HREM-Filters Pro/Lite

with
Realtime Upsampling Filter

User's Guide

DigitalMicrograph Plugin
for
Image Filter Functions

Pro: Commercial Software
Lite: Free Software

1. Introduction

HREM-Filters Pro/Lite is a plug-in for use in Gatan's DigitalMicrograph (GMS 2.x or later). However, we will recommend you to use the latest version.

This HREM-Filters Pro/Lite User's Guide is written to provide information on the basic functions of the HREM-Filters Pro/Lite software, 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.

Note: *HREM-Filters Lite* is free software, so anyone can use this software without a license. However, HREM Research Inc. does not renounce a copyright of this software.

Technical Support

General enquiries on the HREM-Filters should be sent to:

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

Copyright Statements

© Copyright 2006-2024 HREM Research Inc.

All rights reserved. This manual is protected by international copyright laws and treaties. Unauthorized reproduction and distribution of this manual, or any portion of it, will be prosecuted to the maximum extent possible and may result in severe civil and criminal penalties.

DigitalMicrograph is a trademark of Gatan Inc.

2. Installation

This chapter describes hardware and software requirements to run the HREM-Filters Pro/Lite plug-in and an installation procedure of the plug-in.

2.1 Requirements

The HREM-Filters Pro/Lite 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 HREM-Filters Pro is commercial software and thus requires a license key (a USB dongle), while the HREM-Filters Lite is free software and thus requires no license key.

2.1.2 Software requirement

The following is a list of the software requirements necessary to run the HREM-Filters Pro/Lite plug-in:

- **DigitalMicrograph (GMS 2.x or later)**
- **USB Key Driver (only required for HREM-Filters Pro)**

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 "Gatan/PlugIns"of ProgramData (hidden folder).

- **HREM-Filters Pro or HREM-Filters Lite Plug-in (.gtk and .dll)**
- **HREM Mouse Tool Plug-in (Free-ware available at www.hremresearch.com)**
- **IPU Plug-in (Free-ware available at www.hremresearch.com)**
- **USB Key Driver (only required for HREM-Filters Pro)**

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

Installing HREM-Filters Pro or HREM-Filters Lite Plug-in
HREM-Filters Pro or HREM-Filters Lite (.gtk and .dll) can be installed by drag-and-drop copy to the folder "Gatan/PlugIns" of ProgramData (hidden folder).

Installing HREM Mouse Tool Plug-in
This is a free plug-in. Please download the plug-in from the PRODUCT/DM Free Plugins page and install it according to the ReadMe file.

Installing IPU Plug-in
This is a free plug-in. Please download the plug-in from the PRODUCT/DM Free Plugins page and install it according to the ReadMe file.

When the DigitalMicrograph is launched after placing the plug-ins in the PlugIns folder, HREM-Filters Pro/Lite commands will appear under "Filters" menu and the Mouse tool will be appeared as an addition to the standard tools.

Installing Key Driver
The user key driver should be installed by following the instructions given by the key driver installer (**only required for HREM-Filters Pro**).   The key driver installer comes with HREM Filters Pro, or you can find it on our web site.

3. Getting Started…

Using the HREM-Filters Pro/Lite is very simple. All the operations are menu driven, and process the front *active* image. This chapter briefly explains each command.

3.0 Essentials

3.0.1 Noise model

The noise model is very important to extract a signal from a noisy image. Thus, HREM-Filters Pro supports two noise models: Amorphous noise and Random noise. Here, the amorphous noise means the noise from non-periodic substrate (amorphous material), while the random noise corresponds to white noise or statistical noise (Poisson noise).

The amorphous model will use a smoothed background in Fourier space, and be applicable for the most of the cases. However, the random model will be useful for an ADF STEM image or an elemental map, where the statistical noise is significant.

How amorphous noise model works

The background of the filter for the amorphous noise model is estimated as a lower-bound of the image spectrum. During the filter operation only the spectrum that is higher than the background is contribute the filtered image. Thus, the amorphous noise model will effectively extract a periodic structure.

However, non-periodic structures, such as a grain boundary or defect(s), will contribute to the image spectrum in the similar way that amorphous material contribute to the image background. Thus, such non-periodic structure will be washed out using the amorphous noise model.

How random noise model works

The filter based on the random noise model adopts an *iterative* procedure, where the low-frequency information is protected by Gaussian low-pass filter, and the rest of information is passed to the Wiener/Difference filter. Then, the noise in higher frequency component will be progressively removed, while keeping the lower frequency components as much as possible. Therefore, the filter based on the random noise will keep non-periodic structures more than the filter based on the amorphous model. Furthermore, you can choose the best one from the output stack, since this filter is iterative.

3.0.2 Resolution and Information Limit

The concept of Information Limit is important to filter-out the noise in keeping signal information in the image. Here, we assume that all the signal information exists only within the Information Limit as shown in the example below:
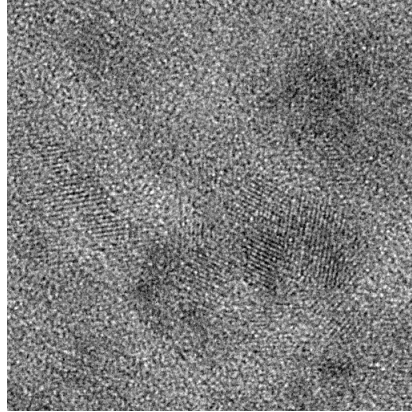

TiO2 nano-particles
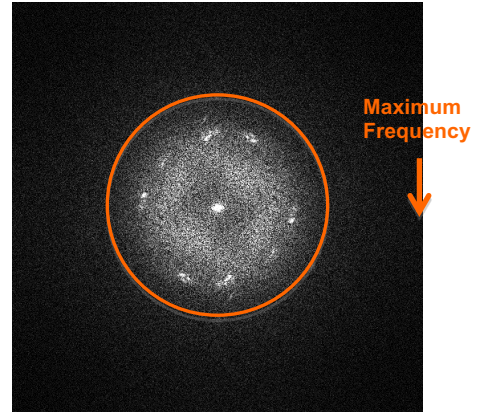
Fourier transform

Resolution and Information Limit are closely related. If you change one value, the other value will be changed. When the image is calibrated, you will see a Resolution in a physical unit, say nm. If not, the unit of Resolution is pix (pixels). When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value for Resolution. Alternatively, you can input the value for Information Limit in terms of the Maximum Frequency (Nyquist Limit) of the Fourier transform.
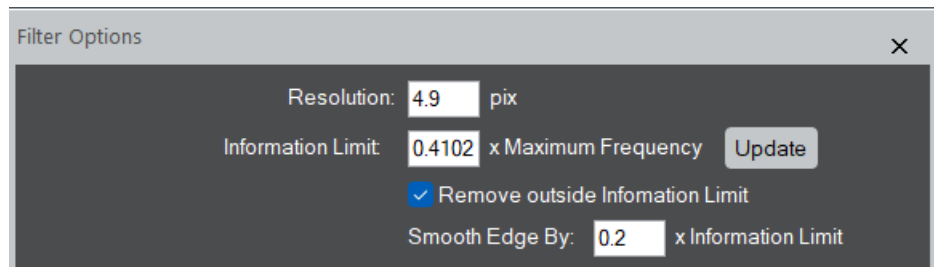
The default value of the Information Limit is 0.5. If the circle is too small or too large, you can adjust the radius of the circle by changing the value of the Information Limit. When you change the value for Resolution or Information Limit, it is advisable to push Update button to confirm its size in the Fourier transform.

If you want, you can remove high frequencies outside the Information Limit, which corresponds to high-frequency noise.

The Information Limit is essential for the Random Noise model, since the Low-pass Gaussian width is defined in terms of the Information Limit.
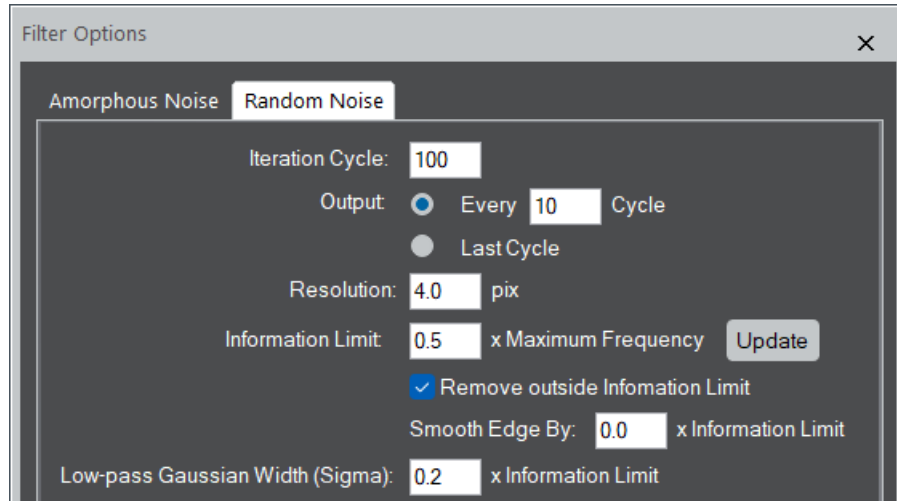

Since the random noise model works iteratively, there are some patemeters to be specified.

Iteration Cycle: This determines the maximum number of iterations

Output: This specified the cycle of result outputs or the output only at the last cycle.

Low-pass Gaussian Width (Sigma): The half-width of the smoothing Gaussian in Fourier space is specified here.

TIPS: A Low-pass Gaussian Width between 0.1 and 0.5, an Iteration Cycle of 100 and Output interval of 10 cycles will be suitable. After a few ten cycles, however, it becomes difficult to visually recognize any changes in the image. Nevertheless, the Fourier transform confirms that the random noise continues to decrease even after several ten cycles.

3.1 HREM-Filters
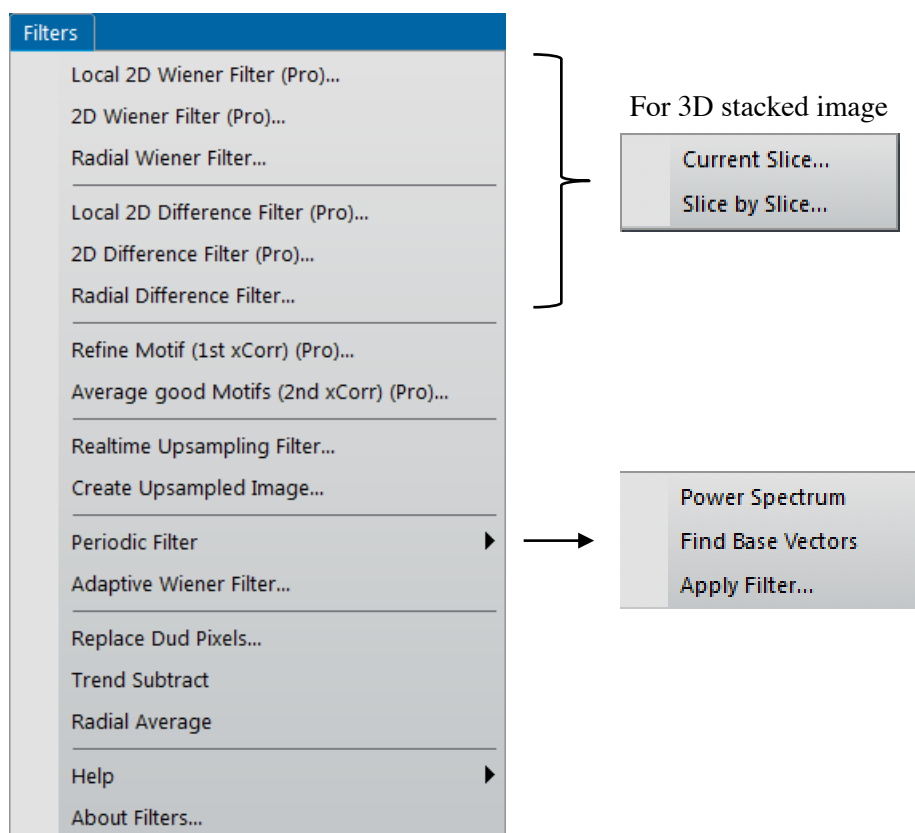
HREM-Filters Pro/Lite Menu.

The commands with (Pro), such as Local 2D Wiener Filter (Pro), indicate that they are available only for HREM-Filters *Pro*. Other commands can be used by both *Pro* and *Lite* versions, although some capabilities indicated by (Pro Only) in the dialog are applicable only for HREM-Filters *Pro*.

When the front data is a 3D stack, the submenu will appear, where you can choose a target from the *Current Slice* and all the slices (*Slice by Slice*).

We will use as an example the following image of crysotile, a clay mineral, taken by Prof. Kogure, Univ. of Tokyo. This is not an ideal crystal showing a simple translational symmetry, and thus clearly shows a power of Filters Pro.
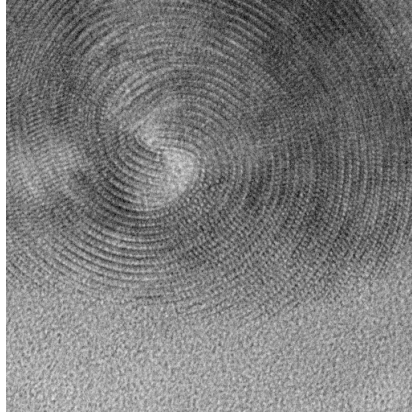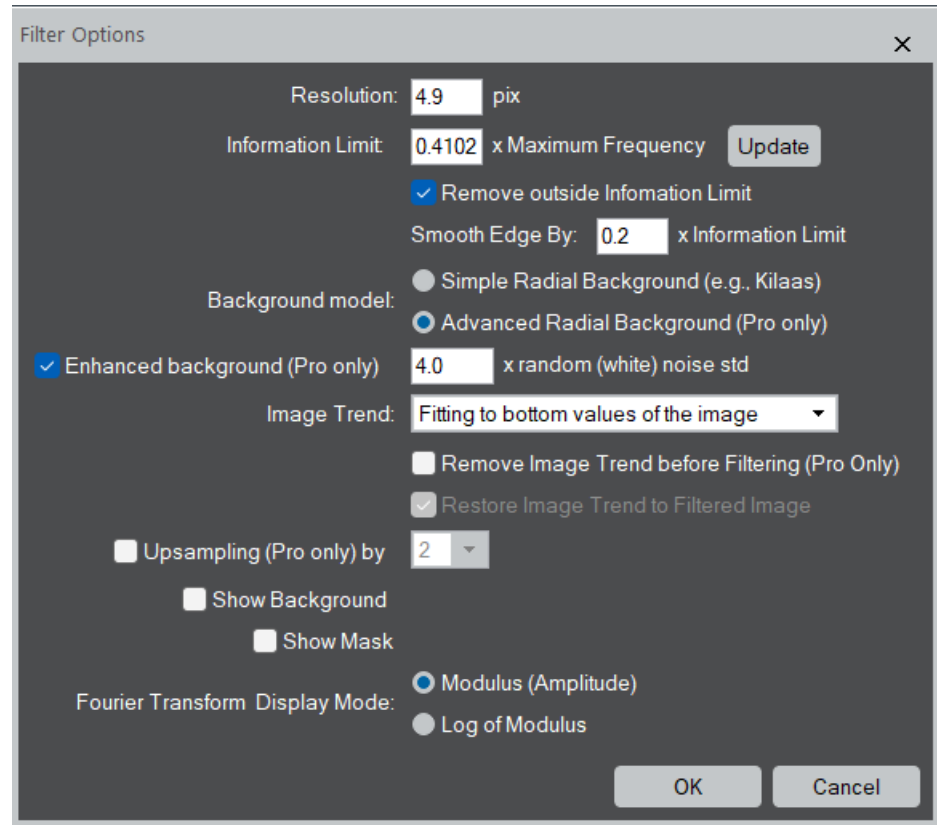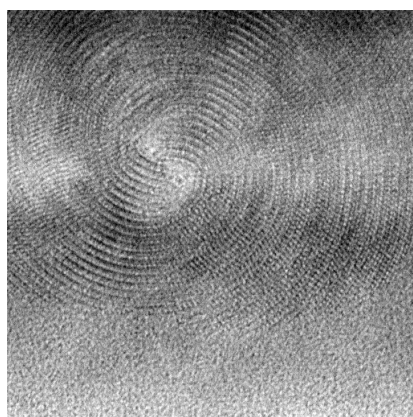

Original Image (crysotile)
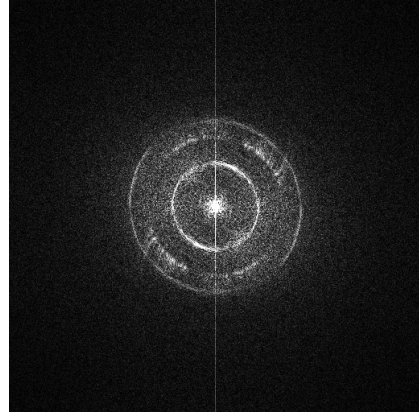
Fourier transform

3.1.1 Radial Wiener/Difference Filter

A radial background of the Wiener/Difference filter is estimated by rotationally averaging a Fourier transform of the whole image.
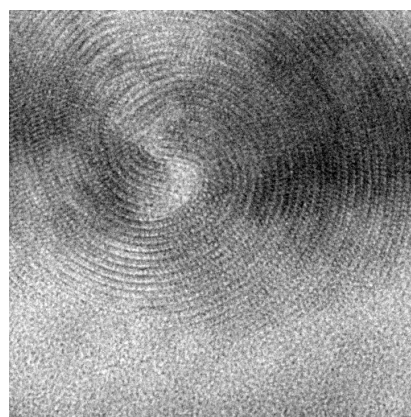

Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value here. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.
Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).
Smooth Edge By:	This defines the value for Smooth Edge.

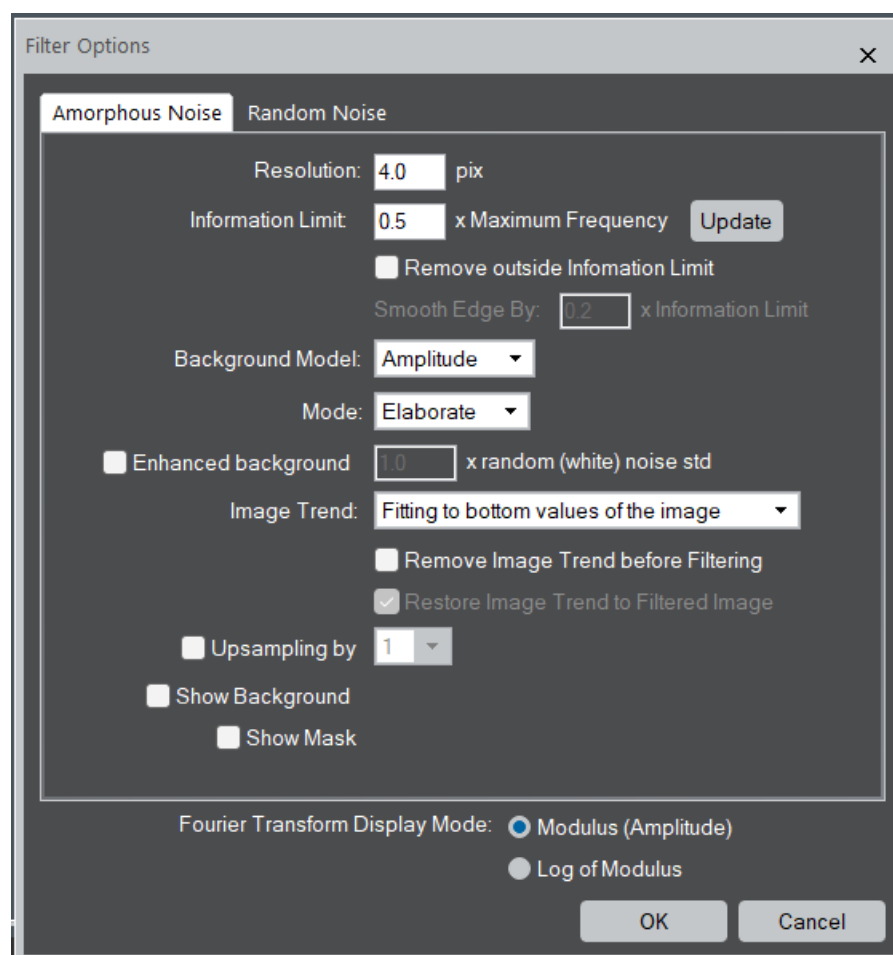|	
Background model:	The choice of the Radial Background model.
	Lite can use *Simple Radial Background* obtained by rotational average of the intensity (e.g., Kilaas).
	Advanced Radial Background that is available for *Pro* only is a smooth version of the Simple Radial Background. Usually, this background is *far superior* to the Simple Radial Background.
Enhanced background (Pro only)	If checked, the background is increased by the factor multiplied by the std of the random noise.
Image Trend:	The choice of the Image Trend model.
	Fitting to bottom values of the image: a smooth 2D image that is not higher than the image values. This distribution is estimated by using non-negative least-squares.
	Gaussian blurred image: Gaussian blur of the original image.
Remove Image Trend before Filtering (Pro Only):	If checked, the image trend is subtracted before applying Wiener filter.
Restore Image Trend to Filtered Image	If checked, the image trend is restored to a filtered image. This becomes active only when the image trend is subtracted before filtering.
Upsampling (Pro only)	If checked, the filtered image will be up-sampled by the selected factor.
Show Background:	If checked, the background of the Wiener/Difference filter will be displayed.
Show Mask:	If checked, the Wiener/Difference filter mask will be displayed.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

Radial Wiener filtered image   Difference from the original image

3.1.2 2D Wiener/Difference Filter (Pro Only)

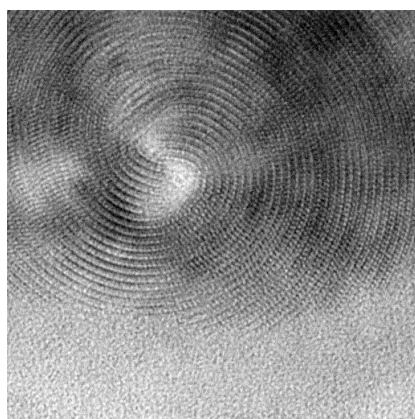There are two noise models: Amorphous noise and Random noise.

3.1.2.1 Amorphous noise

A smoothed two-dimensional trend of Fourier transform of the whole area is used as a background of the Wiener/Difference filter.
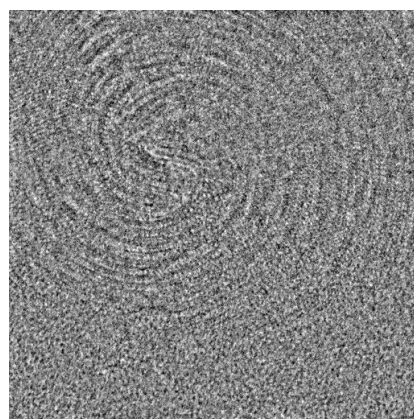

Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value here. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.

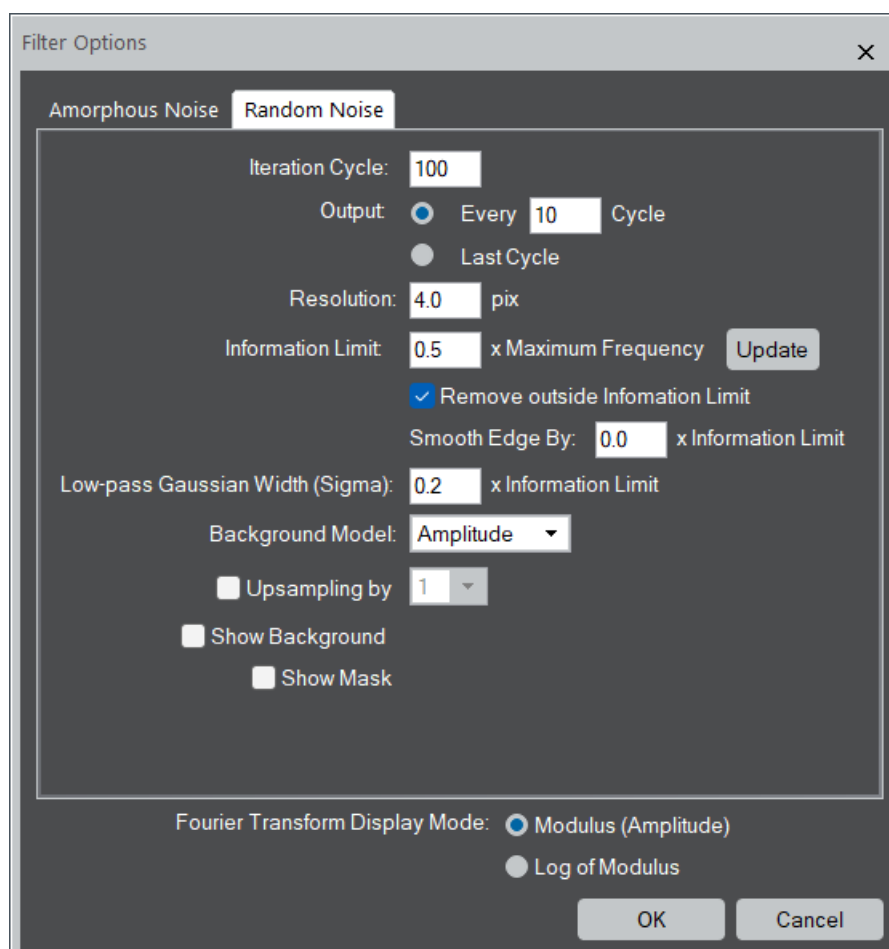|	
Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge)
Smooth Edge By:	This defines the value for <u>Smooth Edge</u>.
Background Model:	The background of the filter will be estimated from the Amplitude or Intensity.
Mode:	The choice of the 2D background estimation scheme from *Quick* and *Elaborate*.
Enhanced background	If checked, the background is increased by the factor multiplied by the std of the random noise.
Image Trend:	The choice of the Image Trend model.
	Fitting to bottom values of the image: a smooth 2D image that is not higher than the image values. This distribution is estimated by using non-negative least-squares.
	Gaussian blurred image: Gaussian blur of the original image.
Remove Image Trend before Filtering	If checked, the image trend is subtracted before applying Wiener filter.
Restore Image Trend to Filtered Image	If checked, the image trend is restored to a filtered image. This becomes active only when the image trend is subtracted before filtering.
Upsampling	If checked, the filtered image will be up-sampled by the selected factor.
Show Background:	If checked, the background of the Wiener/Difference filter will be displayed.
Show Mask:	If checked, the Wiener/Difference filter mask will be displayed.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

2D Wiener filtered image

Difference from the original image
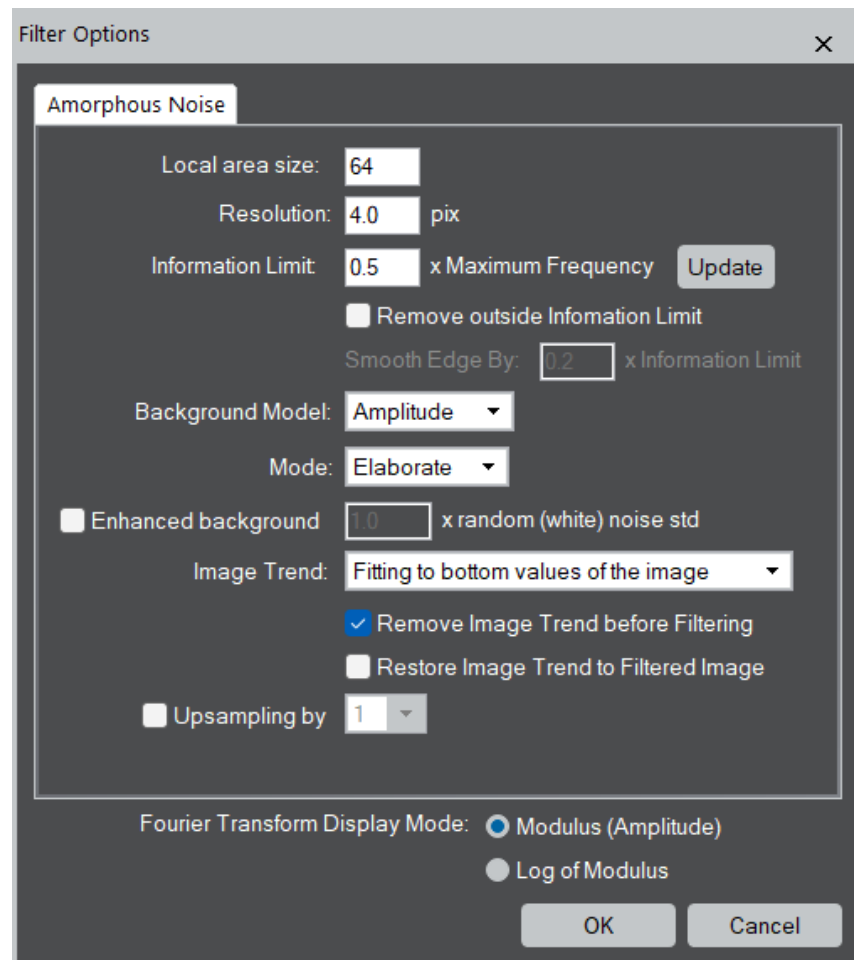
3.1.2.2 Random noise

Iteration Cycles:	This determines the maximum number of iterations
Output:	This specified the cycle of result outputs or the output only at the last cycle.
Resolution:	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value here. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.

Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge)
Smooth Edge By:	This defines the value for <u>Smooth Edge</u>.
Low-pass Gaussian Width (Sigma):	The half-width of the smoothing Gaussian in Fourier space is specified here. A large Gaussian width requires a longer iteration.
Background Model:	The background of the filter will be estimated from the Amplitude or Intensity.
Upsampling	If checked, the filtered image will be up-sampled by the selected factor.
Show Background:	If checked, the background of the Wiener/Difference filter will be displayed.
Show Mask:	If checked, the Wiener/Difference filter mask will be displayed.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

TIPS: A Low-pass Gaussian Width between 0.1 and 0.5, an Iteration Cycle of 100 and Output interval of 10 cycles will be suitable. After a few ten cycles, however, it becomes difficult to visually recognize any changes in the image. Nevertheless, the Fourier transform confirms that the random noise continues to decrease even after several ten cycles.
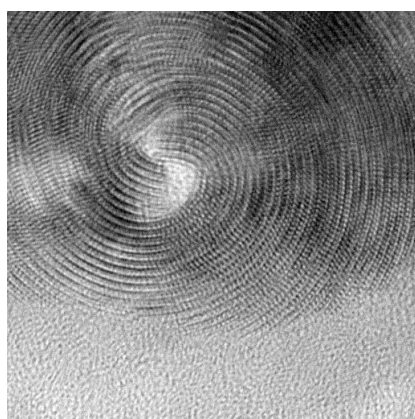
3.1.3 Local 2D Wiener/Difference Filter (Pro Only)

A background of the Local Wiener/Difference filter is locally estimated by smoothed two-dimensional trends of Fourier transform of local areas. The size of the area is controlled by the **Local area size** parameter below.
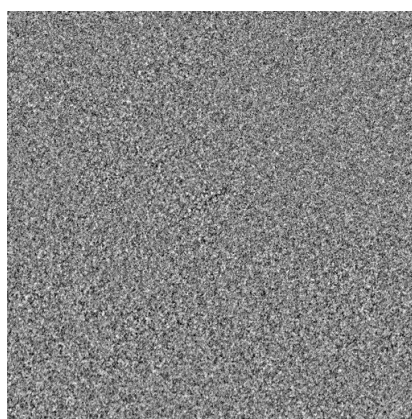

Local area size:	Size of the local square area.
Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value here. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking the Update button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.

|	
Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).
Smooth Edge By:	This defines the value for <u>Smooth Edge</u>.
Background Model:	The background of the filter will be estimated from the Amplitude or Intensity.
Mode:	The choice of the 2D background estimation scheme from *Quick* and *Elaborate*.
Enhanced background	If checked, the background is increased by the factor multiplied by the std of the random noise.
Image Trend:	The choice of the Image Trend model.
	Fitting to bottom values of the image: a smooth 2D image that is not higher than the image values. This distribution is estimated by using non-negative least-squares.
	Gaussian blurred image: Gaussian blur of the original image.
Remove Image Trend before Filtering	If checked, the image trend is subtracted before applying Wiener filter.
Restore Image Trend to Filtered Image	If checked, the image trend is restored to a filtered image. This becomes active only when the image trend is subtracted before filtering.
Upsampling	If checked, the filtered image will be up-sampled by the selected factor.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

Local 2D Wiener filtered image   Difference from the original image

3.2 Motif Average

Motif averaging is a real space technique to obtain a noise-filtered image from an image of periodic structure. Here, we call a small region "motif," for which we search similar regions of the same size over the whole image. Then, we will take an average over the regions with high similarities. Usually, the similarity is measured by cross-correlation of the image and the motif.

3.2.1 Refine Motif (First cross-correlation)

At first assign the original motif using a Rectangle ROI as shown below:
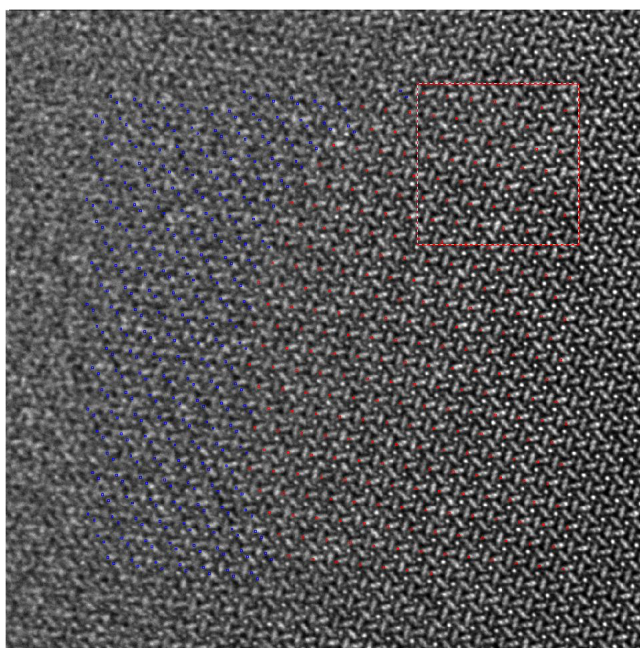
Next, launch the "Refine Motif" command. Then, the dialog below to set search conditions will appear:
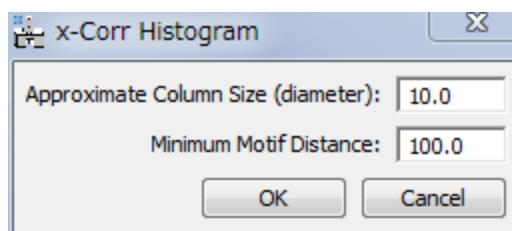

Here, "Approximate Column Size" is a diameter of each atomic column in pixels, and "Minimum Motif Distance" is an approximate distance between the motifs in pixels, not a size of the motif.

When the OK button is pressed, the histogram of cross-correlation of the whole image and the motif will appear.
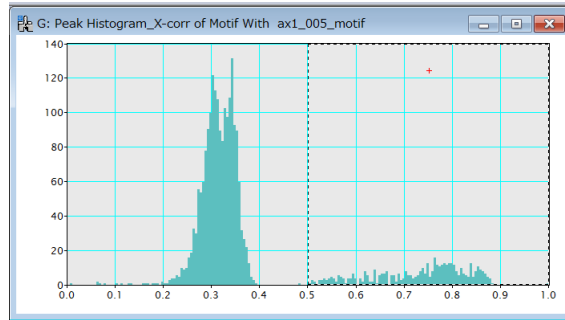
You can change the minimum and maximum values, and the number of bins to be displayed in the HREM Histogram palette. The found peaks are displayed in blue, and the peaks above the threshold in red. The peak threshold can be changed by adjusting the left range of the range ROI in the histogram.

When you change the thresold setiting, press "OK" in the HREM Histogram palette. Then, the original motif and the refined motif averaged over the selected patches will be displayed as shown below:
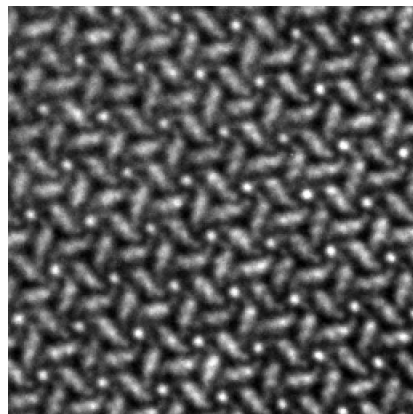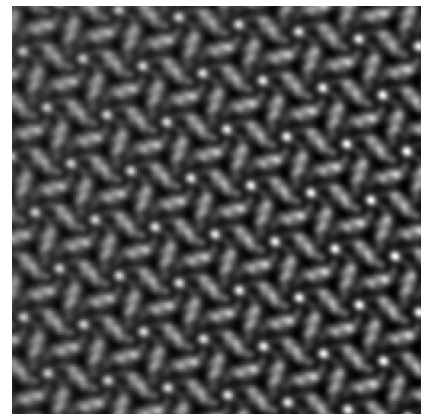

Original motie   Refined motif

### 3.2.2 <u>Average good Motifs (Second cross-correlation)</u>

This is the second step of "Motif Averaging," where the cross-correlation of the whole image with the refined motif is calculated, and an averaged image over the good motifs will be finally obtained.

To obtain the averaged image, launch "Average good Motifs" command when the <u>Refined Motif</u> is a front image. Then, the similar histogram and HREM Histogram pallet will appear. Adjust the threshold by watching the peak color, blue or red, over the whole image. If needed, you can change the minimum and maximum values, and the number of bins in the HREM Histogram palette.

When you satisfy the thresold setiting, press "OK" in the HREM Histogram palette. Then, the averaged image over the good motifs will be displayed as shown below:
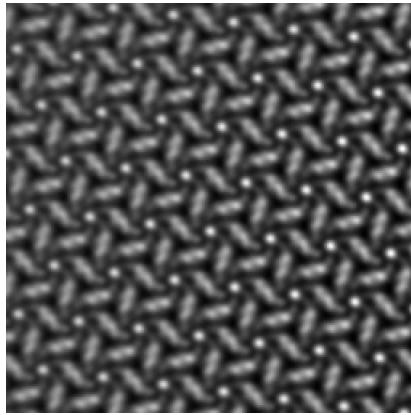
The figures below show the Fourier transforms obtained from the whole original image and the averaged image over the good motifs, respectively. Here, you can see the averaged motif keeps all the periodic information of the original image, and further shows some extra spots, whose effects on the image are difficult to be detected by eyes.
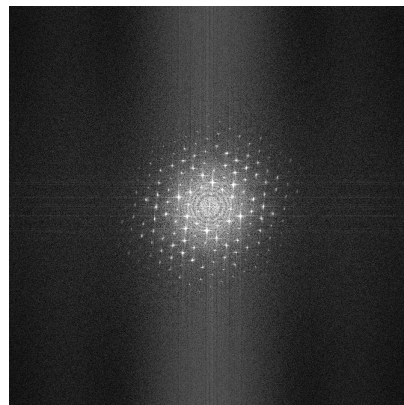
FT of the whole image   FT of the motif averaged image
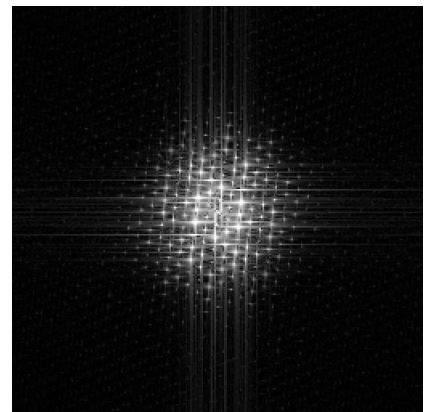
3.3 Realtime Upsampling Filter

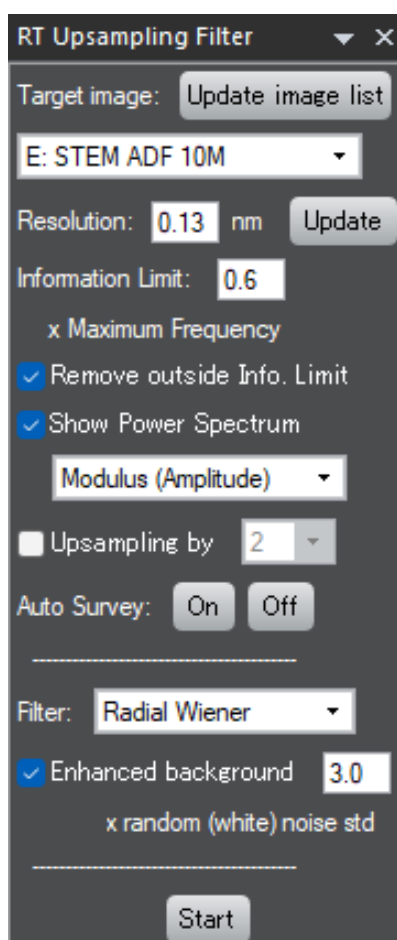The real-time (up-sampling) filter will assist an operator in performing experiments especially at a low dose condition. This filter can be used to adjust microscope condition, such as astigmatism and defocus, by looking the sample itself on the noise filtered image in live.

NOTE: To use the real-time noise filter capability you need <u>the license of the Runtime Module</u>. However, this tool can be used even when you don't have the Runtime license, when you install the HREM-Filters Pro/Lite. In this case, however, the filter selection is set to "None." Namely, you can use this tool without a filter capability to display a smoothed image in live by upsampling the selected image in the view mode.

3.3.1 <u>RT Upsampling Filter Palette</u>

<u>Open the RT Upsampling Filter palette</u>
The Realtime Upsampling Filter palette will be opened by selecting "RT Upsampling Filter" from Window->Floating Windows, or selecting "Realtime Upsampling Filter" from the HREM Filters menu.

<u>Select a target image</u>
The target image can be selected from the image pull-down list. If necessary, the image list can be updated by using "Update image list" button. The target image may be a STEM image, or a TEM image in the view mode.

> **TIPS**: If there is a ROI on the target image, only the area in the ROI is processed. This capability is very useful for a high frame-rate large TEM image. The position and the size of the ROI can be changed at any time, but the filtered image will change only when the target image is updated.

<u>Set the processing parameters</u>
"Resolution" and "Enhanced background factor" are important parameters that affect the filter performance.

Resolution/Information Limit
Resolution/Information Limit can be adjusted by looking the Power Spectrum of the image as usually done by using the command: HREM-Filters->Radial Wiener/Difference Filter. If you already done using the filter command, you can use the latest parameters used by the filter command by the "Load" button. Conversely, you can store these parameters for a later use by "Save" button.

When the target image is calibrated, the corresponding scale unit will be displayed, and you can use a fixed "Resolution" even when the magnification is changed. Contrary, if the target image is not calibrated, the unit "pix" is displayed and "Resolution" should be modified manually when the magnification is changed.

Remove outside Info. Limit
If checked, the noise outside of the Information Limit (Resolution) will be excluded.

Show Power Spectrum
Initial setting of this selection is ON. If you want to hide the Power Spectrum window, you can do by unselect this check box.
A pull-down allows you to select the display mode for the Power Spectrum from Modulus and Log of Modulus. Since display mode does not influence processing, you can select the mode you want.

Upsampling by
If checked, you can upsample the original image by a selected factor (2/3/4).

Auto Survey: ON, OFF
Using ON and OFF buttons you can change the Auto Survey status of the filtered image.

Following two settings are available only for the user who has the license for the ***Real Time Filter module***.
   Filter mode
   You can select "Radial Wiener" or "Radial Difference" filter. If you don't have the license, "None" will be shown here.
   Enhanced background

You can reduce the random noise (quantum noise/Poisson noise) by increase the background level by a selected factor.

Start the filter
The Realtime Upsampling Filter will be started by pressing the "Start" button. Then, this button will change to "Stop," by which you can terminate the processing.
When the Start button is pressed, a filtered image will be displayed in a separate window, and be updated when the target image is revised.

NOTE: If the image update is quicker than a required processing time, some of the frames during the processing will be skipped and not processed. This will usually happen for a high frame-rate TEM image that is larger than 512x512 pixels. By using a small ROI, you can decrease the required processing time and increase a number of frames (fps) that will be processed.

Off-line use of the Realtime filter tool

You can use this tool for off-line processing, when you select an already acquired image stack. When you push "Start" for an acquired image stack, the upsampled image for a current (selected) slice is displayed, and the upsampled image will be updated when the slice is changed, say by the slice player.

The next figure demonstrates what you can expect from the real-time noise filter on a live experiment (on-line use). You can observe a crystal structure even from a single frame with an average dose rate as low as 0.25 el/pix/frame at several frames per second for the ROI of 512 x 512.
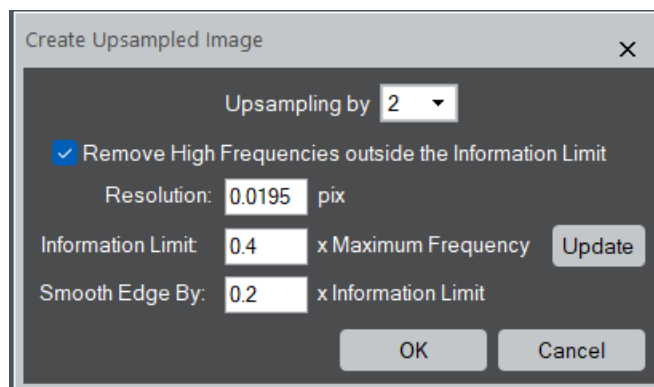
Furthermore, the up-sampling capability allow you to use a lower magnification for image acquisition while observing an up-sampled smooth image in live, and to examine the image acquisition conditions and/or the sample area to be acquired.
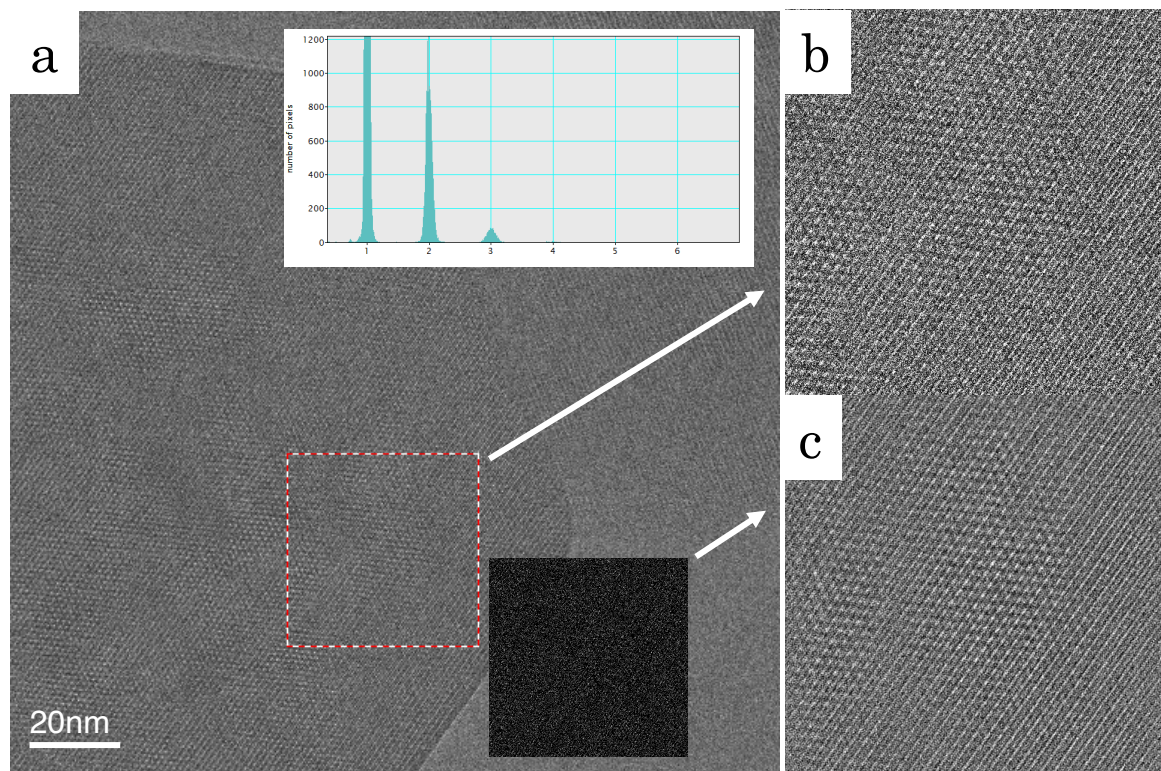
This figure illustrates the off-line use of the noise filtering of low dose TEM images of MOF taken at 300kV (Courtesy of Xiaoxiao Cao, Gatan China.). The left pane (a) shows an area of 2kx2k pixels acquired with a Gatan K2 camera working at Electron Counting mode, where consecutive ten frames are accumulated using the slice tool to reveal the sample feature. The top right pane (b) is an enlarged part of the ROI (512 x 512) in the left pane. The almost dark inset in (a) shows a single frame of the same region, which does not show any structure. The histogram in (a) of this single frame indicates that an average dose rate is as low as of 0.25 el/pix/frame. Surprisingly, the image (c) obtained from this *single* frame reveals the crystal structure using this real-time filter. It may be noteworthy that the noise filtered image (c) of the single frame is better than the accumulated image (b) over 10 frames.

3.3.2 Create Upsampled Image

This command will create an unsampled image/image stack from the observed image/image stack. When creating the unsampled image, you can delete the noise beyond the resolution/information limit.


Upsampling by	If checked, the filtered image will be up-sampled by the selected factor.

Remove High Frequencies outside the Information Limit

	If checked, high frequencies will be removed according to the setting below:
Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value here. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking the Update button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.
Smooth Edge By:	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).

3.4 Other Filters

3.4.1 Periodic Filter
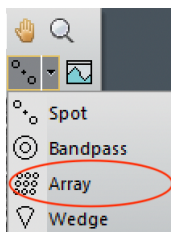
DigitalMicrograph has Periodic Mask (Array) tool for Fourier filtering. However, it is not easy to define two base vectors precisely for Periodic Filter using the standard Periodic Mask tool, especially when the base vectors are short. Therefore, we provide useful commands assisting to find a precise base vectors for a Periodic Filter using the HREM mouse tool, or the standard Periodic Mask tool.
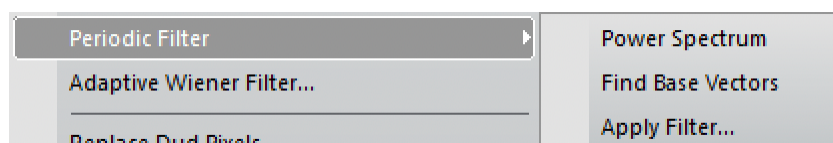

The first step of Periodic Filter is to create a Power Spectrum of the front image, where we put the HREM Mouser points or the Periodic Mask.

The "Find Base Vectors" command will find a set of accurate base vectors using the HREM Mouse tool, or using the DigitalMicrograph's Periodic Mask (Array) tool.
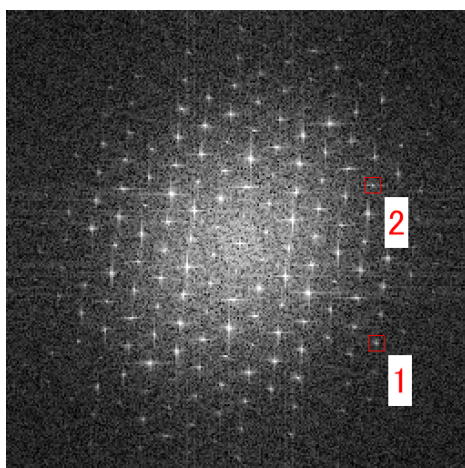
Another command "Apply Filter…" is an extended version of standard "Apply Mask…" under the Process menu, and gives a filtered image.

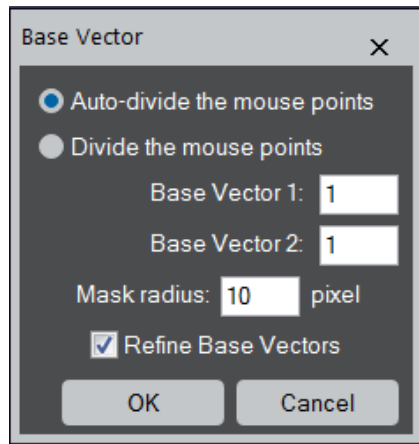### 3.4.1.1 Find Base Vectors (Using Mouse tool)
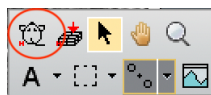
This command will find a precise base vectors for Periodic Filtering using the Mouse tool.

1. Select two spots along two base vectors by using the Mouse tool.

2. Choose "Find Base Vectors" command, then the following dialog will appear:

Here, you can choose "Auto-divide the mouse points" to leave the command to find the best Base Vectors, or "Divide the mouse points" to define the Base Vector lengths by dividing the distances to the mouse points by the specified numbers. You can specify here the mask radius, which can be changed later using the Periodic Mask tool. If you check "Refine Base Vectors," then the base vectors along the specified direction will be estimated precisely based on a least-square technique. Please note that user has to specify two base vectors that cover all the lattice points.

When the OK is pressed, the Periodic Mask will be added to the Power Spectrum as shown below, if the good base vectors are found. Make sure the base vectors are correct. In some case, only a part of the spots is covered by the Periodic Mask. Then, you have to try again by adjusting the positions of the mouse points.
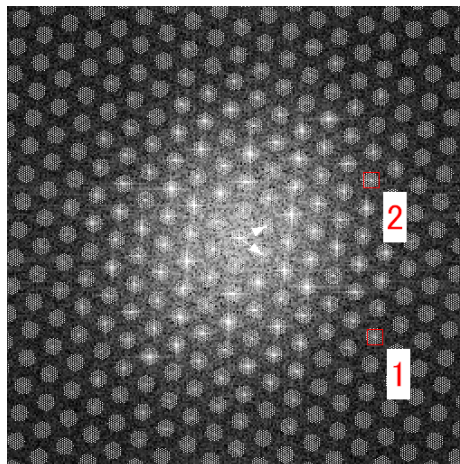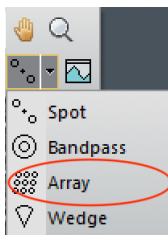

If the command fails to find the correct base vectors, you will get a following message:
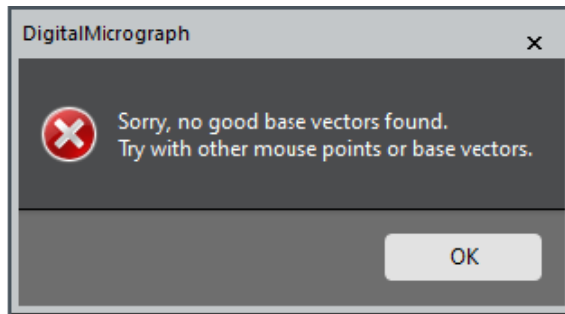
Then, you may want to try other set of lattice points using the Mouse tool.

3. If you want, you can adjust a mask size using the Periodic Mask tool.

## 3.4.1.2 Find Base Vectors (Using Periodic Mask tool)

This command will help you to find a precise base vectors of a standard Periodic Mask (Array) tool.

1. Place the standard Periodic Mask tool on the Power Spectrum.

2. Move the arrowheads of the Periodic Mask tool onto any spots on the *directions* of two base vectors.

3. (Optional) Put a Point ROI on one spot. This will impose a condition on the base vectors. See the TIPS below.

4. Choose "Find Base Vectors" command, then the true base vectors along the specified direction will be estimated precisely based on a least-square technique.   Please note that user has to specify a set of correct directions to cover all the lattice points.

Make sure the base vectors are correct. In some case, only a part of the spots is covered by the Periodic Mask. Then, you have to try again by adjusting the positions of the arrowheads of the Periodic Mask tool.

If the command fails to find the correct base vectors, you will get a following message:
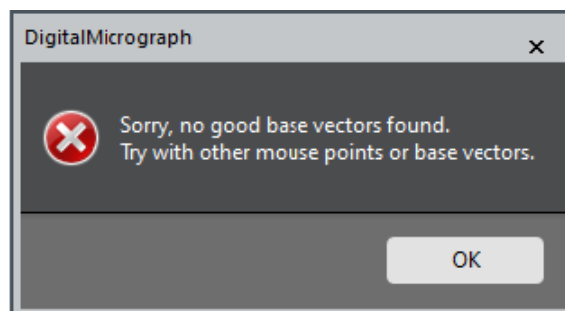
Then, you may want to adjust the positions of the arrowheads or to use other set of lattice points. Before trying another lattice points, you may

also want to try with the Option (Step 2) using the same lattice points.

5. If you want, you can adjust a mask size using the Periodic Mask tool.
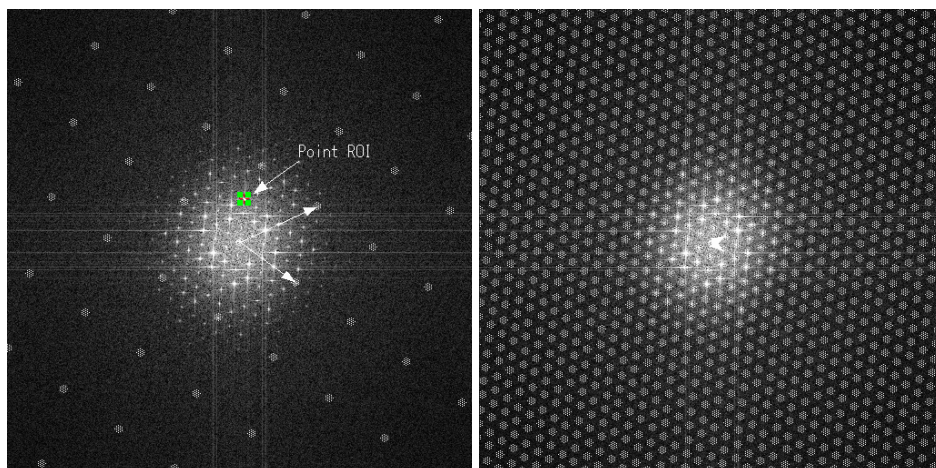
The arrowheads of the Periodic Mask (Array) tool are placed on the lattice points along the base vector directions. Note an optional Point ROI.

The best base vectors are estimated and an array of mask is placed at all the lattice positions on the Power Spectrum.

TIPS: The Point ROI is required to specify the correct base vector when the symmetry of the image gives extinct spots along the base vector. In such a case, place the point ROI on one of the allow spots along the base vector.

NOTE: The same procedure described here to find the base vector will work for the Fourier transform of the image. Then, the "Apply Mask" command of the Process menu will be used.

3.4.1.3 Apply Filter…

This is an extended version of the command "Apply Mask…" under the Process menu of DigitalMicrograph. There are several options that will reduce random noise from the final filtered image.
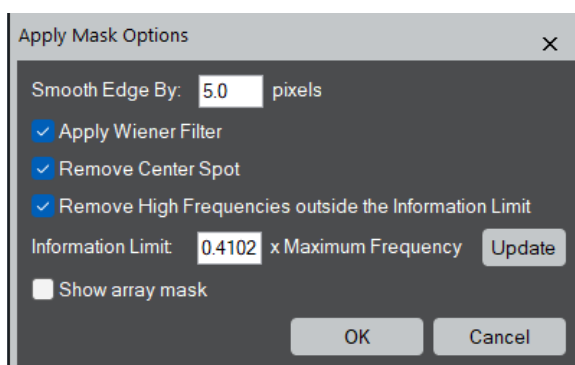
Apply Wiener Filter: Amplitude of the spot is modified by a Wiener estimate

$$F \Rightarrow \frac{|F|^2 - |F_b|^2}{|F_b|^2} F$$

where F_b is an average amplitude around each spot.

Remove Center Spot: Amplitude around the center spot is set to zero except the origin single point.

Remove High Frequencies outside the Information Limit
If checked, high frequencies outside the Information Limit will be removed.

Information Limit: The Information Limit given by a fraction of the Maximum Frequency of the image.

Update By clicking this button, you can verify the Information Limit on the power spectrum.
NOTE: When you change the value of the information limit, click the button again to check the size of the circle.

Show Array Mask If checked, the Array Mask will be shown over diffraction spots. The Array Mask should be hidden, when you adjust the red circle showing the information limit.

When the OK button is pressed, the filtered image will be shown on the new window after applying Periodic Mask to the Fourier transform of the image.

If you want to see the applied mask, you can check it by simply calculating the Fourier transform of the filtered image.

3.4.2 Adaptive Wiener Filter

This command applies a linear filter (local average) to an image *adaptively* according to the local image variance. The sizes of a local average and local variance can be controlled by "Adaptive Average" and "Noise Estimation", respectively. If the variance is large, the filter performs less smoothing, while the variance is small, the filter performs more smoothing.

The adaptive filter is more selective than a simple local average filter, preserving edges and other high-frequency parts of an image.
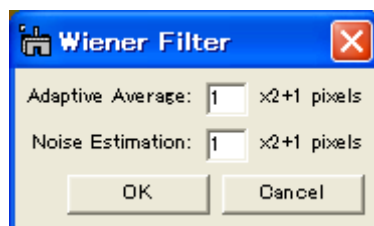
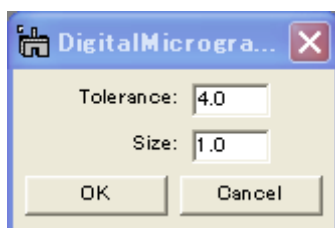# 3.5 HREM-Filters Utilities

3.5.1 Replace Dud Pixels

This command will remove dud image points due to bad pixels of a CCD camera or due to uncontrollable x-ray or cosmic ray. The values of the dud pixels will be replaced by a local mean. This is an automatic version of **Zapper** tool of DigitalMicrograph's standard tools.

The size of a cluster of dud points can be controlled by the **Size** parameter. The **Tolerance** controls a degree of singularity in terms of a local standard deviation.   This will work ideally for small isolated clusters.

For a long connected dud image pixels, an area that includes the dud pixels may be indicated by a **ROI** tool manually. Then, the dud pixels will be replaced by a local mean, when a pixel differs from the local mean by a specified **tolerance** times the variance of the area.
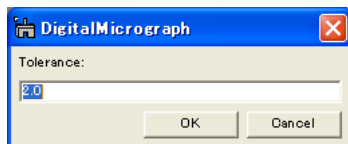
3.5.2 Trend Subtract

This command will remove a smoothed trend of an image, and makes a structural detail to be recognized more clearly. When an image size is large, Filters Lite will take more time to get a result compared with Filters Pro.
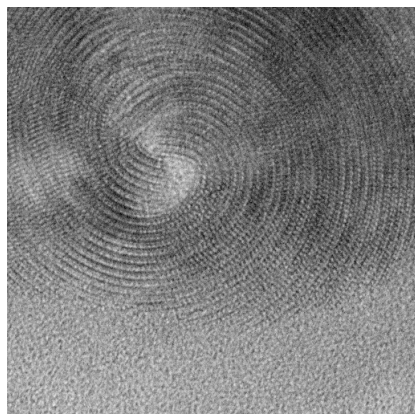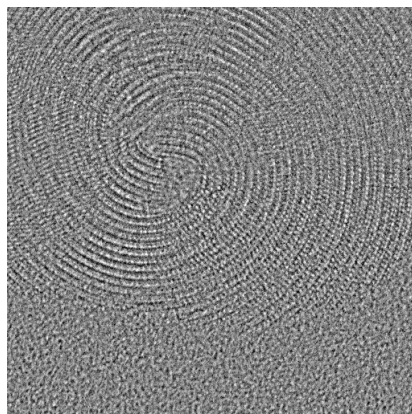
Original Image (crysotile)   Trend Subtracted imag

3.5.3 Radial Average

This command will calculate an average profile over the pixels on the same radial distance from its image center. If the image is complex number such as a Fourier transform of an image, a modulus will be averaged.

This command will also calculate a standard deviation profile, although the profile is hidden by default. You can see the standard deviation profile by choosing "Show std. dev." on a context menu that will appear by clicking a right mouse button on the "std. dev." legend.
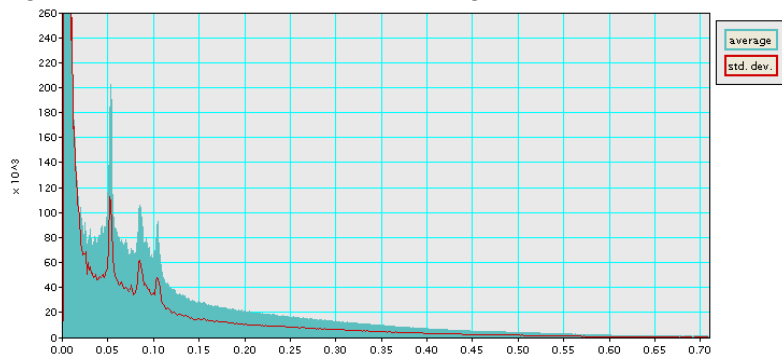
Radial average profile (Standard deviation profile is set to "show.")

4. Filter Description

4.1 Fourier Transform

An observed signal F_o in Fourier transform may be written as a sum of a true signal F_c due to a crystal part and a background F_b due to a non-crystal part: $F_o = F_c + F_b$. If we assume the true signal and the background are mutually independent, then we may be able to write $\left|F_o\right|^2 \approx \left|F_c\right|^2 + \left|F_b\right|^2$.

4.2 Wiener Filter

The Wiener filter seeks a solution that minimizes the summed square difference between the true signal F_c and its estimate $\hat{F}_c$ resulting

$$\hat{F}_c = \frac{\left|F_c\right|^2}{\left|F_c\right|^2 + \left|F_b\right|^2} F_o \approx \frac{\left|F_o\right|^2 - \left|\hat{F}_b\right|^2}{\left|F_o\right|^2} F_o = \frac{\left|F_o\right|^2 - \left|\hat{F}_b\right|^2}{\left|F_o\right|} e^{i\phi_o},$$

where ϕ_o is the phase of the observed signal F_o and $\hat{F}_b$ the estimate of the background. Here, we assume F_c and F_b are independent. If $\left|F_o\right| - \left|\hat{F}_b\right| \leq 0$, $\hat{F}_c$ is set to zero.

4.3 Difference Filter

The Difference filter (the background subtraction filter) is simply given by

$$\hat{F}_c = \left(\left|F_o\right| - \left|\hat{F}_b\right|\right) e^{i\phi_o},$$

where ϕ_o is the phase of the observed signal F_o and $\hat{F}_b$ the estimate of the background. If $\left|F_o\right| - \left|\hat{F}_b\right| \leq 0$, $\hat{F}_c$ is set to zero.

Reference: R. Kilaas, *J. Microscopy* 190 (1998) 45-51.

4.4 Background Estimation

In order to use either filter we have to estimate a background contribution $\hat{F}_b$. A radial average background has been commonly used. Here, we propose new backgrounds.

1. Radial Background
Normally, the background is estimated as a rotational average of the Fourier transform of the whole image assuming that the contribution from amorphous (non-periodic) materials varies slowly.

Reference: L.D. Marks, Ultramicroscopy 62 (1996) 43-52; R. Kilaas, *J. Microscopy* 190 (1997) 45-51.

2. Two-Dimensional Background
A radial background will not work, when structure information appears at the same distance from the origin in Fourier space. Thus, we developed a novel approach based on P-spline fitting to estimate a smoothed two-dimensional background in Fourier space.

Reference: P.H.C. Eilers et al., *Computational Statistics and Data Analysis* 50 (2006) 61-76.

3. Local Two-Dimensional Background
When an orientation of periodic structure is different locally, the background estimated for the whole image is not adequate. Thus, a set of two-dimensional backgrounds in Fourier space is estimated by dividing an image into local small areas.

4. Periodic Mask Background
A periodic mask is frequently applied to a Fourier transform of a lattice image. We may be able to modify a simple periodic filter to a Wiener type filter, where a background is estimated for each diffraction spot from a surrounding area of each mask.

Quick Reference Guide

The HREM-Filters Main Menu
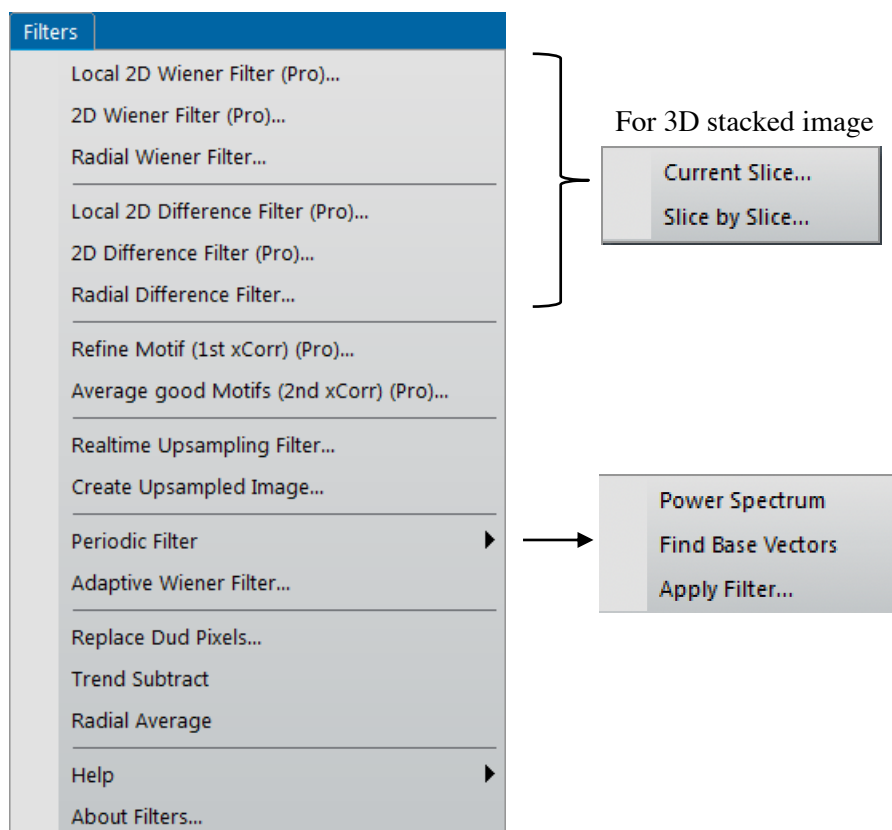
The commands in the HREM-Filters menu are described below.

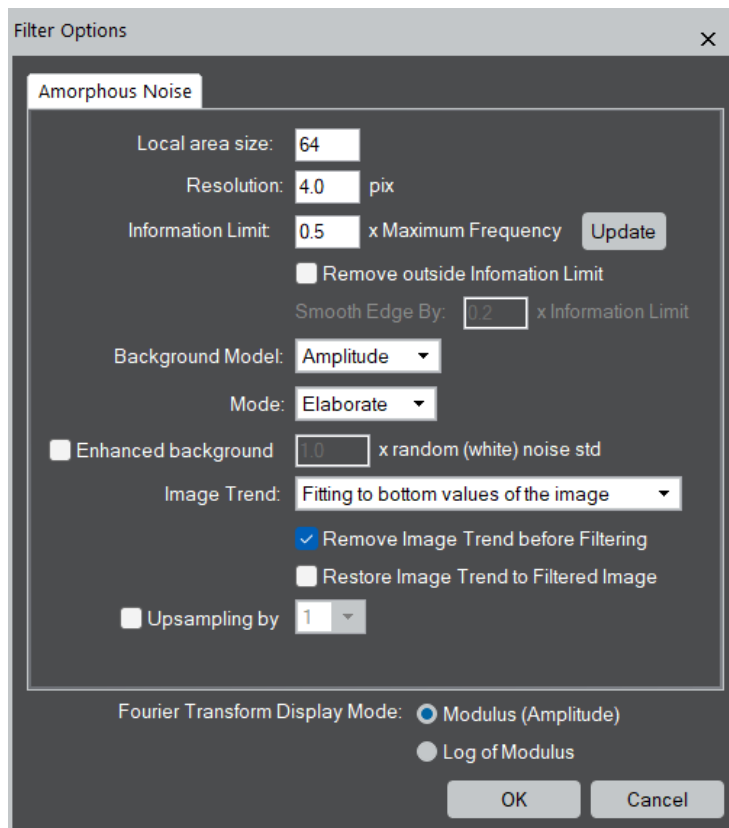| Command	Description
Local 2D Wiener Filter	Calculates a Wiener filtered image using 2D local backgrounds
2D Wiener Filter	Calculates a Wiener filtered image using a 2D background
Radial Wiener Filter	Calculates a Wiener filtered image using a radial background
Local 2D Difference Filter	Calculates a Difference filtered image using 2D local backgrounds
2D Difference Filter	Calculates a Difference filtered image using a 2D background
Radial Difference Filter	Calculates a Difference filtered image using a radial background

Refine Motif	Calculates a cross-correlation of the whole image with the given motif, and give a refined motif for the next command.
Average good Motifs	Calculates a cross-correlation of the whole image with the refined motif, and give an averaged image over he good motifs (image patches).
Realtime Upsampling Filter	Opens RT Upsampling Filter tool, which will assist an operator in performing experiments especially at a low dose condition.
Create Upsampling Image	Creates unsampled image/image stack from the observed image/image stack.

Periodic Filter (see sub menus)	Commands to assist/extend Periodic Filter
	  Find Base Vectors
	  Apply Mask

Adaptive Wiener Filter	Performs a linear filter (local average) adaptively according to the local image variance.
Replace Dud Pixels	Replaces dud pixels with a local average automatically according to the local image variance.
Trend Subtract	Subtracts an image trend (global background)
Radial Average	Calculates a rotational average and std. deviation of a Fourier transform

When the front data is a 3D stack, the submenu will appear, where you can select to process Current Slice or Slice by Slice (all the slices).

Local 2D Wiener/Difference Filter Menu

Filter Options Dialog

Amorphous Noise Tab

Component	Description
Local area size:	Size of the local square area.
Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value her. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click the button to check the size of the circle on the power spectrum.
Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).
Smooth Edge By:	This defines the value for Smooth Edge.

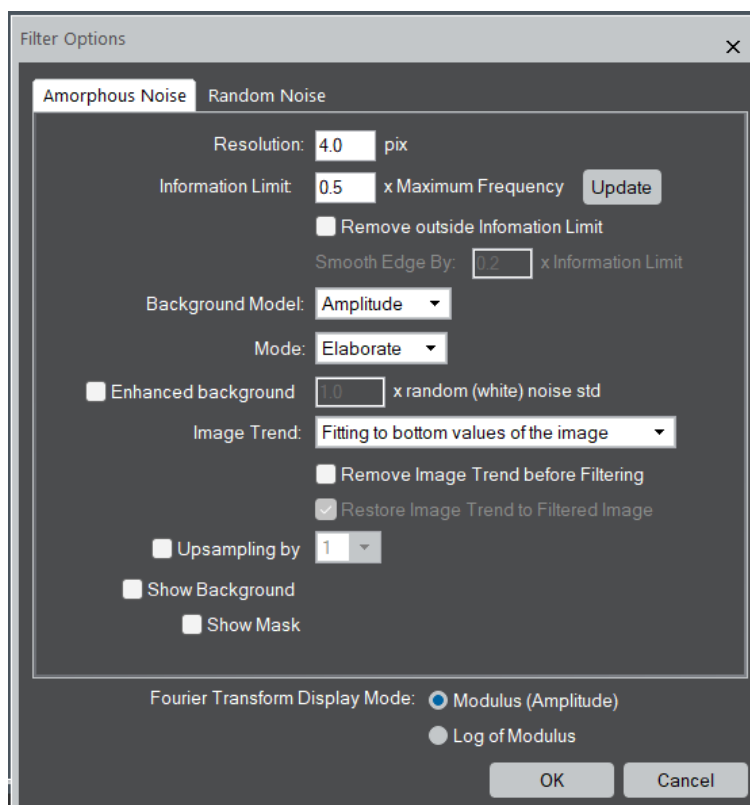| Background Model:	The background of the filter will be estimated from the Amplitude or Intensity.
Mode:	The choice of the 2D background estimation scheme from *Quick* and *Elaborate*.
Enhanced background	If checked, the background is increased by the factor multiplied by the std of the random noise.
Image Trend:	The choice of the Image Trend model. *Fitting to bottom values of the image*: a smooth 2D image that is not higher than the image values. This distribution is estimated by using non-negative least-squares. *Gaussian blurred image*: Gaussian blur of the original image.
Remove Image Trend before Filtering	If checked, the image trend is subtracted before applying Wiener filter.
Restore Image Trend to Filtered Image	If checked, the image trend is restored to a filtered image. This becomes active only when the image trend is subtracted before filtering.
Upsampling	If checked, the filtered image will be up-sampled by the selected factor.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

2D Wiener/Difference Filter Menu

Filter Options Dialog

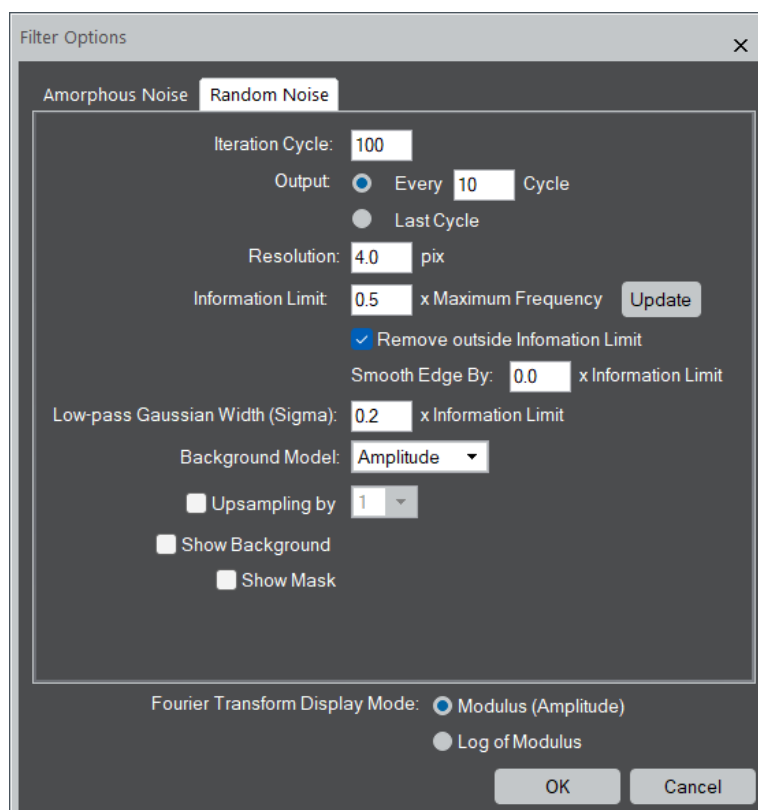There are two noise models: Amorphous noise and Random noise.

Amorphous Noise Tab

Component	Description
Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value her. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click the button to check the size of the circle on the power spectrum.

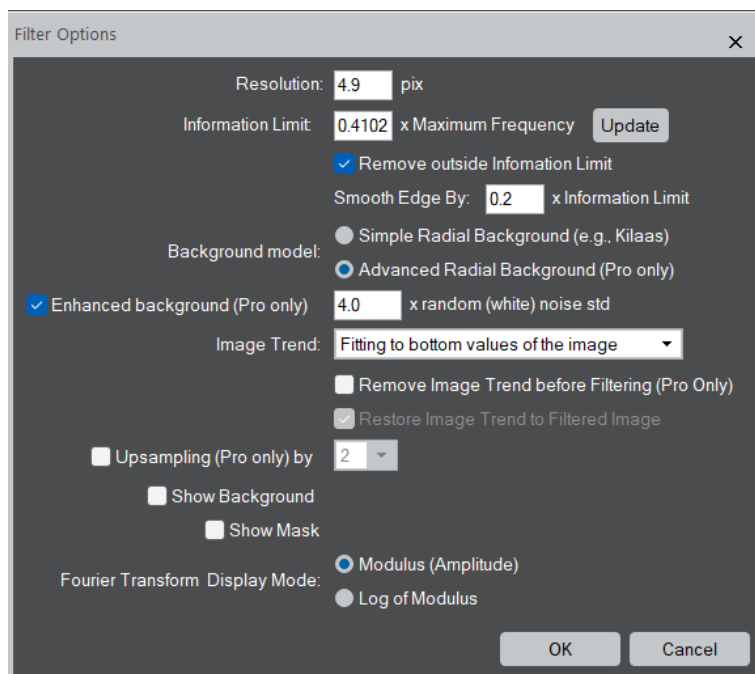| Remove outside the Information Limit Smooth Edge By:	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge). This defines the value for Smooth Edge.
Background Model:	The background of the filter will be estimated from the Amplitude or Intensity.
Mode:	The choice of the 2D background estimation scheme from *Quick* and *Elaborate*.
Enhanced background	If checked, the background is increased by the factor multiplied by the std of the random noise.
Image Trend:	The choice of the Image Trend model. *Fitting to bottom values of the image*: a smooth 2D image that is not higher than the image values. This distribution is estimated by using non-negative least-squares. *Gaussian blurred image*: Gaussian blur of the original image.
Remove Image Trend before Filtering	If checked, the image trend is subtracted before applying Wiener filter.
Restore Image Trend to Filtered Image	If checked, the image trend is restored to a filtered image. This becomes active only when the image trend is subtracted before filtering.
Upsampling	If checked, the filtered image will be up-sampled by the selected factor.
Show Background:	If checked, the background of the Wiener/Difference filter will be displayed.
Show Mask:	If checked, the Wiener/Difference filter mask will be displayed.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

Random Noise Tab

Component	Description
Iteration Cycles:	This determines the maximum number of iterations

Output:
   Each xx Cycles
   Last Cycle
	Specifies the cycle of result outputs or the output only at the last cycle.

Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value her. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click the button to check the size of the circle on the power spectrum.
Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).
Smooth Edge By:	This defines the value for Smooth Edge.

Low-pass Gaussian width (sigma):	The half-width of the smoothing Gaussian in Fourier space is specified here. A large Gaussian width requires a longer iteration. **TIPS**: A Low-pass Gaussian Width between 0.1 and 0.5, an Iteration Cycle of 100 and Output interval of 10 cycles will be suitable. After a few ten cycles, however, it becomes difficult to visually recognize any changes in the image. Nevertheless, the Fourier transform confirms that the random noise continues to decrease even after several ten cycles.
Background Model:	The background of the filter will be estimated from the Amplitude or Intensity.
Upsampling	If checked, the filtered image will be up-sampled by the selected factor.
Show Background:	If checked, the background of the Wiener/Difference filter will be displayed.
Show Mask:	If checked, the Wiener/Difference filter mask will be displayed.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

# Radial Wiener/Difference Filter Menu

Filter Options Dialog

Dialog

Option	Description
Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value her. Since the resolution may not depend on the magnification, it is convenient to use this when the image is calibrated.
Information Limit:	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click the button to check the size of the circle on the power spectrum.
Remove outside the Information Limit	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).
Smooth Edge By:	This defines the value for Smooth Edge.

Background model:	The choice of the Radial Background model.
	Lite can use *Simple Radial Background* obtained by rotational average of the intensity (e.g., Kilaas).
	Advanced Radial Background that is available for *Pro only* is a smooth version of the Simple Radial Background. Usually, this background is far superior to the Simple Radial Background.
Enhanced background (Pro only)	If checked, the background is increased by the factor multiplied by the sdt of the random noise.
Image Trend:	The choice of the Image Trend model.
	Fitting to bottom values of the image: a smooth 2D image that is not higher than the image values. This distribution is estimated by using non-negative least-squares.
	Gaussian blurred image: Gaussian blur of the original image.
Remove Image Trend before Filtering (Pro only)	If checked, the image trend is subtracted before applying Wiener filter.
Restore Image Trend to Filtered Image	If checked, the image trend is restored to a filtered image. This becomes active only when the image trend is subtracted before filtering.
Upsampling (Pro only)	If checked, the filtered image will be up-sampled by the selected factor.
Show Mask:	If checked, the Wiener/Difference filter mask will be displayed.
Show Background:	If checked, the background of the Wiener/Difference filter will be displayed.
Fourier Transform Display Mode	You can select the display mode between Modulus (Amplitude) and Log of Modulus.

Realtime Upsampling Filter Menu

RT Upsampling Filter Palette

The Realtime Upsampling Filter palette will be opened by selecting "RT Upsampling Filter" from Window->Floating Windows, or selecting "Realtime Upsampling Filter" from the HREM Filters menu.
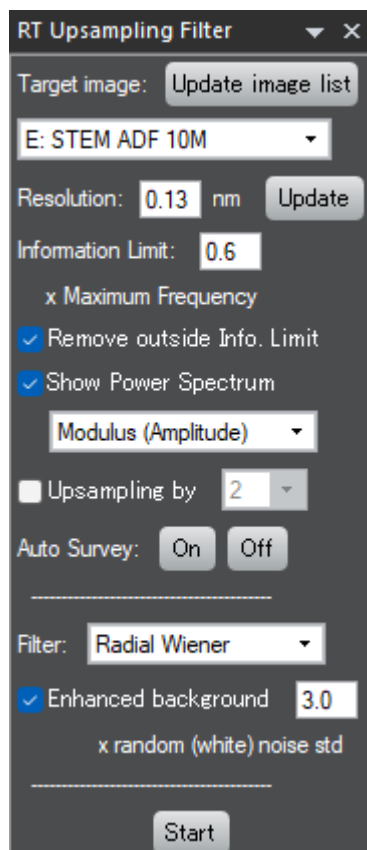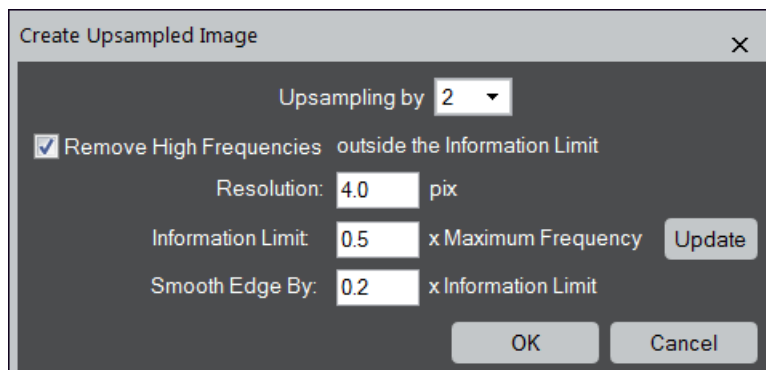

Option	Description
Target image	The target image can be selected from the image pull-down list. If necessary, the image list can be updated by using "Update image list" button. The target image may be a STEM image, or a TEM image in the view mode.
Resolution/Information Limit	Resolution/Information Limit can be adjusted by looking the Power Spectrum of the image. The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click the button to check the size of the circle on the power spectrum.

Remove outside Info. Limit	If checked, the noise outside of the Information Limit (Resolution) will be excluded.
Show Power Spectrum	Initial setting of this selection is ON. If you want hide the Power Spectrum window, you can do by unselect this check box. A pull-down allows you to select the display mode for the Power Spectrum from Modulus and Log of Modulus. Since display mode does not influence processing, you can select the mode you want.
Upsampling by	If checked, you can upsample the original image by a selected factor (2/3/4).
Auto Survey ON, OFF	Using ON and OFF buttons you can change the Auto Survey status of the filtered image.
Start	The Realtime Upsampling Filter will be started by pressing the "Start" button. Then, this button will change to "Stop," by which you can terminate the processing.
Following two settings are available only for the user who has the license for the **Real Time Filter module**.	
Filter mode	Filter mode can be selected from "Radial Wiener" or "Radial Difference" filter. If you don't have the license, "None" will be shown here.
Enhanced background	You can reduce the random noise (quantum noise/Poisson noise) by increase the background level by a selected factor.

Create Upsampled Image dialog

An unsampled image/image stack can be created from the observed image/image stack. When creating the unsampled image, you can delete the noise beyond the resolution/information limit.

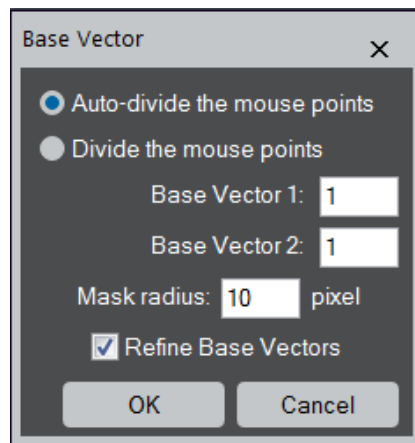| Option	Description
Upsampling by	If checked, the filtered image will be up-sampled by the selected factor.
Remove High Frequencies outside the Information Limit	
	If checked, high frequencies will be removed according to the settings below:
Resolution	When you know the resolution of the micrograph in a physical unit or in pixels, you can directly input the value here.
Information Limit	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.
Smooth Edge By:	If checked, high frequencies outside the Information Limit will be smoothly attenuated from one to zero between (Information Limit)*(1- Smooth Edge) and (Information Limit)*(1+ Smooth Edge).

Periodic Filter Menu

Option	Description
Find Base Vectors	Assists to find a precise base vectors for a Periodic Filter using the HREM mouse tool, or the standard Periodic Mask tool.
Apply Mask…	Apply a periodic mask with Wiener filter and/or low-pass filter. This command is available for *Pro* only.

Find Base Vectors – Base Vectors Dialog

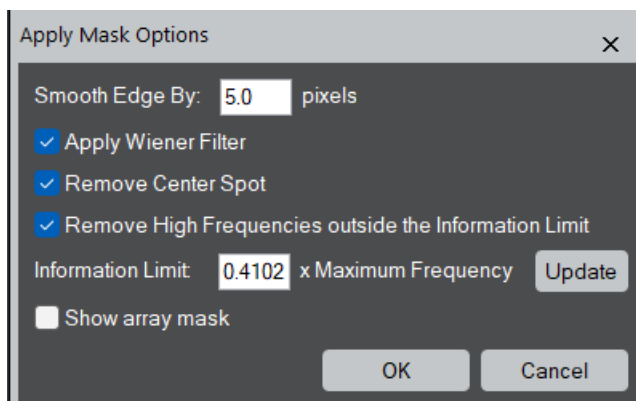When two mouse points are placed on the two spots along the two base vectors, the dialog below will appear.

Dialog

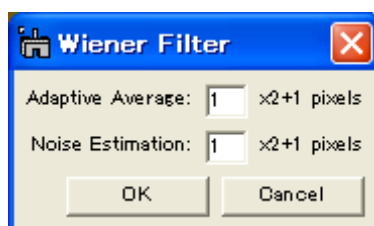| Option	Description
Base Vector 1	The order (index) of the mouse point #1 for the base vector 1.
Base Vector 2	The order (index) of the mouse point #2 for the base vector 2.
Mask Radius	The mask radius for each spot in pixels.
Refine Base Vectors	The base vector can be refined with a least-square fitting by checking this box. Use this capability except you intentionally want to use the mouse points without the least-square refinement.

Apply Mask Menu - Apply Mask Options Dialog

Dialog

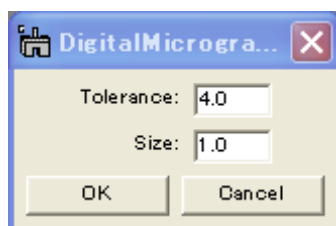| Option	Description
Smooth Edge By	The width of smoothing of each spot (same as DM - Process/Apply Mask command).
Apply Wiener Filter	If checked, Wiener filter is applied to each spot by estimating the background for the spot.
Remove Center Spot	If checked, the whole mask area of the center spot will be removed (filtered out)
Remove High Frequencies outside the Information Limit	
	If checked, high frequencies outside the Information Limit will be removed.
Information Limit	The Information Limit given by a fraction of the Maximum Frequency of the image.
Update	By clicking this button, you can verify the Information Limit on the power spectrum. **NOTE**: When you change the value of the resolution or information limit, click this button to check the size of the circle on the power spectrum.
Show Array Mask	If checked, the Array Mask will be shown over diffraction spots. The Array Mask should be hidden, when you adjust the red circle showing the information limit.

Adaptive Wiener Filter

Dialog

Option	Description
Adaptive Average	Defines an area of local average
Noise Estimation	Defines an area for local variance estimation

Replace Dud Pixels

Dialog

Option	Description
Tolerance	Controls a degree of singularity in terms of a local standard deviation
Size	The size of a cluster of dud points.