FAQ
Frequently Asked Questions

This chapter will answer to
Frequently Asked Questions
with Q&A style

Dynamical Scattering Calculation（MultiGUI）

Q001: How to use Atom Parameter Editor?

Q002: How to use "Occupancy"?

Q003: I saw the example, where an angle of lattice parameter is zero (o)…

Q004: How many phase gratings can we use?

Q005: How many slices can we divide a unit cell (or a super-cell) into?

Q006: How is a phase grating (transmission function) evaluated?

Q007: How to specify the range of scattered waves to be included in the multislice calculation?

Q008: What is a slice thickness for [011] or [111] incidence?

Q009: How to specify an incident beam direction?

Q010: Why is the incident beam direction with c=0 not allowed?

Q011: How to treat an incident beam direction with c=0?

Q012: How is an atom scattering factor for electrons calculated?

Q013: Can we use scatter factor for ions?

Q014: How to specify a thermal factor (thermal vibration effect)?

Q015: How does thermal factor affect an atomic scattering factor?

Q016: How do we use "Unitary test"?

Q017: What kind of propagation function is used in calculation?

Q018: What is three-dimensional effect?

Q019: How to include three-dimensional effect in multislice calculation?

Q020: How to specify model symmetry (symmetry operations)?

Q021: I can't read atom parameters from a text file.

Q022: How to create an atom parameter file (text data)?

Q023: What is a format of atom parameter file (test data)?

Q024: How does an atomic potential contribute to a projected potential?

Image Calculation （ImageGUI）

Q101: My image does not show any contrast.

Q102: Let me know the differences between Simulation Modes.

Q103: When I select "First Order (Envelope)" from Simulation Mode, I can get a correct image, but not with "Second order (TCC)".

Dynamical Scattering Amplitude Output （DFOutGUI）

Q201: Why is a reflection specified using only two indexes? How can we relate these indexes to a normal three-index system?

Q202: How is the phase displayed?

CBED Extension

Q301: High angle area is not displayed.

Q302: Does HOLZ lines appear under the projection approximation?

Q303: Can we calculate a Large-angle CBED (LACBED, Tanaka pattern)?

Q304: How can we improve HOLZ line accuracy?

STEM Extension

Q401: An output from STEM image does not seem to represent a model structure

Q402: How to select a super-cell size?

Q403: Computation becomes extremely slow, when a model size becomes large.

Q404: What is a range to be included for scattering calculation? Does this range depend on the model size?

Q405: What is a strategy to shorten computation time?

Dynamical Scattering Calculation （MultiGUI）

Q001

How to use Atom Parameter Editor?

A

1. Click "Edit" button from Atom Parameters pane. Then, the following "Atom Parameter Editor" window will appear. In this example, the parameters for two atoms are already registered.
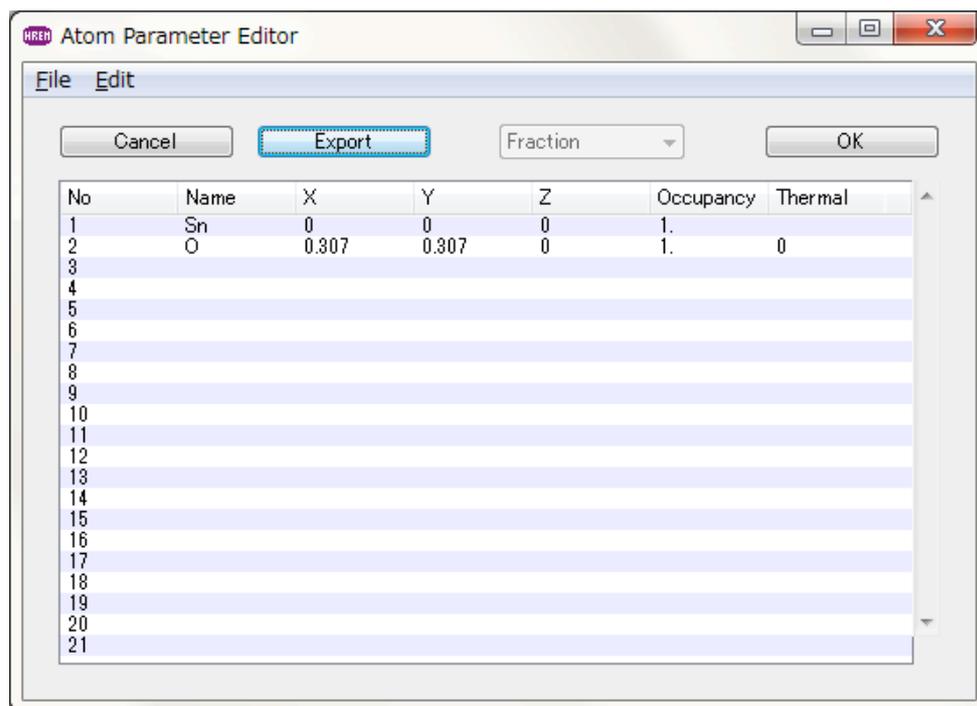
2. Input the following parameters for each atom in separate row.
   - "Name": Atom identifier including an element name. You can add figure(s) before or after the element name to identify each atom.
   - "x", "y" and "z": Atom positions in terms of a unit cell length.
   - "Occupancy": Average probability of occupying the site (normally one).
   - "Thermal": Thermal parameter, namely Debye-Waller factor. If this parameter is zero (0), "Overall Thermal Factor" will be used.

3. When you finish entering the parameters for all the atoms, click "OK" to save the data and close the window. You can click "Cancel" to abort an input at any time.

NOTE   You can save atom parameters as a text file by clicking "Export." Then, you can edit its content easily using your favorite text editor. You can import atom parameters in a text file using "Import" in the "Atom Parameters" pane of MultiGUI. Please check also Q023.

Q002

How to use "Occupancy"?

A "Occupancy" is a probability, with which the element occupy the site as an average over many unit cells. Since each element cannot occupy the site in fraction, occupancy is normally one (1). However, in a disordered structure, for example, a specific site will be occupied more than one element, and an occupancy of each element becomes less than one,

For a special atom position, the symmetry operation generates an atom at the original atom position. "Multiplicity" (the total number of symmetry-generated atoms at the same position) is automatically taken into account by xHREM, so you may not necessary to set "Occupancy" to 1/"Multiplicity" as sometime required by other software.

Q003

I saw the example, where an angle of lattice parameter is zero (o)…

A You can specify an angle in terms of cosine. Thus, zero means 90 degree. However, you should not mix a degree and cosine, so a mixed set of three angles, say 0, 0, 120 are not acceptable.

TIPS Cosine of the angle is used inside the program.

Q004

How many phase gratings can we use?

A You can use up to 1000 different phase gratings. The sequence of the phase grating to be used in calculation will be easily is specified by using "PG Sequence Editor".

Q005

How many slices can we divide a unit cell (or a super-cell) into?

A Since the maximum different phase grating is 1000, you can divide the unit cell (your model structure) into 1000 slices.

Q006

How is a phase grating (transmission function) evaluated?

A A phase grating is directly evaluated by assigning a projected potential of the slice to a complex exponential function. Here, the direction of potential projection is not perpendicular to the slice, but along the incident beam direction.

Q007

How to specify the range of scattered waves to be included in the multislice calculation?

A The range of scattered waves included in the multislice iteration is specified by "Range" parameter of "Dynamical Calculation" pane of the Preferences window.

Q008

What is a slice thickness for [011] or [111] incidence?

A Normally, the slice thickness is measured perpendicular to the slice (this is a physical thickness of the slice). However, the length of a slice measured along the incident beam direction is more important from electron scattering point of view.

For example, the scattering conditions are different even for the same incident beam direction of [011], when the incident surfaces is (001) or (011). xHREM can handle such differences.

xHREM uses the slice that is always parallel to the entrance surface, but projects the potential along the incident beam direction.

If you are interested in knowing more details, please consult the paper:
K. Ishizuka, *Acta Cryst.* A38 (1982) 773-779.

Q009

How to specify an incident beam direction?

A An incident beam direction t is specified by three unit cell vectors in the real space as follows: $t = d_1 a + d_2 b + d_3 c$

For example, the incident beam direction parallel to c-axis is defined as [0, 0, 1]. If the incident beam direction is not specified by a simple sum of three unit cell vectors, it is not a good condition to take an EM image.

NOTE In an experiment of electron diffraction, the incident beam direction may be specified by the Laue point, which corresponds to the Ewald sphere center projected on the observation diffraction plane.

TIPS Given the incident beam directions specified in real and reciprocal unit cell

$$t = d_1 a + d_2 b + d_3 c$$
$$= r_1 a^* + r_2 b^* + r_3 c^*$$

each coefficient can be easily evaluated as follows:

$$d_1 = t a^* = r_1 a^{*2} + r_2 b^* a^* + r_3 c^* a^*$$
$$r_1 = t a = d_1 a^2 + d_2 b a + d_3 c a$$

Q010

Why is the incident beam direction with c=0 not allowed?

A xHREM assumes that an incident surface is the (001) plane (the c-plane of an input unit cell). Thus, the incident beam direction with c=0 means that the electron beam is parallel to an entrance surface, which is not occurred in practice.

TIPS You can specify an incident surface of the specimen, on which an electron beam impinges. Therefore, using xHREM it may become possible to treat a surface effect that is usually neglected by other programs.

Q011

How to treat an incident beam direction with c=0?

A An incident beam direction with c=0 in terms of an input unit cell is not accepted (see Q010). To handle this problem, you can transform the coordinate system from "Preferences" dialog under Edit menu, and make the entrance surface include the c-axis.

MultiGUI takes care of all the necessary transformations, such as atomic coordinates, symmetry operations, an incident beam direction and so on, and creates a correct data set for calculation.

Q012

How is an atom scattering factor for electrons calculated?

A Atom scattering factor (ASF) can be chosen from the following two types in the "Atom Scattering Factor" pane of "Preferences".

Doyle-Turner: ASF for electrons is calculated from x-ray ASF using the following Mott's formula:

$$f_e(s) = 0.023934\{Z - f_x(s)\}/s^2; \quad s = \sin\theta/\lambda$$

Here, x-ray ASF is approximated by a sum of Gaussians, whose coefficients are tabulated in *International Tables for x-ray Crystallography*, Vol. IV. It should be noted that Doyle-Turner ASF is valid only up to s=2.0.

Weikenmeier-Kohl: This form factor is valid also for high-angle scattering beyond s=2.0. Thus, this form factor can be used to estimate absorption potential due to thermal diffuse scattering (TDS).

Q013

Can we use scatter factor for ions?

A In principle, the answer is YES. However, the current GUI does not support such cases, and you have to modify manually the data (.DA1) created by MultuGUI. Please contact our user support for detailed steps.

Q014

How to specify a thermal factor (thermal vibration effect)?

A Effect of thermal vibration is taken into account by using a Debye-Waller thermal factor.

- When you want to use a different thermal factor to each atom, you can specify each thermal factor at "Thermal" column of atom parameters.

- When "Thermal" parameter of individual atom is zero, the thermal factor specified at "Overall Thermal Factor" will be applied to that atom,

TIPS For simplicity, you may want to use the same thermal factor for all the atoms in the model. In this case, specify the thermal factor in "Overall Thermal Factor" and leave blank (or set to zero) at "Thermal" column of each atom.

Q015

How does thermal factor affect an atomic scattering factor?

A An atomic scattering factor (ASF) is attenuated by a Debye-Waller thermal factor B as a function of a scattering angle θ:

$$\exp\left\{-B\left(\frac{\sin\theta}{\lambda}\right)^2\right\}$$

You may note that high-angle scattering is more affected by thermal vibration than low-angle scattering.

Q016

How do we use "Unitary test"?

A Without absorption there is no decrease of electrons. Thus, the total sum of electron density distribution or electron diffraction distribution is always constant. However, if an enough scattering area is not included in scattering calculation, some electrons tends to scatter outside of the scattering area, and the total sum of diffracted electrons will decrease with a sample thickness. Therefore, Australian group introduced the Unitary Test to check calculation conditions for their reciprocal-space multislice formula.

However, xHREM uses the multislice formula (in mixed-space) based on Fast Fourier Transform (FFT), and thus the total sums of both electron density distribution and electron diffraction distribution are identical, and always equal to unity. Therefore, a usual way of Unitary Test has no meaning.

The Unitary Test of xHREM calculates the total sum of electron diffraction distribution excluding intensities at the outermost pixels. Therefore, if an enough scattering area is not included in scattering calculation, the total sum of scattering distribution will decrease with a sample thickness. However, since this attenuation is mild, the Limit of Unitary Test should be very close to one to make the test effective.

NOTE When you include absorption due to thermal diffuse scattering (TDS) using Weikenmeier-Kohl atomic scattering factors, a number of electrons will actually decrease due to absorption. Thus, if you don't set the Unitary Test limit sufficiently low, a computation will stop in the middle of multislice iteration (scattering calculation) owing to the Unitary Test.

Q017

What kind of propagation function is used in calculation?

A xHREM uses the propagation function that corresponds to a spherical wave, not a propagation function with parabola approximation. If you are interested in knowing more details, please consult the paper: K. Ishizuka, *Acta Cryst.* A38 (1982) 773-779.

Q018
What is three-dimensional effect?

A Three-dimensional effect is such that relative atom positions along the incident direction of an electron beam affect scattering intensity distribution,

Q019
How to include three-dimensional effect in multislice calculation?

A Three-dimensional effect may be included in multislice calculation, when relative atom positions along the incident direction of an electron beam are taken into account by dividing a unit cell (model structure) into a multiple slices.

NOTE How accurate the multislice formulation can take into account a three-dimensional effect is still an open question.

Q020
How to specify model symmetry (symmetry operations)?

A The way to specify symmetry operations follows the rule used in *International Tables for Crystallography.*

- yxz components of symmetry operation will be separated by a comma (,).
- each symmetry operation will be separated by a semicolon (;).
- end of all the symmetry operation is a period (.).

Example:
x, y, z; y, x, z+1/2.

Q021
I can't read atom parameters from a text file.

A Please make sure that you are specifying parameter entries in a correct order.

Q022
How to create an atom parameter file (text data)?

A Input a name, coordinates (x, y, z), occupancy and thermal factor for each atom in a single line using an editor or a word processor.   A serial number can be added at the beginning of each line. Each parameter will be separated by a comma (,) or any number of spaces (blanks). Thus, you don't need to align the column position of each parameter.

Example

Name	X	Y	X	Occupancy	Thermal
Sn1	0	0	0	1.0	0
O1	0.307	0.307	0	1.0	0

NOTE Name should include an element name. You can add a number to the element name to distinguish different atoms of the same element.

Save a created data to a text file (sample-name.atm).

Q023

What is a format of atom parameter file (test data)?

A Atom parameter file is a text file, each line of which contains a name, coordinates (x, y, z), occupancy and thermal factor. A number can be added at the beginning of each line. Each parameter will be separated by a comma (,) or any number of spaces (blanks). Thus, you don't need to align the column position of each parameter.

The order of parameters in the text file may be arbitrary, since the order of parameters can be specified as shown below, when you read them.
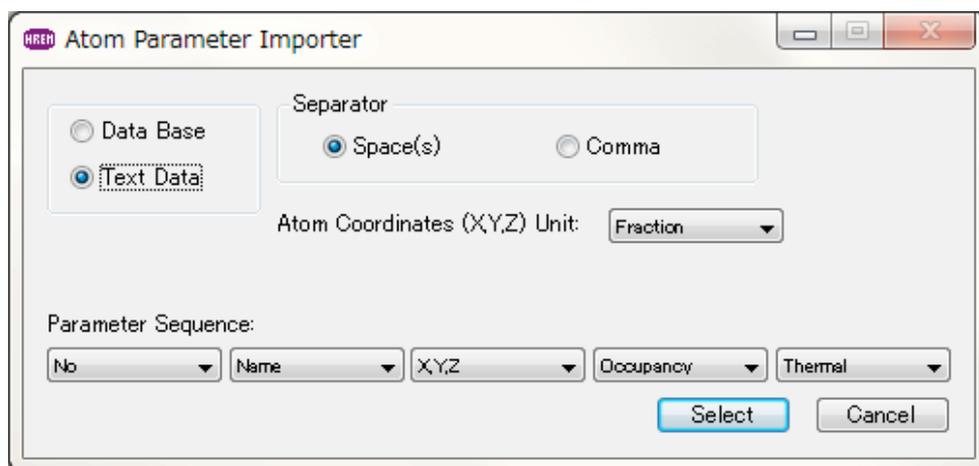
Unit of the atom coordinates can be selected using Atom Coordinates Unit pull-down. This function is especially useful, when you create a atomic model using a third-party model building application.

Q024

How does an atomic potential contribute to a projected potential?

A When a whole unit cell is treated as a single slice (projection approximation), a whole atomic potential will be projected.

When a unit cell is divided into a multiple slices, in principle, only the part of potential belongs to a slice should be projected. However, xHREM will project the whole atomic potential to the slice, which the center of atom (atom coordinate) belongs to. In this way, we can use the projection theorem of Fourier transform to efficiently project an atom potential.

Image Calculation （ImageGUI）

Q101

My image does not show any contrast.

A Please check an aperture radius for image calculation. The smallest fringe spacing that will contribute to image formation depends on the unit (s or d*), which you can select from "Preferences" window. (Note: 2s = d*)

The smallest fringe spacing = 1/2s = 1/d*

Especially, when you have forbidden reflections, please check whether allowed reflections are included within the aperture.

Q102

Let me know the differences between Simulation Modes.

A Simulation Mode determines the way to treat partial coherence.

Using xHREM you can choose a commonly used technique using Envelope functions, or a more elaborate technique using Transmission Cross-coefficient (TCC).

The technique using TCC, except a small model, requires more computation time than the technique using Envelope functions.

Q103

When I select "First Order (Envelope)" from Simulation Mode, I can get a correct image, but not with "Second order (TCC)".

A In the case of "Second order (TCC)" the spatial frequencies of twice of the objective aperture radius will be included in image calculation. This is because interference terms between scattered waves that pass the objective aperture should be included in image calculation.

Thus, "Second order (TCC)" calculation requires the Fourier space that is twice of the aperture size, although "First Order (Envelope)" calculation requires the Fourier space that corresponds to the aperture size. Here, image calculation uses the same area (the same size of Fourier space) used by scattering calculation.

When the Fourier space used for image calculation is not enough, "Range" parameter of "Dynamical calculation" pane should be increased from the "Preferences" window of MultiGUI, and scattering calculation should be done again. The Fourier space used for image calculation cannot be modified by changing "Range" from the "Preferences" window of ImageGUI.

Note Except you don't specify an exceptionally small "Range" for scattering calculation, this situation will not occur.

Dynamical Scattering Amplitude Output（DFOutGUI）

Q201 Why is a reflection specified using only two indexes? How can we relate these indexes to a normal three-index system?

A Multislice calculation determines scattering amplitudes using two-dimensional slices (Phase Gratings). Thus, a wave function calculated is two-dimensional, and its Fourier transform is also two-dimensional. The two indexes specifies a reflection in 2D reciprocal space.

This 2D index can be converted to a normal 3D index by finding a relation between the 3D reciprocal lattice and the 2D reciprocal lattice. The same technique can be used to find a relation for Higher Order Laue Zone (HOLZ).

Q202 How is the phase displayed?

A All the phases are shifted by $-\pi/2$, and thus the phase of scattered wave from a thin sample corresponds to the phase of crystallographic structure factor (the phase of the incident wave is displayed as $-\pi/2$).

In crystallography the phase of structure factor is zero or π for the structure that has a center of symmetry (Namely, the structure factor is real, and will be positive or negative value). xHREM makes the phase of scattered wave from a thin sample correspond to the phase of crystallographic structure factor.

CBED Extension

Q301

High angle area is not displayed.

A The output range of CBED pattern is specified by "Range" of "Dynamical Structure Factor" in "Output Control" pane. Please check the unit (s ot d*) and the specified output value.

Q302

Does HOLZ lines appear under the projection approximation?

A Yes, HOLZ lines will appear close to the correct positions even under the projection approximation. However, their intensities may not be accurate.

Q303

Can we calculate a Large-angle CBED (LACBED, Tanaka pattern)?

A In LACBED experiment, a sample is placed off the electron beam focus point. Then, only the transmitted beam selected by an aperture is recorded.

Since xHREM calculates a CBED pattern by creating the focused probe at the specimen entrance surface, LACBED cannot be obtained.

Q304

How can we improve HOLZ line accuracy?

A In order to get a fine HOLZ line, use a higher "Resolution" of "Calculation Control" of the CBED dialog. Please consult the CBED Manual for a calculation step for each resolution setting.

In order to obtain a CBED pattern with an accurate position and intensity of HOLZ lines, the 3D effect (see Q019) should be properly included. Thus, a unit cell should be divided into a multiple slices.

Q401

An output from STEM image does not seem to represent a model structure.

A

At first, check a projected model structure using Model Viewer (Model View of MultiGUI). If the projected model is displayed correctly, then check a scan step. If the scan step is larger than 0.3 A, you may not get a smoothed atomic structure.

NOTE: If a displayed projected model structure is not correct, even when input atom parameters and a selected space group are right, then the symmetry operations of the selected space group may be wrong. If you find such an error, please report your finding to our support.

Q402

How to select a super-cell size?

A

The size of a super-cell determines a sampling interval of Fourier space (an inverse of super-cell size corresponds to a calculation step of scattering distribution). Therefore, a super-cell size of larger than 5 nm (scattering calculation step of less than 0.2 /nm) should be employed for a good simulation.

1. *Crystal model*

If a unit cell of the model is less than 5 nm, select "Standard" from "Super-cell size." Then, the input unit cell will be automatically repeated to create an approximately 5-nm super-cell. If a unit cell of the model is larger than 5 nm, select a size of super-cell larger than the unit cell.

2. *Interface or a defect model*

Select an appropriate size of super-cell that is larger than the longer edge of the structure model. Other short direction will be automatically repeated to fill the selected super-cell.

3. *Model with no periodicity, such as a nano-particle*

Select an appropriate size of super-cell that can accommodate the whole model.

Q403

Computation becomes extremely slow, when a model size becomes large.

A

STEM calculation requires all the phase gratings at each scan point. Therefore, even when a part of phase gratings cannot be loaded into the mail memory (RAM), all the phase gratings should be read from an external memory for each scan points in the case of a large model. Since computation speed of a contemporary PC is astonishingly fast, a total computation time will be extremely deteriorated due to this data access.

To avoid this defect you have to install more RAM. If the total size of phase gratings becomes more than about 2GM, you may have to use the 64-bit version (*STEM Extension Pro*) that supports a 64-bit OS to handle more memory.

Q404

What is a range to be included for scattering calculation? Does this range depend on the model size?

A

In order to evaluate probe propagation under elastic scattering, calculation including s=2.5/A (d*=5.0/A) is normally sufficient. This range does not depend on the model size.

Q405

What is a strategy to shorten computation time?

A

Since STEM simulation requires scattering calculation at each scan point, a total computation time tends to become very long. The current version of STEM Extension supports Multi-CPU (core). Thus, if you use a PC with a multi-CPU, you can reduce a total computation time by a factor that is approximately a number of CPU (Core).

A further reduction of computation time will be obtained, if you use a cluster version (*STEM Extension Cluster*) that uses multiple computers simultaneously.