ReciPro Manual

Contents

1. Overview

ReciPro is a software package for various crystallographic calculations, simulation of diffraction patterns and high-resolution TEM images, etc., from crystal structure information.

Please send us your comments and suggestions via email (seto@crystal.kobe-u.ac.jp) or via Issue on GitHub (https://github.com/seto77/ReciPro/issues).

1.1. License

This software is distributed under the MIT license (https://github.com/seto77/ReciPro/blob/master/LICENSE.md). Anyone is free to use this software, free of charge, provided that they accept the following conditions.

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- There is no warranty for this software. The author assumes no responsibility for any problems that may arise from the use of this software.

1.3. System requirements

To run ReciPro, you need to have
- Windows OS running .Net Framework 4.8 or higher
- Graphics with support for OpenGL 1.3 or higher[1]

.Net Framework 4.8 can be installed from Microsoft homepage; if you have the latest update in Windows 10, you should already have .Net Framework 4.8 installed.

Also, some of ReciPro features may require large computational resources. To improve the speed, we use multi-threading and GPU usage as much as possible. We recommend you to use a computer with the following specs for better performance.

- Windows 10, 64 bit version
- 16GB or more memory
- CPU with 8 or more cores (especially when performing electron diffraction kinetics calculations)
- External GPU with support for OpenGL 1.5 (especially when using Structure Viewer)

1.3. Main features of ReciPro

Full GUI

All operations in ReciPro are done through a graphical interface. Most of the input and output of files are drag & drop.

Crystal list

ReciPro allows you to handle multiple crystals at once. There is no need to create files and run many windows for each crystal.

The software "CSManager"[2], developed by the same author, allows you to import a huge number of crystal structures easily.

Space groups

ReciPro has a built-in database of space groups. The database includes symmetry elements, Wycoff positions, extinction rules, etc. for the 230 space groups contained in International Tables for Crystallography Volume A (henceforth referred to as ITA), plus a subset (530 symbols) of space groups (Hall symbols[3]).

Atomic information

ReciPro contains information on valence, radius, characteristic X-ray energies and isotope ratios for elements from 1 (H) to 98 (Cf). Parameters necessary for the approximation of the atomic scattering factors for X-rays and electrons are incorporated in ReciPro. Parameters of scattering lengths for neutrons are also incorporated in ReciPro.

Flexible setting of crystal rotation

ReciPro allows the user to set the orientation of the crystal to a crystal axis index, a crystal plane index, or to rotate the crystal to any orientation with the mouse. The crystal rotation state can also be used synchronously to simulate crystal structure, stereonet or single crystal diffraction.

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[1] OpenGL is a library for graphics hardware. Most of the currently used PC supports OpenGL 1.3, but unfortunately, it seems that OpenGL 1.3 may not be available in the following cases.
- Running Windows OS in the Parallel desktop environment from Mac OS
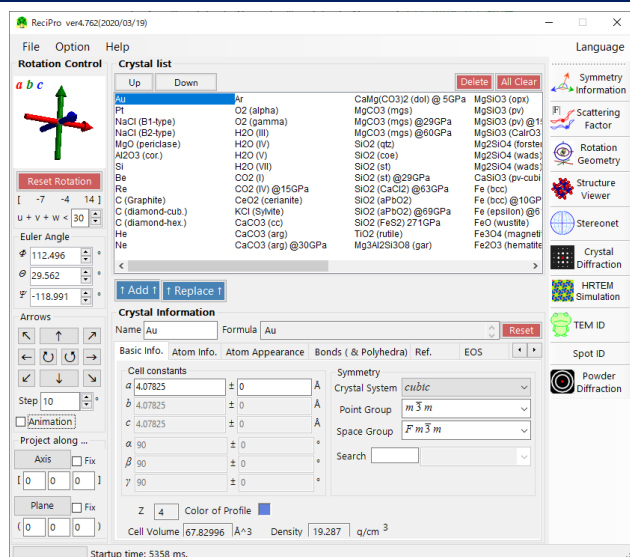- Using Windows with Remote Desktop
You can use ReciPro even if OpenGL 1.3 is not available, but OpenGL drawing functions will be disabled.

[2] CSManager can be downloaded from https://github.com/seto77/CSManager/releases/latest

[3] About Hall symbol notation, see "1.4. Symmetry in reciprocal space" in "International tables for crystallography, Volume B (ITB)".

2. Main window

When ReciPro is successfully launched[4], the main window appears. In the window, the user selects the crystal to be calculated, rotates the crystal, and invokes various other functions. This window can be divided into following types

- File menu (top of page)
- Rotation control (left part)
- Crystal List (upper center)
- Crystal Information (bottom center)
- Functions (right part)

The details are described below.

2.1. File menu

File
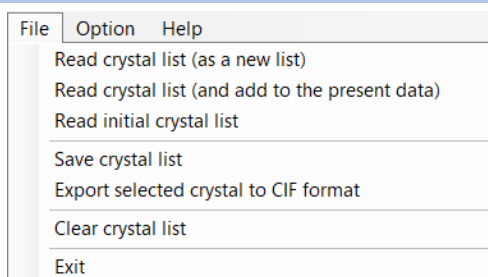
Read crystal list (as new list)
Reads a new crystal list file (*.xml). The already loaded crystal list will be deleted.

Read crystal list (and add to the present data)
Reads a new crystal list file (*.xml). The loaded crystal list is appended to the current list.

Read initial crystal list
Reads the list of crystals loaded at startup again.

Save crystal list
Saves the current crystal list.

Export the selected crystal to CIF format
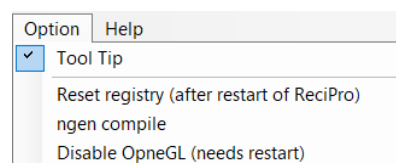Saves the currently selected crystals as a CIF format.

Clear crystal list
Clear all current crystal lists.

Exit
Exit the application.

Option

Tool tip
When checked, the tooltip will be displayed.

Reset registry (after restart of ReciPro)
Reset the registry on reboot. The registry contains information such as window size, wavelength, and camera length. Resetting the registry may be useful if the software becomes unstable for some reason.

ngen compile
By pre-compiling your program, you can speed up the startup time. However, the effect is not so great.

Disable OpenGL (needs restart)
Check to turn off the OpenGL feature. ReciPro uses OpenGL 1.3 or later to draw in three dimensions. However, if you are using an older PC, remote desktop environment or Windows emulation on Mac, the OpenGL version may be less than 1.3. In that case, please check this item.

Help
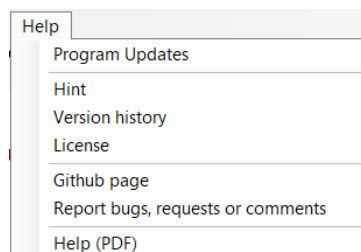
Program updates
Check if a new version has been released and if so, update it.

Hint
Deprecated.

Version history
Shows the version history of ReciPro.

License
Shows the license of ReciPro.

Github page
Opens the Github top-page of ReciPro.

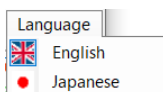### Report bugs, requests, or comments
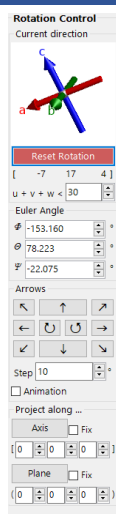Opens an issue page of the Github.

Help (PDF)
Shows this PDF file.

Language

Switch between languages. Currently, only English and Japanese are supported. Need to reboot after switching.
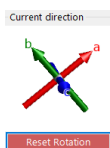
2.2. Rotation control

This control allows you to view/set the rotation status of the selected crystal.

Current direction

The current rotation state of the crystal is displayed. By mouse-dragging this area, you can rotate the crystal.

The axis of the crystal is shown as
- red: a-axis
- green: b-axis
- blue: c-axis

Reset rotation

The crystal orientation is reset to the "initial state", which means that the c-axis is perpendicular to the screen and the b-axis faces upward when projected on the screen[5].

Zone axis

Displays the zone axis corresponding to the direction perpendicular to the screen.

You can also specify the range of indices to be displayed. For example, if you set u+v+w < 30, it will display the closest indices, where the sum of u, v, and w absolute values do not exceed 30[6].

Euler angles

Set the crystal orientation in terms of Euler angles. Euler angles are expressed in three angles, and ReciPro defines the three angles as follows:
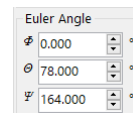- Ψ: Z-axis rotation
- θ: X-axis rotation
- Φ: Z-axis rotation

The rotation operation is performed in the order of Ψ, θ, and Φ. See 3. Rotation geometry and Appendix for a detailed explanation of the coordinate system.

Arrows

When you press the arrow buttons, the selected crystal will rotate in the direction of the arrow by the angle Step.
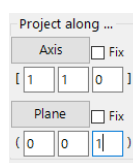
And if you check the "Animation" checkbox, the crystal will rotate continuously at the specified rotation speed.

Project along...

The crystal rotation is set along the specified zone axis or crystal plane.

When "Fix" is checked, the rotation operation is performed with the axis or plane spatially fixed.[7]

Axis

Sets the direction of the specified zone axis to the vertical front of the screen. If the plane is perpendicular to this axis, the direction of the plane is set to the upward direction of the screen.

Plane

Sets the direction of the normal of the specified crystal plane to the vertical front of the screen. If the Axis is set to 0, the axis of the crystal band will be set to face upward on the screen.

2.3. Crystal List
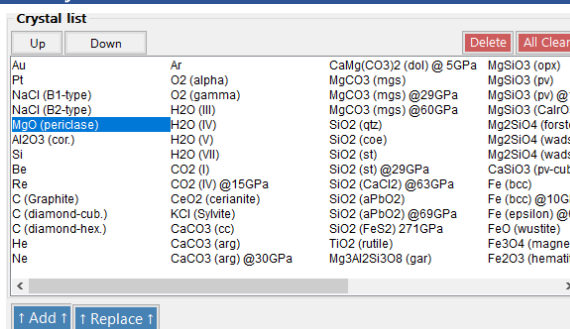
The list should be about 80 crystals in the initial state after installation.[8] When you select a crystal from the list, detailed information is displayed on the bottom screen ("Crystal Information) and the crystal is set for calculation.

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[5] The symbols and definitions for Eulerian angles are the same as those used in Oxford EBSD software (formerly HKL's CHANNEL5). Therefore, users of Oxford EBSD can input the angle output as it is.

[6] For example, a slight rotation of the crystal from the [0 0 1] axis will result in a higher order index such as [1 0 100]. If you want to avoid the case, set the sum of u + v + w to a smaller value.

[7] This feature is useful when one of the diffraction spots in the picture has been clearly indexed.
Please note that the direction of the crystal axis/plane is only fixed when using the mouse drag or arrow buttons to rotate the crystal. If Euler angles are entered directly, the specified axis/plane is not fixed.

[8] The list of crystals is automatically saved when ReciPro is closed, and will be automatically loaded the next time you start ReciPro.

Up/Down

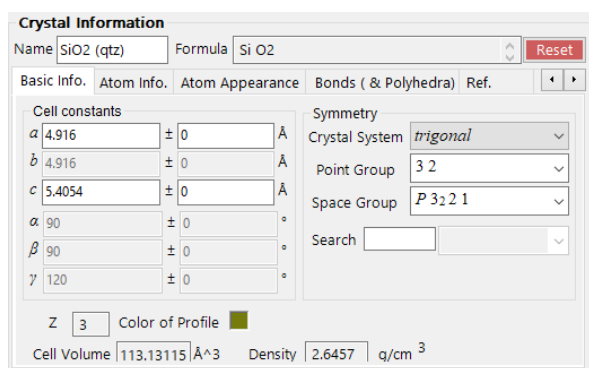Moves the order of the selected crystals up/down.

Delete/All clear

Removes the selected crystal from the list. Alternatively, removes all crystals from the list.

Add/Replace

The crystal is added to the end of the list. Alternatively, it replaces the crystal with the selected crystal in the list.

2.4. Crystal Information

Crystal lattice parameters, symmetry, and atomic position can be set and displayed in this area. By dragging and dropping CIF or AMC file to this area, you can load any crystal.

Whenever you make any changes to the crystal, you must press the "Add" or "Replace" button. If you do not press this button, the crystal will not be saved in the crystal list and your changes will be lost.

This section is very long and will be explained in detail on another page.
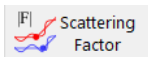
2.5. Functions

Symmetry information

Displays information about the symmetry of the selected crystals and provides a crystallographic calculation function. See here.
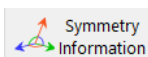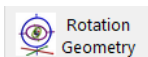
Scattering factor

Lists the crystal planes and calculate the structure factors. See here.

Rotation geometry

Displays and analyzes the rotational state (matrix) in 3 dimensions. See 3. Rotation geometry.

Structure viewer

Draws crystal structure, coordination polyhedral, unit cell, lattice planes, and etc. using OpenGL. See 4. Structure viewer.。
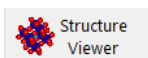
Stereonet

Draws the direction of the crystal plane or axis on a stereonet. See 5. stereonet.

Crystal diffraction

Simulates electron and X-ray diffraction patterns. See 6. Crystal diffraction.

HRTEM simulation

Simulates HRTEM (High resolution TEM) based on the Bethe method. See 7. HRTEM simulation.
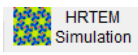
TEM ID

Indexes diffraction spots. See 8. TEM ID.
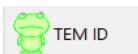
Spot ID

Displays electron diffraction images, and searches, indexes, and fits the diffraction spots. See 9. Spot ID
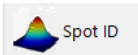
Powder diffraction

Simulate and fit polycrystalline diffraction patterns. See 10. Powder diffraction

3. Rotation geometry

This provides a function to represent the rotational state of a crystal as a 3x3 matrix and to convert it to a different Eulerian coordinate system.

ReciPro provides three Eulerian angles, Ψ, θ, and Φ, in Z-X-Z order, to represent the rotational state of a crystal. However, this expression does not necessarily correspond to the rotation axis of the goniometer in the actual optical system.

Converting the Eulerian angle in ReciPro to an arbitrarily defined Eulerian angle supports the adjustment of the goniometer in the laboratory.

3.1. ReciPro coordinate system (ZXZ)

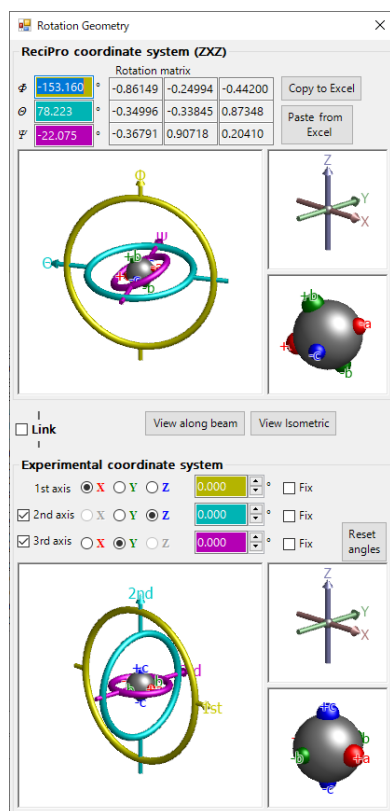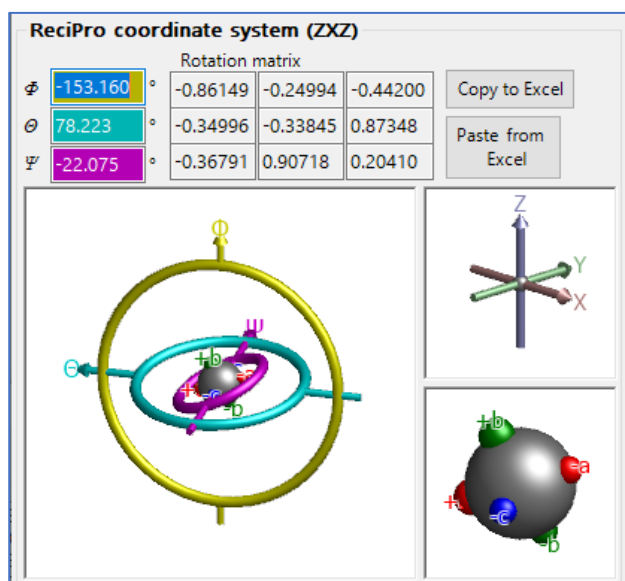The upper half of the windows shows the rotation state of the crystal represented by the "ReciPro coordinate system".

The values of Φ, θ, and Ψ are synchronized with the Euler angle set in the Main window.

"Rotation matrix" shows the 3x3 rotation matrix corresponding to the current rotation state.
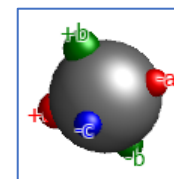
OpenGL windows

The OpenGL window is a three-dimensional representation of the current rotation situation, and the window with three toruses (doughnuts) shows the situation of the three rotation axes. The arrow through the yellow torus corresponds to the axis of rotation of the Euler angle Φ, which is the upper (1st) axis of rotation in the goniometer. The light blue arrow is the middle (2nd) axis of rotation corresponding to θ, and the pink arrow is the lower (3rd) axis of rotation corresponding to Ψ.
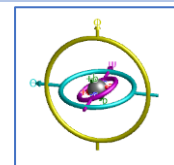
The red, green and blue arrows in this window represent the X, Y and Z axes in real space Cartesian coordinates. Note that the arrows displayed in this window are not the same as the arrows displayed in the Rotation control of the Main window (crystal axis).
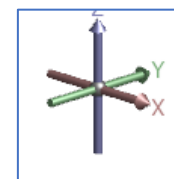
The gray sphere in the center of the goniometer represents the state of the object as it rotates. The red, green, and blue spheres represent the direction of the object; when Φ, θ, and Ψ are all zero, the red, green, and blue spheres are in the same direction as the Cartesian coordinates +X, +Y, and +Z in real space, respectively. Varying Eulerian angles cause the object to rotate in various directions.

The window drawn in OpenGL can be rotated by dragging the left mouse button. Please note that this operation does not rotate the crystal itself, but only changes the projection direction of "Rotation geometry". If you want to rotate the crystal itself, you need to rotate it from the main window.

Copy to Excel

Copy 3x3 rotation matrix to the clipboard in a tab-separated format that can be pasted into Excel.

Paste from Excel

When Excel-formatted 3x3 tab-separated numbers are copied to the clipboard, you can set it as a rotation matrix.

View along beam / isometric

The former is the same as the projection orientation of the Main window. That is, the yellow axis of rotation (Z-axis in Cartesian coordinate system) is perpendicular to the screen[9]. The latter projects in an isometric orientation. Note that the crystal is not rotating, but only in the projection direction.

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[9] The term "View along beam" is used because the Z-axis of the real space coordinate corresponds to the beam direction of X-rays and electrons.

3.2. Experimental coordinate system
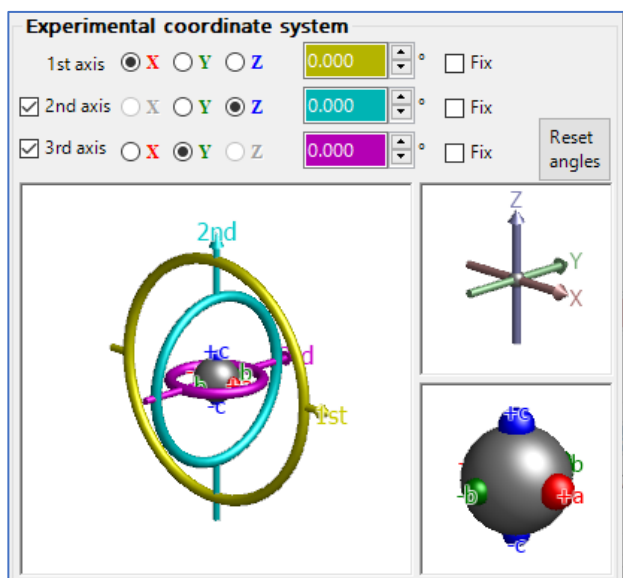
The lower part of the "Rotation geometry" is where you define the Euler angle on the arbitrary axis of rotation and get/set the rotation state of the goniometer. This is called the "Experimental coordinate system".

The description of the objects is the same as that of the "ReciPro coordinate system".

1st, 2nd, 3rd axes

Select the rotation axes of the goniometer from ±X, ±Y and ±Z for the upper (1st), middle (2nd) and lower (3rd) levels.[10] When you change the selection, the graphics will also change accordingly.

The Euler angles for each axis of rotation are displayed in yellow, light blue, and pink text boxes. Alternatively, you can enter the value directly in the text box.

3.3. Link

This is a great feature of "Rotation geometry". If you check "Link", you will see "ReciPro coordinate system" and "Experimental coordinate system " and adjust their Euler angles to match each other so that the object's orientation is consistent with each other. That is, it provides information on the Euler angles for a goniometer represented by a differently defined axis of rotation than ReciPro.

For example, suppose that the laboratory goniometer is adjusted so that the a-axis of a crystal is aligned with the direction of X-ray incidence and the b-axis with the horizontal direction. Enter the Eulerian angle of the laboratory goniometer in the experimental coordinate system. Furthermore, rotate the crystal in the main window of ReciPro and set the vertical direction of the screen to the a-axis and the horizontal direction to the b-axis. If Link is checked in this state, this means that when you point the crystal to a different orientation in the Main window, the angle of the goniometer that achieves the orientation will be displayed.

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[10] The goniometer of ReciPro corresponds to 1st : +Z, 2nd : +X, 3rd : +Z.
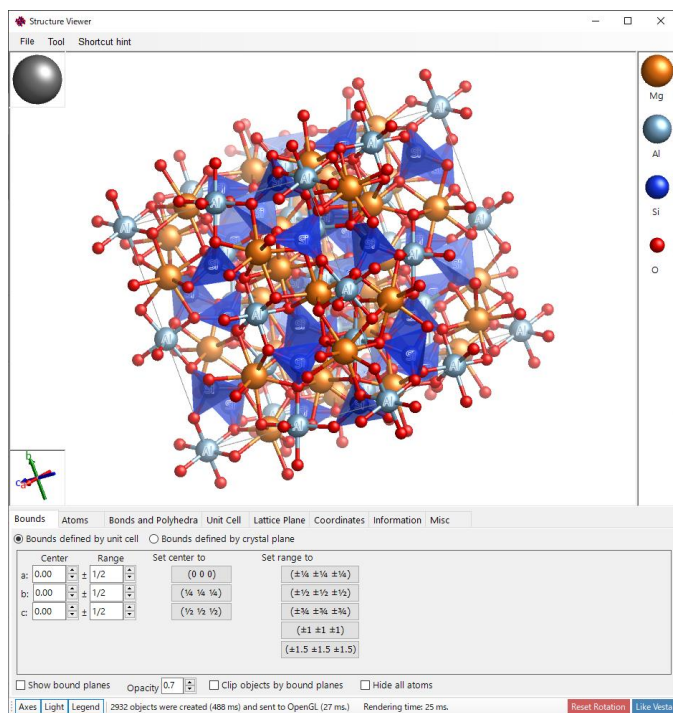
4. Structure Viewer

"Structure Viewer" draws the crystal selected in the main window as a three-dimensional image. This function uses Open GL and requires a video card to draw the crystal.

4.1. Main area

In the upper part of the main area, the crystal structure is drawn. In the upper left, the direction of the light source is shown. The direction of the crystal axis is shown in the lower left. On the right, the legend of the atoms is shown.
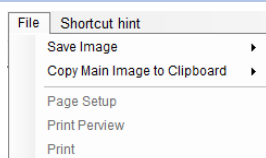
Mouse operation

The following mouse operations are accepted.
- Left drag: rotation.
- Center drag: translation
- Right up/down or wheel: zoom
- Left double click: select/unselect the atom
- Right click:
- CTRL + Right double click: Change perspective <-> orthogonal projection.
- CTRL + Right up/down: Change degree of perspective.

4.2. File menu

File

Save image

Saves the drawn image to a file.

Copy main image to clipboard

Copy the image to the clipboard, CTRL+SHIFT+c does the same action.

Shortcut hint

Displays shortcut hint.

4.3. Tab menu

4.3.1. Bounds

In this tab, you can specify the drawing range of the crystal. There are two ways to set the range: by the unit cell or by the crystal face. You can switch between these two ways using the radio buttons at the top.

Bounds defined by cell

In this mode, the a, b, and c-axes of the unit cell are the unit of the drawing range.

The "Center" is the central fractional coordinate and the "Range" is the upper/lower limit for each axis.

For frequently used values, you can use the preset buttons on the right side.

Bounds defined by crystal planes

In this mode, you can specify the area to be drawn based on the crystal plane. If the input bounds is incomplete and a spatially closed region cannot be defined, ReciPro will automatically set the bound to one unit cell and draw it.

Bound list

When you want to disable the boundary plane temporarily, check the leftmost checkbox in the list.

When you want to add a new bound plane, click the "Add" button, when you want to replace it, click the "Replace" button, when you want to delete an existing plane, click the "Delete" button.

If you want to permanently save the changes you have made, you have to press the "Add" or "Replace" button in the "Main Window" as well. Please do so. Otherwise, when you change the selection of the crystal list in the "Main Window", the changes you have made will be lost.

H k l indices

Set the bound plane by the Miller index. The check box enables to include the crystallographic equivalent of the plane you set[11].

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[11] For example, if {110} is checked for a cubic crystal, the bounds are set to the following 12 planes (1 1 0), (1 -1 0), (-1 1 0), (-1 -1 0), (1 0 1), (1 0 -1), (1 0 1), (-1 0 -1), (0 1 1), (0 1 -1), (0 1 -1), (0 -1 1), and (0 -1 -1).

Distance from origin

The distance from the center of the crystal to the bound face is set. The unit of distance is selectable between "d" and "Å". In the former case, the distance is the input value multiplied by the d-value of the crystal face (in the case of the figure, d x 1.5 = 9.949 Å). If you choose the latter, the input value will be the absolute distance in Å scale. If you change one of them, the other will be changed automatically.

Show bound planes / Opacity

Shows the bound planes or not. When checked, you can set its transparency in Opacity (0 is transparent and 1 is opaque).

Clip objects by bounds planes

If checked, the inside area specified by bounds will be drawn, and objects that intersect with the bounds will be clipped.

Hide atoms

If checked, all atoms, bonds and polyhedra will be hidden.[12]。

4.3.2. Atoms

In this tab, you can set the coordinates and appearance of the atoms.

Atom list

	Label	Element	X	Y	Z	Occ.	Multi.	Wyck. Let.	Site Sym.
	MgX1	12: Mg	1/2	1/2	1/4	1	8	b	2.22
	MgX2	12: Mg	5/8	1/4	3/8	1	32	g	1
	MgY	12: Mg	1/2	1/4	1/8	0.26	16	c	-1

The list of atoms in the crystal is displayed. The list can be manipulated by using "Add", "Replace", and "Delete". If you want to temporarily hide an atom, uncheck the leftmost checkbox in the list.

If you want to permanently save your changes, be sure to click on "Add" or "Replace" in the "Main Window" to make the changes permanent. Please do so. Otherwise, when you change the selection of the crystal list in the "Main Window", the changes you have made will be lost.

Element & Position

Label

Enter the label of the atom.

Element

Set the elements.

X, Y, Z

Enter a real number from 0 to 1, or a fraction such as 1/2 or 2/3.

Occ

Set the occupancy of an atom, which should be a real number between 0 and 1.

Origin shift

Shifts atomic position. Press preset buttons, or enter custom values and press the "Apply custom shift" button.

Appearance

Set the radius, color, and texture of an atom to be drawn.

Radius

Set the atomic radius.

Atom color

Set the color of the atom.

Material

Set the textural properties of atoms in the drawing.

Apply to same elements

Appears only when the "Appearance" tab is selected. The set properties (ionic radius and foreground color) will be applied to all the atoms of the same elemental species.

4.3.3. Bonds (& Polyhedra)

In this tab, you can enter information about the bond and polyhedron.

Bond list

	Center	Vertex	Max len.	Min len.	Bond color	Polyhedron
☑	14: Si	8: O	2.2	0		
☑	13: Al	8: O	2.2	0		

The bond information is displayed. You can manipulate the list by using "Add", "Replace" or "Delete" buttons. If you want to temporarily disable a bond, you can uncheck the leftmost checkbox in the list.

If you want to permanently save your changes, be sure to click on the "Add" or "Replace" button in the "Main Window" to make the changes permanent. Please do so. Otherwise, when you change the selection of the crystal list in the "Main Window", the changes you have made will be lost.

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[12]By checking both "Show bound planes" and "Hide atoms", an arbitrary crystal outline can be drawn. That is, you can represent the shape of the crystal.

Bond property
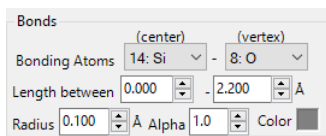
Set bond properties.

Bonding Atom (center)

Sets the elemental species that make up the bond. It will be center for the polyhedron.

Bonding Atom (vertex)

Sets the elemental species that make up the bond. It will be vertices for the polyhedron.

Length between ...

Sets the lower and upper limits of the bond length. If the bond length exceed/below this threshold, it is not object to drawing.

Bond Radius

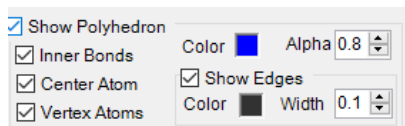Sets the bond thickness (radius) to be drawn.

Alpha

Sets the transparency of the bond to be drawn.

Polyhedron property

Show Polyhedron

When checked, the lower control becomes active and displays the polyhedron made up of bonds (if the polyhedron is valid).

Inner Bonds

When checked/unchecked, the bonds in the polyhedron is visible/invisible.

Center Atom

When checked/unchecked, the center atom of the polyhedron is visible/invisible.

Vertex Atoms

When checked/unchecked, the vertex atoms of the polyhedron are visible/invisible.

Color

Set the transparency of the cell planes.

Alpha

Set the transparency of the cell planes.

Show Edge

Checking this box displays the polyhedron's edges (lines connecting the vertices).
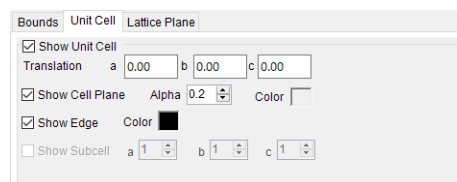
Color

Set the color of the polyhedron edges.

Width

Set the line width of the polyhedron edges.

4.3.4. Unit cell

In this tab, you can set up the drawing of the unit cell. If "Show unit cell" is checked, the unit cell will be drawn in the unit cell.

Translation

Every space group has a default origin. If you want the center of the unit lattice to move from the space group origin, set the translation amount in the a, b, and c axis directions.
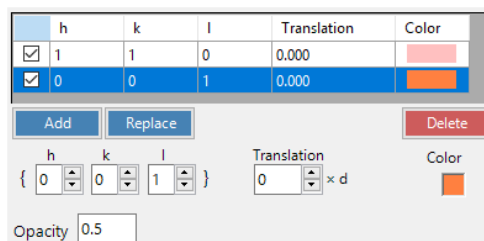
Show cell plane

Specify whether to draw the six faces that make up the unit lattice. If you want to draw them, you can set the color and transparency of the faces.

Show edges

Specify whether or not to draw the edges of the unit cell. You can also set the color.

4.3.5. Lattice plane

In this tab, you can set up the settings for drawing the lattice plane. A list of lattice planes is displayed at the top. You can operate the list by using the "Add", "Replace" and "Delete" buttons. To disable the lattice plane drawing, you can uncheck the leftmost checkbox in the list.

If you want to permanently save the changes made in this tab, you must also click on "Add" or "Replace" in the "Main Window" to make the changes permanent. If you have not done so, you will lose your changes when you change the selection of the crystal list in the "Main Window". Otherwise, when you change the selection of the crystal list in the "Main Window", the changes you have made will be lost.

H k l indices

Specify the lattice plane with the Miller index.

Translation

Use when you want to move the lattice plane in translation.

4.3.6 Coordinate information
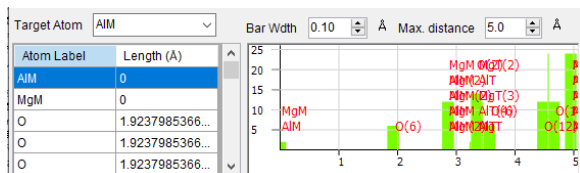
Information about the coordination of atoms.

Table (Left side)

The table on the left shows what kind of atoms are around the specified target atom and at what distance.
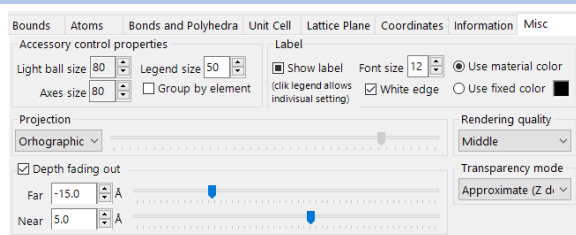
Graph (right side)

This is a graphical representation of the information in the table on the left. You can estimate the coordination number of target atom by adjusting "Bar width" to an appropriate thickness.

4.3.7. Information
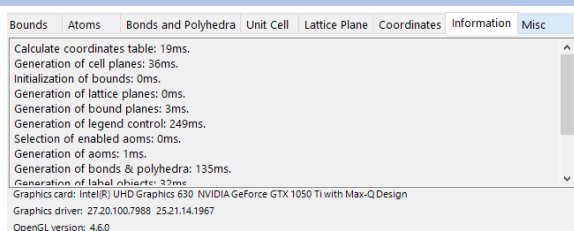
The information of the selected atom is displayed. This is under construction.

4.3.8. Misc.

Accessory panel properties

Set the size of accessory panel. If you check the "Group by element" checkbox, the legend will be displayed for each element instead of the label.

Label

Configure settings related to the atomic label. You can change the font size and color.

Projection

You can set the projection method. "Orthographic" produces a perfectly parallel projection (infinity projection). "Perspective" produces a perspective projection from the viewpoint distance set in the track bar.

Depth fading out

Fade out objects that are farther away in the depth direction." Objects farther away than the "Far" value will be completely transparent, and objects closer than the "Near" value will be completely opaque. The intermediate objects will be set to a transparency range of 0-1.

Rendering quality

Select the drawing quality. The higher the quality, the slower the rendering process will be, so choose the appropriate quality for your GPU's performance.

Transparency mode

Select an algorithm for calculating the overlap of translucent objects (atoms and polyhedra).

"Approximate" may result in inaccurate rendering depending on the placement of the objects, but it is fast. "Perfect" calculates the transparency accurately, but is very slow, so an external GPU card is required.

4.4. Toolbar

The object to be drawn can be selected from the toolbar at the bottom of the "Structure viewer".

Crystal Axes

Displays the orientation of the axes. The size of the axes reflects the lattice constant. You can also rotate with the mouse in this box.

Lightning ball

Specify the position (direction) of light. You can change the position of the light by dragging left.
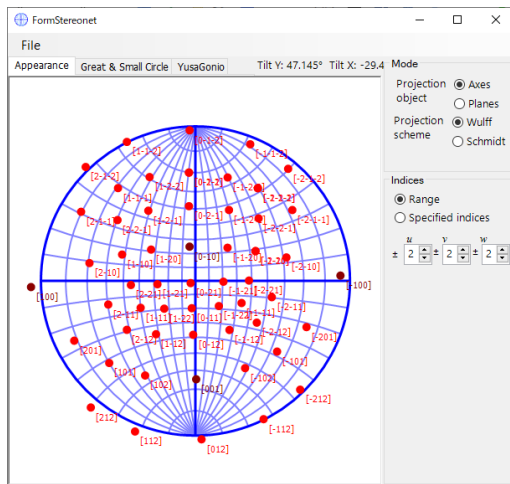
Legend

Displays the legend of the atom. You can choose to label the letters displayed, or use the element name from the Misc tab.

Like Vesta

Change the atomic color/size and bond settings to make it look similar to the well-known Vesta software.

5. Stereonet

"Stereonet" function displays the directions of the crystal planes and crystal axis using stereo-net projection.
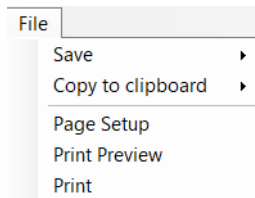
5.1. Main area

In the main area, the stereonet projection of the crystal face and crystal axis of the selected crystal is displayed.

Mouse operation

The following mouse operations are accepted.
• Left drag: rotation.
• Right click: zoom out
• Right up/down or wheel: zoom in.

5.2. File menu

Save or copy the displayed stereonet.

5.3. Mode

Projection object

Select "Axis" or "Plane".

Projection Scheme

Wulff: This option is for calculating equal-angle projection. This method preserves the angle relation, but does not preserve the area (solid angle).

Schmidt: This option is for calculating equal-area projection. This method preserves the area (solid angle), but does not preserve the angle relation.

5.4. Indices

Sets the crystal planes/axes to be drawn.

Range

In this mode, you can specify a range of [u v w] or {h k l} indices.

Specified indices

In this mode, you can specify particular axes of the crystalline planes/axe. After inputting index, it can be added to the drawing list by the "Add" button. You can delete it by the "Remove" button. When "including equivalent indices" is checked, all crystallographically equivalent planes/axes will be drawn.

5.5. Tab menu

Appearance

Size

Set the size of points and letters. "String Size" adjusts the size of index letters, and "Point Size" adjusts the size of the points.

Color

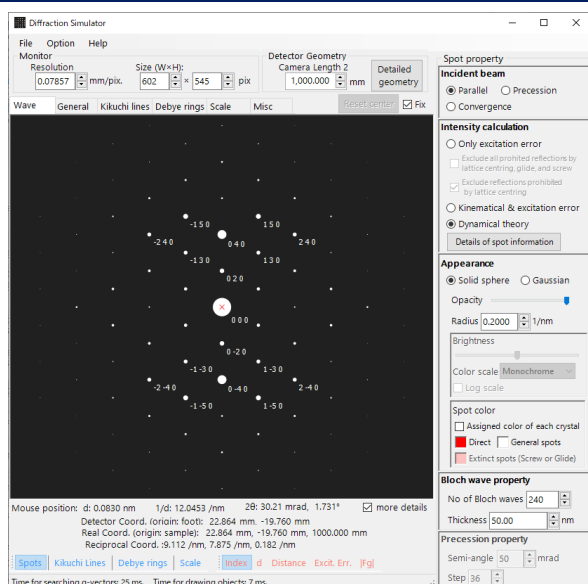Sets the colors of points, letters, stereonet outlines, etc.

Outline

Specifies how the stereonet outline is displayed.

Great and Small Circle

Draws large circles and small circles. Specify by the index of the zone axis or the index of the two crystal planes.

6. Crystal diffraction

"Crystal diffraction" function simulates single-crystal X-ray diffraction or electron diffraction.

6.1. Main area

A diffraction pattern is simulated in the area displayed in the center of the screen.

マウス操作

The following mouse actions are supported
- Left drag: Rotate
- Center drag: Translation
- Right drag: Zoom in
- Right click: Zoom out
- Left double click: Click on the left double click to display the detailed information of the selected spot

Mouse position

The information corresponding to the mouse position will be displayed. Checking "More details" shows more detailed information.

6.2. File menu
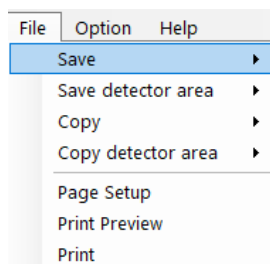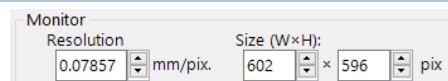

Save / Save detector area

Saves the displayed image.

Copy/ Copy detector area

Copies the displayed image.

6.3. Monitor / Detector geometry

Monitor

Resolution

The size of pixel (mm). This value is just a matter of display scale and does not have to be the actual value. This parameter is changed by scaling with mouse.

Size

The pixel numbers of width and height of the drawing area. Depending on your display resolution, you may not be able to set any values.

Detector geometry
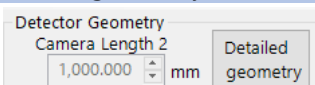
Camera length 2

The distance from the sample to the detector.

Detailed geometry

Opens the optics setting window. In more detail, see 6.7. Detector geometry.

6.4. Tab menu

Wave
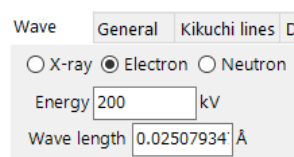
Set the properties of incident wave.

X-ray

Specify X-rays as the source.

To select characteristic X-rays, specify the element type and transition condition (Siegbahn notation).

When you want to select the X-ray from synchrotron radiation, specify "Element" as 0 and enter the energy or wavelength.

Electron

Enter the energy or wavelength.

Neutron

Enter the energy or wavelength.

General

Set the color of spots, letters, chrysanthemum lines, etc.

Kikuchi lines

Wave	General	Kikuchi lines	Debye rings	Scale	Misc

☐ Kikuchi line color (Ecxess)   Threshold 0.400 ⬍ nm⁻¹
■ Kikuchi line color (Defect)   Line Width ▬●▬

It becomes active when "Kikuchi lines" is selected in the Tool bar.

Threshold

The calculation is performed on Kikuchi lines with d-values greater than this value.

Debye rings

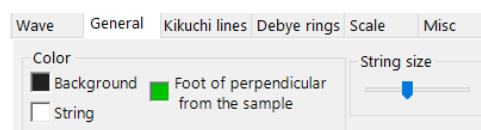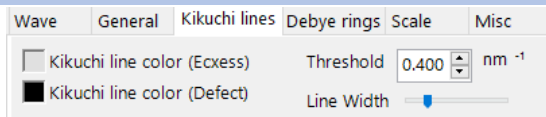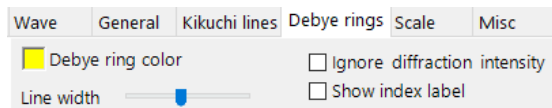| Wave	General	Kikuchi lines	Debye rings	Scale	Misc

🟨 Debye ring color   ☐ Ignore diffraction intensity
Line width ▬●▬   ☐ Show index label

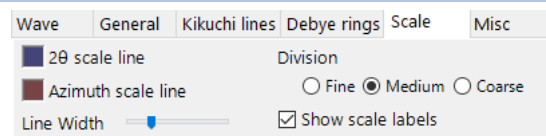It becomes active when "Debye ring" is selected in the Tool bar。

Ignore diffraction intensity

If checked, all Debye rings are drawn in the same color, ignoring the crystal structure factor.

Show index label

If checked, the index appears near the ring.

Scale

Wave	General	Kikuchi lines	Debye rings	Scale	Misc

■ 2θ scale line   Division
■ Azimuth scale line   ○ Fine ◉ Medium ○ Coarse
Line Width ▬●▬   ☑ Show scale labels

It becomes active when "Scale" is selected in the Tool bar.

2θ /Azimuth scale line

The former means direction of scattering angle, and the latter means direction of azimuth. You can change the color of the scale lines.

Line width
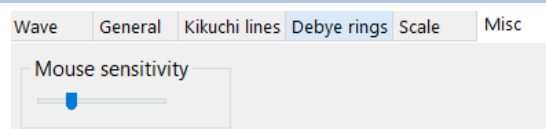
Set the thickness of the scale line.

Division

Set the scale line division.

Show scale labels

Select whether or not to display labels on the scale line.

Misc

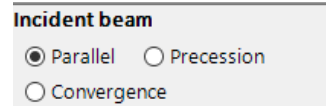| Wave	General	Kikuchi lines	Debye rings	Scale	Misc

Mouse sensitivity
▬●▬

Mouse sensitivity

Sets the sensitivity when you rotate the crystals by the mouse.

6.5. Spot property

It becomes active when Spot is selected in the Tool bar.

Incident beam

Incident beam
◉ Parallel   ○ Precession
○ Convergence

Select the type of incident beam.
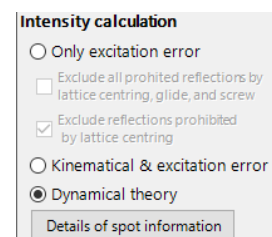
Parallel

Simulate a parallel incident beam.

Precession

Simulates precession incident beam. This mode is only available when you select electrons as the wave source (i.e., precession electron diffraction). When you select this mode, the "Intensity calculation" is automatically set to "Dynamical theory".

Convergence

Simulates a converging incident beam. This mode is only available when you select electrons as the wave source. When you select this mode, the "Intensity calculation" is automatically set to "Dynamical theory", and the "CBED setting" window is launched.

Intensity calculation

Intensity calculation
○ Only excitation error
  ☐ Exclude all prohited reflections by lattice centring, glide, and screw
  ☑ Exclude reflections prohibited by lattice centring
○ Kinematical & excitation error
◉ Dynamical theory
  Details of spot information

Select the method for calculating the intensity of the diffraction spot.

Only excitation error

The intensity is calculated based on the excitation errors (i.e., the geometric distance between the Ewald sphere and the reciprocal lattice points); the smaller the excitation error, the higher the intensity, with the maximum value being the value of Radius (see below). becomes small and zero when the excitation error exceeds Radius.

Kinematical & excitation error

In addition to the excitation error, the crystal structure factor is also incorporated in the diffraction intensity.

Dynamical theory

The dynamic diffraction theory (the Bethe's method) is used to calculate the diffraction intensity. This option is only available when electron is selected as the wave source.

Appearance

Set the display method of the diffraction spot.

Sold sphere / Gaussian

If "Solid sphere" is selected, the reciprocal lattice point is assumed to be a sphere of radius R. The cross section between the sphere and the Ewald sphere is the diffraction spot, which is drawn as a solid circle. The area of the circle corresponds to the diffraction intensity.

In the case of "Gaussian", the reciprocal lattice point is assumed to be a 3D Gaussian function with a certain σ (the standard deviation, or the RMS width) and a certain intensity I (the integral over the whole 3-dimensional space)[13]. The distribution appearing in the cross section of the 3D Gaussian and the Ewald sphere is the diffraction spot, which should be drawn as a 2D Gaussian. The integral of the 2D Gaussian function corresponds to the diffraction intensity.

Opacity

Set the transparency of the diffraction spot to be drawn.

Radius

The value corresponds to the radius of the reciprocal lattice point. The value (hereinafter referred to as R) affects the display of the diffraction spot as follows.

1. "Gaussian" case
   - "Only excitation error" case
     Assuming a 3D Gaussian function where σ is R and the integral is [Brightness] value, the intensity distribution (2D Gaussian) appearing in the cross section of the 3D Gaussian and the Ewald sphere is displayed as a diffraction spot. In this mode, the crystal structure factor is ignored.
   - "Kinematical & excitation error" case
     Assume a 3D Gaussian function where σ is R and the integral is [Brightness] × [relative intensity based on the kinematic theory].
   - "Dynamical theory" case
     The 2D Gaussian function, where σ is R and the integrated intensity is [Brightness] x [relative

intensity based on the dynamic theory], is displayed as the diffraction spot[14].

2. "Solid sphere" case
   - "Only excitation error" case
     Assuming a sphere of radius R centered at the inverse lattice point, the cross section of the sphere and the Ewald sphere is displayed as a diffraction spot. The crystal structure factor is ignored.
   - "Kinematical & excitation error" case
     Assume a sphere with a radius of R × [relative intensity based on the kinematic theory]^(1/3)[15].
   - "Dynamical theory" case
     The radius of the diffraction spot is R × [relative intensity based on the dynamic theory]^1/2. This means that the area of the displayed diffraction spot is directly proportional to the intensity based on the dynamic theory.

Brightness

If "Gaussian" is selected, it will be active. Adjust with the scale bar.

Color scale

Select "Gray scale" or "Cold-warm color".

Log scale

If checked, the intensity will be displayed as a log scale.

Spot color

Set the color of the diffraction spots.

Bloch wave property

This property is active when "Dynamic theory" is selected.

No of Bloch waves

This parameter configures the number of Bloch waves to include in the dynamic diffraction intensity calculation. This value is used if you have selected "Dynamic theory" as the "Intensity calculation" mode.

Thickness

Set the sample thickness.

---

[13] The general presentation of 3-dimensional Gaussian function centered at the origin is as follows;

$$f(x, y, z) = \frac{I}{\sigma^3 (2\pi)^{3/2}} \exp(-\frac{x^2 + y^2 + z^2}{2\sigma^2})$$

The integral of the above f over the whole 3-dimensional (x, y, z) space equals to I.
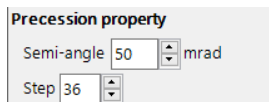The cross section of f truncated by $z = Z$ plane is as follows;

$$f'(x, y, z = Z) = \frac{I}{\sigma^3 (2\pi)^{3/2}} \exp(-\frac{Z^2}{2\sigma^2})\exp(-\frac{y^2 + z^2}{2\sigma^2})$$

The integral of f' over the whole x, y 2-dimensional (x, y) space is $\frac{I}{\sigma\sqrt{2\pi}}\exp(-\frac{Z^2}{2\sigma^2})$.

[14] The effect of excitation error is incorporated in the dynamic theory calculation.

[15] The volume of the sphere is multiplied by 1/3 to make it proportional to the kinematic relative diffraction intensity.

Precession property

Precession property

Semi-angle `50` mrad

Step `36`

This part is active when "Incident beam" is selected as "Precession".

Semi-angle

Sets the semi-angle of the incident electron in precession electron diffraction.

Step

The precession electron diffraction is simulated by adding up parallel beams. The number of the parallel beam directions is set here.

6.6. Toolbar

`Spots` | `Kikuchi Lines` | `Debye rings` | `Scale` | `Index` d `Distance` `Excit. Err.` `|Fg|`

Spots

Toggles between show/hide diffraction spots.

Kikuchi lines

Toggles between show/hide Kikuchi lines

Debye rings

Toggles between show/hide Debye rings[16]。

Scale

Toggles between show/hide scale lines.

Index / d / Distance / Excit. Err / |Fg|

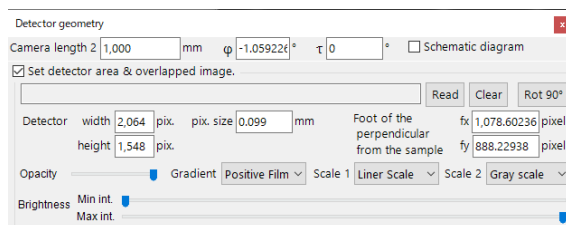Check the labels that appears near the spot.

6.7. Detector geometry

Configure the detailed settings for the detector.

Schematic diagram

A schematic diagram explaining the meaning of the parameters is displayed. See A.2.. for details.

Set detector area & overlapped image
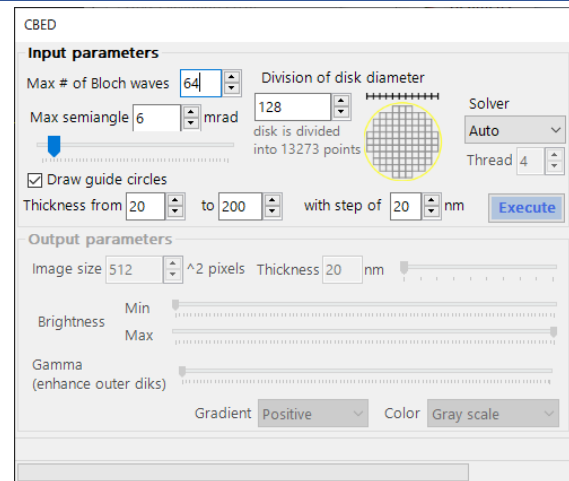
The number and size of detector pixels can be set to superimpose a detector image on the simulated diffraction pattern or to display only the detector image border. The detector area is displayed as a green rectangle.

If you want to superimpose an image, click the Read button to read the image. Then set the pixel size and foot to the correct values. You can also adjust the image's transparency, color scale and brightness.

If you want to display only the border of the detector, set the pixel size, number of pixels and foot without loading the image.

---

[16] Debye rings are essentially a collection of diffraction spots that appear when the sample is polycrystalline.

6.8. CBED setting

CBED is a large resource-intensive calculation. Therefore, the calculation is not done in real time." Press the "Execute" button to execute the calculation.

Input parameters

Max # of Bloch waves

Set how many Bloch waves should be included in the CBED calculation. Since the calculation time is proportional to the cube of the number of Bloch waves, the calculation time will be longer if you include a large number of Bloch waves.

Max semiangle

The convergence angle of the electron beam.

Draw guide circles

Displays guide circles that show the size of the CBED disk, which is useful for determining the Max semiangle.

Division of disk diameter

This parameter specifies the resolution of the CBED disc, which is the number of pixels multiplied by $\pi/4$. The number of pixels is proportional to the computation time, so the computation time increases when a large value is specified.

Thickness from ## to ## with step of

CBED simulations can be performed for multiple set sample thicknesses. Since this software uses the Bethe method, the calculation time is almost the same as when the thickness is varied.

Solver

The Bethe method calculation consumes a large amount of resources to solve the eigenvalue problem. You can select following options as a solver for the eigenvalue problem.

- "Auto" choose one of the following three options automatically, depending on your environment.
- "MKL" uses Intel's MKL library (https://software.intel.com/en-us/mkl).
- "Eigen" uses the Eigen open source library (https://gitlab.com/libeigen/eigen).
- "Managed" uses the Mathnet open source library

(https://github.com/mathnet/).

In the author's experience, Eigen tends to be fastest when the number of Bloch waves is small (< ~500) and MKL is fastest when the number of Bloch waves is large (> ~500).

6.9. Diffraction spot information
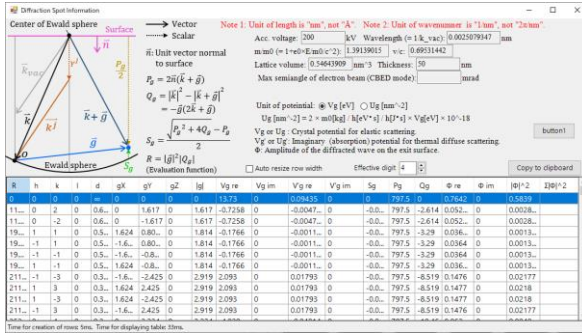
This windows shows detailed information about the diffraction spots calculated by the Bethe's dynamic theory. The meanings of the symbols are shown in the schematic diagram on the top left.

7. HRTEM simulation
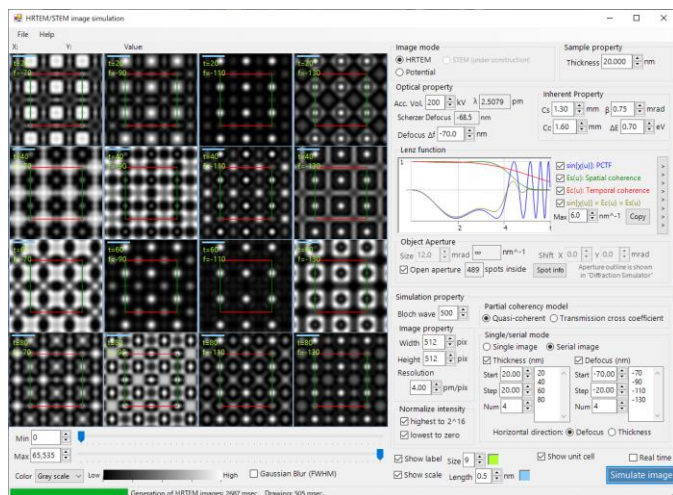
"HRTEM simulation" simulates TEM lattice fringe images for the selected crystal and orientation specified in the main window. Potential can also be simulated.

Click "Simulate image" button at the bottom right to run the simulation.

7.1. Main area

The simulated image is displayed. You can zoom in by right-clicking or right-dragging on the image.

Min/Max

Set the maximum and minimum brightness of the image. You can also use the track bar to adjust it.
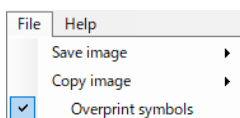
Color

Choose between "Gray" scale or "Cold-Warm" scale.

Gaussian blur

画像に対して、ガウス関数によるフィルター(ぼかし)をかけます。ぼかしの範囲はピクセル単位で指定します。

7.2. File menu

File

Save the image or copy it to the clipboard." When the "Overprint symbols" is checked, the scale and labels will be overprinted into the image.

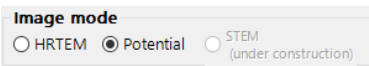### Help

Basic concept of HRTEM simulation

You can refer to the basic principle of HRTEM calculation as a PDF.

Calculation Library

Select the library you want to run the HRTEM simulation in. Native code is usually faster. If the native code does not work, ReciPro always use the managed code.

7.3. Image mode

Select either HRTEM or Potential mode; STEM mode is

currently under development and not yet active.

7.4. Sample property
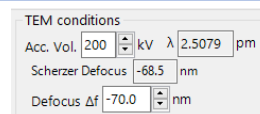
Set up the sample properties of the electron microscope.

Thickness

Set the sample thickness.

7.5. Optical property

Set up the optical properties of the electron microscope.

TEM condition

Set the acceleration voltage (Acc. Vol.) and defocus value. When you change the acceleration voltage, the relativistically-corrected wavelength is displayed on the right. Also, Scherzer defocus is displayed below based on the acceleration voltage and Cs value.
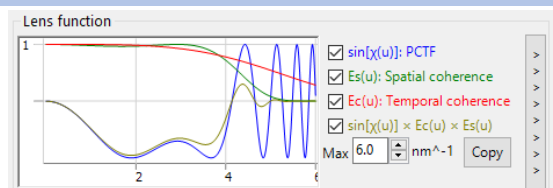
Inherent Property
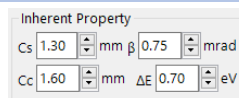
Set the parameters inherent to the electron microscope.
・Cs: Spherical aberration coefficient
・Cc: Chromatic aberration coefficient
・β: Illumination semi angle due to the finite source size effect
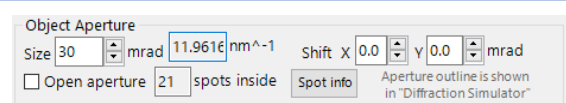・ΔE: 1/e width of electron energy fluctuations

Lens function

The lens function is displayed. By setting the upper limit of the u value, you can change the drawing range.
・Sin[χ(u)]: Phase contrast transfer function (PCTF)
・Es(u): Spatial coherence envelope function
・Ec(u): Temporal coherence envelope function

Objective Aperture

Set up the size and position of the objective lens aperture.

When the "Diffraction Simulator" is launched, you can check the size and position of the aperture.

Size

Set the size of the objective lens aperture in mrad. If you want to open the aperture, check "Open aperture".

The number of diffraction spots considered in the Bethe's method will change depending on the aperture condition you set. The maximum number of spots is limited to the value set in the "Simulation property" section.
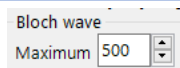
Shift

Sets the horizontal position of the objective lens aperture in mrad.

Spot info.

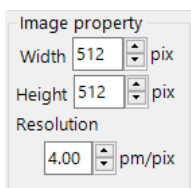Displays detailed spot information.
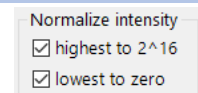
7.6. Simulation property

Bloch Wave

Set the maximum number of Bloch waves used in the calculation.
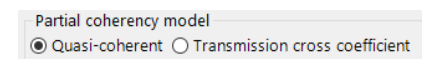
Image Property

Set the number of pixels and resolution of the image to be simulated.

Normalize Intensity

Set how to normalize the intensity of the image to be simulated.

Partial Coherent model

It is displayed when the image mode is HRTEM.

When calculating the HRTEM image, you can choose whether the wave interference is calculated based on the Quasi-coherent model or the transmission cross coherent model. The latter is a more accurate simulation, but the calculation is slower.
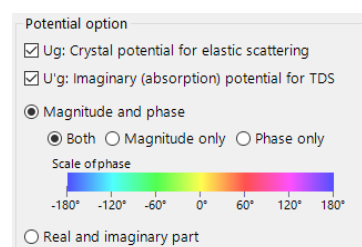
Single/Serial mode

It is displayed when the image mode is HRTEM.
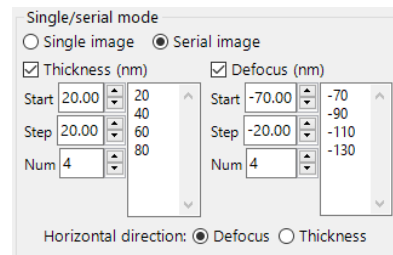
"Single image" mode simulates a single image based on the sample thickness set in "Sample Property" and defocus set in "Optical Property".

"Serial image" mode generates serial images for multiple thicknesses and defocuses set according to the values of Start/Step/Num.

Potential option

It is displayed when the image mode is "Potential".

The selected potential (Ug, U'g) becomes the target of the simulation. You can also select the potential display method from "Magnitude and phase" or "Real and imaginary part".

7.7. Appearance
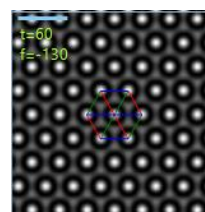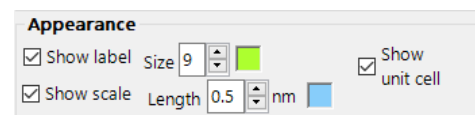
Label

Set whether the label (t: thickness [nm], f: defocus [nm]) will be displayed or not, and the size and color of the label.

Scale

Set whether to display the scale bar or not, and the length and color of the scale bar.

Unit cell

Set whether the unit grid cell is displayed or not. Red, green and blue lines correspond to crystal axes a, b and c, respectively.

8. TEM ID

"TEM ID" is used to index the selected area electron diffraction (SAED) pattern obtained with transmission electron microscopy.

Enter the TEM observation conditions and the geometry of the diffraction spot, and press the "Search zone axes" button to search for the candidate crystal axes.

8.1. TEM condition

Enter the TEM observation conditions.

8.2. Photo1, 2, 3

Enter the geometry of the diffraction spots.

If you want to enter the length between the spots on the detector, enter a value in the mm box.

If you know the d-value, enter the value in the unit of Å or nm^{-1} box.

8.2.1. Three sides
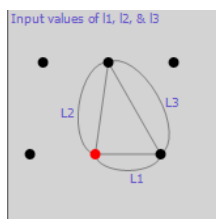
In this mode, you can enter the length of the three sides of a triangle with the direct spot as one vertex.

8.2.2. Two sides and an angle
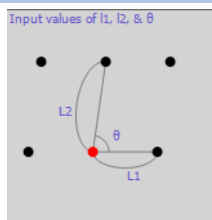
In this mode, you enter the length of the two sides, including the direct spot, and the angle between them.

9. Spot ID
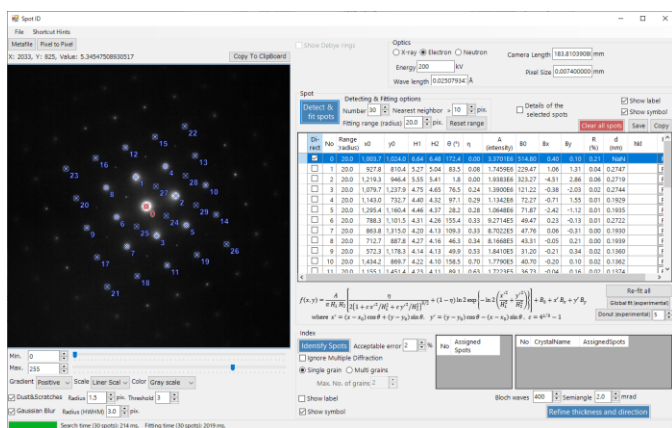
The module detects and indexes the spots in the diffraction image.

7.1. Main area

Displays the image. You can drag and drop the image or load it from the "File" menu.

You can zoom out by right-clicking or right-dragging the mouse to zoom in. In addition, the following mouse actions are acceptable.

Single left click: Select a spot.
Double left clicks: Add a spot
Ctrl+Left double click: Add direct spot
Ctrl+right single click: Remove spot

Min/Max

Set the maximum and minimum brightness of the image. You can also use the track bar to adjust it.

Gradient

Select "Positive" or "Negative".

Scale

Select "Linear" or "Log" scales.

Color

Select "Gray" scale or "Cold-Warm" scale.

Dust & Scratch

Remove exceptional bright/dark spots in the image consisting of one or several pixels. You can set the detection range in pixels and the detection threshold.

Gaussian blur

Applies a filter (blur) by Gaussian function to the image. The blur range is set in pixels.

7.2. Optics

Enter the incident source, energy/wavelength, camera length and detector pixel size.

If dm3/dm4 file (Gatan Digital micrograph file) is loaded, these values will be set automatically using the information in the file.

7.3. Spot

Di-rect	No	Range (radius)	x0	y0	H1	H2	θ (°)	η	A (intensity)	B0	Bx	By	R (%)	d (nm)	hkl	Fit
✓	0	20.0	1,003.7	1,024.0	6.64	6.48	172.4	0.00	3.3701E6	514.80	0.40	0.10	0.21	NaN		Fit
	1	20.0	927.8	810.4	5.27	5.04	83.5	0.08	1.7459E6	229.47	1.06	1.31	0.04	0.2747		Fit
	2	20.0	1,219.3	946.4	5.55	5.41	1.8	0.00	1.9383E6	323.27	-4.51	2.86	0.06	0.2719		Fit
	3	20.0	1,079.7	1,237.9	4.75	4.65	76.5	0.24	1.3900E6	121.22	-0.38	-2.03	0.02	0.2744		Fit
	4	20.0	1,143.0	732.7	4.40	4.32	97.1	0.29	1.1342E6	72.27	-0.71	1.55	0.01	0.1929		Fit
	5	20.0	1,295.4	1,160.4	4.46	4.37	28.2	0.28	1.0648E6	71.87	-2.42	-1.12	0.01	0.1935		Fit
	6	20.0	788.3	1,101.5	4.31	4.26	155.4	0.33	9.2714E5	49.47	0.23	-0.13	0.01	0.2722		Fit
	7	20.0	863.8	1,315.0	4.20	4.13	109.3	0.33	8.7022E5	47.76	0.06	-0.31	0.00	0.1930		Fit
	8	20.0	712.7	887.8	4.27	4.16	46.3	0.34	8.1668E5	43.31	-0.05	0.21	0.00	0.1939		Fit
	9	20.0	572.3	1,178.3	4.14	4.13	49.9	0.53	1.8410E5	31.20	-0.21	0.34	0.02	0.1360		Fit
	10	20.0	1,434.2	869.7	4.22	4.10	158.5	0.70	1.7790E5	40.70	-0.20	0.10	0.02	0.1362		Fit
	11	20.0	1,155.1	1,451.4	4.23	4.11	89.1	0.63	1.7223E5	36.73	-0.04	0.16	0.02	0.1374		Fit

$$f(x,y) = \frac{A}{\pi H_1 H_2}\left[\frac{\eta}{2\{1 + c\,x'^2/H_1^2 + c\,y'^2/H_2^2\}^{3/2}} + (1-\eta)\ln 2\exp\left\{-\ln 2\left(\frac{x'^2}{H_1^2} + \frac{y'^2}{H_2^2}\right)\right\}\right] + B_0 + x'\,B_x + y'\,B_y$$

where $x' = (x - x_0)\cos\theta + (y - y_0)\sin\theta$, $y' = (y - y_0)\cos\theta - (x - x_0)\sin\theta$, $c = 4^{1/3} - 1$

By the "Detect & fit spots" button, the software automatically detects diffraction spots in the image and fits them with the 2D Pseudo-Voigt function[17]. The fitting result is displayed in the table.

Detect & Fitting options

Number

Set the maximum number of spots to be detected.

Nearest neighbor

Set the minimum distance between the spots to be detected.

Fitting range

Set the range of the detected spots to be fitted with the 2D Pseudo Voigt function, in pixel units of radius.

Reset range button

Re-set the fitting range of the spots in the table.

Show label/symbol

Select whether or not the labels and symbols of the detected spots will be displayed as an overlap in the image.

Clear all spots

Removes all spots in the table.

---

[17] In ReciPro, the following fitting functions are used.

$$f(x,y) = \frac{A}{\pi H_1 H_2}\left[\frac{\eta}{2\{1 + c\,x'^2/H_1^2 + c\,y'^2/H_2^2\}^{3/2}} + (1-\eta)\ln 2\exp\left\{-\ln 2\left(\frac{x'^2}{H_1^2} + \frac{y'^2}{H_2^2}\right)\right\}\right] + B_0 + x'\,B_x + y'\,B_y$$

where $x' = (x - x_0)\cos\theta + (y - y_0)\sin\theta$, $y' = (y - y_0)\cos\theta - (x - x_0)\sin\theta$, $c = 4^{1/3} - 1$

The first term in square brackets, $\eta/2\{1 + c\,x'^2/H_1^2 + c\,y'^2/H_2^2\}^{3/2}$), is the 2-dimensional Cauchy distribution function. The second term, $(1 - \eta)\ln 2\exp\{-\ln 2\,(x'^2/H_1^2 + y'^2/H_2^2)\}$, is 2-dimensional Gaussian function.

x_0, y_0 are the center coordinates of the spot. θ is the rotation angle from x, y axes to x', y' axes. H_1, H_2 are half width at half maximum along x' and y' axes respectively. η means the mixed ratio of Cauchy distribution function and Gaussian function. A corresponds to the integral value of this function. The part of $B_0 + x'\,B_x + y'\,B_y$ means the background plane.

During fitting, each parameters are optimized by an iterative approximation using the modified Marqurt method.
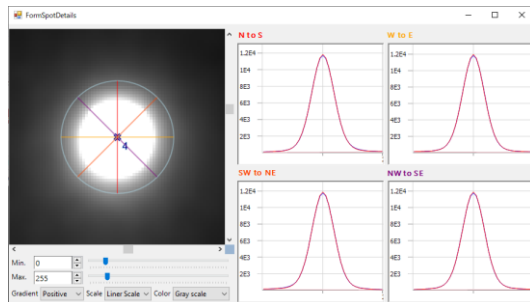
Save/Copy

Save/copy the table information in the Excel format (tab separated values).

Re-fit all

Re-fitting is done for all spots in the table.

Details of the selected spots

When you check the box, a separate window will appear as shown below.

In this window you can see the selected spot on the left side and the profiles of the four directions on the right side. The blue lines are the observed data and the red lines correspond to the fitting results.

7.4. Index

By "Identify spots" while the spots are detected, the spots will be indexed to the crystal selected in the main window.

Acceptable error

Set the tolerance of error.

Single grain/Multi grains

Choose whether to index as a single crystal or multiple grains. If you choose Multi grains, you can specify the maximum number of crystals to be considered.

Show label/symbol

Select whether or not the labels and symbols of the indexed spots will be displayed overlaid on the image.

Refine thickness and direction

Applying dynamic theory of electron diffraction (the Bethe's method), refine the sample thickness and crystal orientation that best matches the detected diffraction intensity

10. Powder diffraction

Under construction

11. Crystal database

The "Crystal database" provides the functions to search and import more than 20,000 crystal structures.

The database is based on the "American Mineralogist Crystal Structure Database". Please read the description in http://rruff.geo.arizona.edu/AMS/amcsd.php carefully, and be sure to cite the following references when using the crystal data:

Downs, R.T. and Hall-Wallace, M. (2003) The American Mineralogist Crystal Structure Database. American Mineralogist 88, 247-250. (pdf file)

11.1. Table

The crystals contained in the database will be displayed. If you have entered the search criteria, only those crystals that meet the criteria will be shown.

When you select a crystal in the table, the information of the crystal is transferred to the "Crystal information" area of the "Main window". If you want to add the crystal to the "Crystal list", click the "Add" or "Replace" button.

11.2. Search options

Enter your search criteria. To search, press the "Search" button or enter key.

Name

Enter crystal name.

Element
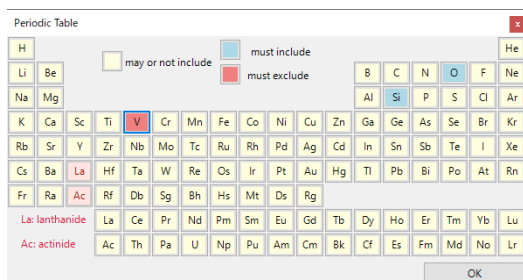
When you press the "Periodic Table" button, a new window will open. Select the element to be searched here. Each element's button changes its status as you press it.

Clicking the "may or not include", "must include", or "must exclude" buttons at the top of the window will change the status of all elements.

Reference

Enter title, journal and author.

Crystal system

Select crystal system.

Cell Param

Enter the cell constants and acceptable error.

d-spacing

Enter the d-spacing and acceptable errors for the strongest crystal diffraction.

Density

Enter the density and acceptable error.

Appendix

A.1. Basic definition of ReciPro coordination

Definition of orientation

Since ReciPro handles various "directions", the definitions are explained below. In ReciPro, right-handed coordinate system is used, and axes are defined as follows:

·   X-axis is to the right of the monitor surface
·   Y-axis is the upward direction of the monitor surface
·   The Z-axis is vertically in front of the monitor surface.

The beam direction corresponds to the direction of the line of sight looking at the monitor, which in the above coordinate system corresponds to the -Z axis direction.
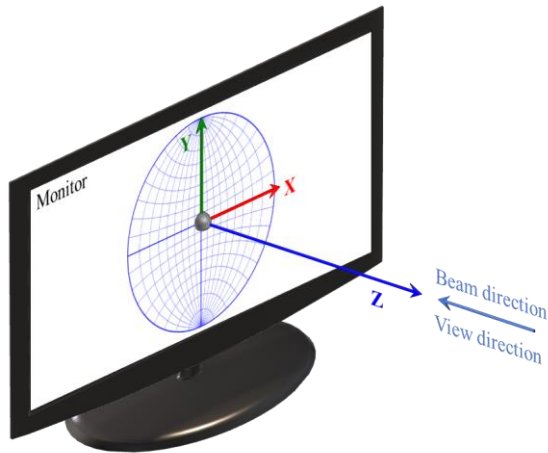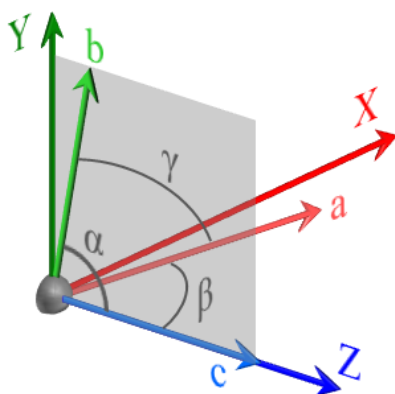
Most of the operations performed in ReciPro are only in the direction (i.e. the 3x3 rotation matrix) and do not require awareness of the position of the origin. However, with the "Crystal diffraction" function, the origin position must be explicitly considered. See A.2. for more details.

Initial crystal direction

ReciPro defines the initial orientation of the crystal   as shown in the figure above[18]. That is, the orientation of the

•   The c-axis is aligned with the Z-axis direction
•   The b-axis lies on the YZ plane and is close to the

Y-axis
•   The a-axis is the direction determined by the b- and c-axes

In other words, the direction in front of the monitor corresponds to the [001] crystal axis, and the right direction on the monitor corresponds to the normal direction of (100) crystal plane. Note that c-axis (= [001] crystal zone axis) always corresponds to the Z-axis, but in some crystal system a- and b-axis do not necessarily correspond to the X- and Y-axis[19].

Euler angles
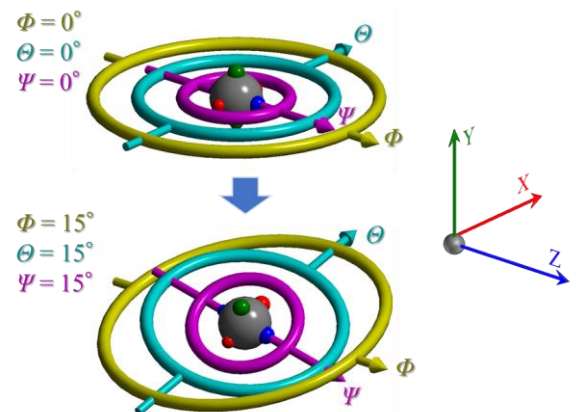
In ReciPro, crystals can be rotated in various directions. Euler angles are used to represent the crystal orientation. The Euler angles in ReciPro uses three symbols, Φ, θ and Ψ as shown the above. When the angles Φ, θ, and Ψ are all zero (upper figure), the directions of the axes of rotation corresponding to those angles are equal to Z, X, and Z, respectively.

Note that the three Euler angles have a master-slave relationship; Φ is the highest (1st) rotation, followed by θ (2nd). Ψ is the lowest (3rd) rotation. The direction of the lower rotational axis depends on the state of the upper rotation. As an example, the lower figure shows a situation where Φ, θ, and Ψ are all set to 15 degrees. The axis of rotation corresponding to angle Φ will always coincide with the Z axis, but the axis of rotation corresponding to angle θ and angle Ψ will generally not coincide with any of X, Y, or Z.

A.2. Definition of coordination in "Crystal diffraction"

"Crystal diffraction" simulates a diffraction pattern on a detector and displays it on your monitor. The detector is a finite-sized plane created by a collection of pixels, The detector is placed at a fixed distance from the sample (scattering matter), and it may be inclined with respect to the incident beam. In order to accurately simulate this situation, information such as the geometric relationship between the detector and the sample and the pixel size/number of pixels of the detector is important.

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[18] This definition is compatible with Oxford's EBSD software.

[19] In the cases of cubic, tetragonal, or orthogonal, the initial orientation of the a-, b-, and c-axes coincide with the X-, Y-, and Z-axes, respectively. In the cases of hexagonal, trigonal, or monoclinic, the b- and c-axes coincide with the Y- and Z-axes, respectively, but the a-axis does not coincide with the X-axis. In the case of triclinic, the c-axis coincides with the Z-axis, but a- and b-axes never coincide with the X- and Y-axes.
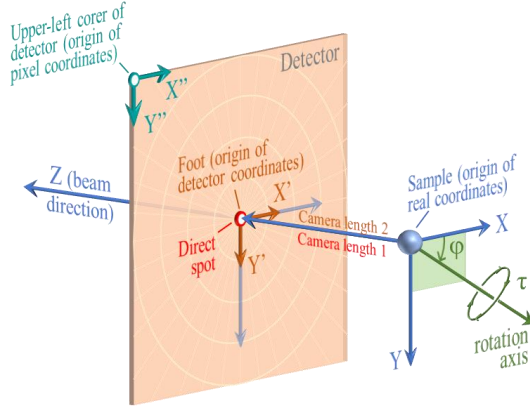
| Before rotation | After rotation |
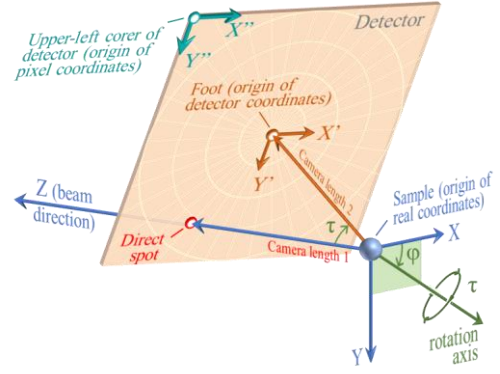
First, consider a situation where the detector is not tilted (i.e., the normal of the incident beam and the detector plane are the same), as shown in the above figure.

"Real coordinates" is a 3-dimensional Cartesian coordinate system in mm scale with sample as the origin. The Z axis is always the same as the beam direction (note that the definition differs from A.1.[20]) The direction of the X axis is right facing the Z axis and the direction of the Y axis is downward. The minimum distance of the detector (i.e. the distance between the sample and the direct spot [= the foot of the perpendicular from the sample, or "Foot"]) is defined as "Camera length 1" or "Camera length 2".

"Detector coordinates" is a two-dimensional Cartesian coordinate system in mm scale with the "foot" as the origin. X' axis is to the right of the detector plane and Y' axis is to the bottom.

"Pixel coordinates" is also a two-dimensional coordinate system with the top-left point of the detector as the origin, is in pixel scale. As in "Detector coordinates", the right direction of the detector plane is the X" axis and the down direction is the Y" axis.

Next, let's consider the situation where the detector is tilted as shown in the above figure.

Two parameters are introduced to represent the inclination of the detector: the direction of the rotation axis (ϕ) and the amount of rotation (τ). The rotation axis is considered to be in the XY plane (Z=0 plane) and the angle from the X axis is defined as ϕ. Then, rotate it around the axis of rotation defined by ϕ by τ in the direction of the right-hand screw.

As a result of the above rotation operation, the "direct spot" and the "foot" are not aligned with each other[21]. In ReciPro, the distance between the former and the sample is called "Camera length 1" (C1) and the distance between the latter and the sample is called "Camera length 2" (C2). Note that the origin of the "Detector coordinates" is always "Foot" and the origin of the "Pixel coordinates" is always the upper left corner of the detector. Also note that when the detector is tilted, the X and Y directions do not coincide with the X' and Y' directions.

Call it Camera length 1 (C1) and the distance between the latter and the sample is called Camera length 2 (C2) [22], where the origin of Detector coordinates is always "Foot" and the Pixel Note that the origin of coordinates is always the upper left corner of the detector. Also note that when the detector is tilted, the X and Y directions do not coincide with the X' and Y' directions.

The definitions of each parameter are listed again in the following section.

Real coordinates (X, Y, Z)

Three dimensional coordinates of the experimental setup with millimeter unit. The origin of the coordinates is always the sample position, and Z axis direction is always parallel to the beam direction. If the detector is normal to the incident beam, X & Y axes are parallel to X' & Y' axes, respectively.

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[20] In the "Crystal diffraction" coordinates, the beam direction is defined as +Z, as opposed to -Z in A.1. The Y-axis direction is inverted accordingly. This is to ensure consistency with previous literature and other software. Another reason for this is that the downward direction of an image is usually represented as +Y when handling images on a computer. However, users do not need to be aware of this difference in coordinate system, and ReciPro automatically performs the appropriate coordinate system conversion.

[21] The relation between the foot point (F_X, F_Y) and the direct spot (D_X, D_Y) is as follows;

$D_X = F_X - C_2 \times \sin(\Phi) \times \tan(\tau)$

$D_Y = F_Y + C_2 \times \cos(\Phi) \times \tan(\tau)$

[22] The relation between "Camera length 1" (C_1) and "Camera length 2" (C_2) is $C_1 \times \cos(\tau) = C_2$

Sample

Scattering material by the incident beam. The origin of the real coordinates.

Rotation of detector

The rotation state of the detector is represented by rotation axis direction and angle. The axis is defined on $Z=0$ plane (namely XY plane).

Φ

Angle from X axis to the rotation axis. Right-hand rule.

T

Rotation angle around the rotation axis. Right-hand rule.

Detector coordinates (X', Y')

Two dimensional coordinates on the detector plane with millimeter unit. The origin is the foot (see below). X' & Y' axes are always parallel to X" & Y", respectively.

Foot

The foot of the perpendicular from the sample. If the detector is normal to the incident beam, the foot position is identical to the direct spot. To use overlapped image mode, the foot position should be set in the pixel coordinates.

Camera length 2 (C_2)

Distance from the sample to the foot. The value is defined in millimeter.

Direct spot

Intersection of the incident beam and the detector.

Camera length 1 (C_1)

Distance from the sample to direct spot.

Pixel coordinates (X", Y")

Two dimensional coordinates on the detector plane with pixel unit. X" and Y" directions correspond to pixel arrays of the detector. The origin is always upper-left corner of the detector.

Pixel size

Length of one side of the pixel. The value is defined in millimeter. A square pixel is only acceptable.

Detector width/height

Pixel numbers horizontally/vertically.

A.3. Principle of Bethe method

A.4. Principle of HRTEM simulation