IWFR
for DigitalMicrograph

Iterative Wavefunction Reconstruction

IWFR Manual 2.1

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

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1. Introduction

IWFR (Iterative Wavefunction Reconstruction) is a plug-in for use in Gatan's DigitalMicrograph for GMS 2.x and 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, and 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 about five images. Using the wave function obtained you can correct optical aberrations such as spherical aberration.

The IWFR is in the spirit of the Gerchberg-Saxton algorithm (which uses 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.

At first, the IWFR assumes that the images are taken with a fixed defocus step, and reconstructs the complex wave function at the exit surface. Using the wave function obtained, however, each defocus can be refined (Refine Defocuses routine), and then a new exit wave function can be obtained by using the revised defocuses.

1.2 Summary of IWFR Procedure

The IWFR procedure 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.
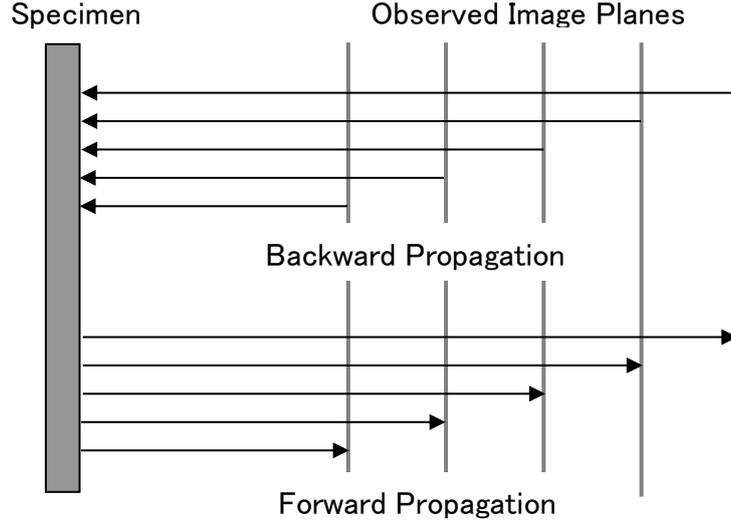
The details of steps of the *original* IWFR process are as follows:

1) Start with a through focal series comprising N experimental images, with the intensity in each plane n denoted by $I_n(\boldsymbol{r})$. The initial phase is set to zero: $\phi_n^1(\boldsymbol{r}) = 0$ 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) *Backward propagation:* 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 $\Delta f = 0$ backward 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) *Forward propagation*: Propagate $\Psi_{avg}^j(\boldsymbol{q})$ to each of the N experimental image planes to obtain $\tilde{\Psi}_n^j(\boldsymbol{q})$, the estimated wave functions in momentum space.

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

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

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

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 $\Psi_{avg}^j(q)$. Otherwise set $\phi_n^{j+1}(r) = \widetilde{\phi}_n^j(r)$ and return to step (2) for iteration $j + 1$.

1.3 References and Technical Notes

L.J. Allen, W. McBride, N.L. O'Leary, M.P. Oxley: Exit wave reconstruction at atomic resolution; Ultramicroscopy 100 (2004) 91-104.

K. Ishizuka: Phase retrieval from image intensities: Why does exit wave restorationf using IWFR work so well?: Microscopy, 62 (2013), S109–S118.

TIPS: It has been verified that the use of the image intensity itself is better to start the IWFR iteration. Thus, the initial backpropagation will be done simply using $I_n(r)$. (See K. Ishizuka: Phase retrieval from image intensities: Why does exit wave restoration using IWFR work so well?: Microscopy, 62 (2013), S109–S118.)

NOTE: Initially a fixed defocus step is assumed during the IWFR iteration. However, each defocus value can be adjusted using the averaged wave function at specimen exit surface. (See Refine Defocuses command.)

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 or more taken directly from the sample.

The defocus distance between the images is assumed to be the same. However, small changes of the defocus intervals can be estimated by the Refine routine, and the revised defocus values will be used in the following IWFR routine.

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
Use the existing image files, which can be opened or imported with DigitalMicropraph (see **Setup Images…**)

3.1 The IWFR Main Menu
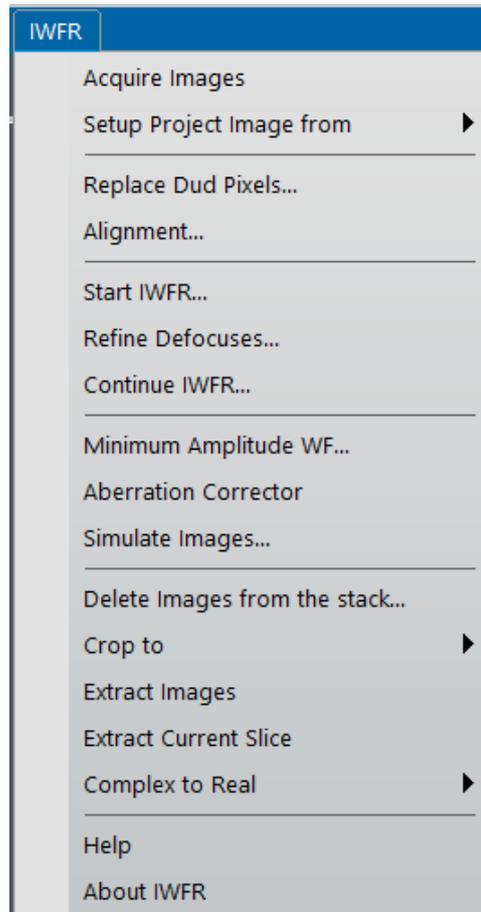
The IWFR plug-in menu.

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.
Start IWFR...	Begins IWFR iteration using the image intensities.

NOTE: This is the original IWFR routine.

|	
Refine Defocuses…	Refines defocus values and image realignment using the Exit Wave determined with Start or Continue IWFR iteration. The result can be fed into Start or Continue IWFR.
Continue IWFR...	Resumes IWFR iteration using the Exit Wave previously determined. This command can be used after Start IWFR or Refine Defocuses.
Minimum Amplitude WF...	Finds a wave function with minimum amplitude modulation by propagating the wave function estimated by the IWFR routine. This routine will estimate the wave function at the exit surface.
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 existing image stack. Using this command you can reduce the number of images to be processed by the IWFR.
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 the current slice of a project stack.
Complex to Real	Converts a complex image to a displayable real image showing 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 one direction of the loop.

3.2.1 Through-Focus Acquisition Setup dialog

This dialog has two tabs: Control and Setup.

Control Tab
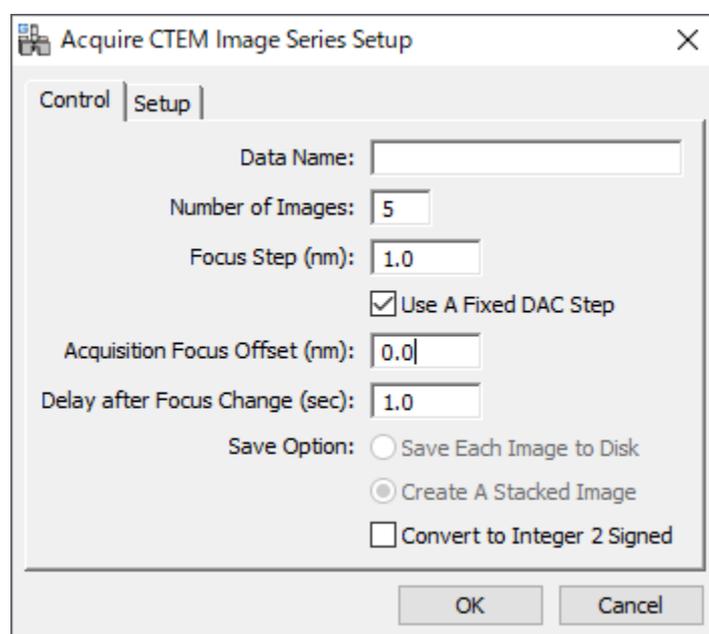
Component	Description
Data Name	Acquired images will be identified with this name and an added sequential number.
Number of Images	Acquired number of images (positive number).
Focus Step	Defocus step between each image (in nm). The closest defocus DAC will be used, so the defocus step may not be exactly the same, if "Use A Fixed DACX Step" is not checked. 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 offset for the 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 as acquired. 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
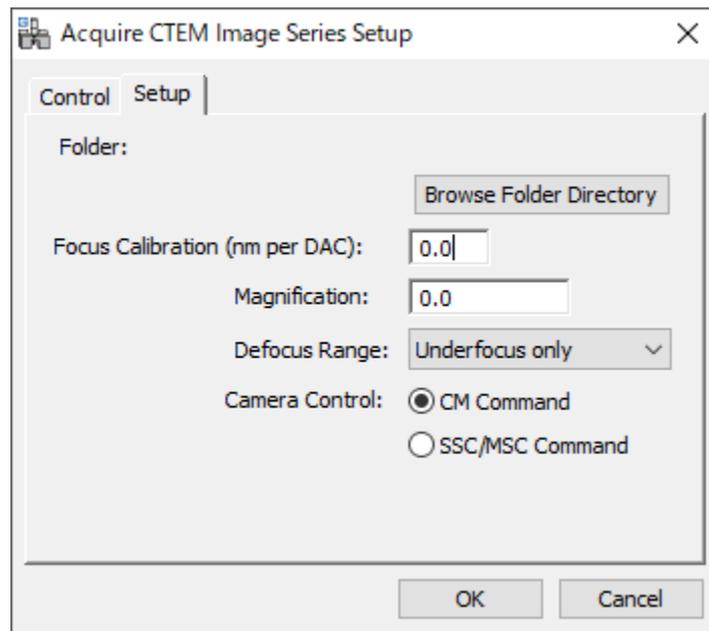
Component	Description
Folder	Acquired images will be saved into this folder, when 'Save Image to Disk' is selected. You can browse the folder directory.
Focus Step	Specifies a focus change in nm produced by a unit DAC change. This will be automatically specified, when you have Gatan's plug-in to measure 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: Archived Images or Image Stack.

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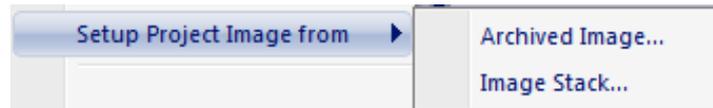
3.3.1 Archived Image...

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 discussed 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
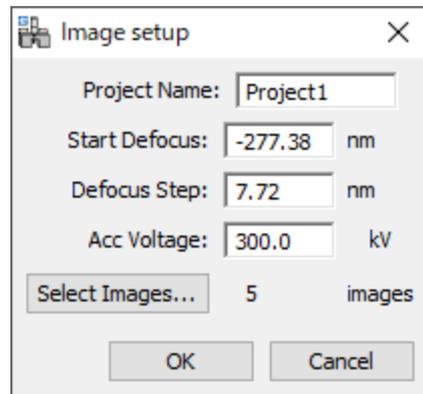
Component	Description
Project Name	Input a suitable name for the project.
Start Defocus	Defocus value for first image in through focal series. **Note**: *Underfocus* is *negative*.
Defocus step	Defocus step between images. Be careful to make sure the sign is correct.
Acc Voltage	Accelerating voltage of the microscope.
Select Images	Opens a **File Open** dialog to select archived images. A number of the selected images will be shown.

File Open Dialog

This is a standard Open dialog, so you can browse a directory and select multiple image files.
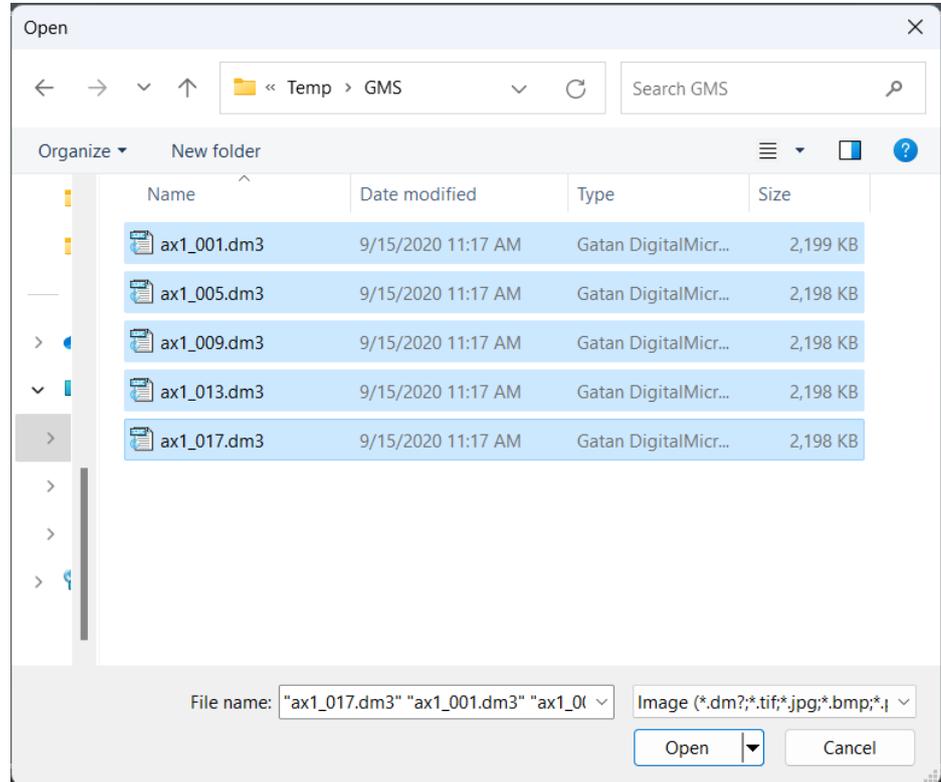

When you select a set of multiple files, all the names of selected files will be shown in the File Name field.   Please note that the files will be read according to the name list sorted by alphabetical order, but not the order shown in the file name field. The easy way to determine the order to be read is to name the image with <base_name>.<image number>.

3.3.2 Image Stack...

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

Setup Project from dialog
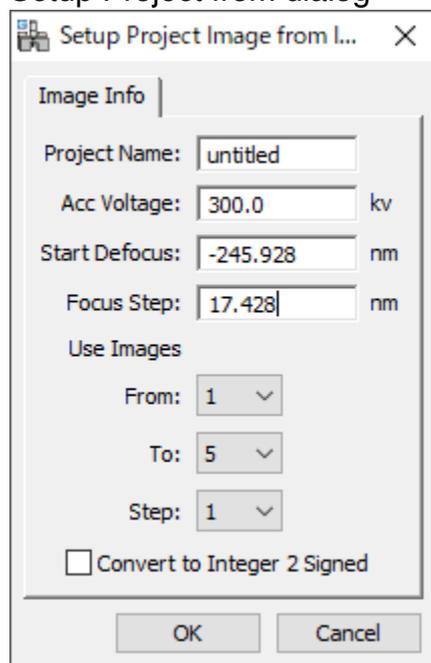
Component	Description
Project Name	Input a suitable name for the project
Acc Voltage	Accelerating voltage of the microscope.
Start Defocus	Defocus value for first image in through focal series. Note: *Underfocus* is <u>*negative*</u>.
Defocus step	Defocus step size between images. Be careful to make sure the sign is correct, depending on the order of stacked stacked image.
Use Images	

From
   To
   Step
	First image
	Last image
	Step (interval)

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 you want, you can crop the result to the Common Area or to the ROI. When the ROI is not present, "Crop to ROI" is disabled.

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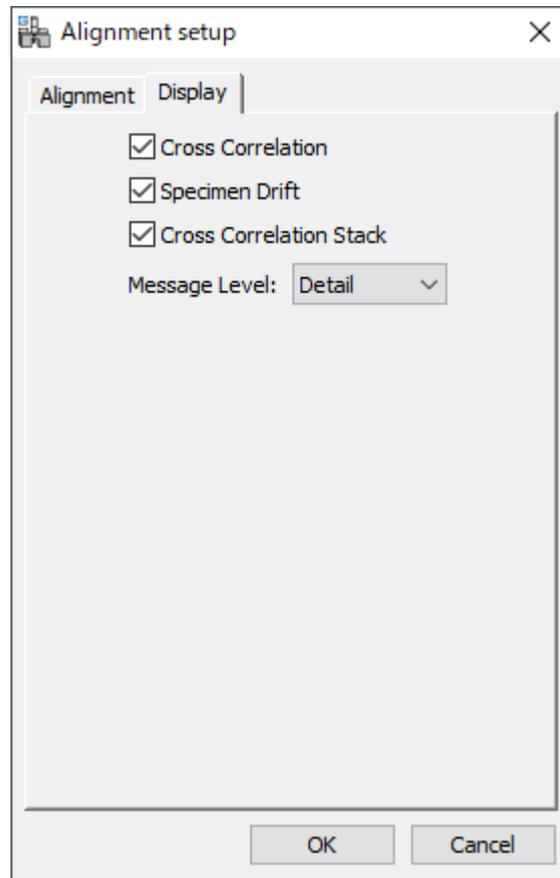
Component	Description
Cross Correlation	Displays cross correlation values between adjacent images.
Specimen Drift	Displays specimen drift values relative to the reference image.
Cross Correlation Stack	Displays 2D cross correlation maps between adjacent images.
Message level	Controls the amount of output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

3.5 Start IWFR... / Continue IWFR…

There are two IWFR commands, namely Start IWFR and Continue IWFR. The former starts the IWFR iteration using the observed intensity, while the latter requires the wave function estimated at the specimen exit surface. Thus, Continue IWFR can be used only after Start IWFR or Refine Defocuses.

Since both commands bring up the same dialogue box with five tabs for IWFR processing, we explain the dialog here only for Start IWFR. When you press 'OK,' the IWFR processing will start.

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

3.5.1 IWFR dialog

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

Control Tab
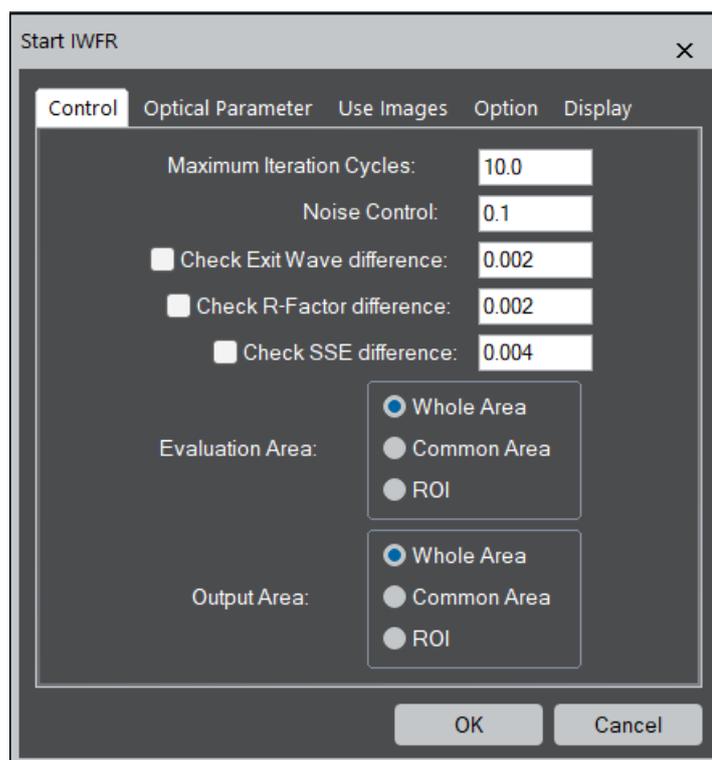
Component	Description
Maximum Iteration Cycles	Maximum number of IWFR iterations (integer).
Noise Control	Noise parameter used in a Tikhonov Filter

Check Exit Wave Difference	Check for convergence by using *relative* Difference of Exit Wave: namely, sum of Abs (Exit Wave Difference) / sum of Abs (Exit Wave).
Check R-Factor Difference	Check for convergence by using *relative* Difference of R-factor: namely, (R-factor Difference) / R-factor.
Check SSE Difference (Sum of Squared Error)	Check for convergence by using *relative* Difference of SSE: namely, (SSE Difference) / SSE.
Evaluation Area	An area to be used for IWFR iteration will be selected here.
Output Area	Output area will be selected here. When the ROI is not present, "Crop to ROI" is disabled. Output area should be equal to or smaller than the Evaluation area.

Optical Parameter Tab

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.
Information Limit	The highest frequency of information that exists in the image, which corresponds to an effective aperture of objective lens.
Use	Selection list of information ranges to be used from Whole, 1/2, 1/3, 1/4.
	Usually, the whole information will be used for the IWFR iteration. However, when the defocus step has an appreciable error, you may want to restrict the range of information for the IWFR Iteration, and then use Refine Defocuses command.

Use Images Tab
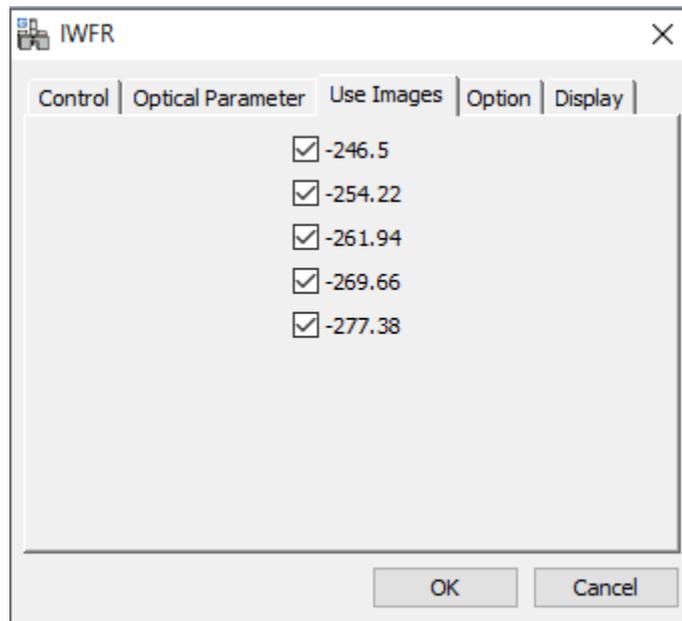
Select a subset of the images in the project to be used for the IWFR.

Option Tab
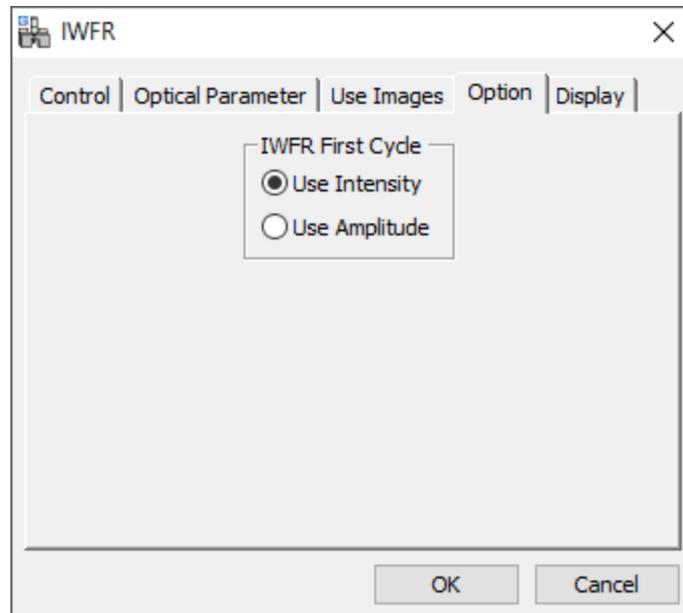
It has been verified that the use of the intensity itself of the observed image is better to start the IWFR iteration, although the *original* IFWR code uses the amplitude of the observed image (sqrt of image intensity). (See References and Technical Notes)

Display Tab
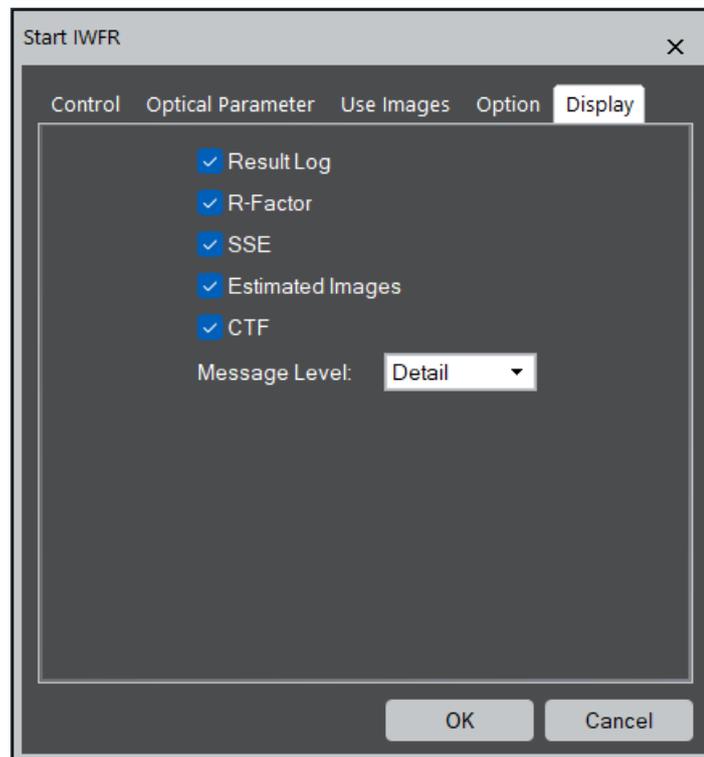
| Component	Description
Result Log	Display exit waves at all cycles as an image stack.
R-Factor	Displays the change of R-factor with the cycle.
SSE	Displays the change of the SSE with the cycle.
Estimated Images	Display calculated image intensities at the final cycle.
CTF	Contrast transfer function of microscope.
Message level	Controls the amount of output messaging to the Results Window. (Minimum/Normal/Detail)

3.6 Refine Defocuses...

This command will refine the image shift and determine each defocus of the image stack using the exit wave and the observed image intensities. The new image stack named as *project-name_*Rn will be created, where *n* is the cycle number of the Refine. The result *project-name_*Rn can be fed into the IWFR reconstruction, namely Start IWFR or Continue IWFR. The IWFR and Refine can be repeatedly performed.

Since this command uses the exit wave, the front image should be a project image (stacked image) after the IWFR has been performed.

3.6.1 Refine Defocuses dialog

Refine Defocuses dialog is similar to the one for Alignment.

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.
Evaluation Area	An area to be used to refine defocuses will be selected here.
Output Area	Output area will be selected here. When the ROI is not present, "Crop to ROI" is disabled. Output area should be equal to or smaller than the Evaluation area.

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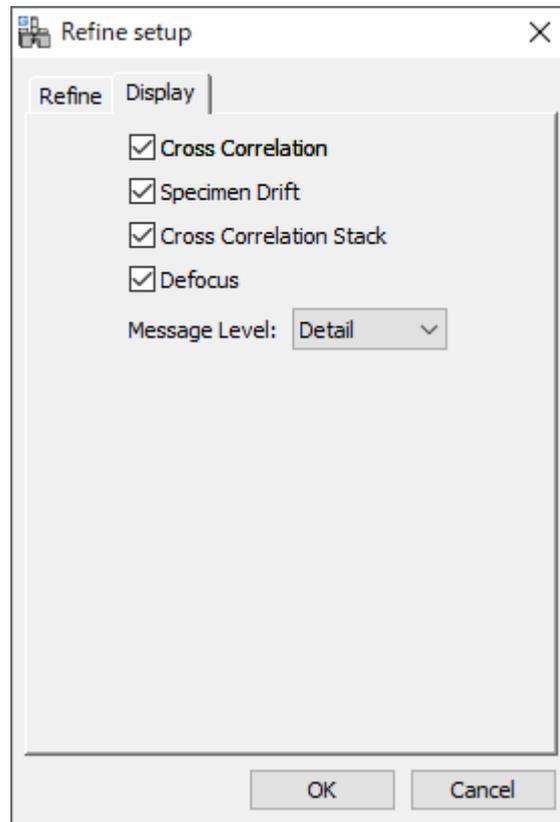
Component	Description
Cross Correlation	Displays cross correlation values between adjacent images.
Specimen Drift	Displays specimen drift values relative to the reference image.
Cross Correlation Stack	Displays 2D cross correlation maps between adjacent images.
Defocus	Displays refined defocuses
Message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

The Refine command will show the refined Defocus in addition to Cross-correlation, Specimen drift,

## 3.7 Minimum Amplitude WF...

This command finds a wave function with the minimum modulation (standard deviation) of image amplitude by propagating a complex wave function obtained by the IWFR command. 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.

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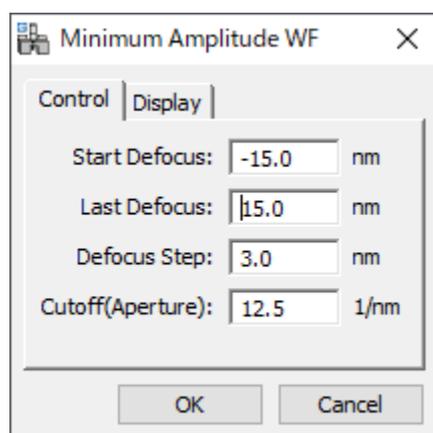
Component	Description
Start Defocus	Start defocus of the defocus range to be searched for a minimum amplitude.
Last Defocus	Last defocus of the defocus range to be searched for a minimum amplitude.
Defocus Step	Defocus step of the defocus range to be searched for a minimum amplitude.
Cutoff (Aperture)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

Display Tab
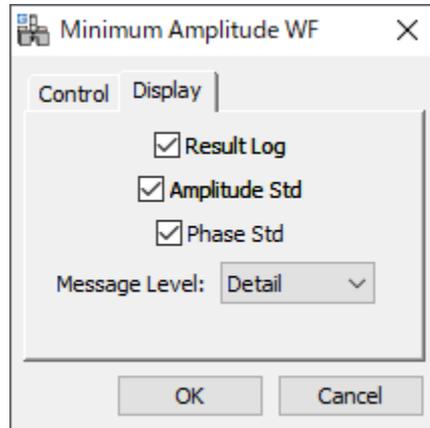
Component	Description
Result Log	Displays complex wave functions at all defocuses.
Amplitude Std	Displays the standard deviation of amplitude of wave function from mean.
Phase Std	Displays the standard deviation of phase of wave function from 0.0.
Message level	Controls the amount of output messaging 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 Palette (Floating window)

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

| Component	Description
Aberration Tabs	See below.
Display	The display mode selection for the complex image from Imaginary /Real /Modulus /Log of Modulus /Phase.
Aberration Figure (Button)	When clicked, "Show Aberration Figures" dialog will open. (see the dialog below).
Apply	The whole image corrected for aberration with the current parameters will be displayed in the new window.

NOTE The rectangular ROI should be placed on the exit wave image to activate the aberration corrector palette. All controls will be in gray, before the ROI is placed.

Aberration Tabs
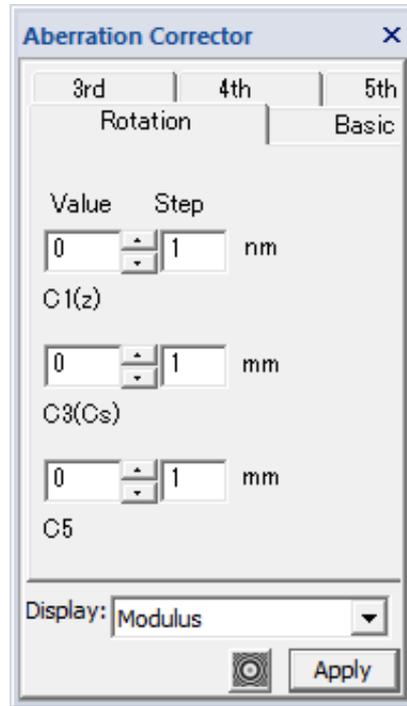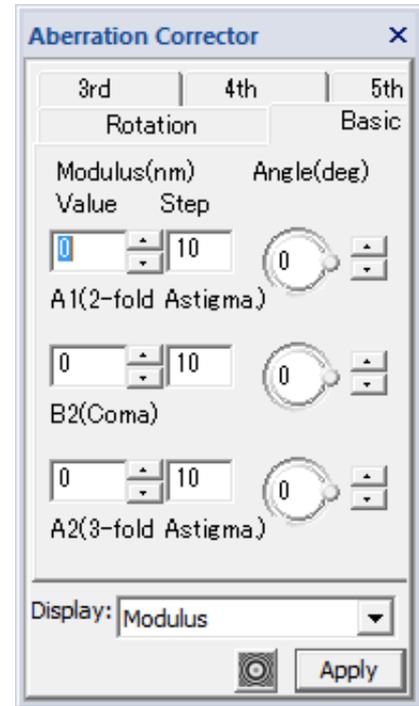
Rotation Tab   Basic Tab (Non-Rotation)

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. You can input directly the step.

Basic Tab (Non-Rotation)

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. You can input directly the step.

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

3.8.2 Aberration figures

The applied aberration figures can be displayed using the "Aberration Figure" button. Since the wave aberration is a complex function, the imaginary part and the phase of the aberration function are displayed as a PCTF (Phase Contrast Transfer Function and a Phase plate, respectively.   When "Show Aberration Figures" button is clicked, the dialog shown below will open:
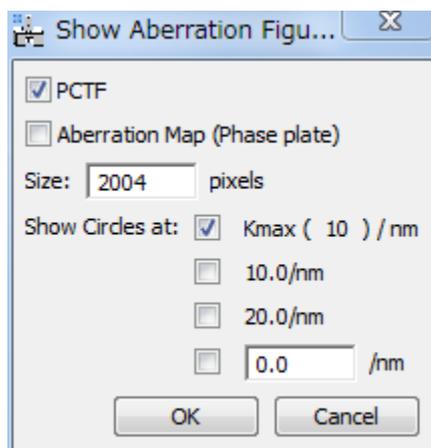
Here, you can choose PCTF and/or Aberration Map, the size of the figure(s) in pixels. You can also draw the circle(s) corresponding to Kmax, 10.0/nm, 20.0/nm and any radius you want.

When you click "OK," the aberration figure(s) will be displayed in a new window(s). These figures will change when the aberration parameters are modified. The figure below shows a typical aberration map (phase plate).
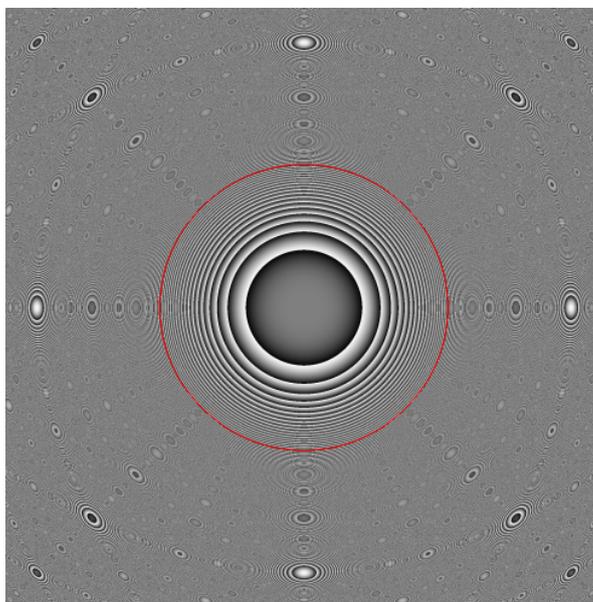
You may note the features at high angle are not real, but result in the moiré effect.

NOTE The aberration figures show only the aberration that is applied to the complex wave function on the front image. Thus, it is not the aberrations that is applied during the image formation.

3.9 Simulate Images...

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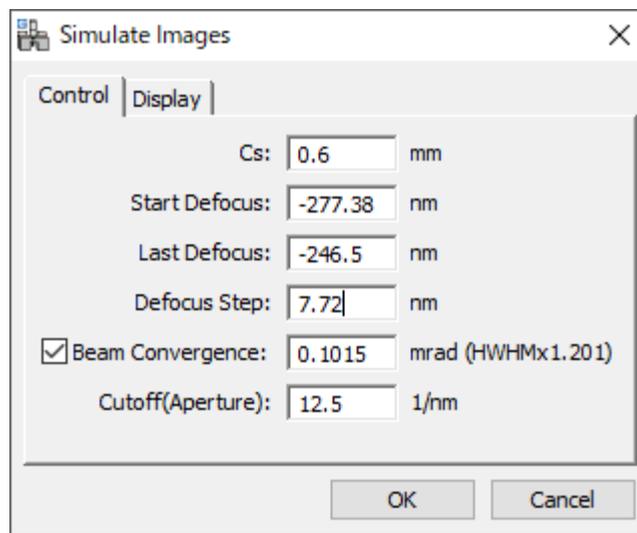
Component	Description
Cs	Third order spherical aberration coefficient
Start Defocus	Start defocus of the defocus range to be simulated.
Last Defocus	Last defocus of the defocus range to be simulated.
Defocus Step	Defocus step for simulation.
Beam Convergence	Beam convergence semi-angle due to finite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

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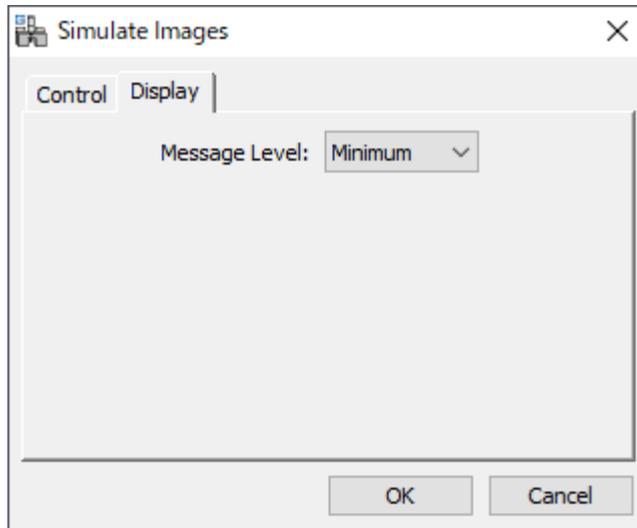
Component	Description
Message level	Controls the amount of output messaging to the Results Window. (Minimum/Normal/Detail)

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.
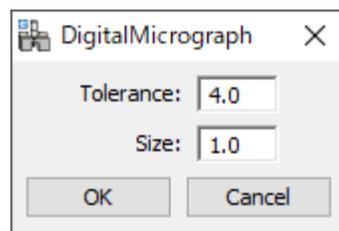
4.2 Complex to Real

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 iteration we approximate Eq. (4) above by

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

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

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

and

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

This allows propagation via

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