LANDYNE Software Suite

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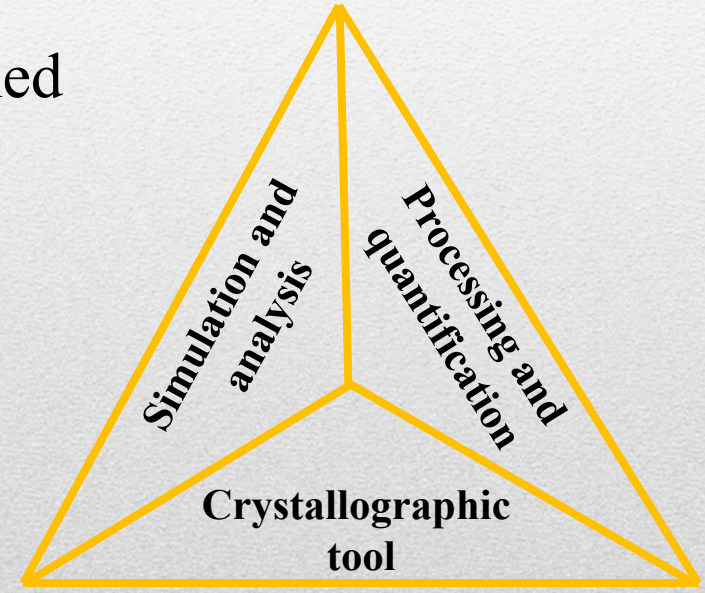
Outline

- Software development
- Online resource
- **Software components**
- Application examples
- Installation with licenses

Website, installation and licenses

Landyne (computer software) was registered in 2010 by XingZhong Li and Jane Li in Lincoln, NE 68521, USA. We made computer software for electron diffraction simulation and crystallographic analysis. There are fourteen software modules in this suite so far. The current version is 5.0.

The Landyne software suite is designed for TEM characteristics of material structure and crystallography.



- As a research tool for analyzing experimental results.
- As a tool for teaching electron microscopy.

Online resource

https://www.unl.edu/ncmn-enif/xzli/
https://landyne.com
Including software package, user manual and related papers.

Installation and licenses

PC, Java JRE and JAI.
YouTube demo videos.
Multiple types of licenses.

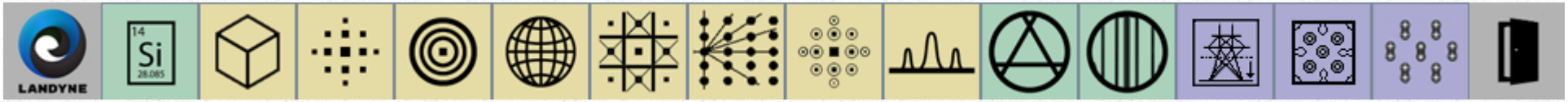
Java and JDK

The program package was complied with Java development kit (JDK) 1.8.0 and above. Java runtime environment (JRE) is needed to run the programs. Java advanced image (JAI) package is needed for ESPOT, SVAT, SAED, PCED, SAKI, QSAED and QPCED for read from and write to files in .tif format.

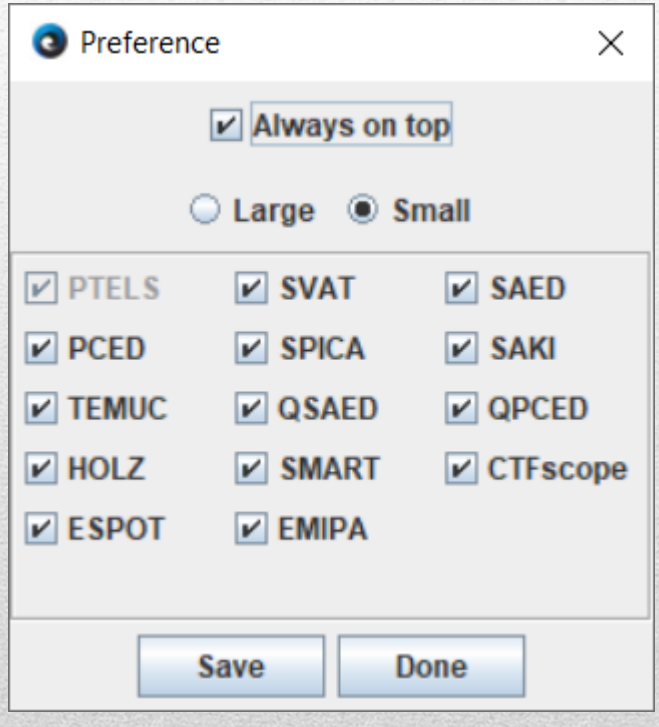
Get JAI1.1.3 from Java official webpage or
http://www.unl.edu/ncmn-cfem/xzli/download

Copy jai_core.jar and jai_codec.jar to
e.g. c:\program files\java\jre1.8.0_31\lib\ext\

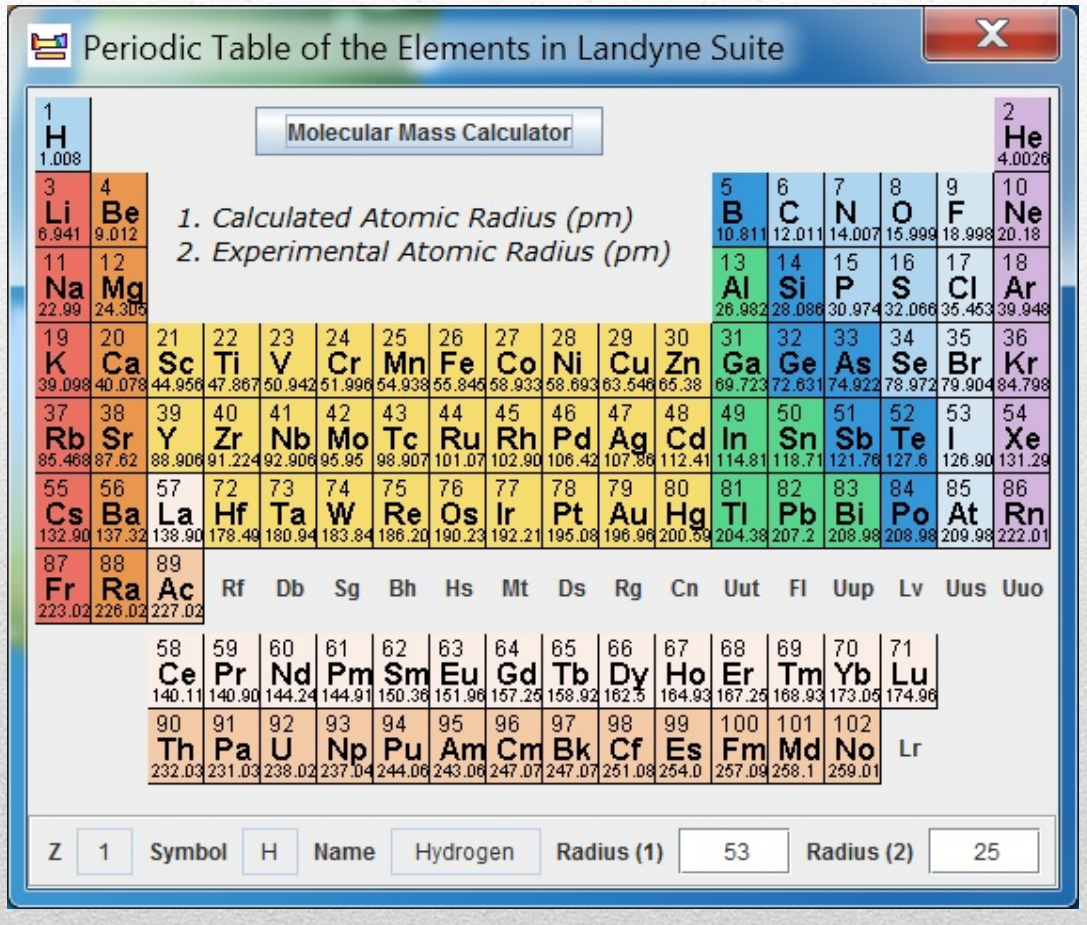
Landyne launcher

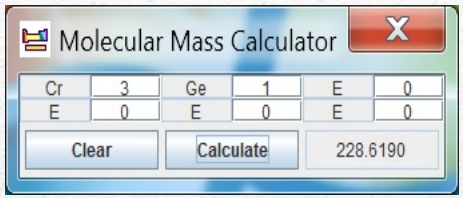


The launcher is a desktop dock for user to run all standalone software in this package conveniently. User can choose the modules from the suite to build a short form or a long form of the launcher.



Periodic Table of Elements for Landyne Suite





Interactive periodic table of the elements

- English label
- Atomic radius
- Molecular mass

Format of crystalline structure file

Keyword	Explanation
[titl]	Description of the structure.
[cell]	Type and parameters of unit cell.
[spgr]	Space group number and symbol.
[natm]	Number of independent atom. Atom label element number x y z occ.
[biso]	Global isotropic temperature factor.
[note]	references and remarks for the data.

Example

```
[titl]    Aluminum
[cell]    F      4.0495  4.0495  4.0495  90  90  90
[spgr]    225    (Fm-3m)
[natm]    1
          Al     13      0.0     0.0     0.0     1.0
[biso]    0
[note]    created for tutorial course, 05, 30, 2017
```

Crystalline structure database

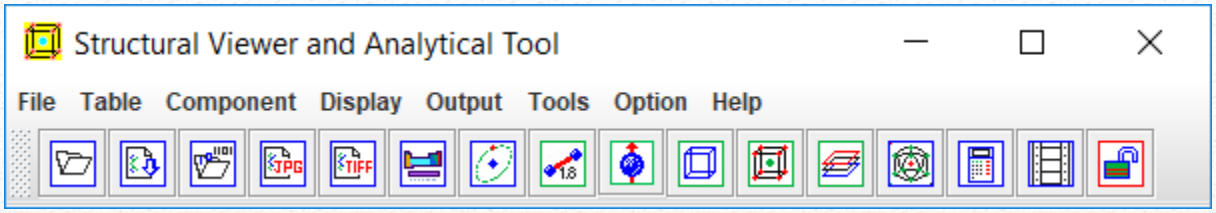
Selected Set of Crystalline Structure Files
Related to X.Z. Li's research work
http://www.unl.edu/ncmn-cfem/xzli/download

The Structure of Materials (Structure Appendix)
By Marc De Graef
http://som.web.cmu.edu/frames.html

Pearson's Handbook: Desk Edition :
Crystallographic Data for Intermetallic Phases
Edition by P. Villars

Crystallography Open Database
http://www.crystallography.net/cod/

ICDD The International Centre for Diffraction Data
http://www.icdd.com/



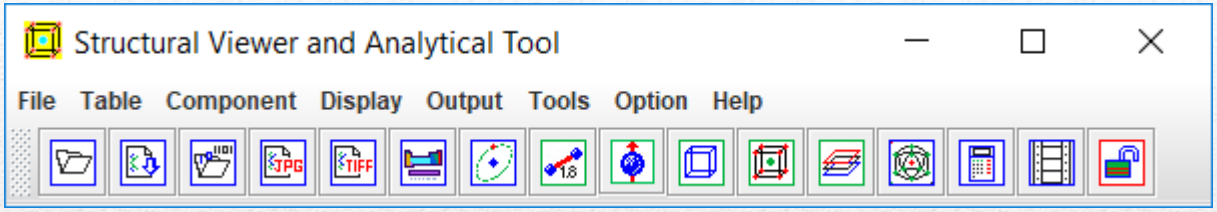
Structural Viewer and Analytical Tool

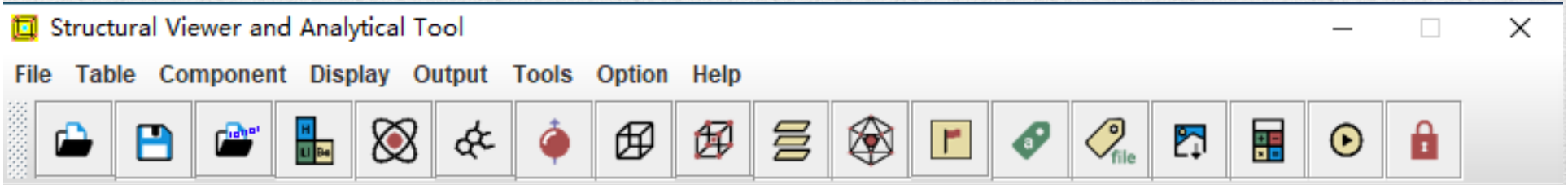
Highlight

- Display of crystal structure in a unit-cell wi/wo chemical bonds and magnetic moments.
- Projection in a selected [uvw] or layer by layer.
- Local structure (or polyhedral clusters).
- Calculation of the chemical composition and the bond length/angle.
- The work on the structure can be saved to a file and reload back.
- Animation including rotation or wobble.
- Image can be saved in GIF, PNG, JPG and TIF formats.

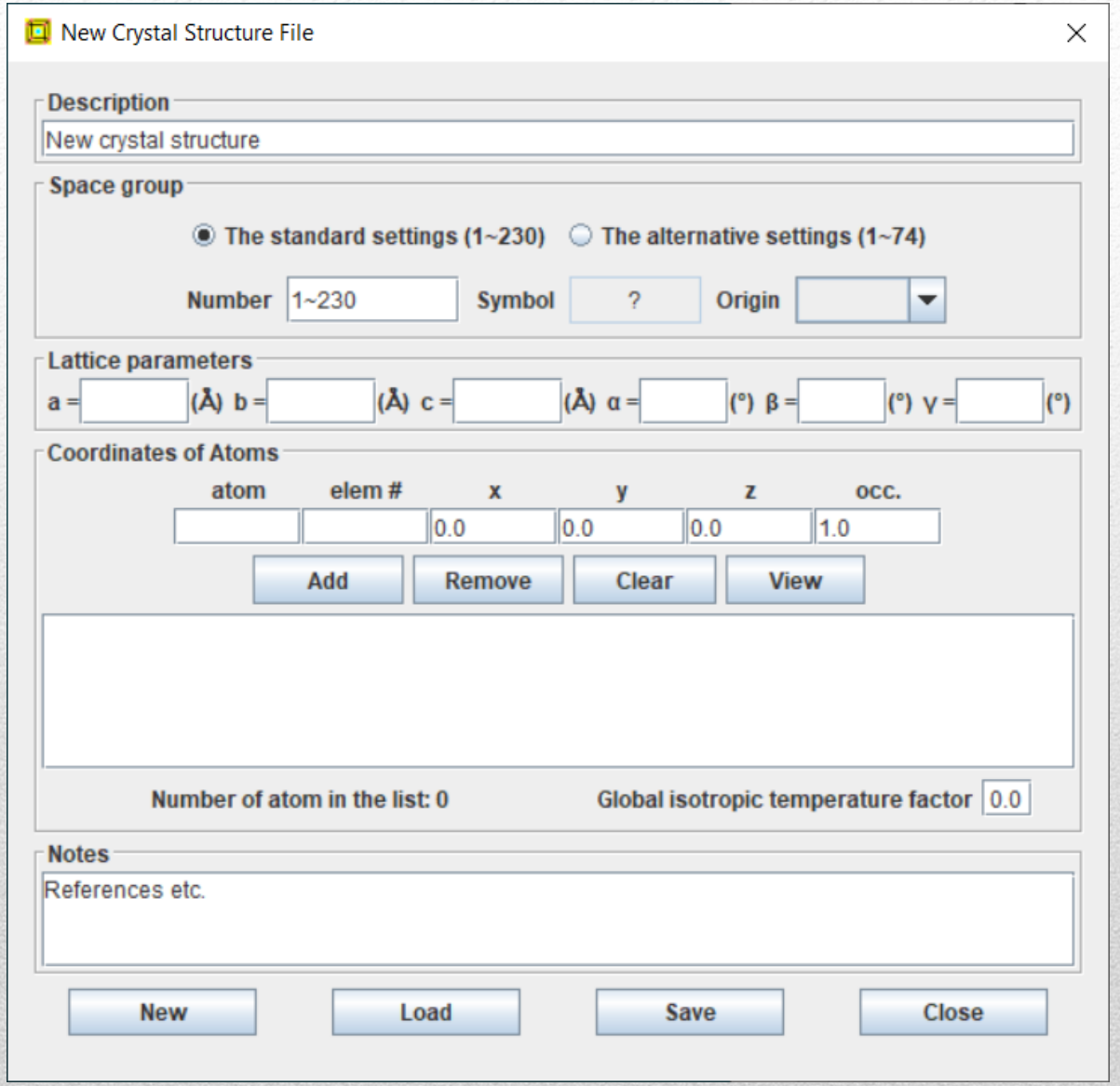
X.-Z. Li, SVAT4 – a computer program for crystal structure visualization and analysis, J. Appl. Cryst. 53 (2020) 848-853.
https://landyne.com/gallery1.php

Structural Viewer and Analytical Tool

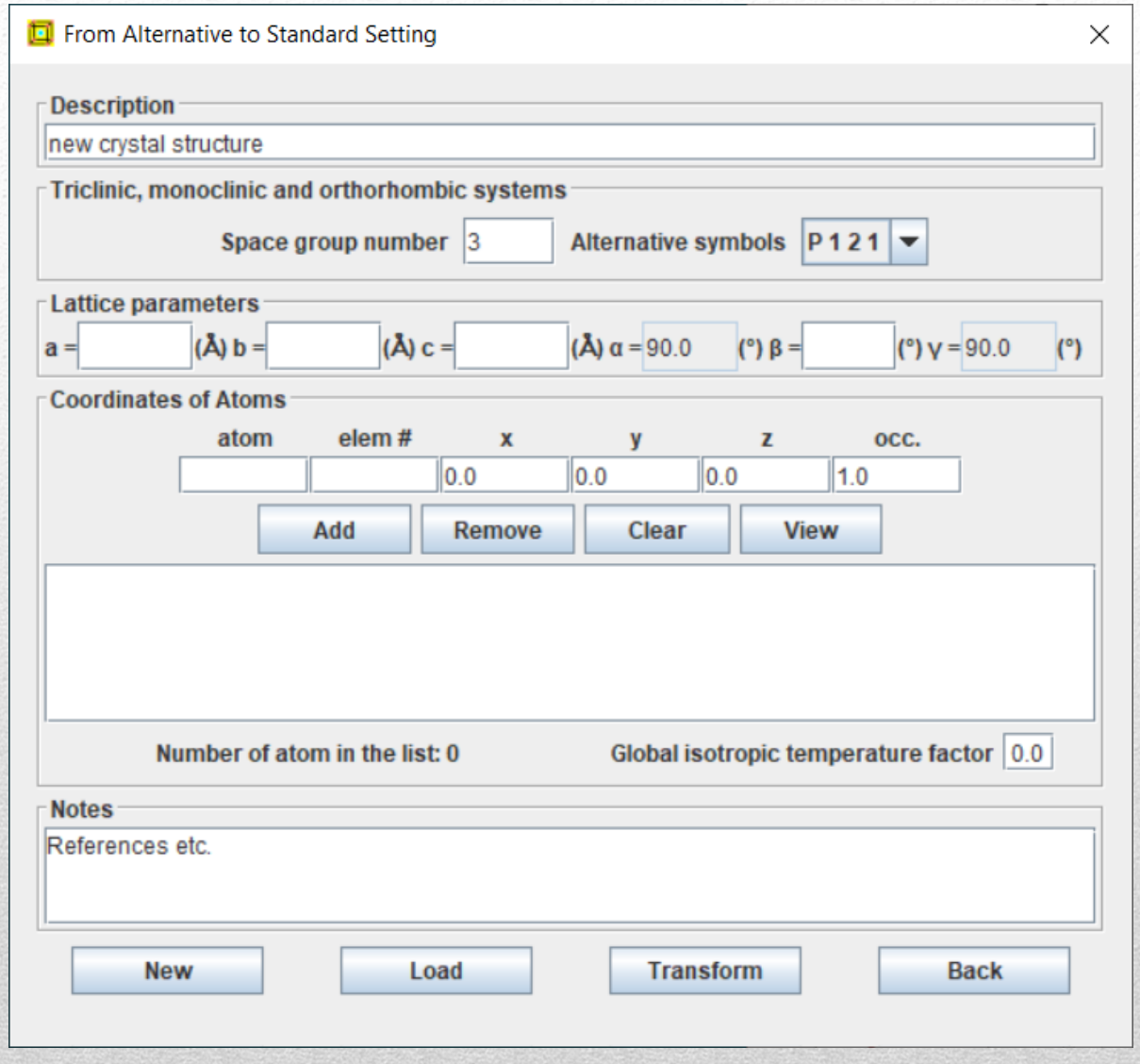




Template for crystalline structure file

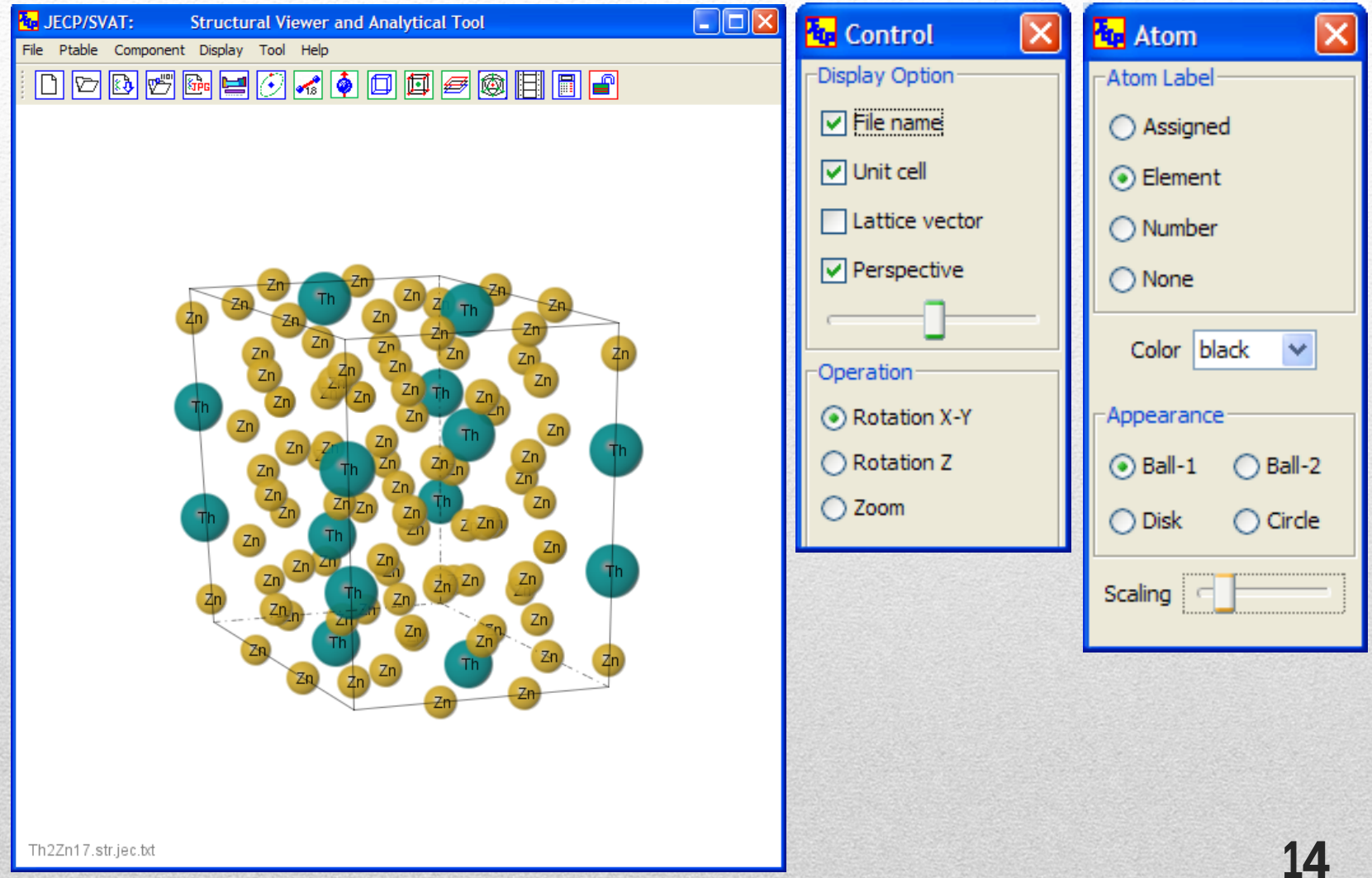


Template for crystalline structure file

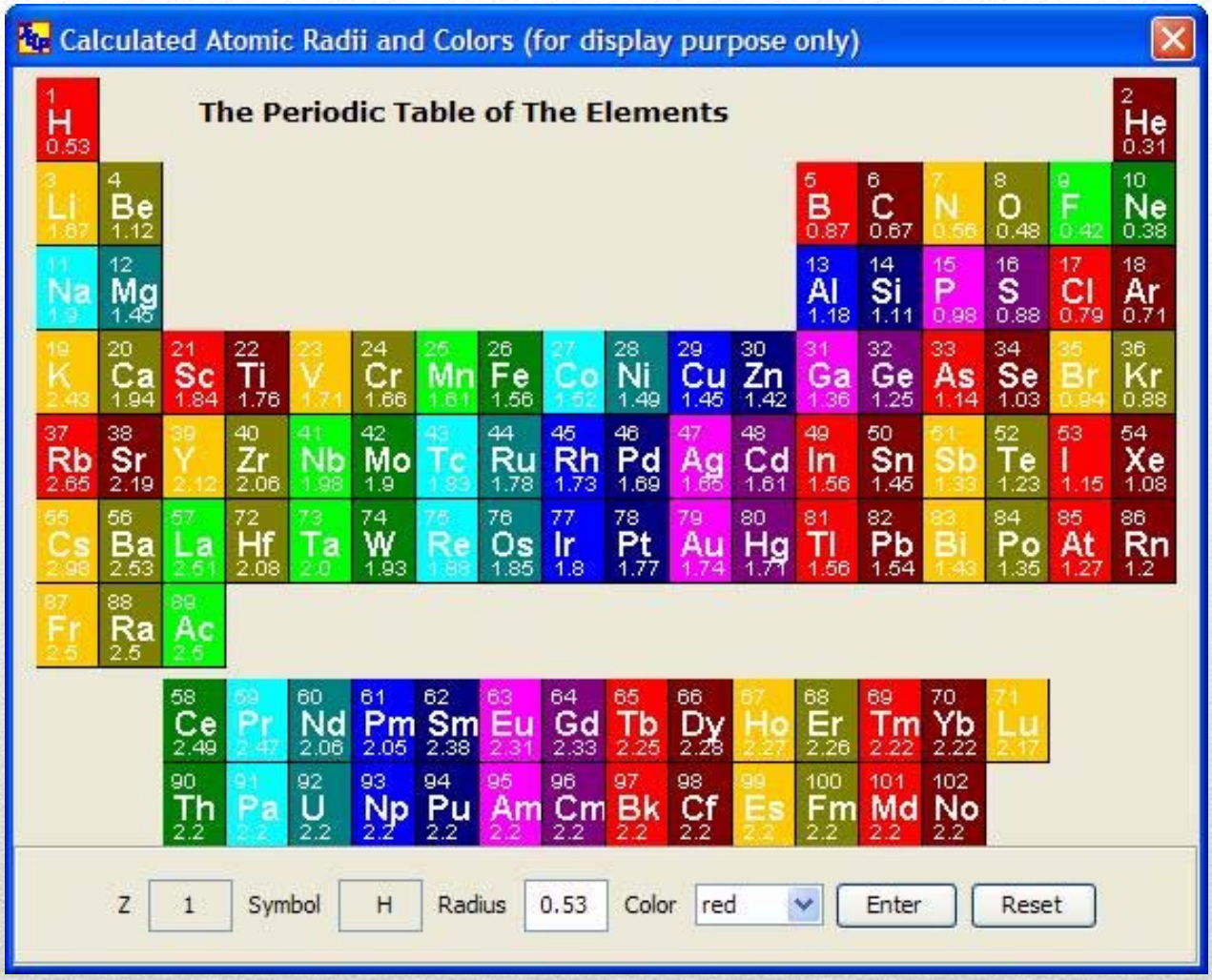


Th_2Zn_{17} rhombohedral structure

Display of crystal structure in a unit-cell.

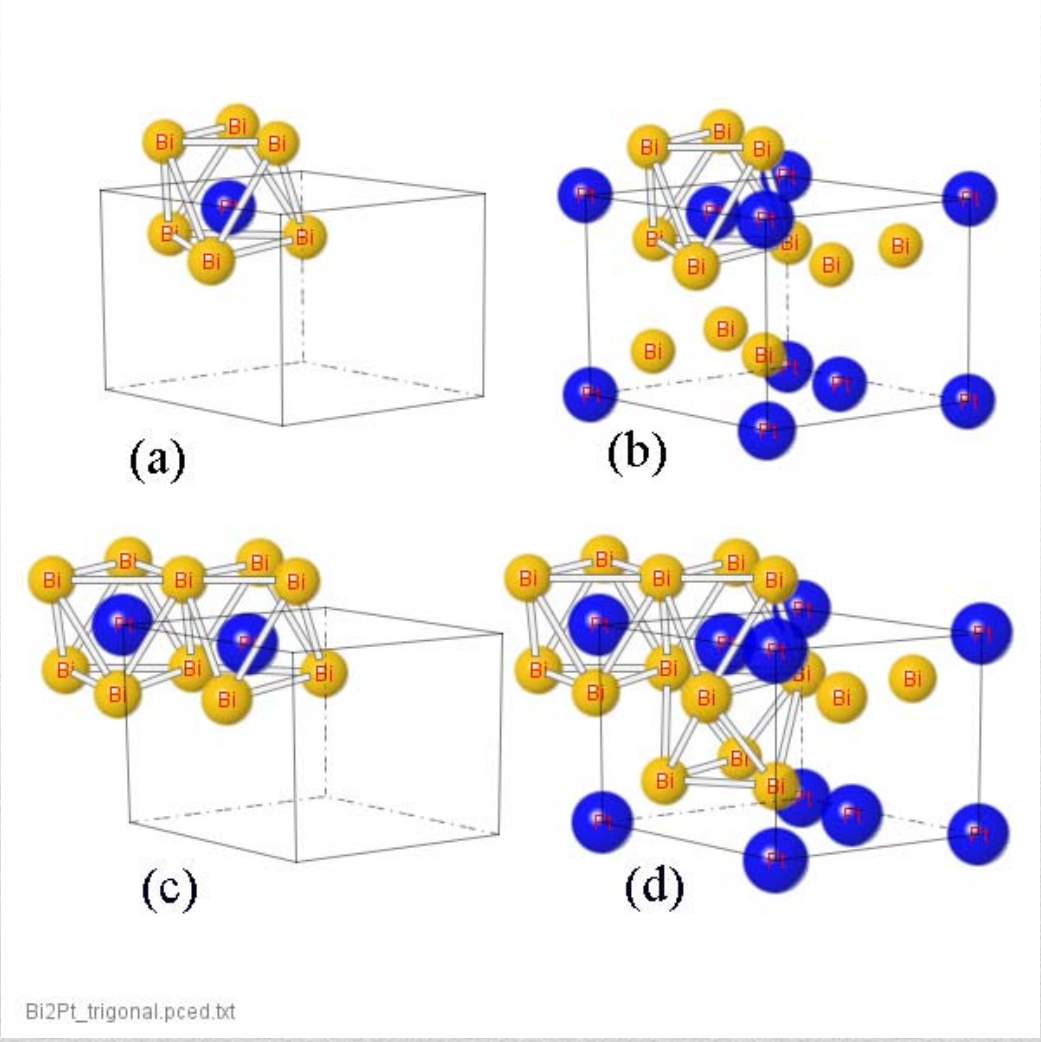


Built-in periodic table of elements



Building-in periodic table for color and atomic radius.

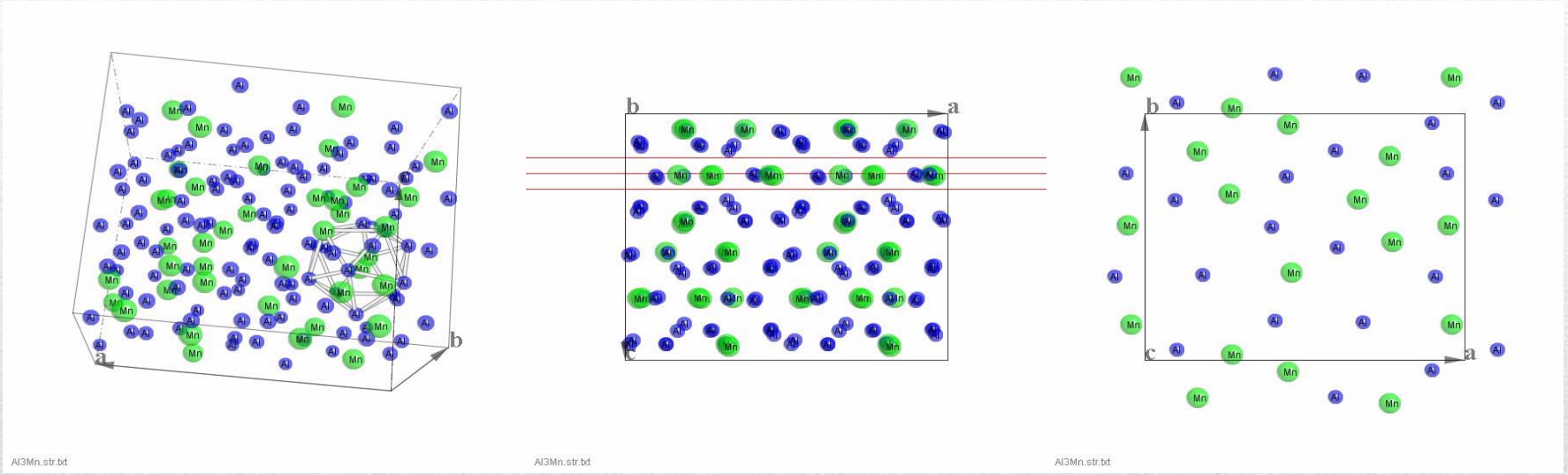
Atom cluster



Local structure or polyhedral clusters.

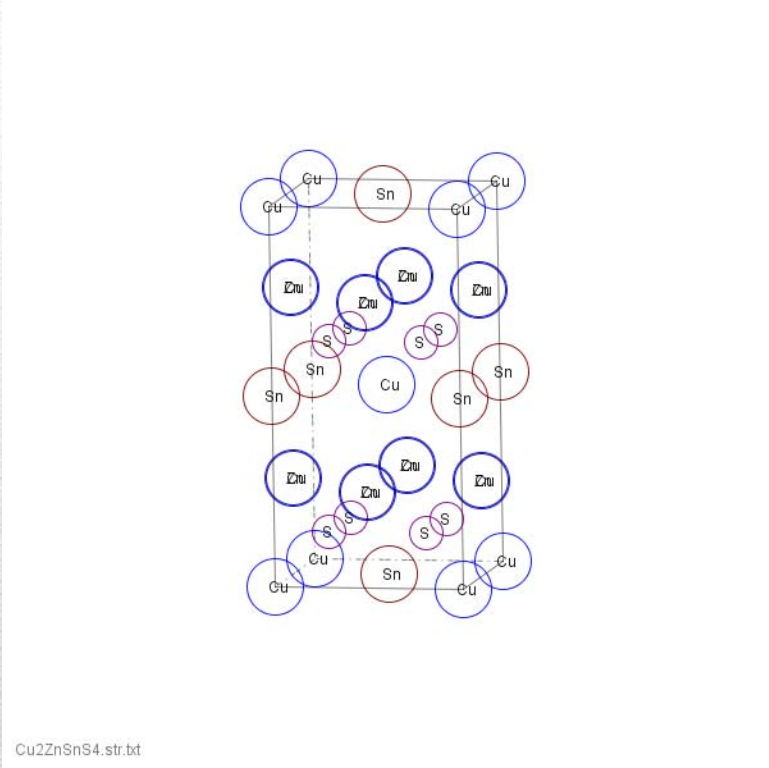
Layer structure

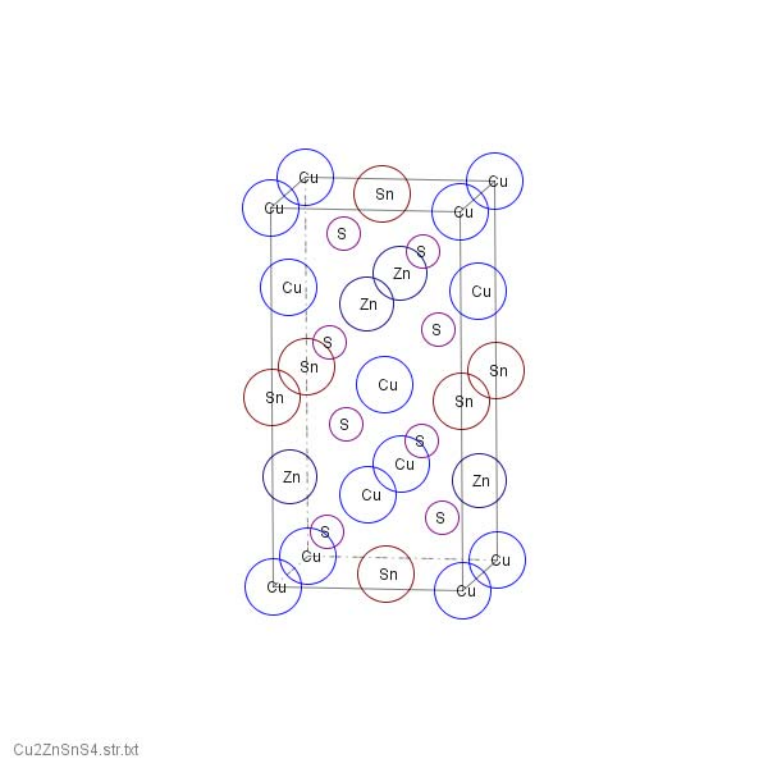
Al_3Mn Projection Layer



Crystal structure can be viewed in layer by layer.

Crystal structure of Cu_2ZnSnS_4





(a) Incorrect input with space group I4 and (b) correct input with space group $I\bar{4}$.

Simulation and Analysis of Electron Diffraction Patterns

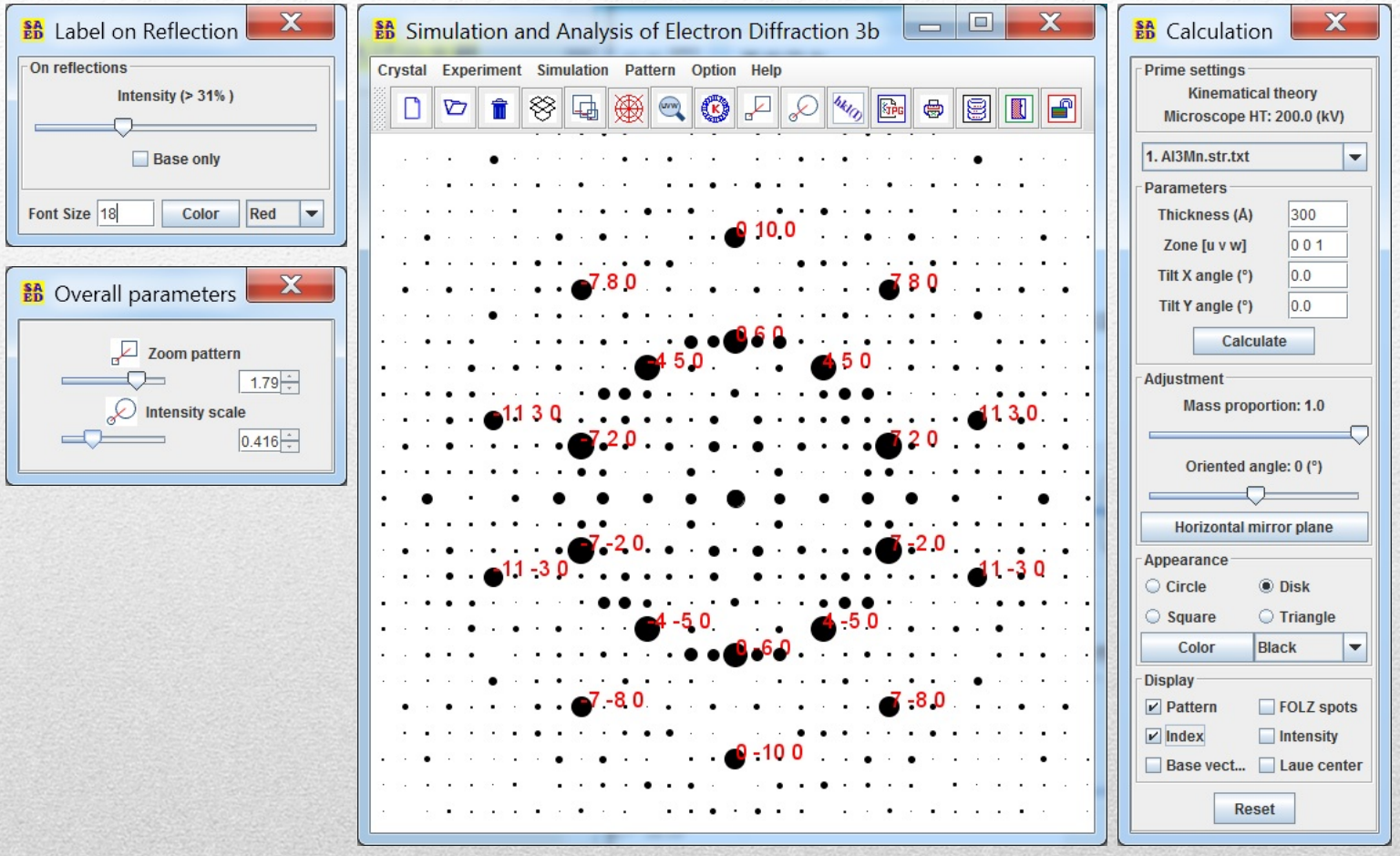
Highlight

- Simulation in kinematical theory and Bloch wave dynamical theory.
- Simulation of composited patterns from multiple phases.
- Simulation of SAED pattern with zero and first order zone.
- Simulation of SAED pattern along/or away from zone axis.
- Simulation of composited patterns of twin crystals.
- Load experimental SAED pattern and for searching the zone axis.
- Save Region of Interest and user-defined TIFF resolution.
- Save electron diffraction data as input data for ESPOT.

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

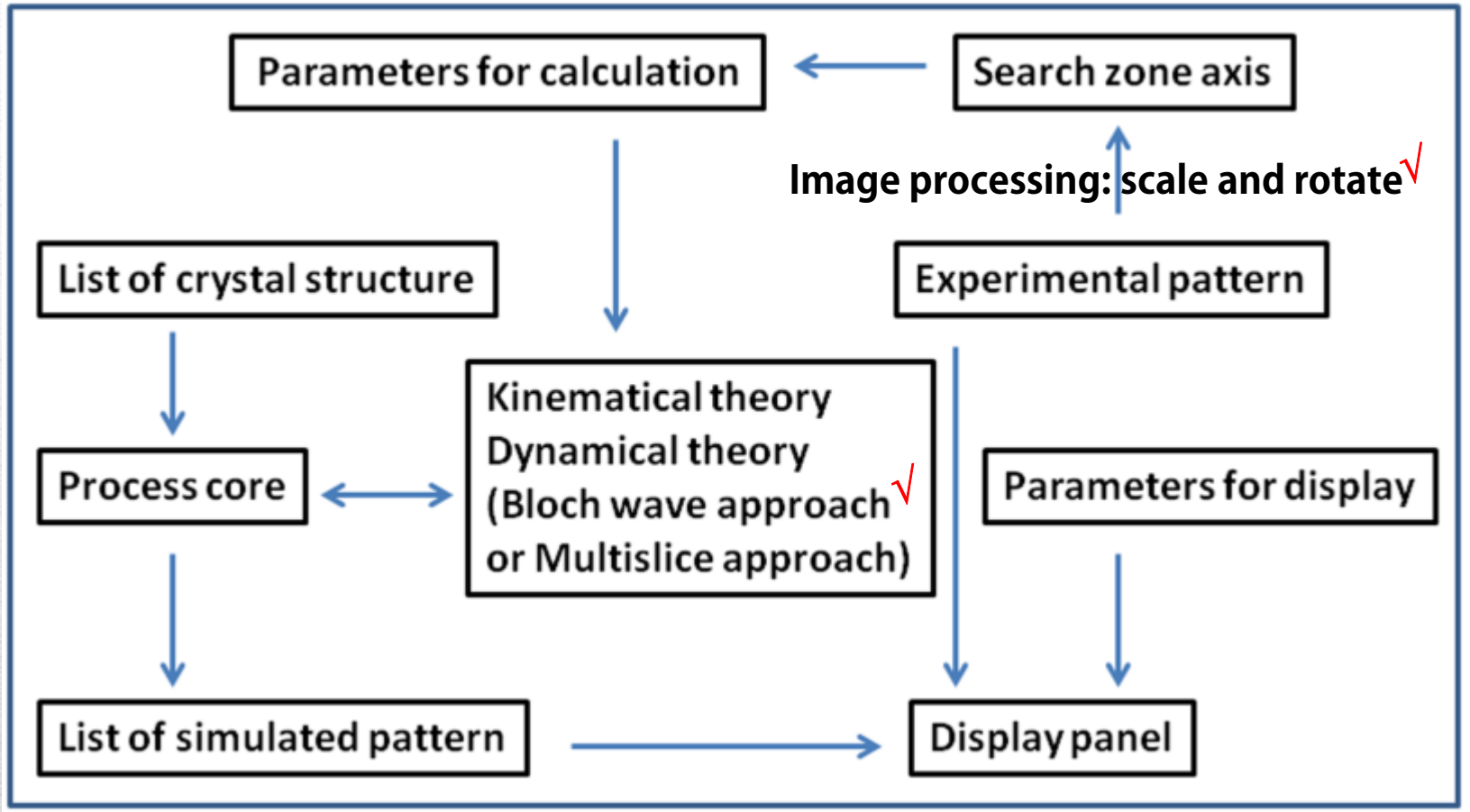
Simulation and Analysis of Electron Diffraction Patterns

SAED simulation of Al_3Mn



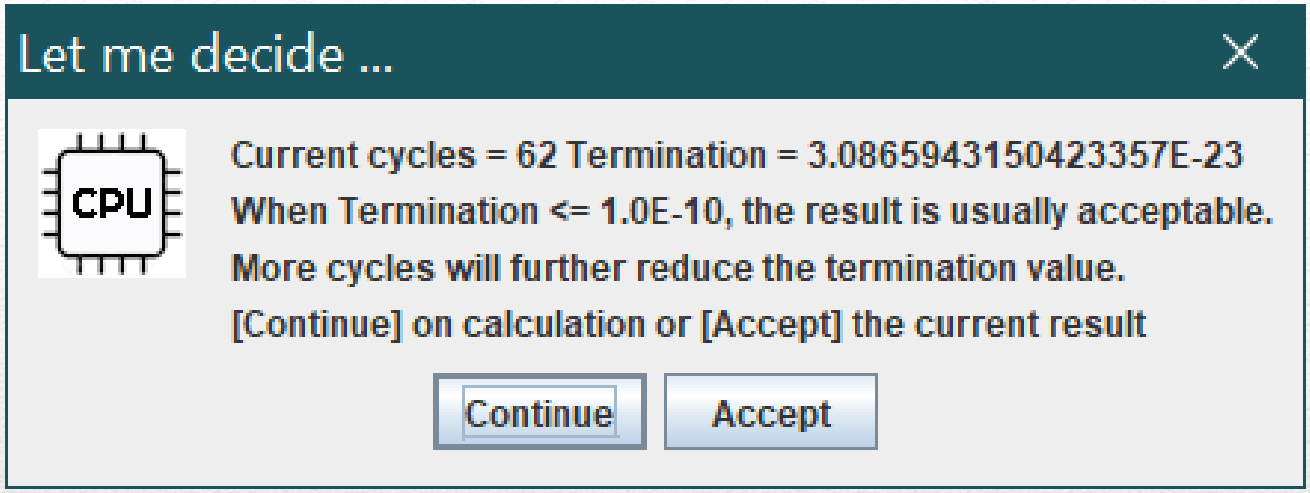
SAED3: X.Z. Li, Microscopy and Analysis, May-June issue (2019) 16-19.

Flow chart of program design



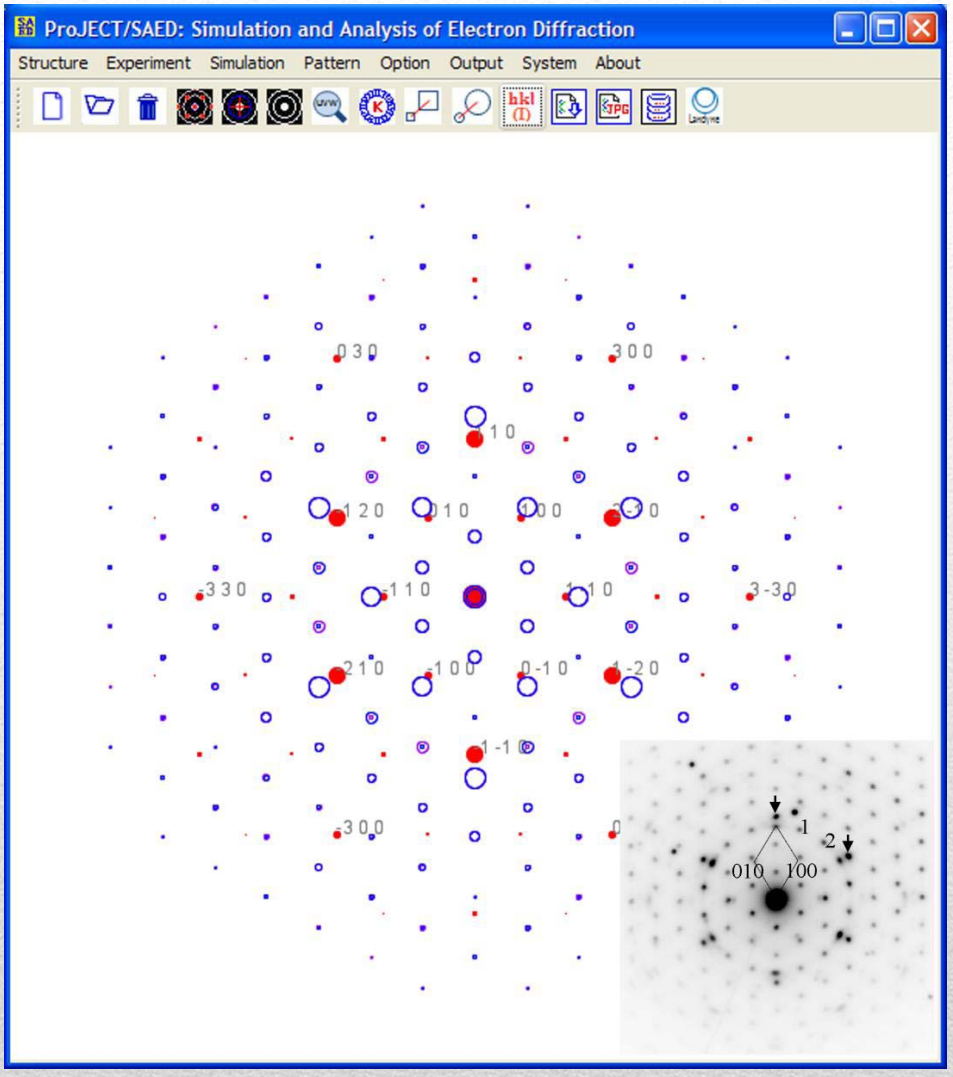
The flow chart of the SAED design.

Time on Blochwave calculation



Snap-shot of an option for user to terminate or continue the calculation. 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; (ii) the software will use previous calculated parameters to simulate a diffraction pattern when only the thickness is changed.

Application on PtBi and γ-$PtBi_2$



PtBi P63/mmc (194)
a = 0.4315 nm c = 0.549 nm

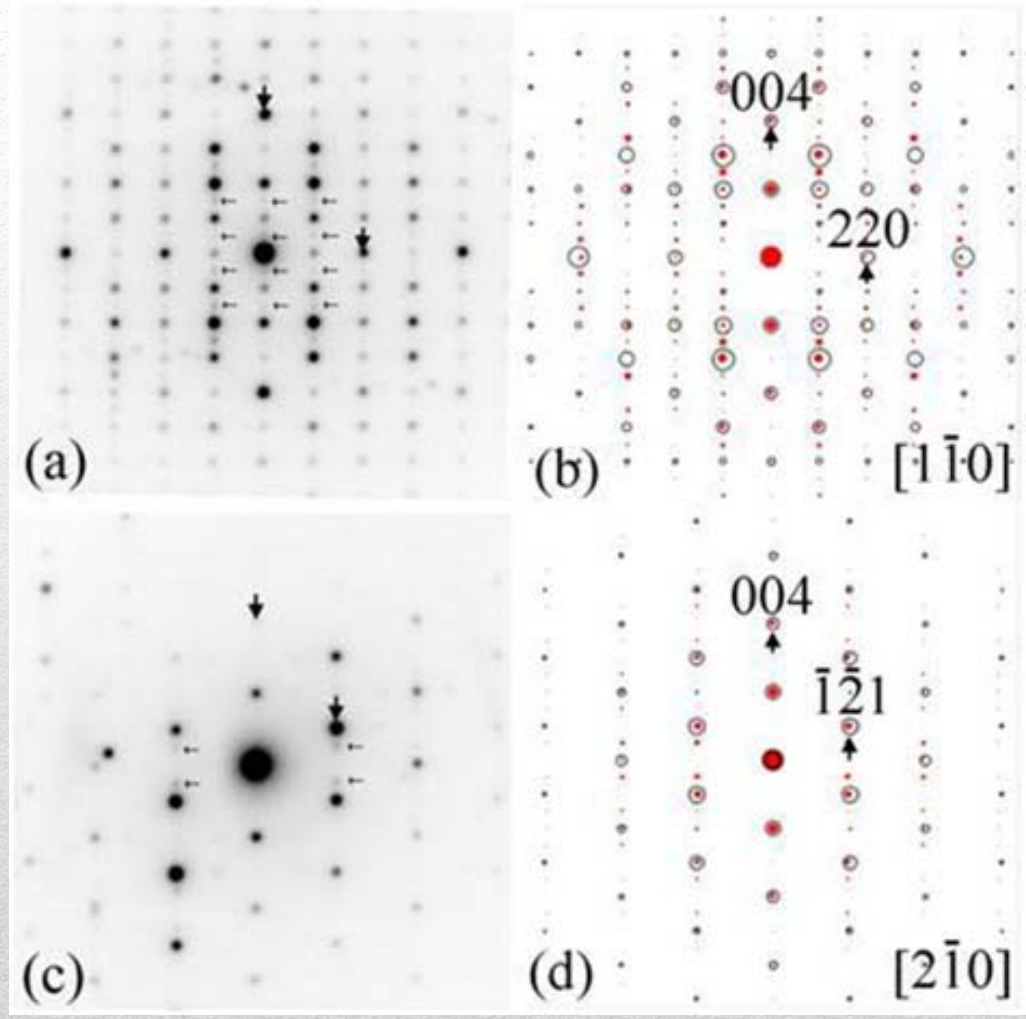
γ–$PtBi_2$ P -3 (147)
a = 0.657 nm c = 0.616 nm

[001] PtBi//[001] γ–$PtBi_2$

(110) PtBi//(100) γ–$PtBi_2$

X.Z. Li *et al*. Philosophical Magazine, 91, 3406 (2011).

Application on α-$PtBi_2$ and β-$PtBi_2$



α-$PtBi_2$ Pbca (61)
a = 0.6732 nm
b = 0.6794 nm
c = 1.3346 nm

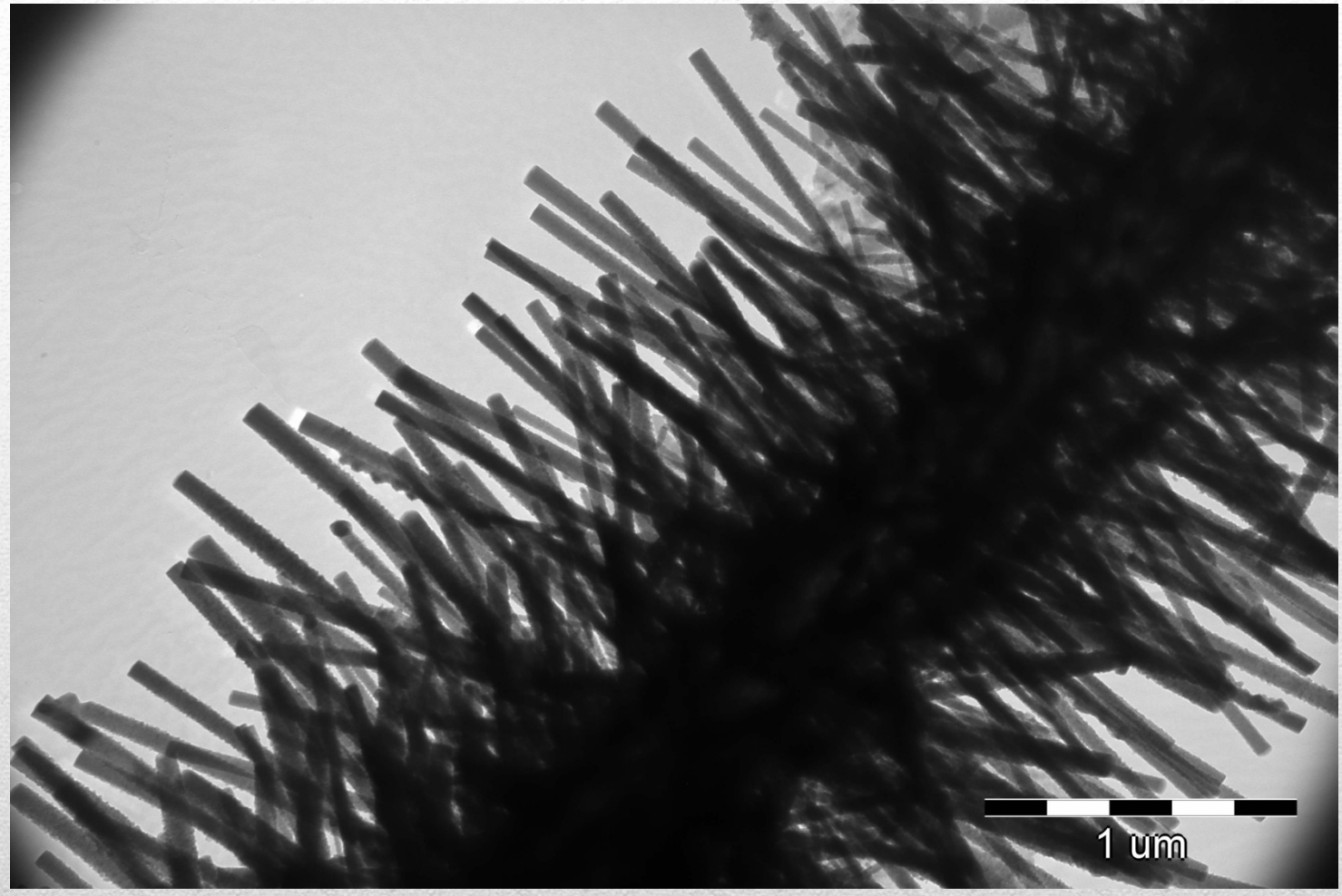
β–$PtBi_2$ P a -3 (205)
a = 0.67014 nm

[001] α-$PtBi_2$//[001] β–$PtBi_2$

(100) α- $PtBi_2$//(100) β–$PtBi_2$

X.Z. Li *et al*. Philosophical Magazine, 91, 3406 (2011).

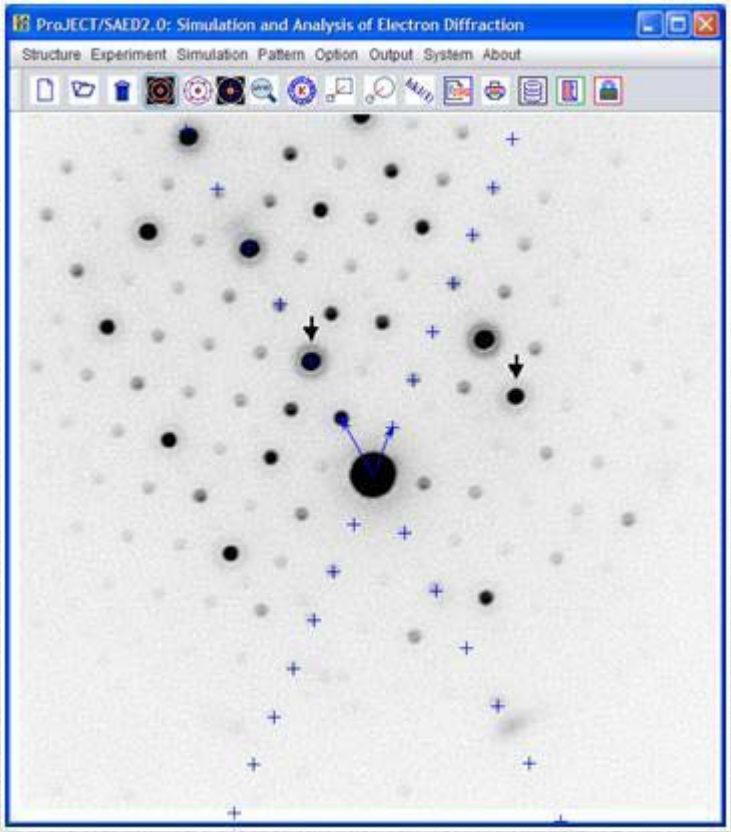
Application to Cu_2S

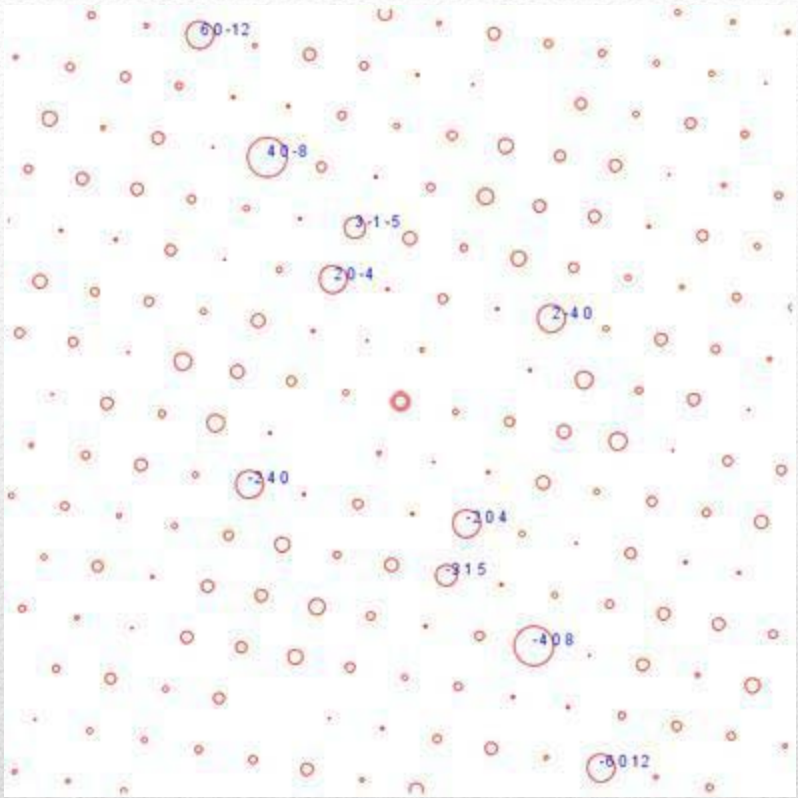


TEM image of the Cu_2S nanowire.

X.Z. Li *et al*. Microscopy and Microanalysis, 18S2, 1470 (2012).

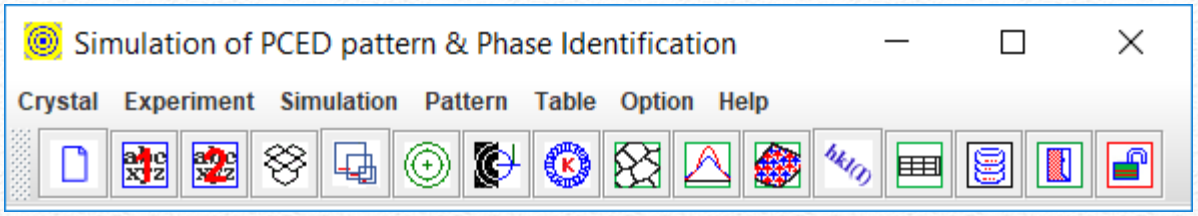
Search for zone axis





Search for the zone axis of the experimental SAED pattern, (a) the experimental SAED pattern of the Cu_2S nanowire and (b) the simulated [211] SAED pattern of the Cu_2S phase.

X.Z. Li *et al*. Microscopy and Microanalysis, 18S2, 1470 (2012).



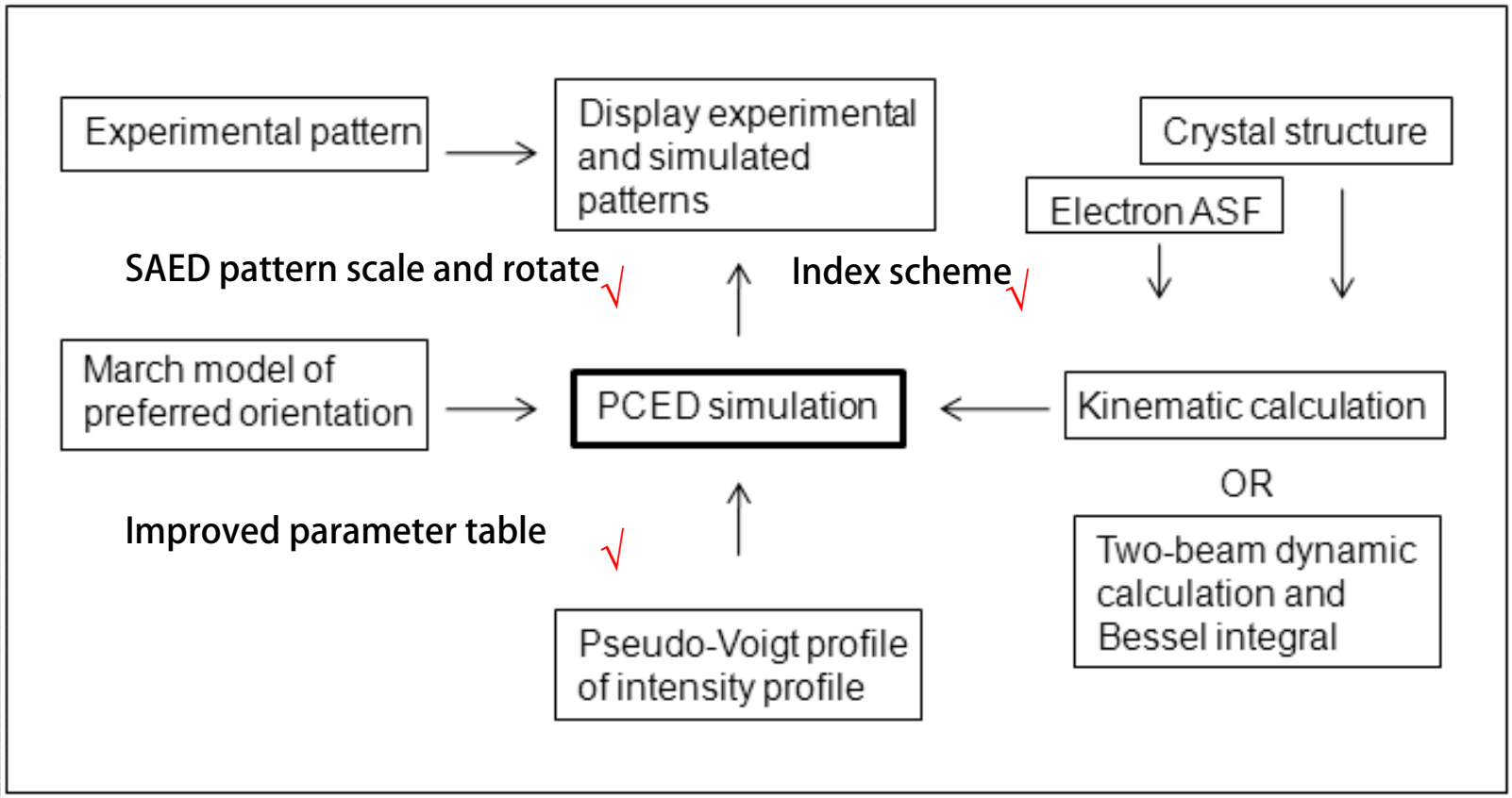
Simulation of Polycrystalline Electron Diffraction Pattern and Phase Identification

Highlight

- Simulation in kinematical theory and in Blackman theory
- Phase identification.
- Texture analysis using March model.
- Phase mass ratio determination.
- Peak shape using pseudo-Voigt profile.
- Miller index and Miller-Bravais index for hexagonal system.
- Save Region of Interest and GIF, PNG, JPG, and TIFF resolution.

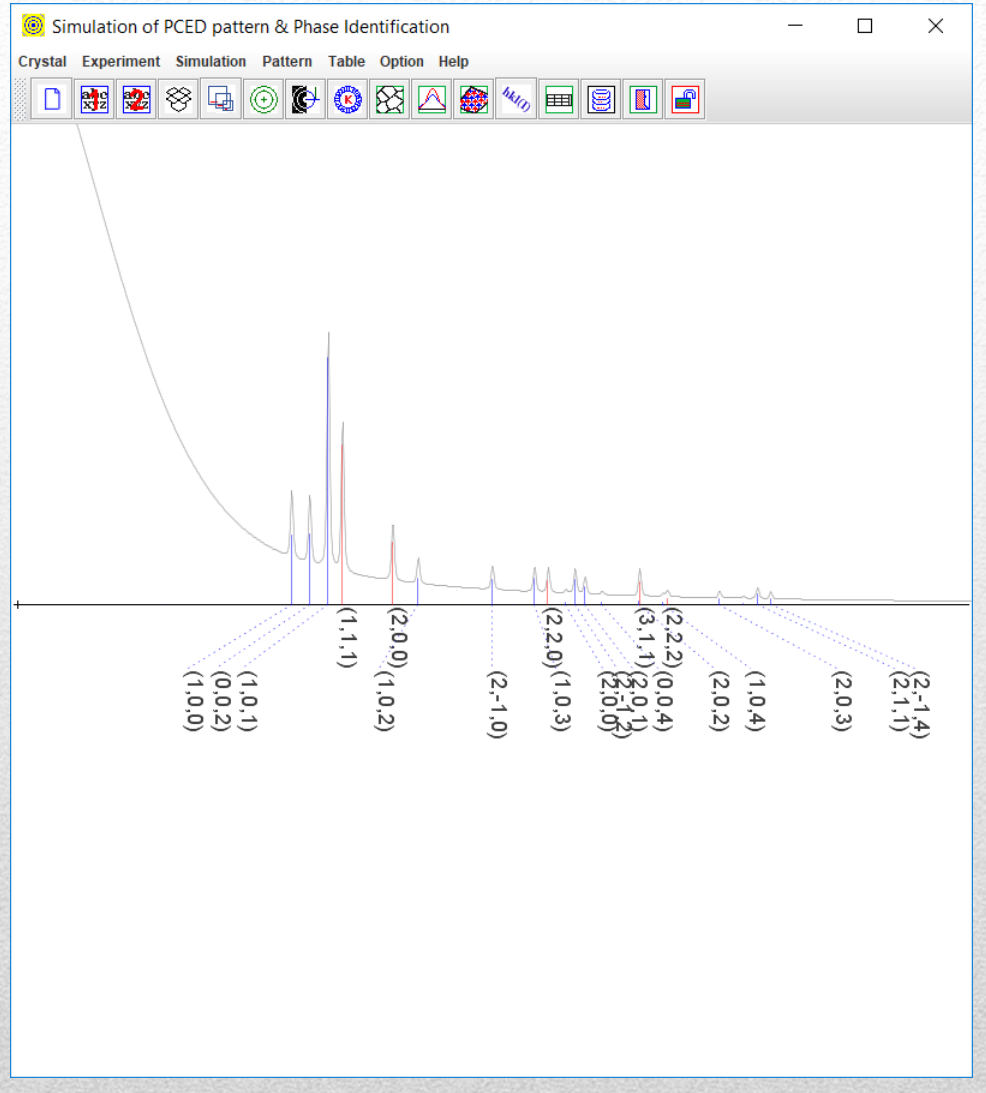
X.-Z. Li, PCED2.0 - A computer program for advanced simulation of polycrystalline electron diffraction pattern, Ultramicroscopy 110 (2010) 297-304.

Flow chart of program design



The flow chart of the PCED design.

Simulation of polycrystalline electron diffraction pattern

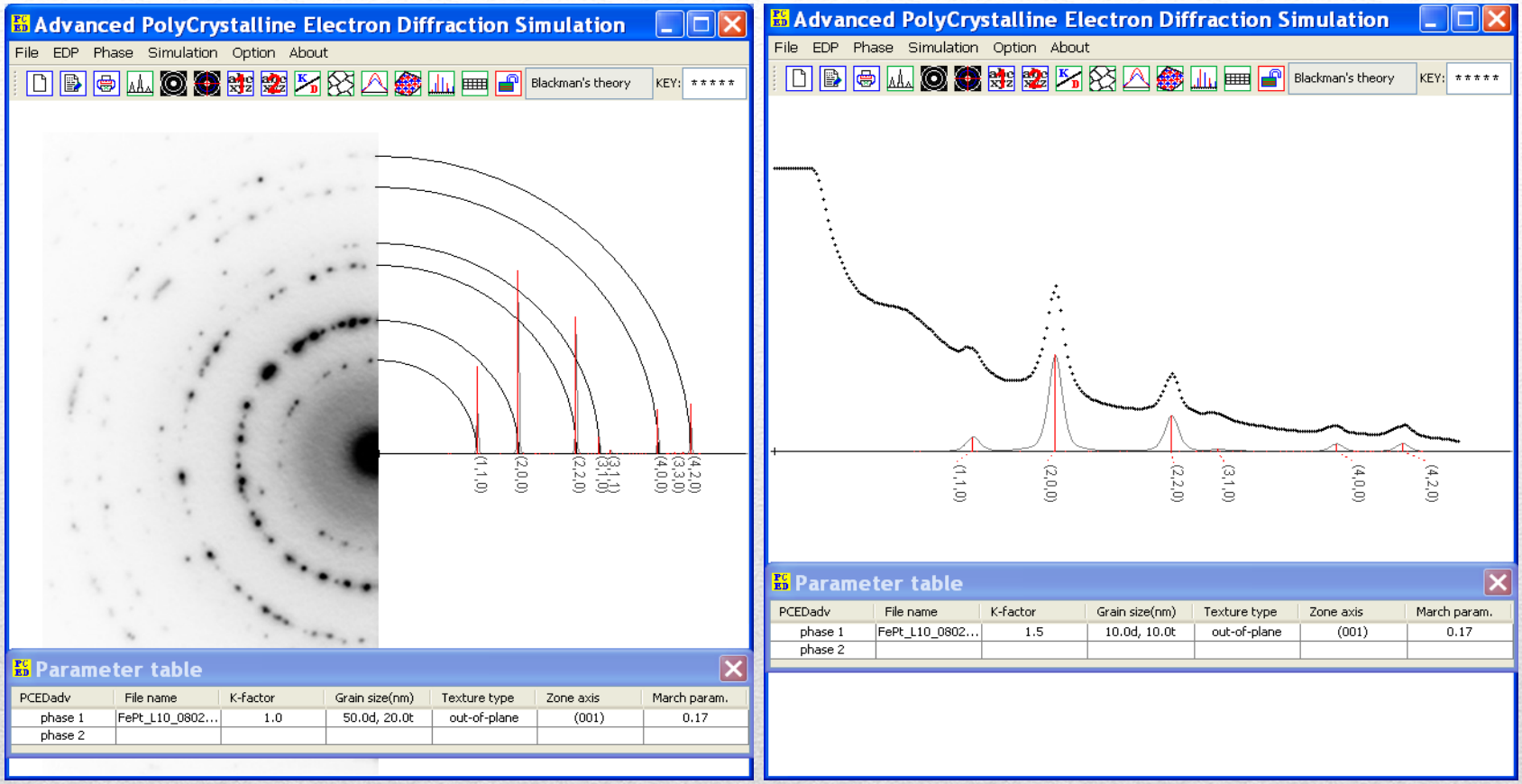


Parameter table

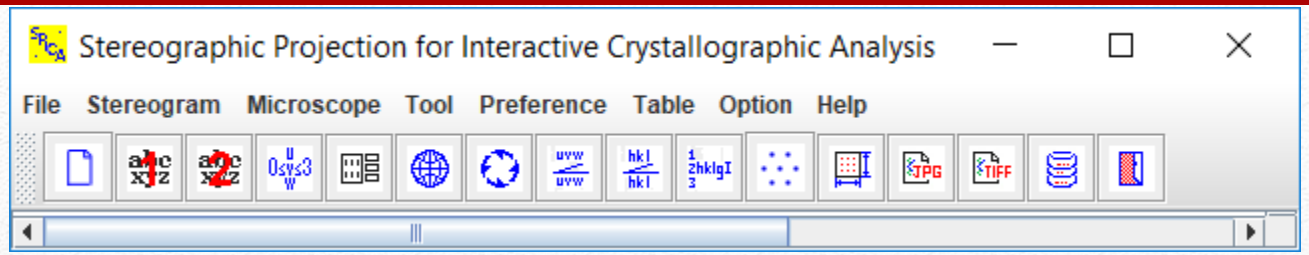
Crystal	Phase 1	Phase 2
File name	Al (default)	Mg (default)
K-factor	1.0	1.0
Grain d(nm)	50.0	50.0
Grain t(nm)	20.0	20.0
Texture	out-of-plane	out-of-plane
Plane (hkl)	001	001
March factor	1.0	1.0

The PCED with simulation of Al and Mg.

Phase identification and semi-quantification



FePt $L1_0$ Phase identification and semi-quantitative matching.



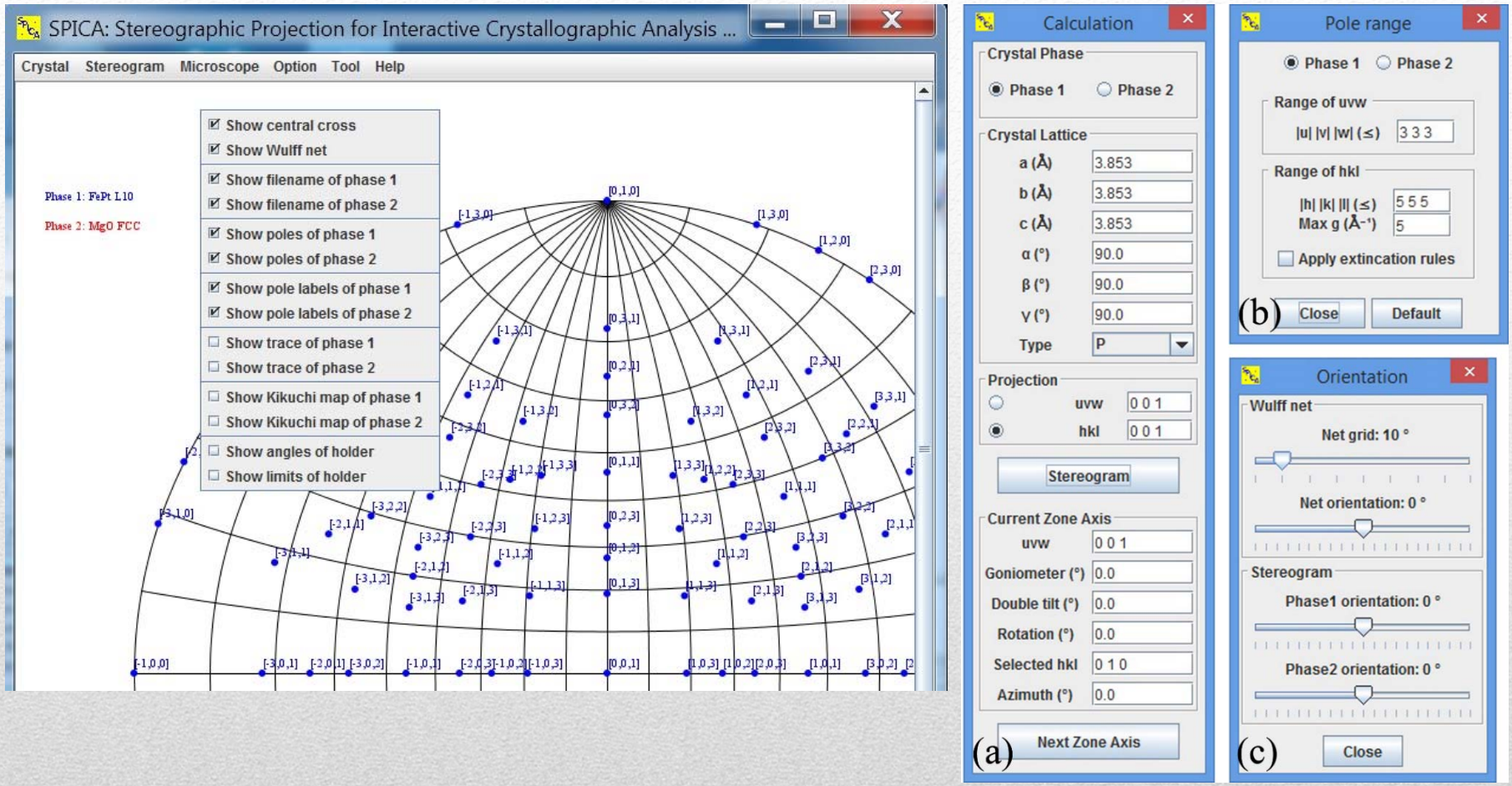
Stereographic Projection for Interactive Crystallographic Analysis

Highlight

- All necessary functions of stereographic projection.
- Calculate two crystal phases simultaneously.
- Display [uvw] labels in various color, size and orientation.
- Display (hkl) labels in various color, size and orientation.
- Generate and overlay two stereographic projections.
- Show Kikuchi maps from the data of (hkl) poles.
- Predicate tilt/rotation angles of zone axes for both double-tilt and rotation TEM holders.

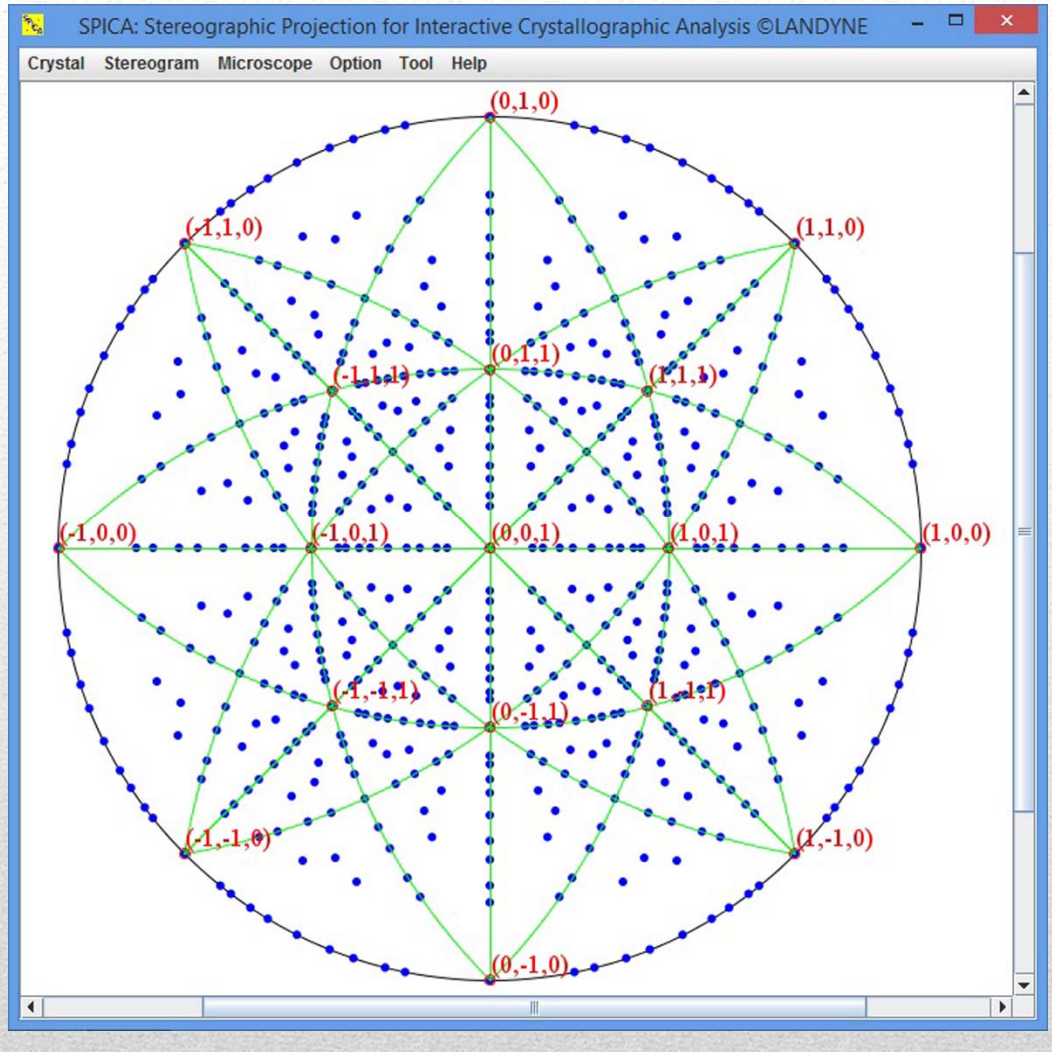
X.-Z. Li, SPICA - Stereographic Projection for Interactive Crystallographic Analysis, J. Appl. Cryst. 49 (2016) 1818-1826

Display and control panels



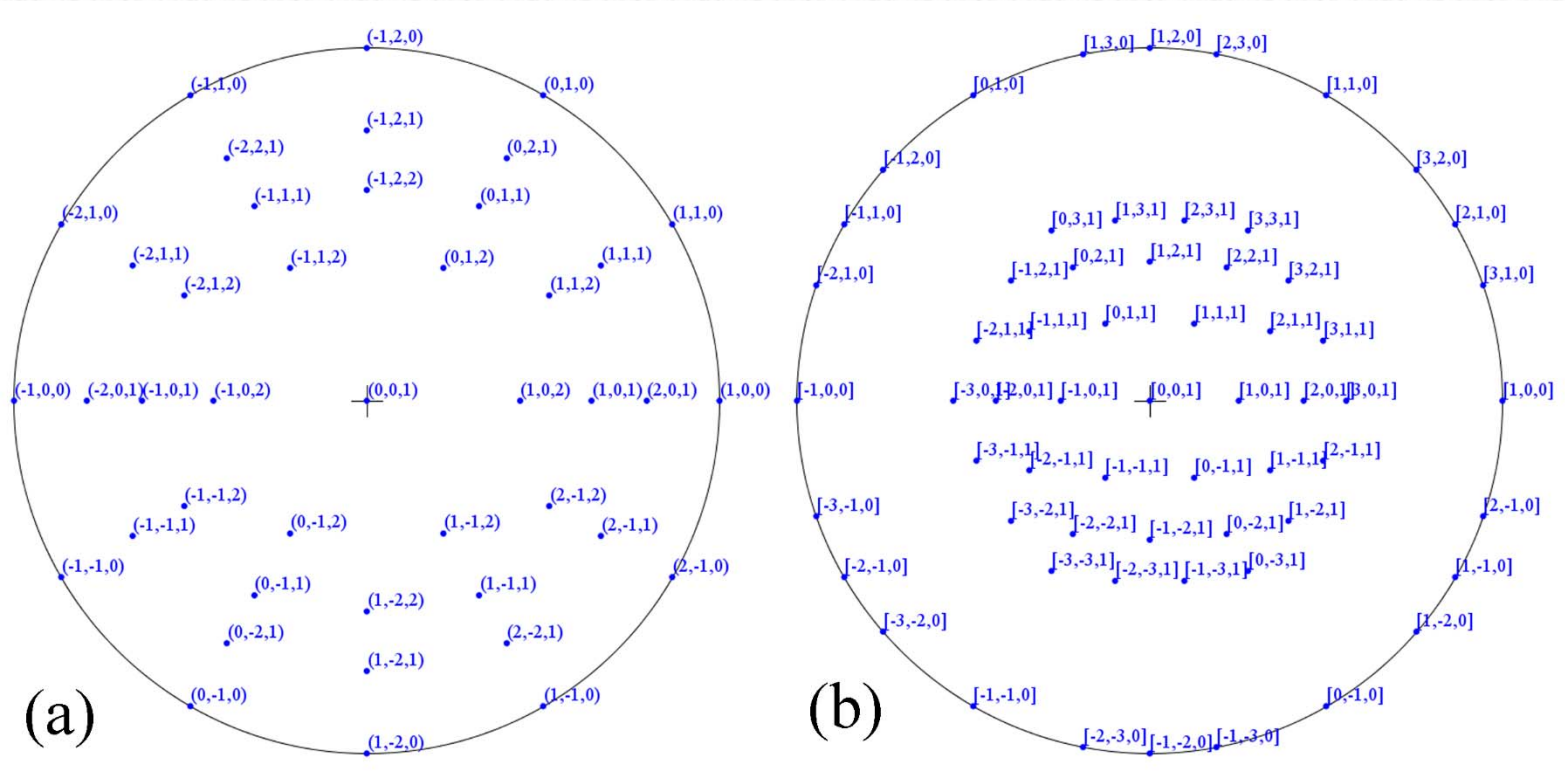
Three basic operational dialogs in SPICA: (a) the calculation dialog, (b) the pole range dialog and (c) the orientation dialog for Wulff net and stereograms.

Stereogram with trace lines



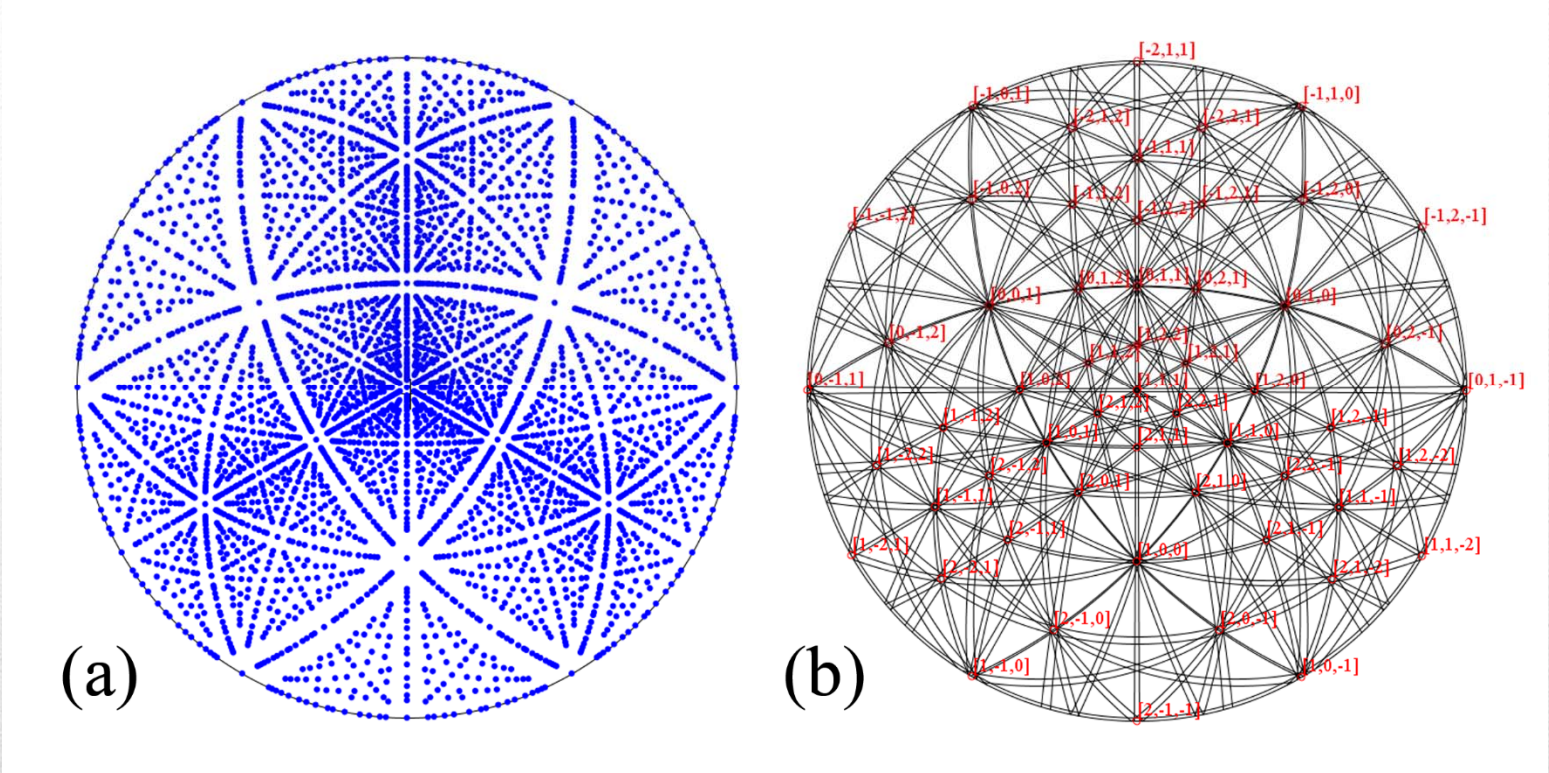
Graphical user interface of SPICA with an (hkl) stereogram of a cubic structure as an example.

Example of the hexagonal Zn



Stereogram of the hexagonal structure of Zn: (a) (h k l) stereogram and (b) [u v w] stereogram. In order to display clearly all indices, the maximum indices were set to h≤2, k≤2, l≤2, u≤3, v≤3 and w≤1.

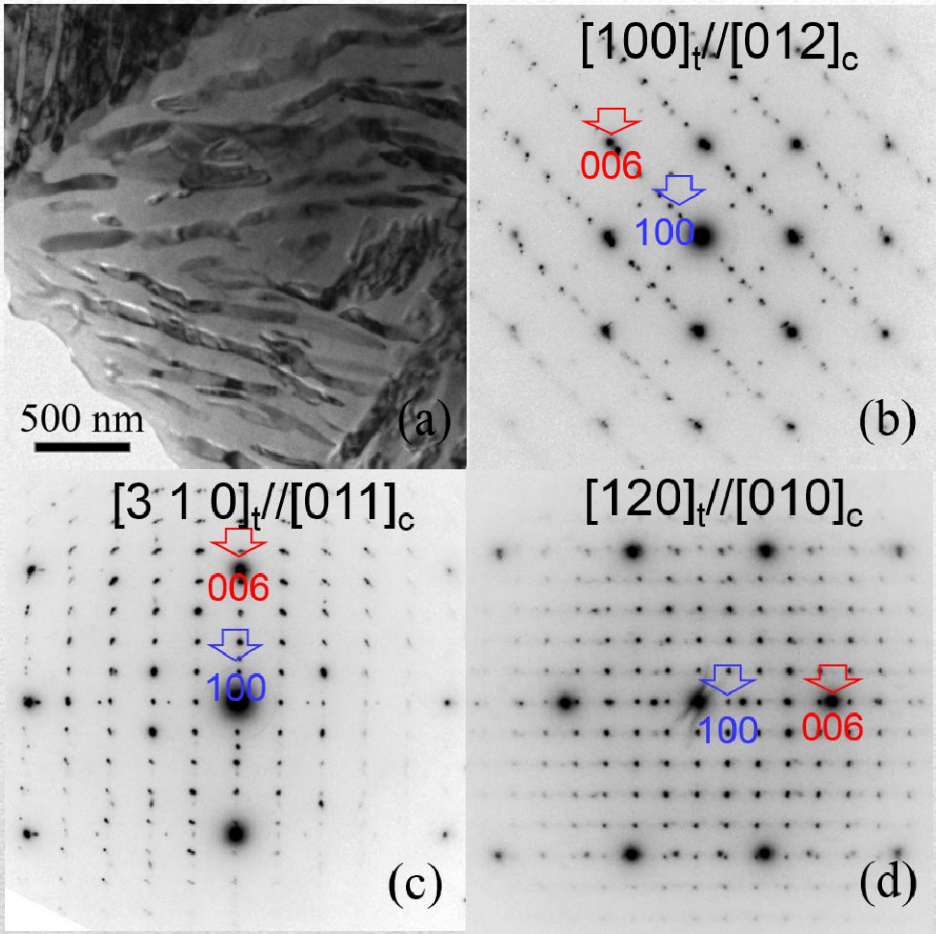
Kikuchi map



Kikuchi maps of a primitive cubic structure with [111] zone axis in the center, (a) generated using the method described by Liu & Liu (2012) and (b) generated using the formula by Young & Lytton (1971) with the wave length of 0.0251 Å (200kV).

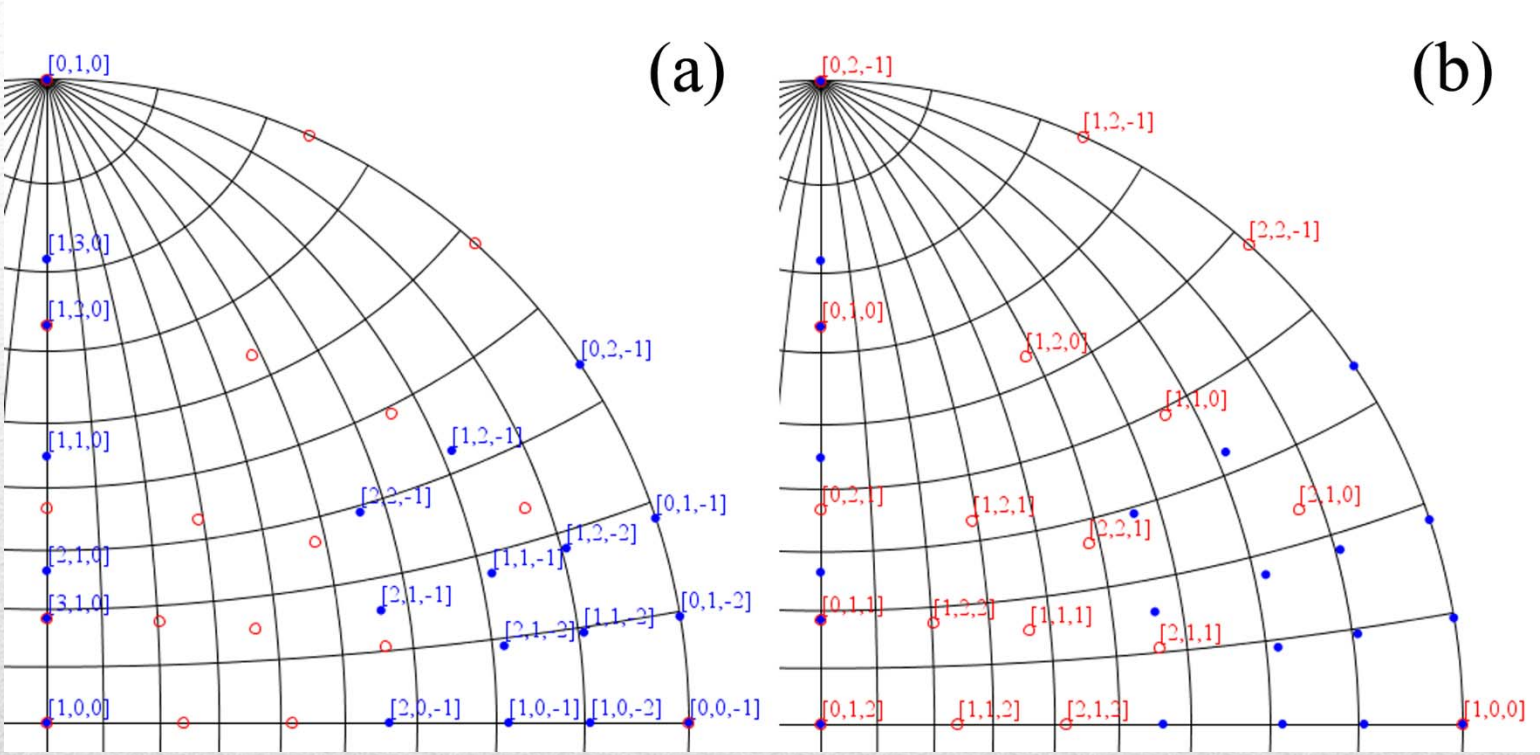
H. Liu, and J. Liu, J. Appl. Cryst. 45, 130-134 (2012).
C.T. Young and J. L. Lytton, J. Appl. Phys. 43, 1408-1417 (1972).

Application to $Mn_2CrGaAl$ compound



Two crystalline phases in $Mn_2CrGa_{0.5}Al_{0.5}$ alloy as the result of a spinodal decomposition: (a) a TEM image of the two phases, cubic phase in light grey and tetragonal phase with strip shape in dark grey, and (b-d) the electron diffraction patterns taken from the two crystalline phases.

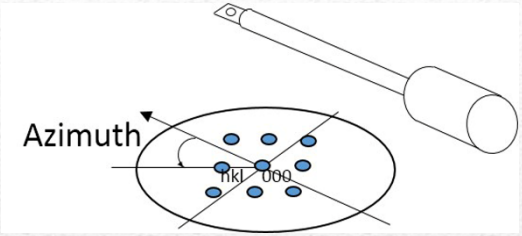
Application to $Mn_2CrGaAl$ compound



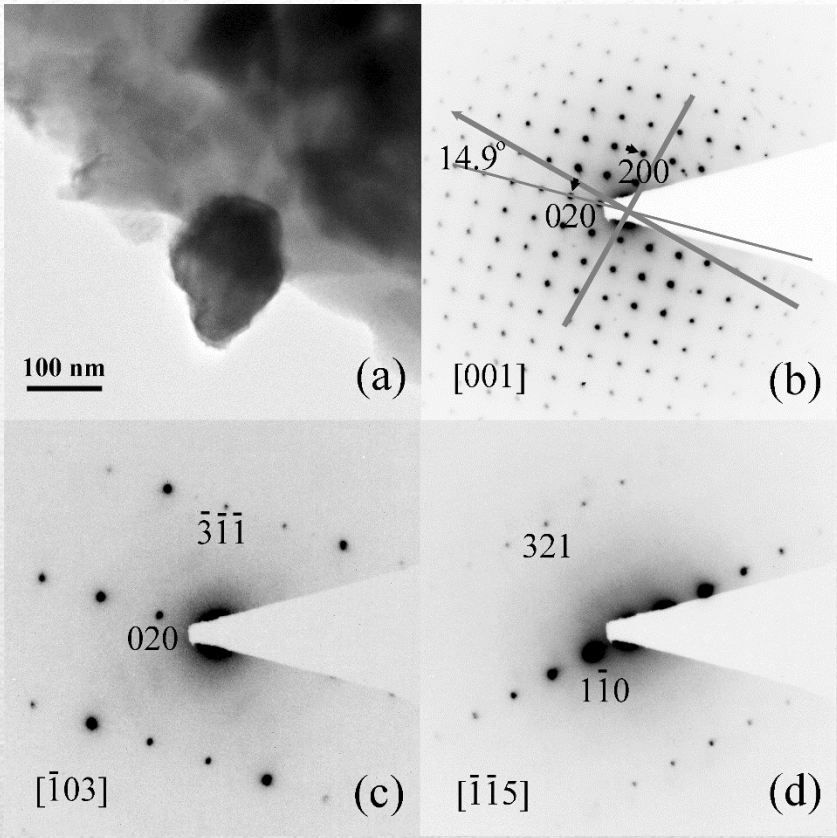
Composite stereogram with (a) the index labels for the cubic phase and (b) the index labels for the tetragonal phase.

X.Z. Li, W.Y. Zhang, and D.J. Sellmyer, submitted to Acta Materialia (2017)

Application to CoFeCrGe compound



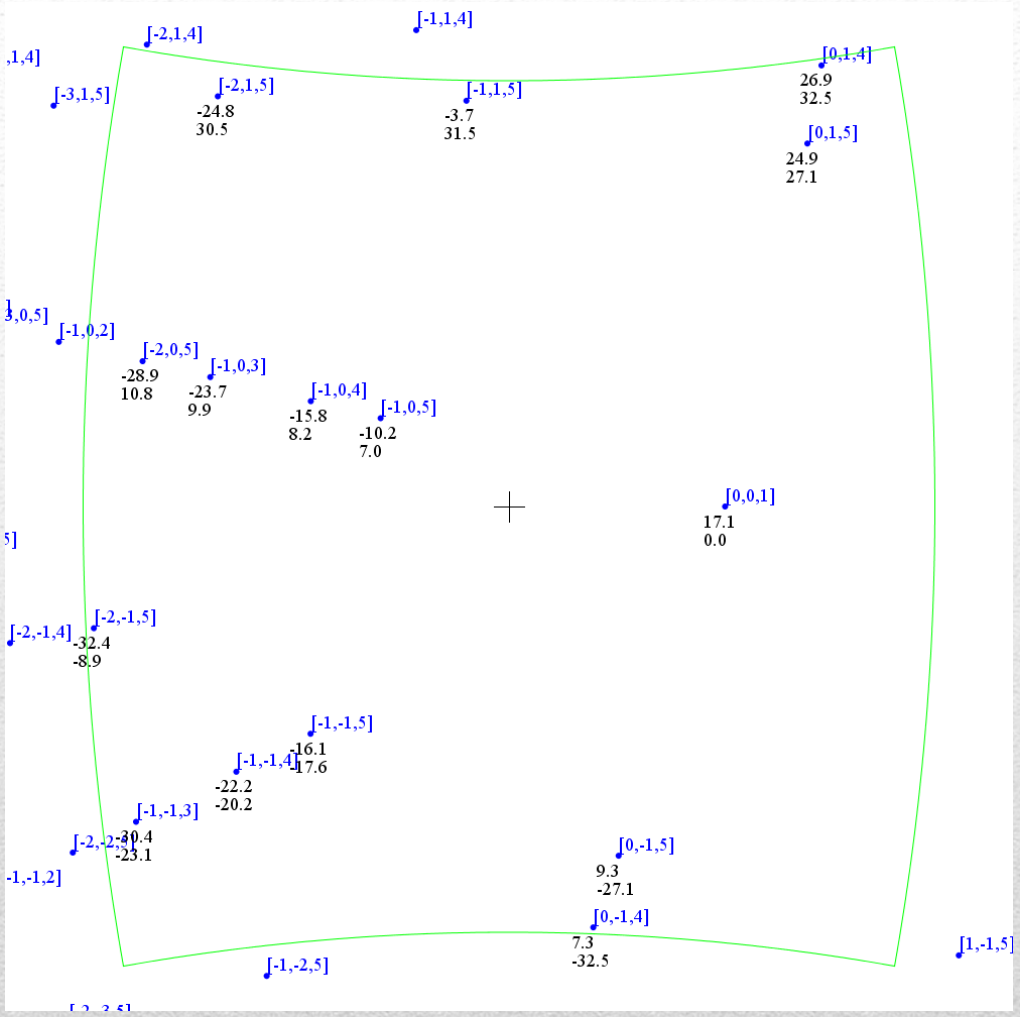
The geometric relation of the observed SAED pattern and the TEM specimen holder for a stereographic projection as a guidance in SAED experiments.



A new tetragonal phase in Co-Fe-Cr-Ge alloy. (a) TEM image of the tetragonal phase with the grain size about 150 nm, (b-d) the SAED patterns of the tetragonal phase.

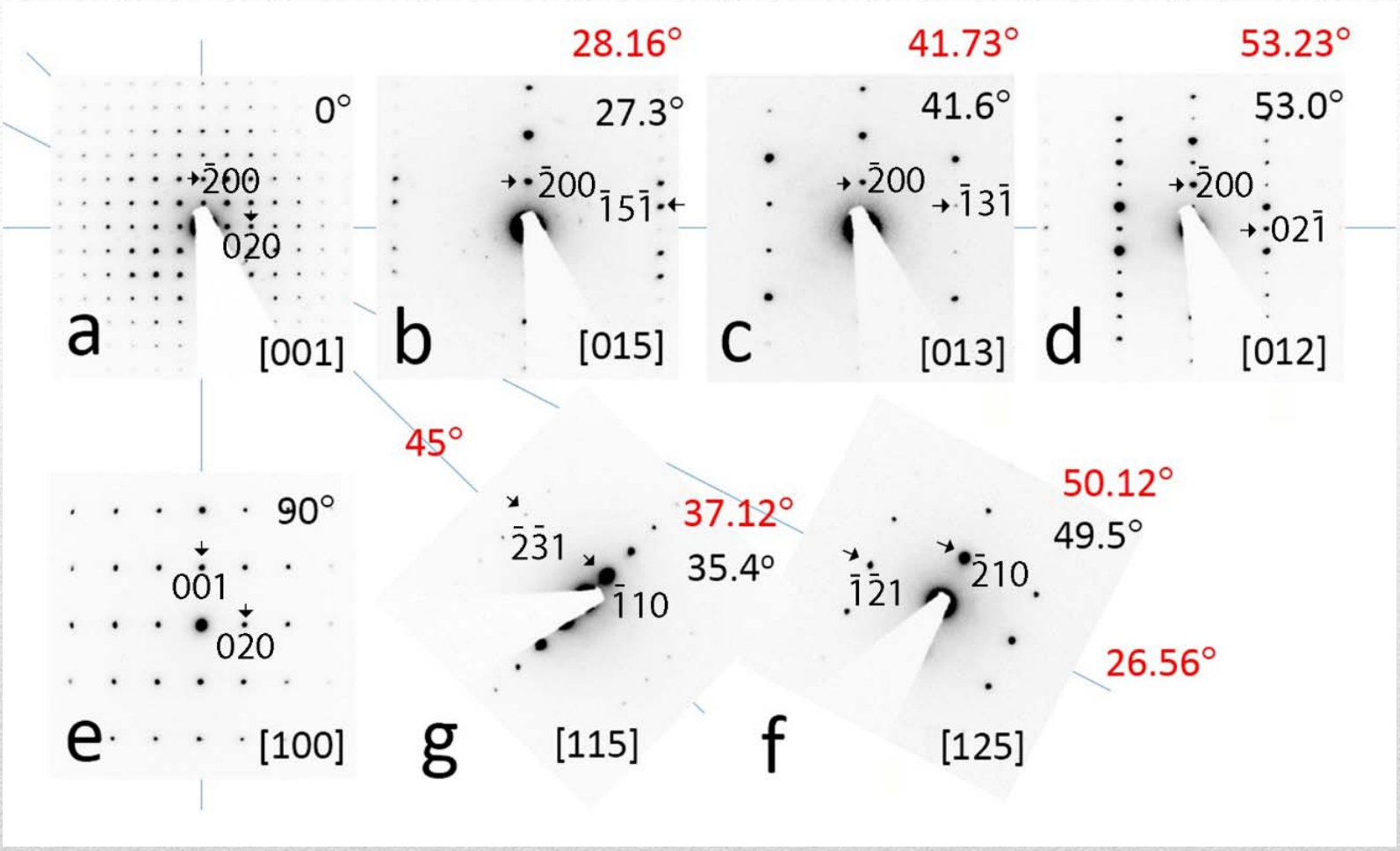
Y.L. Jin, X.Z. Li, and D.J. Sellmyer, Mater. Character. 136 (2018) 302-309.

Application to CoFeCrGe compound

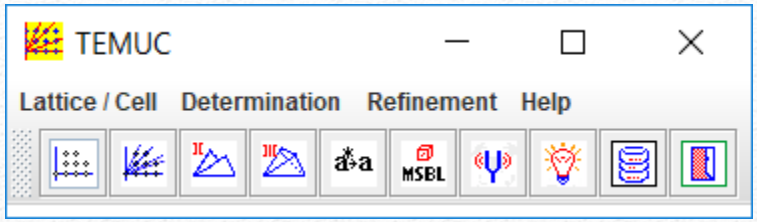


A new tetragonal phase in Co-Fe-Cr-Ge alloy as an example using SPICA to predict the tilt angles for all zone axes within the tilt limitation of the TEM specimen holder.

Application to CoFeCrGe compound



A new tetragonal phase in Co-Fe-Cr-Ge alloy as an example using SPICA to predict the tilt angles for all zone axes within the tilt limitation of the TEM specimen holder.



Unit Cell Determination in Transmission Electron Microscopes

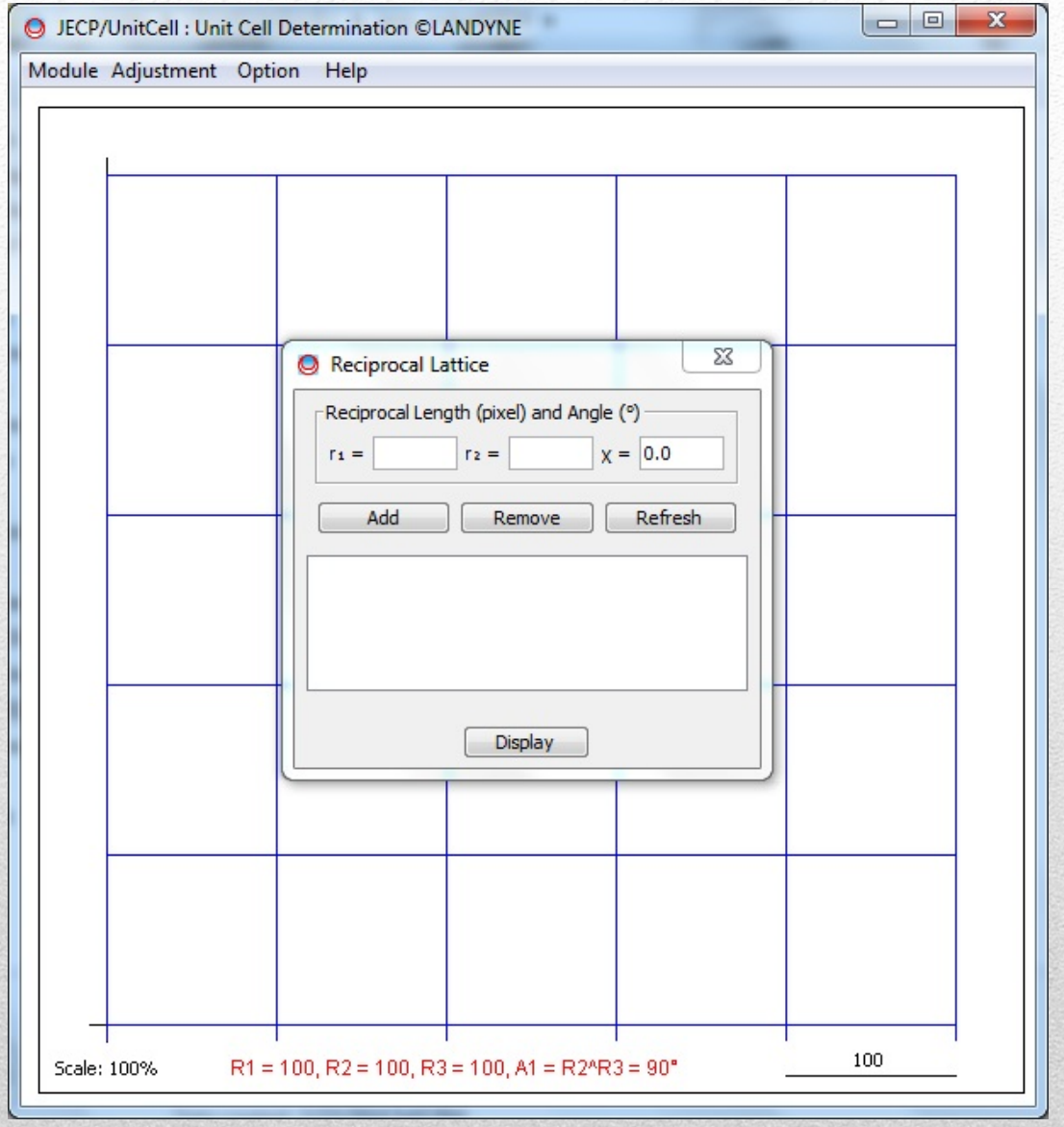
Highlight

Three methods are implemented for Unit-cell determination.

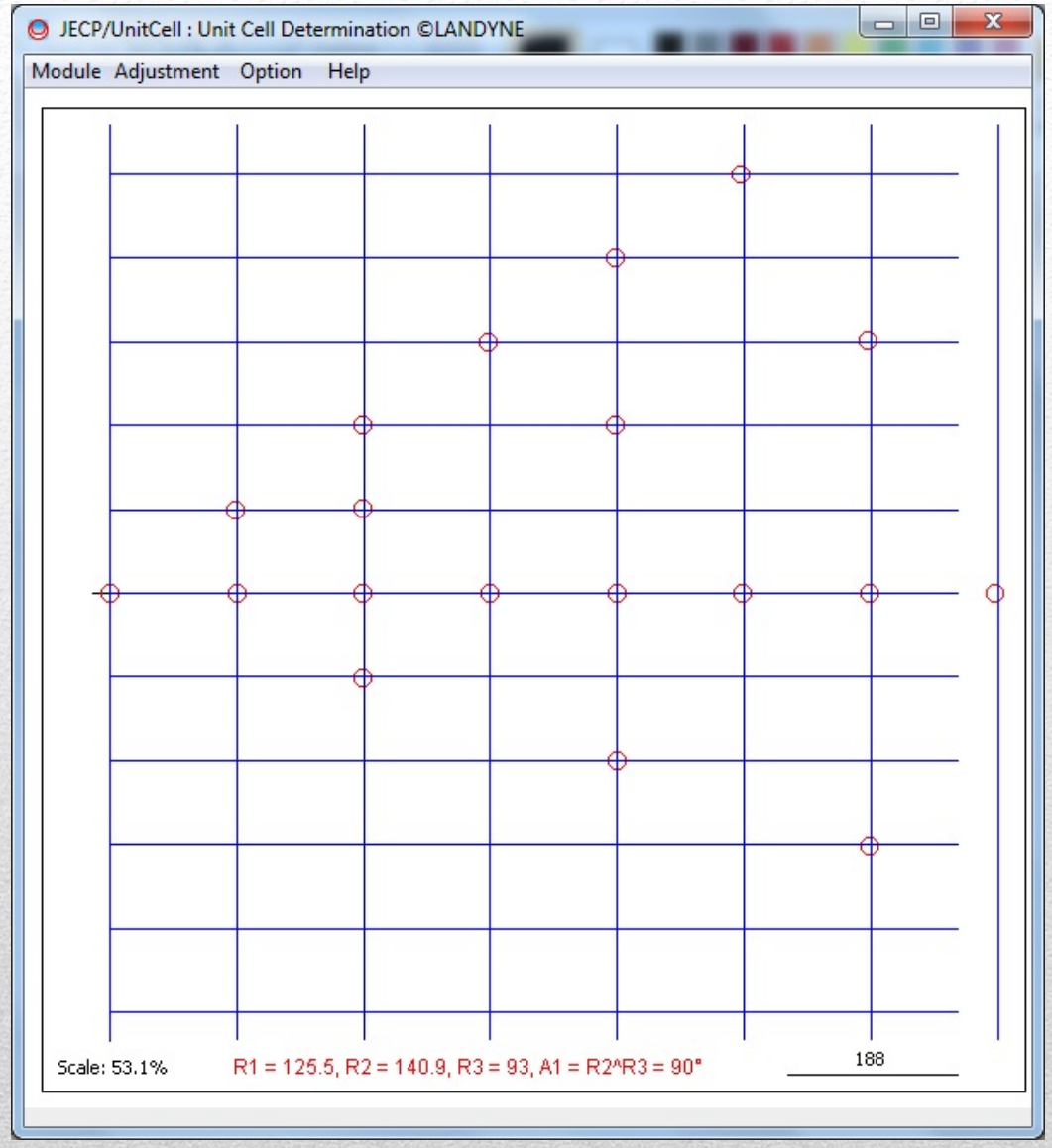
- Reciprocal lattice reconstruction: easy and efficient.
- Reduced cell method: two SAED patterns and angle between them.
- Reduced cell method: three SAED patterns with shared reflections between any two of them.

X.Z. Li, Computer programs for unit-cell determination in electron diffraction experiments, Ultramicroscopy 102 (2005) 269-277.
X.Z. Li, TEMUC3, a computer program for unit-cell determination of crystalline phases in TEM experiments, Micron 117 (2019) 1-7.

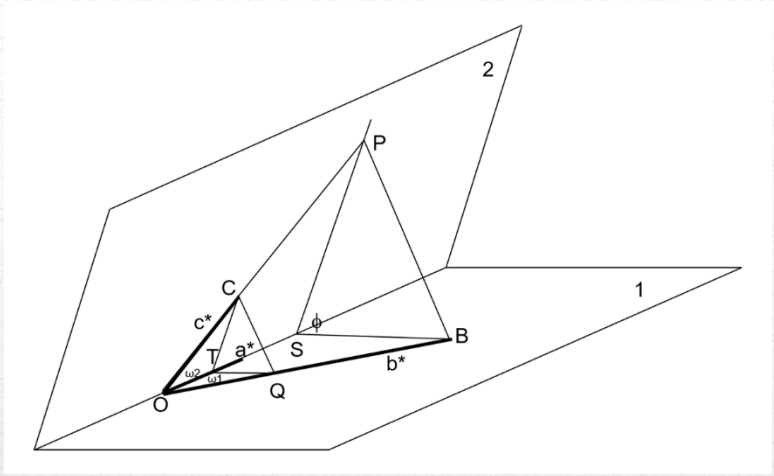
Conventional method

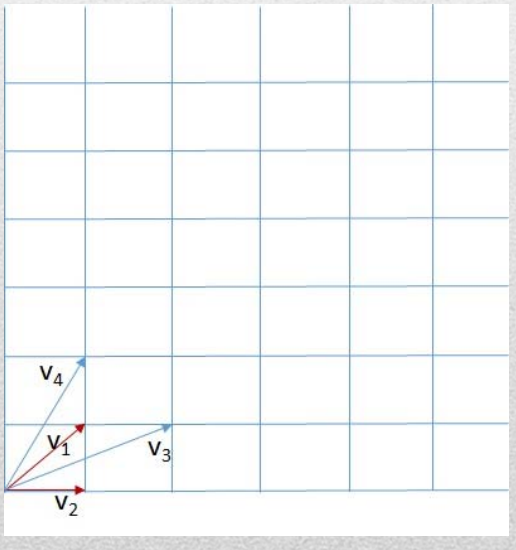


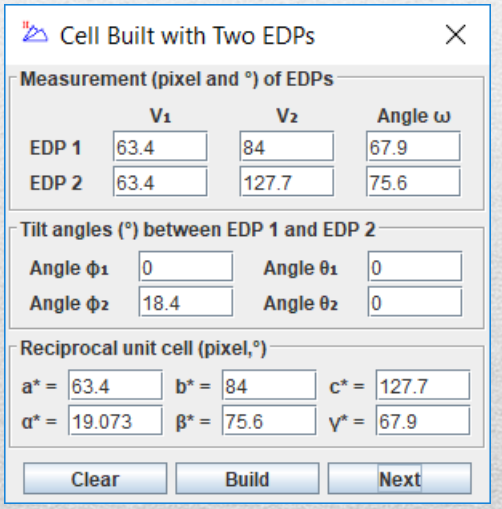
Conventional method



Reduce Cell method I







X.Z. Li, Micron 117 (2019) 1-7.

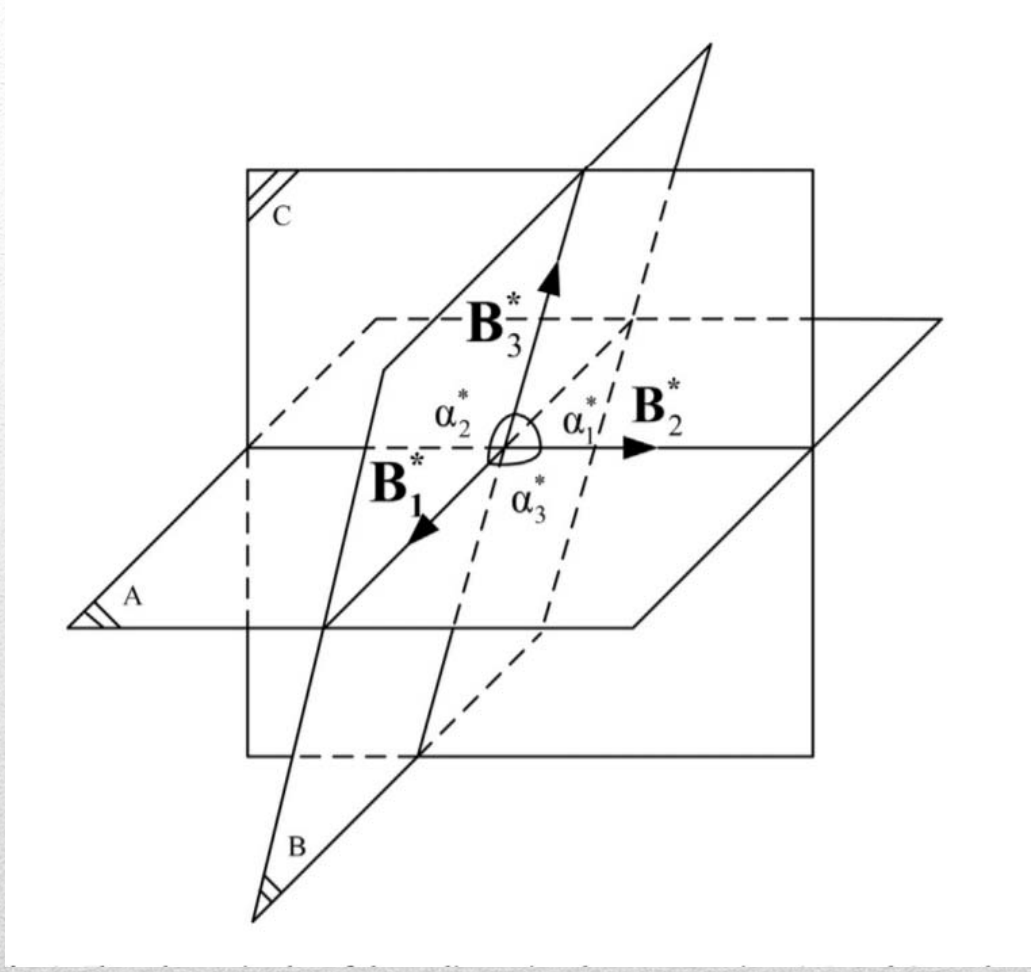
Algorithm I

1. Two SAED patterns with a common axis and tilt angle.
2. Relax the tilt angle in a range.
3. Get the reduced cell.
4. Try another two SAED patterns to get the reduced cell.
5. Compare the closest reduced cell.

---

6. Find the conventional Bravais lattice.

Reduce Cell method II



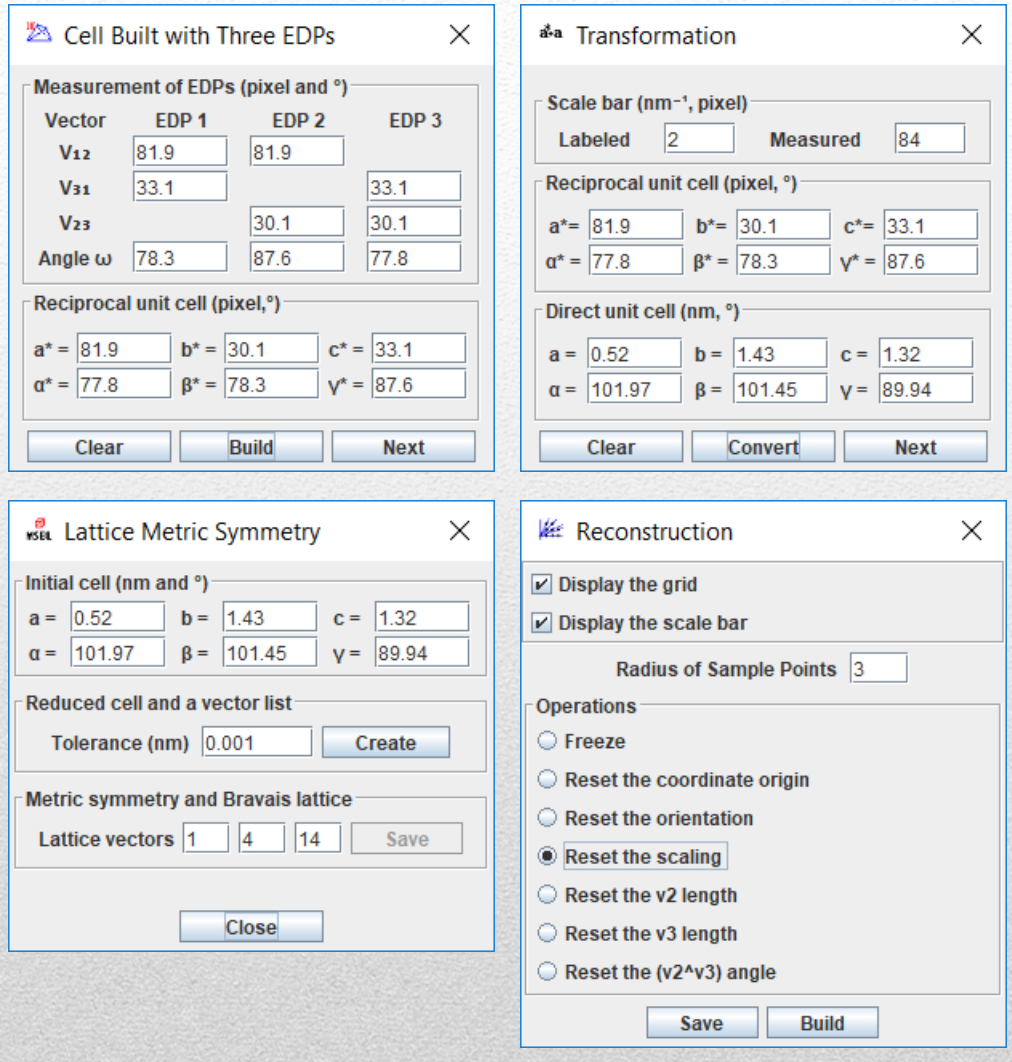
Yi Yang, Canying Cai, Jianguo Lin, Lunjun Gong, Qibin Yang, *Accurate determination of lattice parameters based on Niggli reduced cell theory by using digitized electron diffraction micrograph*, Micron 96 (2017) 9-15.

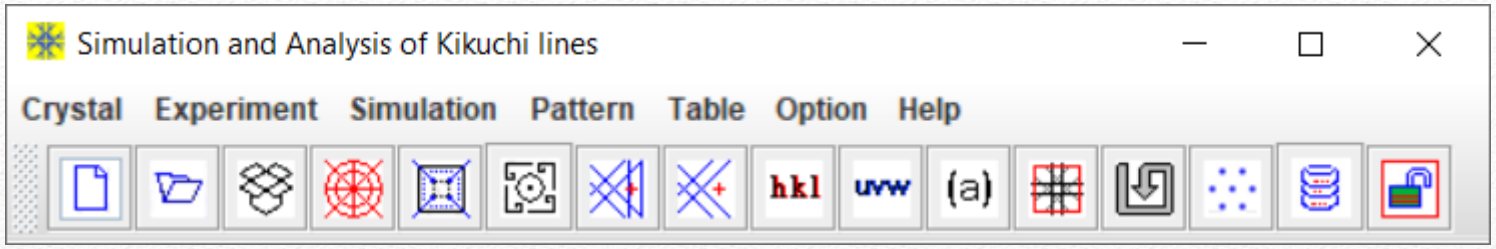
Algorithm II

1. Determination of the basic vectors.
2. Generation of all vectors within a given radius.
3. List the lengths of the vectors after a sorting process.
4. Do 1~3 for a least 3 patterns.
5. Find the common length within a given error threshold.
6. Obtain the cell of the three common vectors.
7. Get the reduce cell.

---

8. Find the conventional Bravais lattice.


Cell Built with Three EDPs
Measurement of EDPs (pixel and °)
Vector EDP 1 EDP 2 EDP 3
V12 81.9 81.9
V31 33.1 33.1
V23 30.1 30.1
Angle ω 78.3 87.6 77.8
Reciprocal unit cell (pixel,°)
a* = 81.9 b* = 30.1 c* = 33.1
α* = 77.8 β* = 78.3 γ* = 87.6
Clear Build Next
Transformation
Scale bar (nm⁻¹, pixel)
Labeled 2 Measured 84
Reciprocal unit cell (pixel, °)
a*= 81.9 b*= 30.1 c*= 33.1
α* = 77.8 β* = 78.3 γ* = 87.6
Direct unit cell (nm, °)
a = 0.52 b = 1.43 c = 1.32
α = 101.97 β = 101.45 γ = 89.94
Clear Convert Next
Lattice Metric Symmetry
Initial cell (nm and °)
a = 0.52 b = 1.43 c = 1.32
α = 101.97 β = 101.45 γ = 89.94
Reduced cell and a vector list
Tolerance (nm) 0.001 Create
Metric symmetry and Bravais lattice
Lattice vectors 1 4 14 Save
Close
Reconstruction
Display the grid
Display the scale bar
Radius of Sample Points 3
Operations
Freeze
Reset the coordinate origin
Reset the orientation
Reset the scaling
Reset the v2 length
Reset the v3 length
Reset the (v2^v3) angle
Save Build



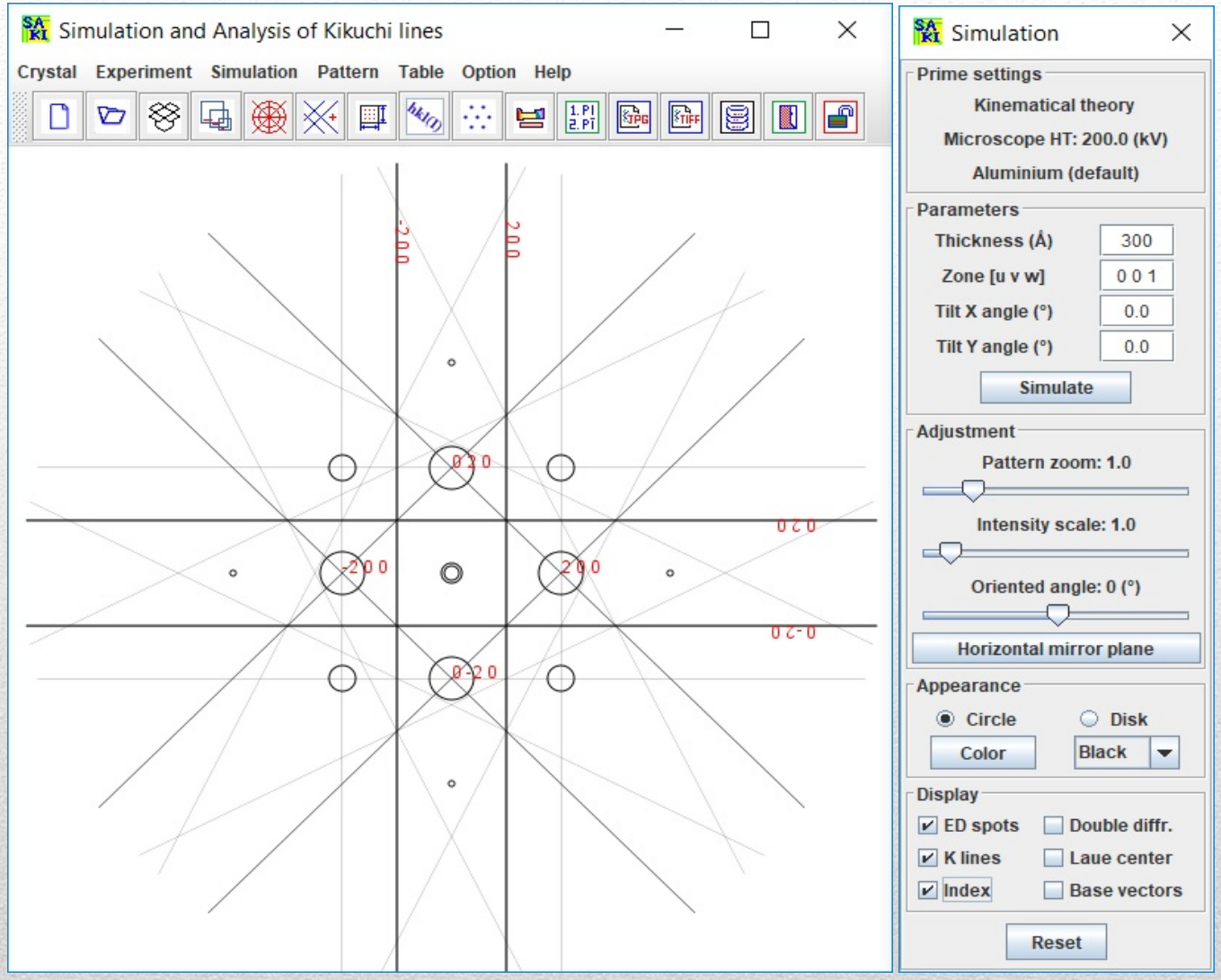
Simulation and Analysis of Kikuchi Patterns

Highlight

- Simulation of Kikuchi patterns with SAED patterns.
- Indices of Kikuchi lines
- Basic image processing of experimental SAED patterns.
- Accurate determination of orientation using a Kikuchi patterns with three poles.
- Simulation of SAED pattern by considering double diffraction effect.
- Save Region of Interest and user-defined TIFF resolution.

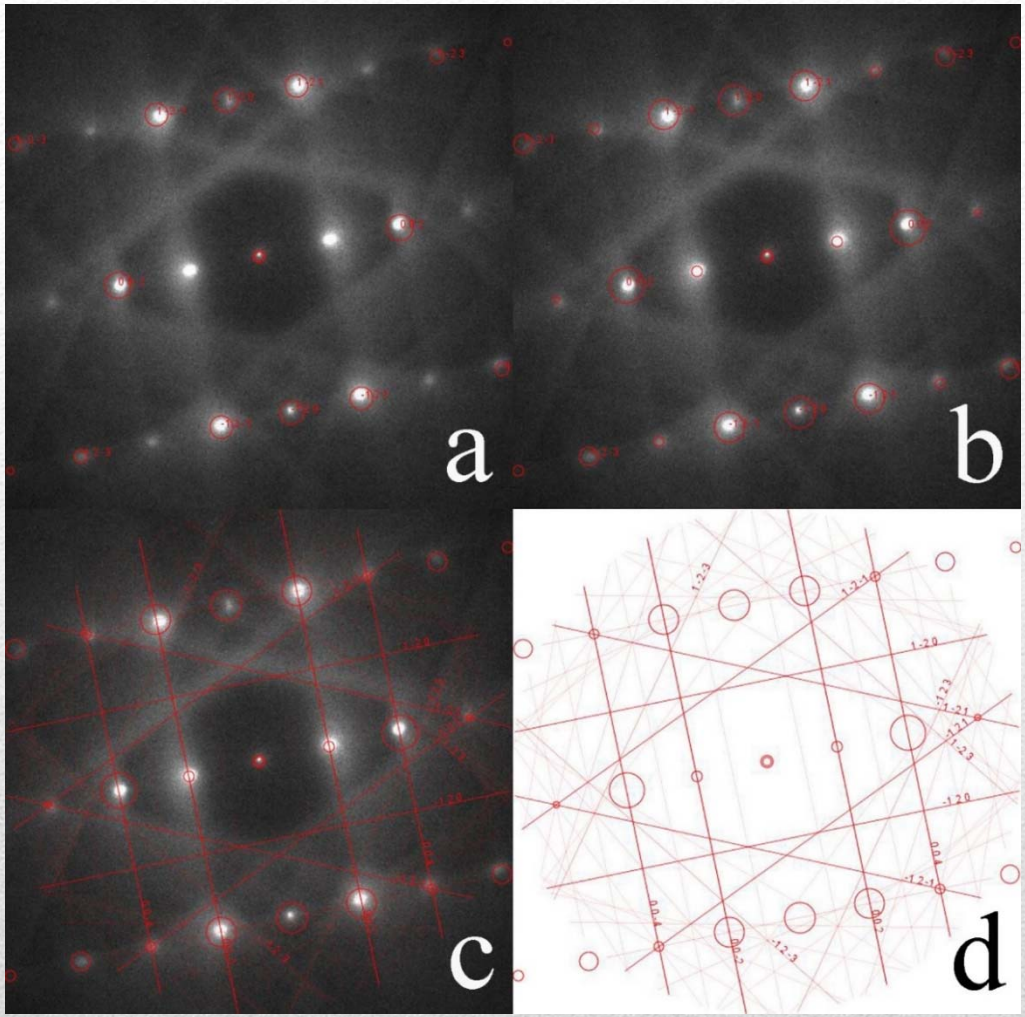
X.-Z. Li, On precise determination of crystal orientation with Kikuchi pattern, Journal of Materials Education, 42 (2020) 99-106.
X.-Z. Li, SAKI, software for simulation and analysis of Kikuchi patterns, Journal of Chinese Microscopy Society, 04 (2021) 398-405.

SAKI: simulation of Kikuchi pattern with index



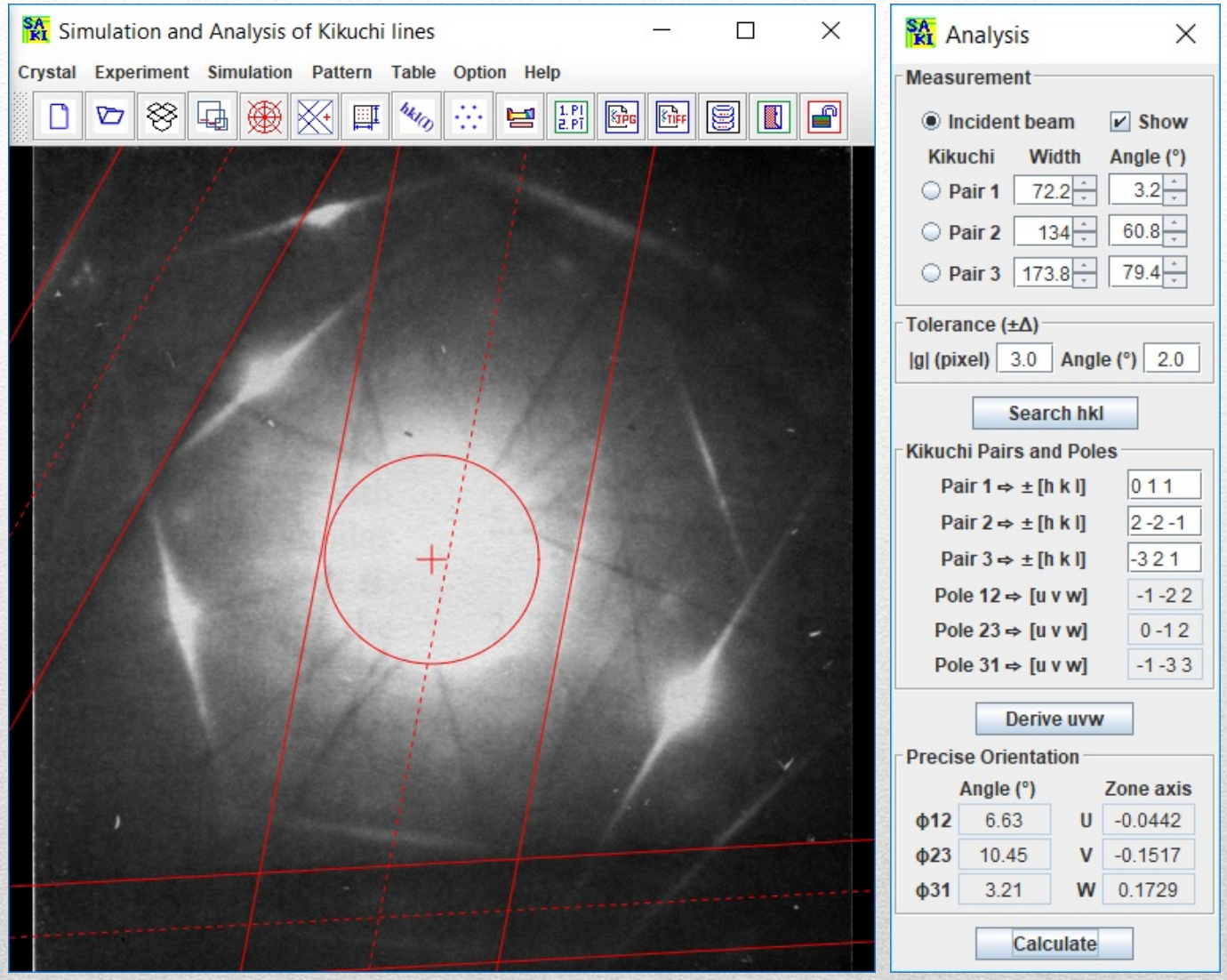
The simulated SAED and Kikuchi pattern with index.

SAKI: simulation of Kikuchi pattern with index



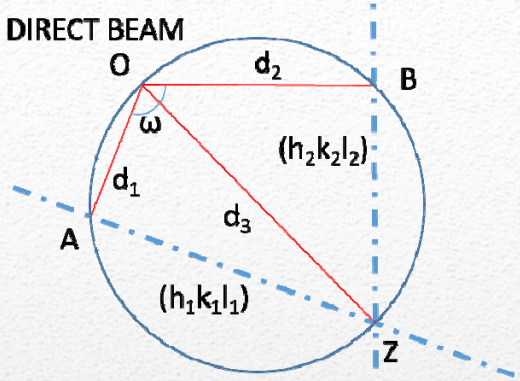
Simulated spot pattern in kinematical diffraction, (b) with double diffraction effect. (c) Simulated Kikuchi pattern supposed on experimental pattern (d) the simulated pattern only for clarity.

SAKI: determination of orientation from three Kikuchi poles

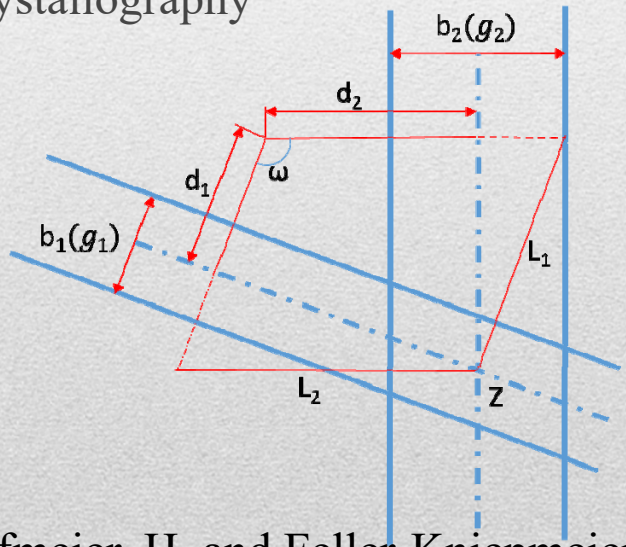


Snap-shot of the main panels in SAKI with analysis of Kikuchi pattern of Mg.

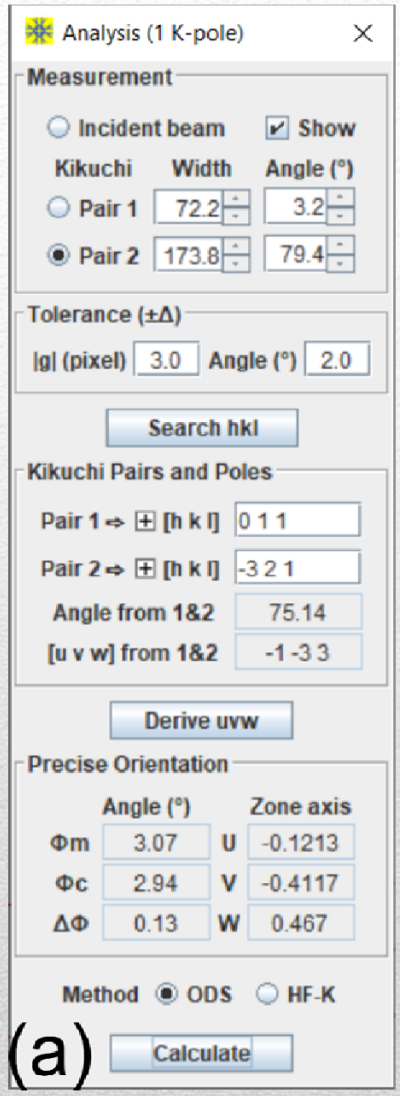
SAKI: determination of orientation from two Kikuchi poles

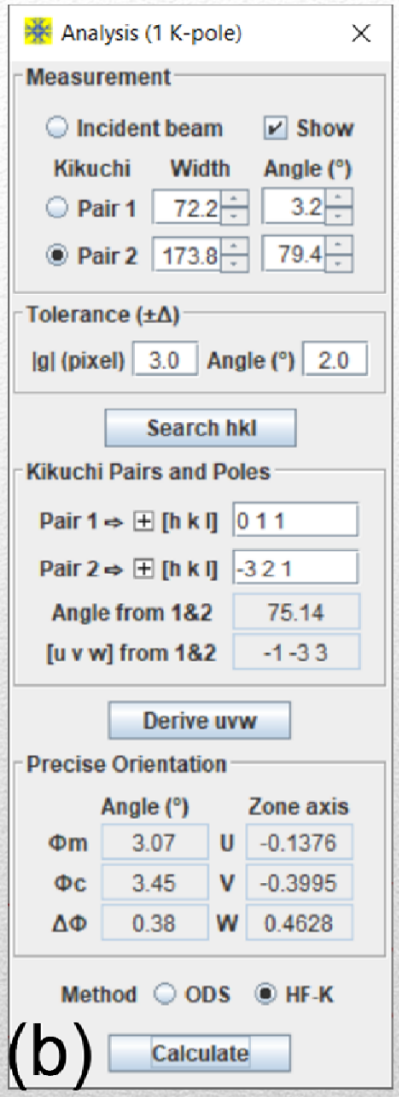


The 14th KH Kuo Summer School on Electron Microscopy and Crystallography

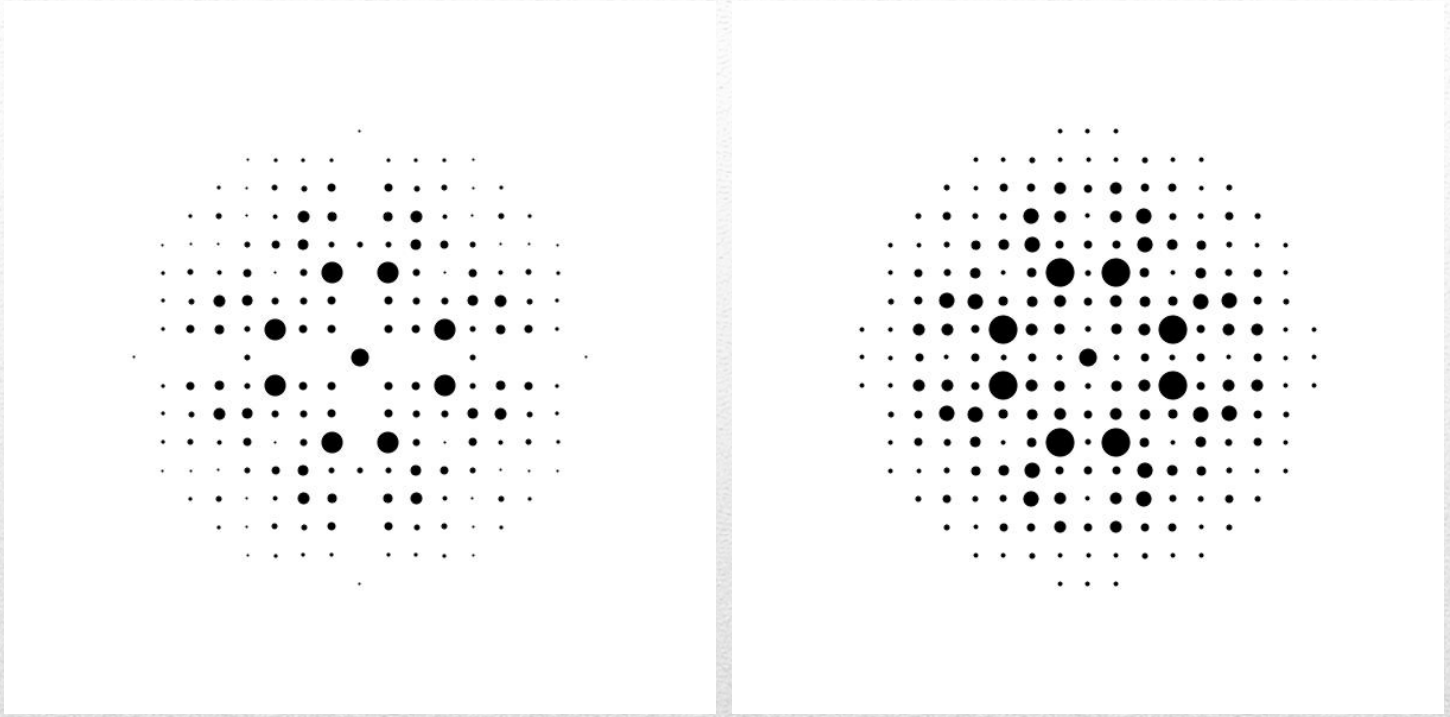


Helfmeier, H. and Feller-Kniepmeier, M. (1977). J. Applied Physics, 48, 3997-3997

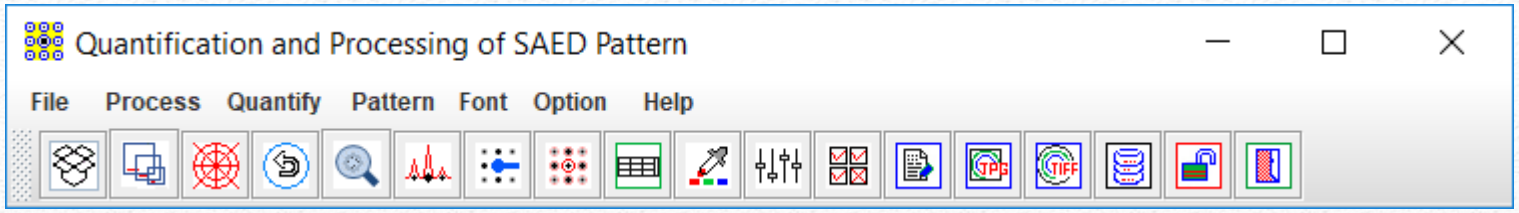




Simulation of double diffraction effect



Crystalline structure: α-Mn, P 4_1 3 2 (213), a = 0.6312 nm.
(a) The simulated SAED pattern and (b) with double diffraction.



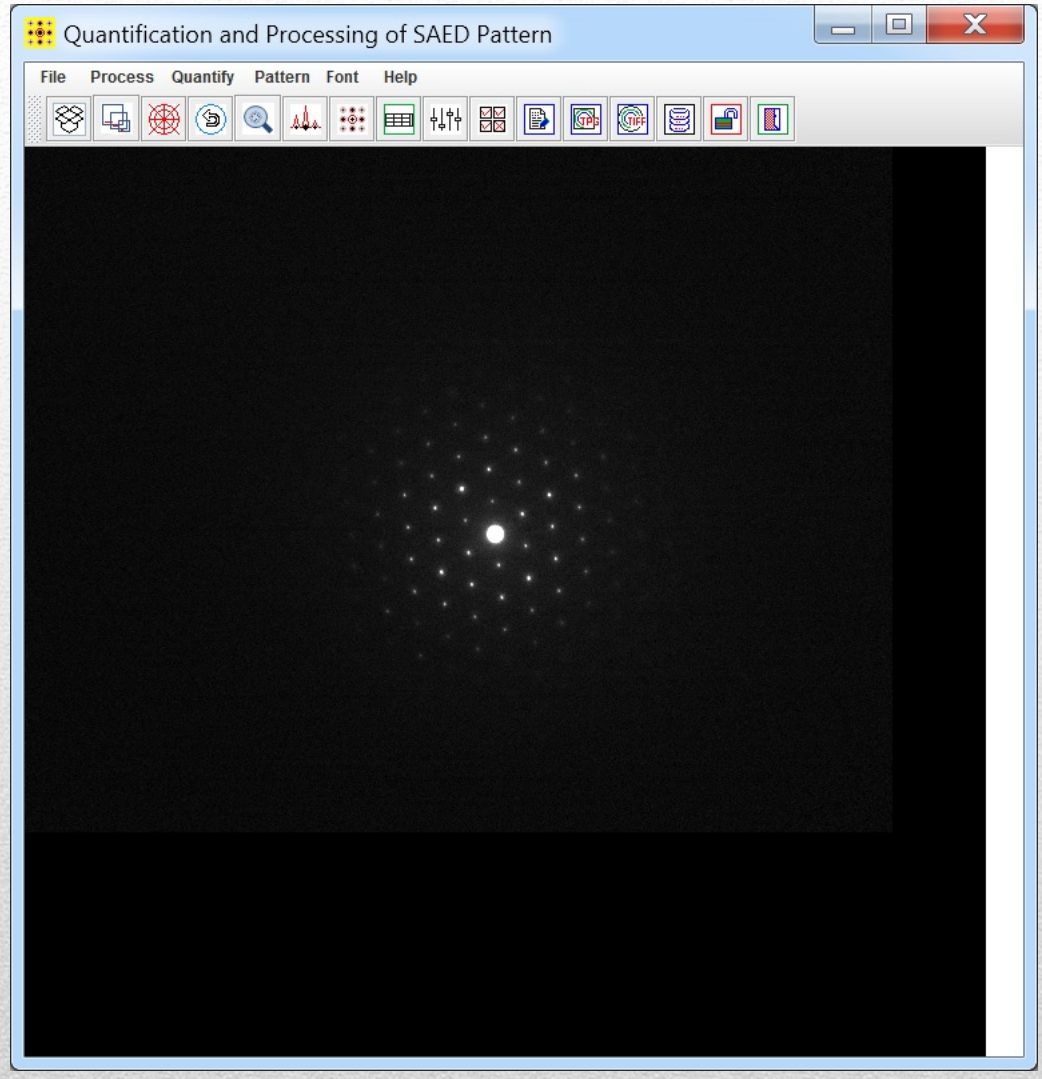
Quantification and Processing of SAED Patterns

Highlight

- Preparation of experimental SAED patterns for publication.
- Precise measurement of the reciprocal lattice spacing.
- Basic image processing of the experimental SAED pattern.
- Retrieval and display of the intensities of SAED patterns of crystal structures and correction by symmetry.
- Line profiles from SAED patterns of crystal structures, including aperiodic crystals.
- Preparation of input data for ESPOT module.
- Save Region of Interest and user-defined TIFF resolution.

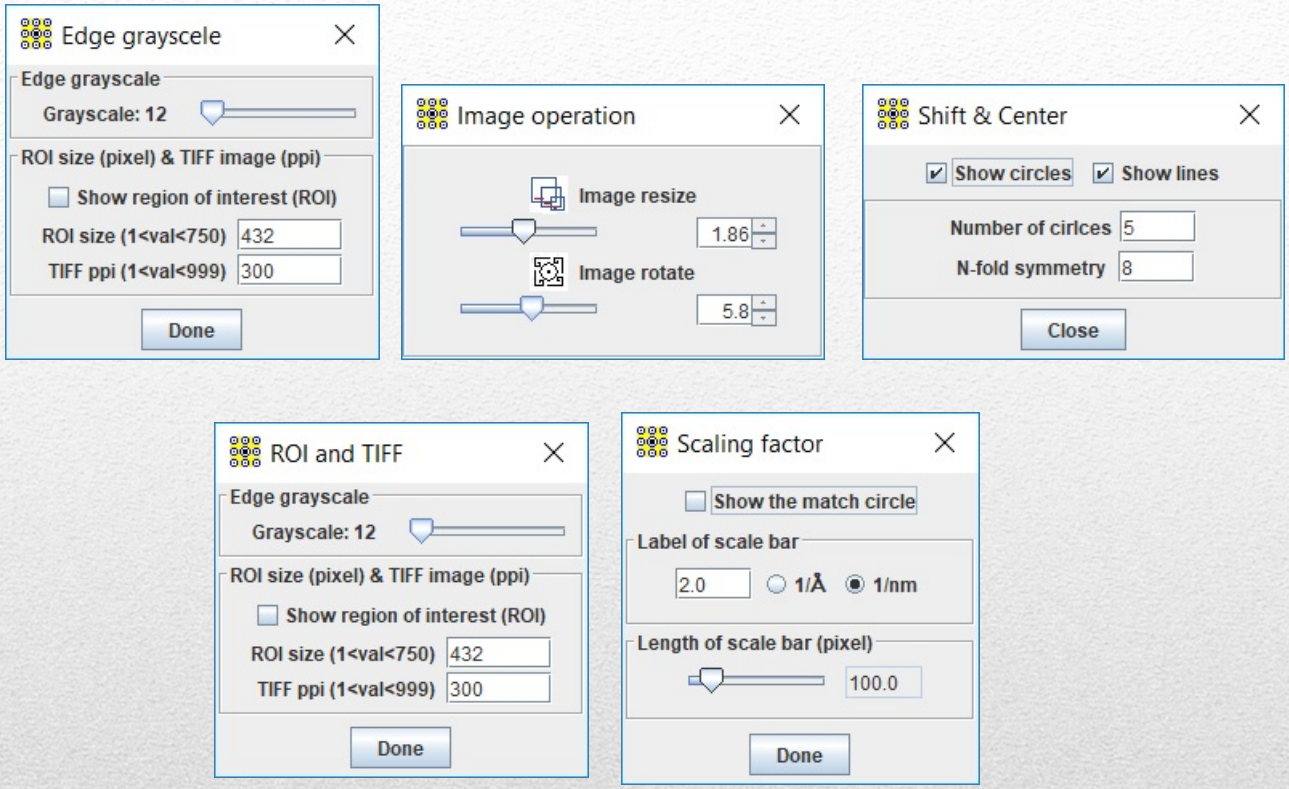
X.-Z. Li, JECP/QSAED, a Computer Program for Quantification of SAED Patterns, Microsc. Microanal. 20S3 (2014) 1486-1487.

QSAED: load an experimental SAED pattern



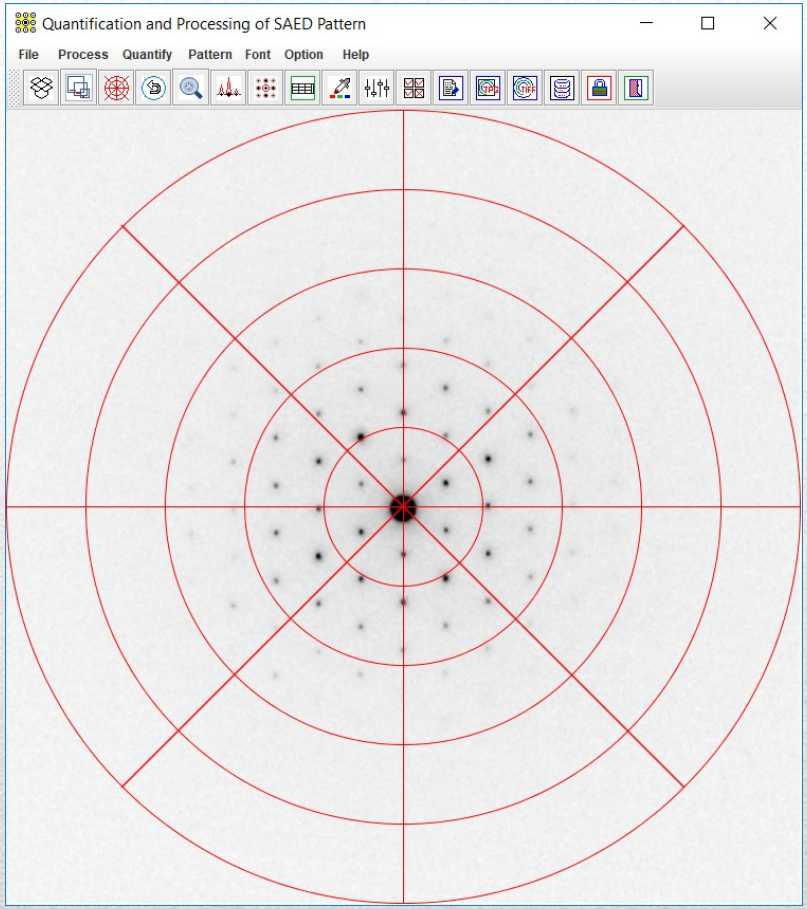
GUI of QSAED with a loaded SAED pattern.

QSAED: operation dialogs



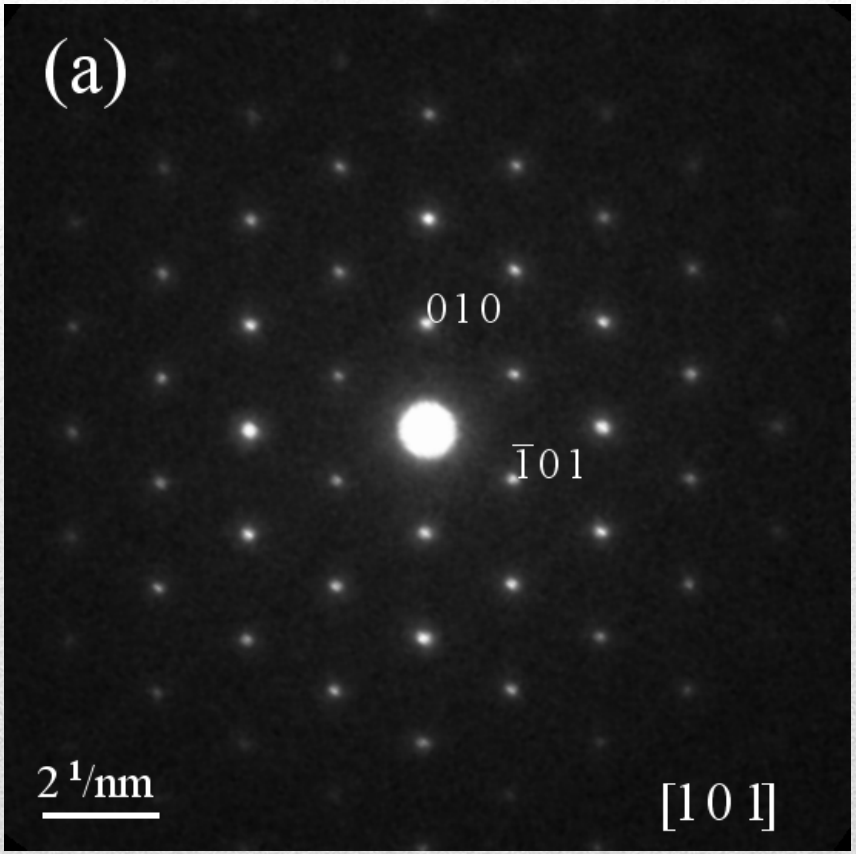
Edge grayscale dialog, resize and rotate dialog, and the shift & center dialog, and scaling factor dialog.

QSAED: load an experimental SAED pattern



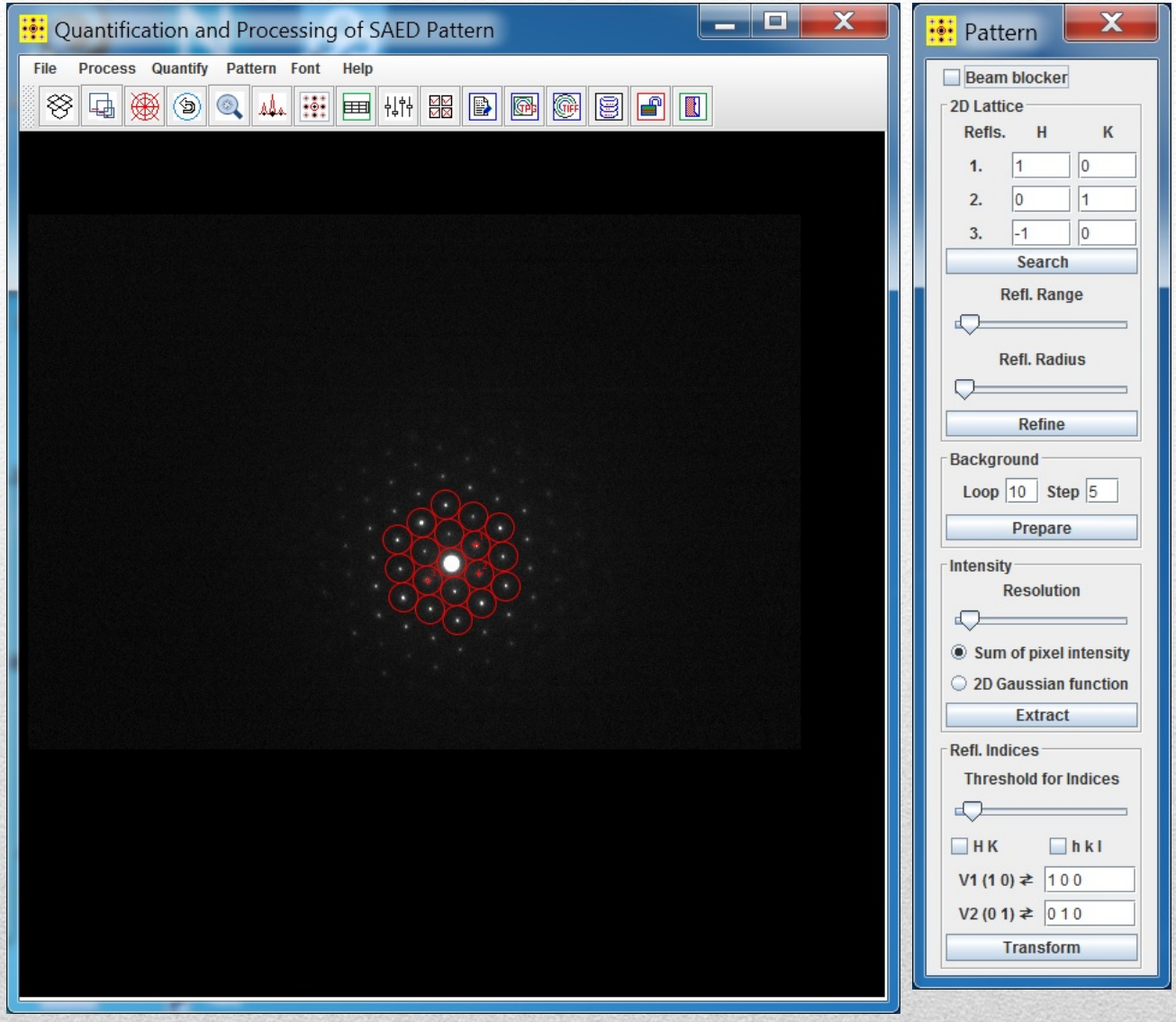
Resize, rotate, center, invert operations on the SAED pattern.

QSAED: fast to prepare the pattern



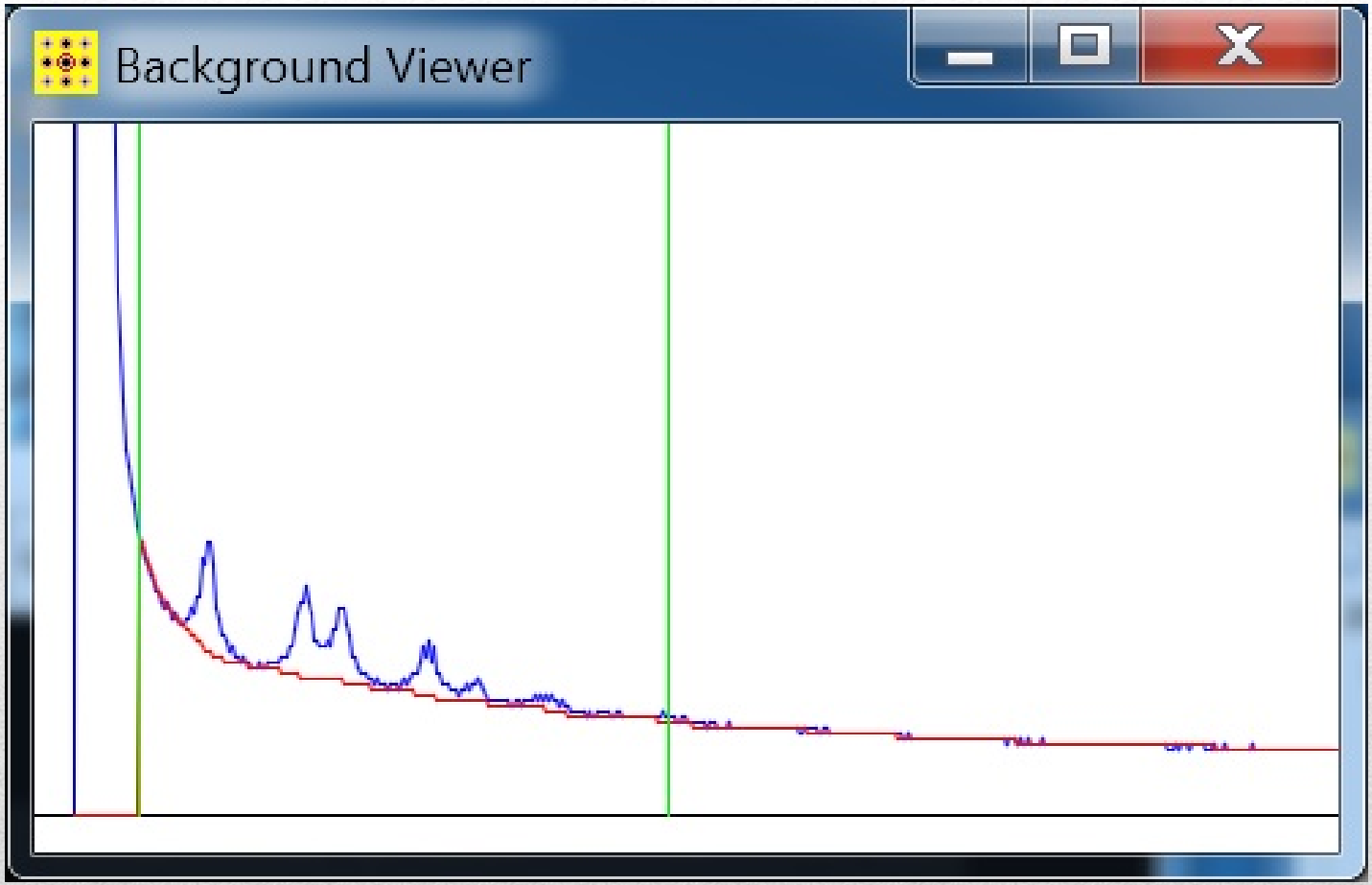
SAED pattern can be easily adjusted for the final report.

QSAED: search for the basic vectors



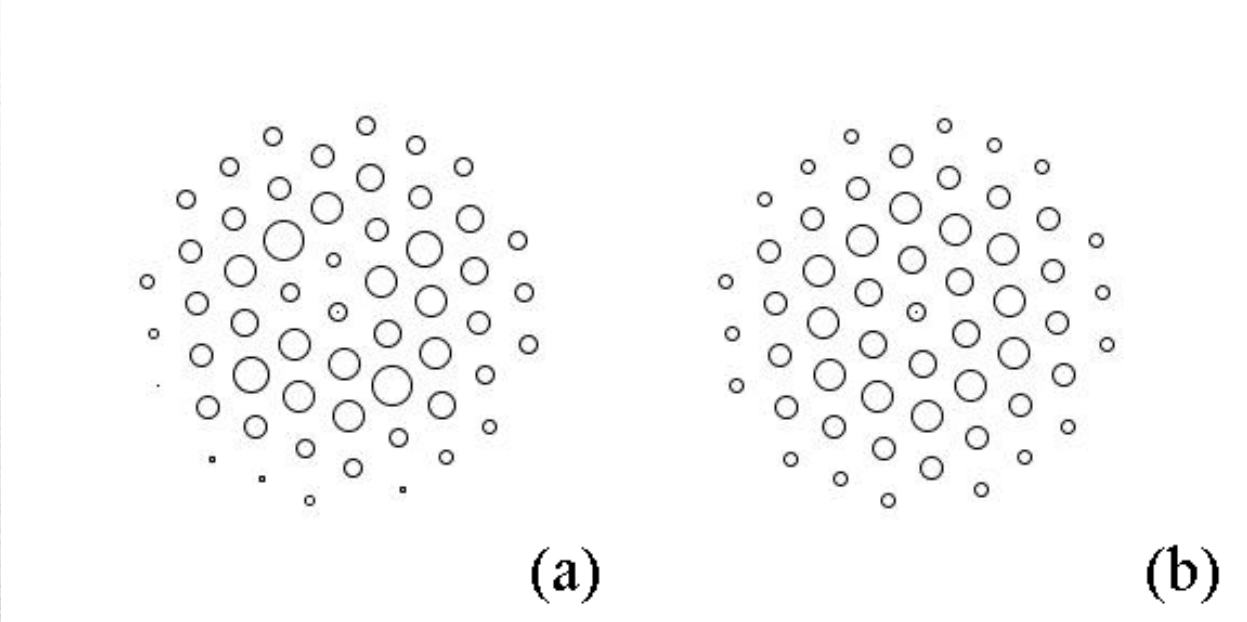
Refinement of reciprocal lattice in QSAED.

QSAED: background intensities



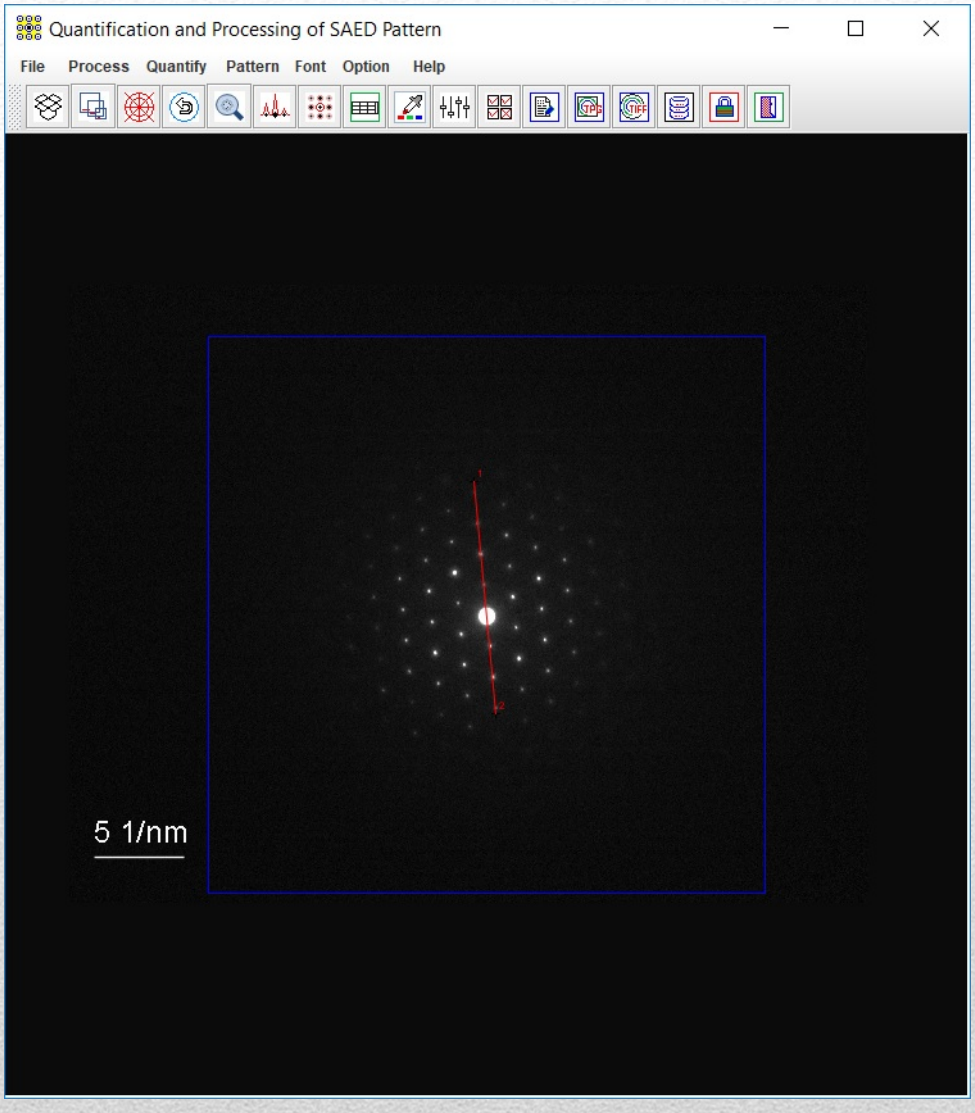
Search background intensities in QSAED.

QSAED: improvement of an SAED pattern



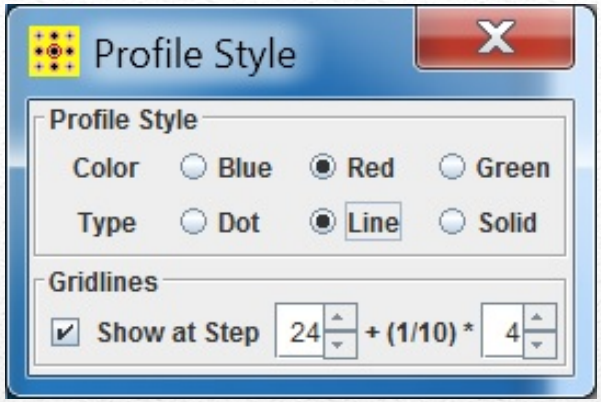
(a) Retrieved intensities and (b) adjusted intensities.

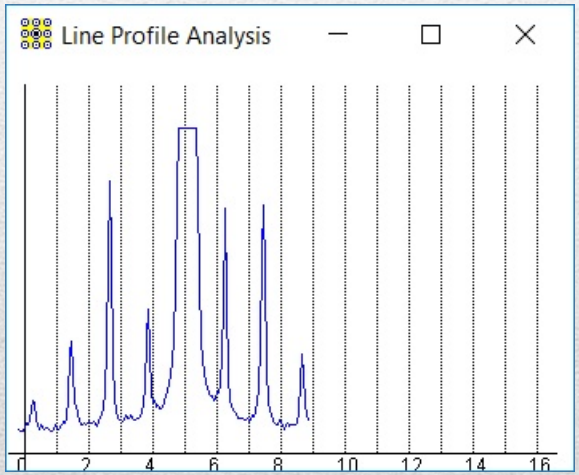
QSAED: retrieve and display the intensities



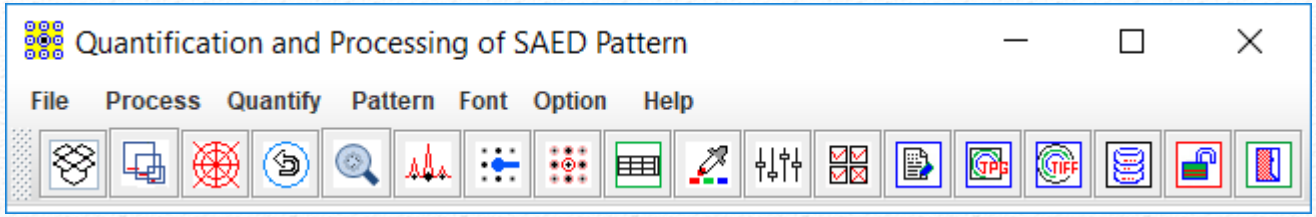
Retrieval of intensities from EDP in QSAED.

QSAED: linear profile retrieve and display





Analysis of line profile from ED pattern in QSAED.



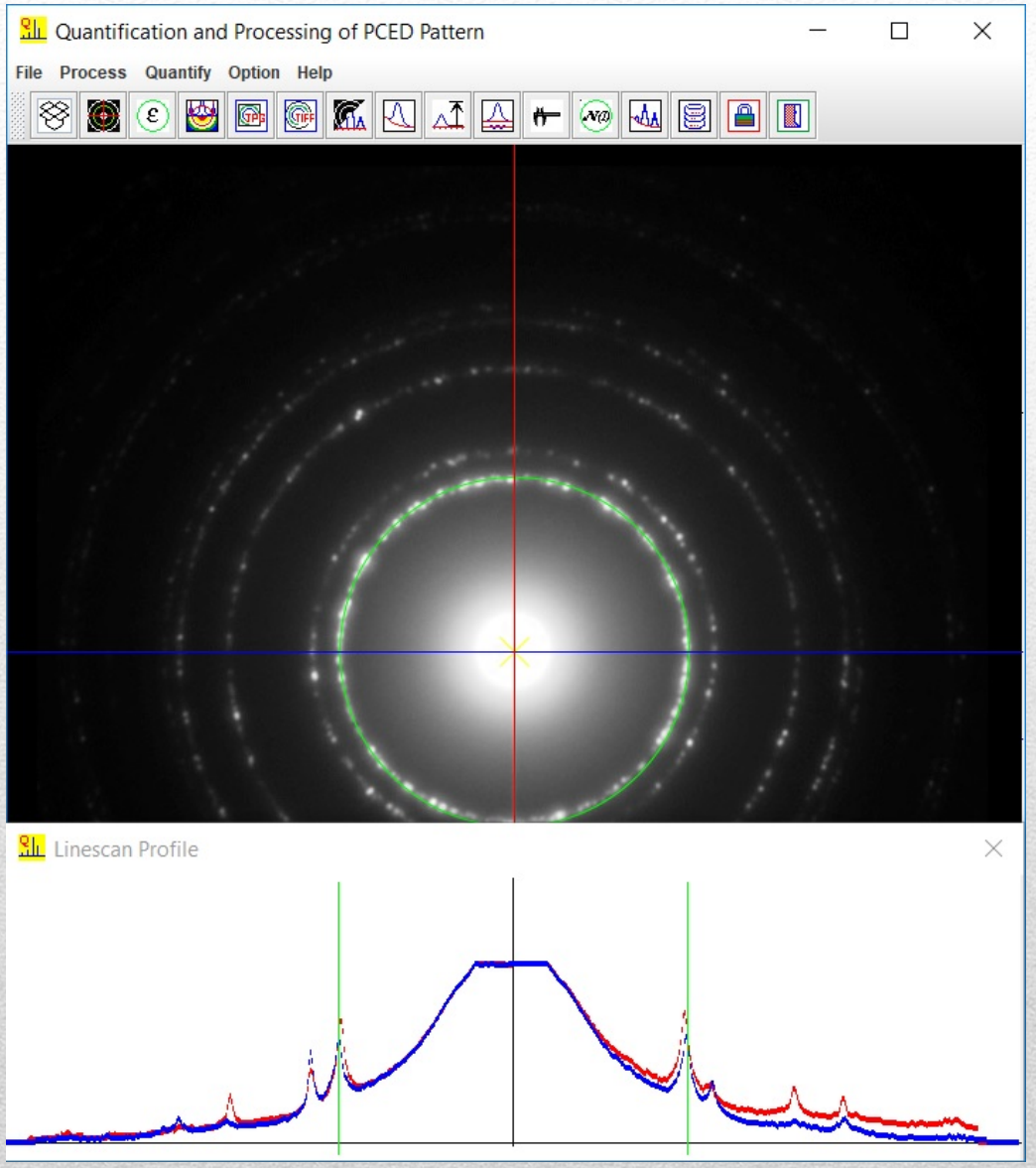
Quantification and Processing of PolyCrystalline SAED Patterns

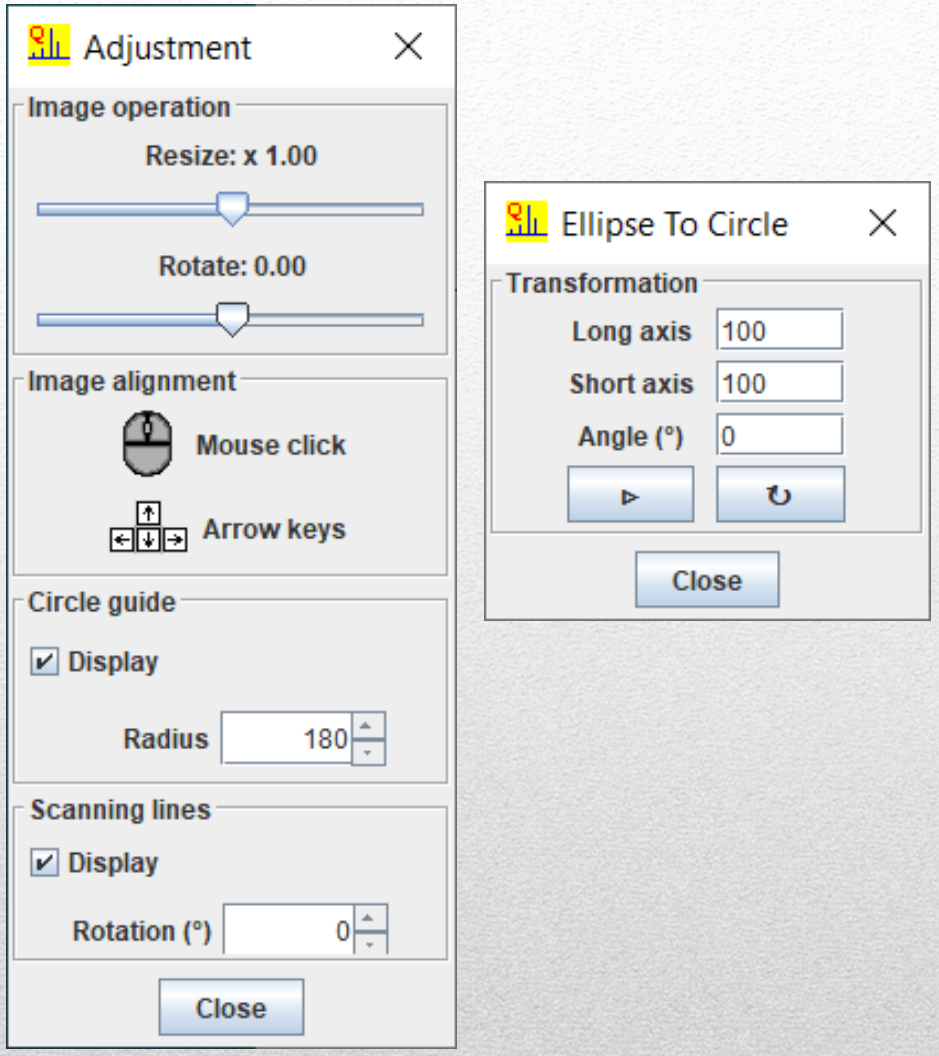
Highlight

- Ellipticity correction.
- Pseudo-color pattern enhancement.
- Max intensity profile and ring highlight.
- Ring intensities -> Intensity profile.
- Background subtraction.
- Profile analysis: peak profile.
- Retrieval of intensities.
- Lattice parameter refinement.

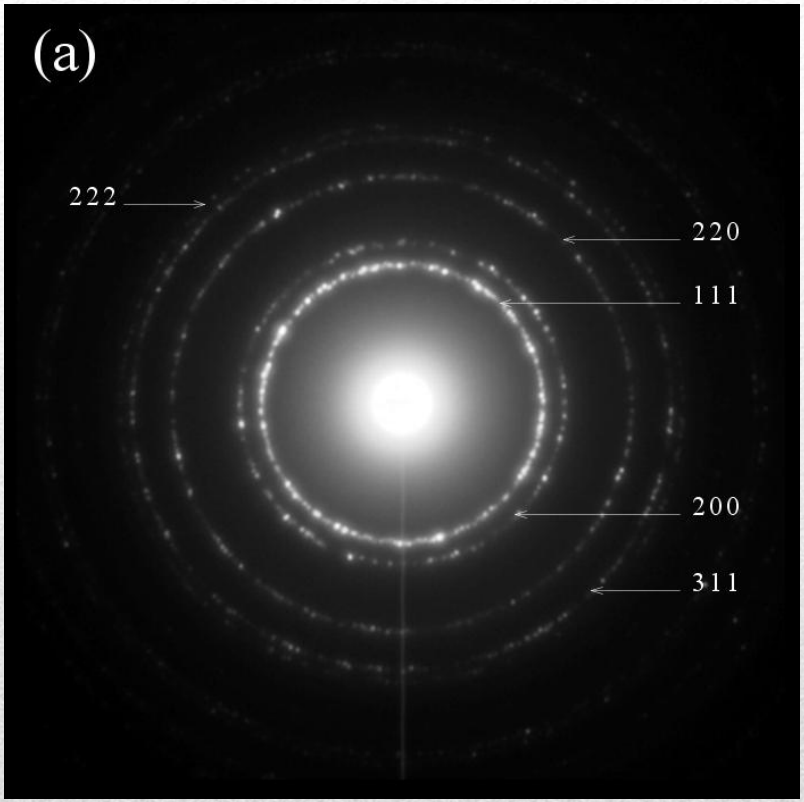
X.Z. Li, QPCED2. 0: a computer program for the processing and quantification of polycrystalline electron diffraction patterns, J. Appl. Crystallogr., 45, 862 (2012).

QPCED


Quantification and Processing of PCED Pattern
File Process Quantify Option Help
Linescan Profile

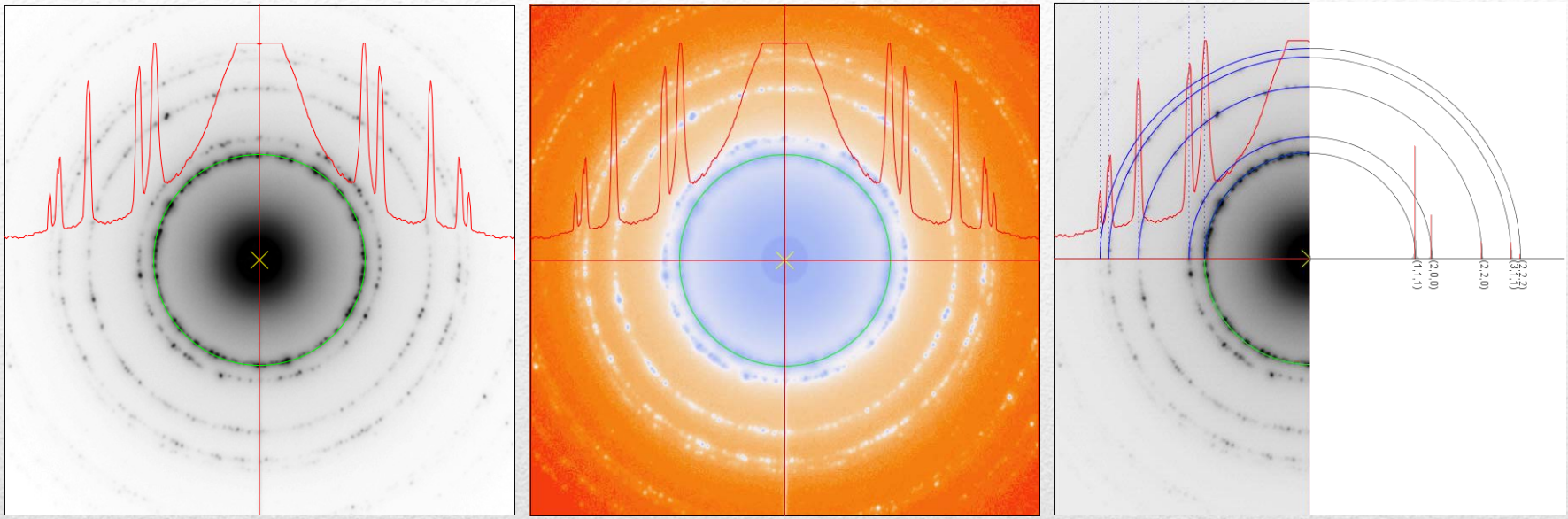


The adjustment dialog and (b) the ellipticity dialog.



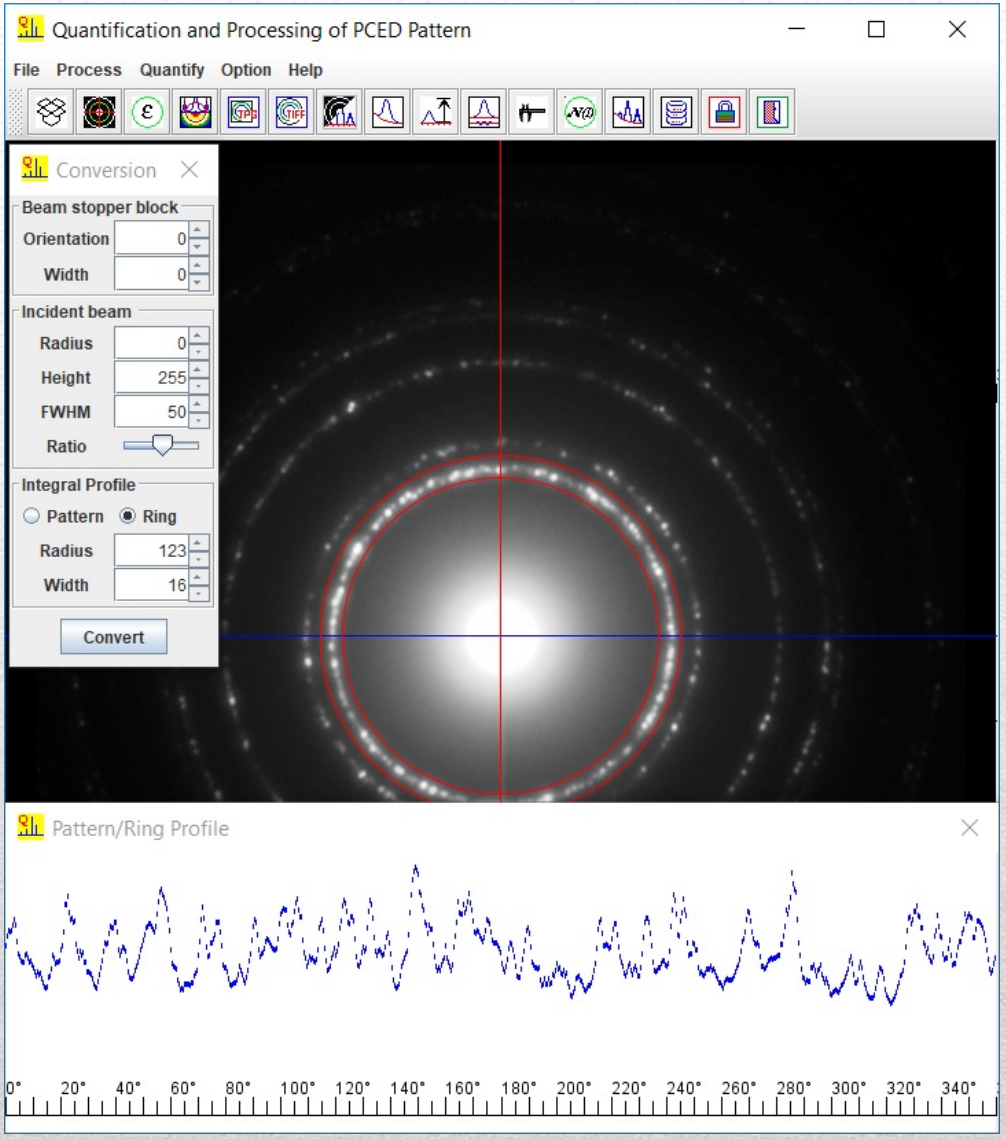
Preparation of a figure for publication.

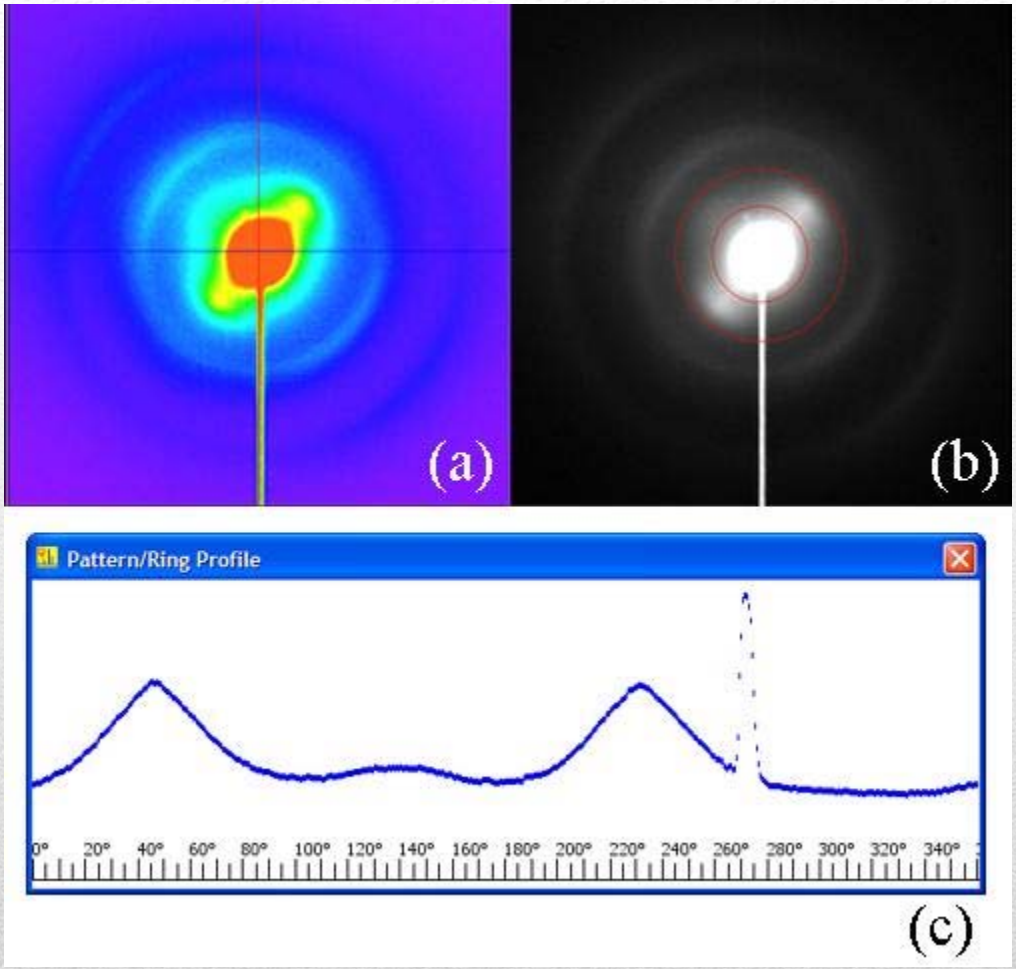
QPCED



The profile of maximum diffraction intensities and pseudo-coloring of an SAED pattern.

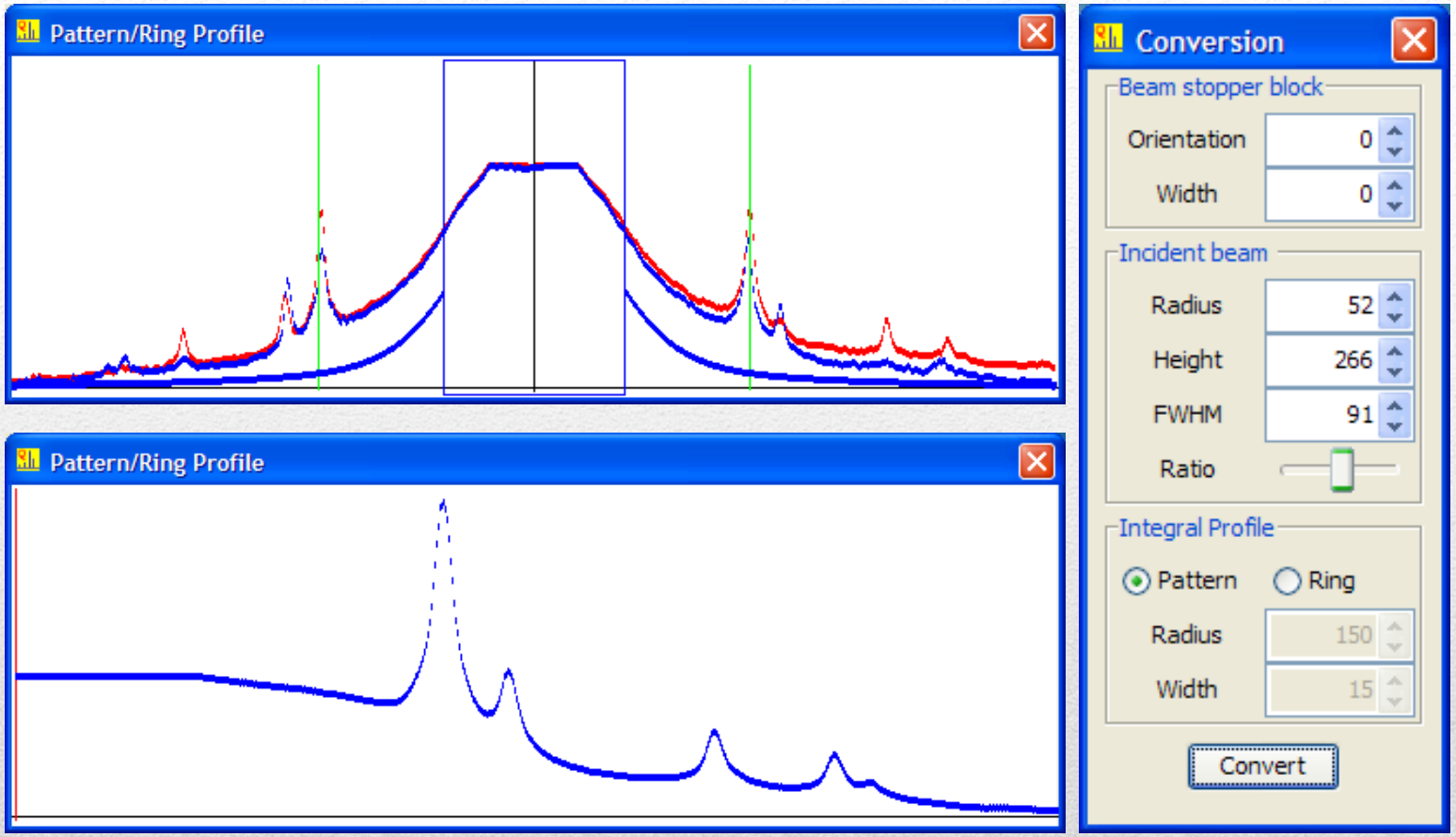
QPCED


Quantification and Processing of PCED Pattern
File Process Quantify Option Help
Conversion
Beam stopper block
Orientation 0
Width 0
Incident beam
Radius 0
Height 255
FWHM 50
Ratio
Integral Profile
Pattern Ring
Radius 123
Width 16
Convert
Pattern/Ring Profile
0° 20° 40° 60° 80° 100° 120° 140° 160° 180° 200° 220° 240° 260° 280° 300° 320° 340°



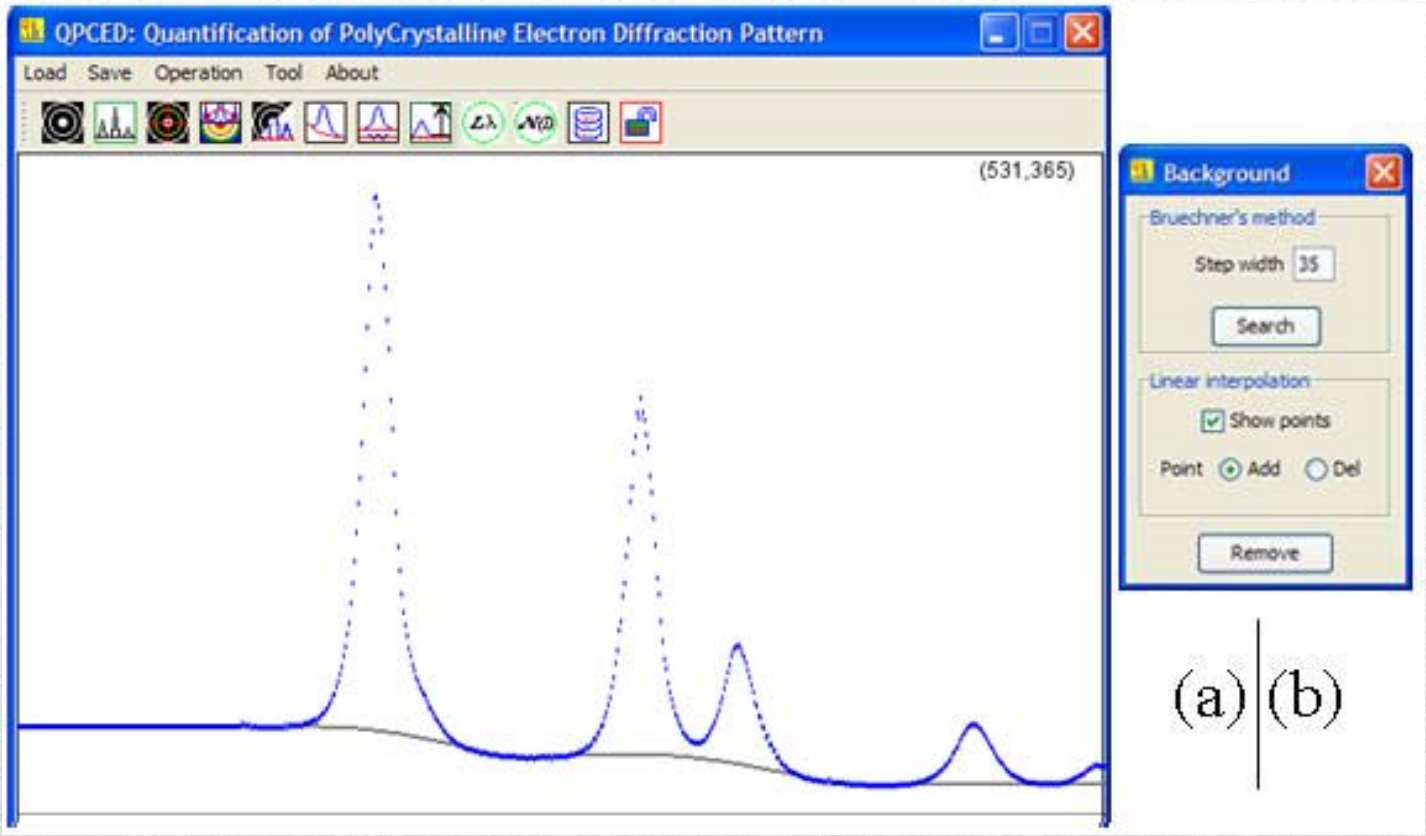
Intensity distribution along diffraction ring due to texture. Carbon fiber composite as an example.

QPCED



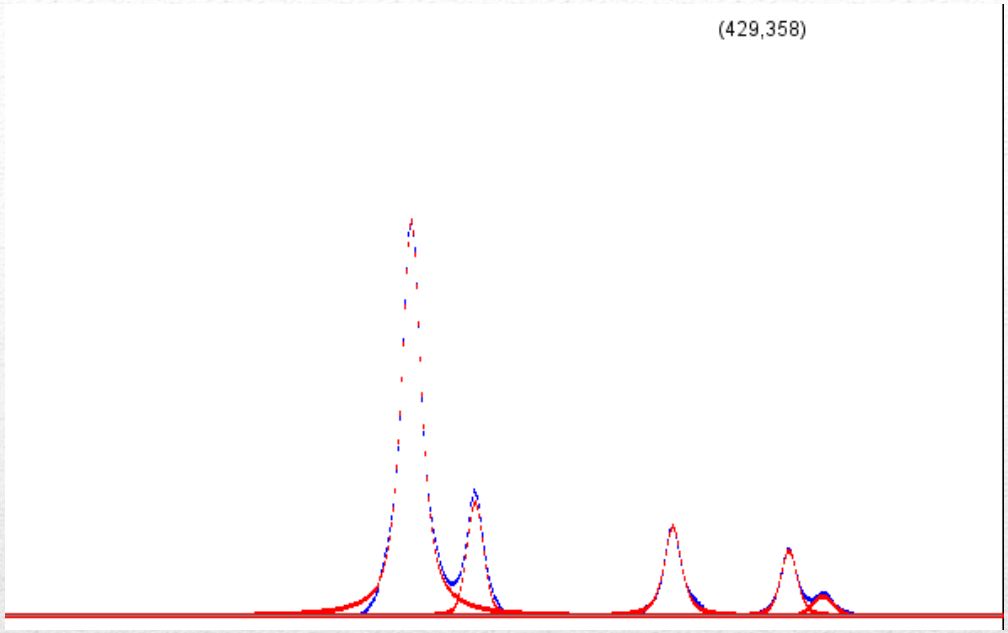
Remove the incident beam and average the intensity profile.

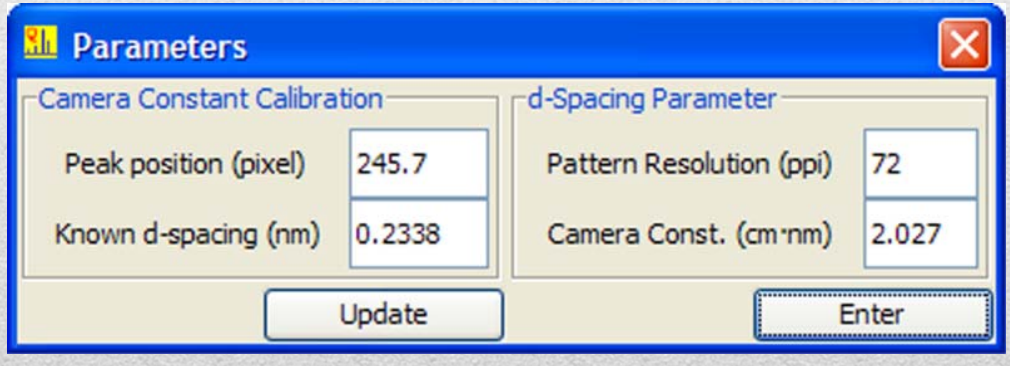
QPCED

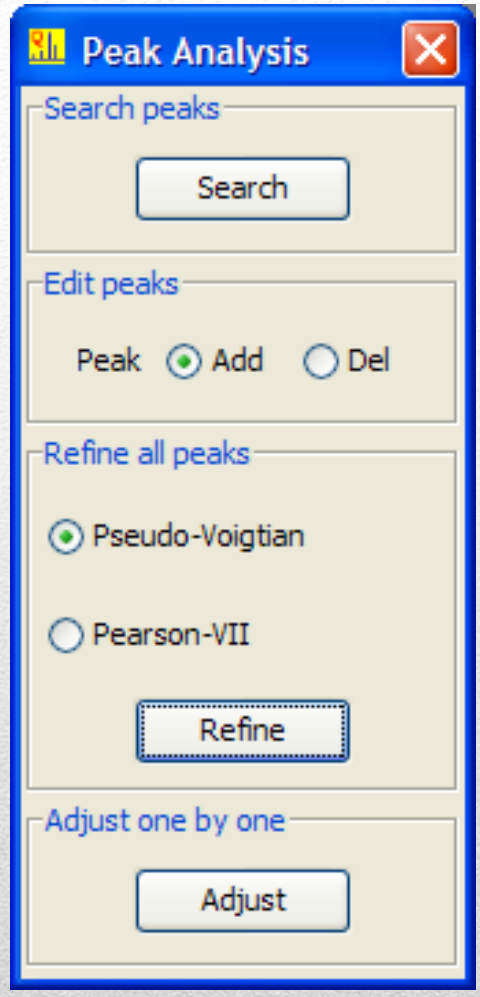


Background can be defined either automatically or manually.

QPCED

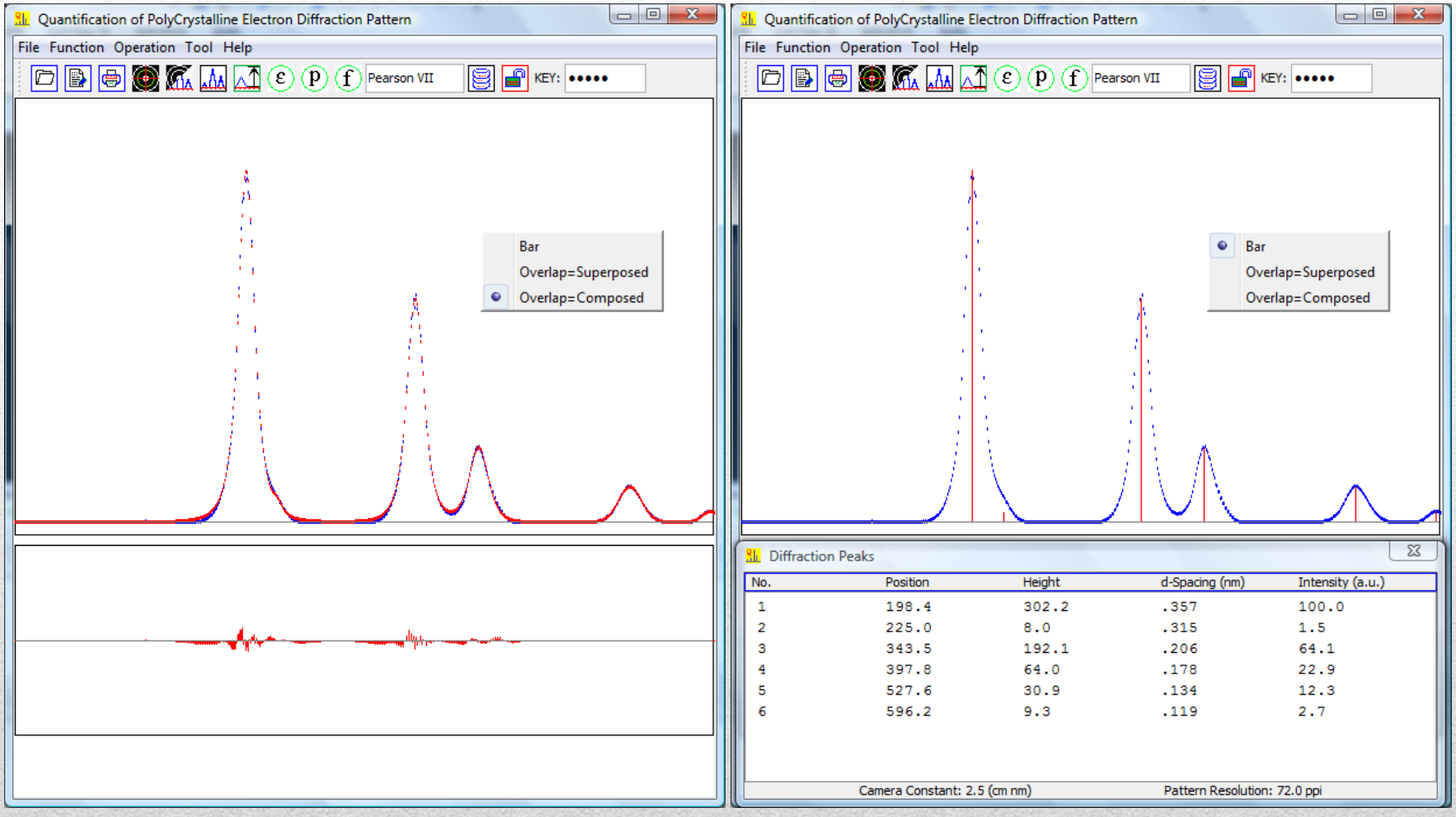




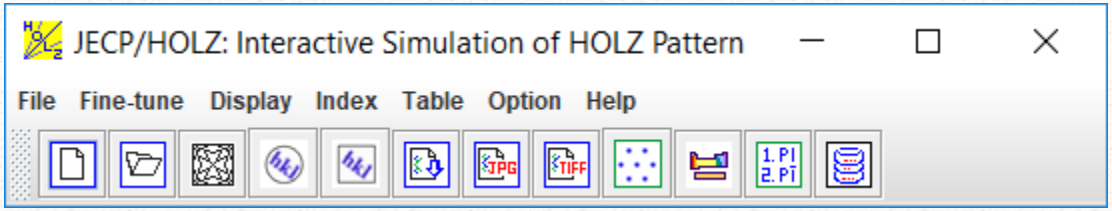


Analysis of the intensity profile by fitting of the diffraction peaks, least-square refinement and manual trial-and-error.

QPCED



Retrieval of the intensities for diffraction peaks.



An Interactive Computer Program for Simulation of HOLZ Pattern with Correction of Dynamical Effect

Highlight

- Simulation of the higher-order Laue zone (HOLZ) lines using kinematical approximation and a first-order dynamic correction.
- Various schemes for indices of the HOLZ lines.
- Dual-view of convergent-beam pattern and HOLZ lines in disk.

X.Z. Li, JECP/HOLZ–an interactive computer program for simulation of HOLZ patterns, J. Appl. Crystallogr., 38, 576-577 (2005).

Formulas of the HOLZ lines under kinematical theory

A HOLZ line in the kinematical approximation is the locus of the Bragg condition for a HOLZ reflection **g**. The incident beam **k** is described as $\mathbf{k}_n$ along **-z** and $\mathbf{k}_t$ in (**x**, **y**) plane. We may think of the HOLZ line as a function of K_t, a vector which originates in the center of the zone axis and extends to a point of interest in the central disk, the trajectory is described by the following two equations (Spencer and Zuo, 1992):

$$g_x k_x + g_y k_y - g_z k_z + \frac{g^2}{2} = 0$$

$$k_z = \sqrt{(k^2 - k_x^2 - k_y^2)}$$

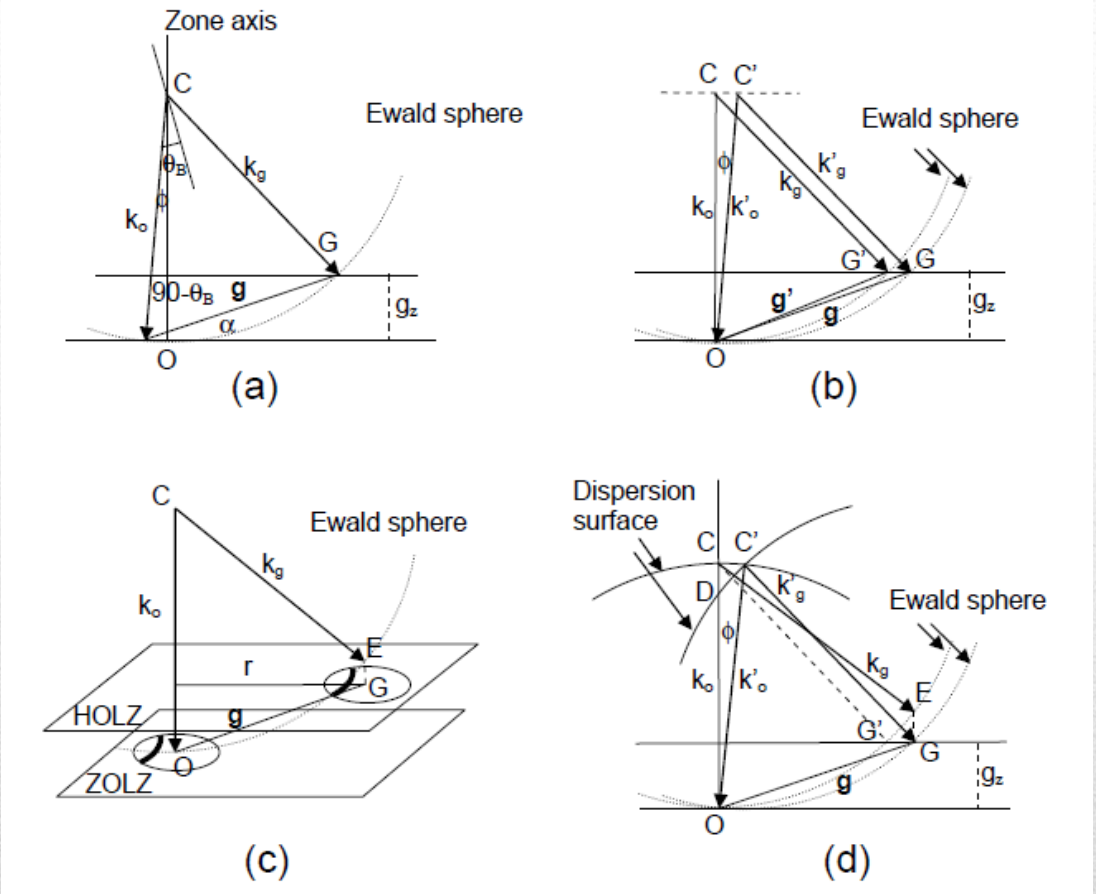
Here: $g^2 = g_x^2 + g_y^2 + g_z^2$

If we use a paraboloid equation, $k_z = k - \frac{k_x^2 + k_y^2}{2k}$ as an approximation of the sphere equation, $k_z = \sqrt{(k^2 - k_x^2 - k_y^2)}$ we end up with an equation for the HOLZ line trajectory (Li, 2007):

$$(k_x + \frac{g_x}{g_z}k)^2 + (k_y + \frac{g_y}{g_z}k)^2 = k^2 + (\frac{g}{g_z}k)^2 - \frac{g^2}{g_z}k$$

J.C.H. Spence, and J.M. Zuo (1992). *Electron microdiffraction*, Plenum Press.
X.Z. Li, *J. Mater. Educ.* 29, 177 (2007).

HOLZ



Schematic diagrams to show the formation of the HOLZ lines based on the kinematic approximation. (a) the rigorous kinematic model, (b) the "kinematically incorrect" model, (c) similar to the (b) scheme, but with curved HOLZ lines, (d) the dispersion surface construction.

Formulas of the HOLZ lines under first-order dynamical correction

In the first-order dynamical correction, it is assumed that only weak interactions occur between HOLZ reflections, the position of a HOLZ line can be approximated by finding the intersection between the zero-layer dispersion surface ($k_1=k_0+\gamma^{(1)}$, here $\gamma^{(1)}$ is the distance of the topmost excited branch of the dispersion surface from the sphere at the zone axis itself) and a plane-wave sphere centered on the HOLZ reflection (Bithell and Stobbs, 1989; Lin et al. 1989; Zuo, 1992).

When the incident beam is far away from a zone axis, the first branch of the dispersion surface can be approximately considered as sphere with radii of $k_1=k_0+\gamma^{(1)}$. Thus, the dynamically corrected HOLZ-line equation is derived as (Li, 2007):

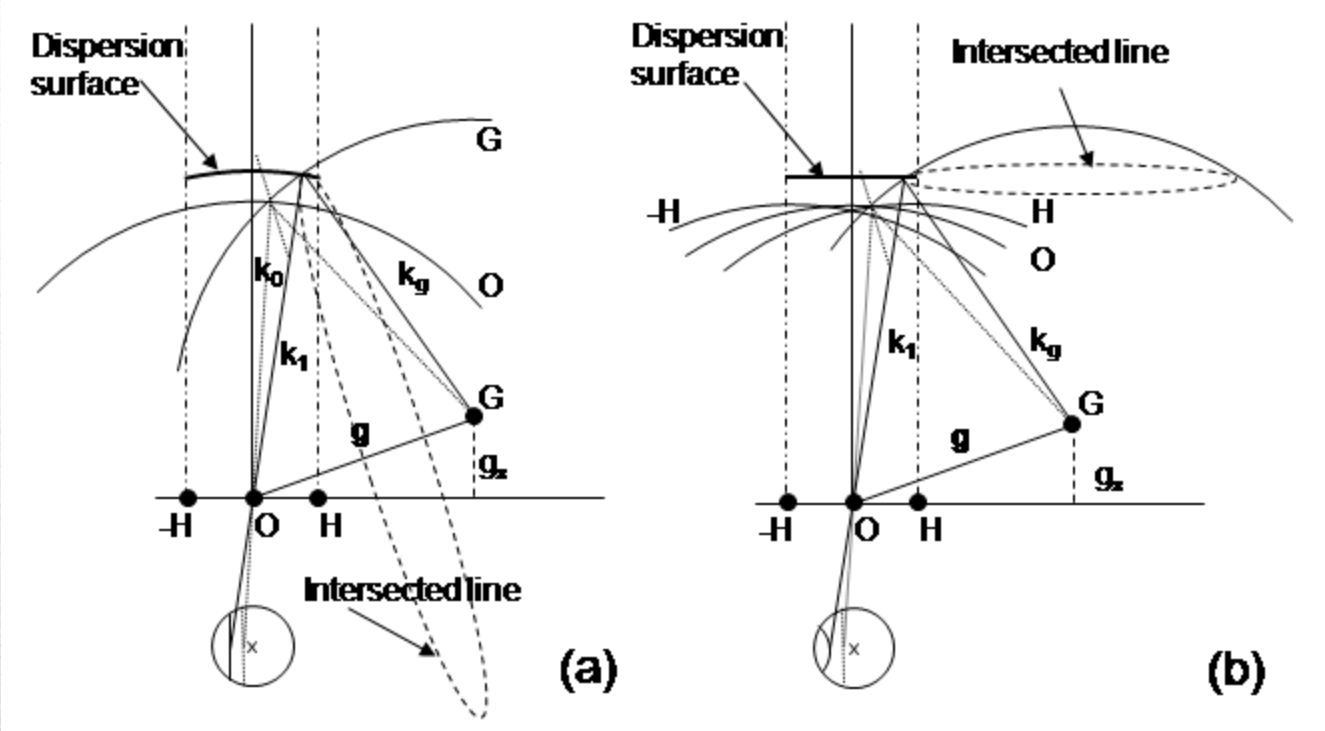
$$g_x k_x + g_y k_y - g_z k_z + \frac{g^2}{2} + g\Delta g = 0 \qquad g\Delta g = (k\gamma^{(1)} + \frac{\gamma^{(1)2}}{2})$$

When the incident beam is near or at a zone axis, the first branch of the dispersion surface can be approximately considered as a flat plane with a distant of $k_1=k_0+g^{(1)}$ to the origin of reciprocal lattice. Thus, the dynamically corrected HOLZ-line equation is derived as (Li, 2007)

$$(k_x+g_x)^2+(k_y+g_y)^2=r^2=k^2-(k_z+\gamma^{(1)}-g_z)^2$$

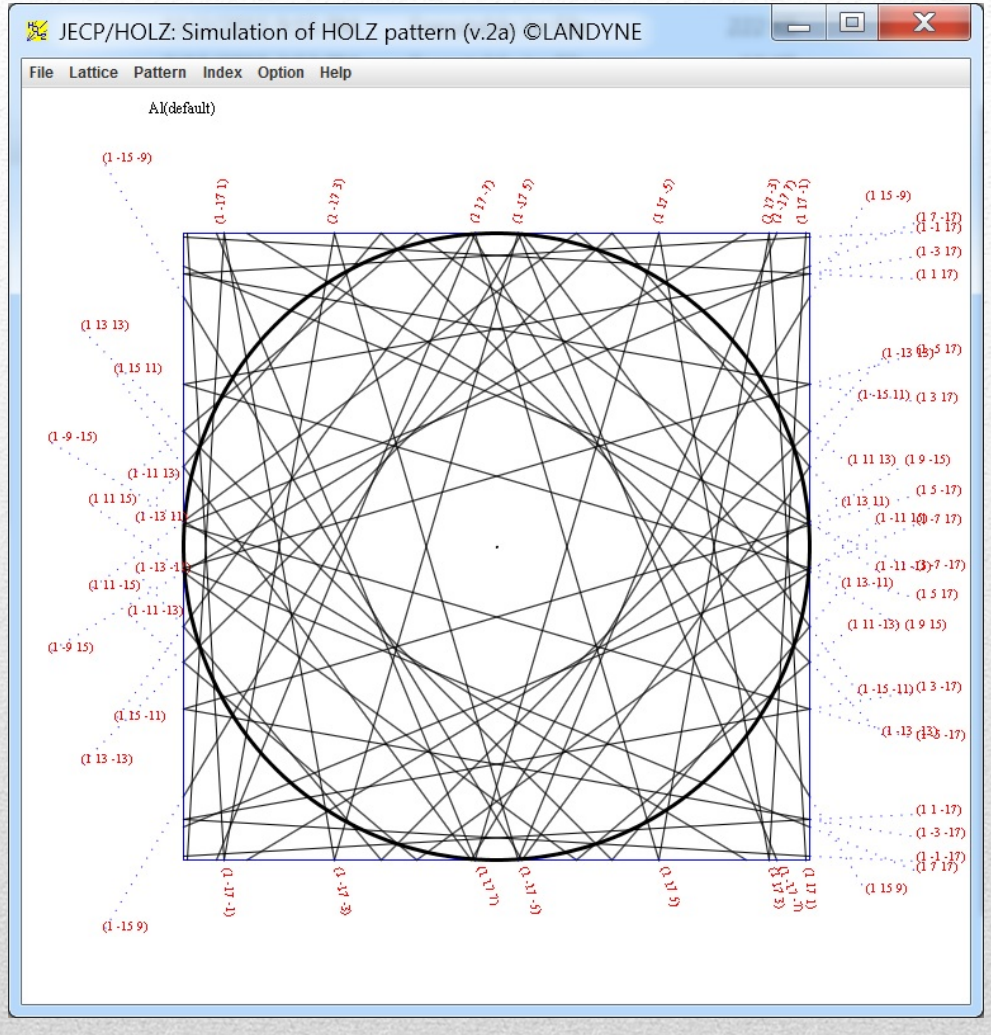
X.Z. Li, J. Mater. Educ. 29, 177 (2007).

HOLZ



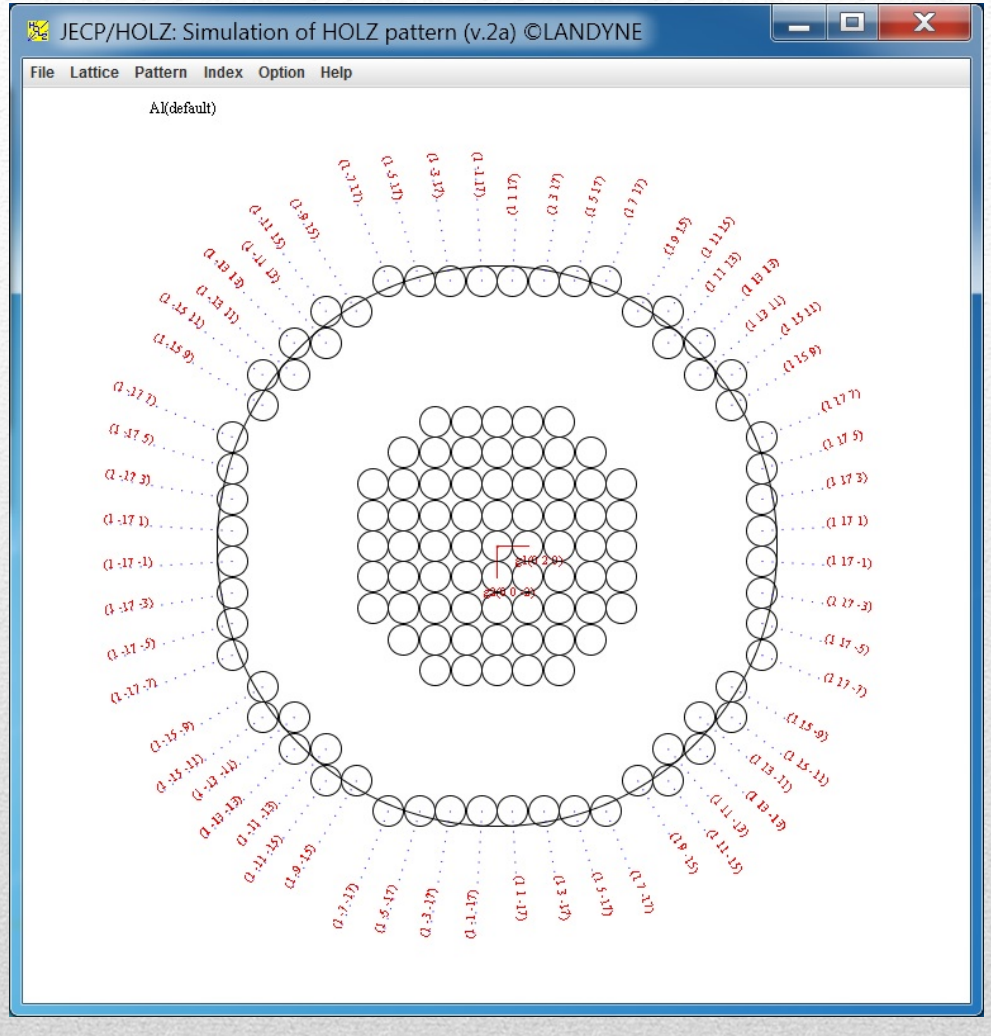
Schematic diagrams of the formation of HOLZ lines using the dispersion surface construction: (a) weak dynamical effect and (b) strong dynamical effect in a zero order Laue zone. The intersected lines are valid within the first Brillouin zones and the extensions of the intersected lines to form circles are for illustration purposes only.

HOLZ



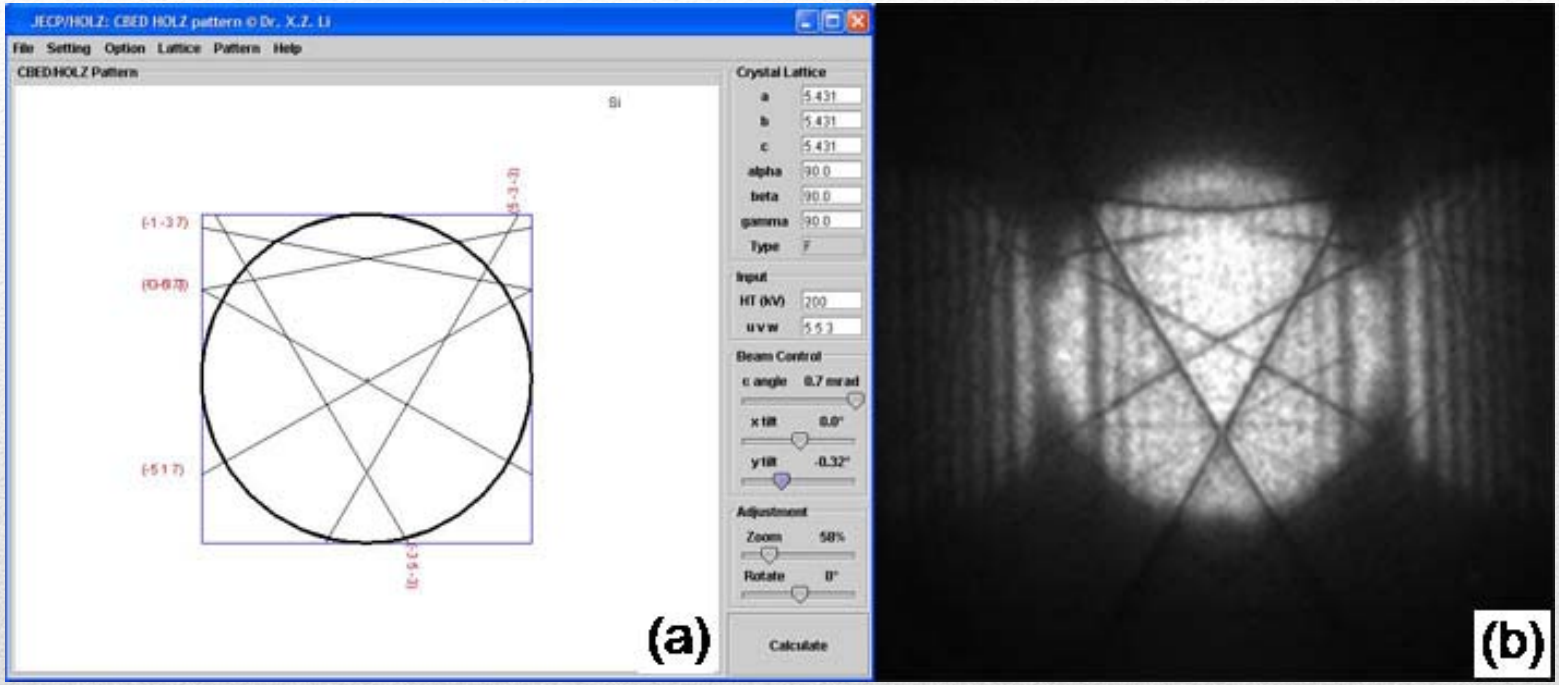
A snapshot of the HOLZ panel with a HOLZ pattern.

HOLZ

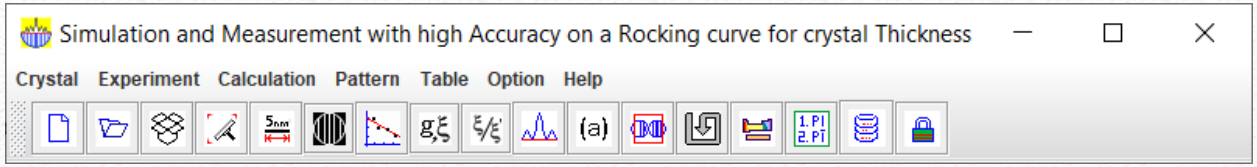


A snapshot of the HOLZ panel with a CBED pattern.

HOLZ



GUI of JECP/HOLZ with (a) a simulated and (b) an experimental HOLZ patterns of Si [553].



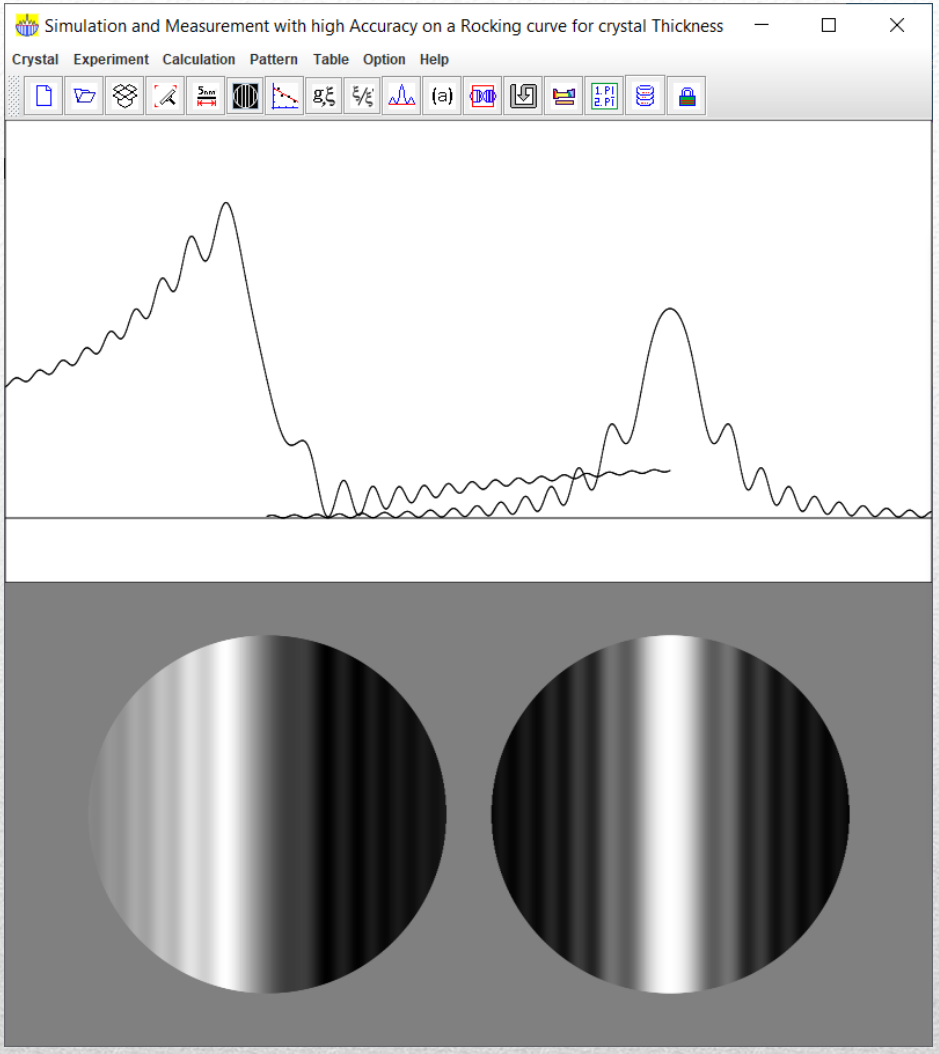
Simulation and Measurement with high Accuracy of a Rocking curve for crystal Thickness

Highlight

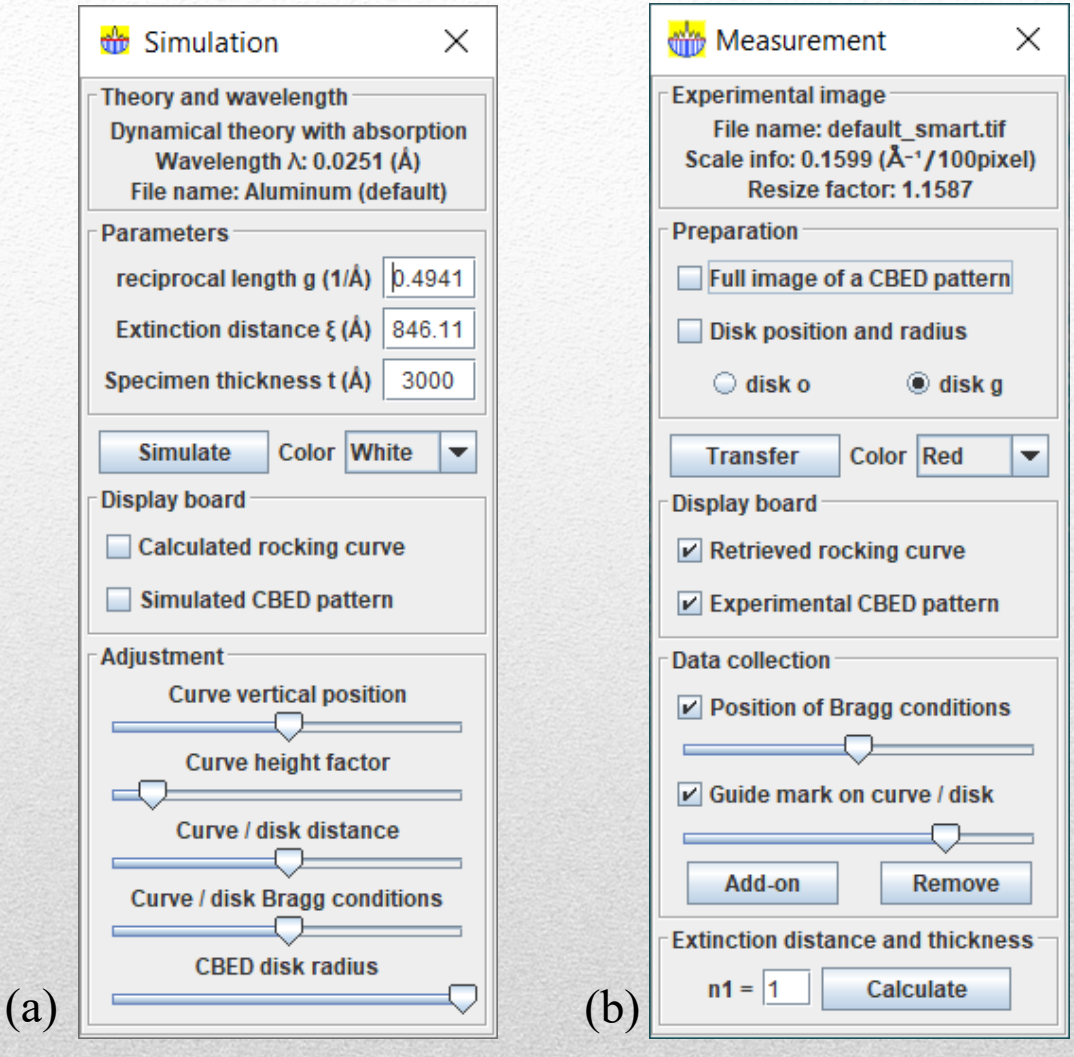
- SMART can be used for the simulation of two-beam CBED pattern, including the absorption effect.
- Computer assisting the measurement of crystal thickness using the experimental two-beam CBED pattern.
- Allow selecting a region of interest on the simulated and experimental CBED patterns to .tif, .jpg. and .gif formats.

X.-Z. Li, Journal of Microscopy and techniques (to be published 2023).

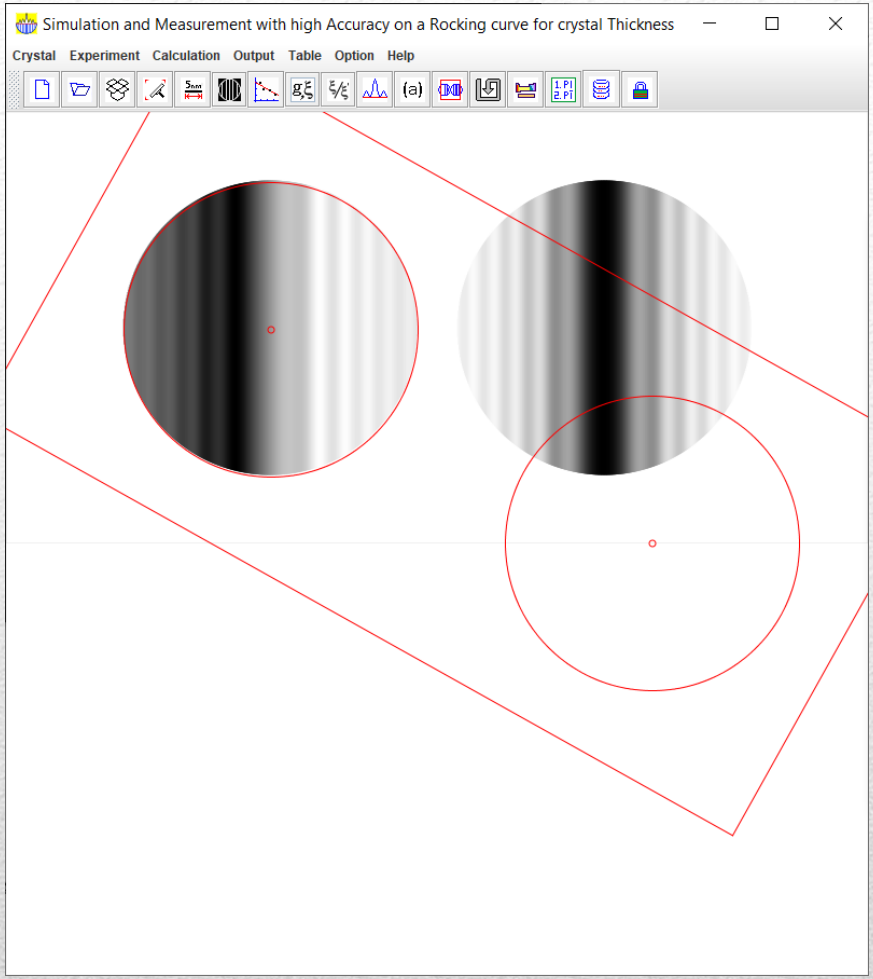
SMART



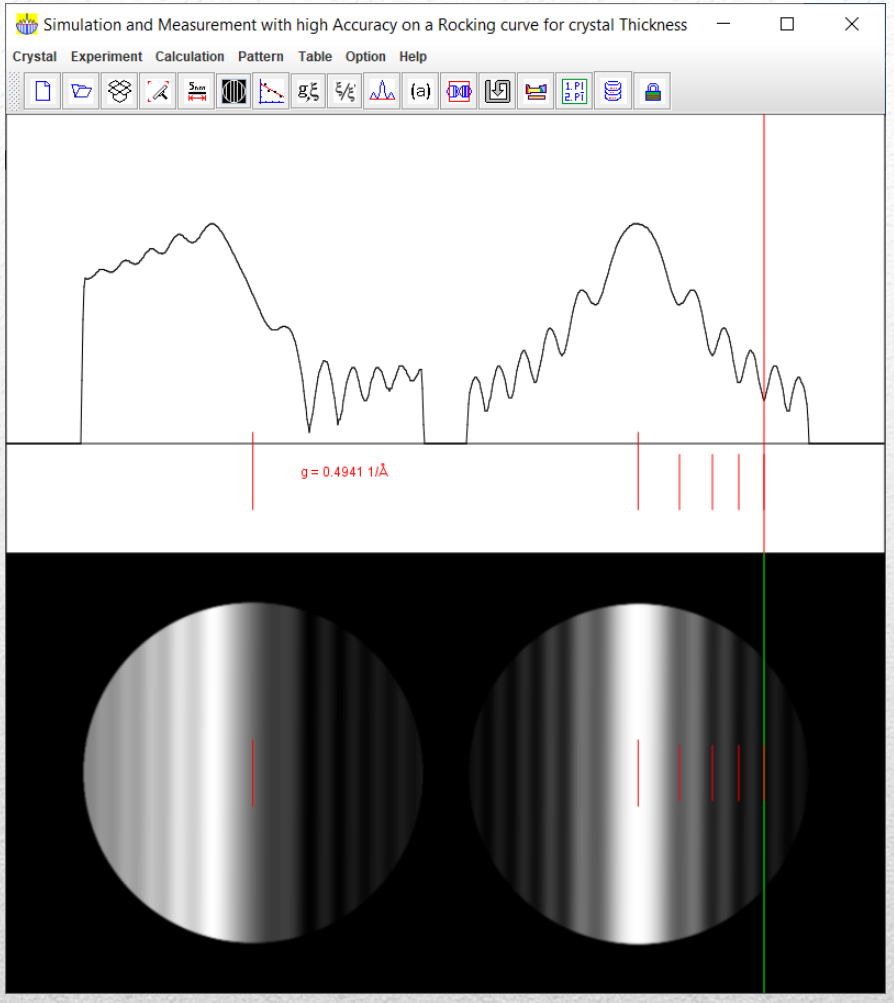
The graphic user interface of SMART. The rocking curve and CBED pattern of Aluminum under the condition of two-beam and g(200).



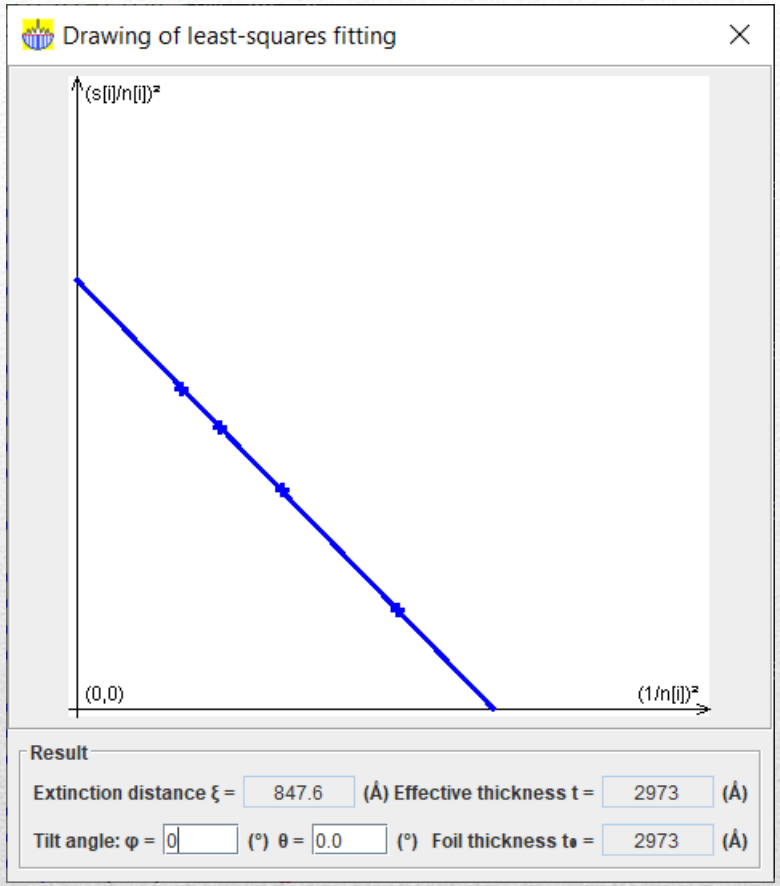
(a) Control panel for simulation and (b) control panel for measurement.



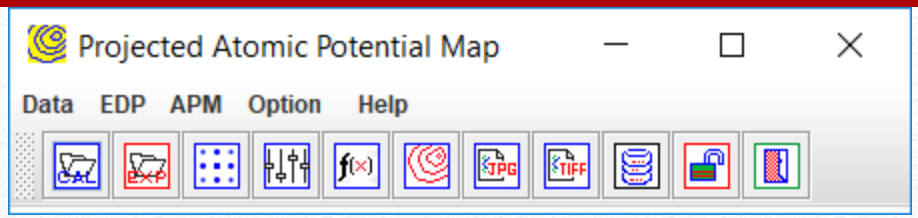
The halfway of the process; only the position and radius of the o disk are defined.



The experimental rocking line and CBED disk. Local minima are marked.



The drawing panel and result table. Selection of n1 (default value =1) and calculate the extinction distance and specimen thickness by the calculate button.



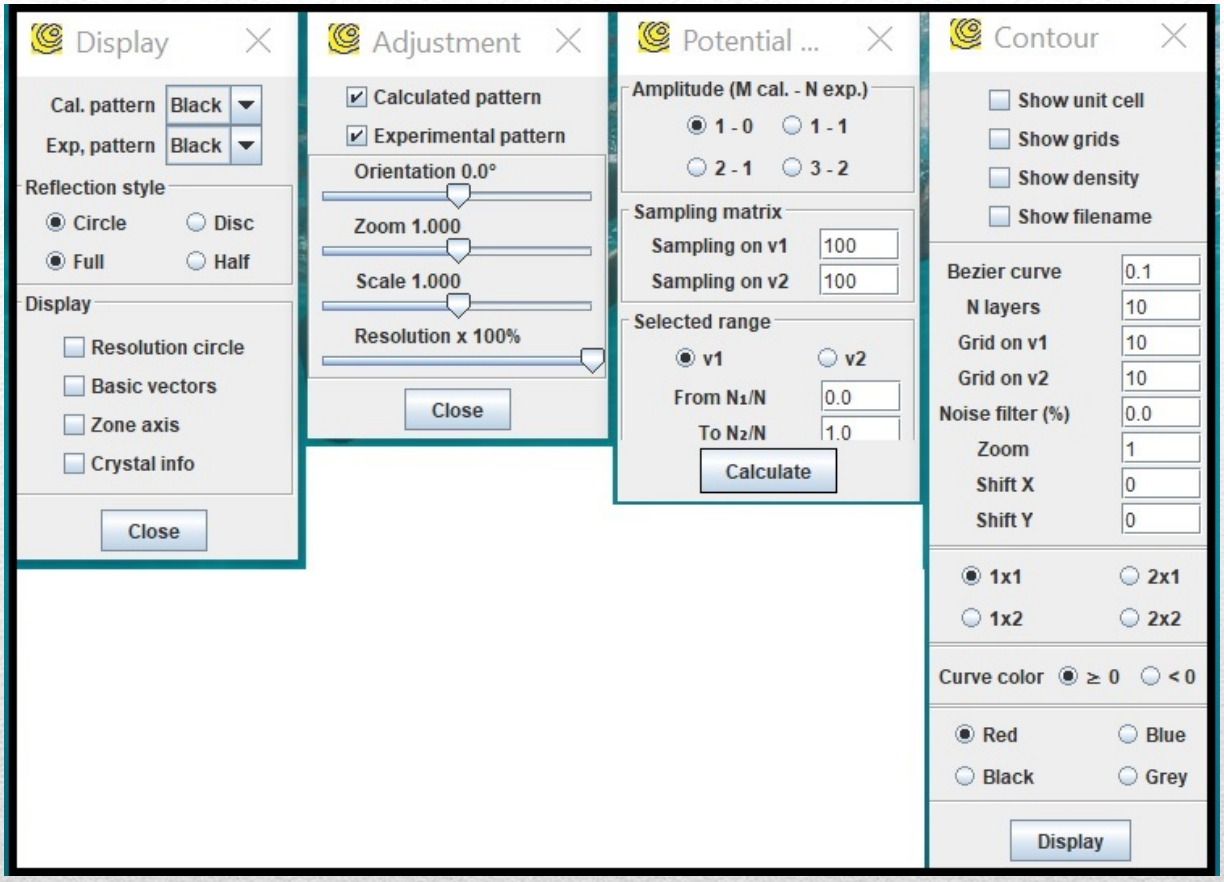
Electrostatic Potential (Difference) Map

Highlight

- ESPOT is an extension of SAED and QSAED.
- It can be used to calculate projected atomic potential map from the calculated diffraction data, which is calculated from SAED.
- With the diffraction data retrieved from experimental pattern using QSAED, the projected atomic potential difference map can be obtained to analyze and improve the structural model.
- Three types of projected atomic potential difference maps are available.

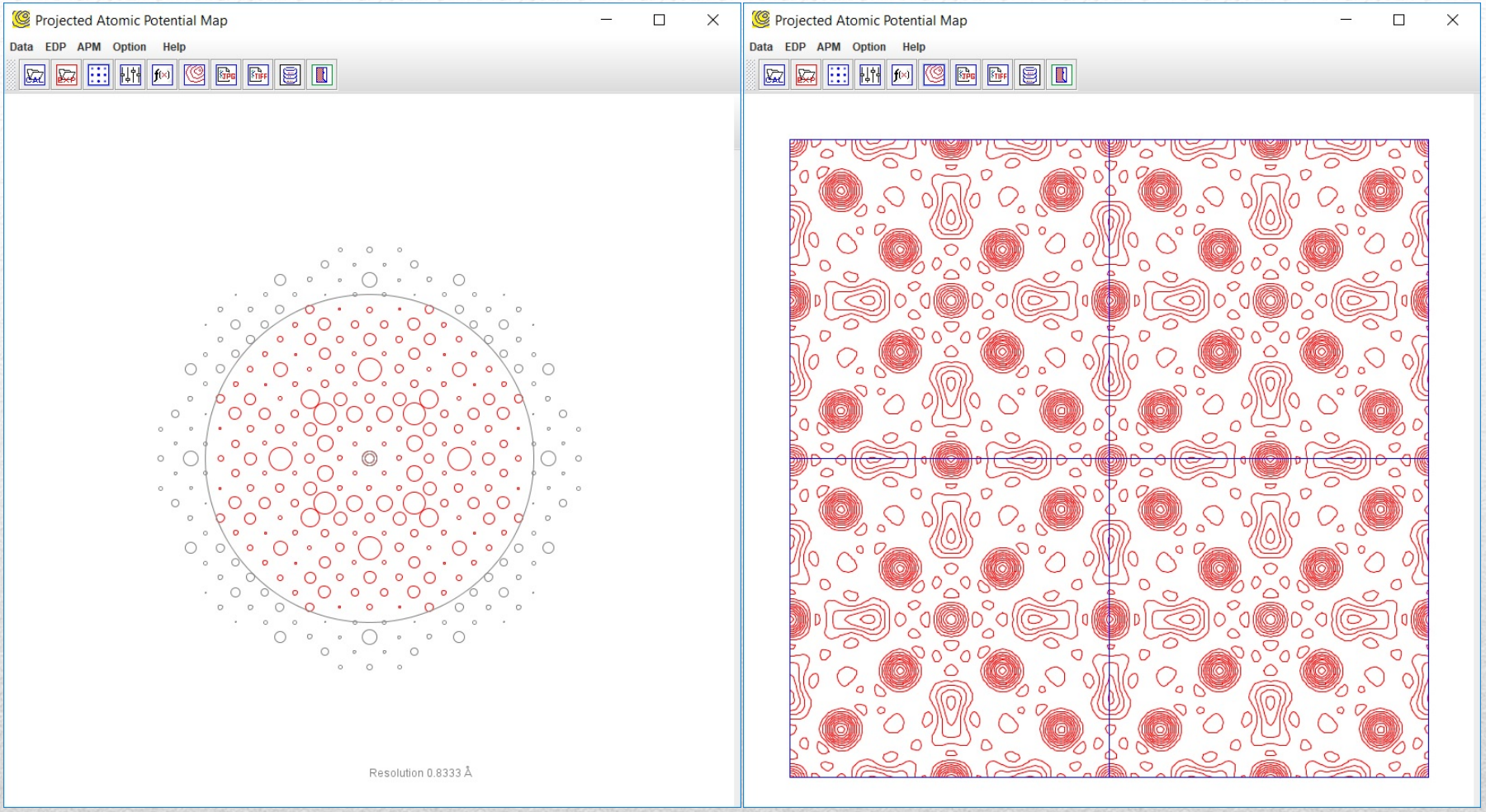
X.-Z. Li, Structural investigation of Zr_2Co_{11} and $Zr_2Co_{11-x}(MoBSi)_x$ phases using quantitative electron diffraction data, J. Applied Cryst., in preparation (2023).

ESPOT



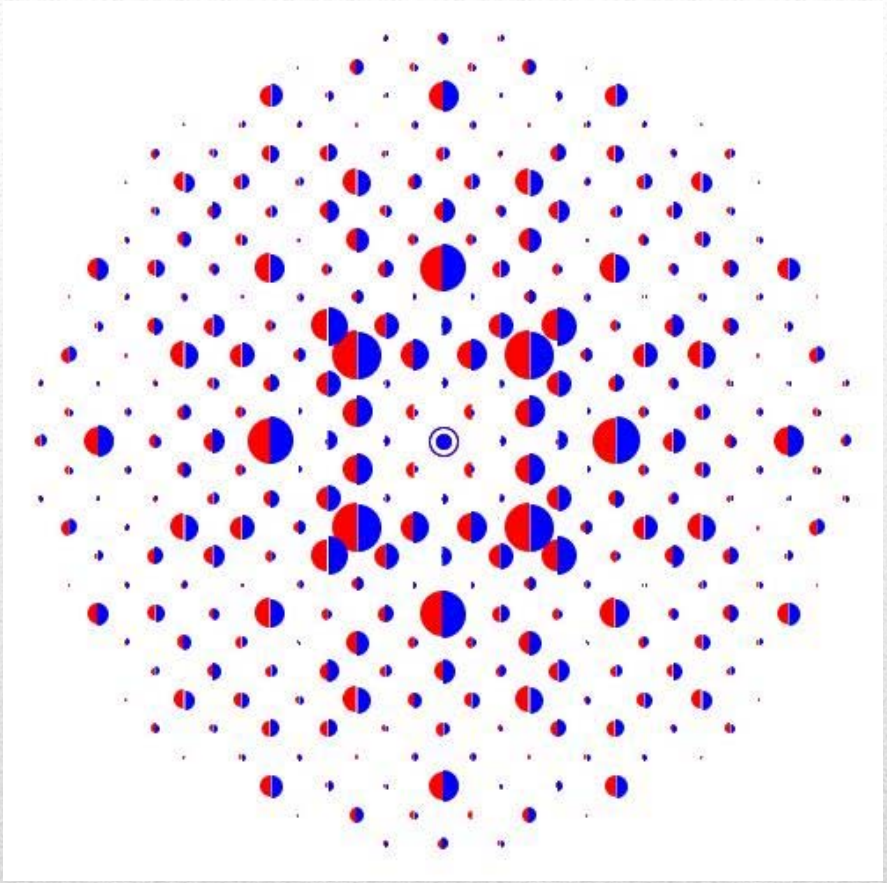
The main operational dialogs of ESPOT.

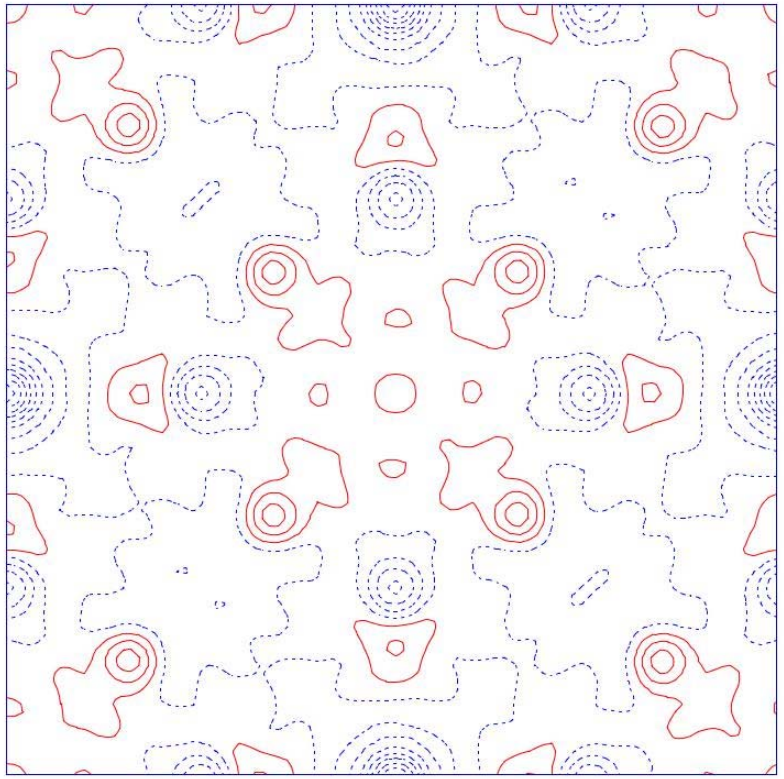
ESPOT



(a) GUI of ESPOT with a calculated diffraction pattern; (b) the GUI of ESPOT with a projected atomic potential map.

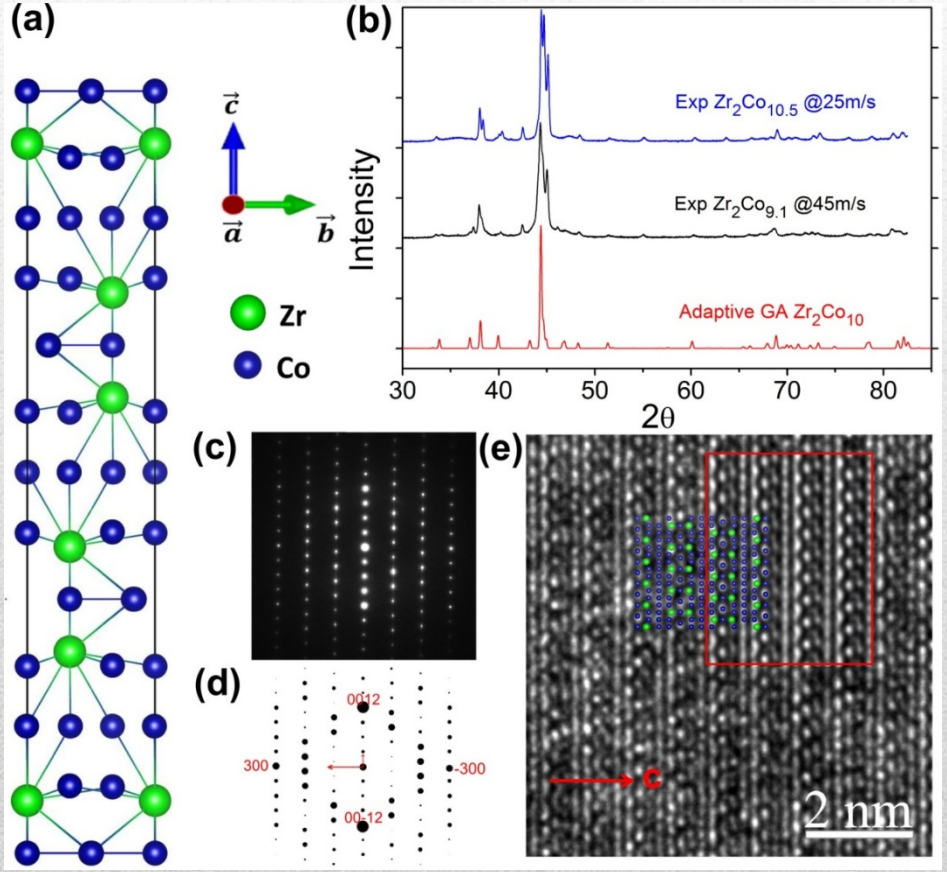
ESPOT





(a) comparison of two diffraction patterns, calculated pattern and (simulated) experimental pattern; (b) the projected atomic potential difference map based on the diffraction data in (a). Missing atoms is revealed in the dot line peaks.

X. Zhao, M. C. Nguyen,1 W. Y. Zhang, C. Z. Wang,1 M. J. Kramer,1 D. J. Sellmyer, X. Z. Li, F. Zhang, L. Q. Ke, V. P. Antropov, and K. M. Ho, Exploring the Structural Complexity of Intermetallic Compounds by an Adaptive Genetic Algorithm, Phys. Rev. Letter, 112 (2014) 045502.

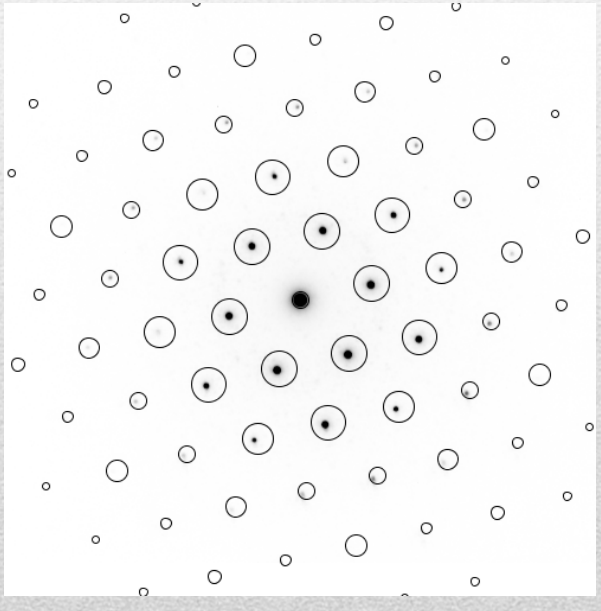


The Adaptive Genetic Algorithm approach is demonstrated by solving a long-standing puzzle in the complex crystal structures of the orthorhombic, rhombohedral, and hexagonal polymorphs close to the Zr_2Co_{11} intermetallic compound.

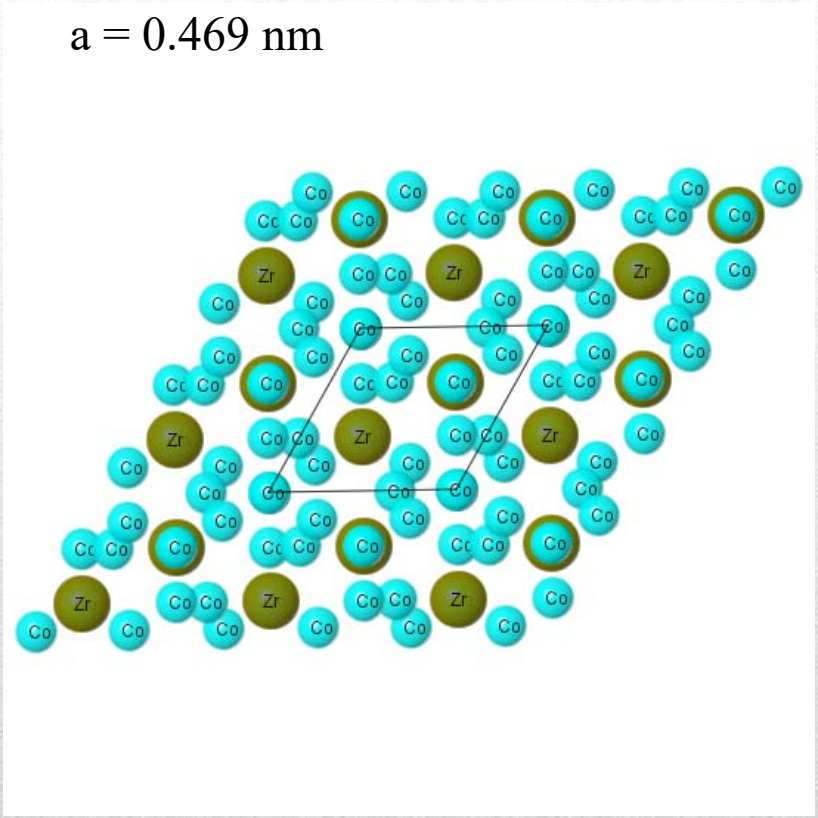
The rhombohedral structure has space group R32 with lattice parameters a = 0.469 and c = 2.40 nm, which match well with experimental data.

对比实验电子衍射强度，我们修改了Zn_2Co_{11}三方晶体相的结构模型。修改后的结构模型可有助于解释Zn_2Co_{11}的同形异构的调制结构的形成。

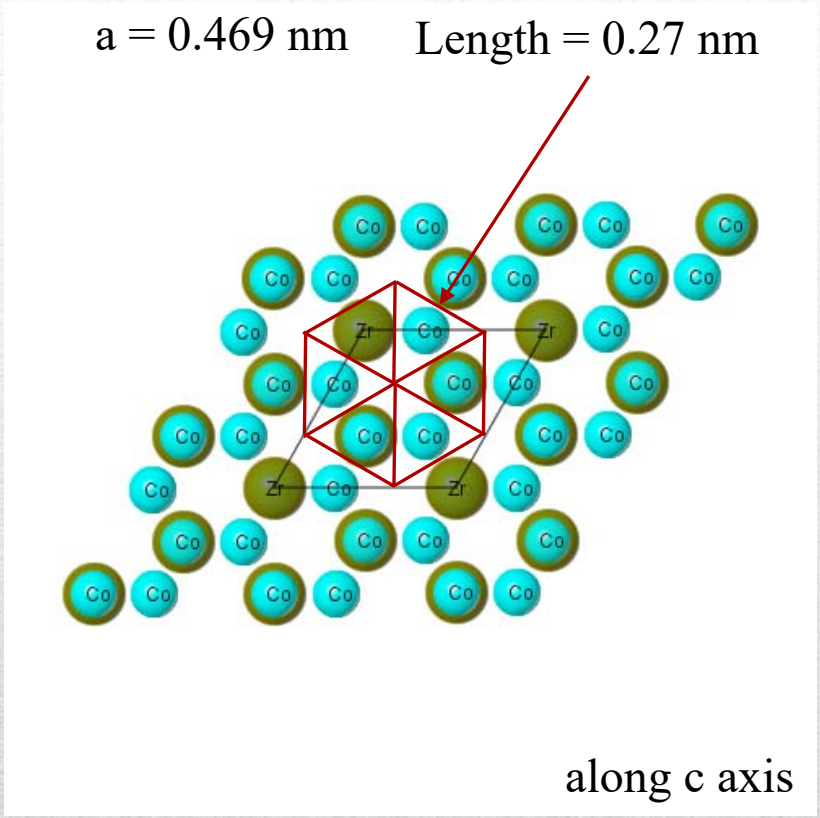
Rhombohedral phase is formed in $Zr_2Co_{11-x}(MoSiB)_x$ alloy.



Rhombohedral phase was synthesized in $Zr_2Co_{11-x}(MoSiB)_x$ alloy.



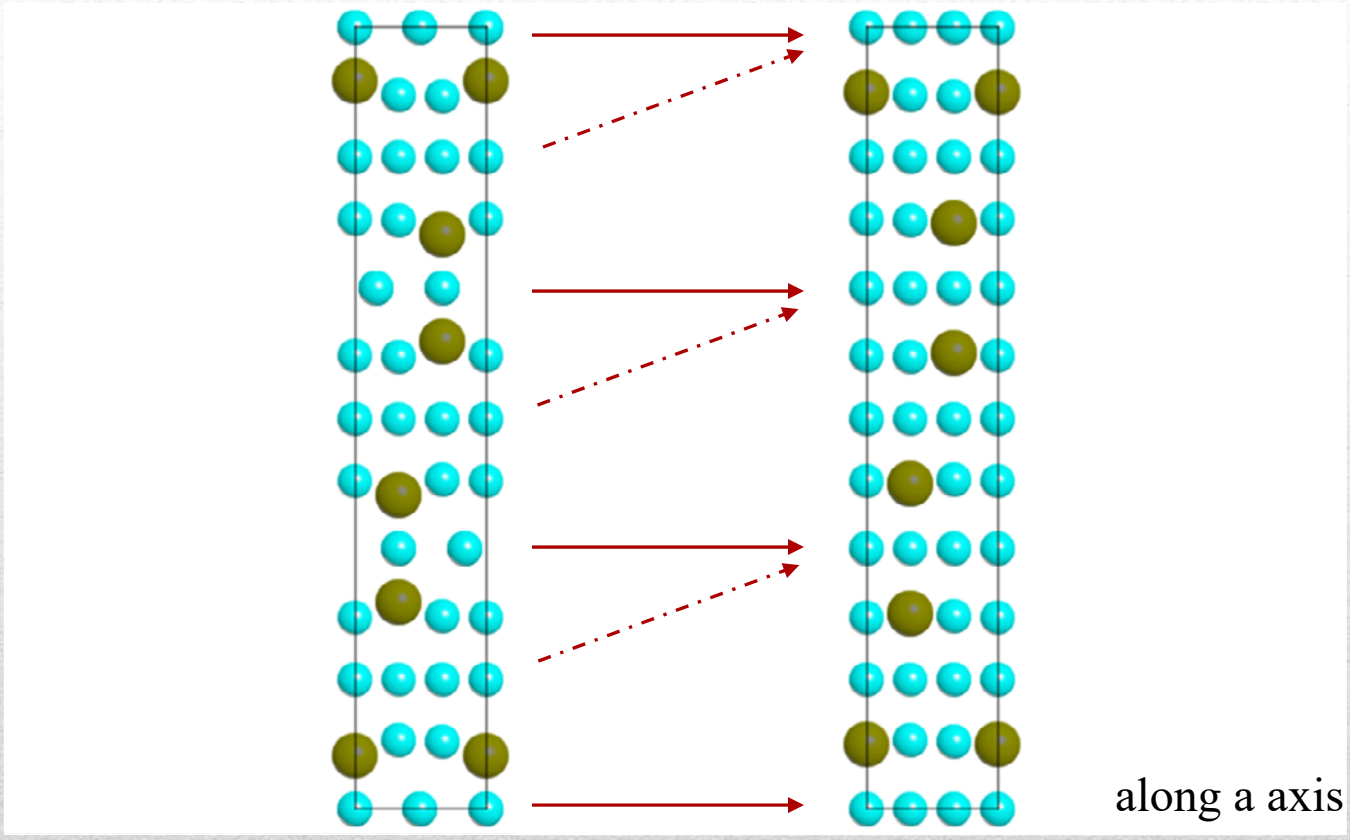
(a)



(b)

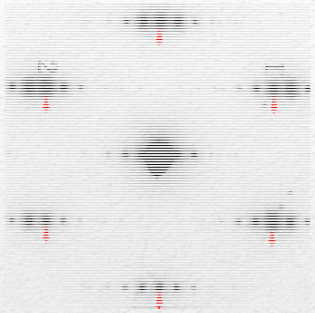
(a) The structural model for Zr_2Co_{11} from AGA and (b) the modification.

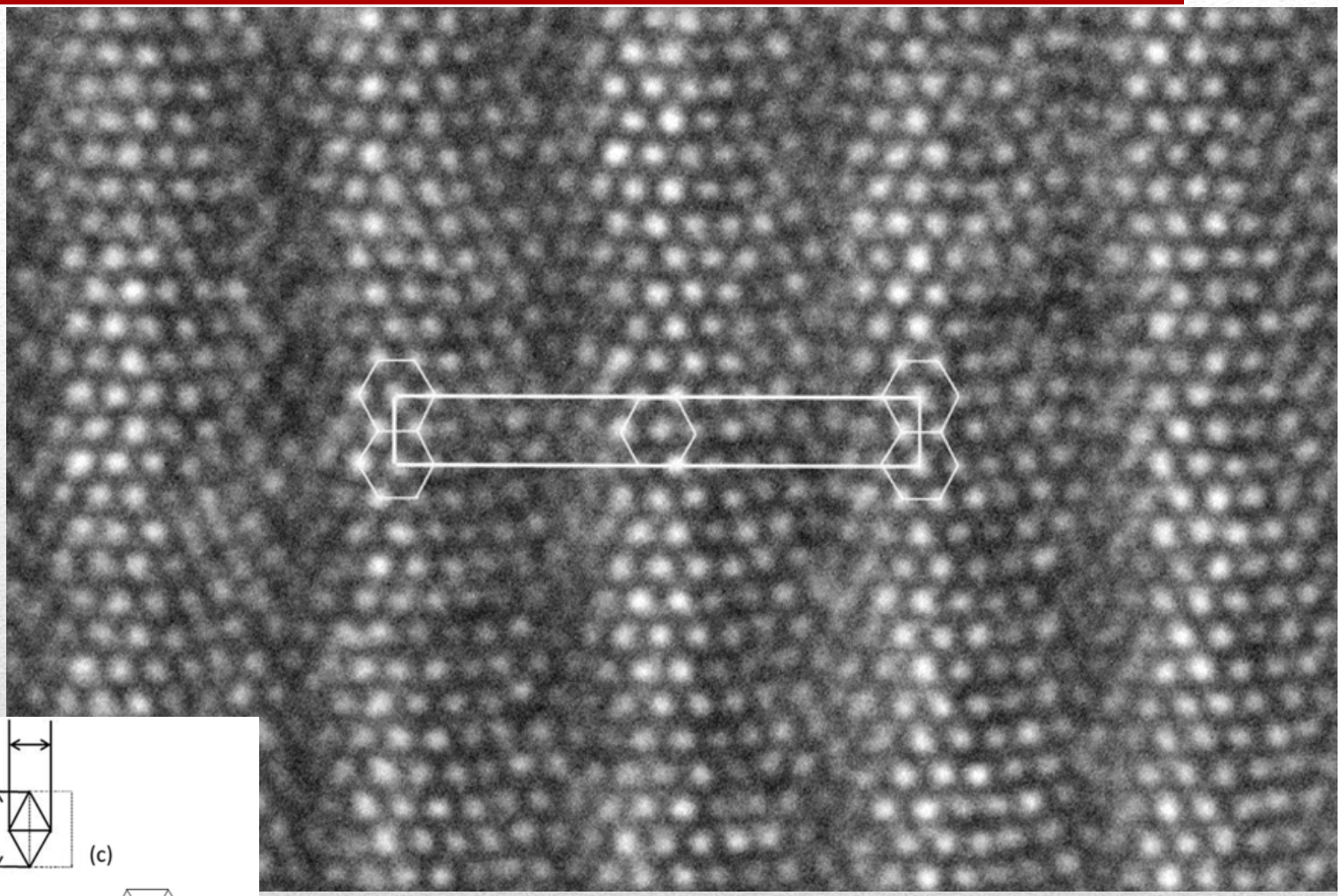
Rhombohedral phase was synthesized in $Zr_2Co_{11-x}(MoSiB)_x$ alloy.

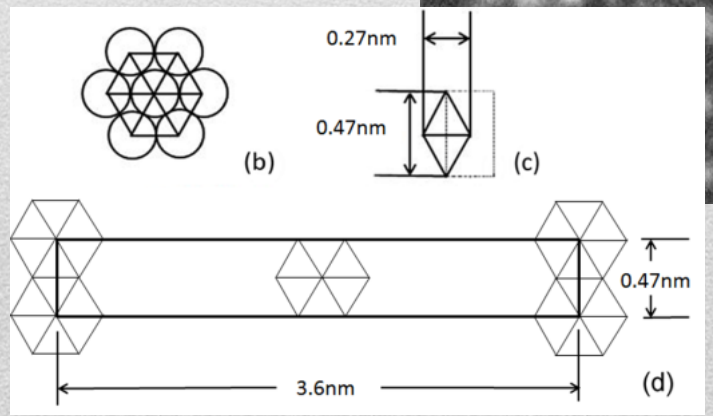


(a) The structural model for Zr_2Co_{11} from AGA and (b) the modification.

Modulated Structure







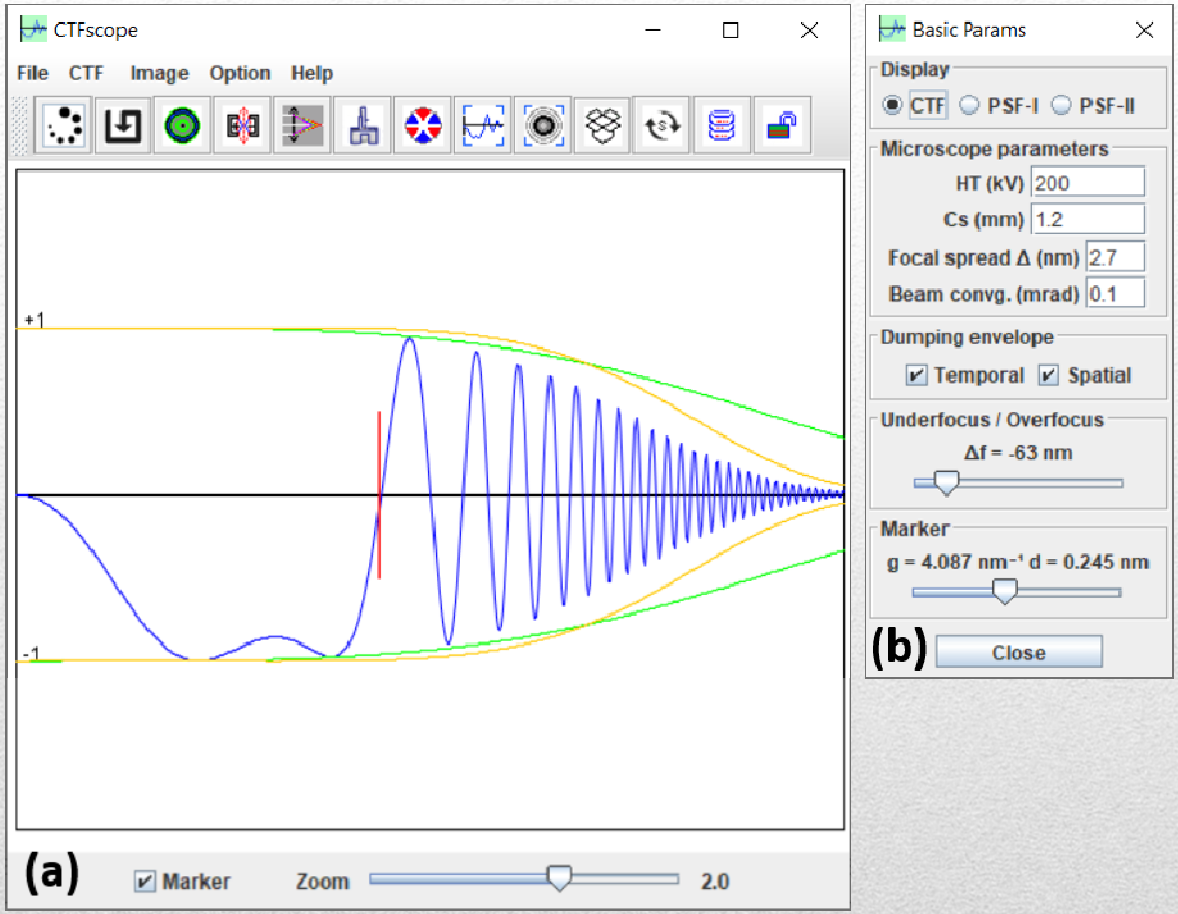
Simulation and Visualization Tool for Contrast Transfer Function

Highlight

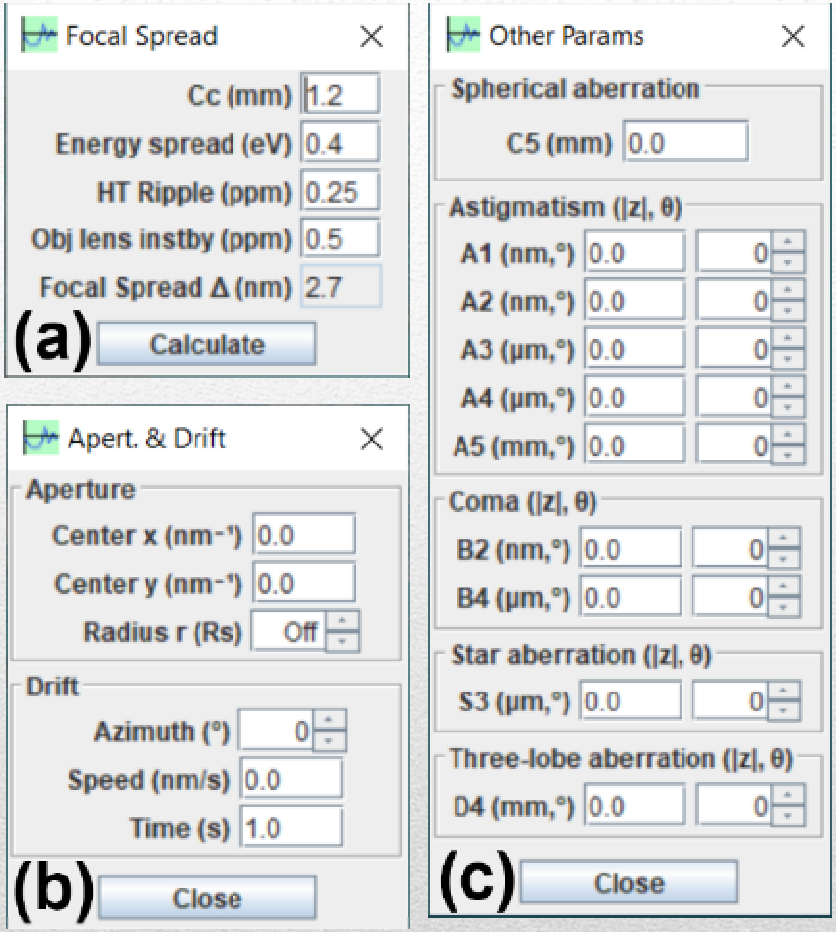
- To calculate the CTF with temporal and spatial dumping envelopes for conventional TEM
- To extend it to various aberrations (up to fifth order) for aberration-corrected (AC)-TEM.
- It includes effects on the CTF and imaging due to the objective aperture and image drift for tutorial purposes.

X.-Z. Li, An Interactive Simulation and Visualization Tool for Conventional and Aberration-corrected Transmission Electron Microscopy, Microscopy Today, Nov.-Dec. issue (2022) 20-27.

CTFscope

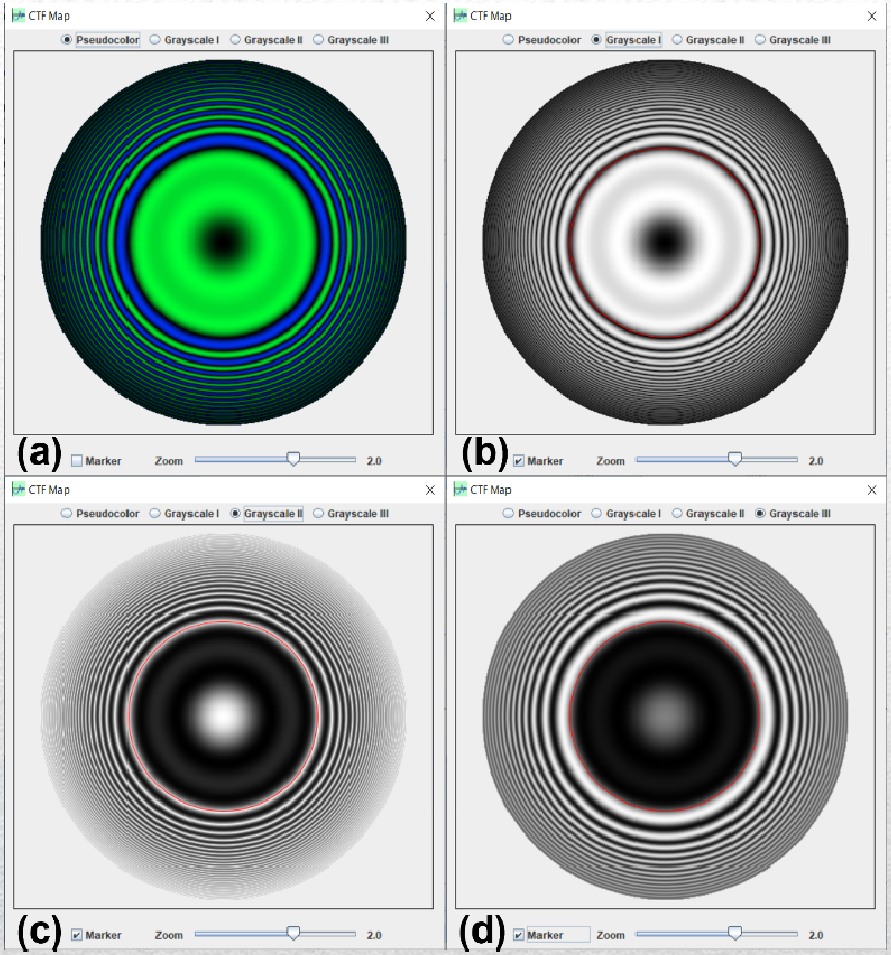


The main frame of the CTFscope with a graphic panel and (b) a dialogue box for microscope setup and optical parameters.



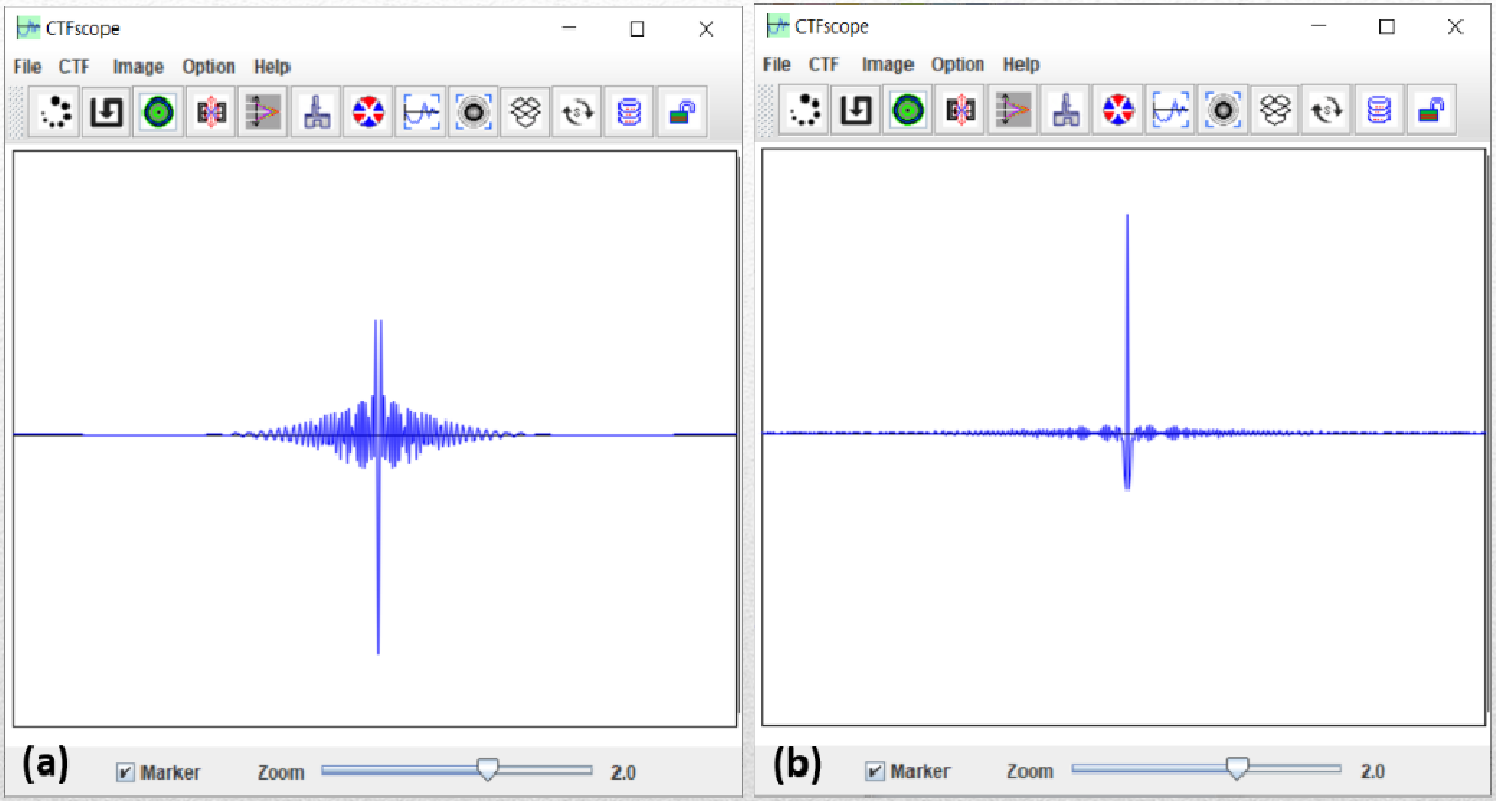
The dialogue boxes for (a) focal spread coefficients, (b) the parameters for an aperture and a continuous drift, (c) astigmatism coefficients, and other higher order aberration coefficients.

CTFscope



The display panel for the calculated CTF in (a) a pseudo color, (b) a grayscale I (from 0 black to $|\pm 1|$ white), a grayscale II (from 0 white to $|\pm 1|$ black) and (d) a grayscale III (from -1 black to 1 white). The circular marker is in (b ~ d).

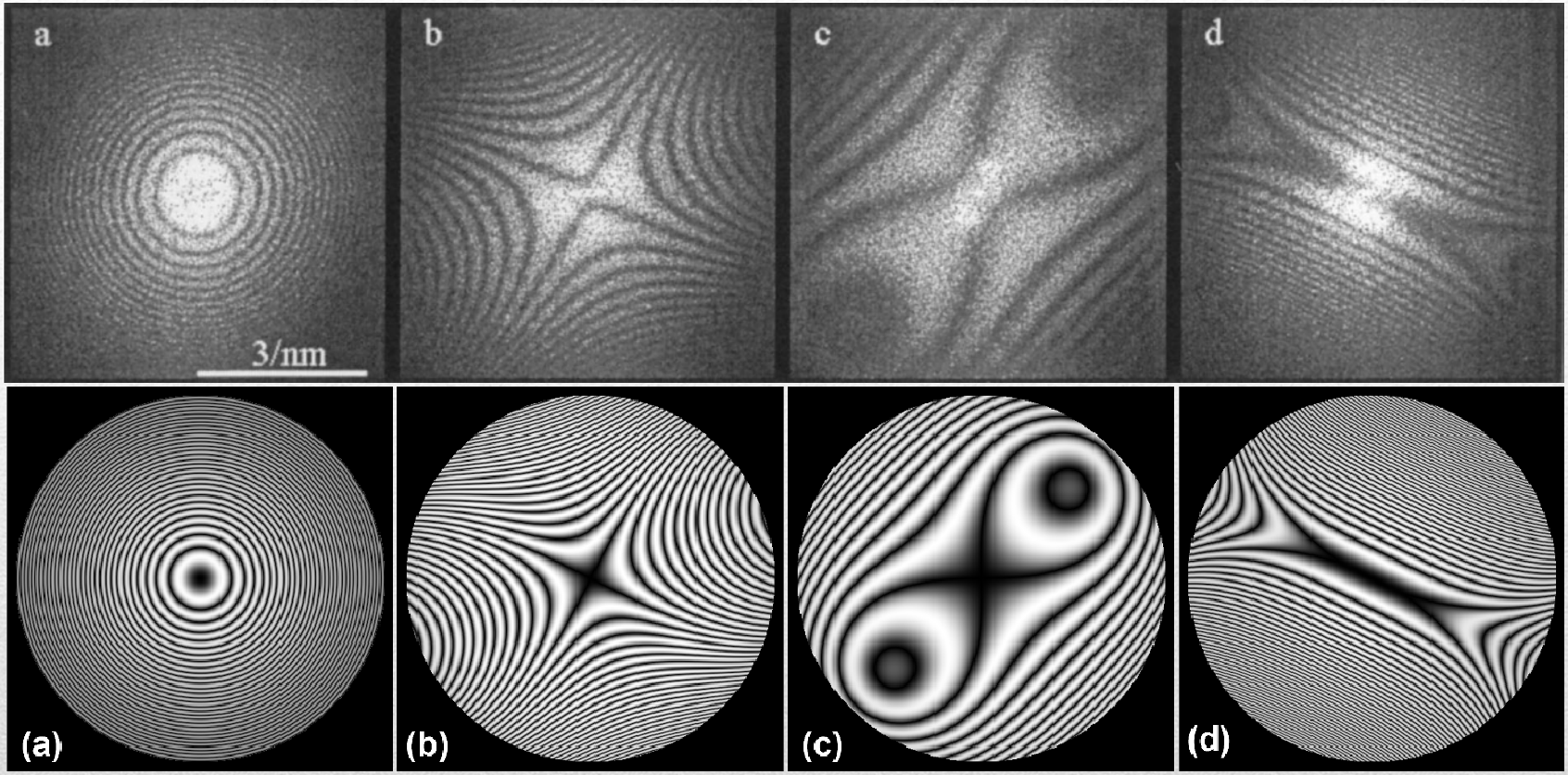
CTFscope



The point spread functions as the Fourier transform of (a) the CTF and (b) |CTF|.

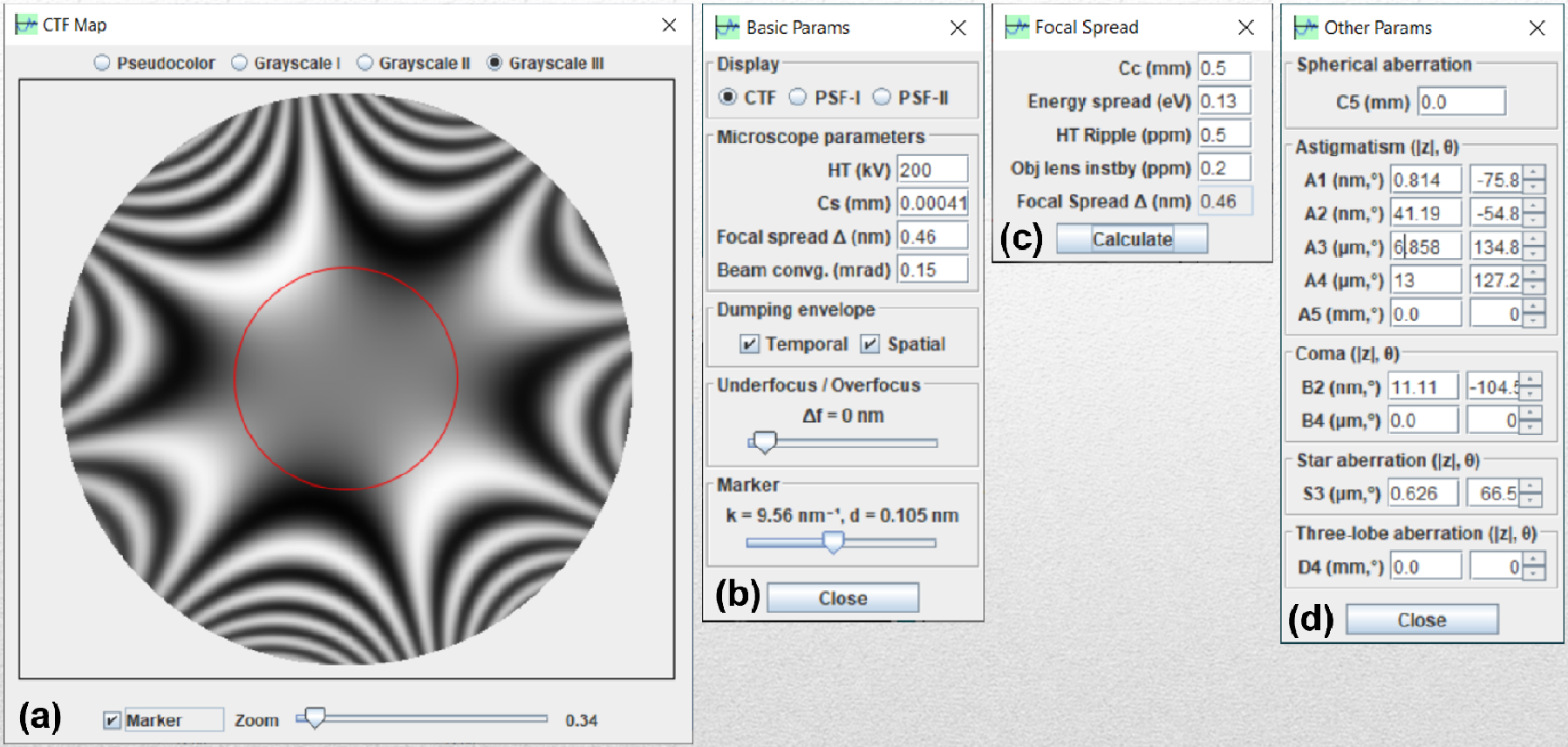
CTFscope

(a) An original image before processing, (b) the processed image using CTF, and (c) the processed image using |CTF|.

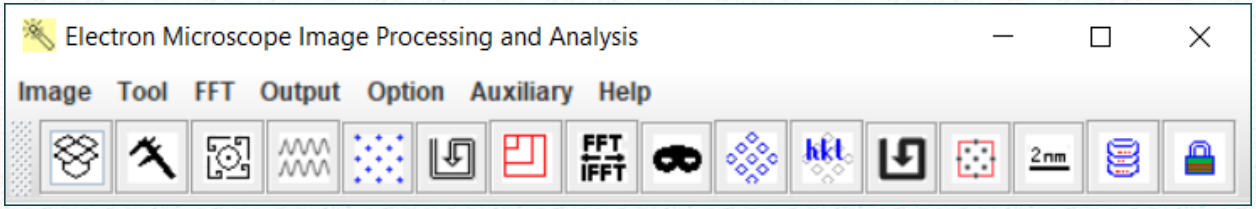


The calculated images using the same parameters in Figure 1 of [S. Uhlemann, M. Haider, Residual wave aberrations in the first spherical aberration corrected transmission electron microscope, Ultramicroscopy 72 (1998) 109-119.]

CTFscope



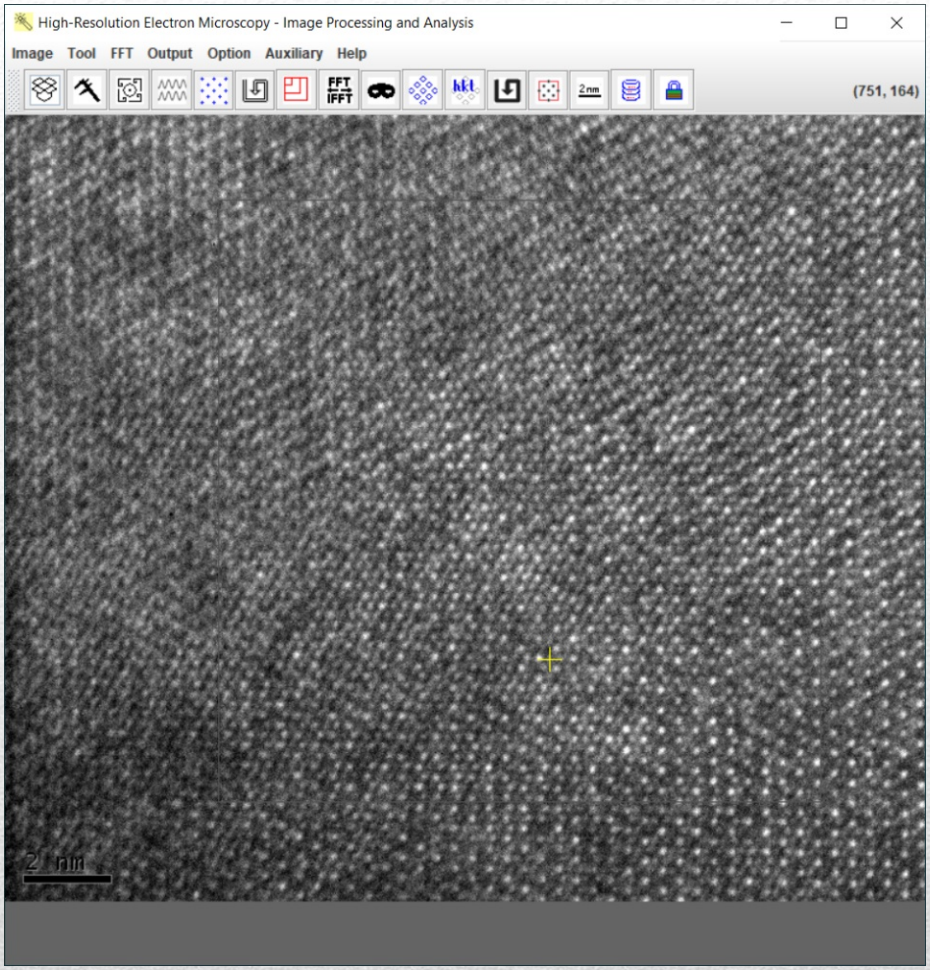
The CTF 2D graph without aperture and drift, calculated using CTFscope using (b-d) the same parameters as those in Figure 4 of reference [S-C Lee, J-M Jeung, S-G Lee and J-G Kim, Journal of Analytical Science and Technology 11 (2020) 31.].



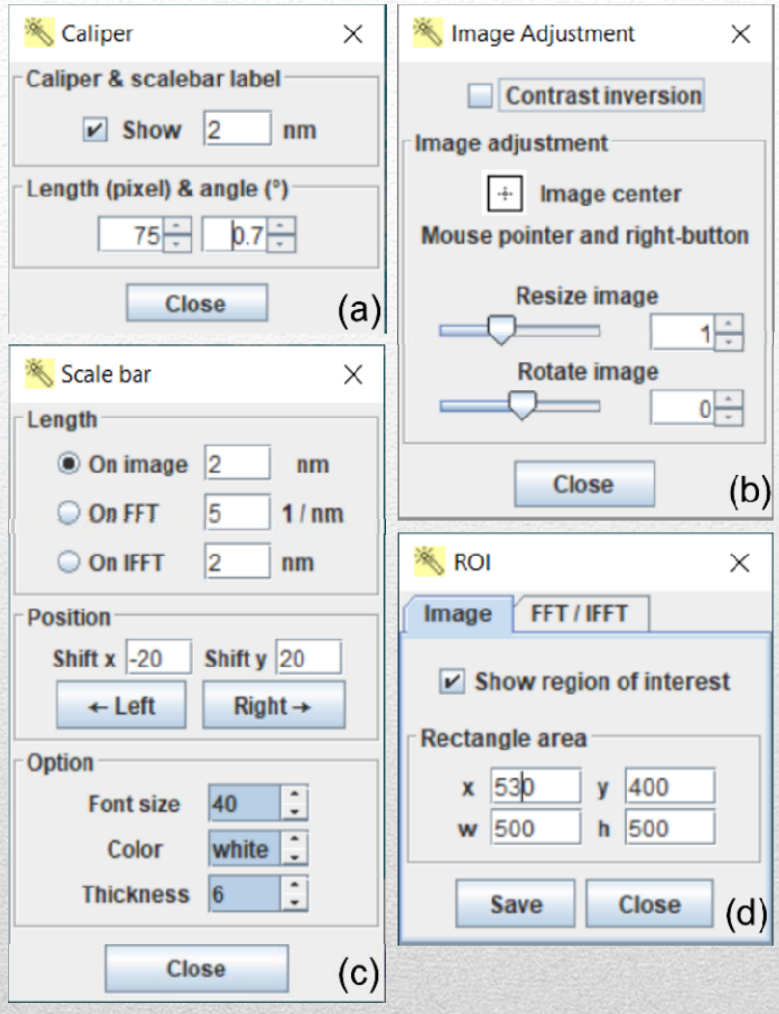
Transmission Electron Microscope Image Processing and Analysis

Highlight

- Convenient tool for selecting area, resizing, and rotation of experimental images.
- Measure the scale bar and transfer to selected image, FFT pattern and IFFT image.
- A series of intensity profiles on HREM images can be retrieved and compared.
- Square and Inscribed circle of an arbitrary length for FFT.
- Varies of masks are available for inversed FFT images.
- Tools for adding scale bars and indices for processed images and FFT patterns.

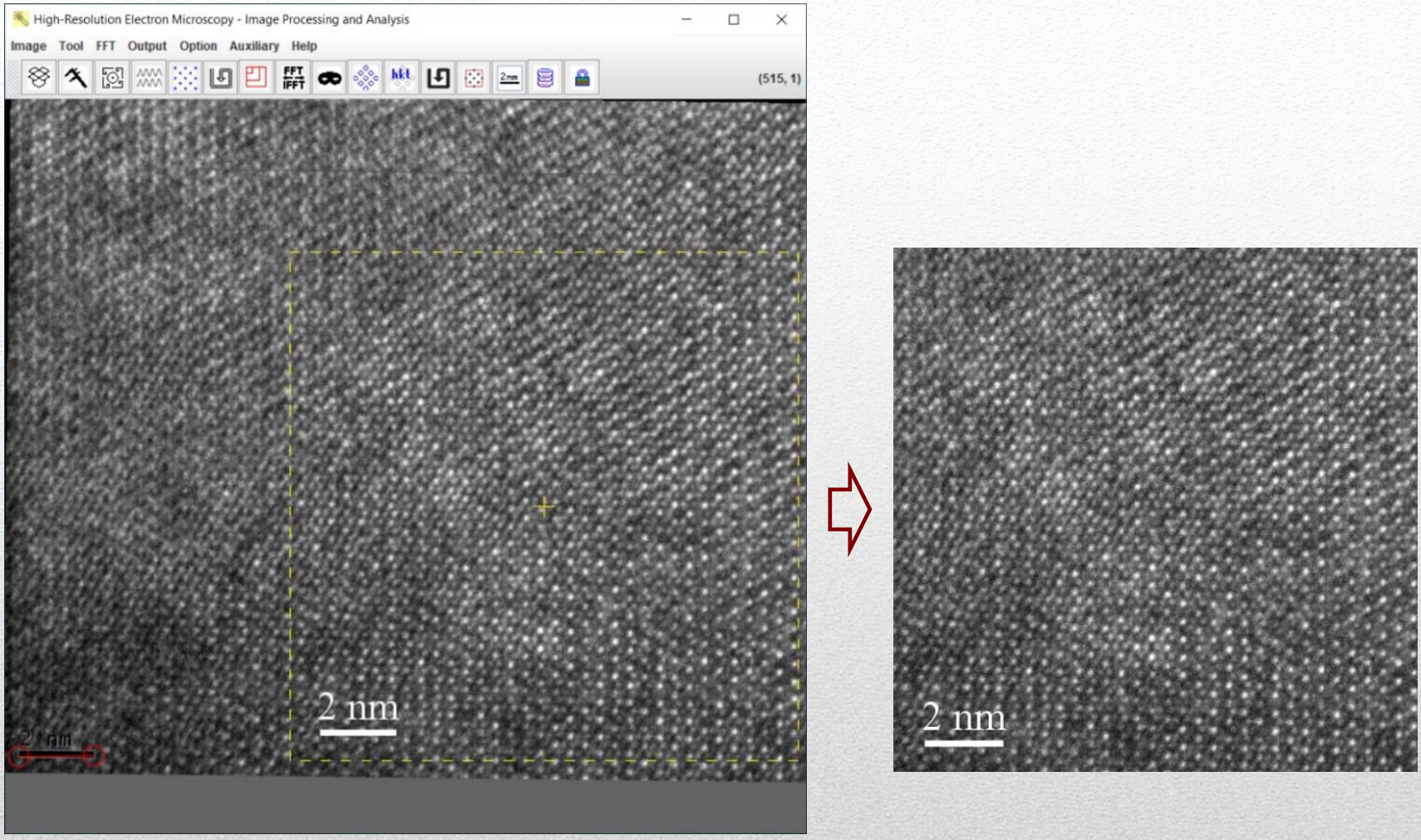


The GUI of HREM-IPA with a drop-down menu and a toolbar menu. The panel shows an electron microscopy image as an example.



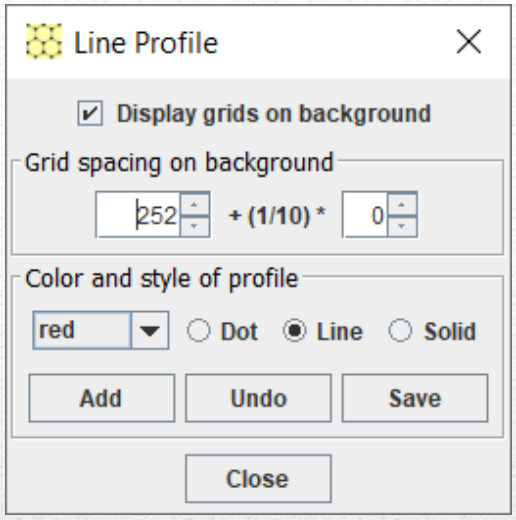
The image operation tools (a) caliper, (b) adjustment, (c) scale bar, and (d) ROI.

EMIPA

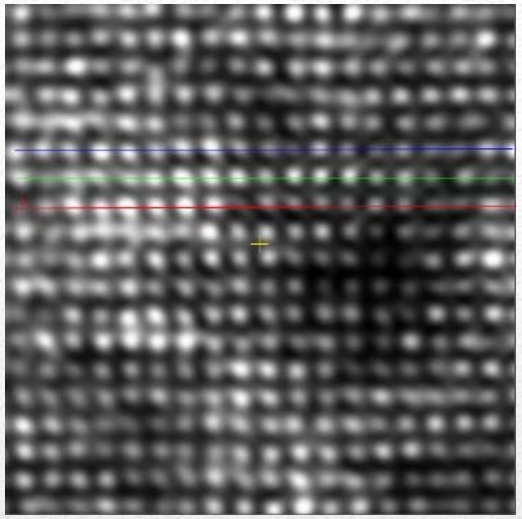


The image is slightly rotated for alignment and calibration on the scale bar. An area is selected and ready for output.

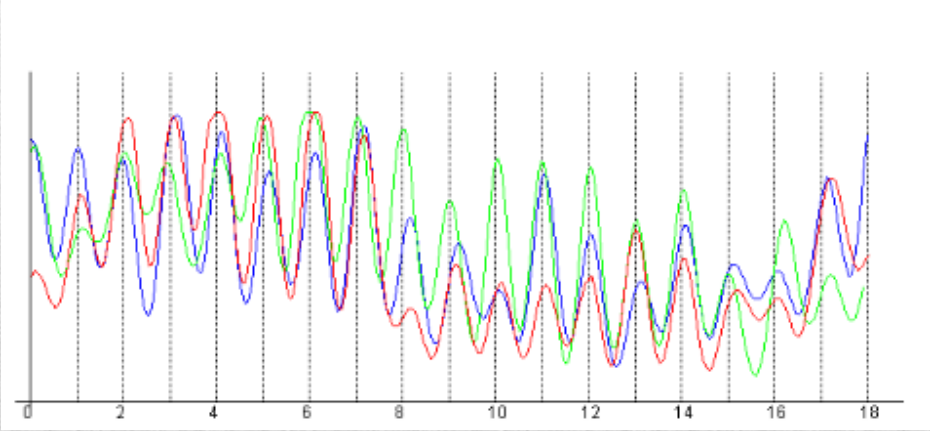
(a)



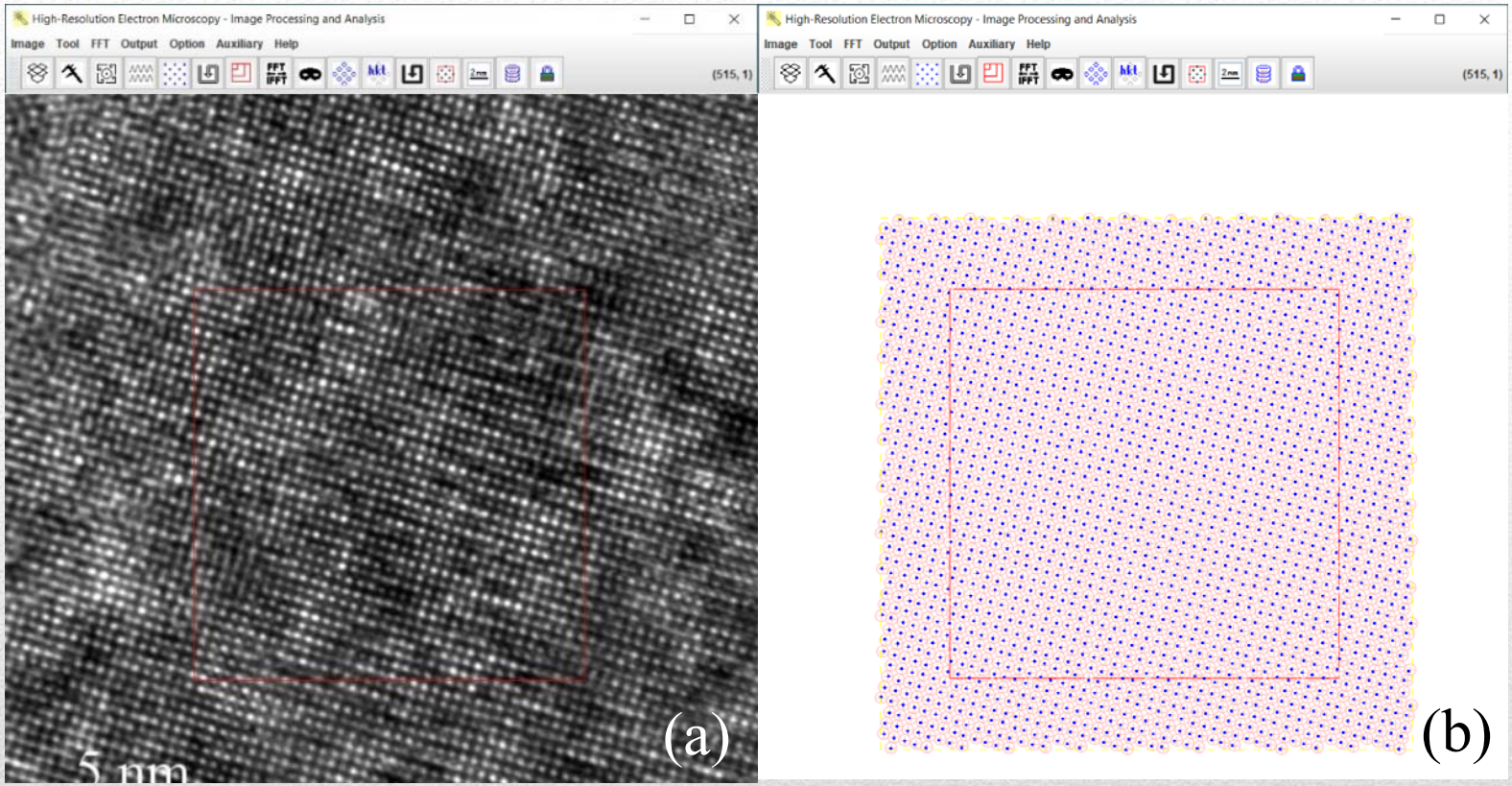
(b)



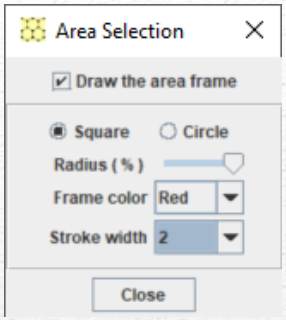
(c)

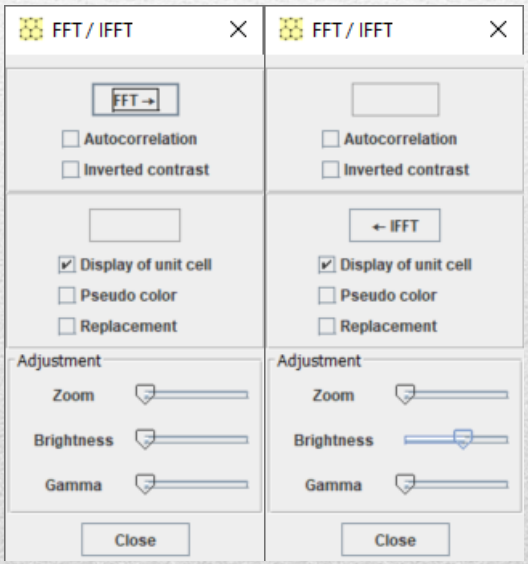


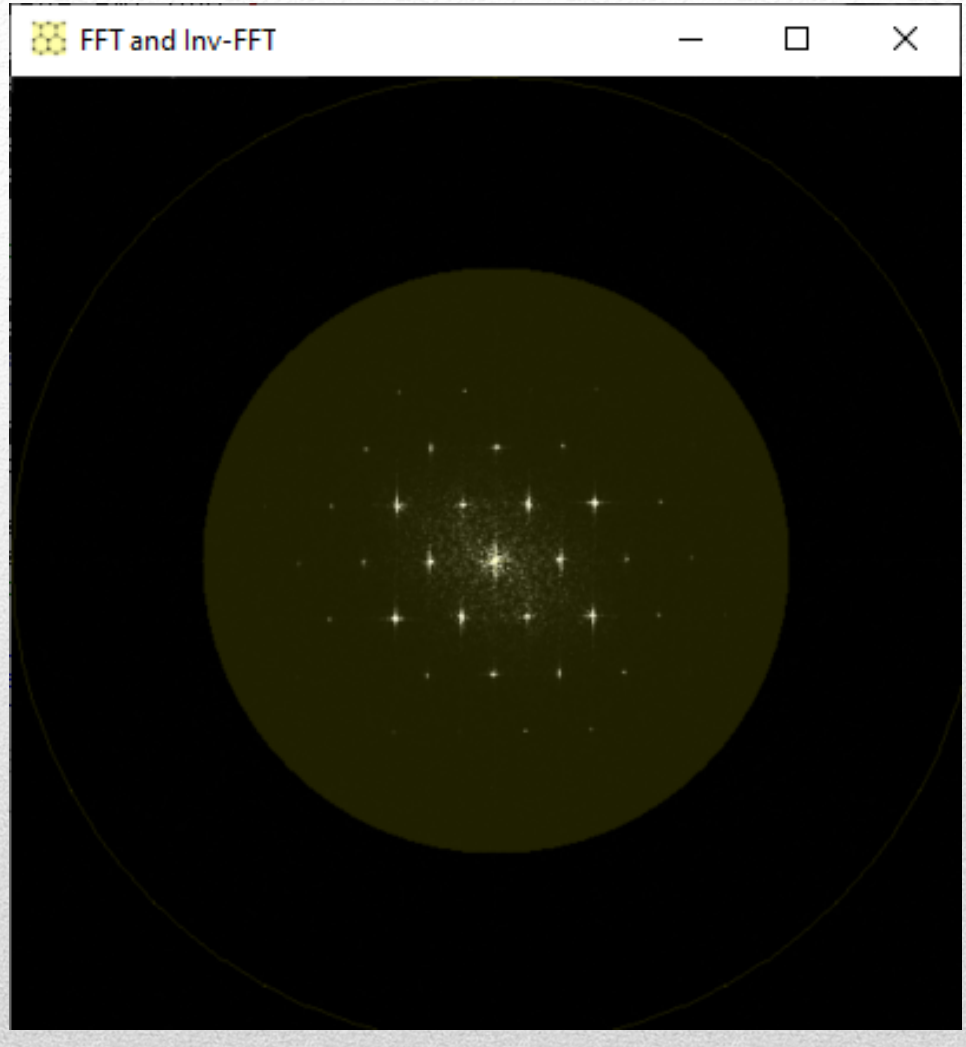
(a) The line profile analysis on an image and (b) the line-scan profile. HREM image was taken in the Mn_2RuSn Heusler alloy.



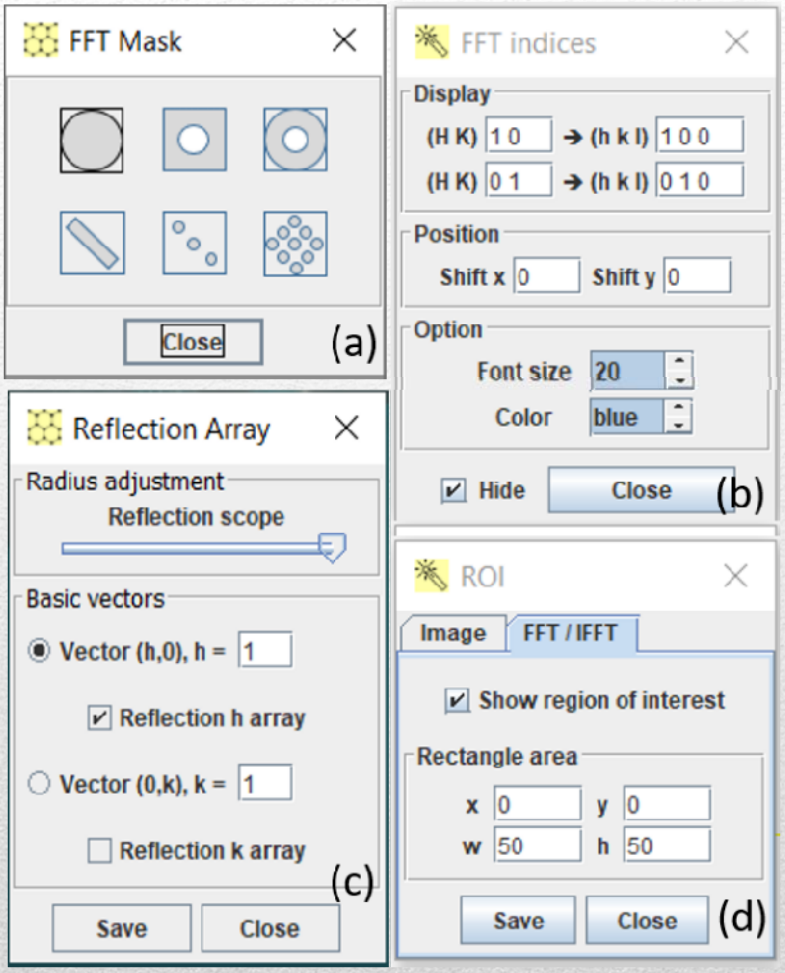
(a) The image HREM image was taken in the Mn_2RuSn Heusler alloy, (b) An array of the image spots can be retrieved from the image.

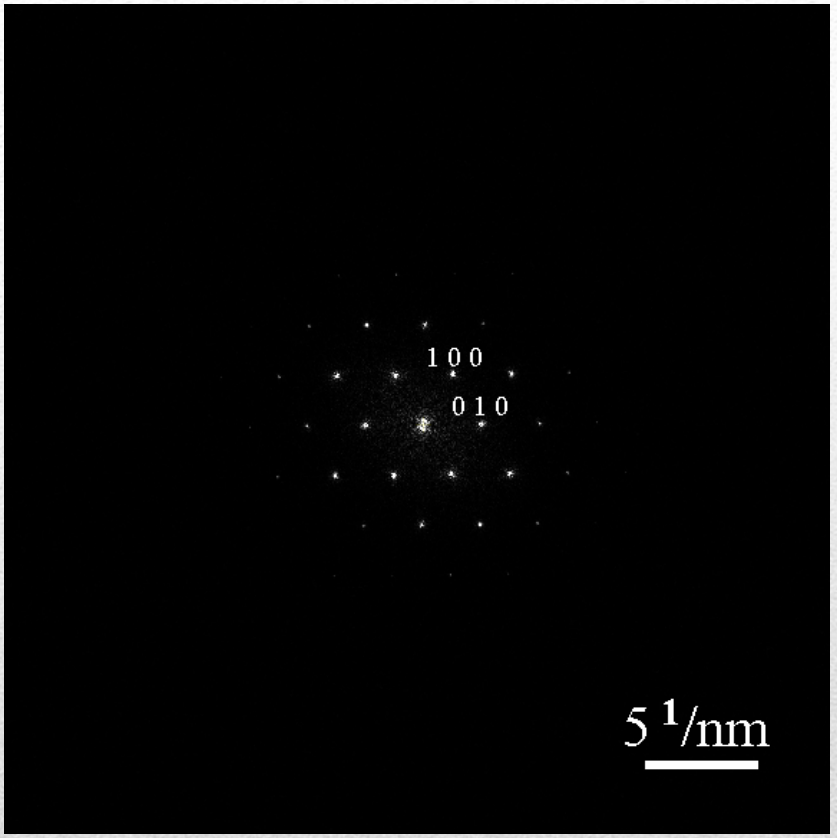




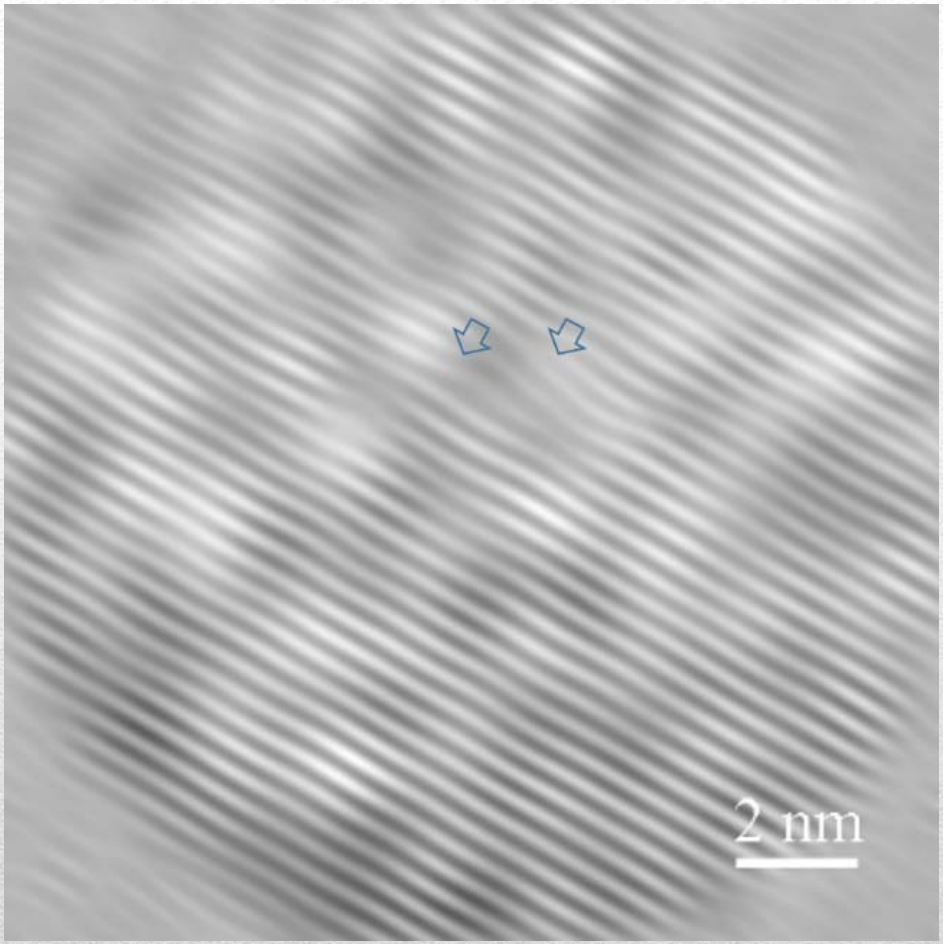


The FFT pattern from the HREM image and a circular mask.

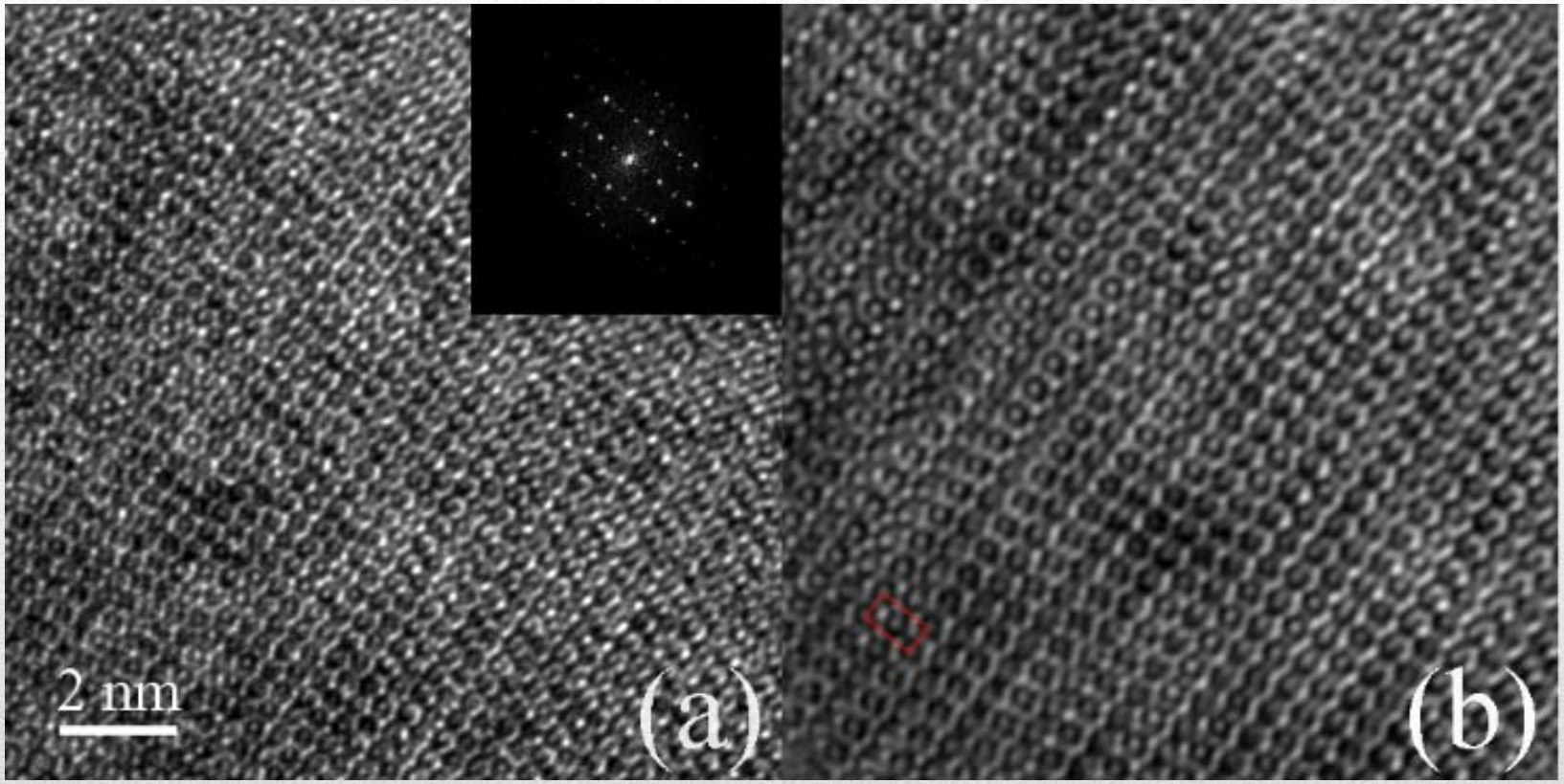




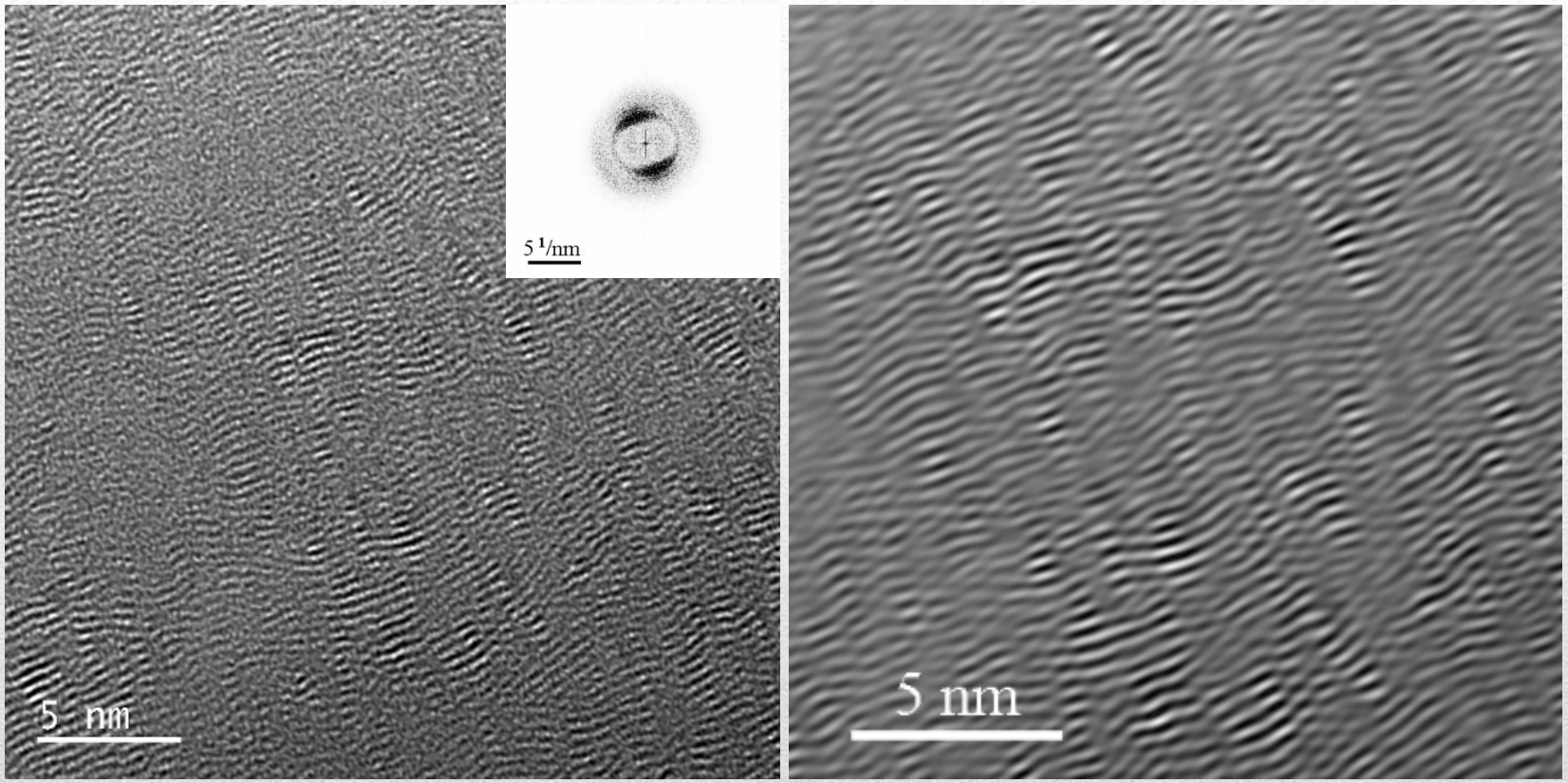
The output of the FFT pattern with two basic indices and a scale bar.



The IFFT pattern by using a mask with a pair of reflections (1 0 0) and (-1 0 0). Two dislocations cores are pointed out by arrowheads.

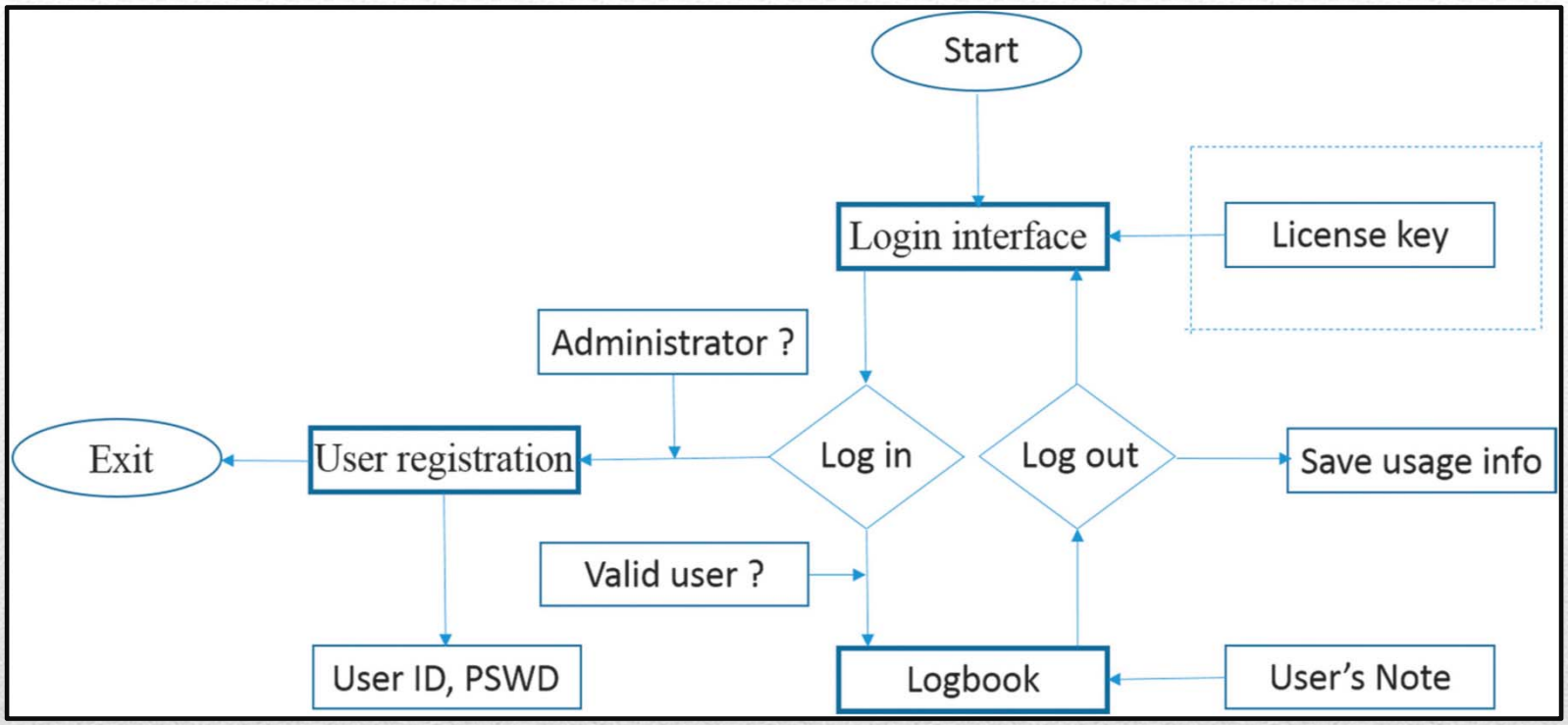


(a) HREM image and (b) the IFFT processing image of the main compound in the $Fe_3Co_3Ti_2$ alloy



An FFT pattern (inserted) and an IFFT image (right side) of the experimental image of graphite fiber (left side).

A Real-Time Logging System for Managing Multiuser Equipment



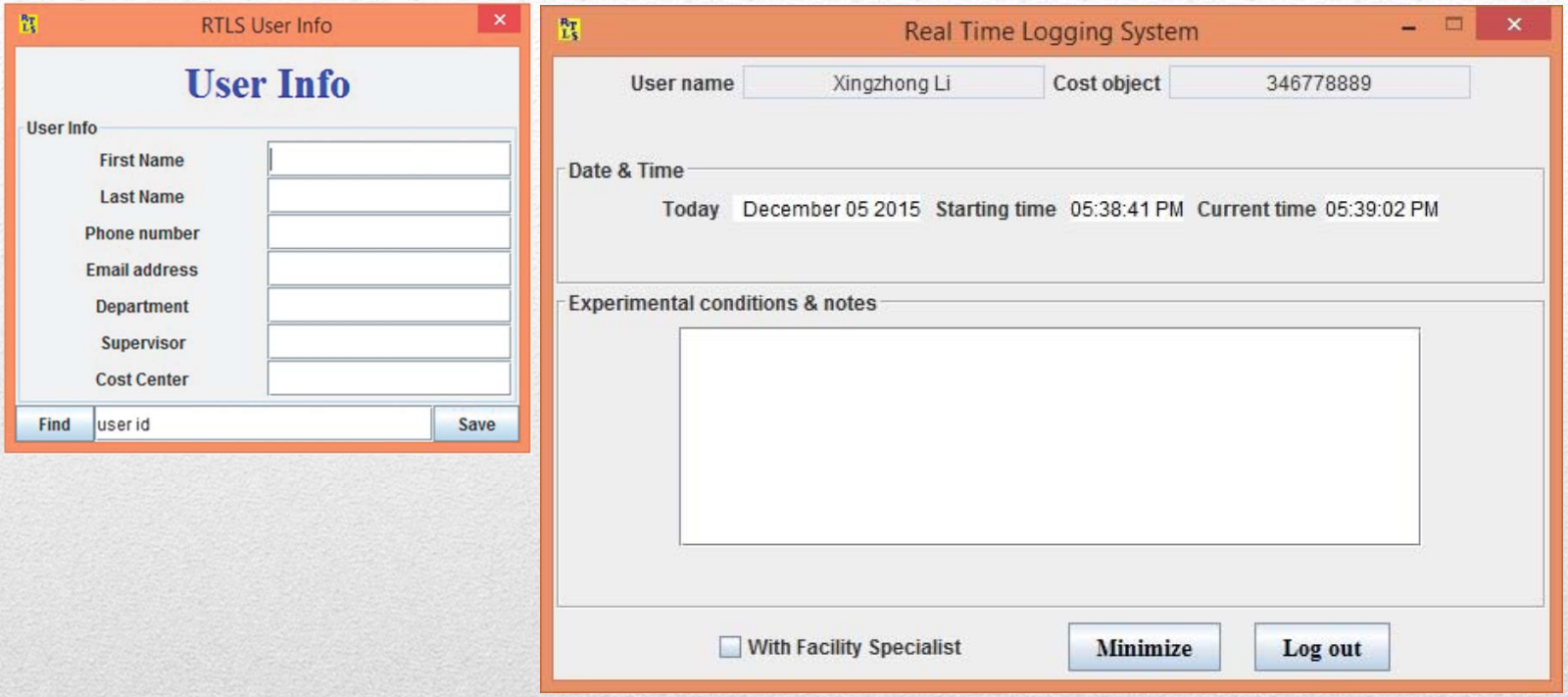
A flowchart of software design for the RTLS. Three main functions are indicated in bold frames.

X.-Z. Li, A real-time logging system for managing multiuser equipment, Microscopy Today, January (2018) 2-4.

A Real-Time Logging System for Managing Multiuser Equipment

X.-Z. Li, A real-time logging system for managing multiuser equipment, Microscopy Today, January (2018) 2-4.

RTLS



X.-Z. Li, A real-time logging system for managing multiuser equipment, Microscopy Today, January (2018) 2-4.

The components in the Landyne and Landyne+ software suites

Software	Description of components in the Landyne suite
PTELS	Periodic table of the elements for the Landyne suite
SVAT	Structural viewer and analytical tool including atom cluster and layer.
SPICA	Stereographic projection for interactive crystallographic analysis.
SAED	Simulation and analysis of electron diffraction (spot) patterns.
PCED	Simulation of PCED (ring) patterns and phase identification.
QSAED	Processing, quantification, and analysis of SAED (spot) patterns.
QPCED	Processing, quantification, and analysis of SAED (ring) patterns.
HOLZ	Simulation of HOLZ pattern including dynamical correction.
SMART	Simulation and measurement of rocking curve for crystal thickness.
SAKI	Simulation and analysis of Kikuchi lines and double diffraction effect.
TEMUC	Lattice determination of unknown structure in TEM/ED experiments.
ESPOT +	Electrostatic potential maps derived from electron diffraction patterns.
CTFscope +	CTF simulation and visualization for conventional and AC-TEM.
EMIPA +	HREM image processing and analysis
EMCIP +	HREM image crystallographic image processing

Microscopy and Microanalysis Meeting 2023

Landyne 5, a Software Suite for Electron Diffraction Simulation and Crystallographic Analysis

Xing-Zhong Li, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588

NCMN

The Landyne suite

Landyne (computer software) was registered in 2010 by X.-Z. Li and Jane Li in Lincoln, NE. We developed a software suite for electron diffraction simulation and crystallographic analysis. The components in the software suite can be classified as three categories according to their functionality, as shown in Figure 1.

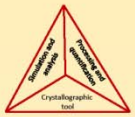


Figure 1. Landyne software suite

Landyne suite in a compressed file, landyne5.7z, can be downloaded from the author's website, listed below with QR codes.

Launcher is a desktop dock for the Landyne software suite. Figure 2 shows a snapshot of the launcher, which allows software components to be selected in the Landyne software suite.

Figure 2. Landyne Launcher.

PTELS is a periodic table of elements for Landyne suite. It provides the radii of the elements. It provides a tool to get the molecular mass.

SVAT is a computer program for interactive visualization of three-dimensional crystal structures, including chemical bonds and magnetic moments. A multitude of functions, e.g., revealing atomic layers and polyhedral clusters, are available for further structural analysis. Atomic sizes, colors, appearances, view directions, orthographic, or perspective views are adjustable. The customized work for the visualization and analysis can be saved and then reloaded. X.-Z. Li. *J. Appl. Cryst.*, 53 (2020) 848-853.

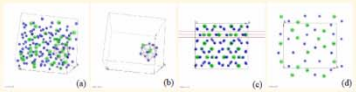


Figure 3. (a) the crystal structure of Al_3Mn phase, (b) a cluster, (c, d) a selected layer structure.

SAED is for simulation of SAED patterns and to find the zone axis of an experimental SAED pattern. X.-Z. Li. *Microscopy and Analysis*, May issue (2019) 16-19.

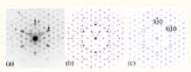


Figure 4. SAED pattern of Pt-Bi thin film, which consists of the twin of γ-$PtBi_2$ and coexisted hexagonal PtBi phase, (a) experimental EDP, (b) simulated EDP and (c) simulated EDP of γ-$PtBi_2$.

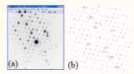


Figure 5. (a) Measurement of basic reciprocal vectors in the experimental EDP of Cu_2S nanofibers. (b) Simulated EDP of Cu_2S in the [2 1 1] zone axis.

QSAED is used to calculate the intensities of experimental SAED of single crystal. X.-Z. Li, *Micros. & Microanal.*, 20S3 (2014) 1486-1487.

- to quantitatively retrieve the intensities of reflections;
- to measure the reciprocal lattice spacing;
- to measure and display and intensity profiles along selected lines;

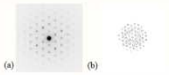


Figure 6. (a) a SAED pattern, (b) retrieved intensities.

PCED is for simulation of polycrystalline electron diffraction patterns and for phase identification. X.-Z. Li, *Ultramicroscopy* 110 (2010) 297-304.

Figure 7. (a) The GUI of the PCED with the simulated electron diffraction pattern of Al (fcc) and Mg (hcp) phases. (b) a calculated panel and (c) a parameter table.

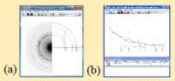


Figure 8. (a) Phase identification using experimental and calculated PCED pattern of Al (fcc), (b) a phase semi-quantification using experimental and calculated the intensity profiles of $FePt\ L1_0$.

QPCED is used to process experimental SAED patterns of polycrystalline phases, including pattern enhancement and ring highlighting, quantitation of intensity profiles from SAED patterns, and from selected rings. X.-Z. Li, *J. Appl. Cryst.* 45 (2012) 862-868.

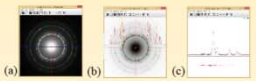


Figure 9. (a, b) Processing and (c) intensity profile of a PCED pattern.

Figure 10. Intensity profile along diffraction ring.

SAKI is for simulation Kikuchi pattern and double diffraction effect on the forbidden reflection spots. It provides tools to determine the precise orientation of crystal grains. X.-Z. Li, *J. Mater. Ed.*, 42:1-2 (2020) 97-104.

Figure 11. SAED and Kikuchi pattern with indices simulated by using SAKI.

Figure 12. SAKI traces the Kikuchi line-pairs for the orientation determination.

Figure 13. Simulated of the Kikuchi patterns comparing with an experimental pattern.

SPICA is used for stereographic projection calculation and interactive crystallographic analysis. X.-Z. Li, *J. Appl. Cryst.*, 49 (2016) 1818-1826.

Figure 14. GUI of SPICA.

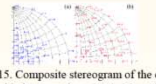


Figure 15. Composite stereogram of the orientation relationship between the α-Mg/γ-$Mg_{17}Al_{12}$.

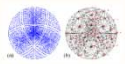


Figure 16. Display of Kikuchi maps.

Figure 17. Calculation of tilt angles in TEM.

TEMUC has been developed for unit-cell determination of crystal phases using electron diffraction data. A user-friendly graphic interface was designed for the following operations, (i) a reciprocal lattice is reconstructed from a tilt series of electron diffraction patterns; (ii) a Niggli cell is generated from the two SAED patterns in a tilt series; iii) a Niggli cell is generated from three electron diffraction patterns, in which each pair shares a common reflection vector; (iv) a conventional unit-cell is converted from a Niggli cell. X.-Z. Li. *Micron*, 117 (2019) 1–7.

HOLZ is used to calculate the HOLZ lines with dynamical correction. X.-Z. Li, *J. Appl. Cryst.*, 38 (2005) 576.

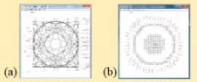


Figure 18. (a) HOLZ simulation and (b) EDP of Si [001].

SMART is for simulation and measurement with high accuracy of a rocking curve for crystal thickness. The simulation of two-beam CBED pattern includes the absorption effect. Computer assisting the measurement of crystal thickness using the experimental two-beam CBED pattern.

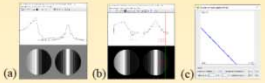


Figure 19. (a) The rocking curve and CBED pattern of Aluminum under the condition of two-beam and g(200). (b) Local minima are marked and (c) The drawing panel and result table.

CTFscope provides a practical tool for CTF simulation, visualization, saving, and edit for graphics and microscopy conditions. which extends to various aberrations (up to fifth order) for AC-TEM. A visualization of CTF is the key to fully understand the application of the function. It also includes the envelope effects due to an aperture and a drift on the CTF and imaging, together with image transformation based on CTF and |CTF| for a tutorial purpose. X.-Z. Li, *Microscopy Today* Nov-Dec. issue (2022) 20-27.

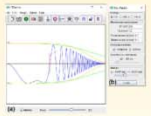


Figure 20. The main frame of the CTFscope.

Figure 21. The calculated CTF diffractograms with various astigmatic values.

ESPOT can be used to calculate the projected atomic potential maps from the calculated diffraction data, which is derived from SAED. In combination with the diffraction data retrieved from the experimental pattern using QSAED, the projected atomic potential difference map can be obtained to analyze and improve the structural model.

Figure 22. (a) A [001] projection of the Fe_3O_4 structure, (b) the simulation of SAED pattern generated from the SAED software, and (c) the projected atom potential map generated from the ESPOT software.

EMIPA provides functions for some basic image manipulations, FFT, a set of masks, and IFFT.

- Convenient tool for selecting area, resizing, and rotation of experimental images.
- A series of intensity profiles on HRTEM images can be retrieved and compared.
- Square and Inscribed circle of an arbitrary length for FFT.
- Varies of masks are available for inversed FFT images.
- Tools for adding scale bars and indices for processed images and FFT patterns.

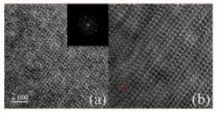


Figure 23. (a) HRTEM image and (b) the IFFT processing image of the main compound in the $Fe_3Co_3Ti_2$ alloy.

https://www.unl.edu/ncmn-emif/xzli/

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https://landyne.com

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