

# TEM/STEM Image Simulation Software

## BesTEM Instruction Manual

<b>1. Home Screen .....</b>	<b>1</b>
<b>2. Default Settings for Various Calculation Conditions at Startup.....</b>	<b>2</b>
<b>3. Read Specimen Data.....</b>	<b>6</b>
<b>4. Crystal/Cluster/Supercell Data 3D Display.....</b>	<b>9</b>
<b>5. TEM Image Calculation .....</b>	<b>12</b>
<b>6. Calculation of Beam Intensity, Ronchigram, STEM Image, and CBD .....</b>	<b>17</b>
<b>7. Crystal Data Making Method .....</b>	<b>23</b>
<b>8. Supercell (Mainly for STEM/CBD calculation) Creation .....</b>	<b>39</b>
<b>9. TEM and STEM Image Calculation of Cluster .....</b>	<b>43</b>

Date prepared/updated: Oct. 29, 2021

\*For purposes of improvement, functions may be changed without notice.

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Production/Sale

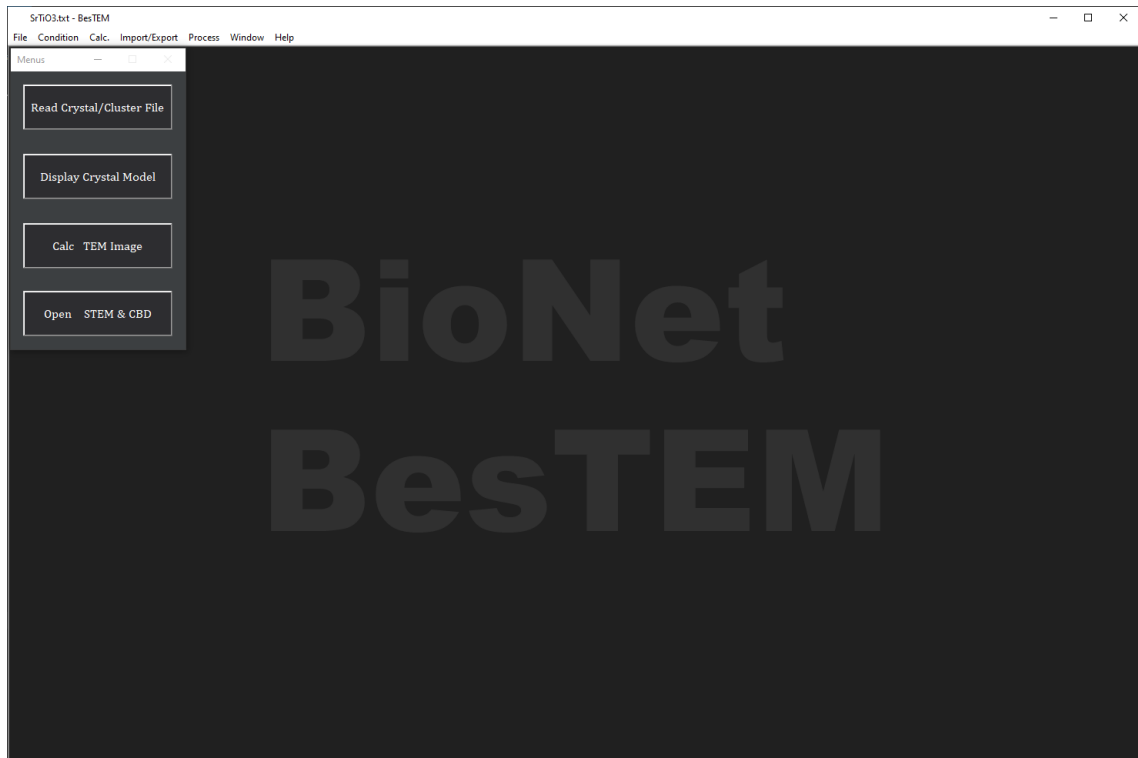
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## 1. Home Screen



When the software starts:

- The **Menu** dialog box will display.
- The crystal data (or the cluster supercell data) in use the last time the software was run will be read.
- Calculation conditions of the basic optical system will default to those in use the last time the software was run.

The **Menu** dialog box offers four buttons:

- To obtain a new read of the Crystal data or Cluster supercell data, click the **Read Crystal/Cluster File** button.
- To display the 3D structure of the current specimen data, click the **Display Crystal Model** button.
- To calculate a TEM image, click the **Calc TEM Image** button.
- To open a dialog box to calculate electron beam strength, Ronchigram, STEM image, and CBD, click the **Open STEM CBD** button.

## 2. Default Settings for Various Calculation Conditions at Startup

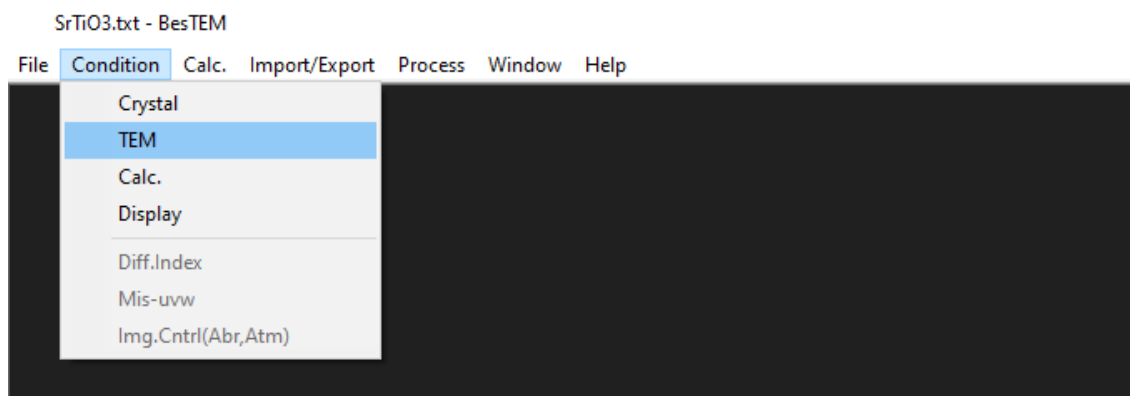
At startup, BesTEM software defaults to certain previously used conditions. If the specimen data file used last time is missing, Si crystal data is automatically created and read.

When setting defaults (optical, calculation, and display conditions) at the time of initial startup, or if you are changing to another setting, perform the following operation:

### 2.1. Optical condition setting

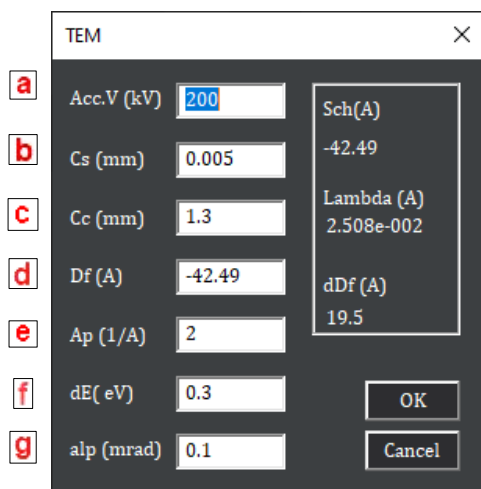
All settings other than **Acc.V (kV)** (accelerating voltage) can be changed after image calculation.

1. From the **Condition** dropdown menu, select **TEM**.



The **TEM** dialog box will appear. In this dialog box, you can set the TEM optical-condition defaults.

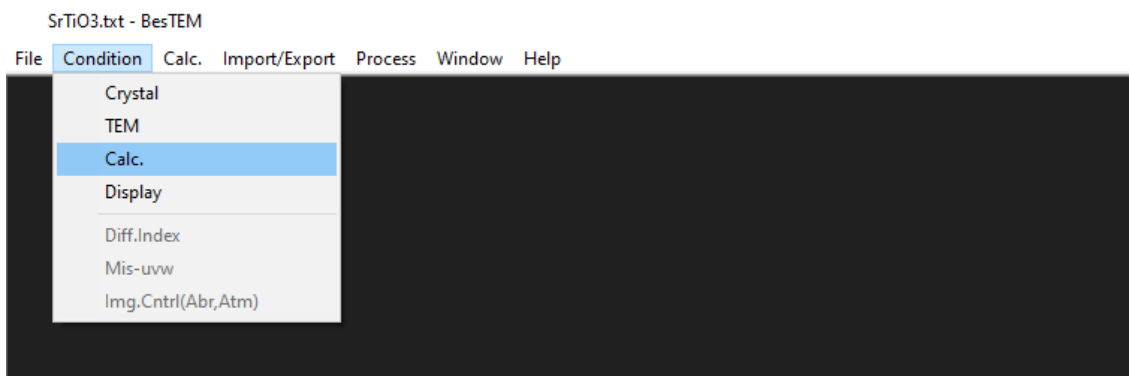
2. Enter each value. When done, click the **OK** button to save.



- (a) Accelerating Voltage
- (b) Spherical aberration coefficient
- (c) Chromatic aberration coefficient
- (d) Defocus amount
- (e) Objective aperture radius
- (f) Energy spread
- (g) Reciprocal source size

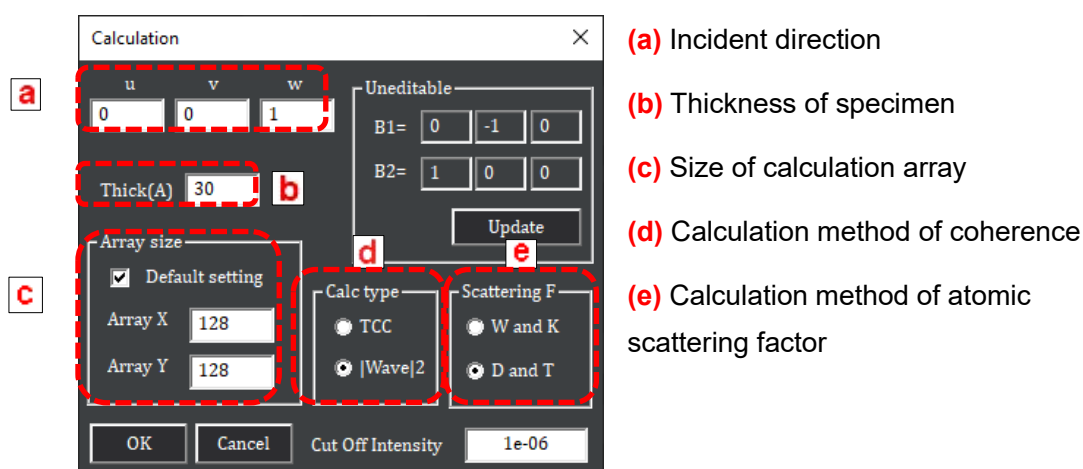
## 2.2. Calculation condition setting

1. From the **Condition** dropdown menu, select **Calc.**



The **Calculation** dialog box will appear. In this dialog box, you can set various calculation conditions.

2. Enter each value. When done, click the **OK** button to save the conditions.



\*These settings are referenced only when the unit cell data is used for calculation. When a cluster or supercell is used instead, the calculation is always performed along the C-axis, and the thickness is the size of the cluster supercell along the C-axis.

\*\*The calculation array size is automatically set to that of the crystal size when **Default setting** is checked. If it is not checked, you must adjust the calculation array size to account for the crystal size each time you load a crystal file.

### References:

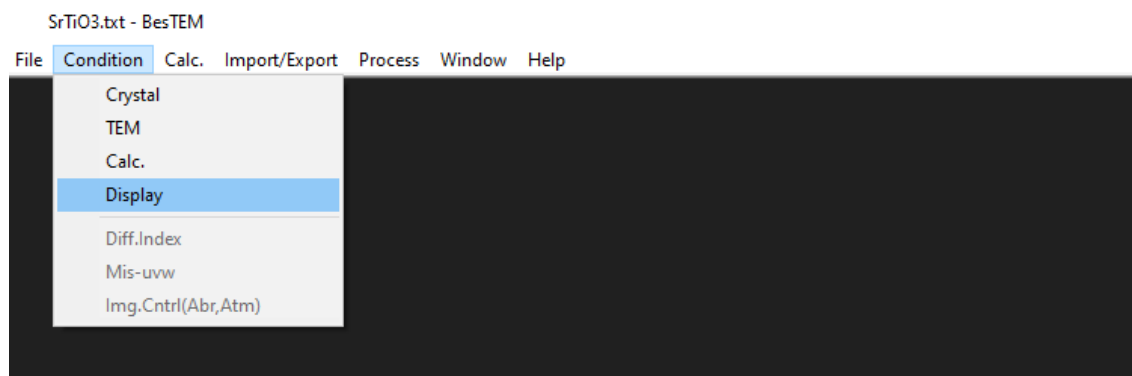
TCC: K. Ishizuka, *Ultramicroscopy* 5 (1980), 55–65

F. Hosokawa et al., *Ultramicroscopy* 167 (2016), 11–20  
Atomic scattering factor: A. Weickenmeier and H. Kohl, *Acta Cryst. A* 47 (1991), 590  
P.A. Doyle and P.S. Turner, *Acta Cryst. A* 24 (1968), 390

### 2.3. Settings for image display and diffraction

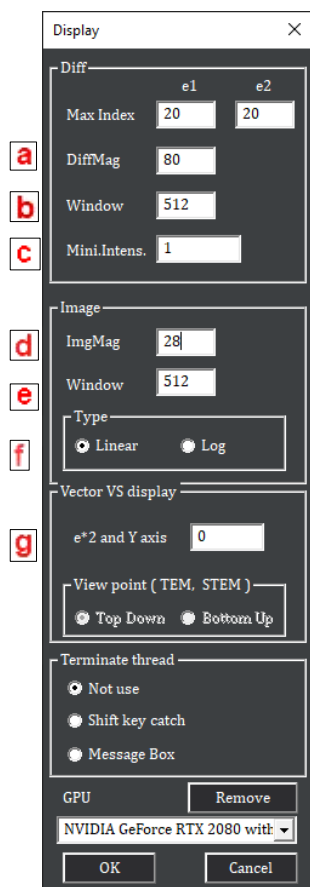
All settings other than **Window** in the **Image** section (window size) can be changed after image calculation.

1. From the **Condition** dropdown menu, select **Display**.



The **Disp** dialog box will appear. In this dialog box, you can set the TEM optical-condition defaults.

2. Enter each value. When done, click the **OK** button to save.



(a) Display magnification of diffraction

(b) Diffraction display window size

(c) Lower limit of display intensity

(d) Image display magnification (number of pixels corresponding to 1Å)

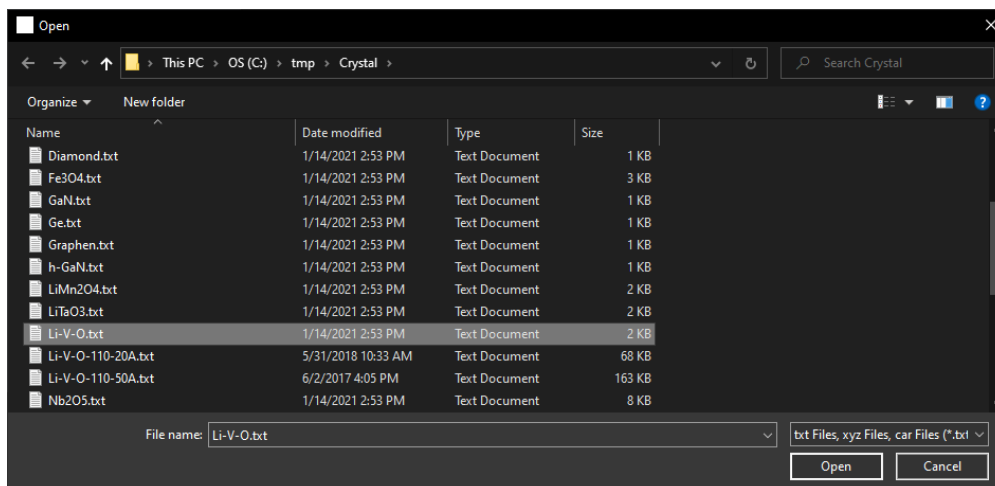
(e) Image display window size

(f) Display method (linear or logarithmic)

(g) Display rotation angle (angle between inverse space vector  $e_2$  and display Y-axis)

### 3. Read specimen data

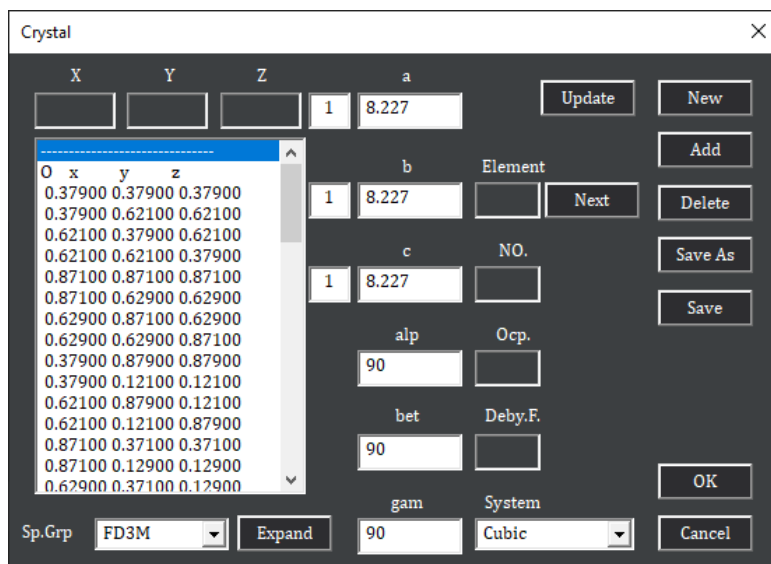
1. From the **Condition** dropdown menu, select **Crystal**.  
Alternatively, from the **File** dropdown menu, select **Open**.
2. Select a crystal file from the menu to open the **Data Import** dialog box.



3. Select data and read file.

#### 3.1 Display of read data

Selecting **Condition > Crystal** opens the **Crystal** dialog box for the loaded data file.



Here, you can edit the unit cell information (**a**, **b**, and **c** space groups;  **$\alpha$** ,  **$\beta$** , and  **$\gamma$**  space groups; crystal **System**) used for calculation.

When you click an element symbol in the list box, the next column of text fields becomes

active, displaying the **Element**, number (**NO.**), site occupancy rate (**Ocp.**), Debye B-factor (**Deby.F.**), and **ionic charge** of the atom contained in the calculation cell are displayed. The site occupancy rate and B-factor can be edited here for each element.

The 'Crystal' dialog box displays a list of atoms with columns for X, Y, and Z coordinates. The first atom is highlighted. To the right, fields for 'a', 'b', 'c', 'alp', 'bet', 'gam', 'Element', 'NO.', 'Ocp.', 'Deby.F.', and 'System' are shown. Buttons for 'Update', 'New', 'Add', 'Next', 'Delete', 'Save As', 'Save', 'OK', and 'Cancel' are present.

O	x	y	z
0.37900	0.37900	0.37900	
0.37900	0.62100	0.62100	
0.62100	0.37900	0.62100	
0.62100	0.62100	0.37900	
0.87100	0.87100	0.87100	
0.87100	0.62900	0.62900	
0.62900	0.87100	0.62900	
0.62900	0.62900	0.87100	
0.37900	0.87900	0.87900	
0.37900	0.12100	0.12100	
0.62100	0.87900	0.12100	
0.62100	0.12100	0.87900	
0.87100	0.37100	0.37100	
0.87100	0.12900	0.12900	
0.62900	0.37100	0.12900	

This screenshot shows the same 'Crystal' dialog box with red dashed boxes and letters highlighting specific features: (a) points to the selected row in the list box; (b) points to the X, Y, Z coordinate fields above the list box; (c) points to the 'Update' button.

(a) In the list box, relative coordinates in the cell are described for each element. If you highlight each coordinate with the mouse, (b) the coordinates will also be displayed in the text fields above the list box. You can edit them in these fields.

(c) The list box has scroll buttons enabled. The **Next** button will automatically scroll to the beginning of the next element.

The data being read can also be checked visually in 3D view. You can open the **3D View** dialog box by clicking **Display Crystal Model** in the home **Menu**, or by choosing **Crystal 3D Viewing** from the **Calc.** dropdown menu.



Menus

Read Crystal/Cluster File

Display Crystal Model

Calc TEM Image

Open STEM & CBD

3D Crystal View

Atom 1

Edit	x	y	z
Select 1	-0.869	-1.289	0.746

Atom 2

Edit	x	y	z
Select 2	-0.869	-1.289	0.746

Distances of 1 - 2

projected	actual	dz
0.000	0.000	0.000

Axis display

☒ Unit cell
 ☒ a<sub>b</sub>c
 ☐ Rotation

Super Cell: Save

Cluster: Save or Imaging

Quit

Origin

X

0.5

Y

0.5

Z

0.5

Select Origin

Reset

Polar control

Amp

103.93

Dir

113.27

Rot

0.0

Check

Draw

UVW control

U

0.43

V

-1.00

W

-0.27

Draw

Reset

Display

Mag

0.54

Size

9

Light up

-0.3

-0.3

1.0

☒ CR/STAL
 

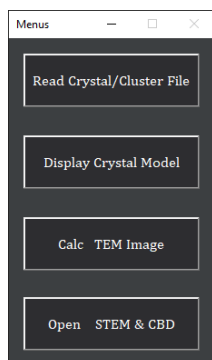
1

1

1

☒ Sphere

#### 4. Crystal/Cluster/Supercell Data 3D Display

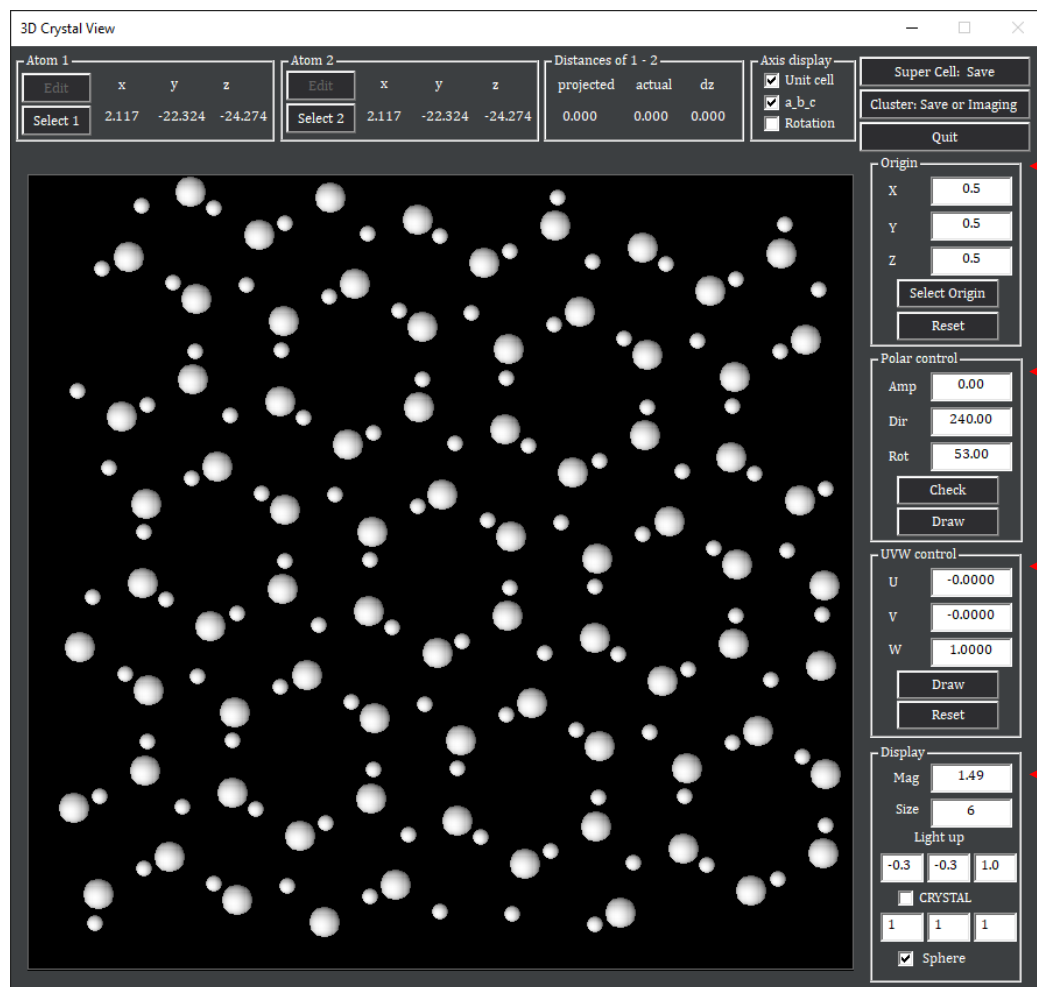


On the home screen, click the **Display Crystal Model** button in the **Menu**.

The **3D Display** box will open, showing a 3D model of the currently loaded data (Crystal or Cluster/Supercell). You can do the following in this in dialog box:

- Manipulate the model rotation by dragging the mouse cursor left (arbitrary direction) or right (up and down).
- Rotate the model by inputting a rotation angle (polar coordinates) or azimuth vector (opposite to the line of sight = perpendicular to the screen)
- Calculate a TEM image of electron incidence from the current line -f-sight direction.
- Create new Cluster data with [001] orientation as the current orientation vector.
- Display the projected distance between any two atoms and distance in real space.  
Create Supercell data from Crystal data.

You can use your mouse wheel to incrementally change the parameters of each text field in the dialog box.



Fixed point of 3D rotation operation:

The default (0.5, 0.5, 0.5) corresponds to the center of the cell.

If you click the **Select Origin** button and then the left mouse button on any atom, that atom will become the center of rotation.

Input 3D display as rotation angle (polar coordinates)

Input D display with direction vector (reverse line of sight)

Display magnification (no unit)

Atom display size (no unit)

Atomic display shading

Repeat display on/off; repeat count

If you click the **Select** button and then click on any atom in the 3D display, that atom will be labeled **Atom**, and its x, y, and z coordinates will be displayed.

The **Edit** button opens the **Crystal file edit** dialog box, where you can edit the atomic coordinates of **Atom**, etc.

Clicking the **Super Cell: Save** button opens the **Super Cell creation** dialog box.

Clicking the **Cluster: Save or Imaging** button opens the dialog box for creating a cluster and calculating a cluster TEM image.

**Atom1 and Atom2:**  
Projection distance on 3D display  
Distance in real space  
Z-axis distance on 3D display

Unit cell display  
**a**, **b**, and **c** axis display  
3D-rotation axis display

Atom 1				Atom 2				Distances of 1 - 2			Axis display		
	x	y	z		x	y	z	projected	actual	dz	<input checked="" type="checkbox"/> Unit cell	<input checked="" type="checkbox"/> a_b_c	<input type="checkbox"/> Rotation
Select 1	2.117	-22.324	-24.274	Select 2	2.117	-22.324	-24.274	0.000	0.000	0.000			

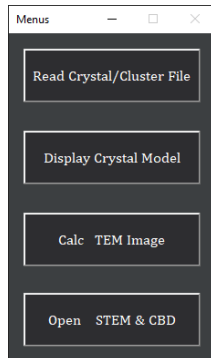
Origin

X: 0.5  
Y: 0.5  
Z: 0.5

Select Origin  
Reset

Exit the **3D Display** dialog box by clicking the **Quit** button.

## 5. TEM Image Calculation

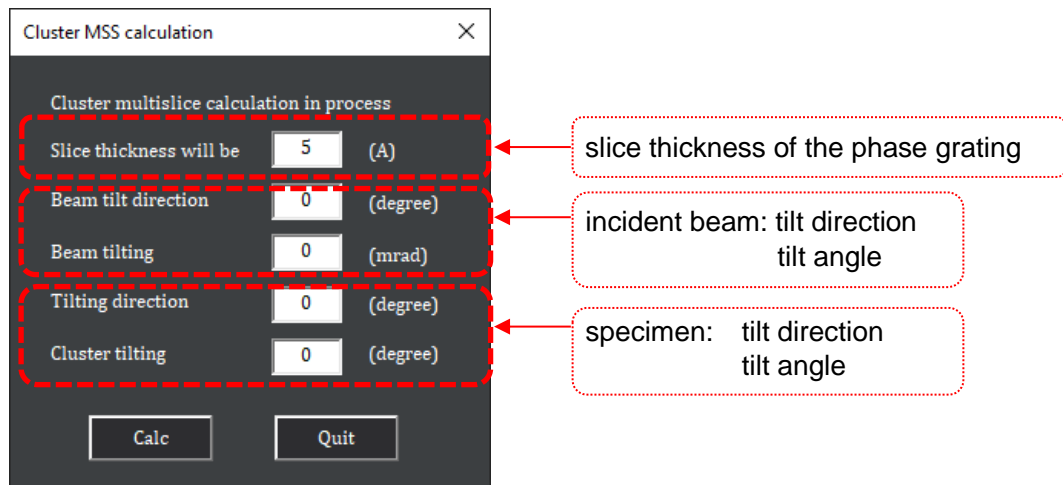


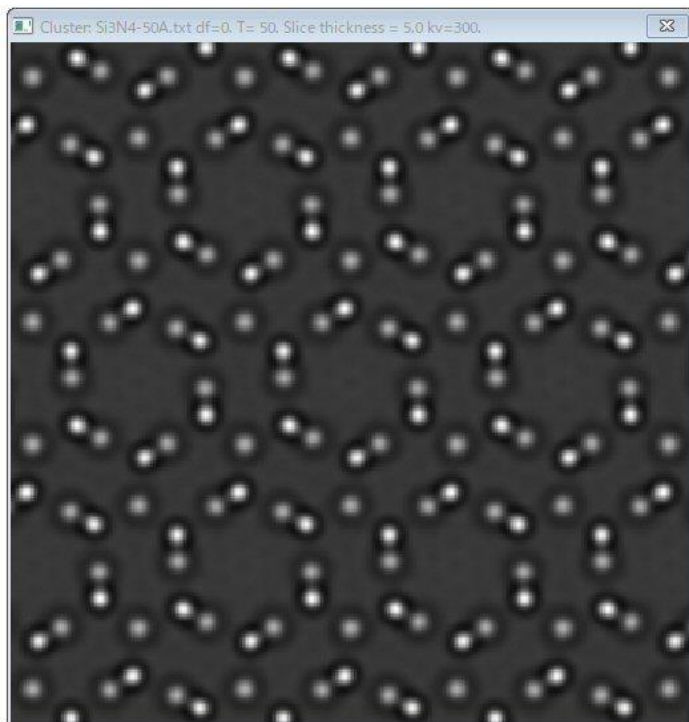
On the home screen, click the **Calc. TEM Image** button in the **Menu**.

If **Crystal** data is read, the TEM image will be calculated with the crystal orientation and the crystal thickness, which are input to the default condition. The slice thickness of the phase grating will be the distance between the crystal's equivalent points in the direction of projection.

If **Cluster / Supercell** data is read, a dialog box for entering the thickness of the phase grating slice will open. Enter the slice thickness and press the **OK** button to calculate the TEM image. (You can also enter the tilt angle/tilt direction of the incident beam and of the sample).

When **Cluster / Supercell** data is read, the **Cluster MSS calculation** dialog box appears:





The figure above is a TEM image calculated from the Supercell data ( $x, y, z = 37.98$  [Å],  $39.465$  [Å],  $50.0$  [Å]) created from the  $[001]$  orientation of  $\beta$ - $\text{Si}_3\text{N}_4$ .

Supercell data is usually created from Crystal data for calculating CBD and STEM images, but it can also be used when you want to calculate TEM images with arbitrary slice thickness. You can also insert or delete atoms at arbitrary coordinates in the supercell, or replace any atom with another atom to perform TEM image calculations.

Once the TEM image has been calculated, the control dialog box for the optical parameters will open automatically. These parameters can be changed by direct input, mouse wheel operation, etc. As parameters are changed, the result is immediately reflected in the calculated TEM image.

Coarse check button: sensitivity switching setting for wheel

### Basic parameters:

**df (Å):** Defocus

**de (eV):** Energy spread

**Cs (mm):** Spherical aberration coefficient  
Fifth-order spherical aberration

**alp (mrad):** Reciprocal source size

**Mag:** Display magnification (pixels / Å)

**Cc (mm):** Chromatic aberration coefficient

**OL Ap (1/Å):** Objective aperture radius

**Sample thickness (Å)** change button

**Edit Atoms** button

**Superimpose Atoms** checkbox

**Display** intensity linear/log radio buttons

### Center Phase Shift (at $g = 0$ ) by phase plate:

**Utilize** checkbox: Phase plate effect on/off

**Phase shift amount** of phase plate  $\phi$

**Shape effect of phase plate:**

- Within radius: no phase change
- Exceeding radius: phase change of  $\phi$

The 'Image Control' dialog box contains the following sections and controls:

- COARSE CONTROL for Button and Mouse Wheel:** A checkbox at the top.
- Basic parameters:** A group box containing:
  - df (Å): 0
  - alp (mrad): 0.1
  - de (eV): 0.4
  - Mag: 21
  - Cs (mm): 0
  - Cc (mm): 1.33
  - C5 (mm): 0
  - OL Ap (1/Å): 1.33
- 2 fold Astigmatism:**
  - dir (deg): 0
  - amp (Å): 0
- Optical mis-alignment:**
  - dir (deg): 0
  - amp (mrad): 0
- OL Ap mis-alignment:**
  - dir (deg): 0
  - amp (mrad): 0
- Image rot/shift:**
  - Rotation: 0
  - Shift x: 0, y: 0
- Sample thickness (Å):** 50.00, with left and right arrow buttons.
- Edit Atoms:** A button.
- Superimpose Atoms:** A checkbox.
- Display:** Radio buttons for 'linear' (selected) and 'log'.
- Show other aberrations:** A button.
- Close:** A button.
- Center Phase Shift (at  $g = 0$ ) by phase plate:**
  - Utilise:** A checkbox.
  - 0.5 pai:** A text label next to a small input field.
  - p/p R, F(mrad):** A group box containing:
    - Radius: 0.1
    - Fringe: 0
    - Fringe factor: 1
  - + for carbon hole:** A text label at the bottom.

**Image Control**

☐ COARSE CONTROL for Button and Mouse Wheel

**Basic parameters**

df (Å) 0

alp (mrad) 0.1

de (eV) 0.4

Mag 21

Cs (mm) 0

Cc (mm) 1.33

C5 (mm) 0

OL Ap (1/Å) 1.33  
0.7519 (Å)

Sample thickness (Å)  
50.00

**2 fold Astigmatism**

dir (deg) 0

amp (Å) 0

**Optical mis-alignment**

dir (deg) 0

amp (mrad) 0

**OL Ap mis-alignment**

dir (deg) 0

amp (mrad) 0

**Image rot / shift**

Rotation 0

Shift x y  
0 0

**Show other aberrations**

**Close**

**Center Phase Shift ( at  $g = 0$  ) by phase plate**

☐ Utilise

0.5 pai

p/p R, F(mrad)

Radius	Fringe	Fringe factor
0.1	0	1

+ for carbon hole

**Annotations:**

- 2-fold astigmatism: direction amplitude
- Optical mis-alignment: direction amplitude
- OL aperture mis-alignment: direction amplitude
- Image rotation  
Image shift
- Click the **==> Show other aberrations** buttons to incorporate higher-order aberrations
- Click the **Close** button to close the dialog box.



Image Control

☐ COARSE CONTROL for Button and Mouse Wheel

Basic parameters

df (Å)

alp (mrad)

de (eV)

Mag

Cs (mm)

Cc (mm)

C5 (mm)

OL Ap (1/Å)

0.7519 [Å]

Sample thickness (Å)

☐ Superimpose Atoms

Display ☒ linear ☐ log

Hide other aberrations

Center Phase Shift (at  $g = 0$ ) by phase plate

☐ Utilise   $\pi$

p/p R. F (mrad)

Radius	Fringe	Fringe factor
<input type="text" value="0.1"/>	<input type="text" value="0"/>	<input type="text" value="1"/>

+ for carbon hole

2 fold Astigmatism

dir (deg)

amp (Å)

Optical mis-alignment

dir (deg)

amp (mrad)

OL Ap mis-alignment

dir (deg)

amp (mrad)

Image rot/shift

Rotation

Shift x  y

Coma

dir (deg)

amp (µm)

3 fold Astigmatism

dir (deg)

amp (µm)

4 fold Astigmatism

dir (deg)

amp (µm)

5 lobe

dir (deg)

amp (mm)

Coma 4th order

dir (deg)

amp (mm)

5 fold Astigmatism

dir (deg)

amp (mm)

6 fold Astigmatism

dir (deg)

amp (mm)

T6 (3fold-6th)

dir (deg)

amp (mm)

Noise

Total dose  e / Å<sup>2</sup>

☐ take effect

The ==> other aberrations buttons allows simulation of higher-order aberrations.

Coma

3 fold Astigmatism

In all fields:

- **dir**: direction
- **amp**: amplitude

4 fold Astigmatism

Star

3 lobe

Coma 4th-order

5 fold Astigmatism

6 fold Astigmatism

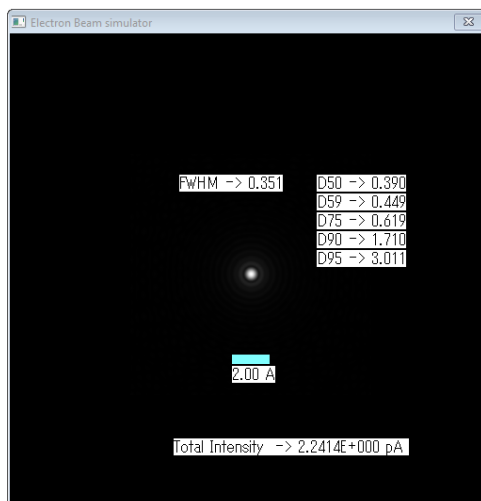
Enter the dose of the electron beam and check the **take effect** to convert the image into a shot noise effect (Poisson noise).

3 fold in 6th-order aberration

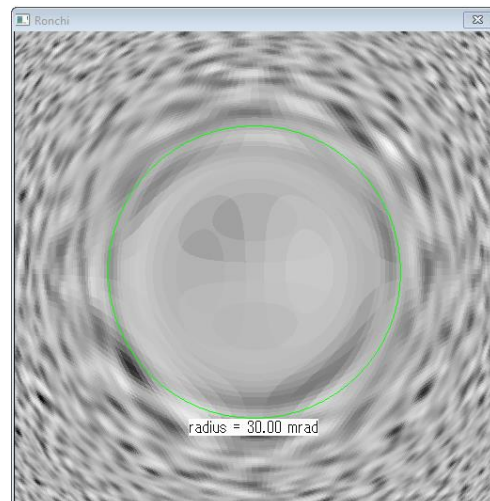
## 6. Calculation of Beam Intensity, Ronchigram, STEM image, and CBD

The **Beam radius calc** dialog box opens in Process / Probe Forming and STEM. (Beam shape, Ronchigram also open at the same time).

Put the mouse cursor into the text field for each value, which you can then change incrementally by scrolling the mouse wheel up (larger) or down (smaller). If (a) **Link to Beam calc.** and **Link to Ronchi calc.** are checked off, beam shape and Ronchigram values respectively will be recalculated as you change the values. When (b) **Link to pixel size** is checked, (c) **pixel size (A / pixel)** is automatically selected for Cs and acceleration voltage.



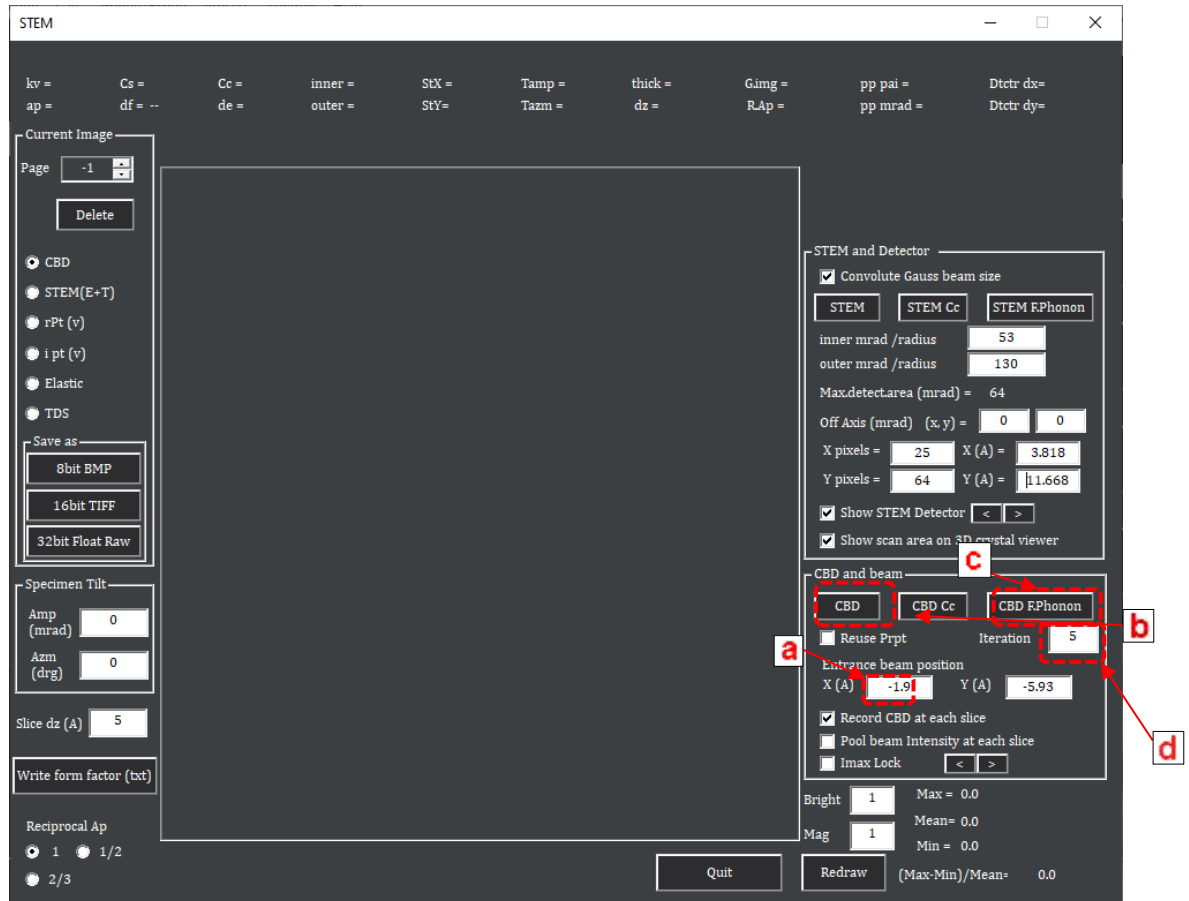
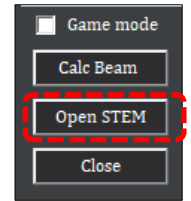
**Beam shape**



**Ronchigram**

## 6.1. STEM and CBD calculation

Click the **Open STEM** button at bottom right of the **Beam radius calc.** dialog box to open the **STEM/CBD calculation** dialog box. To proceed with calculating STEM/CBD, the **Cluster / Supercell** data should be read.



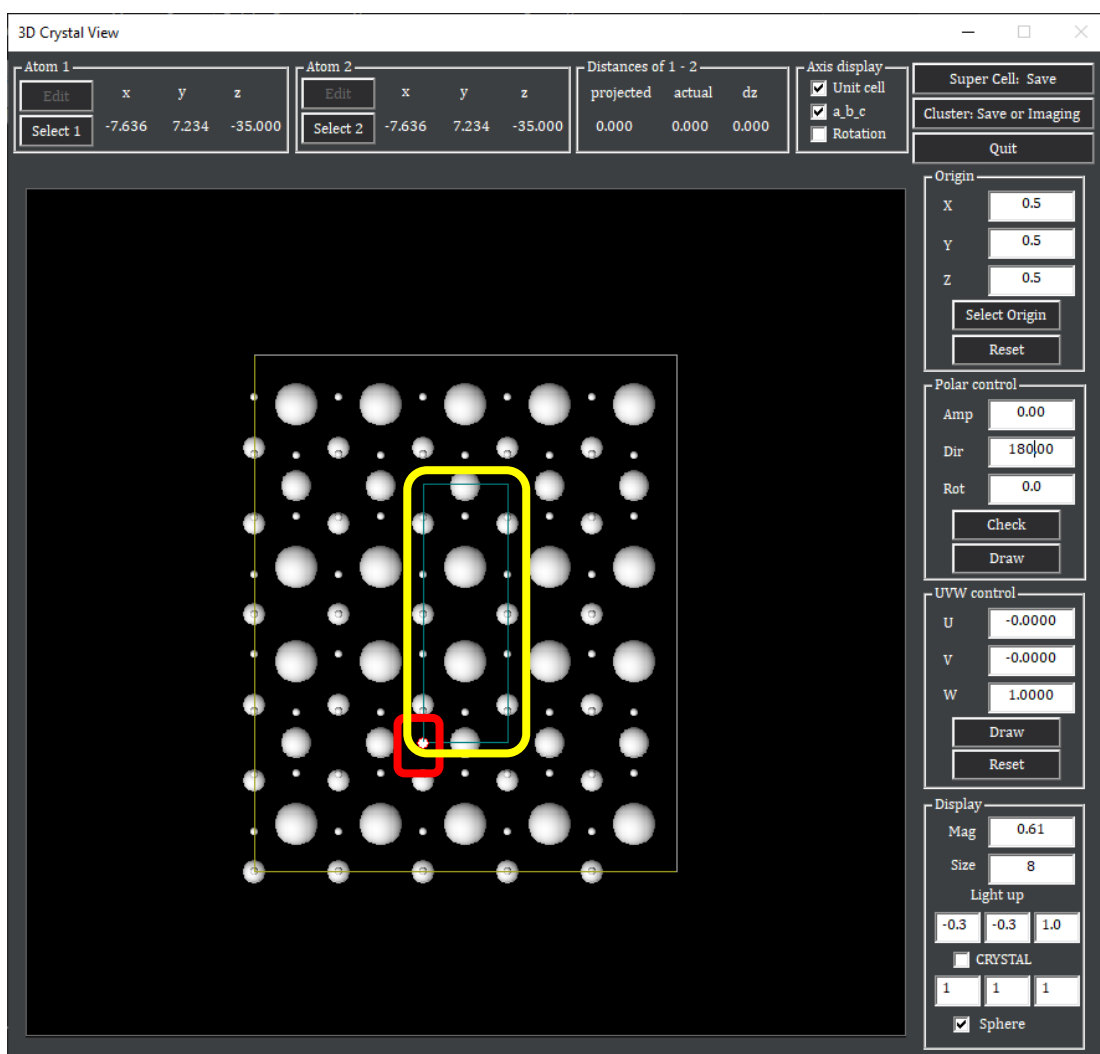
### 6.1.1. CBD calculation

In the **STEM/CBD calculation** dialog box, confirm the parameters of the **Beam radius calc.** dialog box (**kv**, **Cs**, **df**, **CL stop**, other aberrations, etc. Check the beam shape in the beam shape window.

If the **3D Display** dialog box is open, you can check the beam incident position (**x**, **y**; see next page). You can set this value in (a) the text field.

(b) Click the **CBD** button to calculate CBD. The first calculation takes several tens of seconds to calculate the phase grating, but the second phase that can use the same phase grating can be calculated in a few seconds.

(c) Click the **CBD F.Phonon** button to perform frozen-phonon CBD calculation (repeated calculation while shifting atomic position). (d) Enter the number of repetitions.



When both the **3D Display** dialog box and the **STEM/CBD calculation** dialog box are open, the beam **incidence point of CBD** (red box, above) and the **scan area of STEM calculation** (yellow box, above) are displayed. To proceed with STEM/CBD calculations, **Cluster/Supercell** data must be loaded. The calculation direction is limited to [001].

#### 6.1.2. STEM calculation

Check the parameters in the **Beam radius calc.** dialog box (**kv**, **Cs**, **df**, **CL aperture**, other aberrations, etc.). Check the beam shape in the beam shape window.

If the **3D Display** dialog box is open, you can check the scan area of the beam (if it is a crystal, make it equal to a unit cell). The **(a) beam scan area (x, y)** can be set from the input frame (in Å; see next page).

Set **(b)** the **number of divisions of the beam scan area (x, y)** (see next page). This determines the pixel resolution of the STEM image. First of all, it is recommended to use rough calculation

(about 0.2 (Å/pixel)) for the first trial time, since it takes more computation time to improve the accuracy.

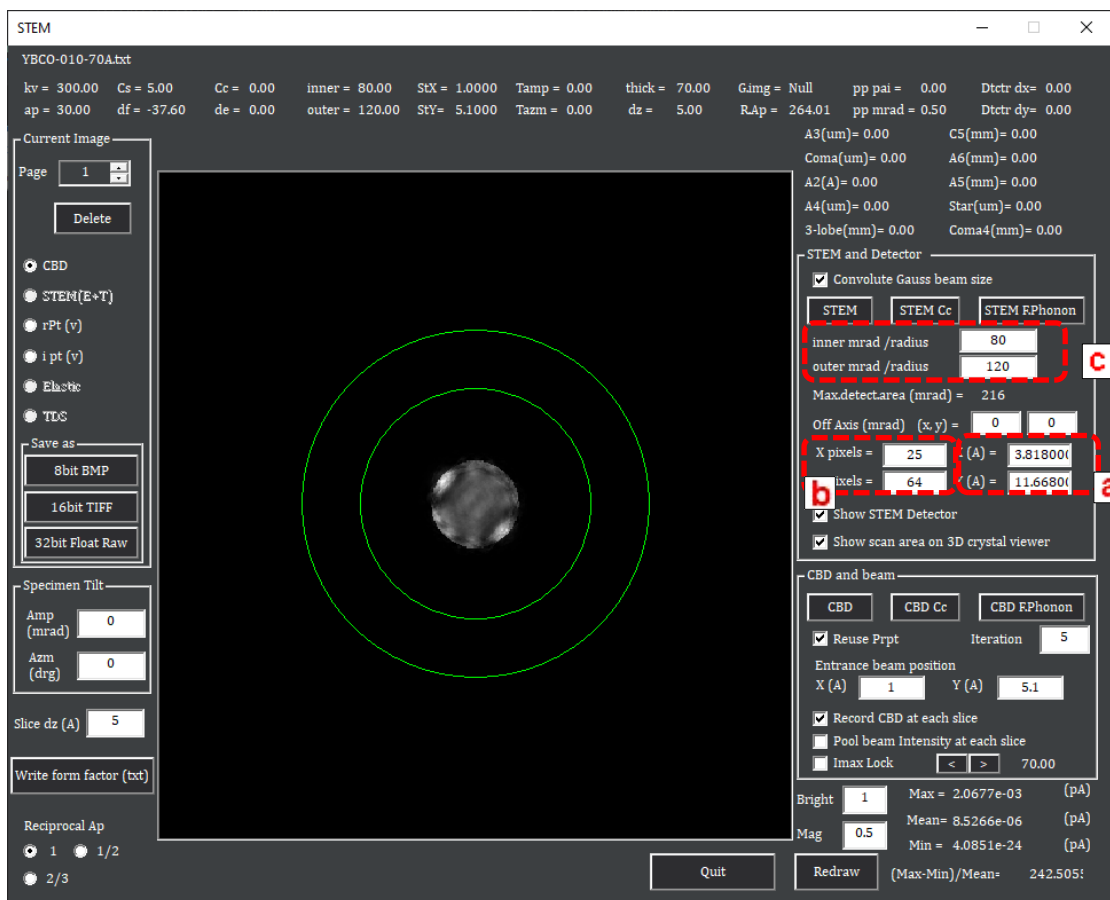
Set **(c)** "inner" and "outer" values for detector size in mrad (detection band between inner and outer). For instance:

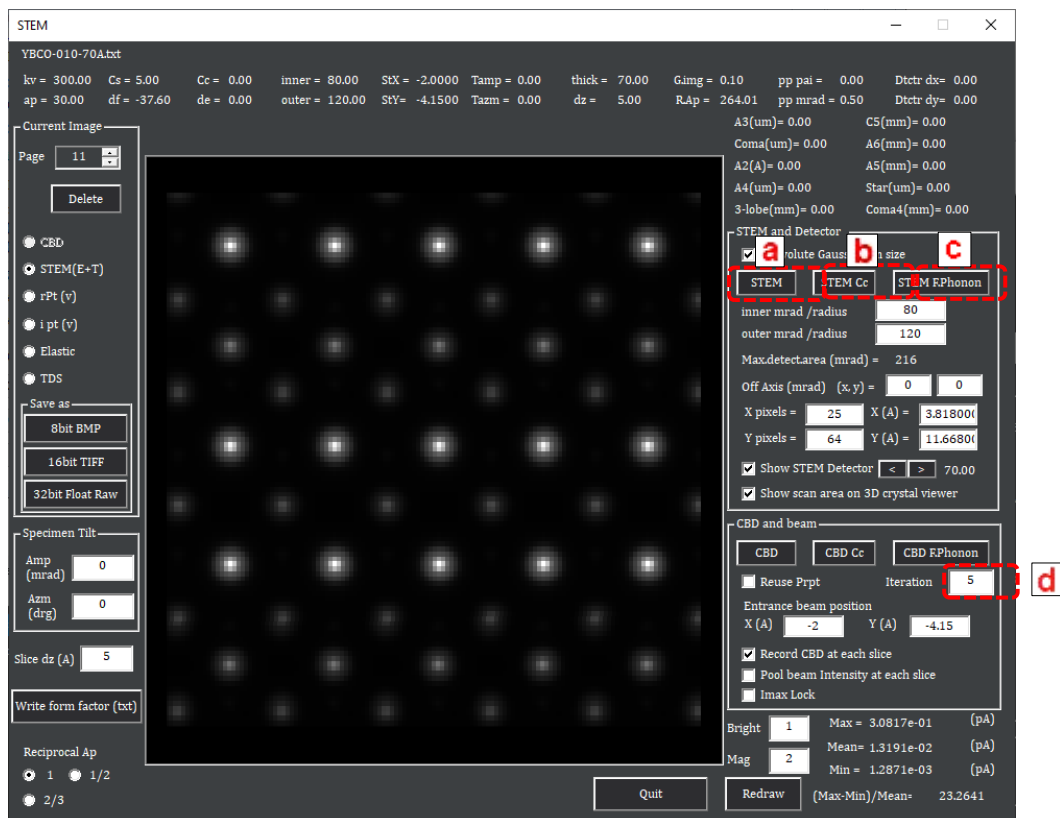
**HAADF settings:** inner > 70, outer > 100

**BF setting:** inner = 0, outer 1 to ~0.2

**ABF setting:** inner = 20 mrad, CL aperture = outer = 30 mrad

The detector position can be confirmed on the CBD calculation display.



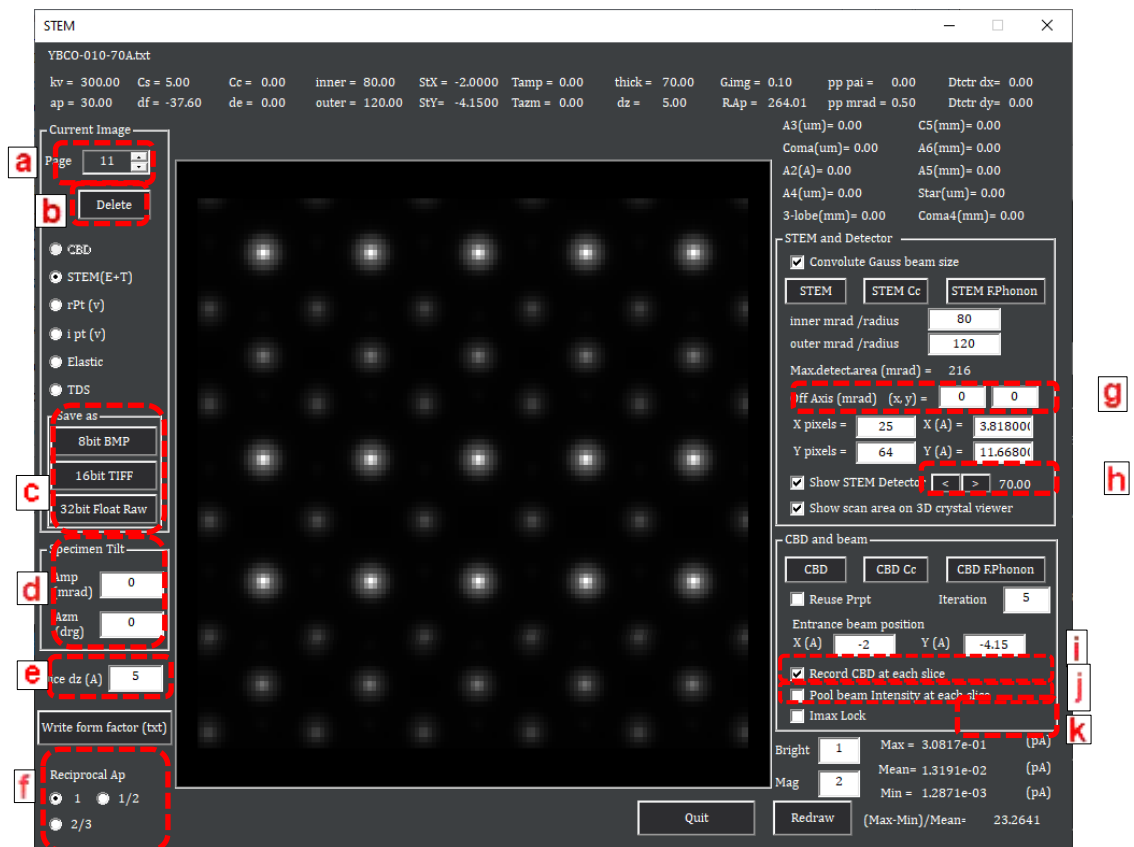


## HAADF

(a) Click the **STEM** button to calculate the STEM image and display the result. Image components of thermal diffuse scattering are calculated using the imaginary potential.

(b) Click the **STEM Cc** button to calculate the STEM image taking into account the effects of chromatic aberration, and then to display the result. This process takes about 10 times longer than calculating with the **STEM** button. Image components of thermal diffuse scattering are calculated using the imaginary potential.

(c) Click the **STEM F.Phonon** button to calculate the effect of thermal diffuse scattering using the frozen-phonon method. The (d) **number of repetitions** in frozen-phonon calculation is the same as the number of repetitions in **CBD F.Phonon**. It takes more time to calculate the number of iterations than it does to calculate imaginary potential.



## ABF

Other features of the **STEM** dialog box:

- Cumulative calculation result (up to 20 past cases) switch button
- Delete** button to clear the current display result
- Save** [current display] **as** 16-bit TIFF, BMP or 32bit Float Raw file
- Specimen Tilt**: value from [001] in the calculation for the **Cluster/Supercell**
- Slice dz (A)**: slice thickness
- Reciprocal Ap**: Magnitude of aperture for propagator in reciprocal space (select **1** for the maximum aperture available for array, or **1/2** or **2/3** of the maximum size.)
- Misalignment of the detector from the axis
- Switching of STEM image recorded for each slice
- Record CBD at each slice**
- Record changes in **Pool beam Intensity at each slice**
- Switch between CBD and beam intensity recorded for each slice. When this is possible, a **Switch** button will appear. Beam intensity is displayed in the beam shape display window associated with the **Beam radius calc.** dialog box.

## 7. Crystal data making method

This section explains how to create Crystal data, using AIA crystal creation as an example.

AIAs:

Crystal system: Cubic

Space group: F-43m

Lattice constant:  $a = b = c = 5.662 \text{ \AA}$ ;  $\alpha = \beta = \gamma = 90^\circ$

Fractional coordinate:

	x	y	z
<b>Al:</b>	0.0	0.0	0.0
<b>As:</b>	0.25	0.25	0.25

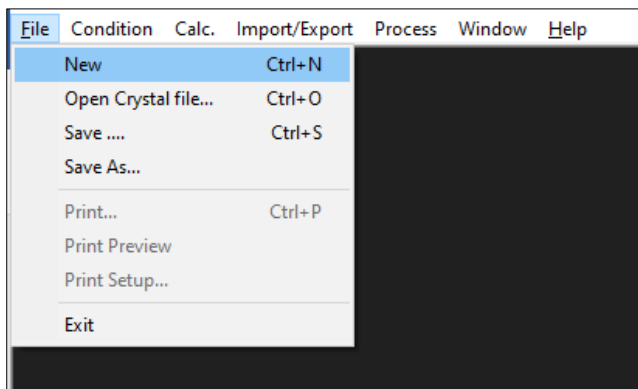
Expanded whole coordinate:

	x	y	z
<b>Al:</b>	0.0	0.0	0.0
	0.0	0.5	0.5
	0.5	0.0	0.5
	0.5	0.5	0.0
<b>As:</b>	0.25	0.25	0.25
	0.25	0.75	0.75
	0.75	0.25	0.75
	0.75	0.75	0.25

B-factor (at 20° C): Al 0.72, As 0.58

Crystal data is data used to calculate a TEM image, and is composed of information of a normal crystal unit cell (crystal system, space group, atomic position, temperature factor, site occupancy, etc.).

When calculating a STEM or TEM image of a cluster, use **Cluster/Supercell** data. This is data that has pseudo-large unit cells and describes the position information of atoms in the unit cell,



temperature factors, etc.

(**Cluster/Supercell** data consisting of repeated crystals can be created from Crystal data.)

From the **File** dropdown menu (left), select **New** to open the **Crystal file editing** dialog box (next page).



The following subsections explain when space groups should or should not be used in coordinate input. Space group notation is described by international symbols and first settings. Also, some characters do not correspond entirely to symbols, and in those instances characters that are close to those symbols in appearance are substituted.

Space group data is filed for each crystal system in the **spg** directory. These data, such as name, number, and symmetrical operations, can be checked with a text editor, but be careful not to overwrite when you save. If you find a notation that appears to be in error, please contact the seller.

### 7.1. When using space group in a coordinate input

1. **(a)** From the **System** dropdown menu, select **Cubic** as the crystal system. **(b)** The values of  $\alpha$ ,  $\beta$ , and  $\gamma$  are automatically set to 90.
2. **(c)** From the **Sp.Grp**-> dropdown menu, select **F-43M**. Specify a space group.
3. **(d)** In the **a** text field at top center, enter the lattice constant **5.662**. **(e)** Click the **Update** button. **(f)** The **b** and **c** values will be automatically set to the same value as **a**.
4. **(g)** Click once to highlight the **?** row of the coordinate display box.

5. (a) In the **Element** text field, enter **Al**. (b) Click the **Update** button. (c) The ? will change to **Al** in the coordinate display box.

The screenshot shows the 'Crystal' window with the following fields and values:

- Coordinate display box:** A table with columns X, Y, Z. The first row is highlighted in blue and contains 'Al', '0.00000', '0.00000', '0.00000'. A red dashed box labeled 'c' is around the 'Al' cell.
- Unit cell parameters:** a = 5.662, b = 5.662, c = 5.662, alp = 90, bet = 90, gam = 90.
- Other parameters:** NO. = 1, Ocp. = 1, Deby.F. = 0, System = Cubic.
- Buttons:** 'Update' is highlighted with a red dashed box and label 'b'. Other buttons include 'New', 'Add', 'Delete', 'Save As', 'Save', 'OK', 'Cancel', 'Expand'.
- Sp.Grp:** F-43M.

6. (a) Keeping the **Al** row still highlighted in the coordinate display box, (b) in the **Ocp.** text field, enter the site occupancy of Al (1 if there is no defect); and (c) in the **Deby.F.** text field, enter the Debye B-factor. (d) Click the **Update** button.

The screenshot shows the 'Crystal' window with the following fields and values:

- Coordinate display box:** The same row as before is highlighted in blue. A red dashed box labeled 'a' is around the entire row.
- Unit cell parameters:** a = 5.662, b = 5.662, c = 5.662, alp = 90, bet = 90, gam = 90.
- Other parameters:** NO. = 1, Ocp. = 1 (labeled 'b'), Deby.F. = 0.72 (labeled 'c'), System = Cubic.
- Buttons:** 'Update' is highlighted with a red dashed box and label 'd'. Other buttons include 'New', 'Add', 'Delete', 'Save As', 'Save', 'OK', 'Cancel', 'Expand'.
- Sp.Grp:** F-43M.

7. (a) In the coordinate display box, highlight the row showing the atomic **x**, **y**, and **z** coordinates for Al. (b) These coordinate values are displayed in the coordinate text fields above the display box. In these fields, enter the fractional coordinate values **0.0**, **0.0**, and **0.0** for Al. (c) Click the **Update** button.

The screenshot shows the 'Crystal' window. At the top, there are text fields for X, Y, and Z coordinates, each containing '0'. Below these is a list box showing a table of atomic coordinates. The first row is highlighted in blue and contains 'Al', '0.00000', '0.00000', and '0.00000'. To the right of the list box are text fields for lattice parameters: 'a' (1, 5.662), 'b' (1, 5.662), 'c' (1, 5.662), 'alp' (90), 'bet' (90), and 'gam' (90). Further right are text fields for 'Element', 'NO.', 'Ocp.', and 'Deby.F.'. At the bottom left is a dropdown for 'Sp.Grp' set to 'F-43M' and an 'Expand' button. At the bottom right are buttons for 'Update', 'New', 'Add', 'Delete', 'Save As', 'Save', 'OK', and 'Cancel'. Red dashed boxes and labels 'a', 'b', and 'c' indicate the areas of interest: (a) the highlighted row in the list box, (b) the 'Update' button, and (c) the 'X', 'Y', 'Z' text fields.

8. (a) With the row of Al atomic coordinates highlighted, (b) click the **Expand** button. (c) Equivalent coordinates of fractional coordinates (**0.0**, **0.0**, **0.0**) of space group F-43M will be generated.

The screenshot shows the 'Crystal' window after clicking the 'Expand' button. The list box now displays multiple rows of equivalent coordinates for Al. The first row is highlighted in blue and contains 'Al', '0.00000', '0.00000', and '0.00000'. The subsequent rows show equivalent coordinates: '0.00000 0.50000 0.50000', '0.50000 0.00000 0.50000', and '0.50000 0.50000 0.00000'. The 'Expand' button at the bottom left is now highlighted with a red dashed box and labeled 'b'. A red dashed box and label 'a' point to the highlighted row in the list box. A red dashed box and label 'c' point to the 'Update' button. The 'X', 'Y', 'Z' text fields at the top still contain '0'. The 'Sp.Grp' dropdown is still set to 'F-43M'.

9. Single click to highlight the row of hyphens (-----) at the top of the coordinate display box.

The screenshot shows the 'Crystal' window. On the left, there is a table with columns 'Al', 'x', 'y', and 'z'. The first row is highlighted with a red dashed box and contains a row of hyphens (-----). Below it are four rows of numerical values. To the right of the table are input fields for lattice parameters 'a', 'b', 'c', 'alp', 'bet', and 'gam', each with a value of 5.662 or 90. There are also input fields for 'Element' (Al), 'NO.' (4), 'Ocp.' (1), 'Deby.F.' (0.72), and 'System' (Cubic). Buttons for 'Update', 'New', 'Add', 'Delete', 'Save As', 'Save', 'OK', and 'Cancel' are visible.

10. (a) Click the **Add** button. (b) This will generate a new atom and one default coordinate (0.0, 0.0, 0.0).

The screenshot shows the 'Crystal' window after clicking the 'Add' button. The 'Add' button is highlighted with a red dashed box and labeled (a). In the coordinate display box, a new row has been added at the top, highlighted with a red dashed box and labeled (b). This row contains a question mark (?) in the 'Al' column and '0.00000' in the 'x', 'y', and 'z' columns. The rest of the interface remains the same as in the previous screenshot.

11. Single click to highlight the newly created atom ? row.

The screenshot shows the 'Crystal' window. On the left, a list of atoms is displayed. The first row is highlighted with a red dashed box and contains a question mark '?' in the 'x' column. Below it, the header 'Al x y z' is shown, followed by four rows of coordinates: (0.00000, 0.00000, 0.00000), (0.00000, 0.50000, 0.50000), (0.50000, 0.00000, 0.50000), and (0.50000, 0.50000, 0.00000). On the right, crystallographic parameters are entered: a=5.662, b=5.662, c=5.662, alp=90, bet=90, gam=90, Element=?, NO.=1, Ocp.=1, Deby.F.=0, and System=Cubic. Buttons for 'Update', 'New', 'Add', 'Delete', 'Save As', 'Save', 'OK', and 'Cancel' are visible.

12. (a) In the **Element** text field, enter **As**. (b) Click the **Update** button. (c) **As** will display instead of ? in the coordinate display box.

This screenshot shows the same 'Crystal' window after the changes. In the atom list, the first row now contains 'As' in the 'x' column, highlighted with a red dashed box and labeled with a red 'c'. The 'Element' text field on the right now contains 'As', highlighted with a red dashed box and labeled with a red 'a'. The 'Update' button is also highlighted with a red dashed box and labeled with a red 'b'. The rest of the interface remains the same as in the previous screenshot.

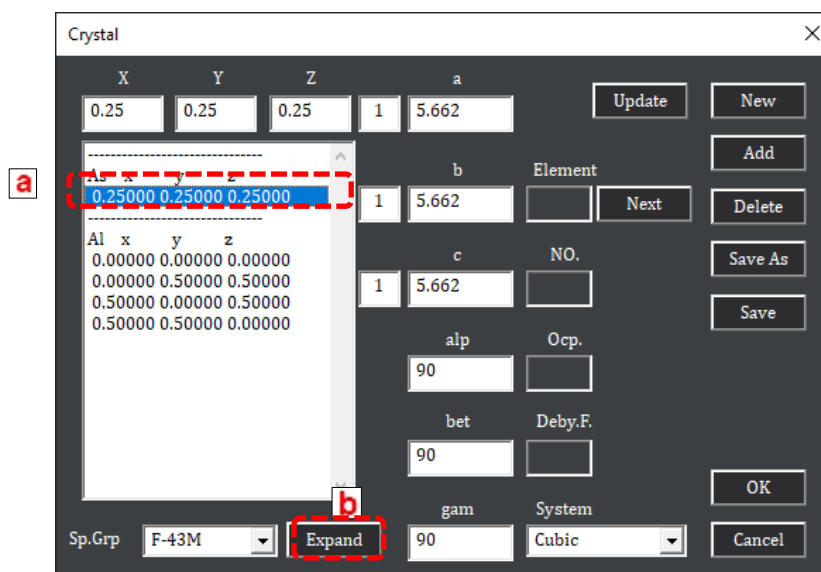
13. (a) In the coordinate display box, highlight the row showing the atomic **x**, **y**, and **z** coordinates for As. (b) These coordinate values are displayed in the coordinate text fields above the display box. (c) Click the **Update** button. (d) Coordinates of As (**0.25, 0.25, 0.25**) will be generated.

The screenshot shows the 'Crystal' window. At the top, there are text fields for X, Y, and Z coordinates, each containing '0.25'. Below these is a table with columns 'x', 'y', and 'z'. The first row is highlighted in blue and contains the values '0.25000', '0.25000', and '0.25000'. To the right of the table are text fields for 'a', 'b', and 'c', each containing '5.662'. Below these are text fields for 'alp', 'bet', and 'gam', each containing '90'. At the bottom right, there are text fields for 'Element' (containing 'As'), 'NO.' (containing '1'), 'Ocp.' (containing '1'), and 'Deby.F.' (containing '0.58'). The 'Update' button is highlighted with a red dashed box. The 'Sp.Grp' dropdown is set to 'F-43M' and the 'System' dropdown is set to 'Cubic'.

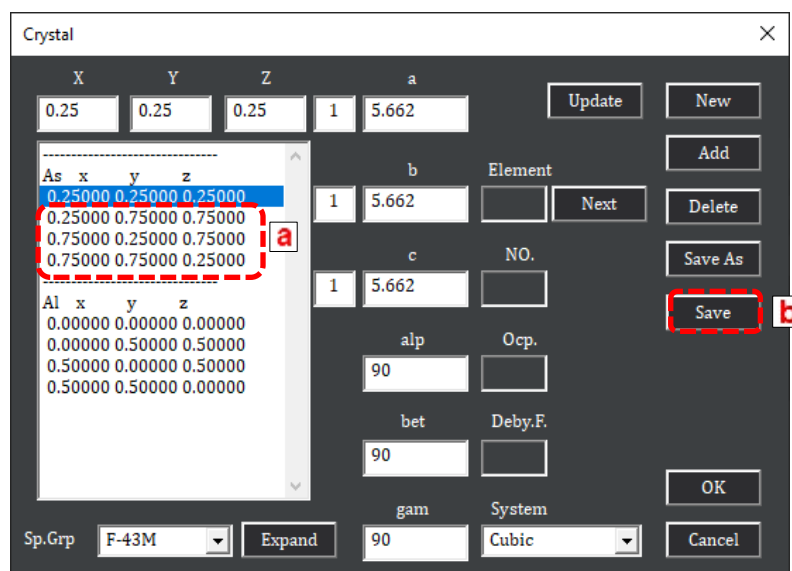
14. (a) Single click to highlight the **As** row in the coordinate display box. With this row highlighted, (b) in the **Ocp.** text field, enter the site occupancy of As (1 if no defect); and (c) in the **Deby.F.** text field, enter the Debye B-factor. (d) Click the **Update** button.

The screenshot shows the 'Crystal' window. The 'As' row in the coordinate display box is highlighted in blue. The 'Ocp.' text field now contains '1' and the 'Deby.F.' text field now contains '0.58'. The 'Update' button is highlighted with a red dashed box. The 'Sp.Grp' dropdown is set to 'F-43M' and the 'System' dropdown is set to 'Cubic'.

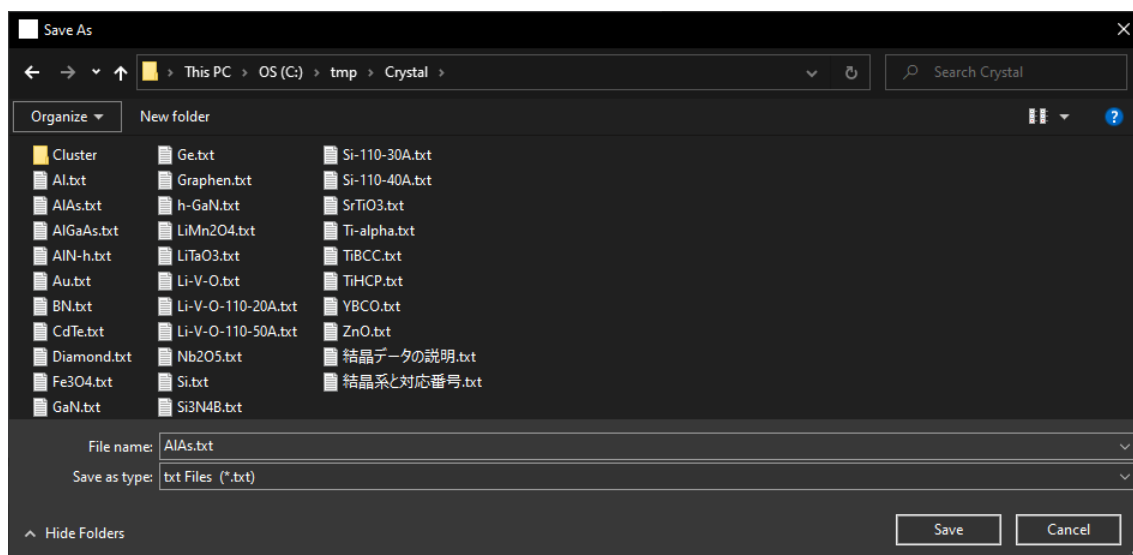
15. (a) Single click to highlight the **As** coordinate (0.25, 0.25, 0.25) row in the coordinate display box.  
 (b) With this row highlighted, click the **Expand** button.



16. (a) The equivalent coordinates of fractional coordinates (0.25, 0.25, 0.25) of space group F-43M will be generated. (b) Click the **Save** button.



17. The **File Save** dialog box will appear. Save the file with a name.





## 7.2. When not using space group in coordinate input

1. (a) From the **System** dropdown menu, select **Triclinic**. (b) In each of the  $\alpha$ ,  $\beta$ , and  $\gamma$  text fields, enter **90**. (c) Click the **Update** button.
2. (d) From the **Sp.Grp**-> dropdown menu, select **P1**.
3. (e) In each of the **a**, **b**, and **c** text fields, enter the lattice constant **5.662**. (f) Click the **Update** button again.

The screenshot shows the 'Crystal' dialog box. The 'System' dropdown is set to 'Triclinic' (labeled 'a'). The 'Sp.Grp' dropdown is set to 'p1' (labeled 'd'). The 'a', 'b', and 'c' lattice constant fields are all set to '5.662' (labeled 'e'). The 'alpha', 'beta', and 'gamma' angle fields are all set to '90' (labeled 'b'). The 'Update' button is highlighted with a red dashed box and labeled 'c' and 'f'. The 'Element' field is set to 'e'. The 'NO.' field is set to '1'. The 'Ocp.' field is set to '1'. The 'eby.F.' field is set to '0'. The 'OK' and 'Cancel' buttons are at the bottom right. The 'Expand' button is at the bottom left. The table on the left shows the following data:

	X	Y	Z
?	x	y	z
0.00000	0.00000	0.00000	0.00000

4. (a) Single-click to highlight the ? row in the coordinate display box. (b) In the **Element** text field, enter **Al**. (c) Click the **Update** button. (d) The ? will change to **Al** in the coordinate display box.

The screenshot shows the 'Crystal' window. On the left, a table displays coordinates for 'Al' at (0.00000, 0.00000, 0.00000). The 'Update' button is highlighted with a red dashed box and labeled 'c'. The 'Element' field is set to 'Al' and labeled 'b'. The 'Sp.Grp' is 'p1' and the 'System' is 'Triclinic'.

5. (a) With the **Al** row in the coordinate display box highlighted, (b) in the **Ocp.** text field, enter the site occupancy of Al (1 if there is no defect); and (c) in the **Deby.F.** text field, enter the Debye B-factor (Al: **0.72**). (d) Click the **Update** button.

The screenshot shows the 'Crystal' window. The 'Al' row in the coordinate display box is highlighted and labeled 'a'. The 'Update' button is highlighted with a red dashed box and labeled 'd'. The 'Ocp.' field is set to '1' and labeled 'b'. The 'Deby.F.' field is set to '0.72' and labeled 'c'. The 'Sp.Grp' is 'p1' and the 'System' is 'Triclinic'.

- Single click to highlight the **Al** atomic coordinates (**0.0, 0.0, 0.0**) in the coordinate display box.

The screenshot shows the 'Crystal' window with the following details:

- Coordinate Display Box:** A table with columns 'Al', 'x', 'y', 'z'. The first row contains '0.000000 0.000000 0.000000' and is highlighted with a blue background and a red dashed border.
- Unit Cell Parameters:**
  - a: 5.662
  - b: 5.662
  - c: 5.662
  - alp: 90
  - bet: 90
  - gam: 90
- Buttons:** 'Update', 'New', 'Add', 'Next', 'Delete', 'Save As', 'Save', 'OK', 'Cancel'.
- System:** Triclinic
- Sp.Grp:** p1

- Click the **Add** button three times in succession.
  - Three new Al coordinates will be generated.

The screenshot shows the 'Crystal' window after three clicks on the 'Add' button. The details are as follows:

- Coordinate Display Box:** The table now contains four rows of 'Al' coordinates, all with values '0.000000 0.000000 0.000000'. The first row is highlighted in blue, and the next three rows are highlighted with a red dashed border and labeled with a red 'b'.
- Buttons:** The 'Add' button is highlighted with a red dashed border and labeled with a red 'a'.
- Other Parameters:** The unit cell parameters, system, and group remain the same as in the previous screenshot.

8. (a) Single click to highlight one of the coordinate lines. (b) Enter the **x**, **y**, and **z** coordinates (e.g., **0.25**, **0.25**, **0.25**) in the coordinate text fields above. (c) Click the **Update** button.

The screenshot shows the 'Crystal' dialog box. At the top, there are three text fields for X, Y, and Z coordinates, each containing '0.25'. These fields are enclosed in a red dashed box labeled (b). Below them is a list box containing several lines of data. The first line, 'Al x y z 0.25000 0.25000 0.25000', is highlighted in blue and labeled (a). To the right of the list box, there are input fields for 'a', 'b', and 'c' (all containing '5.662'), and 'alp', 'bet', and 'gam' (all containing '90'). The 'System' dropdown is set to 'Triclinic'. The 'Update' button is highlighted with a red dashed box and labeled (c). Other buttons like 'New', 'Add', 'Delete', 'Save As', 'Save', 'OK', and 'Cancel' are also visible.

9. Do the same for the other three Al coordinate lines.

This screenshot shows the 'Crystal' dialog box after the fourth coordinate line has been updated. The X, Y, and Z text fields now contain '0.75', '0.75', and '0.25' respectively, and are enclosed in a red dashed box. The list box shows the fourth line, 'Al x y z 0.75000 0.75000 0.25000', highlighted in blue. The 'Update' button is still visible and highlighted with a red dashed box. The other parameters and buttons remain the same as in the previous screenshot.

10. Single click to highlight the row of hyphens (-----) at the top of the coordinate display box.

Crystal

X Y Z

1 5.662

Update New

-----

Al x y z

0.25000 0.25000 0.25000

0.25000 0.75000 0.75000

0.75000 0.25000 0.75000

0.75000 0.75000 0.25000

b Element

1 5.662 Al Next Delete

c NO.

1 5.662 4 Save As Save

alp Ocp.

90 1

bet Deby.F.

90 0.72

gam System

90 Triclinic OK Cancel

Sp.Grp p1 Expand

11. (a) Click the **Add** button. This will generate (b) a new atom and (c) one default coordinate (0.0, 0.0, 0.0).

Crystal

X Y Z

1 5.662

Update New

-----

? x y z

0.00000 0.00000 0.00000

Al x y z

0.25000 0.25000 0.25000

0.25000 0.75000 0.75000

0.75000 0.25000 0.75000

0.75000 0.75000 0.25000

b Element

1 5.662 ? Next Delete

c NO.

1 5.662 1 Save As Save

alp Ocp.

90 1

bet Deby.F.

90 0

gam System

90 Triclinic OK Cancel

Sp.Grp p1 Expand

(a) Add

(b)

(c)

12. Single click to highlight the row for the newly created atom.

Crystal

X	Y	Z
?	x	y z
0.00000	0.00000	0.00000
Al	x	y z
0.25000	0.25000	0.25000
0.25000	0.75000	0.75000
0.75000	0.25000	0.75000
0.75000	0.75000	0.25000

1 5.662

1 5.662

1 5.662

alp 90

bet 90

gam 90

Element ?

NO. 1

Ocp. 1

Deby.F. 0

System Triclinic

Sp.Grp p1

Update New Add Delete Save As Save OK Cancel

13. (a) In the **Element** text field, enter **As**. (b) Click the **Update** button. (c) **As** will replace ? in the coordinate display box.

Crystal

X	Y	Z
As	x	y z
0.00000	0.00000	0.00000
Al	x	y z
0.25000	0.25000	0.25000
0.25000	0.75000	0.75000
0.75000	0.25000	0.75000
0.75000	0.75000	0.25000

1 5.662

1 5.662

1 5.662

alp 90

bet 90

gam 90

Element As

NO. 1

Ocp. 1

Deby.F. 0

System Triclinic

Sp.Grp p1

Update New Add Delete Save As Save OK Cancel

14. (a) Repeat steps 5–9 above to enter site occupancy, Debye B-factor, and coordinate values for **As**. (b) Click the **Save** button.

Crystal

X: 0.5 Y: 0.5 Z: 0

a: 5.662

b: 5.662

c: 5.662

alp: 90

bet: 90

gam: 90

System: Triclinic

Sp. Grp: p1

Expand

Save

As x y z

0.00000 0.00000 0.00000

0.00000 0.50000 0.50000

0.50000 0.00000 0.50000

0.50000 0.50000 0.00000

Al x y z

0.25000 0.25000 0.25000

0.25000 0.75000 0.75000

0.75000 0.25000 0.75000

0.75000 0.75000 0.25000

15. The **File Save** dialog box will appear. Save the file with a name.

Save As

This PC > OS (C:) > tmp > Crystal

File name: AlAs.txt

Save as type: txt Files (\*.txt)

Save

Cancel

Cluster

Al.txt

AlAs.txt

AlGaAs.txt

AlN-h.txt

Au.txt

BN.txt

CdTe.txt

Diamond.txt

Fe3O4.txt

GaN.txt

Ge.txt

Graphen.txt

h-GaN.txt

LiMn2O4.txt

LiTaO3.txt

Li-V-O.txt

Li-V-O-110-20A.txt

Li-V-O-110-50A.txt

Nb2O5.txt

Si.txt

Si3N4B.txt

Si-110-30A.txt

Si-110-40A.txt

SrTiO3.txt

Ti-alpha.txt

TiBCC.txt

TiHCP.txt

YBCO.txt

ZnO.txt

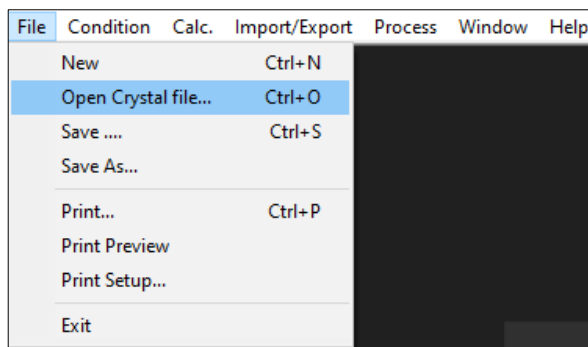
結晶データの説明.txt

結晶系と対応番号.txt

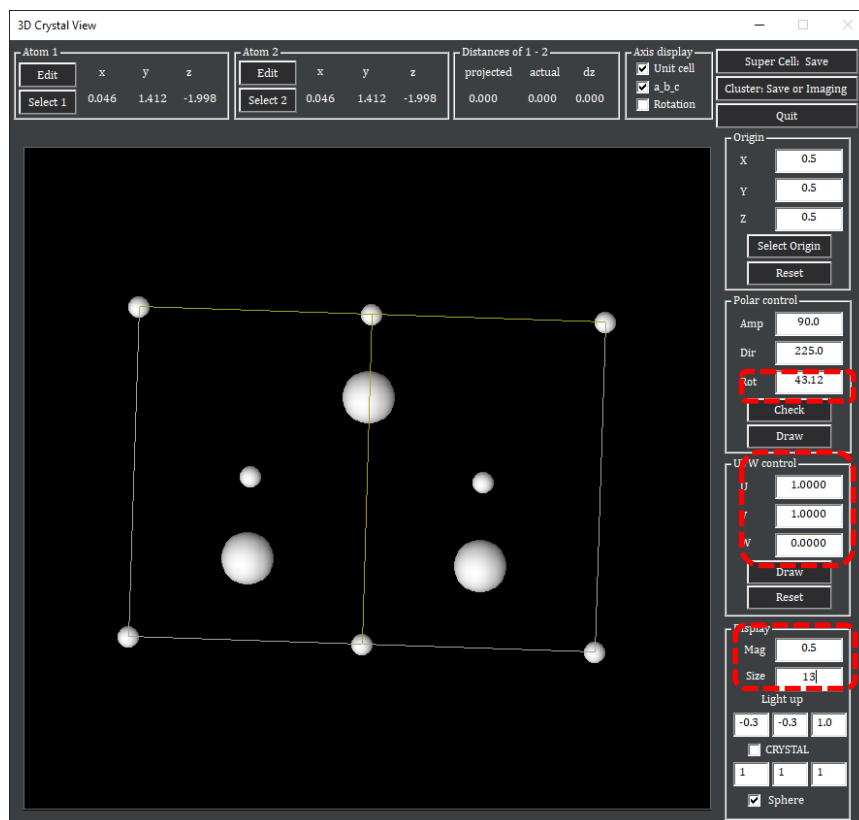
- Note 1.** If the space group is unknown, specify the crystal system as **Triclinic** and the space group as **P1**. In this case, pressing the **Expand** button will not generate equivalent coordinates.
- Note 2.** If the Debye B-factor is unknown, enter **0**. In this case, the calculation proceeds as if the imaginary potential were **0**. The calculation results of **HAADF STEM image** will be different.

## 8. Supercell (Mainly for STEM / CBD calculation) Creation

This section explains how to create a supercell. As an example, we will use a supercell in which the [110] AIA orientation of is the electron incidence orientation, assuming that **AIA** crystal data has already been created.

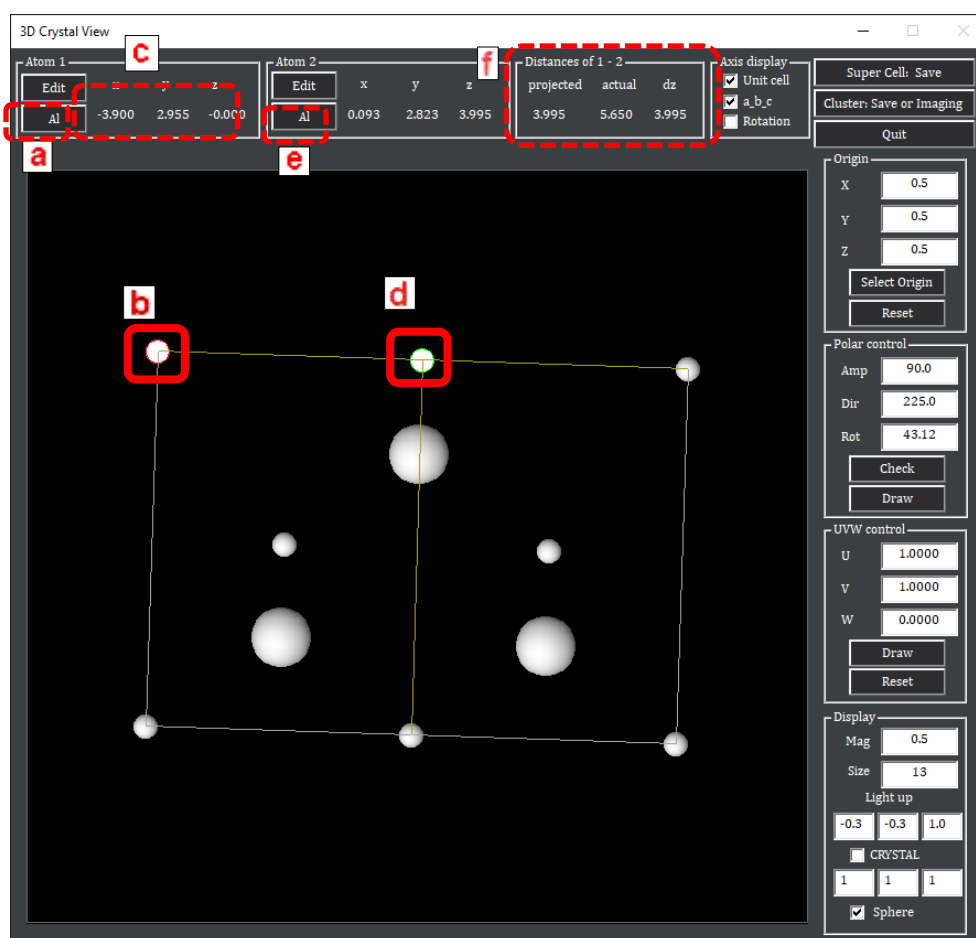


1. From the **File** dropdown menu, select **Open Crystal file...**
2. The **Calc / Crystal 3D Viewing** dialog box will open, displaying a 3D image of crystal data.
3. **(a)** If necessary, change the **Mag[nification]** and **Size** values to improve readability.
4. **(b)** In the **UVW controle** section, enter the electron incidence direction [1 1 0] for **AIA**s from **U V W**. From now on, the horizontal and vertical directions of the display screen will correspond to the **x** and **y** directions of the cell, respectively. Also, since the direction of sight to the screen corresponds to the **z** direction, the [110] orientation of **AIA**s will corresponds to the [001] orientation of the supercell to be created.
5. **(c)** Enter the **Rot** value so that equivalent points are aligned along the axis in both the **x** and **y** directions of the screen. In this case, the equivalent points at 45 or 135 run in the **x** and **y** directions, but in the figure, the value of **Rot** is slightly shifted and entered as 43.12.

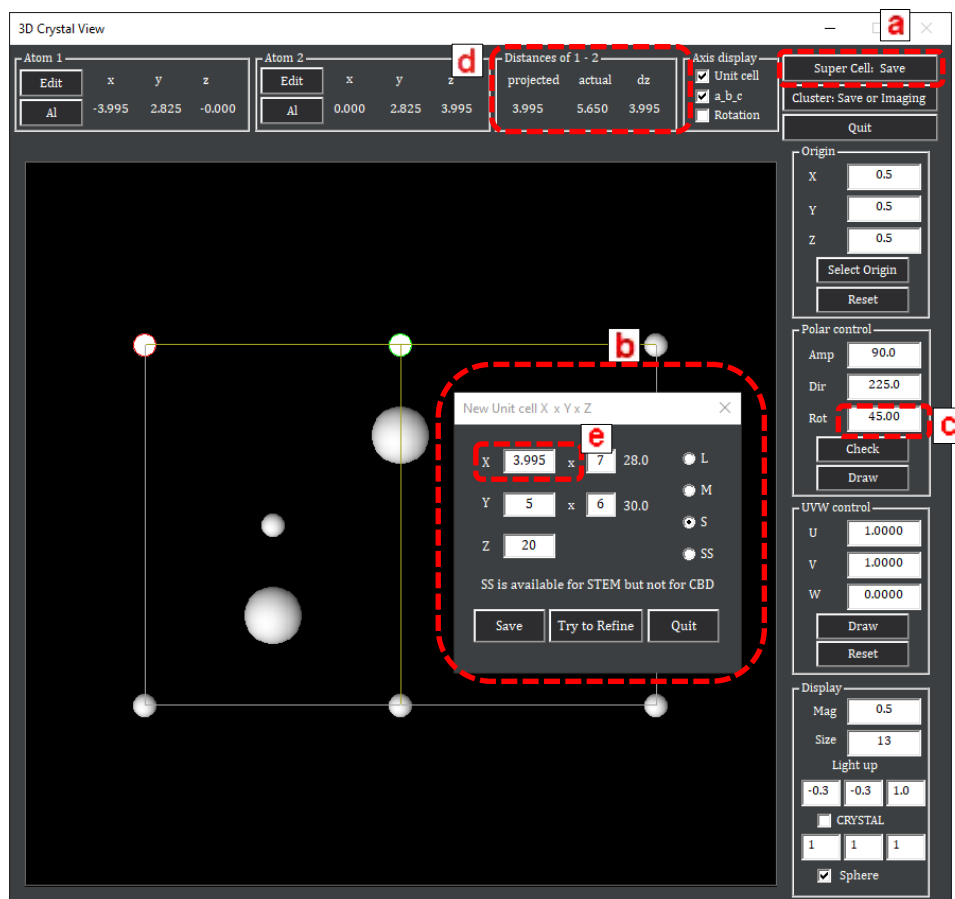




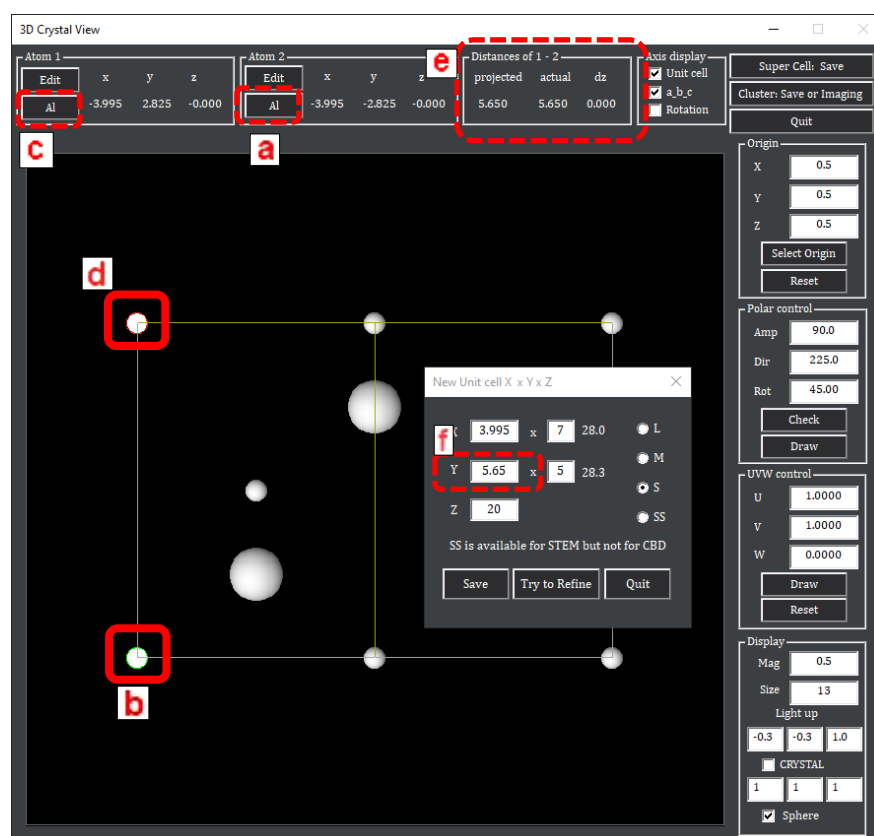
6. Single click **(a)** the second button in the **Atom1** section at top left, and then **(b)** the appropriate atomic coordinates. The atom name will be displayed on that second button, and **(c)** the atom coordinates (**x, y, z**) will be displayed to the right.
7. Similarly, specify **(d)** the atom at the equivalent point in the **x** direction (horizontal direction of the screen) to the atom specified in the **Atom1** frame as **(e)** the **Atom2** frame. When two atoms are specified as **Atom1** and **Atom2**, **(f)** the **distances of 1 – 2** section at top center will display the projection distance of each atom, the distance between them, and the difference in **z** coordinate values (difference in elevation of the viewing direction).



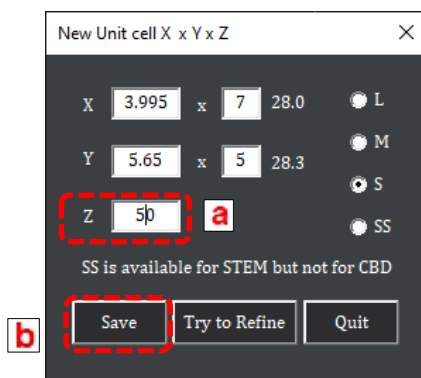
8. Confirm that the two equivalent points specified above (8.1.4, 8.1.5) are almost horizontal.  
**(a)** Click the **Super Cell Save** button.
9. **(b)** A pop-up dialog box for specifying the **Cluster** size will appear. **(c)** The **Rot** value will be refined automatically, so that the two equivalent points will be completely aligned horizontally, and **(d)** the projection distance of these points will be displayed as default and **(e)** as the **X** value in the size specification pop-up dialog box.



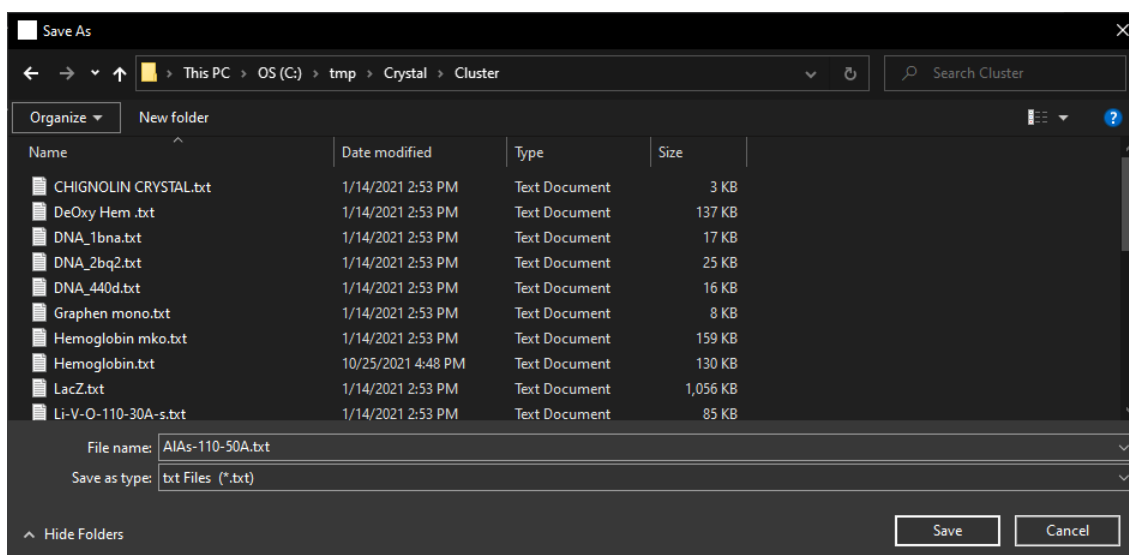
10. (a) Click the second button in the **Atom2** section, and then (b) click the atom at the equivalent point in the **y** direction with respect to (c, d) the atom specified in the **Atom1** section.
11. (e) The **distances of 1 – 2** section at top center will display the updated projected distance of each atom, the updated distance between atoms, and the updated difference in **z**-coordinate values (height difference in viewing direction). Also, (f) the projection distance will be displayed as the **Y** value in the size specification pop-up dialog box.



12. In the size specification pop-up dialog box, (a) enter the size in the **z** direction of the supercell to be created, and then (b) click the **Save** button.



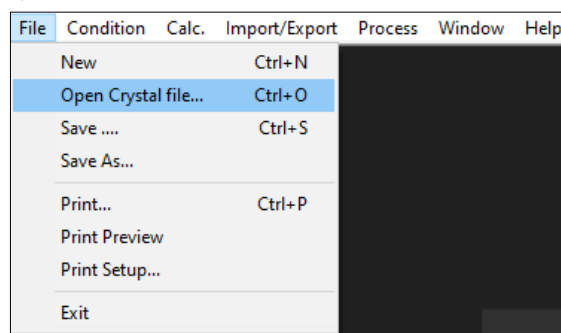
13. The **File Save** dialog box will appear. Save the file with a name.



## 9. TEM and STEM Image Calculation of Cluster

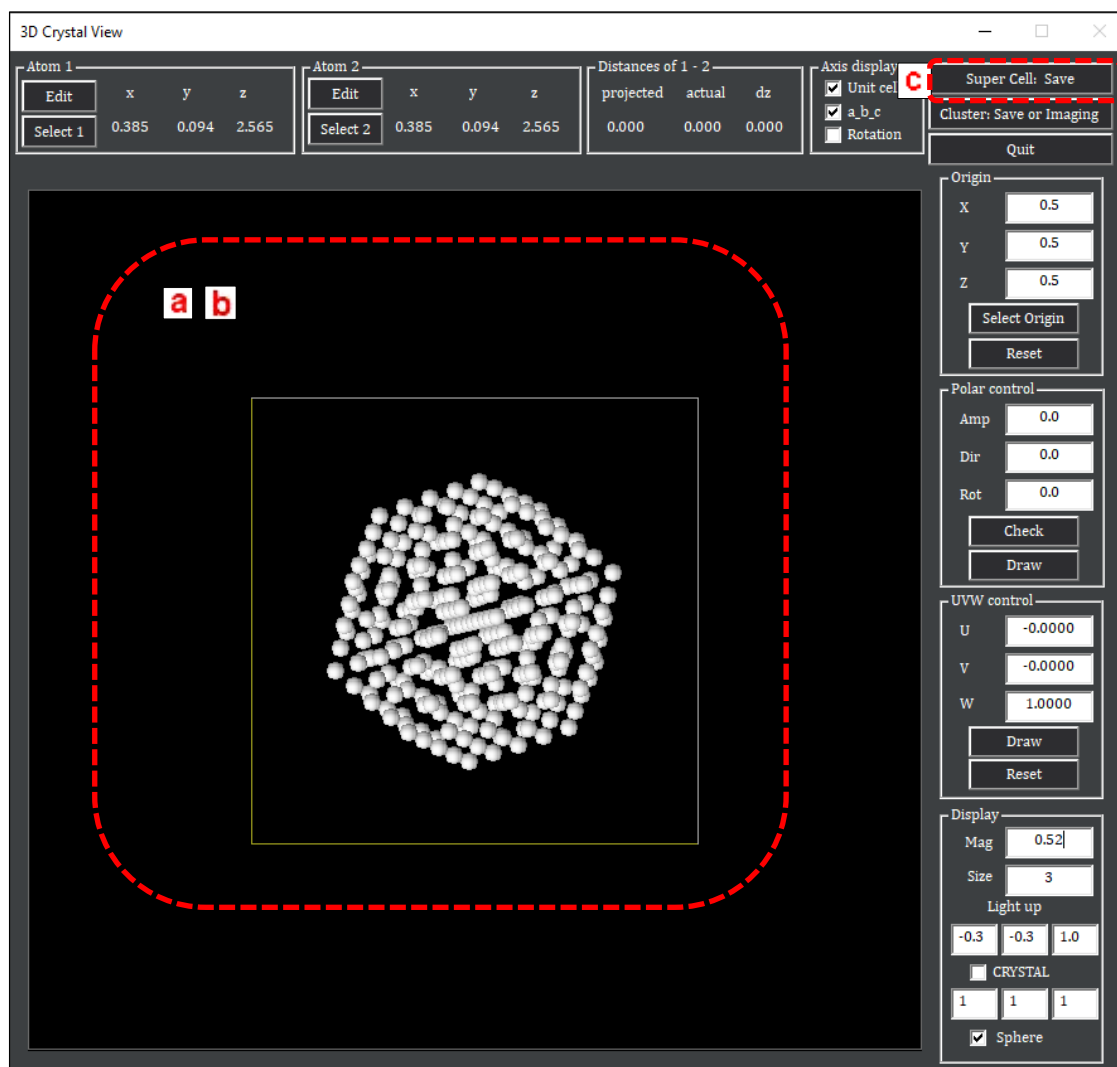
You can calculate TEM and STEM images viewed from any direction from **Cluster** data created by other dedicated software. Cluster data can also read xyz file format and car file format.

1. From the **File** dropdown menu, select **Open Crystal file...**
2. The **Calc / Crystal 3D Viewing** dialog box will open, displaying a 3D image of crystal data.

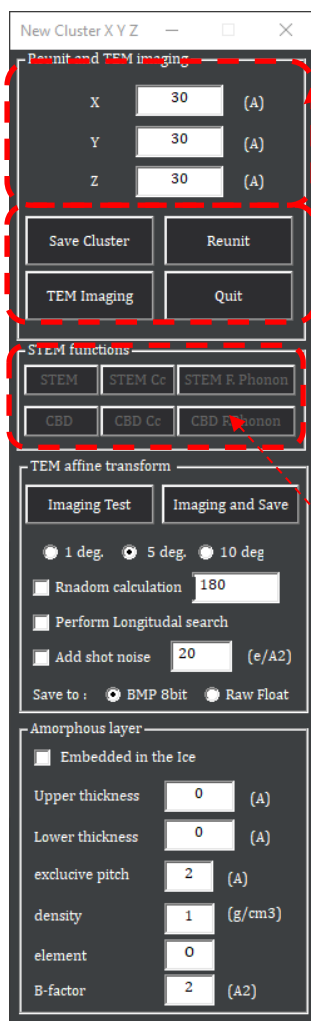


## 9.1 Calculation of TEM image from arbitrary direction

(a) Rotate the **Supercell** data to the desired orientation by dragging with your mouse, (b) set the orientation assumed for TEM observation etc., and (c) click the **Cluster: Save or Imaging** button.



The **New Cluster** dialog box will open, with buttons for supercell resave/TEM image calculation/automatic tilt, multiple TEM or STEM image calculation, etc. from the direction currently displayed.



Specify the size of the Cluster's pseudo unit cell.

The **Reunit** button internally generates coordinates that convert the currently displayed Cluster into display coordinates (**x**: horizontal, **y**: vertical; reverse-gaze direction).

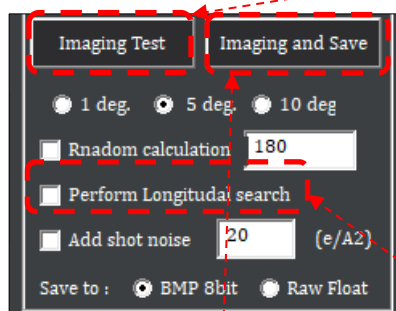
The **Save Cluster** button allows you to save the cluster generated by the **Reunit** button (the **File Save** dialog box will open).

The **TEM Imaging** button (with an intermediate dialog appearing) allows you to calculate the TEM image seen from the viewing direction of the currently displayed Cluster.

Click the **Quit** button to close the **New Cluster** dialog box.

When the **STEM Calculation** dialog box is open, the **STEM imaging** button will be active (see section 6.2 below).

## 9.2 TEM image calculation while rotating the sample automatically



When you click the **Test start** button, the software calculates series of TEM images while automatically tilting the currently displayed Cluster. At this time, you can set the Cluster's inclination interval (**dt**: **1°**, **5°**, **10°**).

When you uncheck **Perform Longitudinal search**, only horizontal inclination (direction is always 0.0) is performed. When the checkbox is checked, the slope value is inclined from 0° to 360° from the horizontal direction (direction = **0.0**), and then the inclination direction is changed counterclockwise by **dt** etc.

When you click the **Imaging and save** button, the inclined TEM image is automatically calculated in the same way as **Test start**, and the series of TEM images are saved. During saving, each TEM image is automatically given a filename as shown in the example on the next page.

Calculated images saved as an automatic tilt series are saved in the following software-generated filename format:

\*\*\*\_Amp\_30.00\_Dir\_0.00\_Rot\_0.00.BMP

In this schema:

- \*\*\* is an arbitrary name entered by the user in the **File Save** dialog box.
- **Amp\_30.00\_Dir\_0.00\_Rot\_0.00** is from an initial cluster direction display state of 0; that is, horizontal direction (**Dir** is set to **0**) and tilt amplitude 30° (**Amp** set to **30.0**).

In other words, the filename indicates the conditions under which the image was calculated.

### 9.3. TEM image calculation with sample embedded in amorphous state

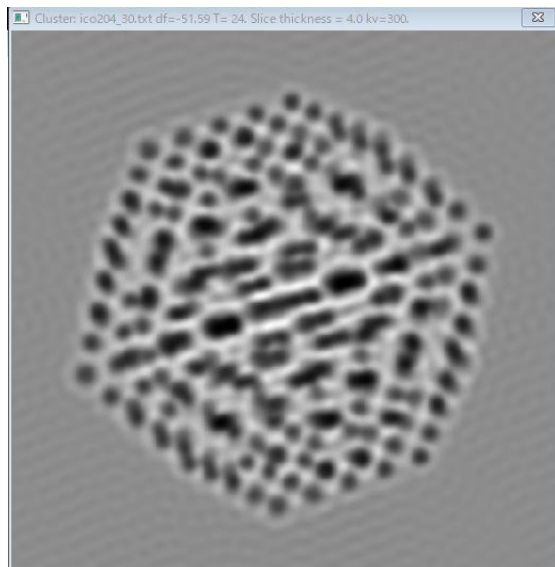
Upper Ice Enter the thickness of the sample amorphous layer

Lower Ice Enter the thickness of the sample amorphous layer below the sample

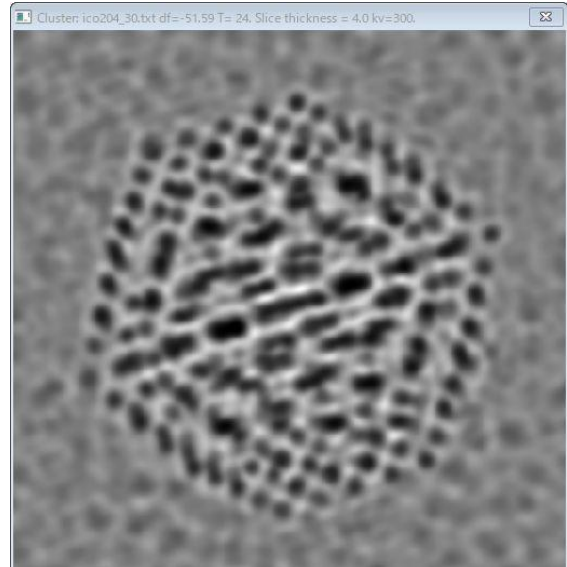
Filed with ice Check that the sample is amorphous density and element. Input the amorphous density and element.

TEM images can be calculated with the sample embedded in an amorphous state. TEM image simulation such as single particle analysis is possible. Multi-slice calculations are also performed for the propagation of electron waves in amorphous materials. By generating coordinate positions with random numbers based on density and elements, an amorphous structure is generated approximately.

## 9.4. Au cluster TEM example



**Au cluster**



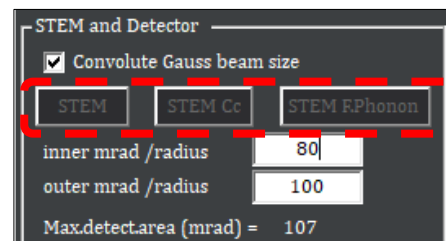
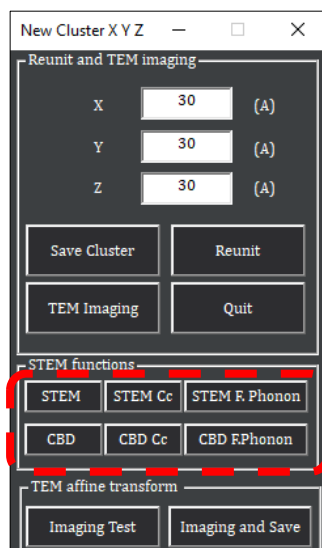
**Au cluster + Amorphous (element C, density) 2.0, upper Floor 20 Å , lower Floor 20 Å、 Embedded state)**

## 9.5. From any direction STEM calculation

STEM Calculation dialogue box (see : 6.1 STEM, CBD Calculation) is open

STEM imaging Button is enabled. STEM For the calculation dialogue box, STEM Calculation

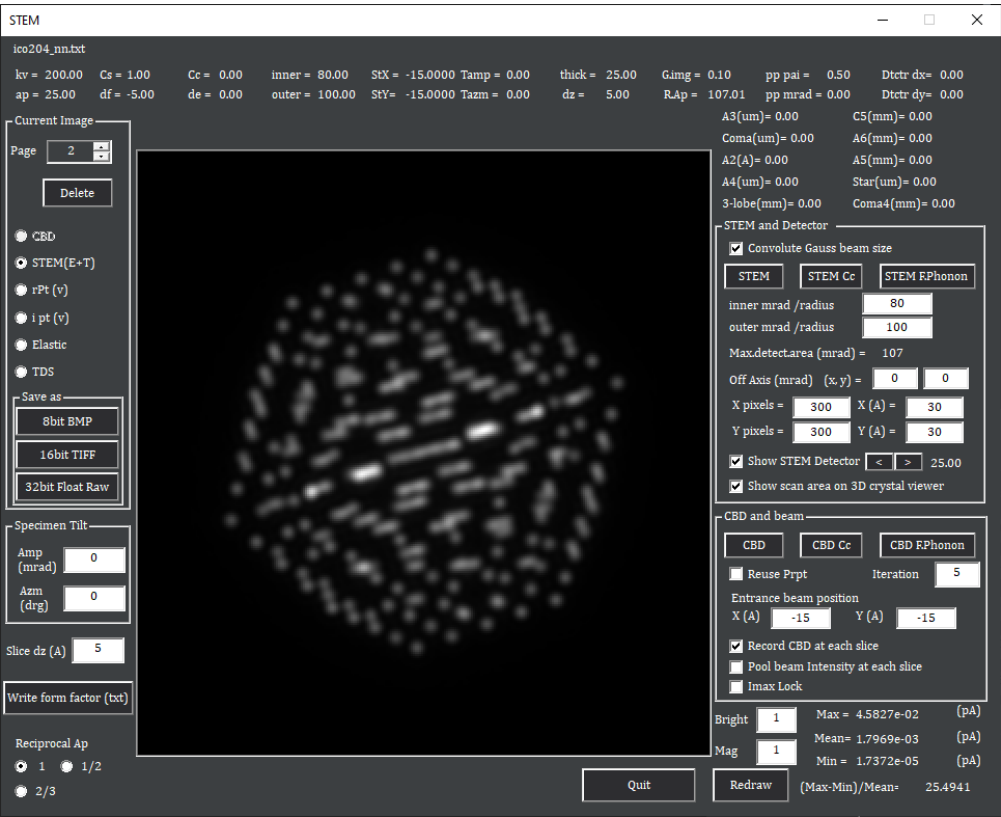
3 One button is disabled.



From the previous info STEM imaging by button, STEM is set in the calculation dialogue box  
STEM According to the calculation conditions, 3D from the viewing direction displayed by the



model STEM image is calculated (STEM In the calculation dialogue box STEM equivalent button.



Au cluster STEM (HAADF) Image simulation example.