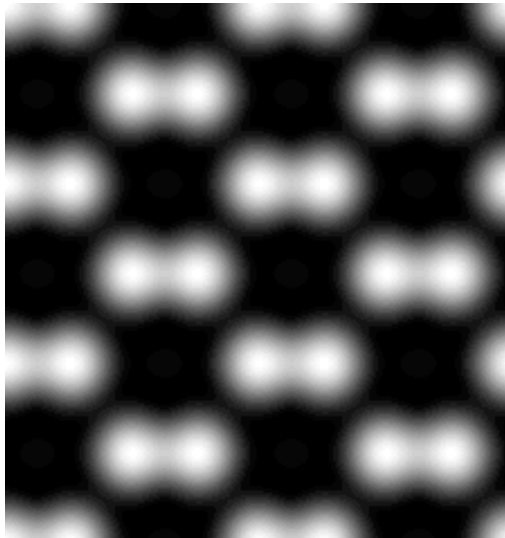


V5.0

*STEM*  
*for xHREM<sup>TM</sup>*  
*(WinHREM<sup>TM</sup>/MacHREM<sup>TM</sup>)*

**Scanning  
Transmission Electron Microscope Image  
Simulation Program**

***User's Guide***



# Scanning Transmission Electron Microscope Image Simulation Program

## *User's Guide*

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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 *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 be 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.

### Concept of STEM Extension

#### 1. User Friendly Graphical Interface

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

2. Reliable and Efficient Algorithm

Thermal Diffuse Scattering (TDS) is believed to be the main source of signal for STEM-HAADF image. STEM Extension will efficiently treat TDS using absorption potentials. Please consult the following paper for a detailed description:

K. Ishizuka: A practical approach for STEM image simulation based on the FFT multislice method, Ultramicroscopy 90 (2001) 71-83.

3. Efficient Computation

STEM image simulation is number crunching, since scattering calculation is necessary at each scanning point. Therefore, the STEM Extension supports multi-core CPU to accelerate computation.

Computation time of STEM image simulation can be reduced to about 1/20 using an efficient interpolation method compared with the original versions.

4. GPGPU Support (Windows only)

The STEM Extension supports NVIDIA GPU to further accelerate STEM performance. Using a single GPU, the computation time can be reduced to one over 10-20 compared with a multi-core CPU. Furthermore, the STEM Extension supports more than one GPU.

## ■ Installation

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STEM 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 STEM program (64bit version) please copy it manually to Programs folder of xHREM (STEMxx.exe is not an installer).

When you purchase STEM 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 use GPU version (Windows Only) (From Ver.5.0)

The NVIDIA GPU(s) can be used for STEM scattering calculation. The calculation module for the GPU is already installed. When any NVIDIA GPU(s) is detected on your PC, the GPU module can be selected in Option Tab of the STEM dialog.

### 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

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### Data Preparation

Most of the data for scattering calculation control will be prepared by using "MultiGUI". A set of data specific to the STEM 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 (GaAs011s.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 STEM simulation, click "STEM" from the Options at the bottom of the MultiGUI WORKSHEET.



Then, the following window will open:

Basic tab

1 → **Optical Parameters**  
 Aperture radius: 11.9 mrad  
 Third order Cs: 0.5 mm  
 Defocus  
 Center Defocus: 354 Angstrom  
 Defocus Step: 0 Angstrom  
 # of over/under foci: 0  
 Defocus Range: 354 To 354 Angstrom  
 Fifth order Cs: 0 mm

2 → **Detector Parameters**  
 Bright Field: 11.9 mrad  
 Annular Dark Field: 56 To 0 mrad  
☒ Optional ADF/ABF: 6 To 11.9 mrad  
☒ DPC (Differential Phase Contrast)

3 → **Scan Control**  
 Scan Mode: Whole Unit  
 Symmetry: cm  
 Calculation step: 0.2 Angstrom  
 Data Output: Every 1 Slices  
 List Output: Y, %SLICE...

OK Cancel

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.)

You can perform calculations at multiple defocuses. Here, you can specify the center defocus, defocus step and a number of defocuses at over- and under-focus sides.

2. Detector Parameters

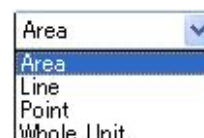
Detector radii of the bright-field imaging and the annular dark-field imaging will be specified here. These radii may be given in mrad, when you select mrad in the Preferences before open this window.

(From v4.4) You can define the optional annular detector. Thus, you can simultaneously calculate ABF or LA-ADF, MA-ADF in addition to HAADF.

(From v4.5) You can control the output for the DPC (Differential Phase Contrast) signals. Here, the DPC signals are calculated as the Center of Mass (CoM) of the diffraction intensity.

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 (top, left; bottom, right) 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: The whole unit area will be calculated assuming an applicable symmetry. Thus, the two-dimensional symmetry group and an approximate scanning step (interval) will be specified. Integral number of scanning points will be calculated internally according to the approximate sampling interval.

The supported symmetries: p1, p2, pm, pg, cm, pmm, pmg, pgg, cmm and p4.



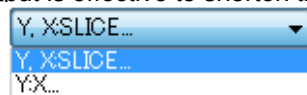
Data Output Cycle: STEM image intensity output interval in terms of the



## STEM for xHREM

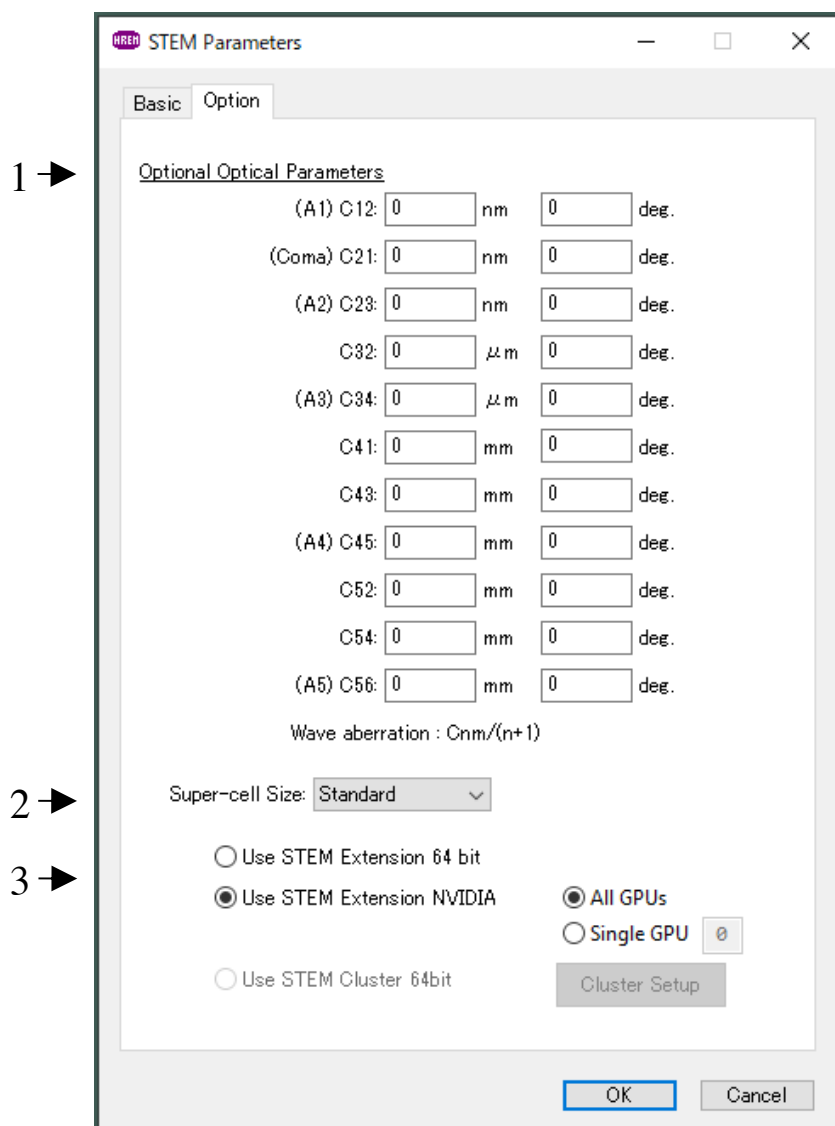
slices.

List Output: the list output showing a scan progress. When a computing time for each slice is very quick, the scan list output may control the overall turnaround time. In this case, a simpler list output is effective to shorten the turnaround time.



When you select the GPU from the Option tab, the list output will be restricted only to Y:X....

### Option Tab



1. High Order Aberration Coefficients

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

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

2. Super-cell Size

Super-cell size used in computation will be selected from the following pull-down list. Normally, “Standard” can be selected here:



The super-cell size in computation should be larger than the input structure model. If the structure mode is smaller than the super-cell size, the input model is repeated to fill the super-cell. Thus, the model size in computation is a multiple of the input model.

3. Execution module Selector

If any NVIDIA GPU is not found, or the Cluster module is not installed in the Program folder, the corresponding selection can not be selected.

Super-cell size and sampling points\*

n	Model	Super-cell size (Target value)	FT space interval (Target value)	Sampling points*
1	Test	12.5 Å	0.08 / Å	128
2	Small	25	0.04	256
3	Standard	50	0.02	512
4	Large	100	0.01	1024
5	Huge	200	0.005	2048
6	Ultimate	400	0.0025	4096

\*The number of the sampling points is estimated for a rectangular unit cell assuming the calculation Range of 5.0/Å (in d\*).

FT space interval = 1/(Super-cell size); Real space interval = 1/2d\*

Sampling points (power of two) > 2d\*/(FT space interval)

## ***STEM for xHREM***

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

**TIPS:** Normally, the Range of  $5.0/\text{\AA}$  (in  $d^*$ ) is enough for calculation using HAADF TDS absorption potentials.

When you use the Frozen Phonon model to emulate TDS (Thermal Diffuse Scattering) without using TDS absorption potential, you have to include in calculation the angle atomic scattering factor until it attenuates sufficiently, say up to  $d^* = 30.0/\text{\AA}$ . Furthermore, using the Frozen Phonon model you have to calculate scattering from many atom coordinates (configurations), and average their intensities to give the TDS, which is not practical.

**TIPS:** For STEM image calculation the super-cell less than “Standard” is not recommended in order to evaluate scattering profile.

**NOTE**      **STEM simulation will use a super-cell with a large number of the sampling points. 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  $s=1.5-2.0/\text{\AA}$  ( $d^*=3.0-4.0/\text{\AA}$ ) or higher will be set by Preferences -> Dynamical calculation > Range. However, “Doyle-Turner“ cannot be used above  $s=2.0/\text{\AA}$ . You have to select “Weikenmeier-Kohl” for a calculation beyond  $s=2.0/\text{\AA}$ .

**TIPS:** Choose “Weikenmeier-Kohl Scattering Factor” from Preferences /Atomic Scattering factor, and check “Including TDS Absorption” box. However, when you want to ignore TDS absorption, and obtain a STEM image using only elastic scattering, you don’t need to check this box. Please note that including **TDS absorption requires a thermal factor (Debye-Waller factor) of each atom.**

2. Set up the optional data for STEM 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 STEM program by choosing "Execute STEM" 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!"

**TIPS:** Calculation of a STEM image by scanning many points will take a long time. Thus, you can stop calculation and continue it layer. In order to resume calculation, choose “Append” from MultiGUI -> Multislice Calculation. When you stop calculation, a calculation will resume from the following scan point on which a full propagation has been completed.

6. 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 set of files depending on the output signal selections. However, all the signal can be accessed by selection 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.

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

The following window will be appeared.

The screenshot shows the 'GaAs011s.SD - xStemImage' window. It has a menu bar with 'File', 'Edit', 'Window', and 'Help'. The 'Title' field is 'GaAs 011'. Below this, the 'Unit Cell' section shows 'a : 4.000 Ang.', 'b : 5.650 Ang.', and 'angle : 0.0000'. The 'Scan Control' section shows 'Whole Unit' with 'a: 0.000 <-> 0.500 / 11 points' and 'b: 0.000 <-> 0.500 / 15 points'. The 'Display Control' section includes 'Defocus: 354', 'Display Mode: STEM Image' with a value of '12' and 'Pixels/Angstrom', 'Display Range: slice: 1', and input fields for 'a: 0.0 <-> 1.0 ( 49 pixels)' and 'b: 0.0 <-> 1.0 ( 69 pixels)'. There are checkboxes for 'Image Tableau' and a 'Tableau Setup' button. The 'Image Mode' section has radio buttons for 'Bright Field', 'Annular Dark Field' (selected), and 'DPC', along with checkboxes for 'TDS' and 'Coherent'. It also shows 'BF Aperture: 0.474', 'ADF Aperture: 2.233 <-> 5.000', and 'ADF/ABF Aperture: 0.239 <-> 0.439'. The 'Interpolation' section has a dropdown set to 'Fourier Transform'. The 'Partial Coherency (Full Width at 1/e)' section has checkboxes for 'Probe Size', 'Defocus Spread', and 'Reverse Contrast', each with a value of '0' and 'Ang.'. The 'Display Limit' section has 'Low: Minimum' and 'High: Maximum' with a 'Survey' button. A 'Generate' button is at the bottom right.

In the case you are using xHREM as a demonstration version, you can use a provided pre-calculated data (GaAs011s.SD).

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).

When multiple defocus data is available, you can select a defocus value (or a center defocus value of Defocus Spread).

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", "Annular Dark Field", "Optional ADF/ABF" (from v4.4) or "DPC" (from v4.6). In the annular detectors, you can also select the image signal(s) from TDS inelastic signal and/or coherent elastic signal.

The "Optional ADF/ABF" can be selected only when you calculate this optional STEM signal. The "DPC" can be selected only when you calculate the DPC signal.

5. Click "Generate" to display a gray scale image.

In order to differentiate the signal source, "BF", "ADF", "ADT" (Optional Annular Detector) or Dv and Dh (DPC signals) is added to the data name.

**TIPS:** You can select one of the two interpolation methods (Fourier Transform/Bi-linear Interpolation) to estimate intensity between the calculated points. Usually, an interpolation using Fourier transform gives smoother image. Thus, a wider step (scan distance) can be used in calculation and a computation time may be substantially decreased.

**TIPS:** Partial coherency due to a probe size as well as a defocus spread can be estimated. Here, Gaussian distributions are assumed for both the probe size and the defocus spread, and a full width at 1/e value is specified.

**NOTE:** In order to estimate partial coherency due to a defocus spread the STEM images at multiple defoci in a sufficient range should be calculated.

**TIPS:** Each pixel value of a gray scale map produced by STEMImage can be output using "Save As..." command as you can do by using ImageBMP. The original data used to produce the gray scale map can also be output using "Save As..." command. Please consult "Numerical Data Output Using ImageBMP" in the xHREM manual for more details.

## ■ Topics

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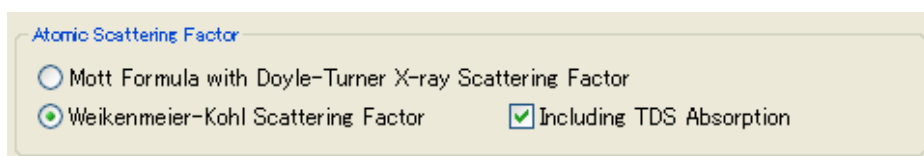
In this section some useful functions as well as advanced topics will be introduced. It is not necessary to read through all the topics at the first time. You may want to study each topic when you need to use it.

### Including TDS Absorption

You can include absorption of elastically scattered wave due to thermal diffuse scattering (TDS) in your dynamical calculation. In this case, however, **thermal displacement parameter (temperature factor; Debye-Waller factor) for each atom in your atomic model is required**. When you don't know a corresponding parameter, an approximate value may be specified.

To include TDS absorption in your dynamical calculation:

1. Launch MultiGUI
2. Choose "Preferences" from Edit menu.
3. Select "Weikenmeier-Kohl Scattering Factor" in "Atomic Scattering Factor" section of the Preferences dialog, and check "Include TDS absorption."



## **Required RAM Size**

For STEM image simulation, scattering calculation is necessary at each scanning point. Then, we have to use all the phase gratings for each scan point. A cotemporary operating system (OS) allows us to use many phase gratings by using a virtual memory management.

However, when a main memory is short to store only a single-phase grating, all the phase gratings should be read from an external memory as a result of roll-in/roll-out. If an external memory is a hard disk, a significant time is required to read the phase gratings into the main memory. Therefore, all the phase gratings should be stored in the main memory for an efficient computation.

Typically, each program can use a roughly 2GB using a 32-bit OS. If the total phase gratings is bigger than this size, you have to use STEM Extension Pro that supports a 64-bit OS.

**TIPS:** In the case of a Standard model with 512x612 pixels, each phase grating requires the following memory:

$$(512 \times 512) \times 8 \text{ (complex)} \times 2 = 4\text{MB.}$$

A larger model uses more phase gratings of larger size, so the total phase gratings will become more than 2GB.

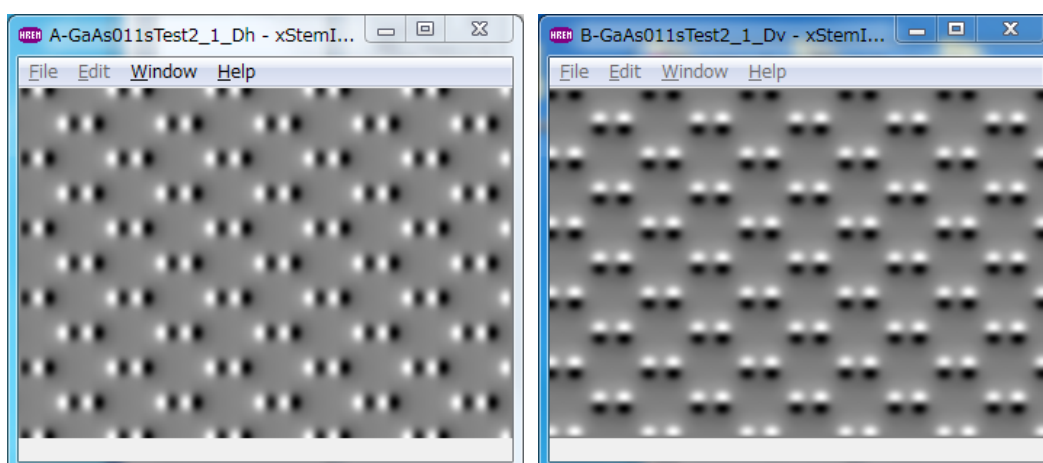


## STEM-DPC (Differential Phase Contrast)

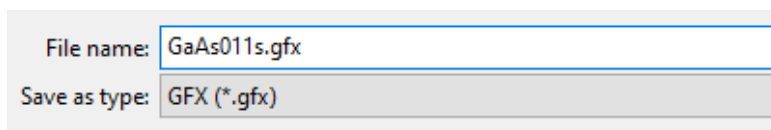
STEM-DPC is the technique to obtain a phase distribution of phase object using a STEM under the thick phase object approximation. A set of the DPC signals represents a vector corresponding to CoM (center of mass) of the diffraction intensity. This vector is a gradient of the phase distribution, which is proportional to a projected potential distribution of the sample.

The DPC images, Dh and Dv, calculated with the STEM Extension correspond to the CoM, which are equivalent to the signal obtained from the **pixelated detector**. To obtain the DPC images corresponding to the experimental ones, however, you have to set the output resolution (pixels/angstrom) and the output range as in the case of other STEM images at the “Display Control” section of the xSTEMImage.

The images below show the DPC images for the GaAs, which correspond to the horizontal (Dh) and vertical (Dv) derivatives of the potential distribution of GaAs in the 011 projection, respectively.



In order to integrate the DPC signals using the qDPC plug-in for DigitalMicrograph, the DPC image data should be firstly read into DigitalMicrograph. You can easily import them to DigitalMicrograph, when you save the DPC images in “gfx” format using File -> Export Data from xSTEMImage as shown below:



**NOTE:** When you output the DPC data from the xSTEMImage GUI using the **Export** command, you don’t need to generate the DPC images in advance, since both Dh and Dv images will be generated and saved at once. On the other hand, when you export the DPC image from the image window, only the corresponding image data, namely Dh or Dv image, will be saved.

## ***STEM for xHREM***

The gfx file can be simply read into the DigitalMicrograph using “Open” command of the File menu. In this case, you may need to select “All file” in the file type option to show the gfx file(s). Or, you can simply drag-and-drop the gfx file(s) to the DigitalMicrograph.

The phase map shown below was obtained from the above two DPC images using “DCT...” command of the qDPC.



**Segmented Detector:** There is a class of the DPC detectors that show the DPC images in real-time. The detectors segmented to four (quadrant) or eight (double quadrants) are commercially available. In this case the DPC signals are not exactly the CoM as given by a pixelated detector, but closely approximate the CoM. Therefore, using the DPC signal obtained with the xSTEM Extension you can get an idea on the phase image obtained by the segmented detector.

### **References**

- [1] qDPC, DigitalMicrograph plug-in: <https://www.hremresearch.com/Eng/plugin/qDPCEng.html> (Microscopy Today 2018 Innovation Award product)
- [2] Ishizuka A., Oka M., Seki T., Shibata N., and Ishizuka K. (2017) Boundary-artifact-free determination of potential distribution from differential phase contrast signals. Microscopy 66, 397-405 (The Japanese Society of Microscopy Award in 2019 paper)
- [3] Ishizuka A. and Ishizuka K. (2020) Observation of Phase Objects using STEM - Differential Phase Contrast (DPC) microscopy, JEOL News 55, 24-31.

## GPU Acceleration (Windows Only)

When you want to use your NVIDIA GPU(s) to accelerate STEM calculation, select “Use STEM Extension NVIDIA” and “All GPU.” If you want to use a specific single GPU, select “Single GPU” and specify the GPU number.



**NOTE:** The name of the GPU and its memory size of all the NVIDIA GPU(s) found on your PC will be enumerated in the list output window opened by MultiGUI as shown below:

```
0 GPU INFORMATION
  Number of NVIDIA GPU: 2
  GPU 0: Quadro P620 / Memory 2048 MB
  GPU 1: Quadro K2200 / Memory 4096 MB
  GPU to be used: All
```

Here, you can check the name of GPU and its number used in the program. The above list output shows the case where all the GPUs will be used.

**NOTE:** Currently, we assume the case where the same GPUs (or the GPUs with the similar computing power) are installed on the PC, and give the same number of scan points to all the GPUs. Therefore, the slowest GPU will control an overall computing time, when “All GPUs” is selected for the case where the computing powers of the GPUs are different. In such a case, it may be more efficient to use only the fastest GPU. (This issue will be resolved in a future release.)

The following extract of the list output shows the progress of scan in the case of 100 x 100 scan points for a full unit cell ( $x = 0.0$  to  $1.0$ ;  $y = 0.0$  to  $1.0$ ). In order to optimize calculation a set of sixteen (16) scan points is given to each GPU. When we use two GPUs, the first 16 points (1 to 16) are calculated by the GPU 0 (1:0), and the next 16 points (17 to 32) are calculated by the GPU 1 (17:1). Then, the GPU 0 calculates the third 16 points (33 to 48) (33:0), and the GPU 1 the fourth 16 points (49 to 64) (49:1), and so on. If the number of the scan points at the end of the scan line is less than 16, some points of the next line will be combined into the group of 16 points: since four (4) points (97 to 100) is left at the end of the first line, twelve (12) points of the next line is combined in to 16 points and calculated by the GPU 0 (97:0). Thus, the next 16 points (13 to 28) of the second line is calculated by the GPU 1 (13:1).

**NOTE:** The numbers before and after the colon (:) indicate the start scan point in each scan line and the GPU to be used, respectively.

## ***STEM for xHREM***

0	STEM PROBE LOOP FOR DEFOCUS:	50.000
Y	--> X	
0.0000	--> 1:0 17:1 33:0 49:1 65:0 81:1 97:0	
0.0101	--> 13:1 29:0 45:1 61:0 77:1 93:0	
0.0202	--> 9:1 25:0 41:1 57:0 73:1 89:0	
0.0303	--> 5:1 21:0 37:1 53:0 69:1 85:0	
0.0404	--> 1:1 17:0 33:1 49:0 65:1 81:0 97:1	
0.0505	--> 13:0 29:1 45:0 61:1 77:0 93:1	
0.0606	--> 9:0 25:1 41:0 57:1 73:0 89:1	
0.0707	--> 5:0 21:1 37:0 53:1 69:0 85:1	
0.0808	--> 1:0 17:1 33:0 49:1 65:0 81:1 97:0	
0.0909	--> 13:1 29:0 45:1 61:0 77:1 93:0	
0.1010	--> 9:1 25:0 41:1 57:0 73:1 89:0	
0.1111	--> 5:1 21:0 37:1 53:0 69:1 85:0	
0.1212	--> 1:1 17:0 33:1 49:0 65:1 81:0 97:1	
0.1313	--> 13:0 29:1 45:0 61:1 77:0 93:1	
0.1414	--> 9:0 25:1 41:0 57:1 73:0 89:1	

**NOTE:** In the above example the scan interval is  $1.0/99 = 0.01010\dots$ , since the full range (0.0 to 1.0) is calculated by 100 of points to simplify the explanation. Thus, the value of Y becomes a multiple of 0.01010. If you use 101 points for a full unit (0.0 to 1.0), the scan interval will become a simple fraction of  $1.0/100 = 0.01$ , and the value of Y becomes a multiple of simple number of 0.01.

# FAQ

## Frequently Asked Questions

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

### 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?

**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 Å, 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 main 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 2GB, 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  $s=2.5/\lambda$  ( $d^*=5.0/\lambda$ ) 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.

Furthermore, from v.5.0 the STEM Extension supports the NVIDIA GPU. The latest GPU has 10-20 times computing power of a multi-core CPU, and gives you the performance equivalent to a cluster of 10-20 PCs at a low cost. Even an old GPU has computing power equivalent to several times of a multi-core CPU, and thus corresponds to a cluster of several PCs. In addition, the GPU module supports more than one GPU.