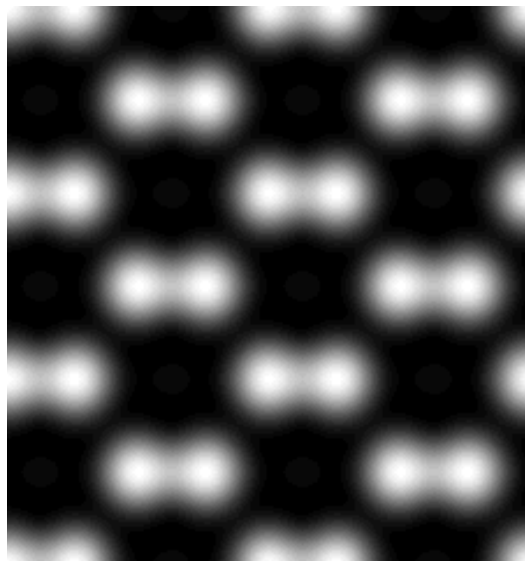


*STEM*  
*for*  
*WinHREM/MacHREM*<sup>TM</sup>

**Scanning  
Transmission Electron Microscope  
Image Simulation Program**

*User's Guide*



**Scanning  
Transmission Electron Microscope  
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***User's Guide***

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Support/Update

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## ■ Introduction

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This is a program to simulate a scanning transmission electron microscope (STEM) image. 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

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STEM 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).



Data



Utility



Programs



Document

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

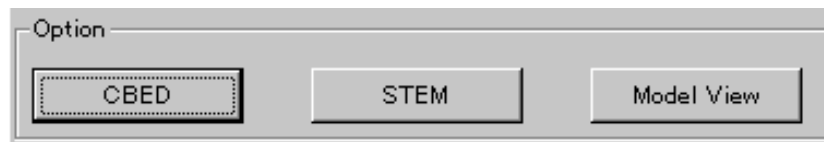
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### Data Preparation

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 STEM 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 SnO<sub>2</sub> will be provided with the program.

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



Then, the following window will open:

## STEM for Win/MacHREM

The image shows a screenshot of the 'STEM Parameters' dialog box. It is divided into four sections, each indicated by a numbered arrow on the left:

- 1 → Optical Parameters:** Contains four input fields: 'Aperture radius' (0.5 /Angstrom), 'Third order Cs' (1.0 mm), 'Defocus' (500.0 Angstrom), and 'Fifth order Cs' (0.0 mm).
- 2 → Detector Parameters:** Contains three input fields: 'Bright Field Outer' (0.1 /Angstrom), 'Dark Field Inner' (0.5 /Angstrom), and 'Dark Field Outer' (1.0 /Angstrom).
- 3 → Scan Control:** Contains a 'Scan Mode' dropdown menu (set to 'Area'), 'Position' X and Y coordinates (each with a range from 0.0 to 1.0 and 11 points), and a 'Data Output Cycle' field (set to 1 Slices).
- 4 → Diffraction Calculation Control:** Contains a 'Resolution' dropdown menu (set to 'Normal').

At the bottom of the dialog are 'Cancel' and 'OK' buttons.

1. Optical Parameters

Input an aperture radius, aberration coefficients. The aperture radius may be given in mrad (You have to select mrad in the Preferences before open this window.)

2. Detector Parameters

## STEM for Win/MacHREM

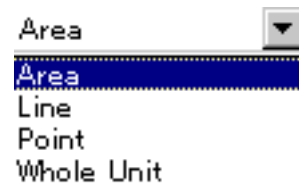
Detector radiuses of the bright-field imaging and the dark-field imaging will be specified here. These radius may be given in mrad (You have to select mrad in the Preferences before open this window.)

**Tips** When you input a zero (0) for Outer Range of Bright Field, the same value specified for the Aperture radius will be used in the program.

**Tips** When you input a zero (0) for Outer Range of Dark Field, the largest value included in the scattering calculation will be used in the program. In this way, you may not need to worry about the outer range of your detector aperture.

### 3. Scan Control

Scan Mode: Scanning scheme will be selected from the list shown below.



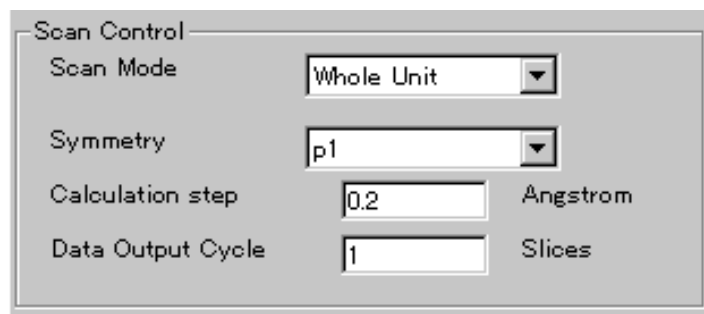
Position: Scanning position(s) will be specified here. The scanning positions will be specified in different ways according to the scanning mode.

**Area:** The ranges of the scanning area and numbers of scanning points along x and y will be specified for this mode.

**Line:** The starting position and the ending position as well as the number of scanning points will be specified for this mode.

**Point:** A single position will be specified for this mode.

**Whole Unit:** For this mode the two- dimensional symmetry group and a calculation step (interval) will be specified.

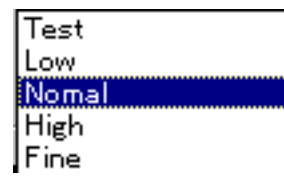


Data Output Cycle: An output interval in terms of the slices.

### 4. Resolution

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

## STEM for Win/MacHREM



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

**NOTE** STEM 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 STEM simulation.
3. Launch STEM program by choosing "Execute STEM" 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.

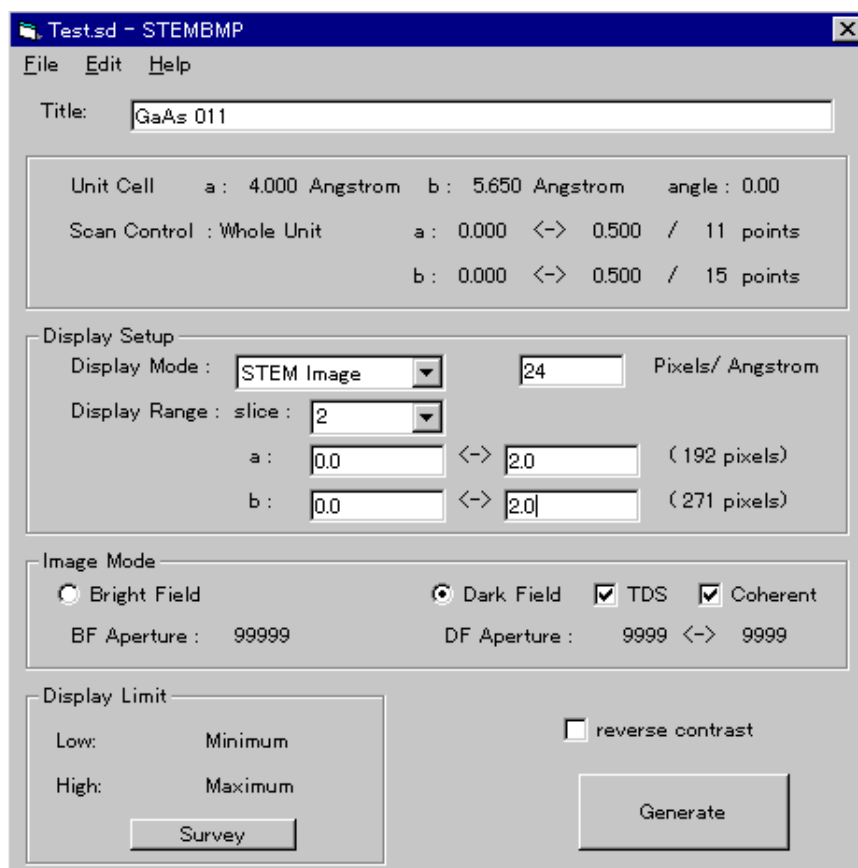
## Gray-scale STEM Images Display

Gray scale STEM images will be generated by using the "STEMImage" utility. The STEM data has been output to a .SD file.

To display a gray scale STEM image, do this:

1. Launch STEMImage.
2. Select a ".SD" file with your sample name in the file selection dialog.  
(Windows) When you can not find your SD file, confirm that the file type specification is "SD Data (\*.SD)."

The following window will be appeared.



3. Select "Display Mode"  
Select a display mode from "STEM Image", "Thickness Map" and "Point." Selectable display mode is depending on the Scan Mode.  
As in this case of a two-dimensional scan image, you have to select the specimen thickness (slice number), a display area and a resolution (Pixels/length).

## *STEM for Win/MacHREM*

When the Scan Mode is "Whole Unit," you can extend the display area more than one unit cell.

4. From "Image Mode" you can select the image type from "Bright Field" or "Dark Field." In the case of the dark field image, you can also select the image signal(s) from TDS inelastic signal and/or coherent elastic signal.
5. Click "Generate" to display a gray scale image.

### STEM Image Quantification

Gray scale STEM 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.