V2.5

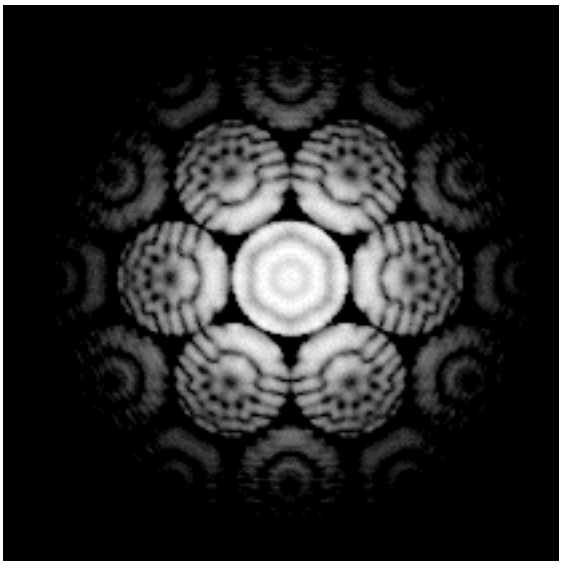
CBED

for

WinHREM/MacHREM™

Coherent
Convergent Beam Electron Diffraction
Simulation Program

User's Guide



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Support/Update
Email: support@hremresearch.com
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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 ***Win/MacHREM™***, a program suite simulating a high-resolution electron microscope image for Windows/PowerMacintosh.

Win/MacHREM™ has the following features.

Concept of Win/MacHREM™

1. User Friendly Graphical Interface

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

WinHREM™/MacHREM™ 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

WinHREM™/MacHREM™ 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 be converted into a standard image format for Windows or Mac OS (Bit map or PICT) and printed as high quality pictures by using Output Graphic Utilities. Photographic quality images as shown below could be obtained by using a high-quality printer.

■ Installation

CBED program is distributed in CD-ROM or on-line. It will include the folders shown below according to the Win/MacHREM folder structure (some folders may not be included, if not necessary).

The program will be used after installing into the hard disk. Please simply copy the content in each folder to the corresponding folder of Win/MacHREM in the hard disk.

TIPS: In the case of the Windows you may want to register a shortcut of the Utility program into "Start menu / Programs / WinHREM." Please consult your computer manual about the procedure to register a shortcut into the start menu.

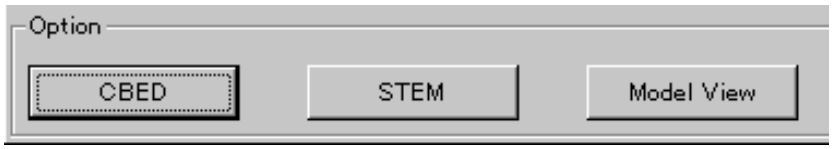
■ Let's Start Tutorials

Data Preparation

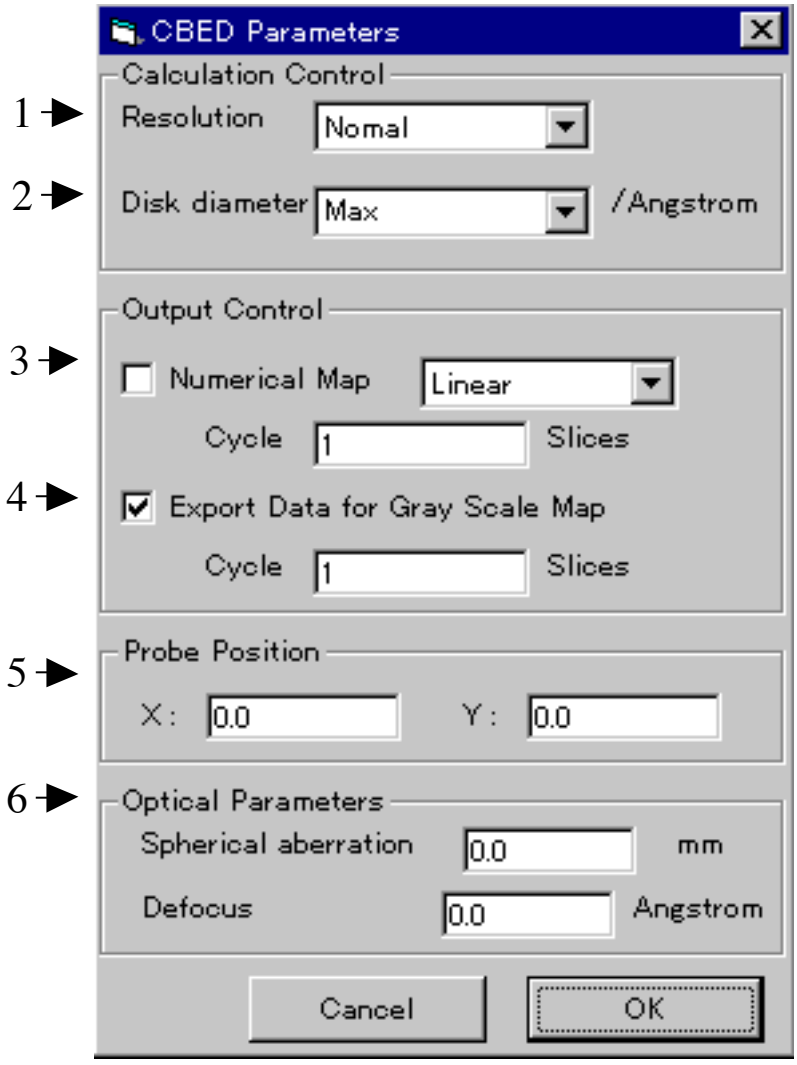
Most of the data for scattering calculation control including the model structure information will be prepared by employing the same worksheet that has been used "MultiGUI" to prepare the data for the dynamical scattering calculation. A set of data specific to the CBED simulation will be specified in the optional windows. Please consult Win/MacHREM User's Manual (MultiGUI Reference) about the general scattering calculation controls.

A sample data for SnO2 will be provided with the program.

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



Then, the following window will open:



1. Resolution

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

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 (d*)	sampling points
1	Test	0.08 / A	128
2	Low	0.04	256
3	Normal	0.02	512
4	High	0.01	1024
5	Fine	0.005	2048

The number of the sampling points shown here are estimated for a rectangular unit cell assuming the limit of the Fourier space of 4.0/A (in d*). For an oblique system the required number of pixels becomes larger than these number shown here.

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.

5. Probe Position

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

6. Optical Parameters

You can also specify a spherical aberration coefficient and a defocus value. This is also an irreverent parameter, if there is no overlap regions between the disks.

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.
2. Set up the optional data for CBED simulation.
3. Launch CBED program by choosing "Execute CBED" from the File menu of the MultiGUI.
4. A window showing the progress of the calculation appears.

   The results will be displayed in the "Input/Output" window for WinHREM, and in the "MacHREM" window for MacHREM.

   When an execution terminates normally, you will get the message "Execution completed. Congratulation!"
5. 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 Win/MacHREM User's Manual about the general usage of ImageBMP.

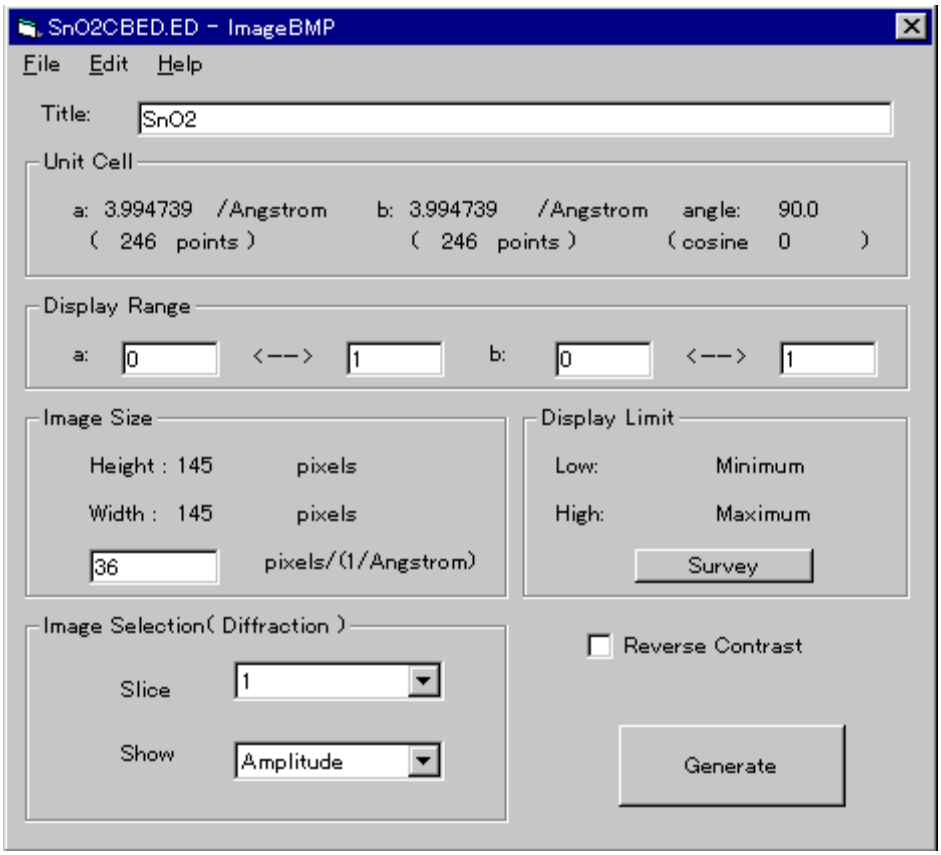
The scattering data for CBED has been output to a .ED file.

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.

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

   The following window will be appeared.



3. Select a specimen thickness (slice number) at which for a CBED pattern to be displayed.
4. Select a display scheme from the "Show" pull-down.
5. When finishing setups, click "Generate" to display a CBED pattern.

CBED Image Quantification

Gray scale CBED patterns generated by using the "ImageBMP" utility can be quantitatively examined as explained for quantification of the HREM images. You can also use the Line Profile capability as explained for the HREM Images. Please consult Win/MacHREM User's Manual about the general usage of ImageBMP.