IWFR
for DigitalMicrograph

Iterative Wavefunction Reconstruction

IWFR Manual 2.0

HREM Research Inc.

Conventions

The typographic conventions used in this help are described below.

Convention	Description
Bold	Used to denote components of the user interface such as buttons, field names, menus, and menu options.
	For example, the **New** button.
Menu...MenuOption	Select the menu from the menu bar then select the menu option from the menu.
	For example, **File...Open** would mean to select the **File** menu and then the **Open** option.
CAPS	Used to denote the name of a key on the keyboard.
	For example, the ENTER key.
Italics	Used to denote emphasis, captions and the result of an action in a procedure.

Technical Support

General enquiries on the IWFR should be sent to:

HREM Research Inc.
Email: support@hremresearch.com
Web: www.hremresearch.com

Copyright Statements

© Copyright 2005-2020 HREM Research Inc.

DigitalMicrograph is a trademark of Gatan Inc.

1. Introduction

IWFR (Iterative Wavefunction Reconstruction) is a plug-in for use in Gatan's DigitalMicrograph for GMS 2.x but works also with GMS 3.x. However, we will recommend you to use the latest GMS.

This IWFR manual is written to provide information on the basic functions of the IWFR plug-in, a procedure for installation of the Plug-In, some general tips on operation. This Guide assumes the user is familiar with image manipulation using DigitalMicrograph as well as Windows operating system.

1.1 What is IWFR?

IWFR stands for Iterative Wave Function Reconstruction, a method that works with a through focal series of HREM images to reconstruct a wave function at the specimen exit surface. Satisfactory results can be obtained with around five images. Using the wave function obtained you can correct optical aberrations such as spherical aberration.

The IWFR method is in the spirit of the Gerchberg-Saxton algorithm (which has originally used a measured *image intensity* and the *diffraction intensity* to retrieve the complex exit surface wave function). Contrary to this, the IWFR uses a set of image intensities measured at different planes (a through-focal series of images) to reconstruct the complex wave at the specimen exit surface (at the zero-defocus plane).

Details of the IWFR algorithm can be found in the following paper: L.J. Allen, W. McBride, N.L. O'Leary and M.P. Oxley: Exit wave reconstruction at atomic resolution. Ultramicroscopy 100 (2004) 91-104.

1.2 Summary of IWFR method

The IWFR method is comprised of iterative cycles of backward-propagation, averaging, forward-propagation and replacing amplitude as schematically shown below. The details of each step are explained below, and the flow chart of the process is summarized schematically in the figure below.
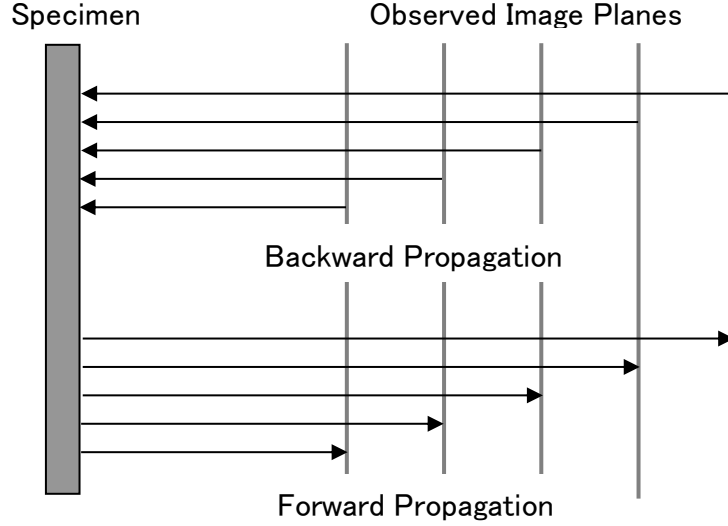
1) Start with a through focal series comprising N experimental images, with the intensity in each plane n denoted by $I_n(\boldsymbol{r})$. Seed the algorithm by guessing a phase for the wave function in each of these planes. In practice we set $\phi_n^1(\boldsymbol{r}) = 0$ for all $\boldsymbol{r}$ in each plane n, where the superscript denotes the first $(j = 1)$ iteration.

2) Construct the wave functions

$$\psi_n^j(\boldsymbol{r}) = \sqrt{I_n(\boldsymbol{r})}\, exp\big[i\phi_n^j(\boldsymbol{r})\big].$$

3) Take a Fourier transform of the wave function in each plane to obtain $\Psi_n^j(\boldsymbol{q})$ and propagate to the nominal exit surface plane $\Delta f = 0$ while also correcting for aberrations in the imaging system. Propagation proceeds via

$$\Psi_{n,0}^j(\boldsymbol{q}) = \Psi_n^j(\boldsymbol{q})\big[T_n(\boldsymbol{q})E_{s,n}^{Coh}E_{\Delta}^{Coh}\big],$$

where $\Psi_{n,0}^j(\boldsymbol{q})$ is the wave function at $\Delta f = 0$ propagated from plane n.

4) Construct the average wave function $\Psi_{avg}^j(\boldsymbol{q}) = (1/N)\sum_{n=1}^{N}\Psi_{n,0}^j(\boldsymbol{q})$.

5) Propagate $\Psi_{avg}^j(\boldsymbol{q})$ to each of the N experimental image planes to obtain $\widetilde{\Psi}_n^j(\boldsymbol{q})$, the estimated wave functions in momentum space.

6) Take an inverse Fourier transform of $\widetilde{\Psi}_n^j(\boldsymbol{q})$ to construct an estimated real space wave function $\widetilde{\psi}_n^j(\boldsymbol{r}) = \sqrt{\tilde{I}_n(\boldsymbol{r})}\, exp\big[i\widetilde{\phi}_n^j(\boldsymbol{r})\big]$ in each plane.

7) Calculate a sum-squared-error (SSE) in each experimental plane using

$$SSE_n^j = \sum_{xy}\left[\sqrt{I_n(\boldsymbol{r})} - \sqrt{\tilde{I}_n^j(\boldsymbol{r})}\right]^2 \Big/ \sum_{xy} I_n(\boldsymbol{r}).$$

The summations are over all pixels in each image.

8) Calculate the average $SSE_{ave}^j = (1/N)\sum_{n=1}^{N} SSE_n^j$.

9) If $j > 1$ and $SSE_{ave}^{j-1} - SSE_{ave}^j < \varepsilon$, where ε is an appropriately chosen convergence parameter, then the wave function reconstruction is complete and the solution is given by the inverse Fourier transform of $\Psi_{avg}^j(\boldsymbol{q})$. Otherwise set $\phi_n^{j+1}(\boldsymbol{r}) = \tilde{\phi}_n^j(\boldsymbol{r})$ and return to step (2) for iteration $j + 1$.

2. Installation

This chapter describes hardware and software requirements to run the IWFR plug-in and an installation procedure of the plug-in.

2.1 Requirements

The IWFR plug-in runs under DigitalMicrograph environment, and the software and hardware requirements are similar to those for DigitalMicrograph itself.

2.1.1 Hardware requirement

The IWFR is commercial software and thus requires a license key (a USB dongle).

2.1.2 Software requirement

The following is a list of the software requirements necessary to run the IWFR plug-in:

- **DigitalMicrograph**.
- **USB Key Driver**

2.2 Software Installation

The following modules should be installed. Please consult the ReadMe file for installation. The following modules should be placed in the folder "PlugIns" under "Gatan" folder at ProgramData.

- **IWFR Plug-in (.gtk and .dll)**
- **IPU Plug-in (Free-ware available at www.hremresearch.com)**
- **Acquire Image Series plug-in (Free-ware available at www.hremresearch.com)**
- **USB Key Driver**

Note: The PlugIns folder should exist under a normal installation of the DigitalMicrograph.

Installing IWFR Plug-in
IWFR plug-in (.gtk and .dll) can be installed by drag-and-drop copy to the folder "PlugIns" under "Gatan" folder at ProgramData.

Installing IPU Plug-in
IPU plug-in is a free plug-in. Please download the plug-in from the Scripts/Plugins page of HREM home page and install it according to the ReadMe file.

Installing Acquire Image Series Plug-in
Acquire Image Series plug-in is a free plug-in. Please download the plug-in from the Scripts/Plugins page of HREM home page and install it according to the ReadMe file.
This plug-in is required only when you want to acquire the images *on-line* from a Gatan CCD camera.

When the DigitalMicrograph is launched after placing the plug-ins the PlugIns folder, the menus "IWFR" and "IPU" will be appeared on the menu bar.

Installing Key Driver
The user key driver should be installed by following the instructions that comes with the key driver installer.   You can find the key driver on our web site.

3. Getting Started…

Using the IWFR plug-in is very simple. All the operations are menu driven, and process the front-most *active* image. This chapter briefly explains each command.

3.0 How to Create an IWFR Project

3.0.1 Projects and Images

An IWFR project is made from a series of images taken from a particular sample. These images are called through-focus images. A project must contain normally five images taken directly from the sample. The defocus distance between them be the same.

The images of the project should be aligned using the Alignment command before launching the IWFR command to reconstruct an exit wave from the sample.

3.0.2 How to Prepare Images

You can use the images directly obtained from your electron microscope for on-line processing or the images previously acquired and saved in the disk for off-line processing.
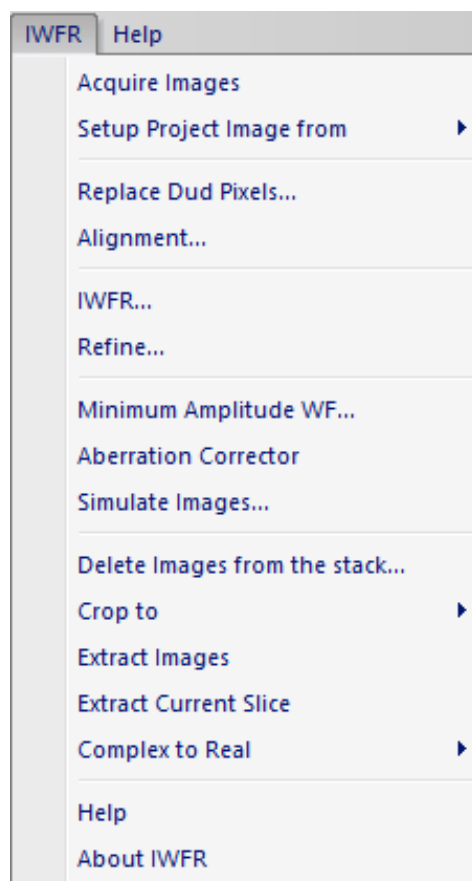
On-line processing
Capture images directly from your electron microscope using Gatan's CCD camera (see Acquire Images...).

Off-line processing
Open the existing image files, which can be opened or imported with DigitalMicropraph (see Setup Images…)

3.1 The IWFR Main Menu

The IWFR plug-in menu.

The options in the IWFR menu are described below.

Option	Description
Acquire Images...	Acquires through-focus images using Gatan camera.
Setup Project Image from	Set up a project image (stacked image) from already acquired through-focus images or a stacked image
Replace Dud Pixels	Replaces bad (defective) pixel values
Alignment...	Aligns a project image.
IWFR...	Executes the IWFR algorithm.

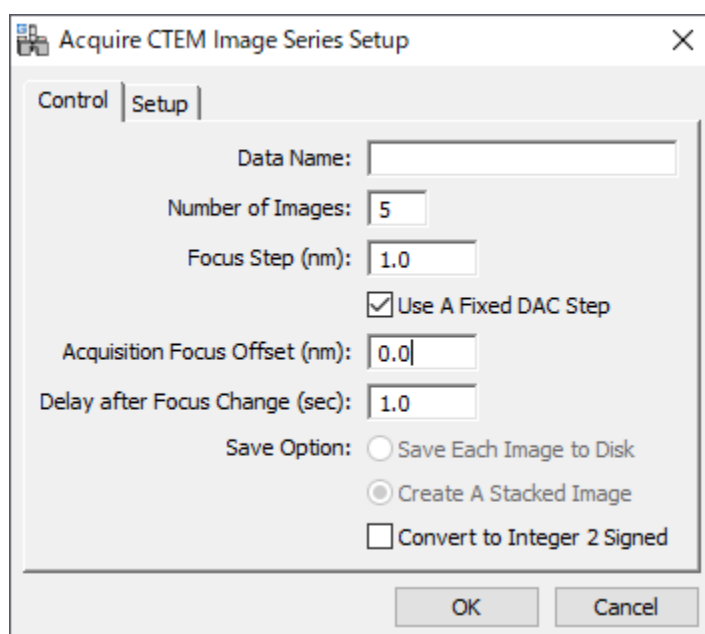|	
Refine…	Refine each defocus step and realign the images. The result can be fed into the IWFR reconstruction.
Minimum Amplitude WF...	Finds a wave function with minimum amplitude modulation
Aberration Corrector	Opens Aberration Corrector window (if not opened).
Simulate Images...	Simulate through-focus images from an exit surface wave function.
Delete Images from the stack…	Deletes some images from the image stack
Crop to	Crops the stacked image to the Common area or the ROI
Extract Images	Extracts all component images from a project
Extract Current Slice	Extracts current slice from a project.
Complex to Real	Converts a complex image to a displayable real image type (Phase/Amplitude/Real/Imaginary).
Help	Open a help document (this file)
About IWFR	Information about IWFR

3.2 Acquire Images...

Opens the Through-Focus Acquisition Setup dialog where you can control image acquisition including a defocus step. When you press 'OK,' a series of images will be acquired automatically.

NOTE   You may have to check an objective lens hysteresis which will affect an actual defocus value. It is advisable to establish a hysteresis loop and collect images along the same direction of the loop.

3.2.1 Through-Focus Acquisition Setup dialog

This dialog has two tabs: Control and Setup.

Control Tab

Component	Description
Data Name	Acquired images will be identified with this name and an added sequential number.
Number of Images	Acquired number of images (positive number).
Focus Step	Defocus step between each image (in nm). The closest defocus DAC will be used, so the defocus step may not be exactly the same. The direction of defocus change will be specified by Defocus Range parameter in the Setup Tab.

|	
Use a Fixed DAC Step	If checked, a fixed DAC close to the specified defocus step will be used.
Acquisition Focus Offset	Specifies the focus change for a first image from the current focus value.
Delay after Focus Change	Settling time after focus change (in sec)
Convert to Integer 2 Signed	Save an acquired image as Integer 2 Signed after converting from an Integer 4 Signed image. Use this option only when your image is known to be expressed as Integer 2 Signed. (Currently, an image will be acquired as Integer 4 Signed and requires a large memory space.)

Setup Tab
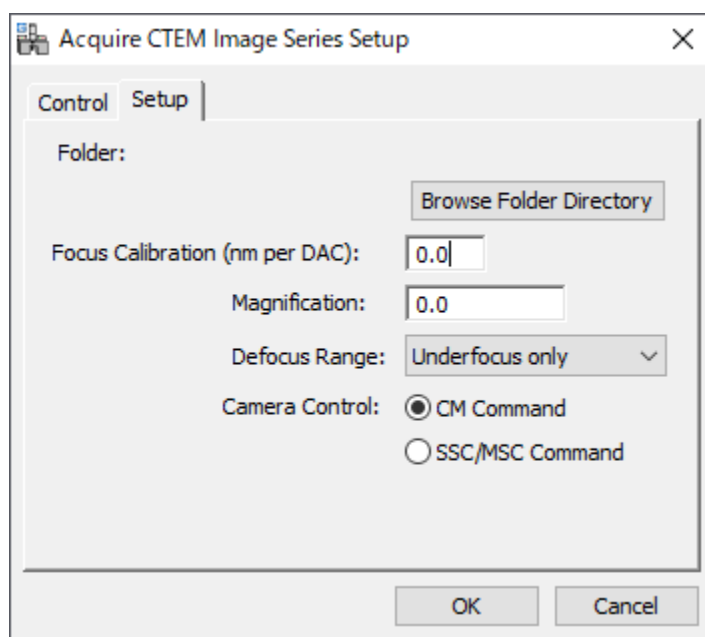
Component	Description
Folder	Acquired images will be saved into this folder, when 'Save Image to Disk' is selected. You can browse the folder directory.
Focus Step	Specifies a focus change in nm produced by a unit DAC change. This will be automatically specified, when you have Gatan's plug-in to measure this value.

Magnification	Image magnification (This will be read from your microscope, if possible.)
Defocus Range	Defocus range and direction of defocus can be selected from: Underfocus only/Overfocus only/Over to underfocus/Under to overfocus. The current defocus is the start defocus or the middle defocus of the Defocus Range depending on the range selection.
Camera Control	If you sre using the very old CCD camera, you may have to use SSC/MSC command.

3.3 Setup Project Image from

If you have already acquired through-focus images, use this command to create a project image (stacked image) to be processed with IWFR command.
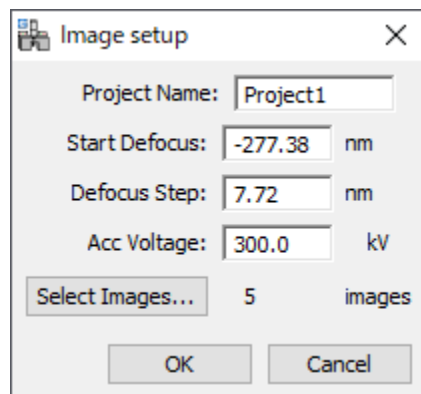
There are two ways to setup the project image.

| Setup Project Image from ▶ | Archived Image... |
| | Image Stack... |
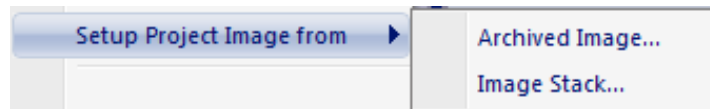
3.3.1 Archived Image...

Information of the project image will be specified using the "Image Setup dialog".

A set of through-focus images can be selected by using the standard Open dialog below.
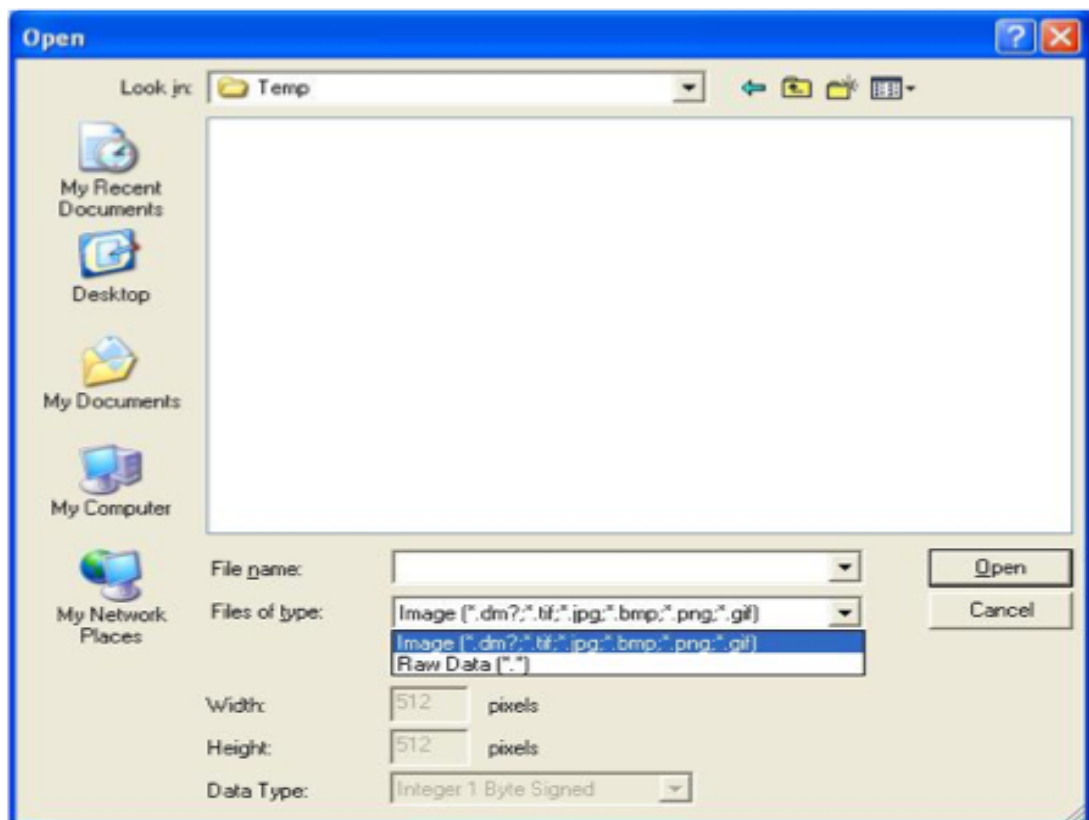
Image Setup dialog

	Image setup	✕
Project Name:	Project1	
Start Defocus:	-277.38	nm
Defocus Step:	7.72	nm
Acc Voltage:	300.0	kV
Select Images...	5	images
	OK Cancel	

Component	Description
Project Name	Input a suitable name for the project
Start Defocus	Defocus value for first image in through focal series. Note: **underfocus** is **negative**.
Defocus step	Defocus step size between images. Be careful to make sure the sign is correct, depending on the order in which you have set up the im
Acc Voltage	Accelerating voltage of the microscope.

Select Images   Opens a File Open dialog to select archived images
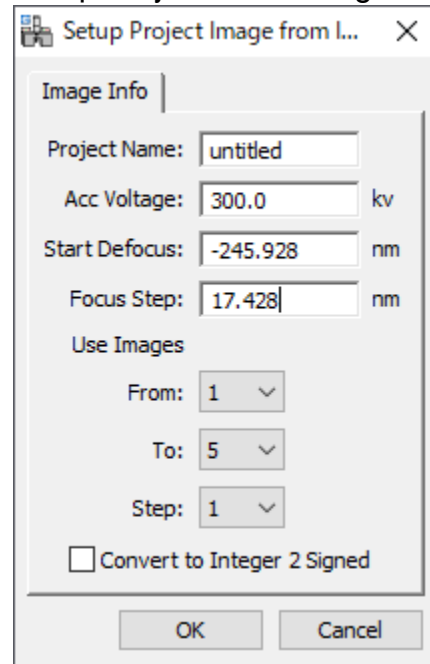
File Open Dialog

This is a standard Open dialog, so you can browse a directory and select multiple image files. When you choose "Raw data" for Files of type, you can read a binary data. In this case, you have to specify the image size (Width and Height), and Data Type.

3.3.2 Image Stack...

When you have already stacked image, use this command to create a project image to be processed with IWFR command.

Setup Project from dialog

Component	Description
Project Name	Input a suitable name for the project
Acc Voltage	Accelerating voltage of the microscope.
Start Defocus	Defocus value for first image in through focal series.
	Note: **underfocus** is **negative**.
Defocus step	Defocus step size between images. Be careful to make sure the sign is correct, depending on the order in which you have set up the im
Use Images	
From	First image
To	Last image
Step	Step (intyerval)
Convert to Integer 2 Signed	Reduces memory requirement by converting the data type from Integer 4 Signed to Integer 2 Signed. Note: The original image should be within the rage of Integer 2 Signed.

3.4 Alignment...

If the front image is a project image (stacked image), this command will align each image by translation using a cross-correlation.
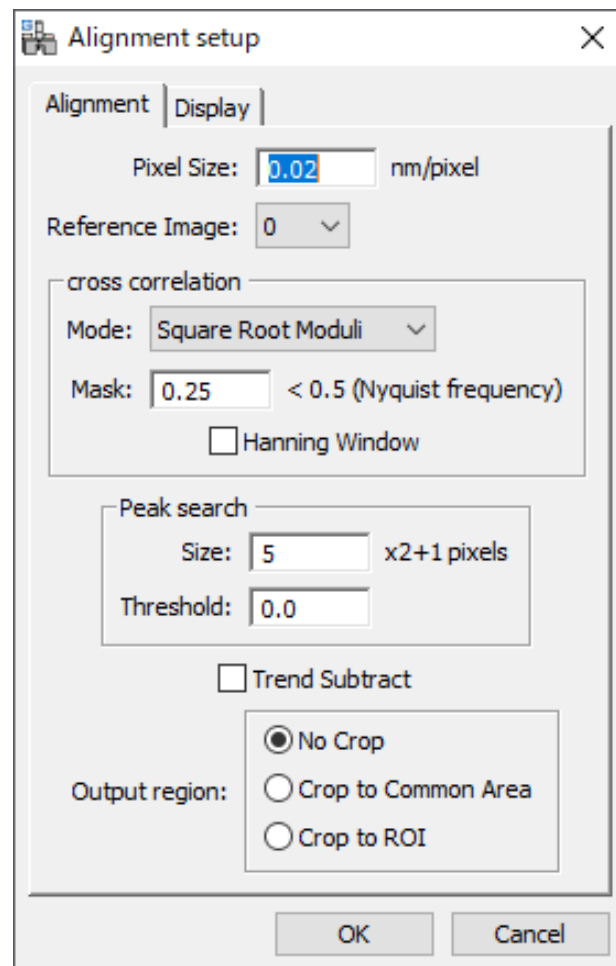
This command brings up a dialogue box for image alignment.

Note You can select an image area for alignment by placing a rectangular ROI on the image.
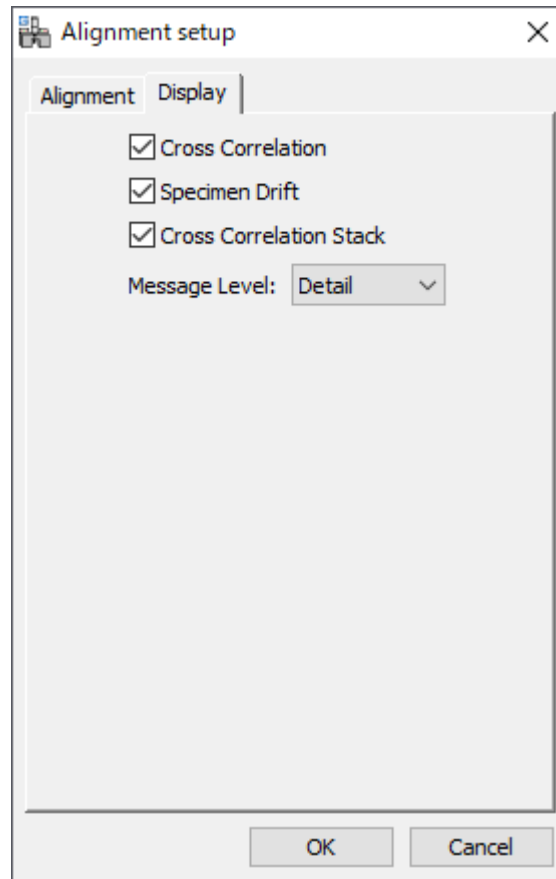
3.4.1 Alignment setup dialog

This dialog has two tabs: Alignment and Display.

Alignment Tab

Component	Description
Pixel Size	Linear size represented by one (square) pixel.
Reference Image	Select a slice number of a good image to start alignment using a cross-correlation.
Cross Correlation	
Mode	Cross-correlation mode will be selected from:
	Conventional: cross-correlation with normal amplitudes.
	Square Root Moduli: cross-correlation with square root amplitudes.
	Phase Only: cross-correlation with unit amplitudes (only phase will be retained).
	None: no alignment will be done.
Mask	Specifies the radius of a low-pass filter in Fourier space (relative to the Nyquist frequency) to reduce high-frequency noise.
Hanning Window	When checked, a Hanning Window will be applied for Fourier transforms used for cross-correlation calculations.
Peak Search	Search conditions for the cross-correlation peak.
Size	Radius of the cross-correlation peak.
Threshold	Intensity below this level will be ignored when estimating a peak center.
Trend Subtract	If checked, a trend (slowly varying feature) is subtracted for alignment to enhance the image feature.
Output region	Output region will be specified here. If the ROI is not present, "Crop to ROI" is disabled.

Display Tab

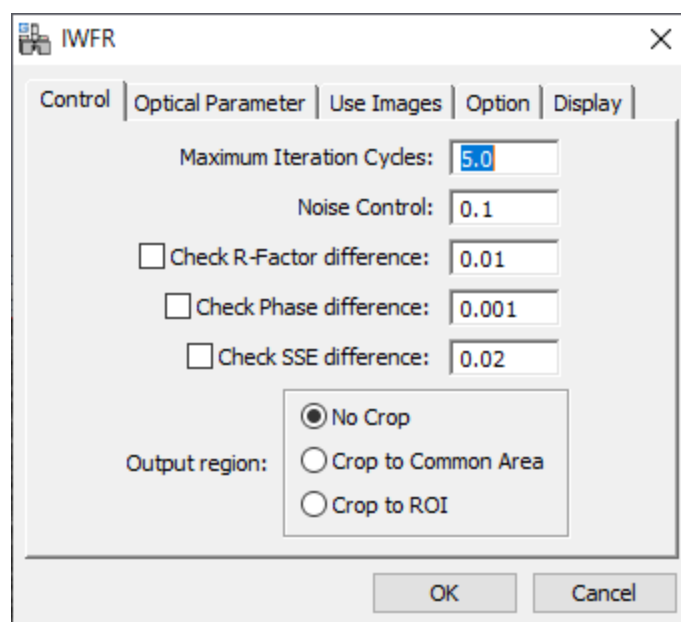| Component	Description
Cross Correlation	Displays cross correlation values between adjacent images.
Specimen Drift	Displays specimen drift values relative to the reference image.
Cross Correlation Stack	Displays 2D cross correlation maps between adjacent images.
Message level	Controls the amount of output messaging to the Results Window. (None/Normal/Detail)

3.5 IWFR...

This command brings up a dialogue box with five tabs for IWFR processing. When you press 'OK,' the IWFR processing will start.

Note When the front project image is not calibrated, a dialog asking a calibration will appear.

3.4.1 IWFR dialog

This dialog has five tabs: Control, Optical parameters, Use images, Option, and Display.
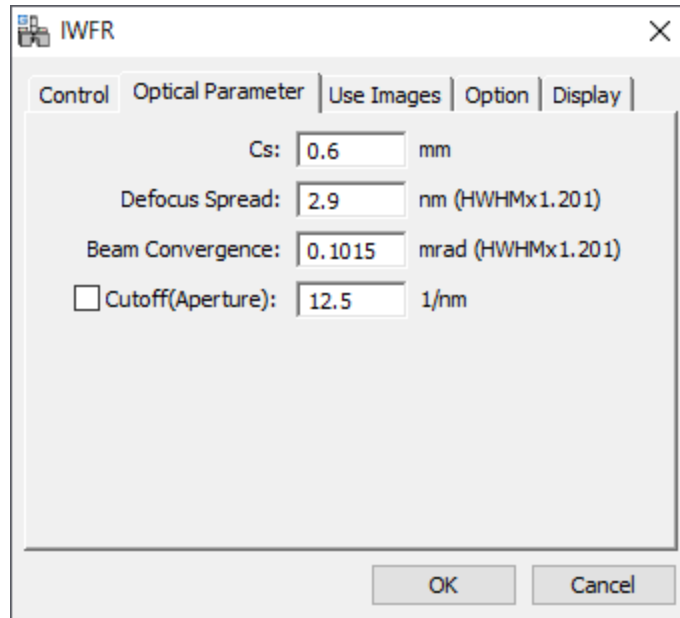
Control Tab

Component	Description
Maximum Iteration Cycles	Maximum number of iterations for the IWFR method (integer).
Noise Control	Noise magnitude used in a Thikonov Filter
Check R-Factor Difference	Check to see whether iterations have converged using the R-factor.
Check Phase difference	Check for convergence by comparing phase at consecutive cycles.
Check SSE difference	Check to see whether iterations have converged using the SSE (sum-squared error).

Output region   Output region will be specified here. The output can be cropped to the Common area and/or ROI. if they are present.

Optical Parameter Tab

IWFR	✕

Control | **Optical Parameter** | Use Images | Option | Display

Cs:	0.6	mm
Defocus Spread:	2.9	nm (HWHMx1.201)
Beam Convergence:	0.1015	mrad (HWHMx1.201)
☐ Cutoff(Aperture):	12.5	1/nm

OK   Cancel

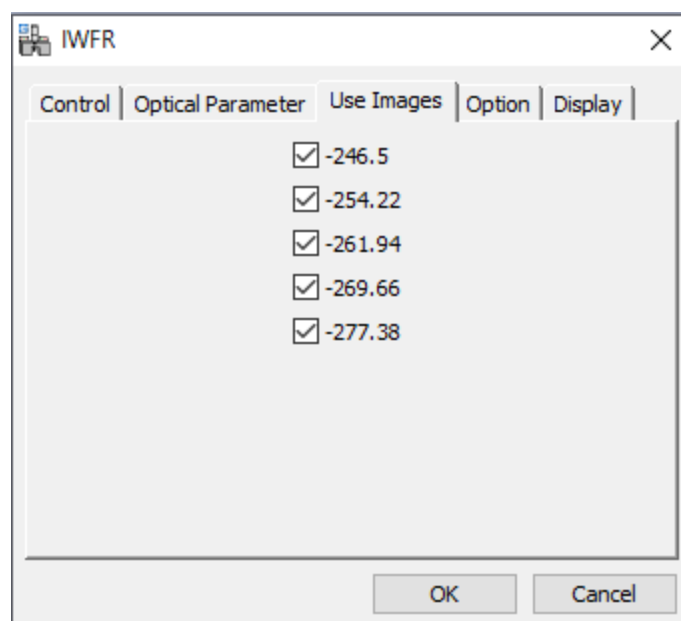| Component	Description
Cs	Third order spherical aberration coefficient
Defocus Spread	Effective defocus spread arising as a result of temporal incoherence.
Beam Convergence	Beam convergence semi-angle due to finite source size.
Cutoff (Aperture)	Effective aperture of objective lens.

Use Images Tab

Select a subset of the images in the project to perform the IWFR.

```
┌─ IWFR ──────────────────────────────── X ─┐
│                                           │
│ Control │ Optical Parameter │ Use Images │ Option │ Display │
│                                           │
│                  ☑ -246.5                 │
│                  ☑ -254.22                │
│                  ☑ -261.94                │
│                  ☑ -269.66                │
│                  ☑ -277.38                │
│                                           │
│                                           │
│                                           │
│                                           │
│                                           │
│                                           │
│                      [  OK  ]  [ Cancel ] │
└───────────────────────────────────────────┘
```

Display Tab

```
┌─ IWFR ──────────────────────────────── X ─┐
│                                           │
│ Control │ Optical Parameter │ Use Images │ Option │ Display │
│                                           │
│               ☐ Result Log                │
│               ☐ R-Factor                  │
│               ☐ Phase                     │
│               ☐ SSE                       │
│               ☐ Estimated Images          │
│               ☐ CTF                       │
│         Message Level: [ Detail      ∨ ]  │
│                                           │
│                                           │
│                      [  OK  ]  [ Cancel ] │
└───────────────────────────────────────────┘
```
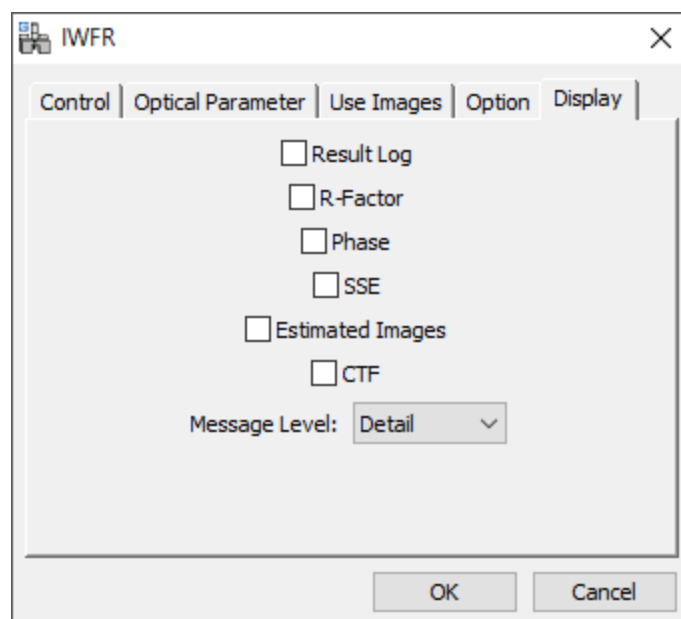
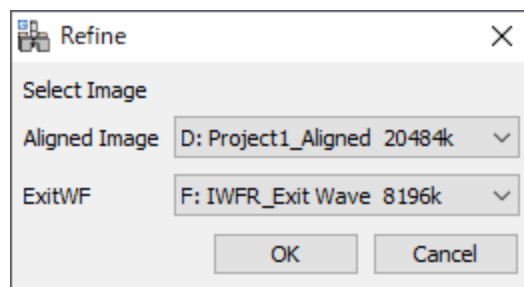| Component	Description
Result Log	Display exit surface waves at all cycles
R-Factor	Displays progress of R-factor.

Phase	Displays progress of convergence in terms of the phase.
SSE	Displays progress of convergence in terms of the SSE.
Estimated Images	Display calculated image intensities at the final cycle.
CTF	Contrast transfer function of microscope.
Message level	Controls the amount of output messaging to the Results Window. (Minimum/Normal/Detail)

3.6 Refine...

This command will refine each defocus and realign the images. The result can be fed into the IWFR reconstruction.

This will pop up the dialog below.

At first, the dialog to select the aligned image to be refined and the exit wave function will be selected.
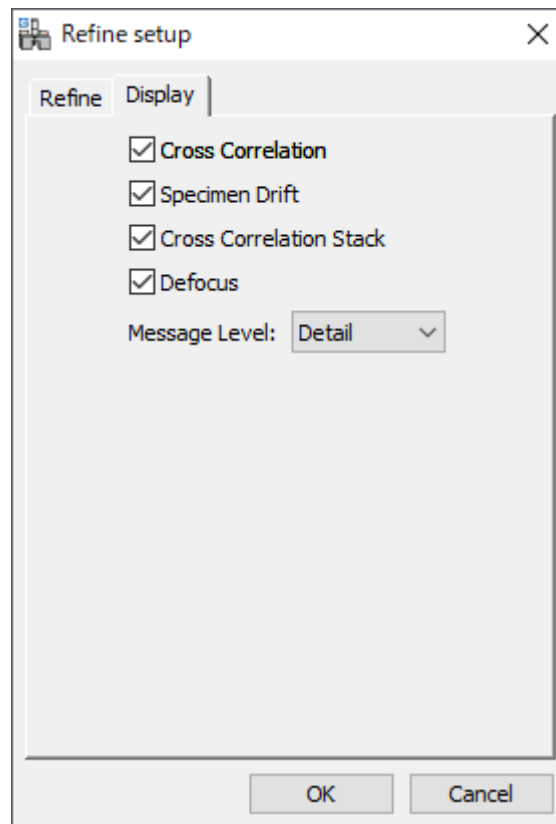

Then, the main dialog for Refine will appear, which is similar to the Alignment dialog.

Refine Tab

Component	Description
Pixel Size	Linear size represented by one (square) pixel.
Cross Correlation	
Mode	Cross-correlation mode will be selected from:
	Conventional: cross-correlation with normal amplitudes.
	Square Root Moduli: cross-correlation with square root amplitudes.
	Phase Only: cross-correlation with unit amplitudes (only phase will be retained).
	None: no alignment will be done.
Mask	Specifies the radius of a low-pass filter in Fourier space (relative to the Nyquist frequency) to reduce high-frequency noise.
Hanning Window	When checked, a Hanning Window will be applied for Fourier transforms used for cross-correlation calculations.
Peak Search	Search conditions for the cross-correlation peak.
Size	Radius of the cross-correlation peak.
Threshold	Intensity below this level will be ignored when estimating a peak center.
Trend Subtract	If checked, a trend (slowly varying feature) is subtracted for alignment to enhance the image feature.
Output region	Output region will be specified here. If the ROI is not present, "Crop to ROI" is disabled.

Display Tab

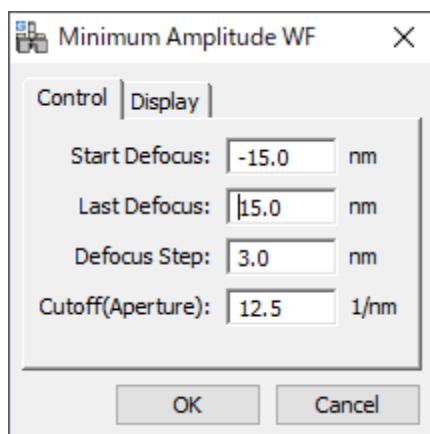| Component	Description
Cross Correlation	Displays cross correlation values between adjacent images.
Specimen Drift	Displays specimen drift values relative to the reference image.
Cross Correlation Stack	Displays 2D cross correlation maps between adjacent images.
Defocus	Displays refined defocuses
Message level	Controls the amount of output messaging to the Results Window. (None/Normal/Detail)

3.7 Minimum Amplitude WF...

This command finds a wave function with the minimum modulation (standard deviation) of image amplitude by propagating a complex (exit) wave function. This command may be used to find the wave function at the specimen exit surface, where the amplitude modulation will be minimum for a phase object. This brings up the Minimum Amplitude WF dialogue box.

3.7.1 Minimum Amplitude WF dialogue

This dialog has two tabs: Control and Display.

Control Tab

Component	Description
Start Defocus	Start defocus of the defocus range to be searched for a minimum amplitude.
Last Defocus	Last defocus of the defocus range to be searched for a minimum amplitude.
Defocus Step	Defocus step of the defocus range to be searched for a minimum amplitude.
Cutoff (Aperture)	Aperture radius in Fourier space (in 1/nm)

Display Tab
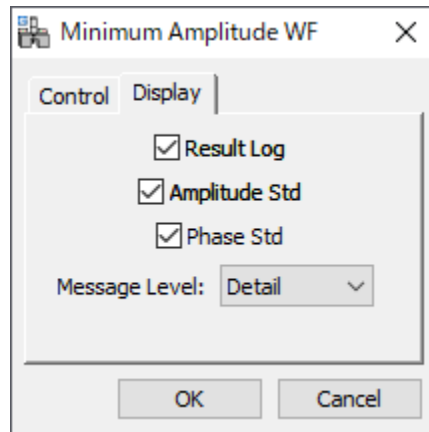
Component	Description
Result Log	Display complex wave functions at all defocuses.
Amplitude Std	Display standard deviation of amplitude of wave function from mean.
Phase Std	Display standard deviation of phase of wave function from 0.0.
Message level	Controls the amount of output messaging to the Results Window. (Minimum/Normal/Detail)

3.8 Aberration Corrector...

This command opens Aberration Corrector window (if not opened).?The aberration corrector becomes active, only when the Rectangle ROI is placed on the image. Aberration correction is applied on the fly to the image within the ROI. The same aberration will be applied to the whole image, when the Apply button is pressed.

Definition of the aberration coefficients: A pre-factor of $1/(n+1)$ is applied to the Modulus of n-th order aberration coefficient. For example, for the second order Coma (B2) the actual modulus is Modules/(2+1).

3.8.1 Aberration Corrector Pallet (Floating window)

This window has five tabs for grouped aberrations and some controls.

Component	Description
Aberration Tabs	See below.
Display	The display mode selection from Imaginary/Real/Modulus/Log of Modulus/Phase.
PCTF Button	Phase Contrast Transfer Function (Imaginary part of the aberration function) will be displayed in a separate PCTF window. The image size will be specified in the Show PCTF dialog.
Apply	Aberration correction with the current selections will be applied to the whole image.

Aberration Tabs
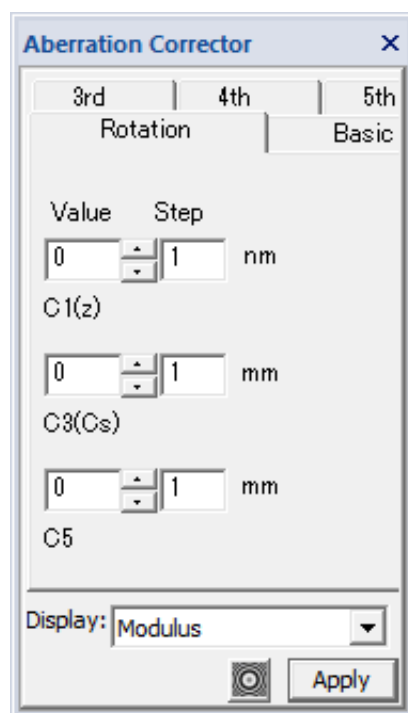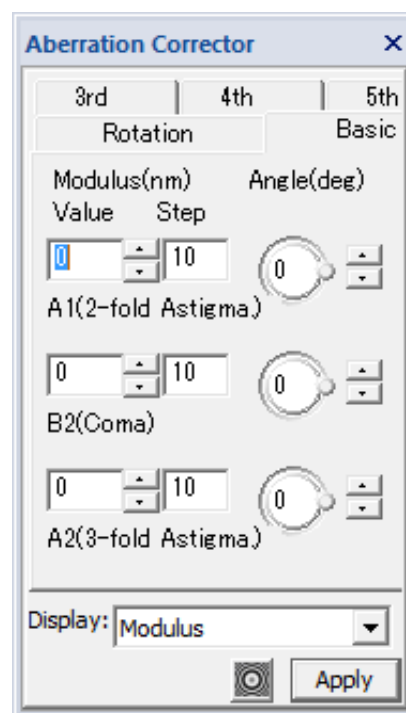
Rotation Tab   Basic/Non-Rotation Tab

Rotation Tab

Rotational aberrations, namely defocus (C1), 3rd order spherical aberration (C3) and fifth order spherical aberration (C5) will be adjusted by a value shown in the Value box. You can input directly a number in the Value box, or up/down by a step in the Step box.

Basic/Non-Rotation Tab

Basic non-rotational aberrations, namely two-fold astigmatism (A1), coma (B2) and three-fold astigmatism (A2) will be adjusted by the Modulus and Angle. The Modulus will be specified directly in the Value box, or up/down by a step in the Step box. The Angle will be specified directly in the circle, or up/down by the arrows.

Other higher-order non-rotational aberrations will be adjusted in the same way for the basic non-rotational aberrations.
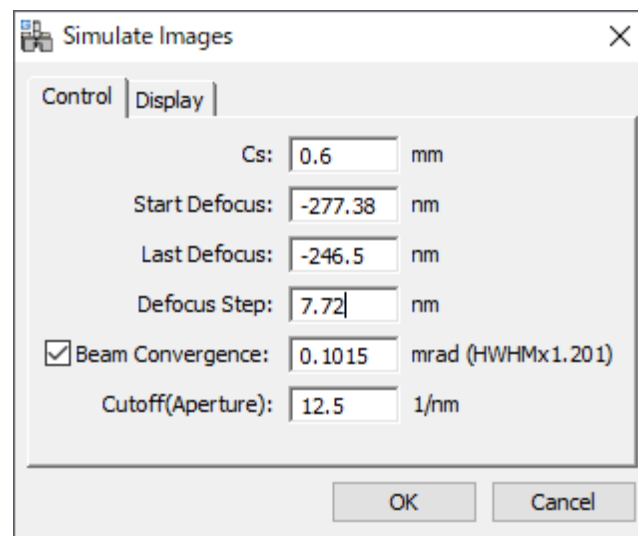
3.9 Simulate Images...

This command simulates through-focus images from an exit surface wave function for selected imaging parameters.
This brings up the Simulate Images dialog box.

3.9.1 Simulate Images dialogue

This dialog has two tabs: Control and Display.

Control Tab

Component	Description
Cs	Third order spherical aberration coefficient
Start Defocus	Start defocus of the defocus range to be simulated.
Last Defocus	Last defocus of the defocus range to be simulated.
Defocus Step	Defocus step for simulation.
Beam Convergence	Beam convergence semi-angle due to finite source size.
Cutoff (Aperture)	Effective aperture of objective lens (in 1/nm).

Display Tab
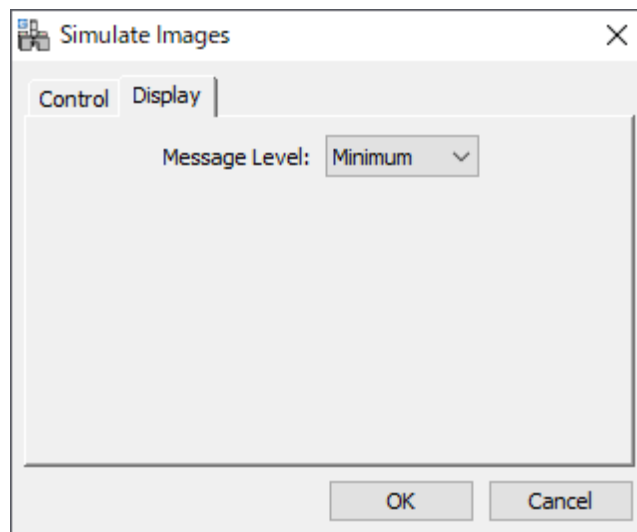
| Component	Description
Message level	Controls the amount of output messaging to the Results Window. (Minimum/Normal/Detail)

4. Utilities

4.1 Replace Dud Pixels

This command will find bad (defective) pixels in the image, whose value deviates from the average of neighbor pixels by the Tolerance times of the std (standard deviation).

The Size defines the neighbor pixels of Size x 2 + 1.
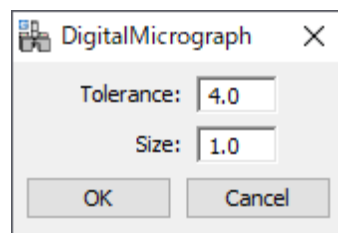
4.2 Delete Images from the stack…

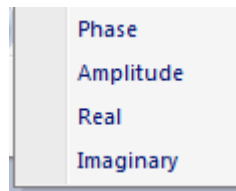This command delete the images from the image stack.

4.3 Crop to

This command crops the stacked image to the Common area or the ROI

4.4 Extract Images, Current Slice

This command extracts the all the images or a single current image of the image stack.

4.5 Complex to Real

Phase
Amplitude
Real
Imaginary

This command creates a real image from a complex image. You can select the type of the real image from the submenu.

5. Appendix

5.1 Focal series with partial coherence

We define the exit surface wave function as

$$\psi_0(\mathbf{r}) = \sqrt{I_0(\mathbf{r})} \exp[i\phi_0(\mathbf{r})], \tag{1}$$

where $I_0(\mathbf{r})$ is the intensity at the exit surface, $\phi_0(\mathbf{r})$ is the phase and $\mathbf{r}$ is a vector perpendicular to the optical axis. The subscript 0 denotes the exit surface.

The momentum space wave function is given by

$$\Psi_0(\mathbf{q}) \equiv F[\psi_0(\mathbf{r})] = \sqrt{I_0(\mathbf{q})} \exp[i\phi_0(\mathbf{q})], \tag{2}$$

where F denotes the Fourier transform and $\mathbf{q}$ is the momentum space variable conjugate to $\mathbf{r}$.

The diffractogram formed by propagation to the nth plane is given by

$$\begin{aligned}
\hat{I}_n(\mathbf{q}) &\equiv F[I_n(\mathbf{r})] \\
&= \int T_n^{CC}(\mathbf{q}' + \mathbf{q}, \mathbf{q}') \Psi_0(\mathbf{q}' + \mathbf{q}) \Psi_0^*(\mathbf{q}') \mathrm{d}\mathbf{q}',
\end{aligned} \tag{3}$$

where the transmission cross coefficient for the nth plane takes the usual form

$$T_n^{CC}(\mathbf{q}' + \mathbf{q}, \mathbf{q}') = T_n(\mathbf{q}' + \mathbf{q}) T_n^*(\mathbf{q}') E_s(\mathbf{q}' + \mathbf{q}, \mathbf{q}') E_\Delta(\mathbf{q}' + \mathbf{q}, \mathbf{q}'). \tag{4}$$

The transfer function of the optical system is defined by

$$T_n(\mathbf{q}) = A(\mathbf{q}) \exp[-i\chi_n(\mathbf{q})], \tag{5}$$

where $A(\mathbf{q})$ is a top hat function describing the objective aperture.

Considering only defocus (positive for over-focus) and third order spherical aberration described by the coefficient C_s we have

$$\chi_n(\mathbf{q}) = \pi\lambda\Delta f_n q^2 + 0.5\pi\lambda^3 C_s q^4,$$ (6)

where λ is the wavelength of the incident electrons.

The spatial and temporal coherence envelope functions are given by

$$E_s(\mathbf{q'} + \mathbf{q}, \mathbf{q'}) = \exp\left\{-\frac{\beta^2}{4\lambda^2}\left[\frac{\partial\chi_n(\mathbf{q'} + \mathbf{q})}{\partial\mathbf{q'}} - \frac{\partial\chi_n(\mathbf{q'})}{\partial\mathbf{q'}}\right]^2\right\}$$ (7)

and

$$E_\Delta(\mathbf{q'} + \mathbf{q}, \mathbf{q'}) = \exp\left\{-\frac{\Delta^2}{4}\left[\frac{\partial\chi_n(\mathbf{q'} + \mathbf{q})}{\partial\Delta f} - \frac{\partial\chi_n(\mathbf{q'})}{\partial\Delta f}\right]^2\right\}$$ (8)

respectively, with β the beam convergence semi-angle and Δ the defocus spread (1/e values).

For the IWFR method we approximate Eq. (4) above by

$$T_n^{CC}(\mathbf{q'} + \mathbf{q}, \mathbf{q'}) = T_n(\mathbf{q'} + \mathbf{q})T_n^*(\mathbf{q'})E_s^{coh}(\mathbf{q'} + \mathbf{q})E_s^{coh*}(\mathbf{q'})E_\Delta^{coh}(\mathbf{q'} + \mathbf{q})E_\Delta^{coh*}(\mathbf{q'})$$ (9)

where $T_n(\mathbf{q})$ is defined in Eq. (5),

$$E_s^{coh}(\mathbf{q}) = \exp\left\{-\frac{\beta^2}{4\lambda^2}\left[\frac{\partial\chi_n(\mathbf{q})}{\partial\mathbf{q}}\right]^2\right\}$$ (10)

and

$$E_\Delta^{coh}(\mathbf{q}) = \exp\left\{-\frac{\Delta^2}{4}\left[\frac{\partial\chi_n(\mathbf{q})}{\partial\Delta f}\right]^2\right\}.$$ (11)

This allows propagation via

$$\Psi(\mathbf{q}) = \Psi_0(\mathbf{q})T(\mathbf{q})E_s^{coh}(\mathbf{q})E_\Delta^{coh}(\mathbf{q})$$ (12)