<u>V4.1</u>
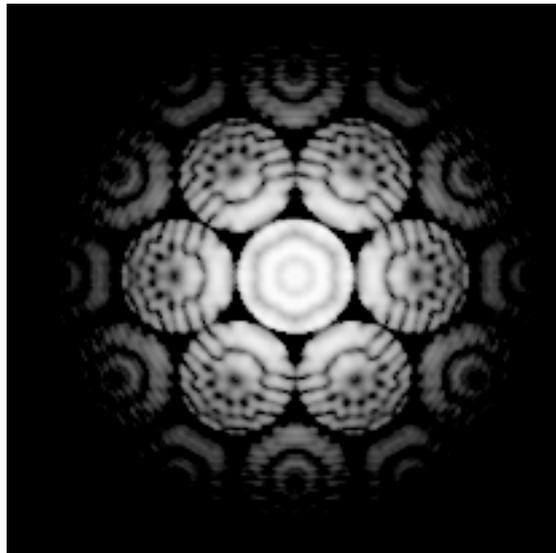
CBED

for xHREM™
(WinHREM™/MacHREM™)

**Coherent
Convergent Beam Electron Diffraction
Simulation Program**

User's Guide

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■ Introduction

This is a program to simulate convergent beam electron diffraction (CBED) patterns. This program is designed as an optional function of ***xHREM™*** ***(WinHREM™/MacHREM™)***, a program suite simulating a high-resolution electron microscope image for Windows/Mac OS.

xHREM™ has the following features.

Concept of xHREM™

1. ### User Friendly Graphical Interface

   xHREM™ employs user friendly Data Generation Utilities based on the Graphical User Interface for Windows or Mac OS.

   xHREM™ is general-purpose software that can be used to simulate all the images expected from any crystal systems, defect structures and interfaces. Although data generation for such general-purpose software normally becomes complex, a novice user can easily generate his/her data by using the graphical Data Generation Utilities with minimum requirements for the special knowledge.

2. ### Reliable and Efficient Algorithm

   xHREM™ emerges from the HREM image simulation programs based on FFT multislice technique developed at Arizona State University, USA (see References).   This is one of the most reliable and efficient HREM image simulation programs.

3. ### High Quality Image Output
   Numerical data such as projected potential, wave function propagating the specimen, simulated image intensities could printed as high quality gray scale maps (Bitmap) by using Output Graphic Utilities.   Numerical value of each pixel of the gray scale can be exported for further analysis with other software.

■ Installation

CBED program (32bit version) and some sample data should be already installed into your hard disk, when you have installed xHREM Simulation Suite.

In the case of CBED program (64bit version) please copy it manually to Programs folder of xHREM (CBEDxx.exe is not an installer).

When you purchase CBED program as an additional order, you have to update your user key. This update can be done by using Remote Update System (RUS). When you send current key information, then we will send back information to update your key.

How to evaluate xHREM without a user key (v4.1 or later)

When a user key is not recognized, xHREM will run as a demonstration version. Then, you cannot calculate dynamical scattering using MultiGUI, However, you can get an experience on how to create an input data using the graphical user interface. Furthermore, for the sample data you can go through the steps for image simulation using the pre-calculated data that are included in the installer.

■ Let's Start Tutorials

Data Preparation

Most of the data for scattering calculation control will be prepared by using "MultiGUI". A set of data specific to the CBED simulation will be specified in the optional windows. Please consult xHREM User's Manual about the general scattering calculation controls.

A sample data for GaAs (GaAs011c.WS1) will be provided with the program.

When you use xHREM as a demonstration version, you cannot save an input data nor execute actual calculation. However, for the sample data you can go through the steps for image simulation using the pre-calculated data.

In order to set up the optional data specific to the CBED simulation, click " CBED" from the Options at the bottom of the MultiGUI WORKSHEET.
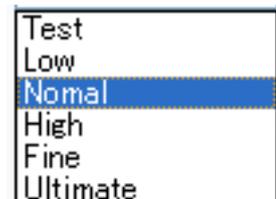
Options

| DIFFUSE | CBED | STEM | Model View |

Then, the following window will open:

Basic tab
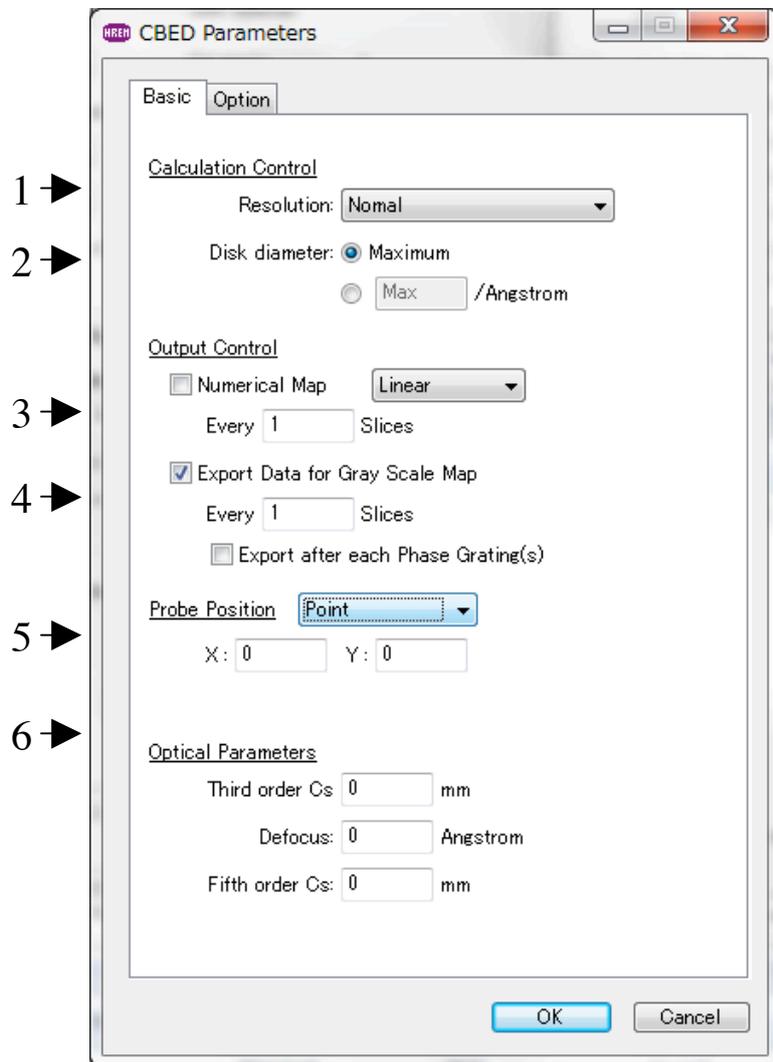
1. Resolution

    Resolution in Fourier space for the scattering calculation will be selected from the following pull down list:

    Usually, "Normal" or a higher resolution should be used. ("Test" and "Low" may be used to check the data.)

A sampling interval in Fourier space (Resolution) determines a model size (super-cell) in computation. A finer sampling interval in Fourier space (higher the resolution) results in a larger super-cell, and the number of sampling points will increase.

TIPS: A high-resolution CBED simulation requires a fine sampling interval in Fourier space, and thus requires a long computation time. Therefore, it is advisable to check the calculation data at a lower resolution before performing a simulation at the final resolution.

Required sampling points and sampling interval of the Fourier space

for each resolution setting

n	Resolution	Sampling interval (Approximate)	Sampling points*	Super-cell size (Approximate)
1	Test	0.08 / A	100 (128)	12.5 A
2	Low	0.04	200 (256)	25
3	Normal	0.02	400 (512)	50
4	High	0.01	800 (1k)	100
5	Fine	0.005	1600 (2k)	200
6	Ultimate	0.0025	3200 (4k)	400

The number of the sampling points shown here is estimated for a rectangular unit cell assuming the Range (a limit of calculation in Fourier space) of 4.0/A (in d).   An approximate number of the sampling points is given by 2 x Range /(sampling interval).

TIPS: The limit of calculation in Fourier space will be specified by "Range" parameter at Preferences/Dynamical calculation. The numbers of the sampling point will increase proportionally with the limit of calculation in Fourier space. For an oblique system the required number of pixels becomes larger than these number shown here.

TIPS: A super-cell size is an inverse of the sampling interval of the Fourier space. The input model will be repeated to conform to the super-cell size. Thus, a model size (super-cell) in computation is a multiple of the input unit size. Then, a real sampling interval is calculated as an inverse of the model size.

2.   Disk diameter

Specify the CBED disk diameter (not a radius), which is equal to the beam convergence. If you want to set the disk largest but not overlapped, you may simply select "Max."

3.   Numerical Map

On/off control for the numerical map output. The output may be "Linear" or "Log" scale. Output interval is specified in terms of slice. Output format defined in the Preferences will be used.

4. `Export Data for Gray Scale Map`

On/off control for the numerical data output onto a file, which is required for generating gray scale CBED patterns. Output interval is specified in terms of slice.

1. `Probe Position: Point/Line`

Probe position in the unit cell can be specified. This is an irreverent parameter, if there is no overlap region between the disks.

`Point:` Single CBED calculation at the specified probe position.

`Line:` Multiple CBED calculations at the probe positions on the specified line. The result at each point will be saved to the separate file. The start and end points, and the number of points will be specified as follows:
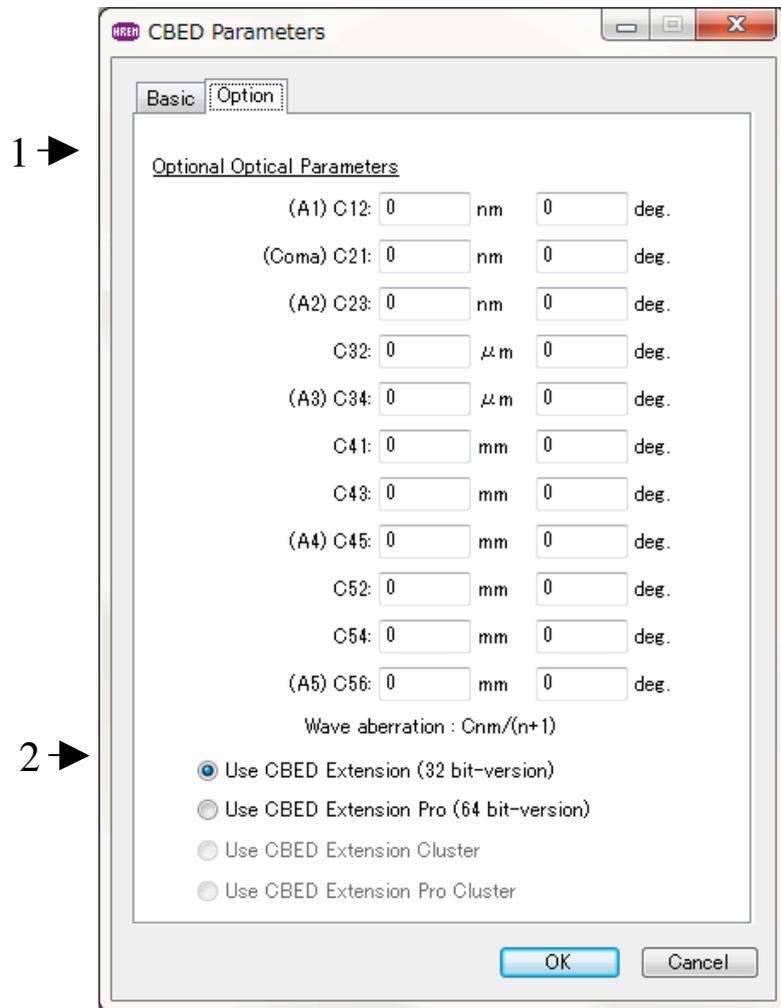
Probe Position	Line ▼		
X: 0	←→	1	/ 5 Points
Y: 0		1	

2. `Optical Parameters`

You can also specify a spherical aberration (third order) coefficient, a defocus value and a fifth order spherical aberration coefficient. This is also an irreverent parameter, if there is no overlap region between the disks.

Option tab

3. Higher Order Optical Parameters

    High order geometrical aberration coefficients up to 5th order can be specified here. Although various definitions of the coefficients appear in the literatures, we simply define them in terms of wave aberration as

    $$\frac{C_{nm}}{(n+1)}\alpha^{(n+1)}\cos m(\phi-\phi_{nm}).$$

4. 32bit/64bit Selector

    If the 64bit module is not installed to Programs folder, you cannot select it. (There are no Cluster versions for CBED)

NOTE: **CBED simulation will use a large number of the sampling points as shown above in real space as well as in Fourier space. Therefore, you will get a huge amount of the list output, when you try to print out the whole area of the potential distribution or the scattering distribution.**

Dynamical Scattering Calculation

1. Create the general scattering calculation controls in the main WORKSHEET.

   TIPS: To calculate elastic scattering to high-angle, a calculation range of s=1.5-2.0/A (d*=3.0-4.0/A) or higher will be set by Preferences -> Dynamical calculation > Range. However, "Doyle-Turner" cannot be used above s=2.0/A. You have to select "Weikenmeier-Kohl" foa a calculation over s=2.0/A.

2. Set up the optional data for CBED simulation.

3. Save the new data using "Save" or "Save As" from the File menu of the MultiGUI. (Before saving the data you can't select the Execute command.)

   When you are using xHREM as a demonstration version, skip the steps after this, since you cannot save an input data nor execute actual calculation.

4. Launch CBED program by choosing "Execute CBED" from the File menu of the MultiGUI.

5. A window showing the progress of the calculation appears.

   When an execution terminates normally, you will get the message "Execution completed. Congratulation!"

6. You can save the result window by choosing "Save As..." from the File menu of the result window.

Gray-scale CBED Images Display

Gray scale CBED patterns will be generated by using the "ImageBMP" utility. Please consult xHREM User's Manual about the general usage of ImageBMP.

The scattering data for CBED has been output to a .ED file.

To display a gray scale CBED pattern, do this:

1. Launch ImageBMP.

2. Select an ".ED" file with your sample name in the file selection dialog.

    When you cannot find your ED file, confirm that the file type specification is "ED Data (*.ED)."

    In the case you are using xHREM as a demonstration version, you can use a provided pre-calculated data (GaAs011c.ED).

    The following window will be appeared.
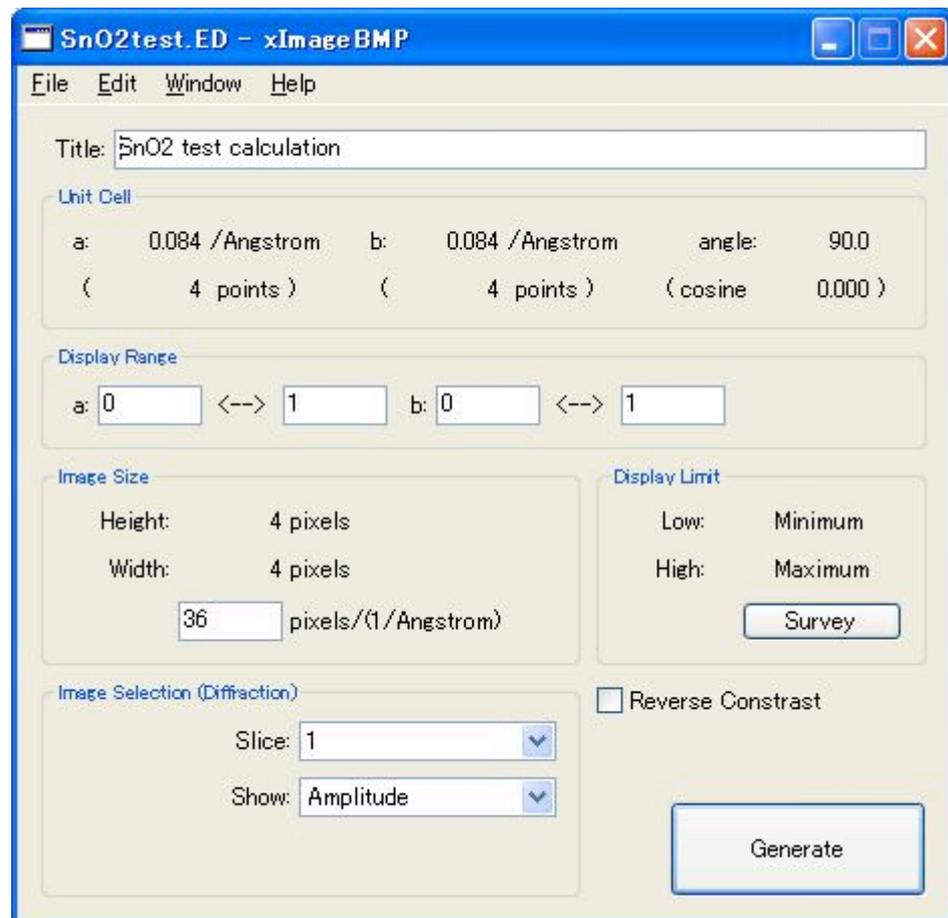
3. Select a specimen thickness (slice number) from "Slice" pull-down.

4. Select a display scheme from the "Show" pull-down.

5. When finishing setups, click "Generate" to display a CBED pattern.