

## Contents

1. Overview.....	2
1.1. License.....	2
1.3. System requirements.....	2
1.3. Main features of ReciPro.....	2
2. Main window.....	3
2.1. File menu.....	3
2.2. Rotation control.....	4
2.3. Crystal List.....	4
2.4. Crystal Information.....	5
2.5. Functions.....	5
3. Rotation geometry.....	6
3.1. ReciPro coordinate system (ZXZ).....	6
3.2. Experimental coordinate system.....	7
3.3. Link.....	7
4. Structure Viewer.....	8
4.1. Main area.....	8
4.2. File menu.....	8
4.3. Tab menu.....	8
4.4. Toolbar.....	11
5. Stereonet.....	12
5.1. Main area.....	12
5.2. File menu.....	12
5.3. Mode.....	12
5.4. Indices.....	12
5.5. Tab menu.....	12
6. Crystal diffraction.....	13
6.1. Main area.....	13
6.2. File menu.....	13
6.3. Monitor / Detector geometry.....	13
6.4. Tab menu.....	13
6.5. Spot property.....	14
6.6. Toolbar.....	15
6.7. Detector geometry.....	15
6.8. CBED setting.....	16
6.9. Diffraction spot information.....	16
7. HRTEM simulation.....	17
7.1. Main area.....	17
7.2. File menu.....	17
7.3. Image mode.....	17
7.4. Sample property.....	17
7.5. Optical property.....	17
7.6. Simulation property.....	18
7.7. Appearance.....	18
8. TEM ID.....	19
8.1. TEM condition.....	19
8.2. Photo1, 2, 3.....	19

9. Spot ID.....	20
7.1. Main area.....	20
7.2. Optics.....	20
7.3. Spot.....	20
7.4. Index.....	21
10. Powder diffraction.....	22
11. Crystal database.....	23
11.1. Table.....	23
11.2. Search options.....	23
Appendix.....	24
A.1. Basic definition of ReciPro coordination.....	24
A.2. Definition of coordination in “Crystal diffraction”.....	24
A.3. Principle of Bethe method.....	26
A.4. Principle of HRTEM simulation.....	26

## 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](mailto: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.

- You are free to copy, distribute, modify, distribute modified versions of this software, use it for commercial purposes, sell it for a fee, and do whatever you want with it.
- If you redistribute this software, you must put the copyright of this software and the full text of this license in the source code or in a separate license notice file included with the source code.
- 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

.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"<sup>1</sup>, 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, Wyckoff 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<sup>2</sup>).

#### 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.

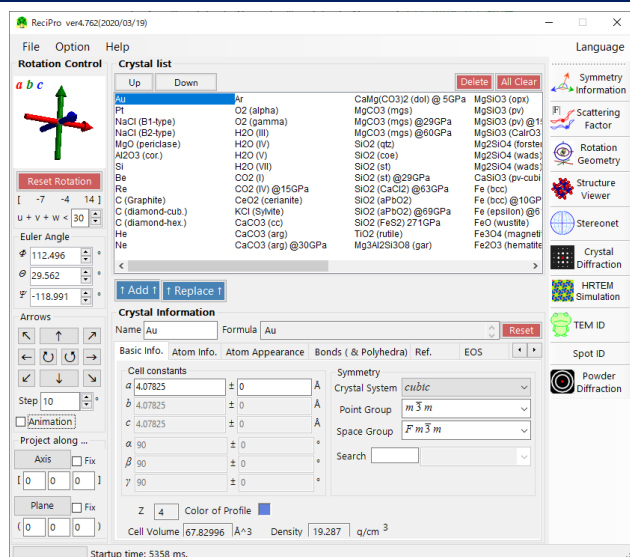
#### Flexible setting of crystal rotation

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.

<sup>1</sup> CSManager can be downloaded from <https://github.com/seto77/CSManager/releases/latest>

<sup>2</sup> About Hall symbol notation, see "1.4. Symmetry in reciprocal space" in "International tables for crystallography, Volume B (ITB)".

## 2. Main window



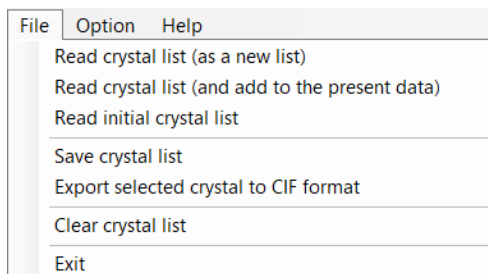
When ReciPro is successfully launched<sup>3</sup>, the main window appears. In the window, the user selects the crystal to be calculated, rotates the crystal, and invokes various other functions. This window can be divided into following types

- 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.

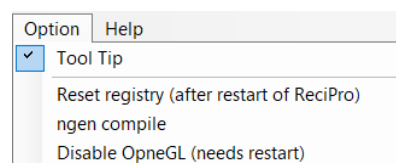
#### Clear crystal list

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.

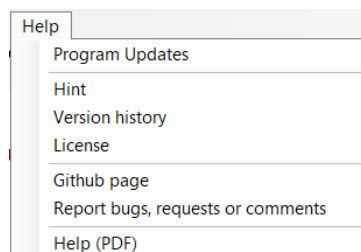
#### ngen compile

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

#### License

#### Github page

#### Report bugs, requests, or comments

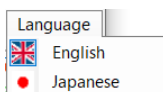
#### Help (PDF)

Show this page.

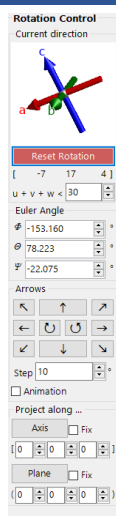
<sup>3</sup> It takes some time to start up, as it loads information about space groups and atoms at startup.

## Language

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



## 2.2. Rotation control



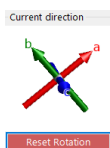
This control allows you to view/set the rotation status of the selected crystal.

### 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

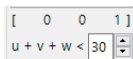
The crystal orientation is reset to the "initial state", which means that the c-axis is perpendicular to the screen and the b-axis faces upward when projected on the screen<sup>4</sup>.

### Zone axis

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

$u+v+w < 30$  indicates the closest azimuth for  $u, v, w$  that does not exceed 30 in absolute terms.

スクリーンに垂直な方向に対応する晶帯軸指数を表示します。 $u+v+w < 30$ とセットした場合は、 $uvw$ の絶対値の総和が30を超えない範囲で最も近い方位を表示します<sup>5</sup>。



### Euler angles

Set the crystal orientation in terms of Euler angles. Euler

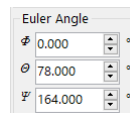
angles are expressed in three angles, and ReciPro defines the three angles as follows:

$\Psi$ : Z-axis rotation

$\theta$ : X-axis rotation

$\Phi$ : Z-axis rotation

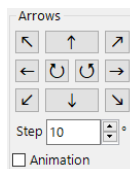
The rotation operation is performed in the order of  $\Psi$ ,  $\theta$ , and  $\Phi$ . See [3. Rotation geometry](#) and [Appendix](#) for a detailed explanation of the coordinate system.



### Arrows

When you press the arrow buttons, the selected crystal will rotate in the direction of the arrow by the angle Step.

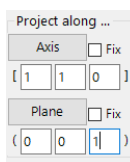
And if you check the "Animation" checkbox, the crystal will rotate continuously at the specified rotation speed.



### 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.<sup>6</sup>



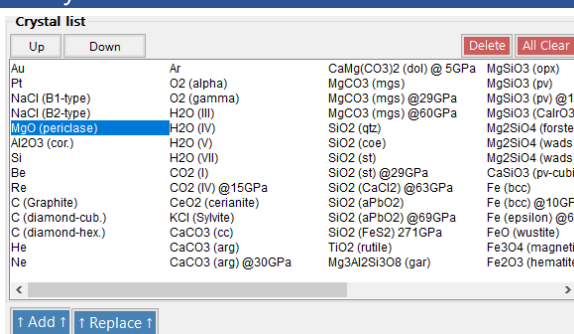
#### Axis

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

<sup>4</sup> 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.

<sup>5</sup> 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.

<sup>6</sup> 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.

installation.<sup>7</sup> 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.

### Up/Down

Moves the order of the selected crystals up/down.

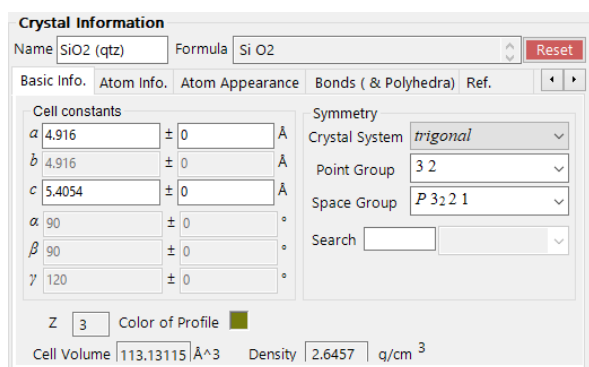
### Delete/All clear

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.

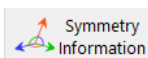
Whenever you make any changes to the crystal, you must press the "Add" or "Replace" button. If you do not press this button, the crystal will not be saved in the crystal list and your changes will be lost.

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

## 2.5. Functions

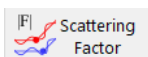
### Symmetry information

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](#).



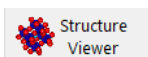
### Rotation geometry

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](#).



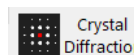
### Stereonet

Draws the direction of the crystal plane or axis on a stereonet. See [5. stereonet](#).



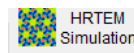
### Crystal diffraction

Simulates electron and X-ray diffraction patterns. See [6. Crystal diffraction](#).



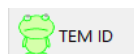
### HRTEM simulation

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



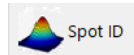
### TEM ID

Indexes diffraction spots. See [8. TEM ID](#).



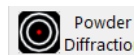
### Spot ID

Displays electron diffraction images, and searches, indexes, and fits the diffraction spots. See [9. Spot ID](#).



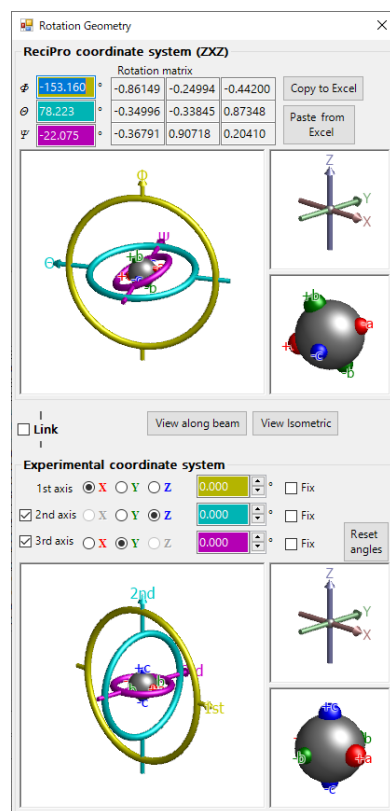
### Powder diffraction

Simulate and fit polycrystalline diffraction patterns. See [10. Powder diffraction](#).



<sup>7</sup> The list of crystals is automatically saved when ReciPro is closed, and will be automatically loaded the next time you start ReciPro.

### 3. Rotation geometry

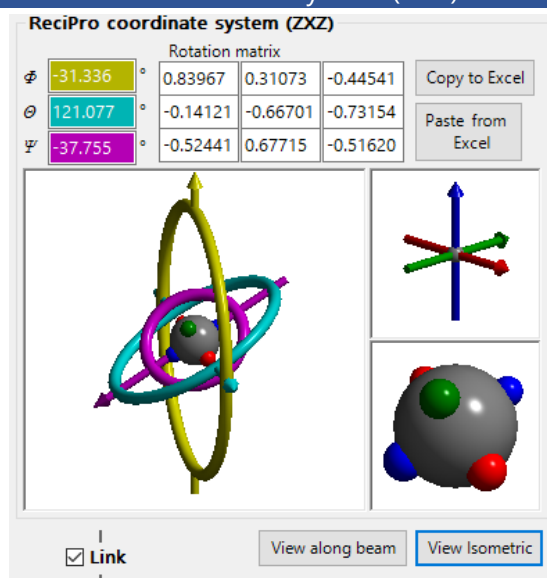


This provides a function to represent the rotational state of a crystal as a 3x3 matrix and to convert it to a different Eulerian coordinate system.

ReciPro provides three Eulerian angles,  $\Psi$ ,  $\theta$ , and  $\Phi$ , 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)



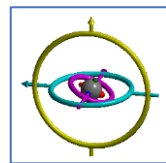
"Rotation geometry" 画面の上半分は、"Reciprocal coordinate system" で表現された結晶の回転状態を表示/設定する部分です。

上部に表示されている  $\Phi$ ,  $\theta$ ,  $\Psi$  の値は Main window で設定されたオイラー角と同期しています。 $\Psi$ ,  $\theta$ ,  $\Phi$  の値を変更したい場合は Main Window 側からおこなってください。

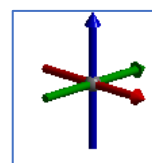
"Rotation matrix" の部分には、現在の回転状態に対応する 3×3 行列の回転行列が表示されます。

#### OpenGL windows

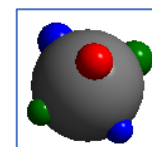
The OpenGL window is a three-dimensional representation of the current rotation situation, and the window with three toruses (doughnuts) shows the situation of the three rotation axes. The arrow through the yellow torus corresponds to the axis of rotation of the Euler angle  $\Phi$ , which is the upper (1st) axis of rotation in the goniometer. The light blue arrow is the middle (2nd) axis of rotation corresponding to  $\theta$ , and the pink arrow is the lower (3rd) axis of rotation corresponding to  $\Psi$ .



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  $\Phi$ ,  $\theta$ , and  $\Psi$  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

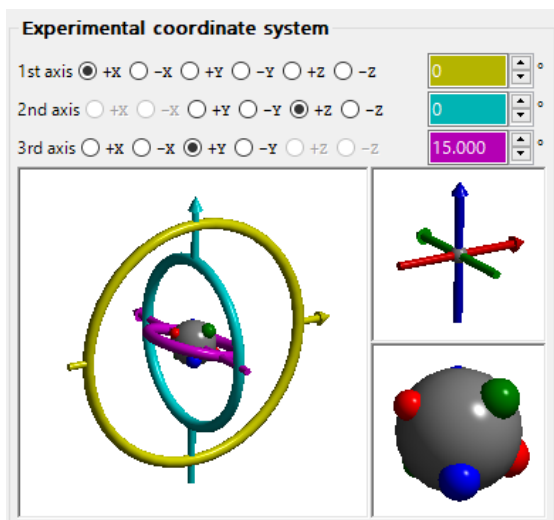
When Excel-formatted 3x3 tab-separated numbers are copied to the clipboard, you can set it as a rotation matrix.

#### 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<sup>8</sup>. The latter projects in an isometric orientation. Note that the crystal is not rotating, but only in the projection direction.

<sup>8</sup> 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".

#### 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup> axes

Select the rotation axes of the goniometer from  $\pm X$ ,  $\pm Y$  and  $\pm Z$  for the upper (1st), middle (2nd) and lower (3rd) levels.<sup>9</sup> 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.

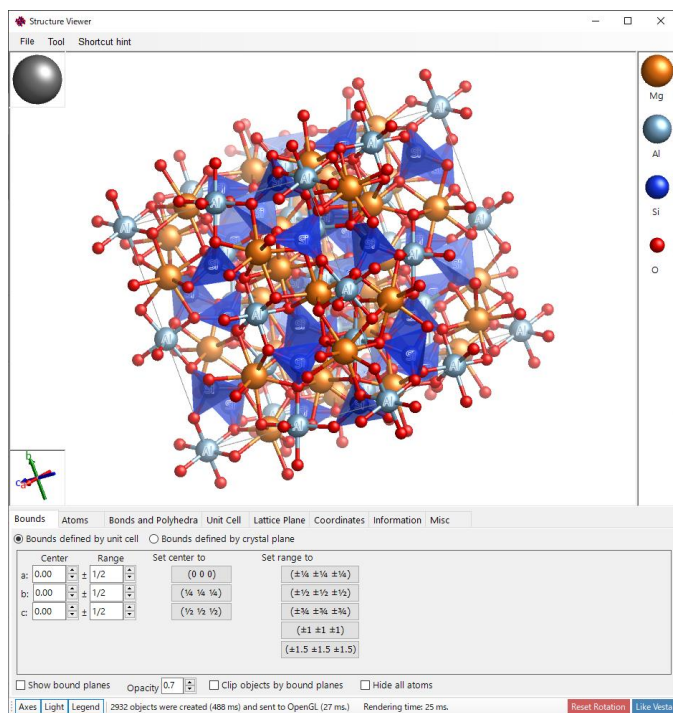


For example, suppose that the laboratory goniometer is adjusted so that the a-axis of a crystal is aligned with the direction of X-ray incidence and the b-axis with the horizontal direction. Enter the Eulerian angle of the laboratory goniometer in the experimental coordinate system. Furthermore, rotate 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.

<sup>9</sup> The goniometer of ReciPro corresponds to 1<sup>st</sup> : +Z, 2<sup>nd</sup> : +X, 3<sup>rd</sup> : +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.

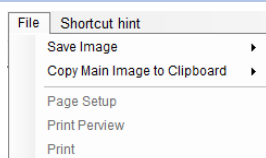
#### Mouse operation

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

☒ Bounds defined by unit cell ☐ Bounds defined by crystal plane

	Center	Range	Set center to	Set range to
a:	0.00	± 0.50	(0 0 0)	(±1/2 ±1/2 ±1/2)
b:	0.00	± 0.50	(1/4 1/4 1/4)	(±3/4 ±3/4 ±3/4)
c:	0.00	± 0.50	(1/2 1/2 1/2)	(±1 ±1 ±1)

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

☐ Bounds defined by unit cell ☒ Bounds defined by crystal plane

	h	k	l	Equivalency	Multiples of d	Distance (Å)	Color
<input checked="" type="checkbox"/>	1	1	1	<input checked="" type="checkbox"/>	1,000	0.663	Green

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<sup>10</sup>.

<sup>10</sup> 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), 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,  $d \times 1.5 = 9.949 \text{ Å}$ ). 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.

Distance from origin  
d x 1.500 (= 9.949 Å)

### 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).

☐ Show bound planes Opacity 0.7

### 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.

☐ Clip objects by bound planes

### Hide atoms

If checked, all atoms, bonds and polyhedra will be hidden.<sup>11</sup>

☐ Hide all atoms

## 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

Add Replace Apply to Same Elements Up Down Delete

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

Element & Position Origin shift Appearance

Label: MgX1 X: 1/2 Occ: 1

Element: 12: Mg Y: 1/2

Z: 1/4

☐ Show error

#### 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

Element & Position Origin shift Appearance

Shift coordinates of all atoms by:

☐ + ☐ - (1/8 1/8 1/8) (1/4 1/4 1/4) (1/4 -1/4 1/4) (1/4 -1/4 0)

(1/4 1/4 0) (0 1/4 1/4) (1/4 0 1/4) (0 1/4 1/8) (0 1/4 -1/8)

Apply custom shift 0.0000 0.0000 0.0000

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

### Appearance

Element & Position Origin shift Appearance

Radius 0.445 Å Color

Ambient 0.1 Diffusion 0.8 Specular 0.7 Shininess 20.0 Emission 0.2 Alpha 1.0

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
<input checked="" type="checkbox"/>	14: Si	8: O	2.2	0		
<input checked="" type="checkbox"/>	13: Al	8: O	2.2	0		

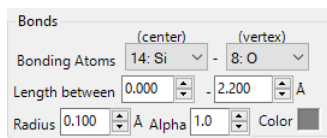
Add Replace Delete

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.

<sup>11</sup> "Show bound planes"と"Hide atoms"を両方チェックすれば、任意の結晶外形を描画することが出来ます。つまり、結晶の形状を表現することが出来ます。

## Bond property



ボンド情報を設定/表示します。

### 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.

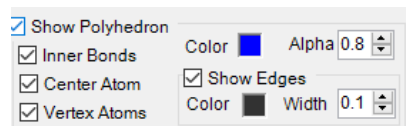
### Bond Radius

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).

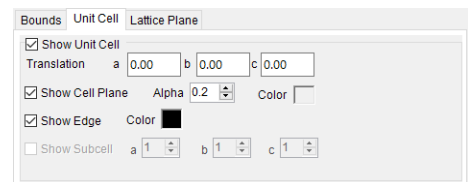
### Color

Set the color of the polyhedron edges.

### Width

Set the line width of the polyhedron edges.

## 4.3.4. Unit cell



このタブでは結晶の単位格子の描画に関する設定を行います。“Show unit cell” をチェックすると、単位格子の描画が行われます。

### 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.

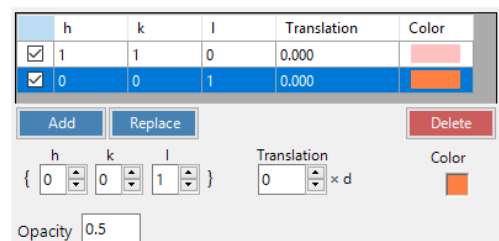
### Show cell plane

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

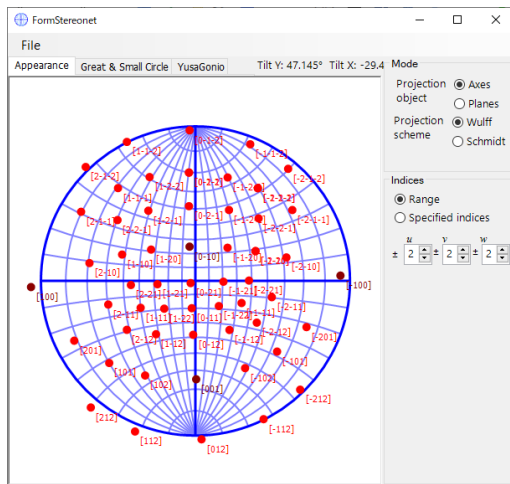
Specify the lattice plane with the Miller index.

### Translation

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



## 5. Stereonet



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

### 5.1. Main area

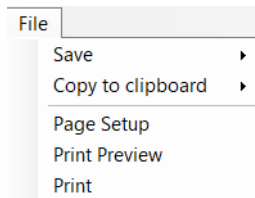
In the main area, the stereonet projection of the crystal face and crystal axis of the selected crystal is displayed.

#### マウス操作

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

Axis: Draw crystal axes.

Plane: Drawing crystal planes.

#### 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.

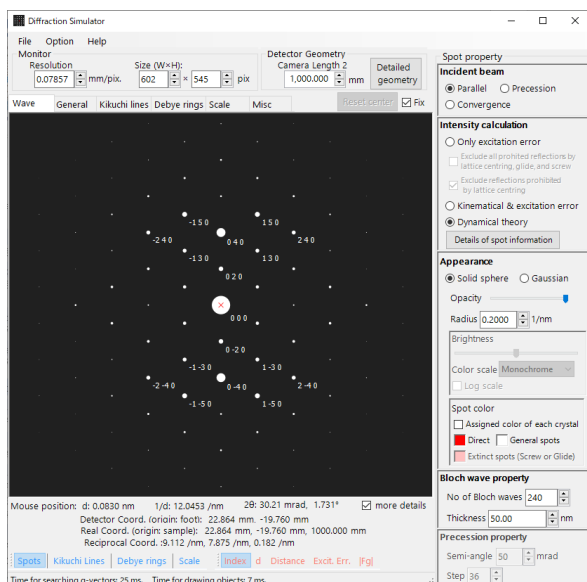
#### Outline

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 は、単結晶 X 線回折あるいは電子回折のシミュレーションを行います。

### 6.1. Main area

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

#### マウス操作

以下のようなマウス操作に対応します。

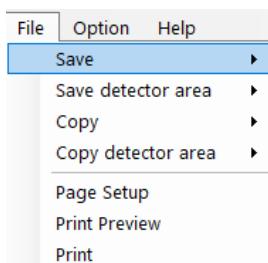
- Left drag: 回転
- Right drag: 拡大
- Right click: 縮小
- Left double click: 選択したスポットの詳細情報を表示

#### Mouse position

Mouse position: d: 0.1025 nm 1/d: 9.7598 /nm 2θ: 24.48 mrad, 1.402° ☒ more details  
Detector Coord. (origin: foot): 13.671 mm, 20.310 mm  
Real Coord. (origin: sample): 13.671 mm, 20.310 mm, 1000.000 mm  
Reciprocal Coord.: 5.449 /nm, -8.096 /nm, 0.119 /nm

Drawing area 内にマウスポインタがある場合、その位置に相当する情報を表示します。“More details”をチェックすると表示領域が拡張し、より細かい情報が表示されます。

### 6.2. File menu



#### Save / Save detector area

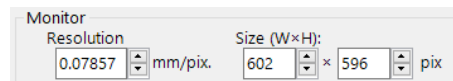
表示されている画像を保存します。後者は detector area を設定している場合にのみ表示されます。

#### Save / Save detector area

表示されている画像を保存します。後者は detector area を設定している場合にのみ表示されます。

## 6.3. Monitor / Detector geometry

### Monitor



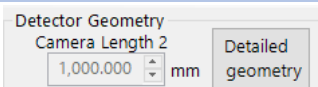
#### Resolution

1 ピクセルあたりの長さ(mm)を設定します。この値は単なるスケールの問題なので、実際の値でなくてもかまいません。マウスによる拡大縮小で変更されるパラメータです。

#### Size

Drawing area の width と height をピクセル数で指定します。お使いのディスプレイの解像度によっては自由な値を設定できない場合があります。

### Detector geometry



#### Camera length 2

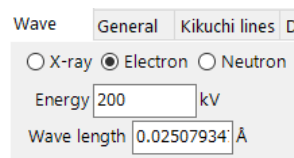
試料から検出器までの距離が表示されます。

#### Detailed geometry

光学系に関する設定画面が起動します。詳しくは [6.7. Detector geometry](#) をご覧ください。

## 6.4. Tab menu

### Wave



入射波を設定します。

#### 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.

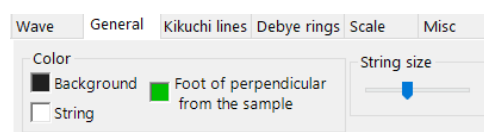
#### Electron

Enter the energy or wavelength.

#### Neutron

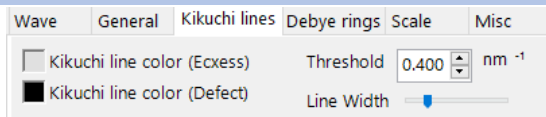
Enter the energy or wavelength.

### General



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

## Kikuchi lines

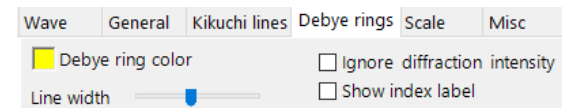


Kikuchi lines に関する設定を行います。[Tool bar](#) で Kikuchi lines を選択しているときにアクティブになります。

### Threshold

この値より大きな d 値をもつ Kikuchi lines を計算対象とします。

## Debye rings



Debye ring に関する設定を行います。[Tool bar](#) で Debye rings を選択しているときにアクティブになります。

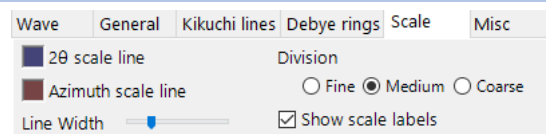
### Ignore diffraction intensity

チェックすると、結晶構造因子を無視して、全てのデバイリングを同一の色で描画します。

### Show index label

デバイリングの面指数を表示します。

## Scale



[Tool bar](#) で Scale を選択しているときにアクティブになります。

### 2θ/Azimuth scale line

前者は散乱角方向、後者は方位角方向を意味しています。それぞれスケールラインの色を変更できます。

### Line width

Scale line の太さを設定します。

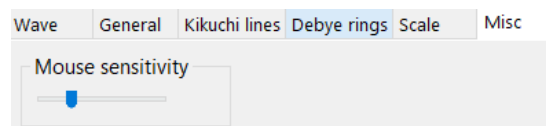
### Division

Scale line の目盛間隔を設定します。

### Show scale labels

Scale line にラベルを表示するかどうかを選択します。

## Misc



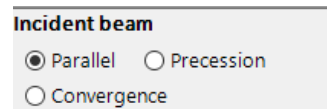
### Mouse sensitivity

マウス操作をする際のマウス感度を設定します。

## 6.5. Spot property

回折スポットの計算、表示などに関する設定を行います。[Tool bar](#) で Spot を選択しているときにアクティブになります。

## Incident beam



Select the type of incident beam.

### Parallel

Simulate a parallel incident beam.

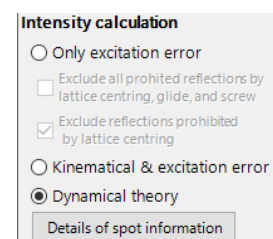
### Precession

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



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

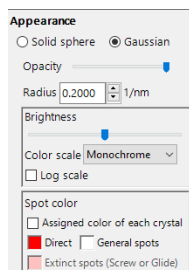
In addition to the excitation error, the crystal structure factor is also incorporated in the diffraction intensity.

### 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 diffraction spot will be displayed as a filled circle, where the area of the circle corresponds to the diffraction intensity.

In “Gaussian”, the spot will be displayed as a two-dimensional Gaussian function. The integral intensity corresponds to the diffraction intensity.

### Opacity

Specifies the transparency of the diffraction spot to be drawn.

### Radius

逆格子点の半径を指定します。ここで指定した値は、次のように回折スポットの表示に影響します。

- Gaussian を選択している場合
- Solid sphere を選択していて、かつ“Only excitation error” あるいは “Kinematical & excitation error” を選択している場合、逆格子点を次の様な半径をもつ球体であると考えて、その球体とエワルド球との断面を回折スポットとして表示します。
  - ✓ Only excitation error を選択している場合は、常に Radius
  - ✓ Kinematical & excitation error を選択している場合は、 $\text{Radius} \times (\text{運動学的な相対回折強度})^{1/3}$
- Solid sphere を選択していて、かつ“Dynamical theory” を選択している場合、表示される回折スポットの半径は、 $\text{Radius} \times (\text{動力学的な相対回折強度})^{1/2}$  になります。

### Brightness

Gaussian を選択した場合にアクティブになります。スケールバーで調節します。

### Color scale

Gray scale か Cold-warm color かを選択します。

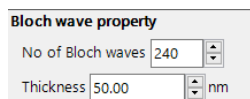
### Log scale

チェックすると強度が Log scale で表示されます。

### Spot color

回折スポットの色を設定します。

## Bloch wave property



“Intensity calculation” として、“Dynamic theory”を選択している場合にアクティブになります。

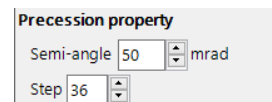
## No of Bloch waves

動力学的回折強度計算の際に取り入れる Bloch wave の数を設定します。この数値は、Incident beam として Parallel あるいは Precession を選択し、Intensity calculation として Dynamic theory を選択している場合に使われます。

## Thickness

試料の厚みを設定します。

## Precession property



“Incident beam”として“Precession”を選択しているときにアクティブになります。

### Semi-angle

Precession electron diffraction における入射電子の半頂角を設定します。

### Step

Precession electron diffraction は、複数の方向からの parallel beam diffraction を足し合わせることによってシミュレーションします。この方向の数を設定します。

## 6.6. Toolbar



### Spots

Toggles between show/hide diffraction spots.

### Kikuchi lines

Toggles between show/hide Kikuchi lines

### Debye rings

Toggles between show/hide Debye rings<sup>12</sup>.

### Scale

Toggles between show/hide scale lines.

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

スポットの近くに表示されるラベルの情報を選択します。

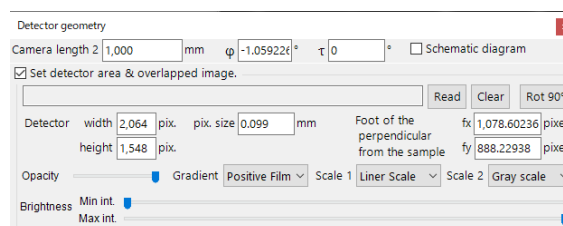
## 6.7. Detector geometry

検出器に関する詳細な設定を行います。

## Schematic diagram

パラメータの意味を説明する模式図が表示されます。詳しくは [A.2](#) を参照してください。

## Set detector area & overlapped image



The number and size of detector pixels can be set to

<sup>12</sup> Debye rings は、本来試料が多結晶体であるときに現れる回折スポットの集合体です。

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

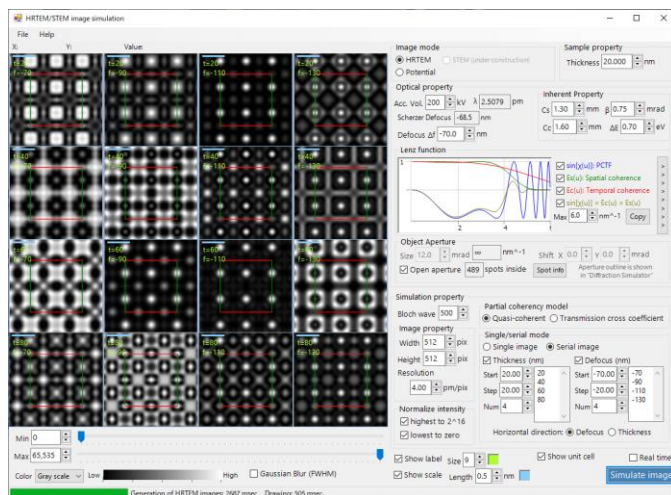
CBED は大きなリソースを必要とする計算です。そのため、リアルタイムで計算は行いません。“Execute”ボタンを押して計算を実行します。

Bethe 法では固有値・固有ベクトルの計算に大きなリソースが消費されます。固有値問題のソルバーとして、

作者の経験によれば、Bloch 波の数が小さい( $< \sim 500$ )  
場合は Eigen が、大きい場合( $> \sim 500$ )は MKL が最も高  
速である傾向があります。

Dynamic theory によって計算された回折スポットの詳細情報を表示します。記号の意味は、左上の模式図を参考にしてください。

## 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

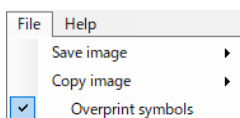
Choose between "Gray" scale or "Cold-Warm" scale.

#### 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



画像の保存、あるいはクリップボードへのコピーを行います。"Overprint symbols"をチェックした場合は、画像にスケールや文字などの情報が書き込まれます。

#### Help

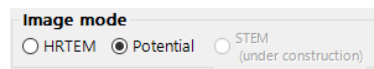
##### Basic concept of HRTEM simulation

HRTEM 計算の原理を PDF で参照することが出来ます。

##### Calculation Library

HRTEM simulation を実行する際のライブラリを選択します。通常は Native code の方が高速です。もし Native code が動作しない場合は、Managed code を使ってください。

### 7.3. Image mode



HRTEM モードか Potential モードを選択します。STEM モードは現在開発中であり、まだアクティブではありません。

### 7.4. Sample property

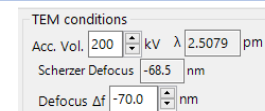
#### Thickness

試料の厚さを設定します。

### 7.5. Optical property

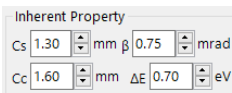
電子顕微鏡の観察条件を設定します。

#### TEM condition



加速電圧 (Acc. Vol.)、デフォーカスを指定します。加速電圧を変更すると、相対論補正された波長が表示されます。また、加速電圧と Cs 値に基づいて Scherzer defocus が表示されます。

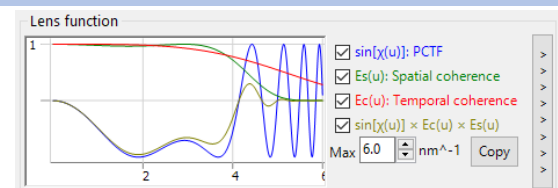
#### Inherent Property



電子顕微鏡に固有のパラメータを設定します。

- Cs: Spherical aberration coefficient (球面収差)
- Cc: Chromatic aberration coefficient (色収差)
- $\beta$ : Illumination semi angle due to the finite source size effect (照射半頂角)
- $\Delta E$ :  $1/e$  width of electron energy fluctuations (エネルギー幅)

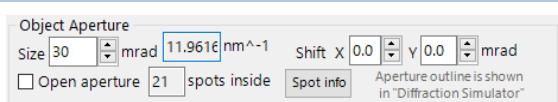
#### Lens function



レンズ関数を表示します。表示する項目は、以下の通りです。u 値の上限を設定することで、描画範囲を変更できます。

- $\text{Sin}[\chi(u)]$ : Phase contrast transfer function (PCTF)
- $E_s(u)$ : Spatial coherence envelope function
- $E_c(u)$ : Temporal coherence envelope function

#### Objective Aperture



対物レンズ絞りの大きさや位置を設定します。Diffraction simulator を起動すると、絞りの大きさや位置を確認することが出来ます。

#### Size

対物レンズ絞りの大きさを、mrad 単位で設定します。

絞りを開放したい場合は、“Open aperture”をチェックします。

設定した絞りの条件によって、Bethe 動力学法において考慮される回折スポットの数が増減します。スポットの上限数は、“Simulation property”で設定された値に制限されます。

#### Shift

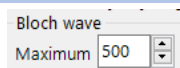
対物レンズ絞りの水平方向の位置を **mrاد** 単位で設定します。

#### Spot info.

詳細なスポット情報を表示します。

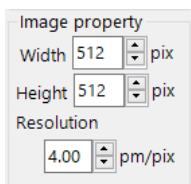
## 7.6. Simulation property

### Bloch Wave

A screenshot of the 'Bloch wave' section in the simulation software. It shows a label 'Maximum' followed by a text input field containing the number '500'.

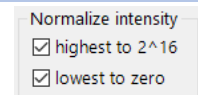
計算に取り込む最大の Bloch 波の数を設定します。

### Image Property

A screenshot of the 'Image property' dialog box. It contains three input fields: 'Width' set to 512 pix, 'Height' set to 512 pix, and 'Resolution' set to 4.00 pm/pix.

シミュレーションする画像のピクセル数と解像度を設定します。

### Normalize Intensity

A screenshot of the 'Normalize intensity' section. It has two checked checkboxes: 'highest to 2^16' and 'lowest to zero'.

シミュレーションする画像の強度のノーマライズ方法を設定します。

### Partial Coherent model

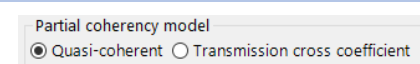
A screenshot of the 'Partial coherence model' section. It shows two radio buttons: 'Quasi-coherent' (which is selected) and 'Transmission cross coefficient'.

Image mode が HRTEM の時に表示されます。

HRTEM イメージを計算する際に、波の干渉を Quasi-coherent モデルに基づいて計算するか、Transmission cross coherent モデルに基づくかを選択します。後者の方が正確なシミュレーションですが、計算速度は遅くなります。

## Single/Serial mode

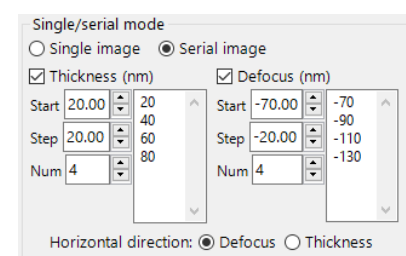
A screenshot of the 'Single/serial mode' dialog. It has two radio buttons: 'Single image' and 'Serial image' (which is selected). Below are two sections for 'Thickness (nm)' and 'Defocus (nm)', each with 'Start', 'Step', and 'Num' input fields. At the bottom, there are two radio buttons for 'Horizontal direction': 'Defocus' (selected) and 'Thickness'.

Image mode が HRTEM の時に表示されます。

Single image モードでは Sample Property で設定した試料の厚みと Optical property で設定したデフォーカスに基づいて一枚の画像がシミュレーションされます。

Serial image モードでは、Start/Step/Num で設定した複数の厚み/デフォーカスに対して画像を生成します。

## Potential option

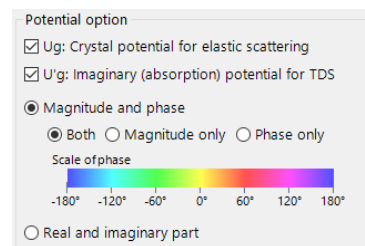
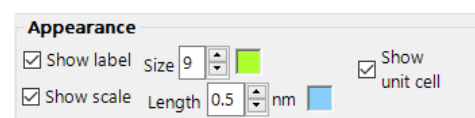
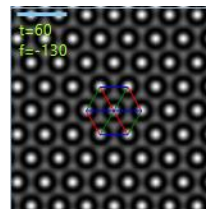
A screenshot of the 'Potential option' dialog. It has two checked checkboxes: 'Ug: Crystal potential for elastic scattering' and 'U'g: Imaginary (absorption) potential for TDS'. Below are three radio buttons: 'Magnitude and phase' (selected), 'Both', 'Magnitude only', and 'Phase only'. There is a 'Scale of phase' color bar ranging from -180° to 180°. At the bottom, there is a radio button for 'Real and imaginary part'.

Image mode が Potential の時に表示されます。

選択された potential がシミュレーション対象となります。また potential の表示方法を“Magnitude and phase”あるいは“Real and imaginary part”から選択します。

## 7.7. Appearance

A screenshot of the 'Appearance' dialog. It has two checked checkboxes: 'Show label' and 'Show scale'. The 'Show label' section has 'Size' set to 9 and a color selection box. The 'Show scale' section has 'Length' set to 0.5 nm and a color selection box. There is also a 'Show unit cell' checkbox.

### Label

ラベル (t: thickness [nm], f: defocus [nm]) を表示するかどうか、およびラベルのサイズと色を設定します。

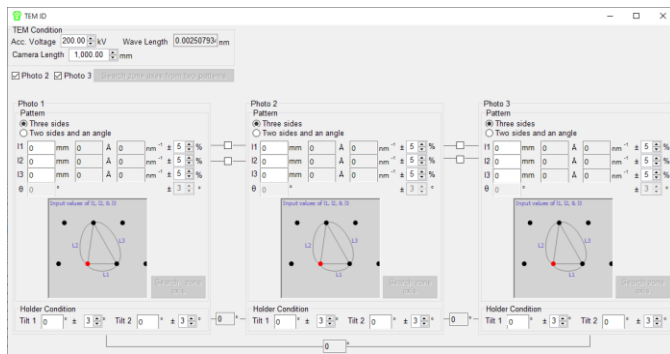
### Scale

スケールバーを表示するかどうか、およびスケールの長さや色を設定します。

### Unit cell

単位格子を表示するかどうかを設定します。画像に表示される単位格子の赤は a 軸、緑は b 軸、青は c 軸に対応します。s

## 8. TEM ID



“TEM ID”では、透過電子顕微鏡の制限視野回折によって得られた回折パターンを指数付けします。

TEM の観測条件および回折スポットの幾何学を入力し、“Search zone axes”ボタンを押すことで、候補の晶体軸が検索されます。

### 8.1. TEM condition

TEM の観測条件を入力します。

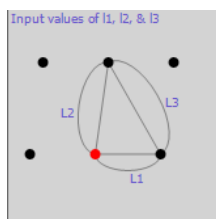
### 8.2. Photo1, 2, 3

回折スポットの幾何学を入力します。

検出器上でのスポット間の長さを入力する場合は、mm 単位のボックスに値を入力します。

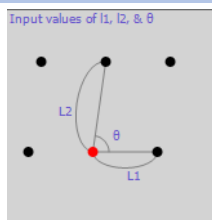
d 値が分かっている場合は、Å 単位あるいは nm<sup>-1</sup> のボックスに値を入力します。

#### 8.2.1. Three sides



ダイレクトスポットを頂点に含む三角形の 3 辺の長さを入力します。

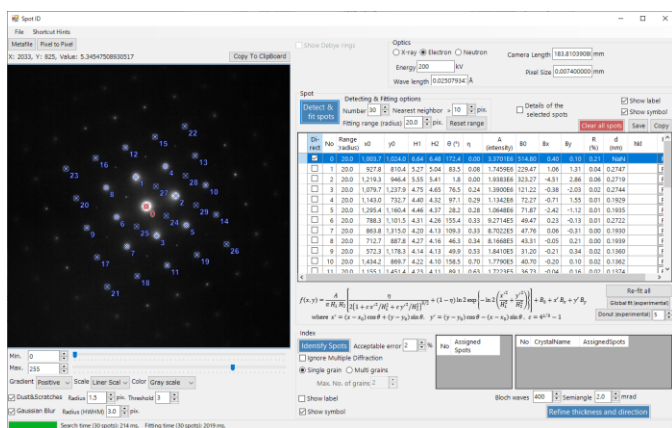
#### 8.2.2. Two sides and an angle



ダイレクトスポットを頂点に含む三角形の 2 辺の長さとその 2 辺がなす角度を入力します。



## 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 click: 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

Optics  
☐ X-ray ☒ Electron ☐ Neutron  
Camera Length 183.81039081 mm  
Energy 200 keV  
Wave length 0.02507934 Å  
Pixel Size 0.007400000 mm

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

Spot  
Detecting & Fitting options  
Number 30 Nearest neighbor 10  
Fitting range (radius) 20.0  
Details of the selected spots  
Clear all spots Save Copy

Di-rect	No.	Range (radius)	x0	y0	H1	H2	θ (°)	η	A (intensity)	B0	Bx	By	R (%)	d (nm)	hkl	Fit
<input checked="" type="checkbox"/>	0	20.0	1.0037	1.0240	6.64	6.46	172.4	0.00	3.370166	514.80	0.40	0.10	0.21	NaN	NaN	FR
<input type="checkbox"/>	1	20.0	927.8	810.4	5.27	5.04	83.5	0.08	1.745966	229.47	1.06	1.31	0.04	0.2747		FR
<input type="checkbox"/>	2	20.0	1.2193	946.4	5.55	5.41	1.8	0.00	1.938366	323.27	-4.51	2.86	0.06	0.2719		FR
<input type="checkbox"/>	3	20.0	1.0797	1.2379	4.75	4.65	76.5	0.24	1.390066	121.22	-0.38	-2.03	0.02	0.2744		FR
<input type="checkbox"/>	4	20.0	1.1430	732.7	4.40	4.32	97.1	0.29	1.134266	72.27	-0.71	1.55	0.01	0.1929		FR
<input type="checkbox"/>	5	20.0	1.2954	1.1604	4.46	4.37	28.2	0.28	1.064866	71.87	-2.42	-1.12	0.01	0.1935		FR
<input type="checkbox"/>	6	20.0	788.3	1.1015	4.31	4.26	155.4	0.33	9.271465	49.47	0.23	-0.13	0.01	0.2722		FR
<input type="checkbox"/>	7	20.0	863.8	1.3150	4.20	4.13	109.3	0.33	8.702265	47.76	0.06	-0.31	0.00	0.1930		FR
<input type="checkbox"/>	8	20.0	712.7	887.8	4.27	4.16	46.3	0.34	8.166865	43.31	-0.05	0.21	0.00	0.1939		FR
<input type="checkbox"/>	9	20.0	572.3	1.1783	4.14	4.13	49.9	0.53	1.841065	31.20	-0.21	0.34	0.02	0.1360		FR
<input type="checkbox"/>	10	20.0	1.4342	869.7	4.22	4.10	158.5	0.70	1.779065	40.70	-0.20	0.10	0.02	0.1362		FR
<input type="checkbox"/>	11	20.0	1.1551	1.4514	4.23	4.11	89.1	0.63	1.722365	36.73	-0.04	0.06	0.02	0.1374		FR

$$f(x,y) = \frac{A}{\pi H_1 H_2} \left[ \frac{\eta}{2 \left[ 1 + c x'^2/H_1^2 + c y'^2/H_2^2 \right]^{3/2}} + (1-\eta) \ln 2 \exp \left\{ -\ln 2 \left( \frac{x'^2}{H_1^2} + \frac{y'^2}{H_2^2} \right) \right\} \right] + B_0 + x' B_x + y' B_y$$
  
where  $x' = (x - x_0) \cos \theta + (y - y_0) \sin \theta$ ,  $y' = (y - y_0) \cos \theta - (x - x_0) \sin \theta$ ,  $c = 4^{1/3} - 1$

Re-fit all  
Global fit (experimental) 5

By the "Detect & fit spots" button, the software automatically detects diffraction spots in the image and fits them with the 2D Pseudo-Voigt function<sup>13</sup>. 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.

<sup>13</sup> In ReciPro, the following fitting functions are used.

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

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,  $\eta/2 \left[ 1 + c x'^2/H_1^2 + c y'^2/H_2^2 \right]^{3/2}$ , is the 2-dimensional Cauchy distribution function. The second term,  $(1 - \eta) \ln 2 \exp \left\{ -\ln 2 \left( \frac{x'^2}{H_1^2} + \frac{y'^2}{H_2^2} \right) \right\}$ , is 2-dimensional Gaussian function.

$x_0, y_0$  are the center coordinates of the spot.  $\theta$  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.  $\eta$  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 Marquart method.



## Save/Copy

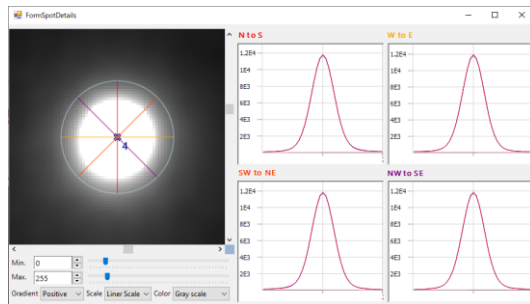
Save/copy the table information in the Excel format (tab separated values).

## 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

Name	Density	Formula	a	b	c	$\alpha$	$\beta$	$\gamma$	Crystal S
Hydrokenosol...	2.5651	Na <sub>2</sub> Si <sub>2</sub> Al <sub>12</sub> O <sub>29</sub> ...	9.87	9.87	9.87	90	90	90	cubic
Abernathyite	9.8707	K U <sub>4</sub> As <sub>2</sub> O <sub>15</sub> ...	7.176	7.176	10.126	90	90	90	tetrag
Abernathyite	9.6511	NH <sub>10</sub> U <sub>4</sub> As <sub>2</sub> ...	7.189	7.189	10.191	90	90	90	tetrag
Abernathyite	9.8554	K O <sub>31</sub> H <sub>15</sub> U...	7.171	7.171	10.048	90	90	90	tetrag
Fluorapophylli...	2.5337	K <sub>1.68</sub> Na <sub>0.32</sub> ...	8.963	8.963	15.804	90	90	90	tetrag
Fluorapophylli...	2.5453	K Ca <sub>4</sub> Si <sub>8</sub> O <sub>3</sub> ...	8.965	8.965	15.767	90	90	90	tetrag
Fluorapophylli...	2.5428	K Ca <sub>4</sub> Si <sub>8</sub> O <sub>3</sub> ...	8.96	8.96	15.8	90	90	90	tetrag
Ahrensite	4.8498	Fe <sub>16</sub> O <sub>8</sub> Si <sub>7</sub> ...	8.234	8.234	8.234	90	90	90	cubic
Hydroxyapop...	2.3556	K Ca <sub>4</sub> Si <sub>8</sub> O <sub>2</sub> ...	8.979	8.979	15.83	90	90	90	tetrag
Hilgardite	2.6936	Ca <sub>2</sub> Cl <sub>85</sub> O <sub>1</sub> ...	11.438	11.318	6.318	90	90.06	90	monoc
Ahrensite	5.5211	Fe Si <sub>4</sub> O <sub>4</sub>	8.236	8.236	8.236	90	90	90	cubic
Anorthite	2.6975	Ca <sub>2.6</sub> Na <sub>1.28</sub> ...	8.1736	12.8736	7.1022	93.462	116.054	90.475	triclin
Anorthite	2.6975	Ca <sub>2.6</sub> Na <sub>1.28</sub> ...	8.1736	12.8736	7.1022	93.462	116.054	90.475	triclin

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.

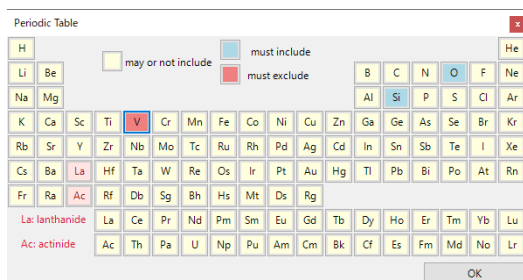
### 11.2. Search options

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.

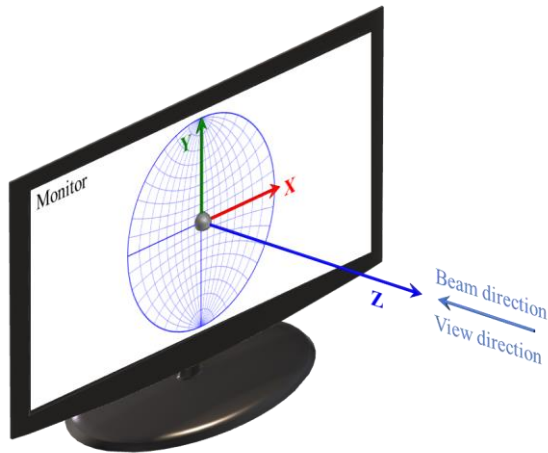
#### Density

Enter the density and acceptable error.

## Appendix

### A.1. Basic definition of ReciPro coordination

#### Definition of orientation



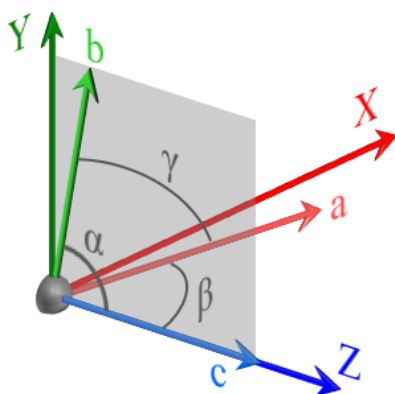
Since ReciPro handles various "directions", the definitions are explained below. In ReciPro, right-handed coordinate system is used, and axes are defined as follows:

- 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<sup>14</sup>. That is, the orientation of the

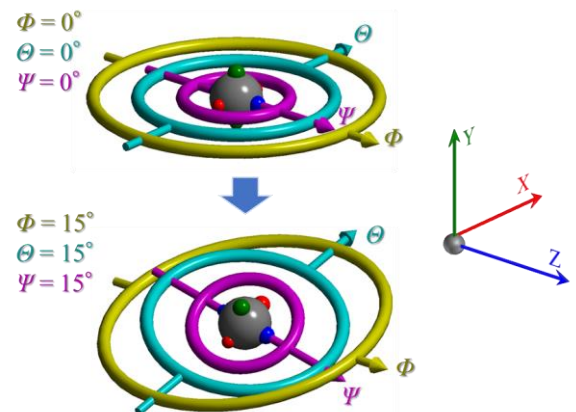
- The c-axis is aligned with the Z-axis direction
- The b-axis lies on the YZ plane and is close to the

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<sup>15</sup>.

#### 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,  $\Phi$ ,  $\theta$  and  $\Psi$  as shown the above. When the angles  $\Phi$ ,  $\theta$ , and  $\Psi$  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;  $\Phi$  is the highest (1st) rotation, followed by  $\theta$  (2nd).  $\Psi$  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  $\Phi$ ,  $\theta$ , and  $\Psi$  are all set to 15 degrees. The axis of rotation corresponding to angle  $\Phi$  will always coincide with the Z axis, but the axis of rotation corresponding to angle  $\theta$  and angle  $\Psi$  will generally not coincide with any of X, Y, or Z.

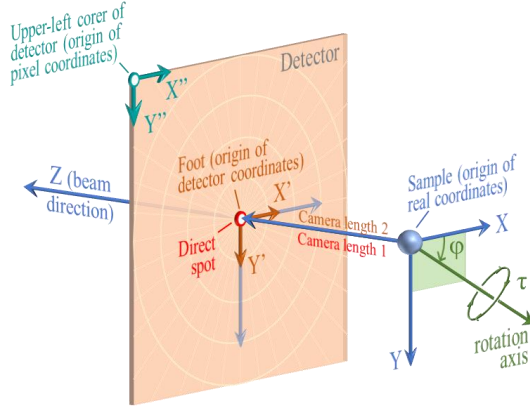
### A.2. Definition of coordination in "Crystal diffraction"

"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.

<sup>14</sup> This definition is compatible with Oxford's EBSD software.

<sup>15</sup> In the cases of cubic, tetragonal, or orthogonol, 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



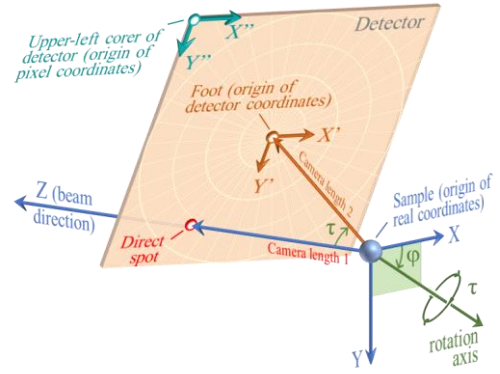
First, consider a situation where the detector is not tilted (i.e., the normal of the incident beam and the detector plane are the same), as shown in the above figure.

"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.<sup>16</sup>) 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.

### After rotation



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 ( $\phi$ ) and the amount of rotation ( $\tau$ ). The rotation axis is considered to be in the XY plane ( $Z=0$  plane) and the angle from the X axis is defined as  $\phi$ . Then, rotate it around the axis of rotation defined by  $\phi$  by  $\tau$  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<sup>17</sup>. 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)<sup>18</sup>, 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.

<sup>16</sup> 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.

<sup>17</sup> The relation between the foot point ( $F_x, F_y$ ) and the direct spot ( $D_x, D_y$ ) is as follows;

$$D_x = F_x - C_2 \times \sin(\Phi) \times \tan(\tau)$$

$$D_y = F_y + C_2 \times \cos(\Phi) \times \tan(\tau)$$

<sup>18</sup> 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).

#### $\Phi$

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