

HRTEM Exit Wave Reconstruction Package

User Manual

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I Installation

The reconstruction package will automatically be available as the hardware key will be programmed to enable the optional package.

The reconstruction package will be accessible through the sub-menu “Exit Wave Reconstruction” under the Process Menu. A separate menu item “Shiske Filter Restoration” will also appear under the Process Menu.

II Introduction

This Package constitutes an extension to MacTempasX (Total Resolution LLC) and provides a number of functions for reconstructing the complex electron exit wave from a series of High Resolution Transmission Electron Microscope (HRTEM) images taken at different foci. The approach used for reconstructing the complex exit wave is based on the Gerchberg-Saxton algorithm.

The Shiske Filter Restoration method is based on an optimum filter approach for restoring the specimen projected potential from a focus series of HRTEM images.

III Reconstruction Package Menu Commands

Process	Text	Window	Help
Image Calculator			⇧⌘C
FFT			⌘F
Linked Fourier Spectrum			⌘F
Hanning Masked FFT			⇧⌘F
Soft Circular Masked FFT			⇧⌘F
Inverse FFT			⌘I
Power Spectrum			
Edit Mask...			⇧⌘M
Apply Mask(s)			⌘M
Fourier Filters			▶
Spatial Filters			▶
Transform			▶
Statistics			▶
Calibrate...			⌘C
Extract From Complex			▶
Correlation / Convolution			▶
Azimuthal Average			▶
Template Matching...			
Peak/Lattice Analysis			▶
Average/Extract Motif...			
Change Image Origin...			
Geometric Phase Analysis...			
Diffraction Pattern Quantification...			
Crystallographic Image Processing...			⌘S
Exit Wave Reconstruction			▶
Shiske Filter Restoration...			
Focus Determination			▶
✓ Always Create New Image			
			Align Image Series...
			Gerchberg-Saxton...
			Low Resolution TIE Method...
			Aberration Correction...

Process (MacTempas process menu)

Exit Wave Reconstruction

Align Image Series...

Gerchberg-Saxton...

Low Resolution TIE Method...

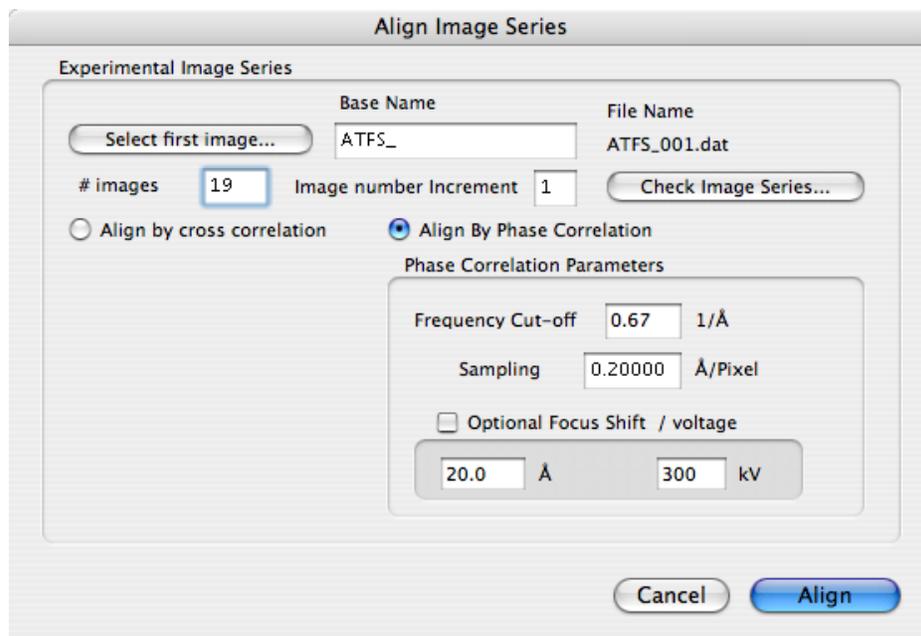
Aberration Correction...

Shiske Filter Restoration...

IV USE OF COMMANDS

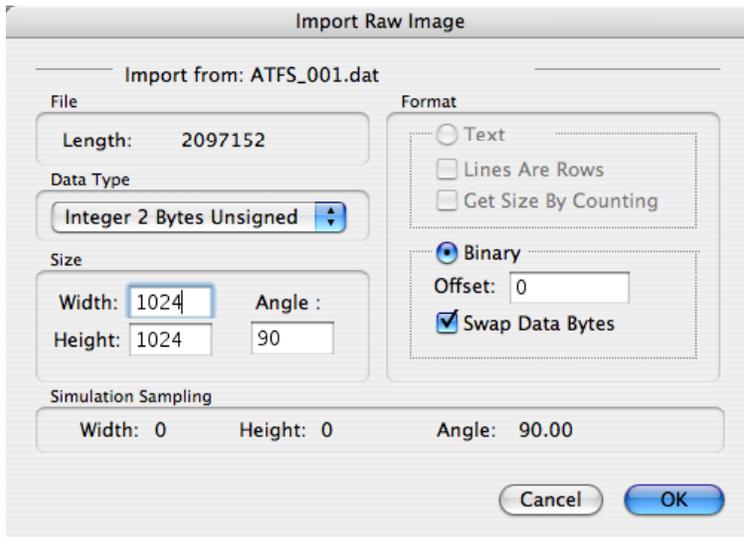
Align Image Series...

Will align a series of images either by the use of the cross correlation function or the phase correlation function. Optionally with the phase correlation function, a known focus step can be used to assist in the alignment procedure.

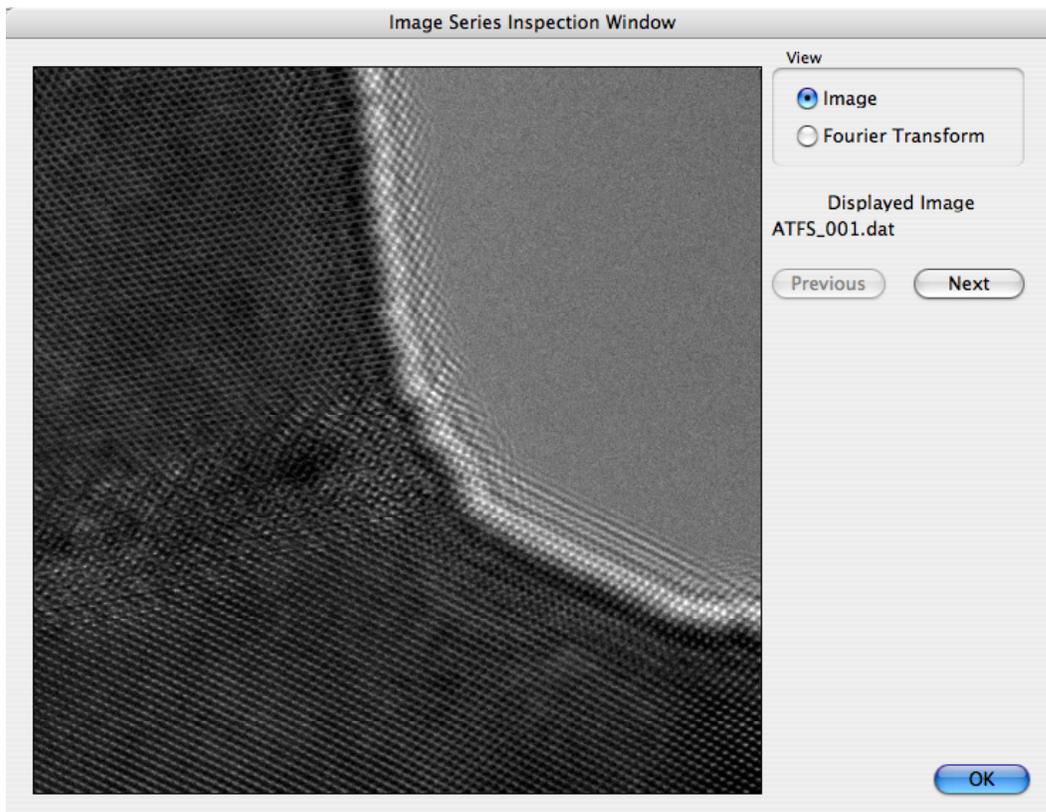


Use **Select first image...** to specify the first image in a series of images. For raw (binary) images, the user needs to specify the data type, any byte offset and any necessary byte swap of the data. Verify that the base name is correct as the software tries to guess the structure of the base name for the series based on the

file name.

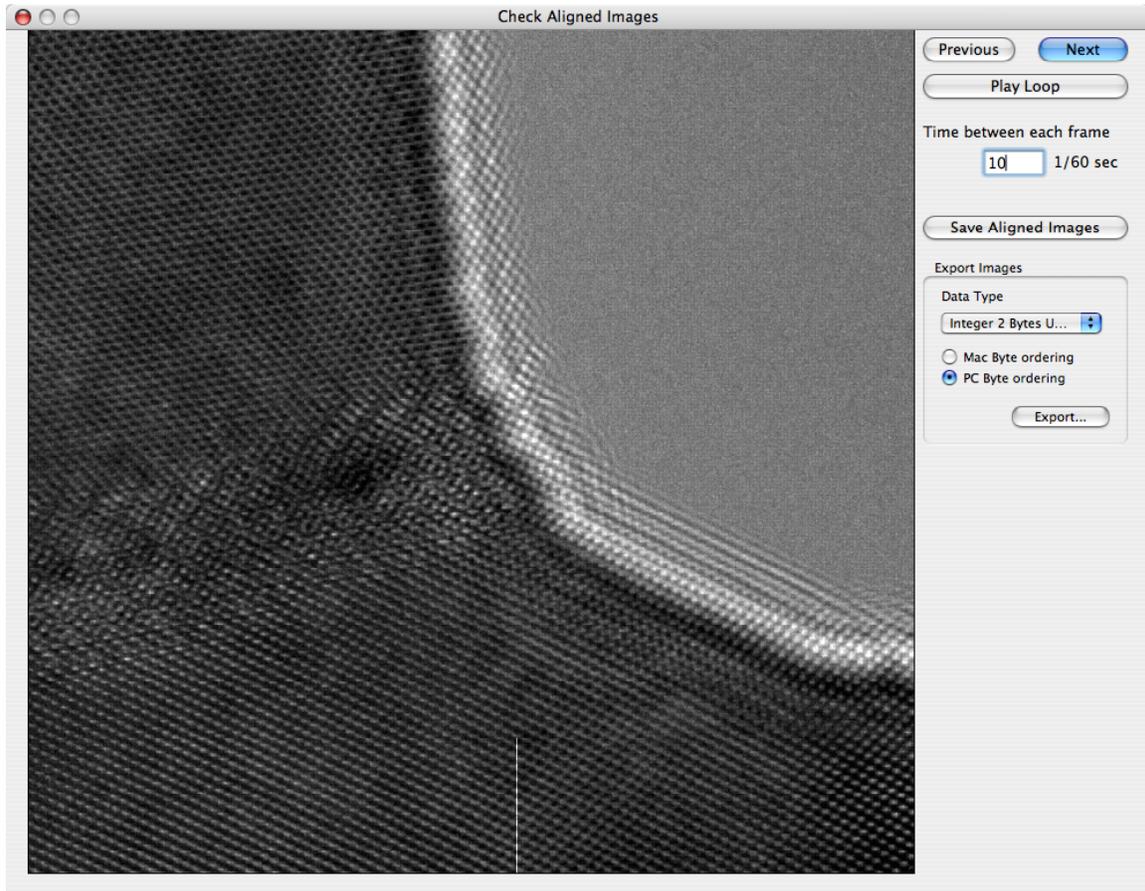


Use **Check Image Series** to verify that the images have been read in correctly and that all the images are suitable for use in the reconstruction



Click **Align** to start the alignment of the image series.

Once the image alignment procedure is completed, the following window is displayed.



To check the alignment, one can step through the images one by one or play the series as a movie with a specified time interval between frames.

The aligned images can be resaved back to the original filenames (**Save Aligned Images**) or exported in a different (or same) format (**Export...**) to a new set of files.

Gerchberg-Saxton...

This is the basic starting point for performing the exit wave reconstruction. The images can be aligned at this point or they can have previously been aligned through the **Align Image Series...** command. Regardless, for experimental images, the align checkbox should be checked as this will allow the software to do further sub-pixel alignment as part of the reconstruction algorithm.

Invoking this menu command brings up the following dialog.

Gerchberg-Saxton Exit Wave Reconstruction

Experimental Image Series

Select First Image... Base Name: ATFS_ File Name: ATFS_001.dat

First Focus [Å]: -2965 # images in series: 19 Sampling [Å/px]: 0.20549

Series Focus step [Å]: 24.0 Max # Iterations/cycle: 10 Customize Reconstruction...

Stop when change in fit is less than: 0.250 % Max # cycles: 3

Simulated Images (no alignment/noise processing) Align

Show live update of reconstructed wave functions Cross correlation

On completion show image/wavefunction amplitudes Phase correlation

Restoration Filter Noise Constant (>0): 0.010000 Cut-off: 0.67 1/Å

Show Aligned Images

Microscope Parameters

Voltage [kV]: 300 Divergence [mrad]: 0.20 PhasePlate (π): 0.00

Cs [mm]: 0.60 Cs5 [mm]: 0.00 R1 [1/Å]: 0.001 R2 [1/Å]: 0.001

Focus Spread [Å]: 30.00 Lens Aperture [1/Å]: 1.25

Pre-Alignment Noise Filter(s)

Wiener Filter Low Frequency Filter 0.10 1/Å

High Frequency Limit 1.50 1/Å

Post Reconstruction Filter

Low Frequency Filter 0.10 1/Å

Cancel Reconstruct

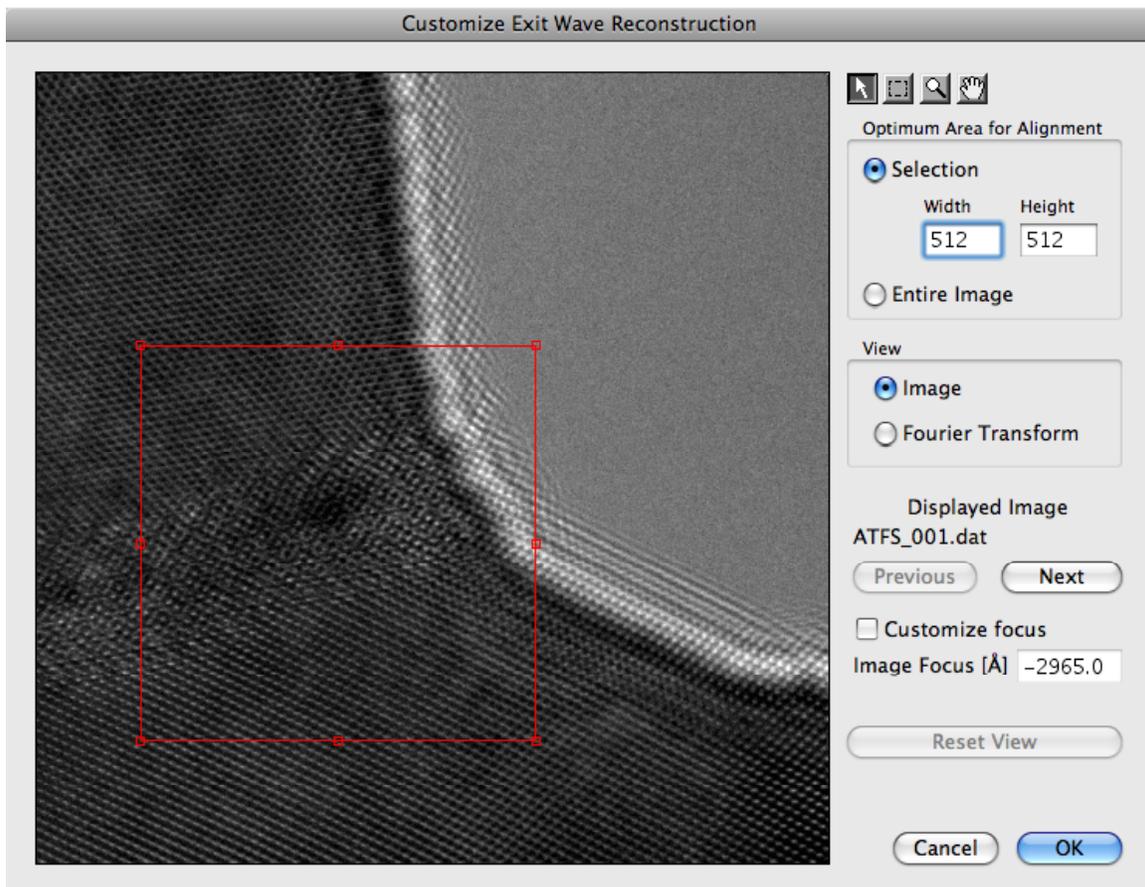
After selecting the first image in the series, the rest of the information needs to be filled out according to the experimental conditions. The image series is specified by the first image to be used in the reconstruction and the number of images in the series. The starting focus and the focus step must be set to correspond to assumed values for the experiment. The software will try to refine the focus values as part of the reconstruction. If the images come with a sampling (as from a calibrated Gatan Image file), the sampling will be set accordingly. Otherwise, the sampling of the image must be specified.

All the Microscope Parameters must be set if they differ from the default values supplied by the software.

The package will normally default to working with experimental images containing noise and in need of alignment. However, this can be over-riden by clicking on the **Simulated Images** checkbox. For experimental images, noise filtering can be applied as well as a high frequency cut off.

Options exist to have a live update of the reconstructed image after each iteration and to show the wave-function amplitudes in the image plane as determined by the algorithm.

By selecting **Customize...** a specified area can be chosen to be used for determining the alignment. By default an area centered in the image and of a dimension which is half of the image dimension is used. Individual focus values for the images can also be set at this point if those are known. As mentioned earlier, the software will try to search for focus values that optimizes the fit between calculated images from the reconstructed exit wave with the experimental images.



Restoration Filter Noise Constant

This constant must be non-zero in order to not blow up noise in regions where the contrast transfer function of the objective lens is very small. The default value will probably suffice in most cases.

Max. Number of Iterations/cycle and Max. Number of Cycles

The reconstruction algorithm is comprised of a series of iterations.

The first step is to compute a starting exit wave from each image back-propagated to the exit plane of the specimen. The exit wave is an average of the exit wave generated from each image in the series. Initially, the amplitude of the complex wave in the image plane is set to the amplitude of each image and a phase of zero. This complex wave is then propagated back to the exit plane through the contrast transfer function of the microscope. The exit wave is then forward propagated through the microscope to yield computed images for each focus value. The computed images are compared to the experimental images and a fit is calculated. This constitutes one iteration, Amplitudes of the propagated waves are reset to those of the image and then propagated back to the exit plane for the next iteration. At the end of one cycle, the software will look for new focus values that optimizes the fit with the experimental images and a new cycle will begin with a new sequence of iterations. The calculation will continue until the number of cycles and iterations have been reached or until the change in fit has reached a set limit. If the limit is not reached within the given number of cycles, the software will ask if the calculation should continue.

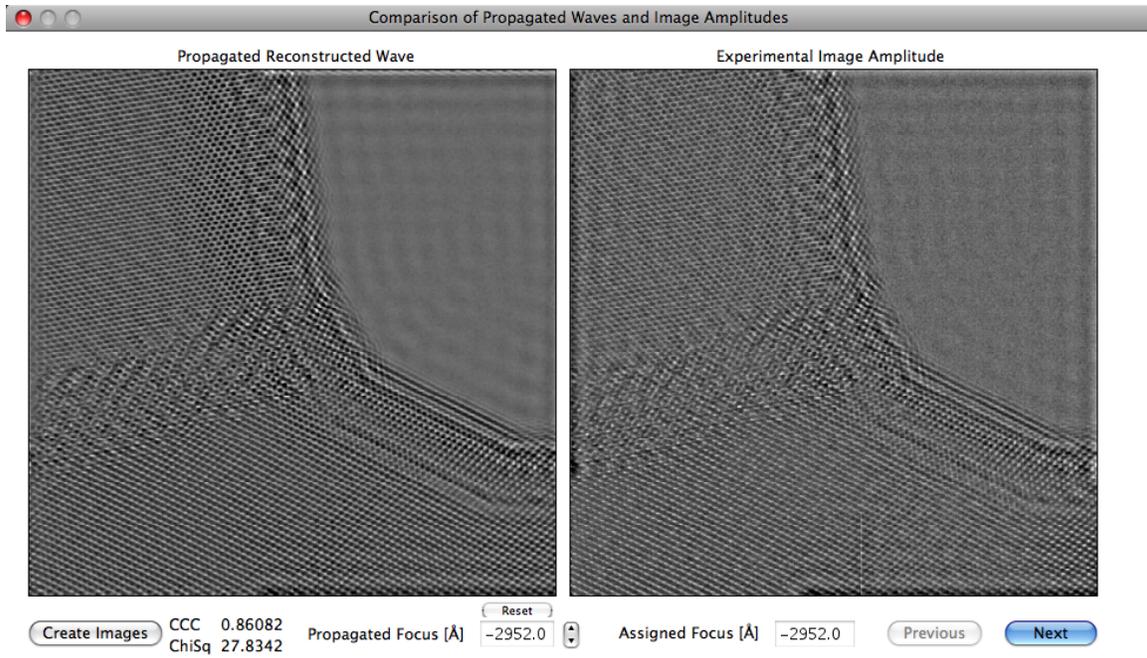
At any point, the calculation can be stopped by pressing "Apple" + "." (Apple period). If this is done once the software has begun the iterations, the current iteration will continue to the end and the reconstructed wave at that point will be shown.

Reconstruct

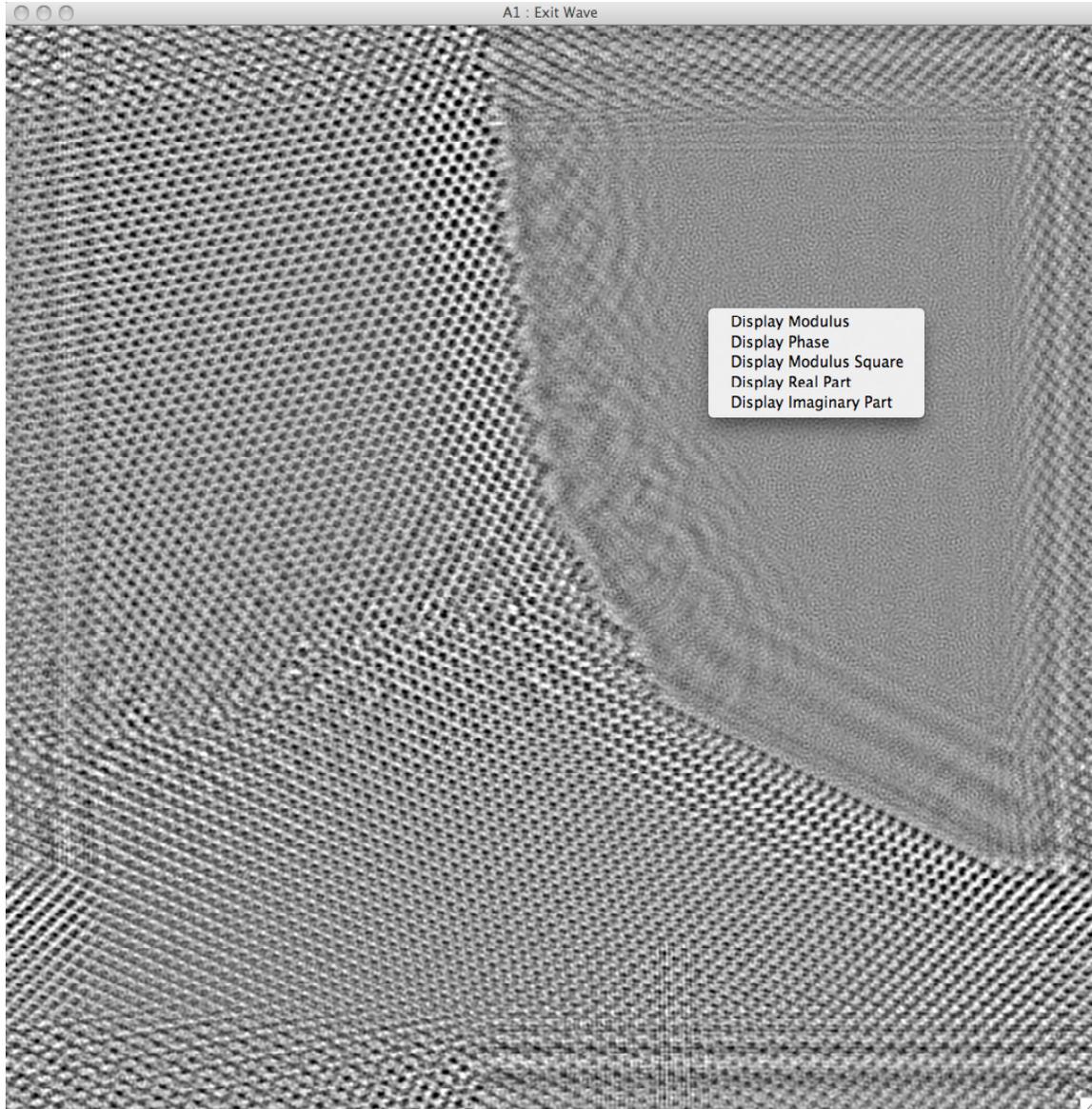
Will as it says start the reconstruction algorithm. The time required for the reconstruction is a function of the image size, the number of images and the number of iterations.

If the option to show amplitudes of computed images is selected, the software will display a window where the computed and experimental images are shown side by side for comparison. This window is shown below.

It should be noted that the values for the cross correlation coefficient and chi-square below are values obtained for the entire image. The reconstruction and refinement algorithm uses values obtained from a central region which is half of the actual image in size or the region specified in the "customize reconstruction" window.



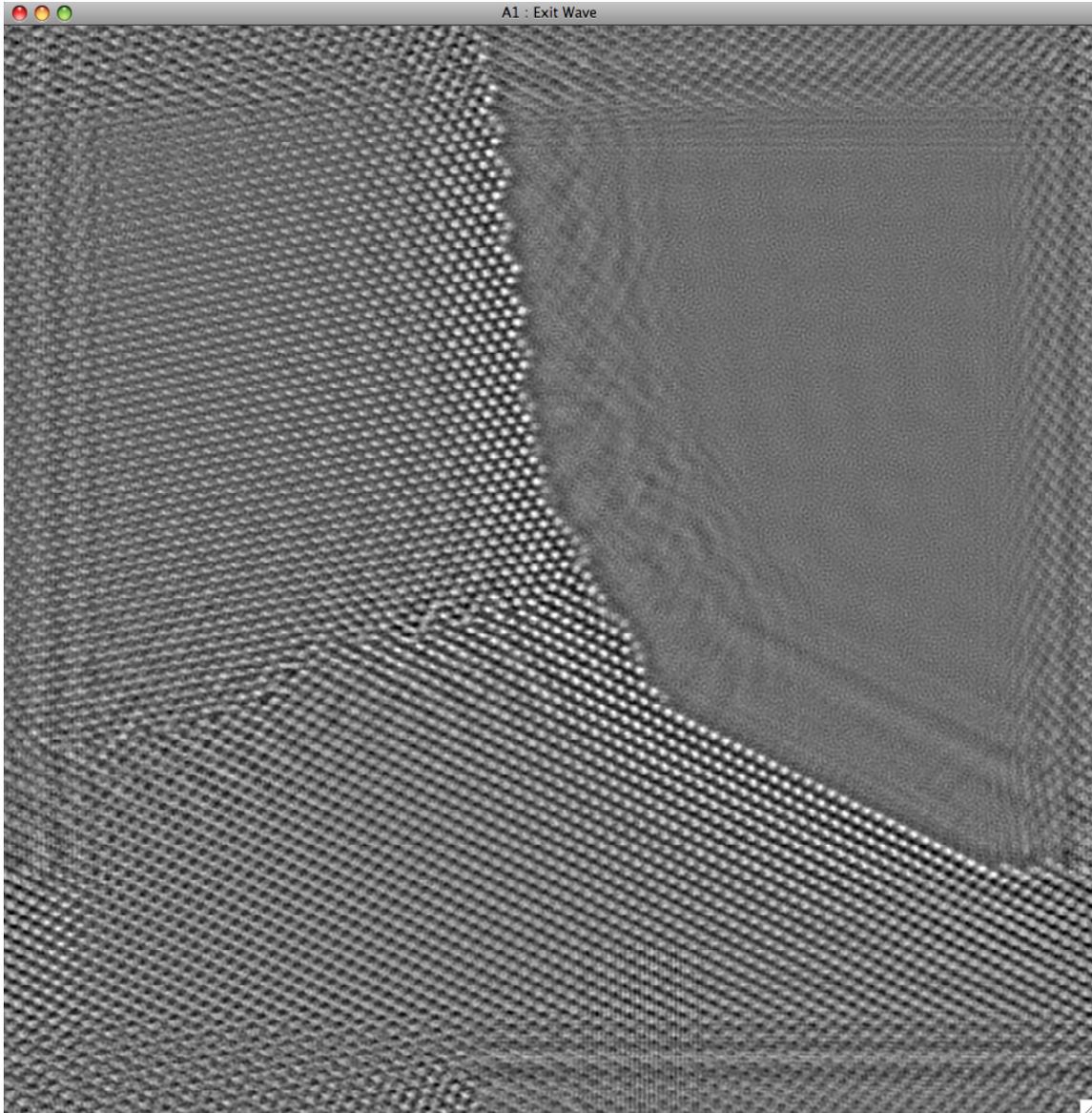
The actual output of the algorithm is a complex reconstructed exit wave.



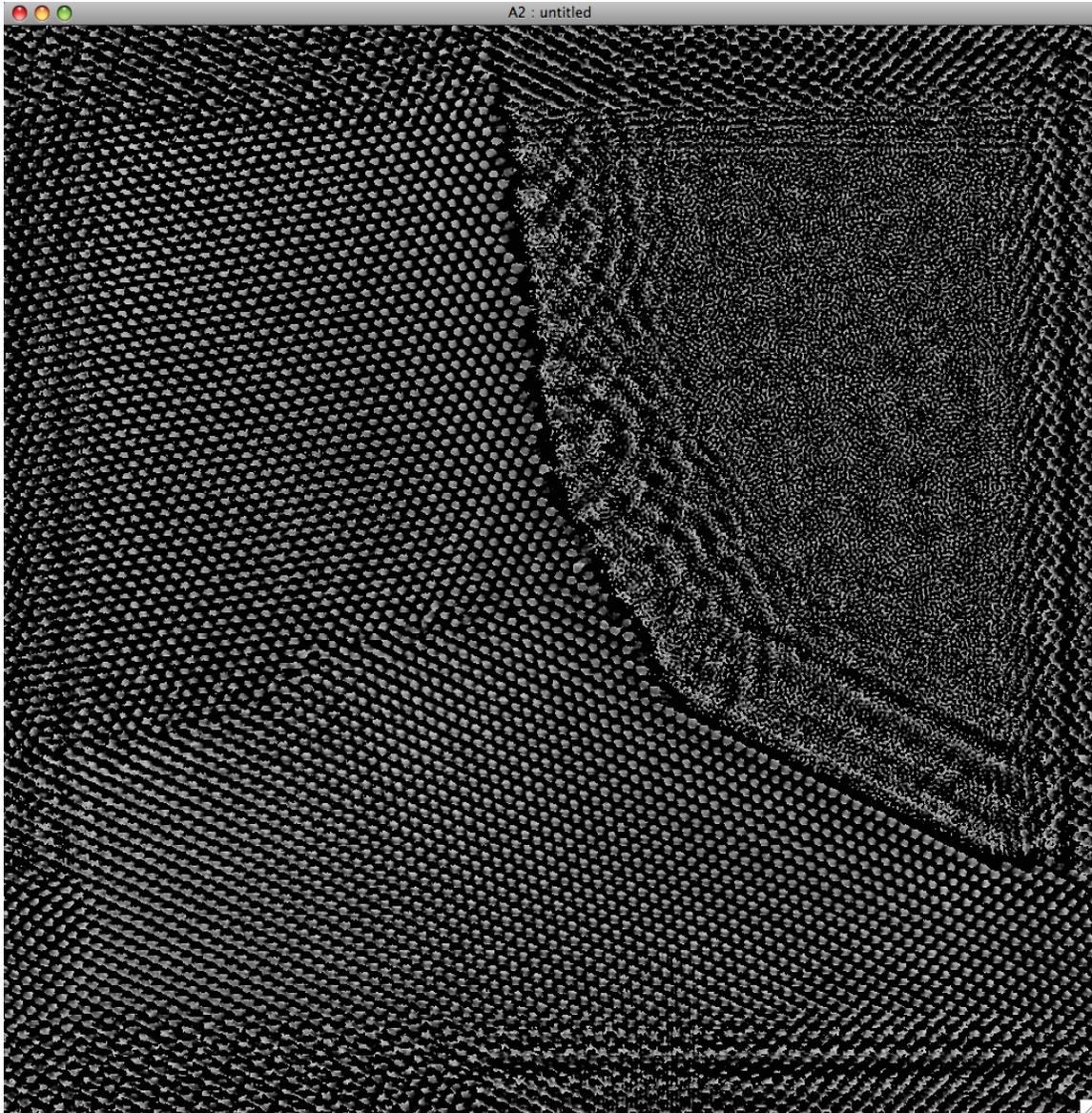
which can be split into an amplitude and a phase image.

The Amplitude image visually would look like the default display of the complex wave. A complex image can be shown in different form. By right button clicking (or Control + click) on the image, a pop-up menu will be displayed allowing the selection of which part of the image to show.

The phase of the exit wave is shown below.



If one were to perform the operation mathematical operation (Exit Wave – 1), the phase of the exit wave should closely correspond to what can be calculated from the s-wave approach. One can do this operation with the image calculator or with the scripting package (if installed). Alternatively, one do a linked Fourier transform of the exit wave, place an annular mask in the Fourier transform and make the inner ring such that it eliminates the inner part of the Fourier spectrum. The resulting phase image for the above calculation would look as shown below in a somewhat contrast enhanced image.

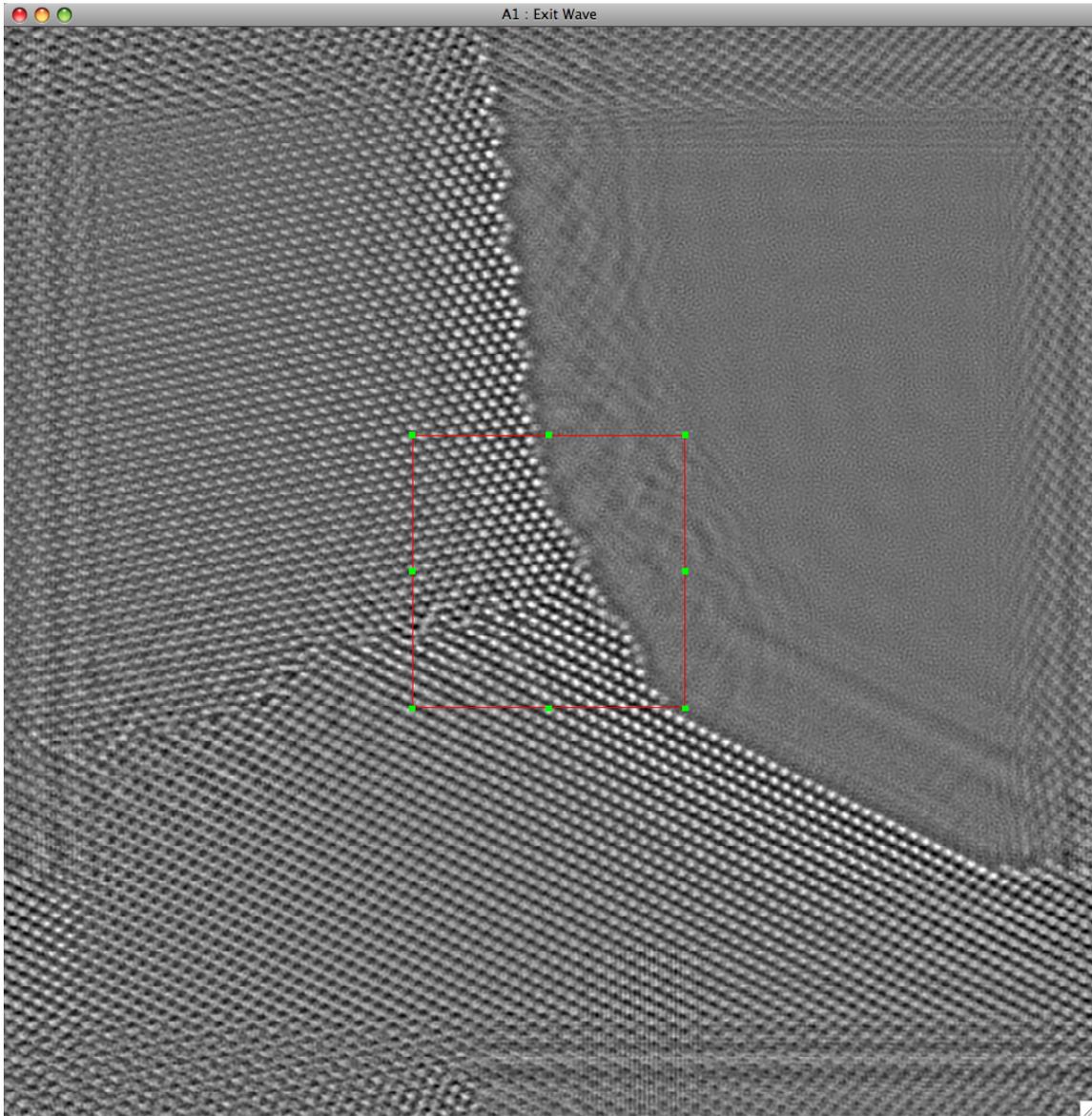


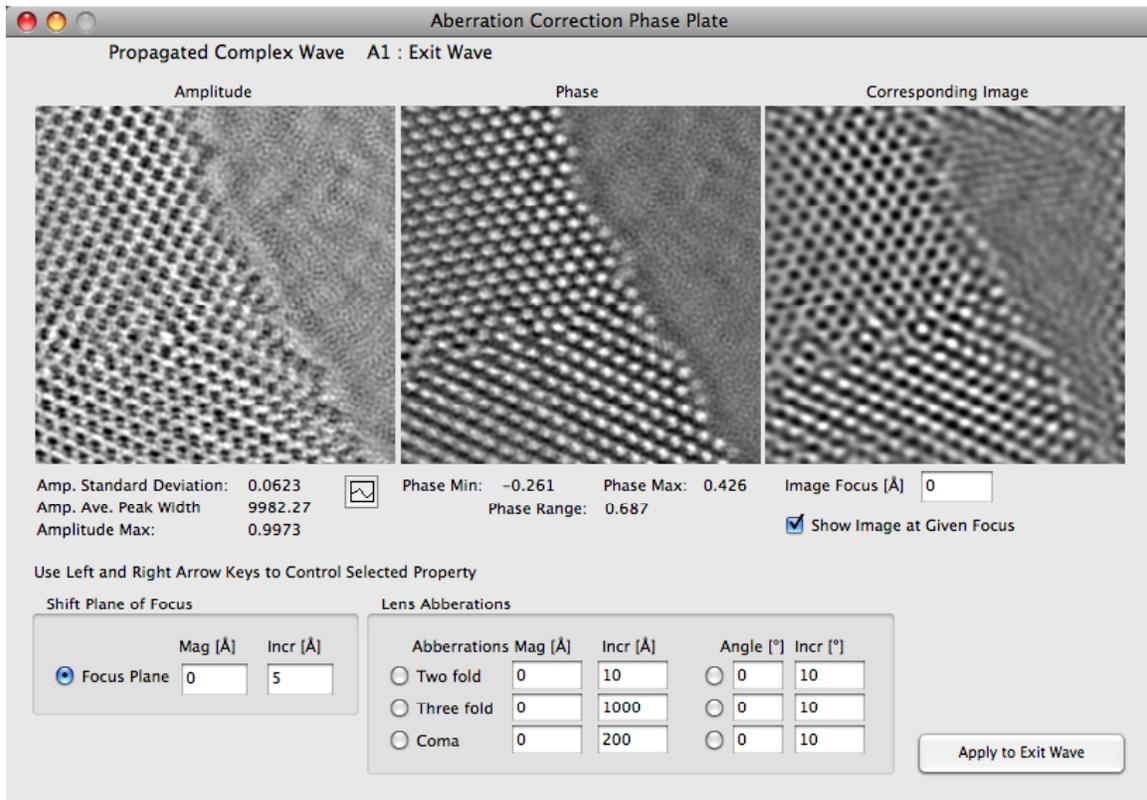
Aberration Correction...

The starting focus value and other aberration coefficients may not be determined initially with optimum accuracy. In order to possibly correct for any change in these parameters, it is possible to apply a phase plate to the reconstructed exit wave.

When the Aberration Correction menu command is invoked, a default selection will be placed on the exit wave. This selection can be moved around. Once invoked, a window shows the amplitude image and the phase image. The user selects which parameter to adjust, and can modify it with the left and right arrow keys. The amplitude and phase image are continually updated for the new values of the selected parameter. Once satisfactory settings are found, the new parameters can be applied to the entire exit wave. If the selection gets deleted,

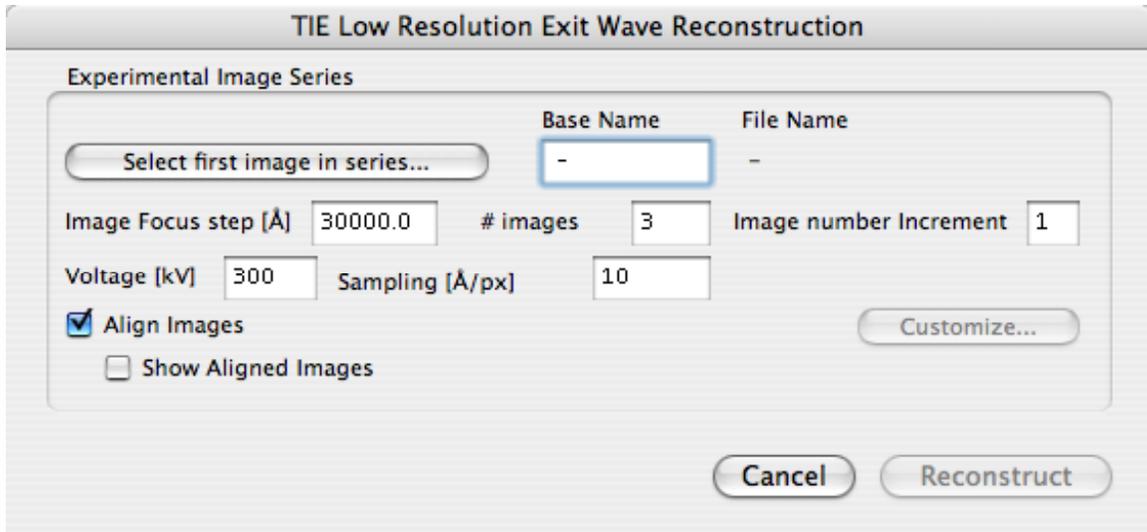
a new default selection is automatically created if the aberration window is open. It is possible to also show the corresponding computed image for any given focus from the current exit wave with the imposed aberration corrections.





Low Resolution TIE Method...

takes take 3 or more low resolution images taken at different values of focus and attempts to reconstruct the complex low resolution exit wave. The algorithm is based on the Transport of Intensity equation and can be used on low resolution images for imaging magnetic domains, etc.



Shiske Filter Restoration...

The Shiske filter relies on the assumption that the observed signal (the image) is related to the object (the projected potential) in a linear fashion through a transfer function. This holds true to a good approximation for the Fourier coefficients of the potential and the image within the validity of the Weak Phase Object Approximation (WPOA). In the WPOA the specimen is thin enough so that the object is thought of as a phase function operating on the phase of the electron wave function. Multiple scattering is ignored and the propagation of the wavefield within the specimen is also ignored. In addition, most of the electrons are considered not scattered (the central beam in the diffraction pattern is strong). Within the WPO approximation one can write

$$I_i(\vec{g}) = V(\vec{g})H_i(\vec{g}) + \eta_i(\vec{g})$$

where H is a transfer function associated with the microscope, V is the potential (projected) of the specimen and I is the fourier coefficients of the recorded image. A noise term is added which is to be considered uncorrelated with the object we are trying to reconstruct. In the equation above, we are stating that we can record a number of different images for different values of the transfer function H and noise, given the same object V.

We want to find the best estimate of the potential given N images recorded at different conditions of the microscope lens. We want to express the estimate by the application of a set of filters such that the estimated potential can be written

$$V_{est}(\vec{g}) = \sum_i F_i(\vec{g})I_i(\vec{g})$$

Thus what we try to find is the optimal solution for a filter function which minimizes the difference between the estimated solution and the “true” potential which we seek to find.

$$\text{Minimize } \left\langle \left| \sum_i F_i(\vec{g}) I_i(\vec{g}) - V(\vec{g}) \right|^2 \right\rangle$$

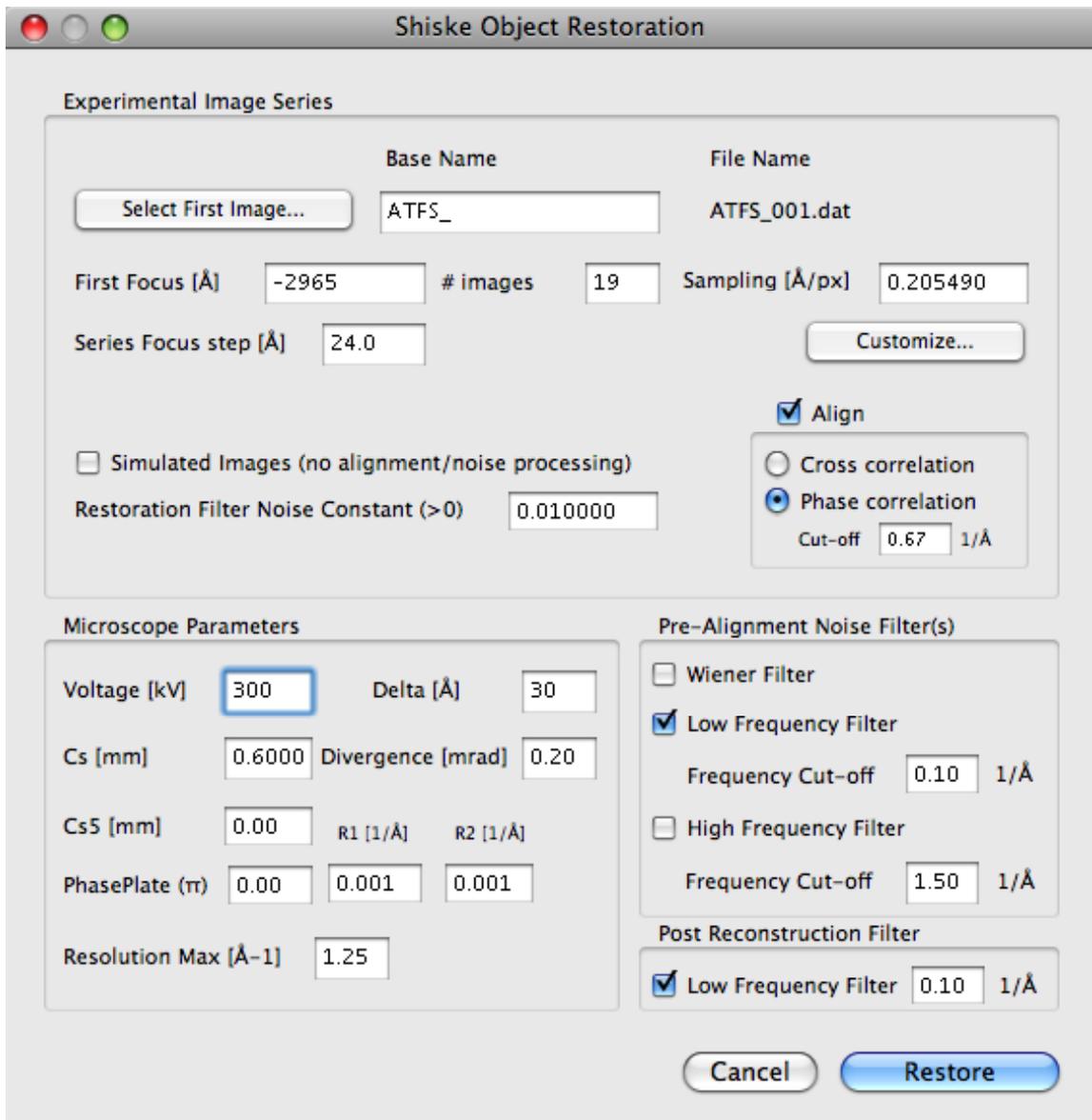
The solution is a filter function operating on each image of the form

$$F_i(\vec{g}) = \frac{H_i^*(\vec{g})}{\sum_i H_i(\vec{g})^2 + N/O}$$

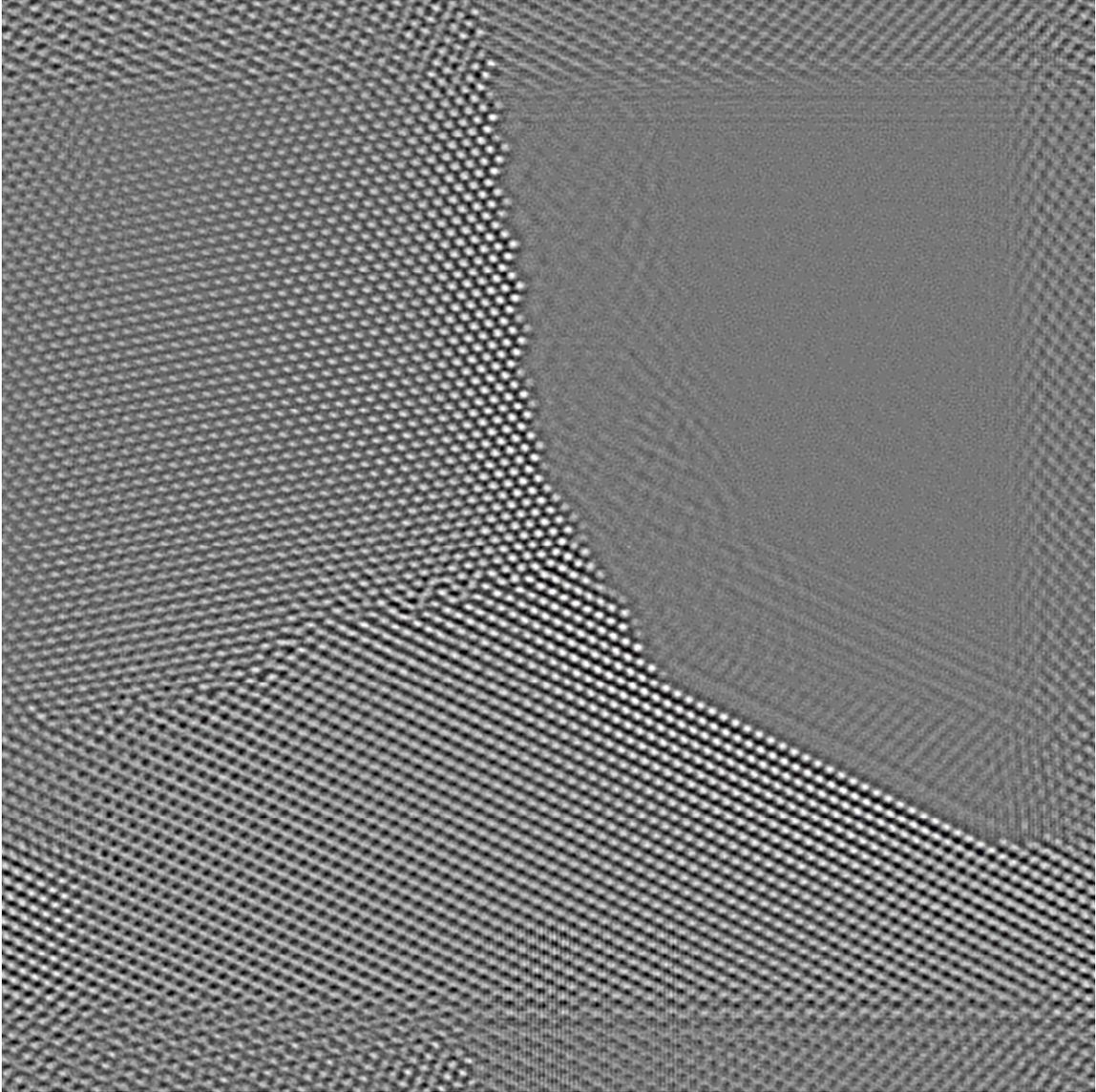
In the WPOA the function H is proportional the contrast transfer function of the microscope.

$$H_i(\vec{g}) \propto \sin(\chi_i(\vec{g}))$$

Below is an example of the use of the Shiske filter restoration on the same experimental images of gold used in the Gerchberg-Saxton exit wave retrieval algorithm.



In the image below, there has been imposed a low frequency cut-off corresponding to 5 Ångströms.

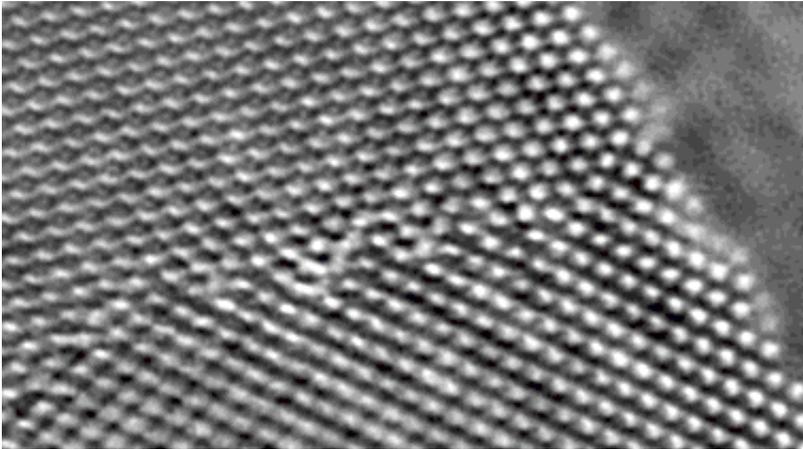


V Comparison of Reconstruction Methods

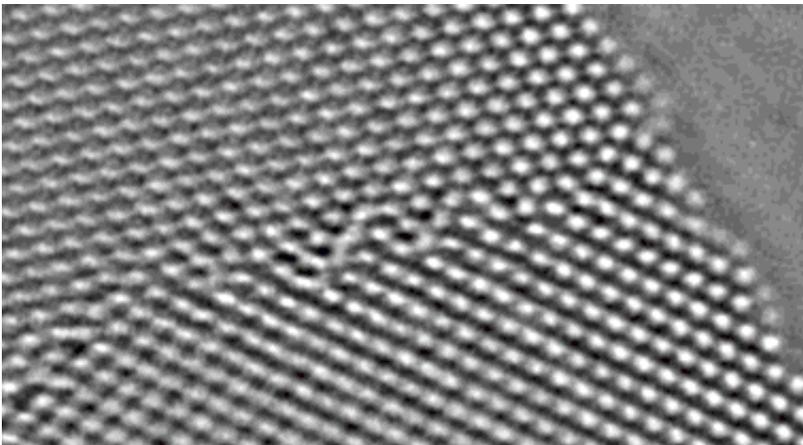
It is interesting to try to compare the solutions one finds by using different methods, in this case the results from True Image, Gerchberg-Saxton and Shiske filtering. True Image and Gerchberg-Saxton attempts to restore the exit wave while Shiske restoration tries to restore the potential. In the images below, we are comparing qualitatively the phase of the exit wave from the two exit wave reconstruction methods with the potential found from the Shiske restoration. This is meant show how in this particular case all the methods would lead to essentially the same interpretation of the atomic structure. No claims are made

to the validity of the approximations underlying the different methods.

True Image



Gerchberg-Saxton



Shiske

