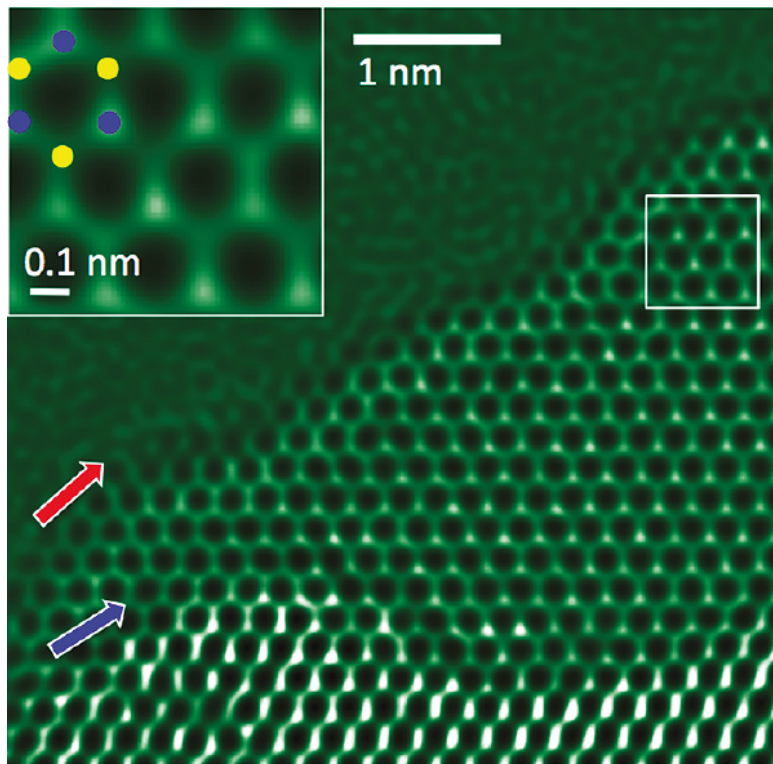# *FTSR for DigitalMicrograph*

Focal and Tilt Series
Exit Wavefunction Reconstruction

FTSR Manual 2.3

HREM Research Inc.

Conventions

The main typographic conventions used in this manual are described below.

Convention	Description
Bold	Used to denote specified elements 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 requires the user 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.
Items in Shaded Boxes	Shaded boxes indicate key references.

Contact Information

General enquiries about FTSR for DigitalMicrograph including software installations should be directed to:

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GMS software can be downloaded from www.gatan.com

To help us answer any queries please make sure you include the FTSR Version Number, Operating System and GMS Version Number with any enquiry.

Technical enquires about focal and tilt series reconstruction not directly related to software installations should be directed to:

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Installation

Software Requirements

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

- DigitalMicrograph (GATAN^{TM}).
  DigitalMicrograph is a part of Gatan GMS (Gatan Microscopy Suite). Currently, there are three versions of the FTSR plug-in respectively for GMS 2.x 64bit, GMS 2.x 32bit and GMS 1.x. The GMS 2.x (32 or 64 bit) can be obtained from www.gatan.com.
- USB Key Driver
- IPU Plug-in (Free-ware downloadable from www.hremresearch.com)

Software Installation

Installing USB Key Driver
The user key driver should be installed by following the instructions provided by the key driver installer. The key driver installer can be downloaded from www.hremresearch.com.

Installing the FTSR Plug-in (also read the file ReadMe.txt)
The plug-in can be installed by "drag-and-drop" copy to the folder "Plugins". The Plugins folder should exist as a subfolder created during a normal installation of DigitalMicrograph.

Installing IPU Plug-in
FTSR uses some functions based on the Intel' MKL (Math Kernel Library) provided by the IPU plug-in. All the files relating the IPU plug-in can be installed by drag-and-drop copy. Please consult the ReadMe file that comes with the IPU plug-in. The IPU plugin can be downloaded from www.hremresearch.com.

When DigitalMicrograph is launched after placing the plug-in into the Plugins folder, FTSR menu commands will appear under "FTSR" menu.

FTSR	Help
Acquire Images	▶
Setup Project Image	▶
Replace Dud Pixels...	
Registration...	
Restoration...	
Minimum Amplitude WF...	
Aberration Corrector	
Check Registration	
Extract All Images	
Extract Current Slice	
Complex To Real	▶
Convert To IWFR	
MTF/NPS Data	▶
Help	▶
About FSR	

Revision Records

New features of version 2.3

Sub-pixel alignment during registration.
The image after "Check Registration" can now be used for restoration.

New features of version 2.2

Process optimization buy sing Intel C++ for GMS 2.x.

New features of version 2.1

You can now use an arbitrary power of the amplitude in the cross-correlation in addition to the current phase-only/square-root amplitude cross-correlation.

New features of version 2.0

FTSR 2.0 is the major upgrade that includes TSR (Tilt Series Reconstruction).

Introduction.

What is FTSR ?

FTSR is a software package that carries out Focal or Tilt Series Reconstruction of the complex wavefunction at the specimen exit surface using either a through focal (FSR) or tilt azimuth series (TSR) of HREM images.

FTSR also contains options for measuring the Modulation Transfer Function of the camera used for data acquisition and for dynamical correction of the effects of residual aberrations on the reconstructed wavefunction.

FTSR runs within the Gatan GMS environment (32 or 64 Bit) as a plugin.

The FTSR software package provides a number of automated functions required to reconstruct the complex exit wavefunction.

I) Automated registration of a dataset of images

II) Determination of the first order aberration coefficients for all individual images. In the case of a suitable tilt azimuth data set these measurements also enable all coefficients in the wave aberration function to be calculated to an order dependent on the size of the dataset used.

III) Removal of the blurring effects of the CCD detector due to an imperfect Modulation Transfer Function [1]. Suitable functions are provided for recording and processing the dataset required to measure the MTF for any Gatan camera.

IV) Compensation of residual aberrations after initial reconstruction using a variable numerical phase plate. For aberration corrected instruments the values of the residual aberrations can be input directly from those estimated by the corrector control software.

The FTSR method described in this manual is based on a linear Wiener filter for the restoration [2], with aberration measurement for individual images based on the PCF/ PCI approach [3,4].

[1] *The Effects of Electron and photon Scattering on Signal and Noise Transfer properties of Scintillators in CCD Cameras Used for Electron Detection*. R. R. Meyer and A. I. Kirkland, Ultramicroscopy, **75**, 23, 1998.
[2] *Super Resolution by Aperture Synthesis: Tilt reconstruction in CTEM*, A.I. Kirkland, W. O. Saxton, K. L. Chau, K. Tsuno, M. Kawasaki, Ultramicroscopy, **57**, 355, 1995.
[3] *A New Method for the Determination of the Wave Aberration Function for High Resolution TEM. 1. Measurement of the Symmetric Aberrations*, R R Meyer, A. I. Kirkland and W O Saxton, Ultramicroscopy, **92**, 89, 2002.
[4] *A New Method for the Determination of the Wave Aberration Function for High Resolution TEM. 2. Measurement of Antisymmetric Aberrations,* R. R. Meyer, A. I. Kirkland and W O Saxton, Ultramicroscopy, **99**, 115, 2004.

Background Theory.

Essential High Resolution Imaging Theory

The wavefunction leaving an object plane, *o*, for monochromatic, axial illumination can be described in terms of a scattered and an unscattered component. For weak scattering the former can be assumed to be significantly larger than the latter and accordingly approximated to unity, as:

$$\Psi_o(\mathbf{x}) = 1 + \Psi_{so}(\mathbf{x}) \tag{1}$$

The recorded intensity in an image plane, *i*, is thus given by:

$$I(\mathbf{x}) = |\Psi_i(\mathbf{x})|^2 = 1 + \Psi_{si}(\mathbf{x}) + \Psi^*_{si}(\mathbf{x}) + |\Psi_{si}(\mathbf{x})|^2 \tag{2}$$

If it is further assumed that the scattering is sufficiently weak to ignore the quadratic term in equation (2) then the Fourier Transform of the image contrast (the fractional intensity deviation) is given as:

$$c(\mathbf{k}) = \psi_{si}(\mathbf{k}) + \psi^*_{si}(-\mathbf{k}) \tag{3}$$

The Fourier transforms of the object and image waves are related by the <u>Wave Aberration Function</u>, *W*(**k**), through:

$$\psi_{si}(\mathbf{k}) = \psi_{so}(\mathbf{k})\omega(\mathbf{k}) \tag{4}$$

where,

$$\omega(\mathbf{k}) = \exp\left[-iW(\mathbf{k})\right] \tag{5}$$

In all of the above derivations a weak object approximation is assumed for simplicity. However more complex object functions can be included [5].

[5] *High Resolution Exit Wave Restoration,* S. J. Haigh and A. I. Kirkland, Chapter 3 (pp 41-72) in "Modelling Nanoscale Imaging in Electron Microscopy", Eds. T. Vogt, W. Dahmen and P. Binev Springer, 2012

Hence in terms of the object wave the Fourier Transform of the image contrast can be rewritten as:

$$c(\mathbf{k}) = \psi_{so}(\mathbf{k})\omega(\mathbf{k}) + \psi^*_{so}(-\mathbf{k})\omega(-\mathbf{k}) + \eta(\mathbf{k}) \tag{6}$$

in which $\eta(\mathbf{k})$ represents the observed noise in an experimental image.

The aim of all exit wave reconstruction algorithms is now to find an estimate of the object wavefunction given a set of observed image contrast transforms, $c(\mathbf{k})$ in the presence of noise and a knowledge of their individual transfer functions, $\omega(\mathbf{k})$.

Restoration Filters

For data available in the form of several differently aberrated images, an optimum solution for $\psi'_{so}(\mathbf{k})$ can be recovered using one of several different restoration filters, based on either linear or non-linear imaging theory. Linear filters, are analytical and have the advantage of computational efficiency, which makes them fast even for large image areas. In contrast, non-linear restoration filters are more generally applicable and in principle are able to deal with thicker specimens where imaging conditions deviate from the simple linear imaging approximation. However, non-linear algorithms require computationally intensive numerical iteration and are therefore slower to calculate.

In the FTSR software, a linear Wiener Filter is applied to a series of images in the presence of noise to give an _optimal estimate_ of the reconstructed wavefunction, expressed in the form of a weighted superposition of the image transforms, c_i, as:

$$\psi'_{so}(\mathbf{k}) = \sum_i r_i(\mathbf{k}) c_i(\mathbf{k}) \tag{7}$$

in which the restoring filters, r_i depend on the complex wave transfer functions, $\omega(\mathbf{k})$ of the individual images as:

$$r_i(\mathbf{k}) = \frac{\Omega(-\mathbf{k})\omega_i^*(\mathbf{k}) - C^*(\mathbf{k})\omega_i(-\mathbf{k})}{\Omega(-\mathbf{k})\Omega(\mathbf{k}) - |C(\mathbf{k})|^2 + \nu(\mathbf{k})}$$

$$\Omega(\mathbf{k}) = \sum_i |\omega_i(\mathbf{k})|^2 \tag{8}$$

$$C(\mathbf{k}) = \sum_i \omega_i(\mathbf{k})\omega_i(-\mathbf{k})$$

The physical effect of equation (7) on a Fourier component transmitted by only a single image is simply to retain it after division by the corresponding transfer function and for components present in all images to average the estimates obtained from any pair of differently aberrated images. For a component not transferred in any image the value of the Wiener filter tends to zero due to the inclusion of the noise to object power ratio, $\nu(\mathbf{k})$. This prevents any amplification of noise in the absence of signal.

It is clear from equation (7) that exit wave restoration is only possible when the imaging parameters for each image and hence the wave aberration functions are known. In addition the individual images have to be accurately registered with respect to a common origin.

In the Final step of the exit wave reconstruction process the exit-plane wavefunction itself is obtained simply by inverse Fourier transformation.

The Wave Aberration Function

For successful exit wave restoration the entire image formation process must be accurately modelled if quantitative data is to be extracted from the restored exit wavefunction. For TEM imaging the objective lens is the key electron optical component and here we briefly describe its influence in terms of a wave aberration function.

For a point object, P_0, imaged using a perfect lens, the wavefield at the back focal plane of the objective lens is spherical and converges to a single point in the image plane, P_{iG}. However, all round, static, purely electromagnetic objective lenses contain positive spherical aberration such that this spherical wavefield is perturbed. Hence, for real lenses, a ray intersects the *image* plane at a point P_i, displaced from P_{iG}. This enables us to define an image aberration as $\delta r = r_i - r_{iG}$. This image aberration is the first differential of the wave aberration function, $W(k)$, which defines the distance between the aberrated and ideal wavefields in the *diffraction* plane.
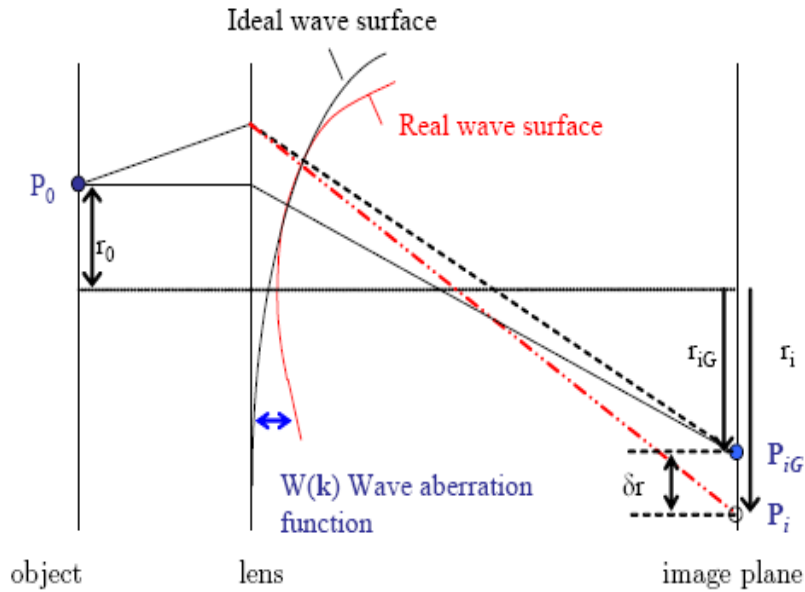
Figure 1. Image formation in a real lens system containing aberrations.

In general, the wave aberration function, $W(k,r,E)$, is a function of the complex reciprocal space vector $k=k_x+ik_y$, position in the image plane r, and the energy distribution of the electrons, E. Variations in W with E are commonly ignored in the *monochromatic approximation* as the electron energy spread is small (~1eV or less at 200kV primary energy, for a field emission source). Furthermore, at high magnification where the field of view is restricted, the dependence of W on r also can be neglected in the *isoplanatic approximation*.

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Applying both of these approximations, *W* can be written in terms of <u>coherent axial aberration coefficients</u> by Taylor expansion of *W* with respect to **k** about the origin of zero scattering as:

$$W(k) = \mathrm{Re}\,\{\, C_{0,1}\lambda\mathbf{k}* + \frac{1}{2}C_{1,2}\lambda\mathbf{k}*^2 + \frac{1}{2}C_{1,0}\lambda^2\mathbf{k}*\mathbf{k}$$

$$+ \frac{1}{3}C_{2,3}\lambda^3\mathbf{k}*^3 + \frac{1}{3}C_{2,1}\lambda^3\mathbf{k}*^2\mathbf{k}$$

$$+ \frac{1}{4}C_{3,4}\lambda^4\mathbf{k}*^4 + \frac{1}{4}C_{3,2}\lambda^4\mathbf{k}*^3\mathbf{k} + \frac{1}{4}C_{3,0}\lambda^4\mathbf{k}*^2\mathbf{k}^2$$

$$+ \frac{1}{5}C_{4,5}\lambda^5\mathbf{k}*^5 + \frac{1}{5}C_{4,3}\lambda^5\mathbf{k}*^4\mathbf{k} + \frac{1}{5}C_{4,1}\lambda^5\mathbf{k}*^3\mathbf{k}^2$$

$$+ \frac{1}{6}C_{5,6}\lambda^6\mathbf{k}*^6 + \frac{1}{6}C_{5,2}\lambda^6\mathbf{k}*^4\mathbf{k}^2 + \frac{1}{6}C_{5,0}\lambda^6\mathbf{k}*^3\mathbf{k}^3 + \frac{1}{6}C_{5,4}\lambda^6\mathbf{k}*^5\mathbf{k} + ...\}$$

(9)

Equation 9 can also be usefully rewritten in polar form, which makes the symmetry of each of the coefficients clear.

The nomenclature used above and subsequently to describe the aberration coefficients is one of several alternatives. In this particular nomenclature the first subscript refers to the order of the coefficient in terms of real space displacements and the second subscript describes the angular symmetry.

However, an older alternative nomenclature exists for the description of the aberration coefficients that follows the Seidel nomenclature using letters to describe the symmetry of the coefficient. These two alternative nomenclatures (see also [6]) are summarised in Table 1 for coefficients, ranked in **k** together with their radial symmetry.

[6] *Aberration Corrected Imaging in CTEM and STEM*, A. I. Kirkland, P. D. Nellist, L. Y. Chang and S. Haigh, Advances in Imaging and Electron Physics, Ed. P W Hawkes, **153**, Chapter 8, 327, 2009.

Aberration Coefficient	Krivanek notation	Typke and Dierksen notation	Order in k	Azimuthal symmetry
Image shift	$C_{0,1}$	A_0	1	1
Two fold astigmatism	$C_{1,2}$	A_1	2	2
Defocus (over focus positive)	$C_{1,0}$	C_1	2	inf
Three fold astigmatism	$C_{2,3}$	A_2	3	3
Axial coma	$C_{2,1}$	B_2	3	1
Four fold astigmatism	$C_{3,4}$	A_3	4	4
Axial star aberration	$C_{3,2}$	S_3	4	2
Spherical aberration	$C_{3,0}$	C_3	4	inf
Five fold astigmatism	$C_{4,5}$	A_4	5	5
Fourth order axial coma	$C_{4,1}$	B_4	5	1
Three lobe aberration	$C_{4,3}$	D_4	5	3
Six fold astigmatism	$C_{5,6}$	A_5	6	6
Fifth order rosette aberration	$C_{5,4}$	R_5	6	4
Fifth order axial star aberration	$C_{5,2}$	S_5	6	2
Fifth order spherical aberration	$C_{5,0}$	C_5	6	inf

Table 1. Coeficients of the wave aberration function ranked in k *with azimuthal symmetry indicated. Notations due to Krivanek and Typke and Dierksen are listed.*

For HRTEM imaging, the effect of the coherent aberrations is to increase the distance travelled by the electron wave, corresponding to a phase change, $\chi(\mathbf{k})$ given by:

$$\chi(\mathbf{k}) = \frac{2\pi}{\lambda} W(\mathbf{k}) \qquad (10)$$

The influence of lens aberrations on the specimen exit wave, $\psi_{so}(\mathbf{k})$, is therefore described by a multiplicative phase factor dependent on the coefficients in the wave aberration function. Accordingly the accuracy to which the coefficients must be known is also a function of resolution (Table 2).

Aberration Coefficients (nm)	Resolution, d (nm)		
	0.12	0.1	0.08
$C_{1,0}$, $C_{1,2}$ (first order in k)	1.43	1.00	0.64
$C_{2,1}$, $C_{2,3}$ (second order in k)	103	59.5	30.5
$C_{3,0}$, $C_{3,2}$, $C_{3,4}$ (third order in k)	6,560	3,160	1,300
$C_{4,1}$, $C_{4,3}$, $C_{4,5}$ (fourth order in k)	392,000	158,000	51,700
$C_{5,0}$, $C_{5,2}$, $C_{5,4}$, $C_{5,6}$ (fifth order in k)	22,500,000	7,530,000	197,000

Table 2. The magnitude of individual aberration coefficients required to produce a $\pi/4$ phase shift for various resolutions.

The PCF / PCI Method for Aberration Measurement

Few of the aberration coefficients defined above are directly observable under axial illumination and aberration determination therefore relies on measurements of one or more possible observables taken as a function of known injected beam tilts.

For an axial focus series (FSR) only the symmetric coefficients $C_{1,0}$ (defocus), $C_{1,2}$ (two fold astigmatism) and $C_{3,0}$ (third order spherical aberration) can be determined ($C_{5,0}$ (fifth order spherical aberration) can in principal also be measured for aberration corrected instruments but it has limited effect except at extreme resolutions). Therefore in order to determine the remaining coefficients it is necessary to acquire a series of images recorded with varying illumination tilts (TSR).

In the FTSR software, values of the aberration coefficients from individual images are calculated from measured values of the defocus and two fold-astigmatism which are evaluated in a two step process using a Phase Correlation Function followed by a Phase Contrast Index Function [3,4].

In the first step, the _relative defocus values_ between images in a focal series are calculated using a <u>Phase Correlation Function</u> (PCF) which also determines the image registration vectors. The PCF is defined as the conventional XCF with the modulus set to unity;

$$PCF(\mathbf{x}) = FT^{-1}\left[F(\mathbf{k}) \frac{c_1(\mathbf{k}) * c_2(\mathbf{k})}{\left| c_1(\mathbf{k}) * c_2(\mathbf{k}) \right|} \right] \tag{11}$$

with $c_i(\mathbf{k})$ the image Fourier transforms and $F(\mathbf{k})$ a rotationally symmetric weighting factor that supresses high frequency noise. This modulus normalisation is important as it suppresses the crystal reflections that make the conventional XCF periodic.

Thus this approach to aberration determination works for crystalline materials and does not require the extended areas of amorphous material that are needed for conventional aberration measurement from fitted diffractograms.

Within the FTSR software it is also possible to use alternative correlation functions for image registration in this first step including the <u>Mutual Correlation Function</u> (MCF) defined by:

$$MCF(\mathbf{x}) = FT^{-1}\left[F(\mathbf{k}) \frac{c_1(\mathbf{k}) * c_2(\mathbf{k})}{\left| c_1(\mathbf{k}) * c_2(\mathbf{k}) \right|^{1/2}} \right] \tag{12}$$

A more General Correlation Function (GCF) is also implemented within the FTSR software given as:

$$GCF(\mathbf{x}) = FT^{-1}\left[F(\mathbf{k}) \frac{c_1(\mathbf{k}) * c_2(\mathbf{k})}{\left| c_1(\mathbf{k}) * c_2(\mathbf{k}) \right|^{1-n}} \right]$$

(13)

where $0 \le n \le 1$.

The optimum use of different correlation functions is determined by the extent of crystalline material in the images to be registered. For images with predominantly crystalline material a value of n close to 0 is optimum and for images with significant amounts of amorphous material a value of n close to 1 is preferred.

For focal series restoration (FSR) the entire data set of images is used in the PCF stage, whereas for tilt series restoration (TSR) the relative defocus values between images in a short (3 member) focal series at each tilt angle are used.

The PCF calculated between two images recorded at different defocus levels therefore consists of a centrosymmetric ring pattern, the exact form of which depends on the relative defocus between them (Figure 2).
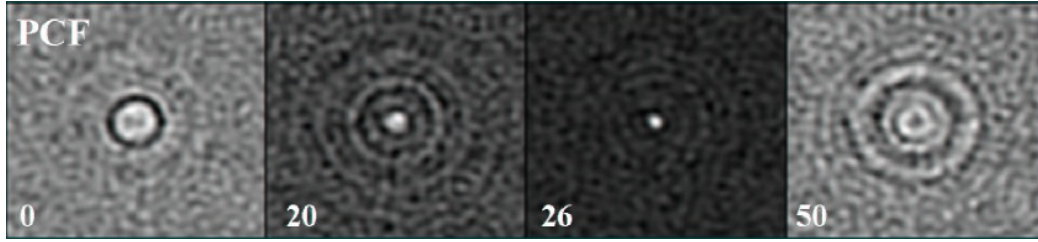
Figure 2. Phase Correlation Functions calculated between two images from a focal series of a crystalline oxide, for different compensated focus differences marked. At the correct compensated focus difference the PCF collapses to a single sharp peak.

It is possible to compensate for the phase shifts giving rise to this ring pattern by the application of a phase factor dependent on the defocus difference thus defining a phase compensated PCF as;

$$PCF(\mathbf{x}) = FT^{-1}\left[F(\mathbf{k}) \frac{\cos(W_{C_1}(\mathbf{k})) c_1^*(\mathbf{k}) c_2(\mathbf{k})}{\left| \cos(W_{C_1}(\mathbf{k})) c_1^*(\mathbf{k}) c_2(\mathbf{k}) + h \right|} \right]$$

(14)

in which the small positive number h prevents a zero denominator and where $W_{c1}(\mathbf{k})$ describes the propagation from the first to the second image in the presence of only a defocus difference C_1. When the value of C_1 used to calculate the phase compensated *PCF* matches the actual focus difference, the phase compensated PCF collapses to a sharp localised correlation peak. Hence, the relative defocus difference between two images can be determined by simply maximising this peak height as a function of the compensated defocus to an accuracy of <1nm.

In the second step an initial image wavefunction, $\psi_{si}(\mathbf{k})$, is evaluated in the plane of a reference image and the absolute values of two fold astigmatism, A_1 and defocus, C_1 are determined using a Phase Contrast Index Function given by;

$$f_{PCI}(\mathbf{k}, C_1, A_1) = -\cos(\arg(\psi_{si}(\mathbf{k})) \_ \arg(\psi_{si}(-\mathbf{k})) + 2W_{C_1, A_1}(\mathbf{k}, C_1, A_1)) \quad (15)$$

Where W_{C_1, A_1} is a wave aberration function including only trial parameters C_1, A_1 and fixed spherical aberration C_3. When these trial parameters are correct, f_{PCI} will tend to unity for all spatial frequencies whereas for mismatched parameters f_{PCI} shows dark bands (Figure 3)
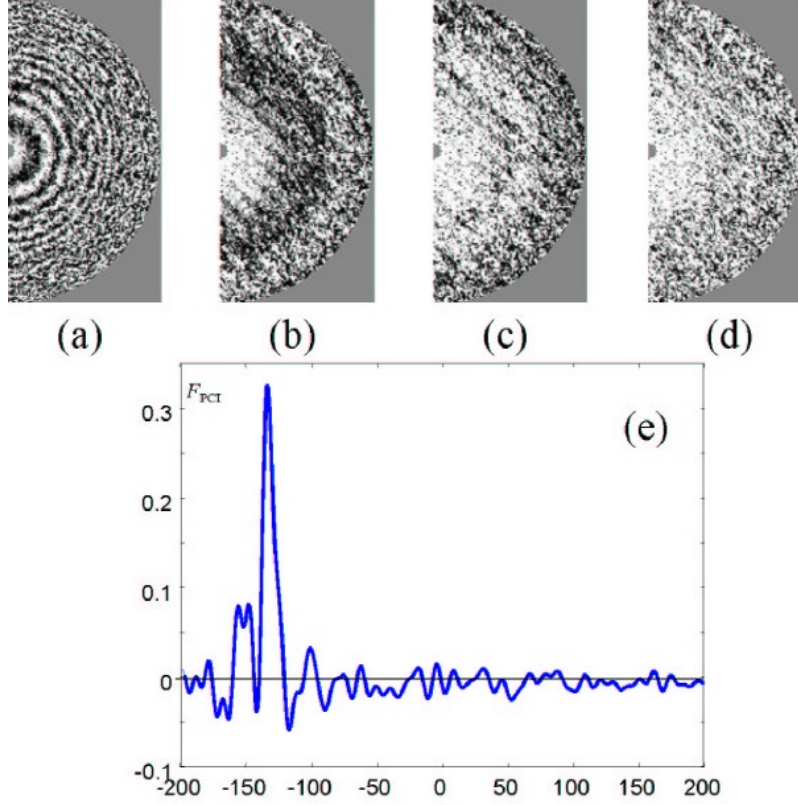
Figure 3. The phase contrast index function, fₚcₗ. For mismatched values of C₁ (a) 50nm, (b) 10nm, (c) 3nm fₚcₗ shows dark rings, whereas at the correct value of C₁, (d) 0nm it is close to one (white) at all spatial frequencies. (e) fₚcₗ plotted as a function of C₁ with a sharp maximum at the correct value of C₁.

In practice the mean phase contrast index, F_{PCI} given by;

$$F_{PCI}(C_1, A_1) = \langle f_{PCI}(\mathbf{k}, C_1, A_1)\rangle_{\mathbf{k}} \quad (16)$$

can be conveniently used, where $<\dots>$ denotes a weighted average over $\mathbf{k}$. This function has a sharp maximum for the correct imaging parameters and hence maximizing this against C_1 and the two components of A_1 allows accurate determination of these parameters.

This method can be extended using measurements of C_1 and A_1 taken under a known set of different illumination directions to evaluate the full set of aberration coefficients by least squares fitting of the parameters to be determined to an overdetermined set of observations available using the linear dependence of the observables on the imaging parameters to yield a unique solution.

Dataset Geometries

Focal Series Restoration (FSR)

A typical focal series dataset consists of between 20 and 30 images.

The key considerations in deciding the acquisition parameters are the *focal range*, the *focal step* and the *number of images* used in total. Suitable values for these depend on the sensitivity of the sample to radiation damage and on the resolution limit and stability of the microscope used.

In setting the *focal range*, the most important factor is that the effective wave transfer function in the final restoration is free from gaps and that it extends to the information limit set by the effects of partial coherence.

The optimum *focal step* between images depends on the resolution required in the final restoration and on the electron optical properties of the instrument used. The focal step affects the individual transfer functions for each image included in the restoration and it is important that this is also chosen to ensure that the effective wave transfer function of the entire series is free from transfer gaps at all spatial frequencies up to the information limit of the microscope.

The radiation resistance of the sample ultimately determines the total *number of images* that can be used for a specific electron dose. For many inorganic materials 30 or more images can be recorded whereas for sensitive organic materials, sample damage can be significant for as few as ten images. However the minimum *number of images* used should not be less than five for accurate exit wavefunction reconstruction. Using more images has the additional benefits of improving the signal to noise ratio in the final restoration and also lessening the effects of non-linear imaging components which reduce as *$(N)^{1/2}$* for *N* images

Uncorrected Microscopes

For <u>uncorrected instruments</u> the information limit set by the effects of partial spatial and temporal coherence is close to the Scherzer resolution limit ($d_{sch}= (C_3^{1/4}\lambda)^{34}$) determined by the effects of finite positive C_3 for thermionic electron sources. However it extends considerably beyond this value for Field Emission Sources with smaller virtual source sizes and reduced energy spreads.

For an instrument fitted with a Field Emission Source a useful *focal range*, extends from the Scherzer Defocus to *ca.* 5 Sch underfocus. The starting Scherzer focus is often recognizable but where it is not, adjusting the microscope to give an image with minimum contrast (Gaussian focus) and then underfocussing the objective lens by the correct amount corresponding to the Scherzer focus (determined by the

accelerating voltage and C_3) gives a suitably accurate starting point if the objective lens focus step is calibrated.

This implies a *focal step* of 1/5 Sch for a 20 member series or less if more images are used.

For instruments with a thermionic source a larger *focal step* can be used over the same *focal range,* which can usefully reduces the overall number of images, without significantly affecting the ultimate resolution of the restoration.

Importantly an ideal dataset should not contain images with low contrast, which may be difficult to accurately register and may subsequently need to be excluded from the reconstruction.

The reduced unit of defocus (Sch) is given by $(C_s\lambda)^{1/2}$

Corrected Microscopes

For aberration corrected instruments two alternative settings for the focal step can be defined.

The Resolution Limited Condition.

For a corrected instrument it is often more useful to define the *focal step* (ΔC_1) in terms of an allowable phase shift (typically $\pi/2$) at the ultimate resolution limit (g_{max}) of the reconstructed exit wave as:

$$\tfrac{1}{2}\, \Delta C_1\ g_{max}^2 < \pi/2 \tag{17}$$

The optimum *focal range* for the above condition is now determined by the *focal step* and the number of images (normally 20-30 images).

As is the case for uncorrected instruments larger numbers of images reduce the effects of non-linear image components in the restoration and help to ensure uniform transfer in the effective wave aberration function used in the restoration.

The C_5 Balanced condition

An alternative focal series dataset suitable for corrected instruments, where the 5th order spherical aberration limits the resolution, relies on balancing the uncorrected positive 5th order spherical aberration with the 3rd order spherical aberration and 1st order defocus to establish the starting point of the focal series

The equations that determine the values of third order spherical aberration and first order defocus, in the presence of a limiting positive fifth order spherical aberration are:

$$C_3 = -2.88(C_5^2\lambda)^{\frac{1}{3}}$$

(18)

$$C_1 = +1.56(C_5\lambda^2)^{\frac{1}{3}}$$

(19)

To apply this condition in practice the user should adjust C_3 to the small negative value as given above (using the corrector control software) and record a focal series with a focal step determined by the allowable phase shift at the ultimate resolution limit of the reconstructed exit wave as defined in the previous section describing the Resolution Limited Condition. It should be noted that this gives a narrow focal range and requires highly stable objective lens control and sample stability to be effective.

Note: For all types of instruments focal drift due to objective lens or sample instabilities should be minimized for successful focal series restorations and it is important to ensure that the focal step used is greater than any residual focal drift between images in the focal series.

Tilt Series Restoration (TSR)

The overall geometry of a Tilt Series dataset consists of several short (3 image) focal series recorded at a number of different tilt azimuths $(\theta_1$ to $\theta_6)$ as shown below.
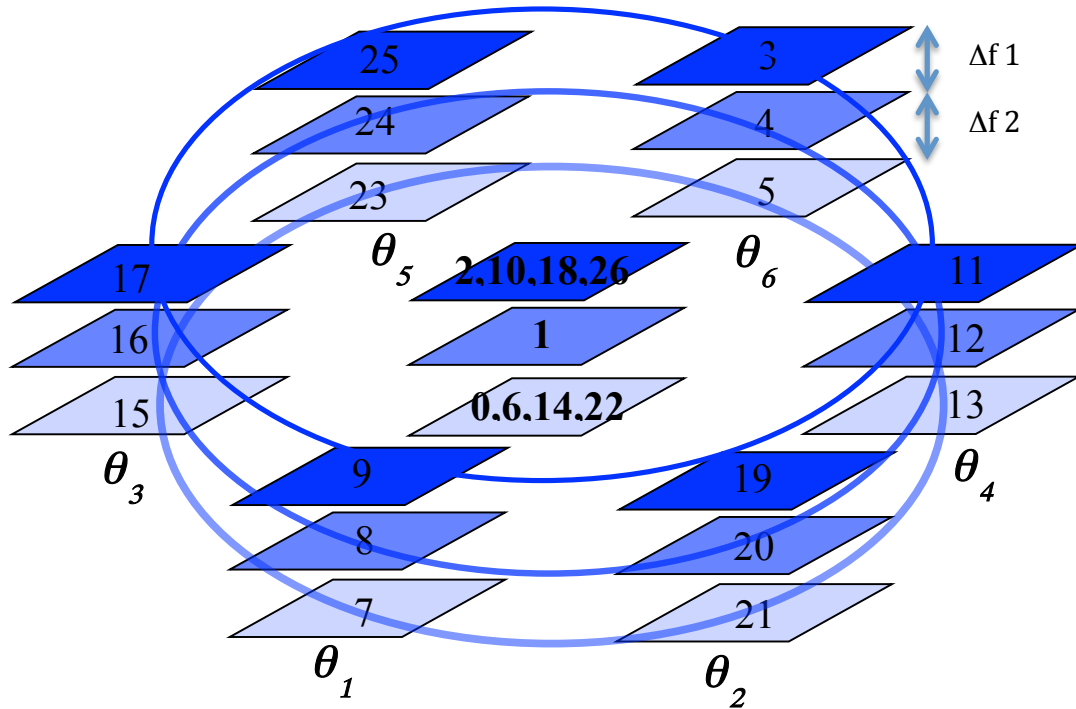
Figure 2. A typical Tilt Azimuth Dataset for 6 tilt azimuths recording a short 3-member focal series at each. Numbers for each image describe the optimum sequence for image acquisition in order to minimize hysteresis in the objective lens and beam tilt coils.

For Tilt Series reconstruction datasets the considerations of sample damage and the reduction in non-linear image components that affect the optimum total number of images described for focal series reconstruction also apply equally.

The order of experimental image acquisition is important in order to avoid errors arising from hysteresis in either the objective lens or beam tilt coils (the order in Figure 2 minimises this effect).

Note*: In the Diagram above the middle image within the short focal series is that used for exit wavefunction reconstruction.*

For tilt series datasets three acquisition parameters are important, firstly the *tilt angle* secondly *the number of images* and finally the *focal step* between images within each short focal series. Currently, the number of images is fixed to 26 as in the above scheme.

Uncorrected Microscopes

For *uncorrected instruments* the *tilt angle* that provides maximum resolution improvement is related to both the defocus of the axial image and the finite spherical aberration [2].

The relationship between the optimum tilt angle and the defocus is given by:

$$C_1 = C_3 \tau^2 \tag{20}$$

where the tilt angle in reduced units is related to the spherical aberration as:

$$\tau = \left(\lambda / C_3 \right)^{\frac{1}{4}} \tag{21}$$

The above equations imply that there is no single optimum tilt angle for reconstruction. For a given defocus, if the tilt angle is too low then the reconstruction offers limited resolution improvement compared to the axial limit and higher tilt angles lead to transfer gaps in the final wave restoration transfer function.

In practice a defocus of 1 Sch ($C_1 = \left(C_3 \lambda \right)^{1/2}$) and a corresponding tilt angle of one reduced unit is a good compromise.

The *focal step* between images in each short focal series is primarily determined by the requirements of the PCF / PCI approach used within the FTSR software. The key requirements are that all three images in the short focal series show high contrast and that the focal steps *(Δf1* and *Δf2*) are not equal and Golden mean ratio between these is generally a good choice. These choices are important to ensure accurate registration and determination of the relative defocus levels within each short focal series.

The number of tilt azimuths used is primarily determined by considerations of sample damage and overall acquisition time. In practice 6 equally spaced tilt azimuths as shown in Figure 2 provide good coverage of Fourier space without needing an excessive number of images.

Corrected Microscopes

For *corrected instruments* the relationship between optimal tilt, the uncorrected parasitic axial aberrations and chromatic effects is more complex.

For this type of instrument the most important difference is that the critical conditioning between the focus of the central image and the tilt angle (equations (20) and (21)) is relaxed and larger tilt angles can therefore be employed than for uncorrected instruments leading to greater resolution improvement.

Ultimately, for corrected instruments the maximum tilt (and hence resolution improvement) that can be obtained is limited by either uncorrected residual axial aberrations, or by partial temporal coherence.

The maximum tilt angle allowed due to uncorrected residual aberrations can be estimated by setting a phase shift limit of *$\pi/2$* as the maximum allowed and measuring the variation in the uncorrected axial aberration coefficients with beam tilt magnitude.

In practice for third order electron-optical correction the residual coefficients are sufficiently small that tilt angles up to 25mrad do not lead to significant phase shifts according to the above criterion.

Appendices

A: Worked Example of Focal Series Reconstruction

This example describes the steps needed to restore the specimen exit wavefunction from a focal series of experimental images of $Nb_{16}W_{18}O_{94}$ (niobium tungsten oxide) acquired using a 300kV JEOL 3000F FEG transmission electron microscope.

In order to restore the specimen exit wavefunction the effects of the imaging system of the microscope must be compensated. These effects include,

1. The coherent aberrations of the objective lens (which in a conventional microscope will be dominated by the effects of the finite positive spherical aberration)
2. The partial coherence due to the finite size of the illumination source and instabilities in the current and voltage power supplies
3. The transfer system of the camera used, described by the Modulation Transfer Function

These parameters will vary from one instrument to another and for a restoration their values must be measured accurately.

The experimental parameters for NbWO Data used in this example are given in the table below. You will need to enter these values later in order to perform the restoration.

Parameter	Value
Accelerating Voltage	**300kV**
Sampling Interval	**0.028nm**
Spherical Aberration (C_3)	**0.6mm**
Nominal Focus Step	**10nm**
Three Fold Astigmatism (A_2) Rectangular Notation	**850, -100nm**
Beam Divergence	**0.15mrad**
Focal Spread	**4nm**
K_{max}	**$10nm^{-1}$**
Start Focus	**-150nm**
End Focus	**+50nm**
Vibration	**0.03nm**

STEP 1) Examine the Images

The data set consists of a focal series of 30 images numbered (100-129) that can be downloaded from:
www.hremresearch.com.

Initially use only images numbered 116 to 126.

It is important to critically assess the quality of images in a restoration data set. If images are poor quality the restoration will not succeed. If the information you are trying to recover is not present in any of the images it will not be present in the restoration and it is not worth spending a large amount of effort trying to retrieve it. To initially assess the image quality open a selection of the images and look at the FFTs (compute the Fourier transform from an image using the FFT command in the 'Process' menu in DigitalMicrograph). The Fourier transforms of the images show the resolution of the highest spatial frequency present in an

image. For example in this dataset the image #125 is blurred and shows better information transfer in one direction than in the other. In some cases it helpful to leave poor quality images out during the restoration step. Similarly, if the sample is obviously changing through the image series it may be necessary to perform the restoration using only a partial dataset of images where any changes are minimised.

STEP 2) Setup Images

Assemble the individual images from the focal series into a "3D block" using the **'FSR Project from Archived Images…'** of **'Setup project images'** under the FTSR main menu. This will show the following dialog:
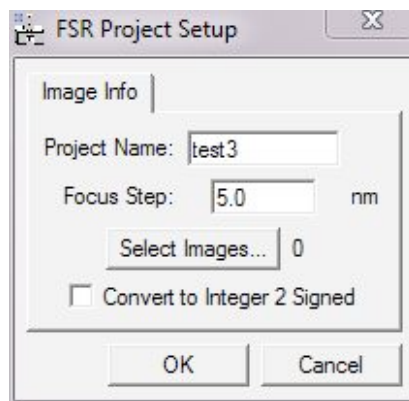
Give the project a suitable name and fill in the **focus step** using the value given above.

Choose which images are to be included in the exit wave restoration. To select multiple images hold down the shift key.
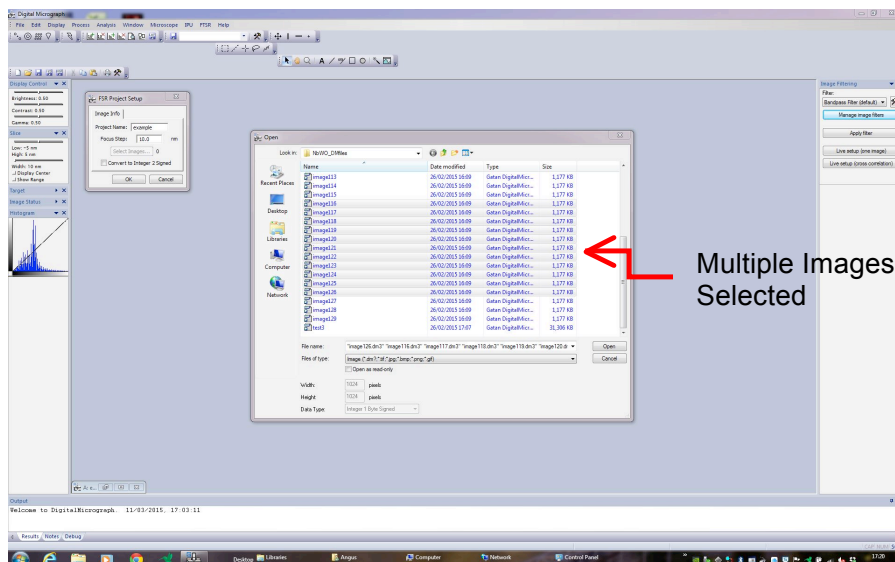
Use the *"Slice Tool"* in DigitalMicrograph to examine the 3D block of images. Click on the small ruler icon in the target window to verify how images in the slice are labeled. It is possible to visually estimate the specimen drift present in the data set by identifying a feature and tracking the position of this feature in each sequential slice. If the specimen drift is too large this will prevent high-resolution information from being recovered. In general the specimen drift should be less than one pixel during the exposure time used to record the image.

NOTE: Creating a slice renames the images starting from slice 0 so it is helpful to keep a careful note of original and new image numbers.
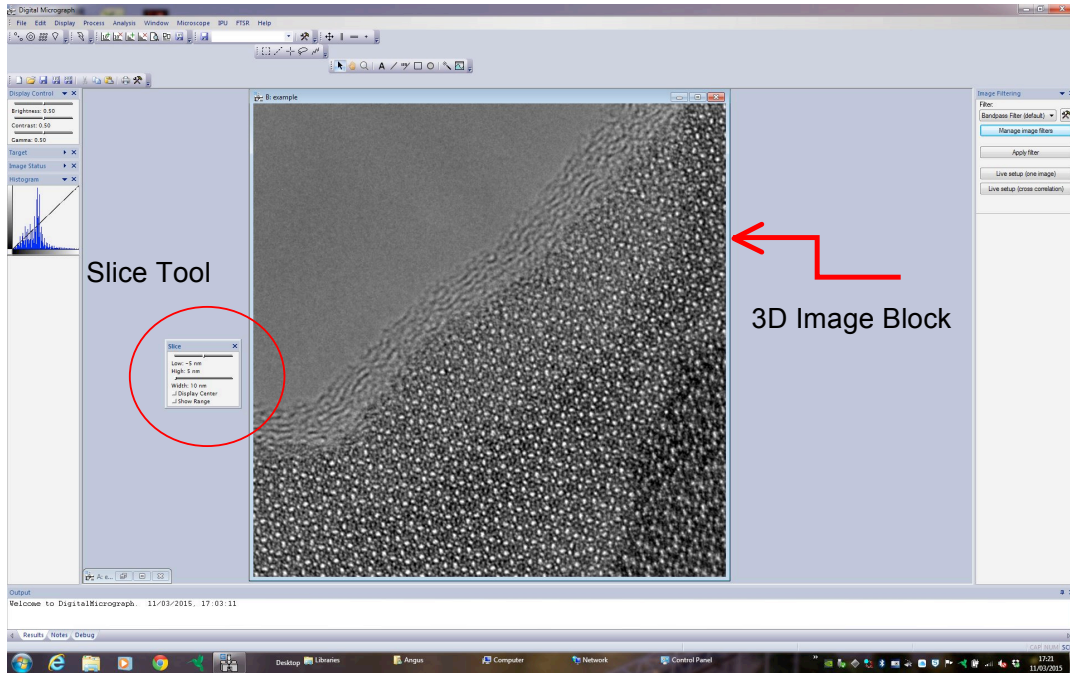
STEP 3) Run FSR Registration

This step measures the drift and focus change of each image relative to the reference image.

First select a small 2^nx2^n region (e.g 512 x 512 pixels, n=9) using the ***ROI tool*** in DigitalMicrograph. The best results are usually obtained when this area contains some amorphous material or a specimen edge together with some of the material of interest to allow accurate cross correlation during the registration. As the defocus of the sample may vary across the field of view it is generally advisable to choose an area as close as possible to the region of interest for the final restoration.

NOTE: A click/drag with the alt key held down will force the ROI tool to select an area of size 2^nx2^n.
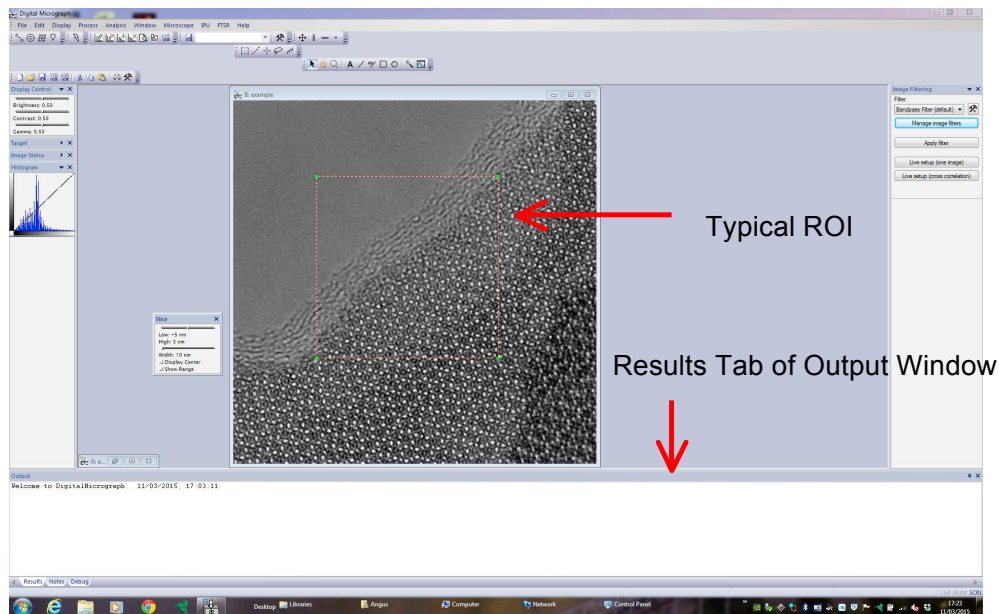
The results of the registration are displayed into the ***Output Window*** in DigitalMicrograph (selecting the ***Results tab***) so this should be open and visible (not obscured by any images). If it is not already open it can be opened by selecting **"Show Output Window"** from the **"Window"** menu in DigitalMicrograph.

With the 3D data block selected, choose **Registration** from the FTSR menu. This displays the FSR Registration Dialog Box. Using the three tabs, **Control, Setup and Option** shown below all the experimental and microscope parameters needed for the registration can be entered.

In the **Control tab** enter the following values:

> The *number of the reference image*[1] and the *numbers of the first and last images*
> > to be used in the registration. The reference image cannot be either the first or the last image in the data set.
>
> The *sampling interval.*
>
> *The value of K_{max}*

At the bottom of the "Control" tab click "Browse" and select the *mtf* (modulation transfer function) and *nps* (noise power spectrum) files for the camera used to acquire the data. These files describe the transfer characteristics of the camera and can be calculated directly within FTSR (see appendix C). For this example suitable MTF and NPS files can be downloaded from:
www.hremresearch.com.

Finally select the **Cross Correlation Mode** (Phase Only (PCF), Square Root Amplitude (MCF) Regular (XCF) or Arbitrary Amplitude Power (GCF) from the drop down menu

---
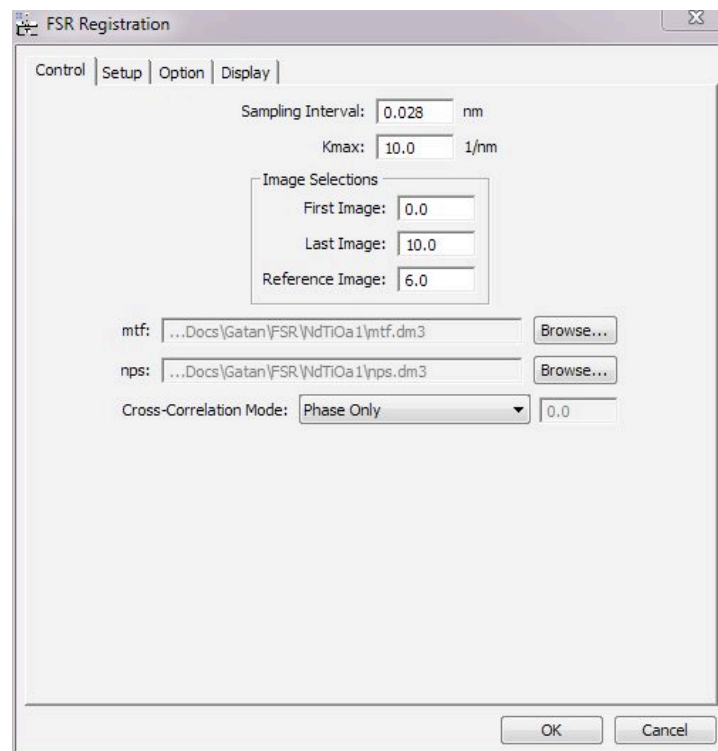
[1] To use the image with the original number 122 as the reference image, where the images named image116 to image126 are to be included in the registration, the images will be referred to as 0,1,2,3 …. 9,10 in the 3D data block. Therefore, the number of the reference image will be 6 as there are 7 images between the first image116, labelled 0, and the reference image122, labelled 6. To convince yourself of this compare the names and slice number of images in the data cube

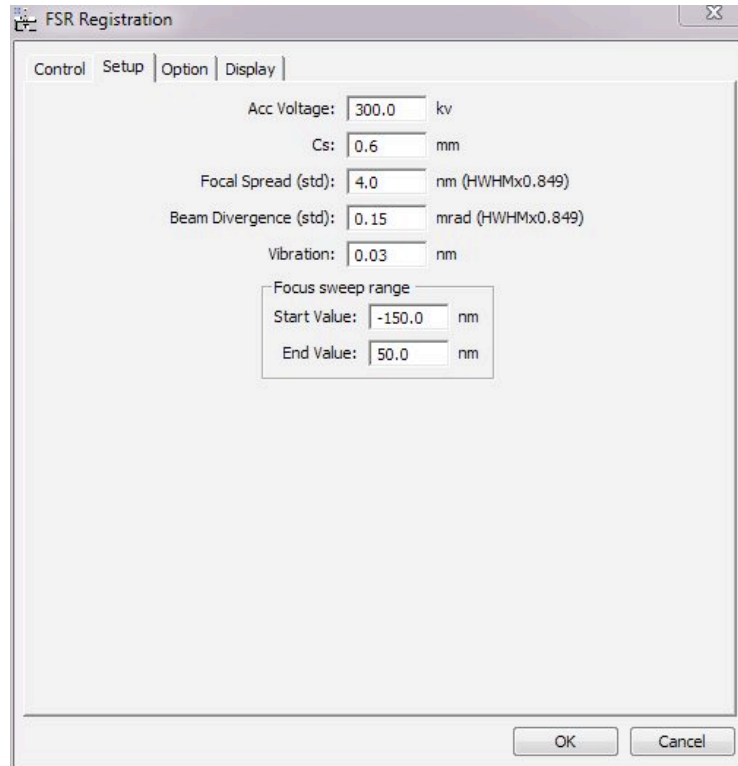In the **Setup tab** enter the following values:

The *Accelerating voltage*
The *value of C_s*
The ***Focal Spread***
The Beam Divergence
The *value of **Vibration***
The values for the ***start*** and ***end focus*** used to search

In the **Option tab** enter the values for any residual uncorrected aberrations present in the dataset using either *rectangular or polar notation*. In this example only the residual value for A_2 is used.
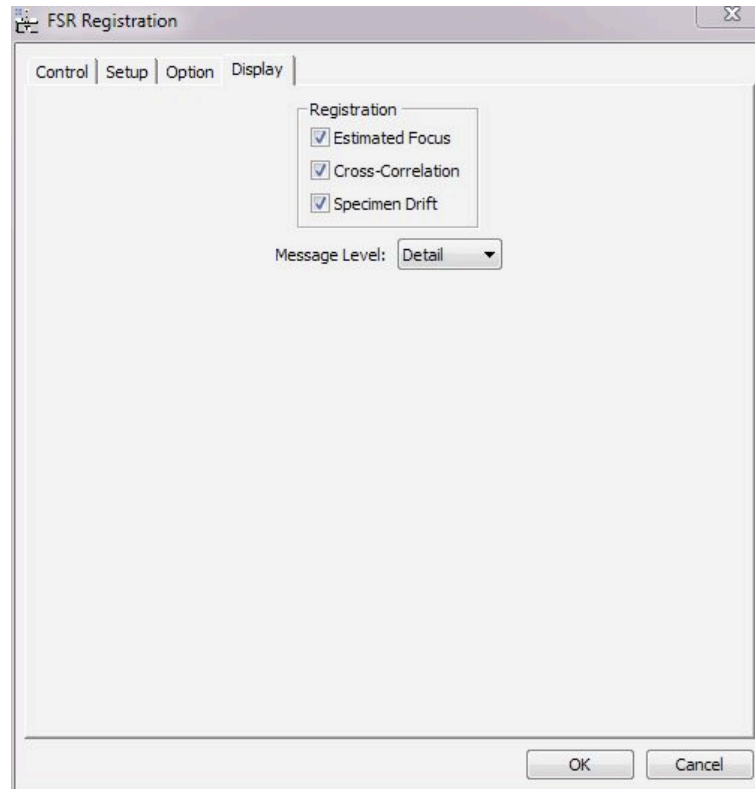
The **Display tab** selects the output of information from the registration process with selection boxes for the *Estimated Focus, Cross Correlation* and *Specimen Drift*. There is also an option to select the *Message Level*.

For this example select all outputs and set the message level to Detail

When you are satisfied you have input all the parameters correctly click *OK* to start the registration process.

The calculation for 11 images, using a 512 x 512 ROI takes about a minute on a standard PC.

While the calculation is proceeding it is useful to watch the results. If you realize a mistake has been made *it is possible to cancel the registration at any stage by holding down the* **SPACE** *bar*.

The first step of the registration uses a phase correlation function to measure the differences in defocus (focal step plus any focal drift) and 'x, y' position (due to specimen drift) between the reference image and the images either side of the reference. It then uses this estimate of the focal difference and specimen drift to find the complex image at the reference plane. Next, the differences in defocus and 'x, y' position from the complex image are measured for each image in the series, and the estimated complex image at the reference plane is updated by adding the contribution from the new image. The best fit for each image with the complex image at the reference plane is output in the *Results tab* of the Output window in DigitalMicrograph.

For example for image 1 the output in the results window is :

fsr_pred_xmpcf image 1 with c1=-68,-52,0.5
image: 1 c1,the=-68,0 x,y,t = 7,2,0.0156433
image: 1 c1,the=-66,0 x,y,t = 7,2,0.0195913
image: 1 c1,the=-64,0 x,y,t = 7,2,0.0232036
image: 1 c1,the=-62,0 x,y,t = 7,2,0.0259503
image: 1 c1,the=-60,0 x,y,t = 7,2,0.0276188
image: 1 c1,the=-58,0 x,y,t = 7,2,0.0277665
image: 1 c1,the=-56,0 x,y,t = 7,2,0.0266799
image: 1 c1,the=-54,0 x,y,t = 7,2,0.0245146
image: 1 c1,the=-52,0 x,y,t = 7,2,0.0214846
image: 1 c1,the=-59,0 x,y,t = 7,2,0.0278797
image: 1 c1,the=-58.5,0 x,y,t = 7,2,0.0278615
Best fit to image 1: c1=-59 x,y,the,t,min = 7,2,0,0.0278797,-0.00288628
adding im 1 pos 7,-9 to rest. c1=-59 a1=0,0 bti=0,0 cs=0.6 a=0 the=0

In the above data **c1** is the defocus difference from the complex image at the reference plane
(-59nm). The specimen drift in pixels is given by **x, y** (in the above output x=7 and y=2) and
the height of the correlation peak is referred to as **t**. In this example, the best fit (highest peak
height) is 0.0278797. Values of **t** less than 0.01 should be considered suspect as the fit may be
too poor to allow the exit wavefunction to be successfully restored.

In the display of the final best fit **a1** is the two fold astigmatism and **bti** is the beam tilt (0,0
for an axial focal series data set).

The final output in the results window is a summary of the fit for all the images relative to the
reference image. e.g. for this example:

Best fit to image 0: c1=-70 x,y,the,t,min = 2,-5,0,0.028546,-0.00300342
adding im 0 pos 9,-14 to rest. c1=-70 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 1 pos 7,-9 to rest. c1=-59 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 2 pos 0,-11 to rest. c1=-48 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 3 pos 3,-11 to rest. c1=-36.5 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 4 pos -1,-10 to rest. c1=-23 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 5 pos -1,-2 to rest. c1=-11.5 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 6 pos 0,0 to rest. c1=0 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 7 pos 0,6 to rest. c1=12 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 8 pos -4,10 to rest. c1=23 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 9 pos -6,13 to rest. c1=34 a1=0,0 bti=0,0 cs=0.6 a=0 the=0
adding im 10 pos -3,14 to rest. c1=45.5 a1=0,0 bti=0,0 cs=0.6 a=0 the=0

In addition to the output window a set of graphs of the key parameters may also be displayed
depending on the selections made in the **Display tab**.

The *Estimated Focus* window plots the focus values of each of the images in the series
against the image number (0-10 in this case). For a focal series with a constant focal step this
plot should be approximately linear like the one below. Significant deviations from linearity
indicate the presence of non-linear focal drift or of errors in the registration and these images
may have to be excluded from the final restoration.
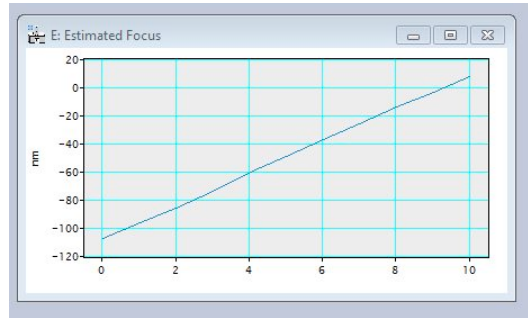
The Cross Correlation window displays the maximum correlation peak height (*t*) for each of the images. As demonstrated in the plot below, the registration of images close to the reference image or near the Gaussian defocus may be lower but values greater than 0.01 generally indicate an acceptable registration. This minimum peak height may vary for different types of specimens.
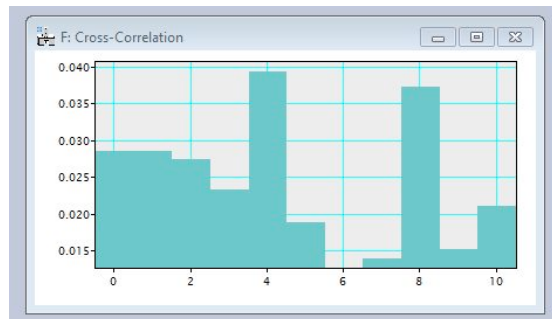
The 'Specimen drift' window shows the relative displacement between each of the images in both the x and y directions. If this is rapidly varying and non-linear, it may mean that the correlation between images is poor or that there is too much drift in the experimental data for high resolution to be achievable in the final restoration.

Do not panic if the registration varies from those shown here. The technique is sensitive to the exact specimen area since it measures local aberrations and these may vary slightly across the field of view. However, if the values are very different go back and check you didn't make any mistake inputting the required values.
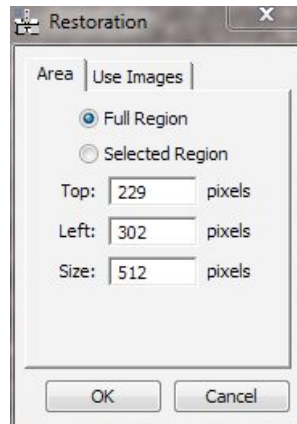
After Registration

After the registration process is finished the registration values can be checked using the **Check Registration** command in the FTSR main menu. This displays the 3D data block of images aligned using the registration values calculated and the accuracy of the registration can be assessed using the *Slice Player* in DigitalMicrograph.

STEP 4) Run FSR Restoration

This step combines the images to form the restored exit wavefunction.

From the **FTSR Menu** select **Restoration**, which displays the restoration dialog

Using the **Area tab** is possible to choose to restore the wavefunction for either the whole field of view, the region for which registration was performed or any selected region specified here using the parameters determined from the registration of the smaller ROI.

The **Use Images tab** allows you to select which images are used in the restoration. In this example all 11 of the images initially used to form the 3D data block are used.
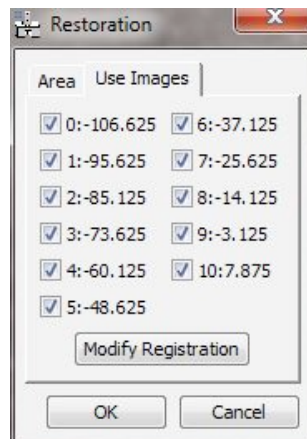
Press **OK** to start the restoration process

Pressing the **Modify Registration Button** displays the dialog below which allows you to alter the calculated registration vectors of any individual image or to exclude specific images. In this example image 6 is the reference and none of the registration vectors are changed.

Modify Registration

Use	Defocus	x-shift	y-shift	Use	Defocus	x-shift	y-shift
✓ 0:	-106.625	8.91148	-13.2918	✓ 6:	-37.125	0.0	0.0
✓ 1:	-95.625	6.2818	-8.30098	✓ 7:	-25.625	-0.49502	6.66581
✓ 2:	-85.125	-0.36096	-10.2098	✓ 8:	-14.125	-3.71559	10.3195
✓ 3:	-73.625	2.24265	-10.1042	✓ 9:	-3.125	-5.32992	13.135
✓ 4:	-60.125	-1.44037	-9.72375	✓ 10:	7.875	-2.80433	14.114
✓ 5:	-48.625	-1.08704	-1.33974				

OK   Cancel
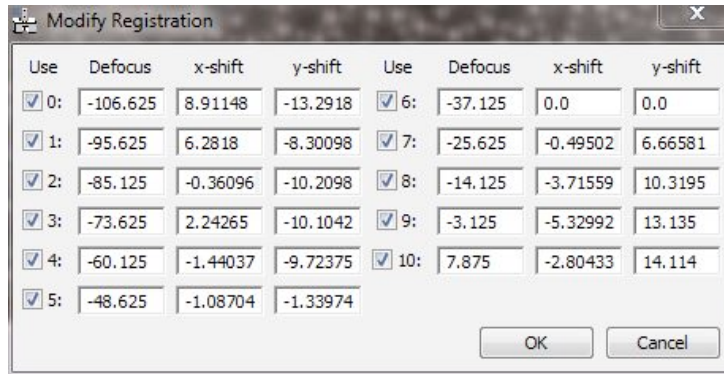
STEP 5) Examine The Restored Object Wavefunction

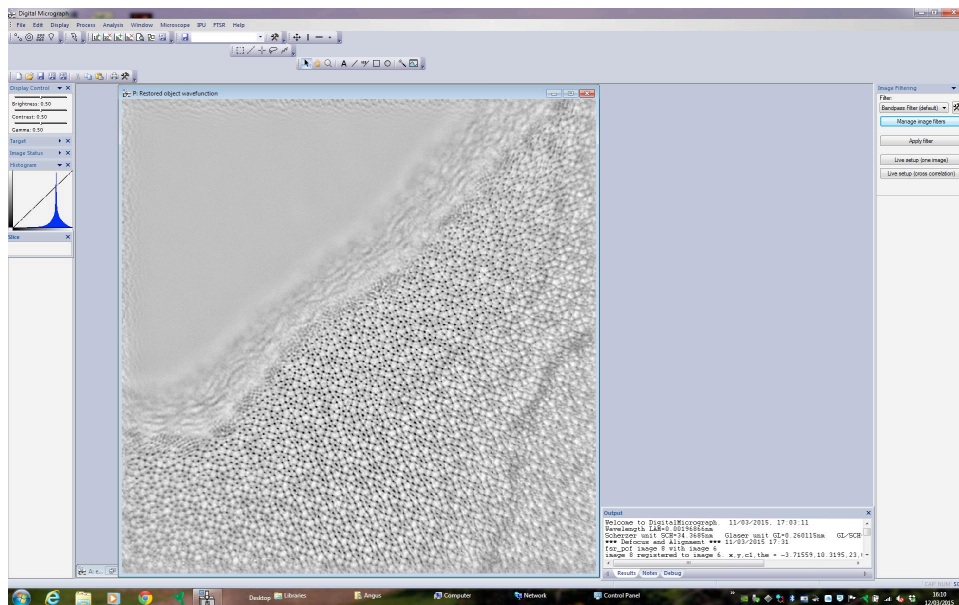The output from the restoration for the whole image area is shown above.

The restored exit wavefunction is complex and the **Phase**, **Amplitude**, **Real** or **Imaginary** parts of this can be displayed by selecting one of these from the **Complex to Real** command in the FTSR main menu.

NOTE: If the restored exit wavefunction is appears completely black it is probably a display problem. To fix this open the *Image Display* window from the *Display Menu* in DigitalMicrograph (or Right Click within the Image Window) and change the survey mode to Whole Image

Finally the restored wavefunction can be adjusted to account for any uncorrected aberration using the **Aberration Corrector** as described in the *Quick Rreference Guide* of this manual. To explore this try running the restoration of the same dataset but without initially inputting the value for A_2

B: Calculating the Sampling Interval

The *Sampling Interval* is the effective width of one pixel in an image and will depend on the magnification of the image. It is important that this is known accurately to allow the restoration to be performed successfully. In general, it is *NOT* sufficient to simply calculate this value from the nominal magnification shown on the microscope. The sampling interval also determines the maximum resolution of your restoration since no image will contain spatial frequencies higher than twice the sampling interval (the Nyquist limit).

The sampling interval can be calculated accurately by taking a lattice image of a sample that has a well characterized lattice spacing e.g. silicon.
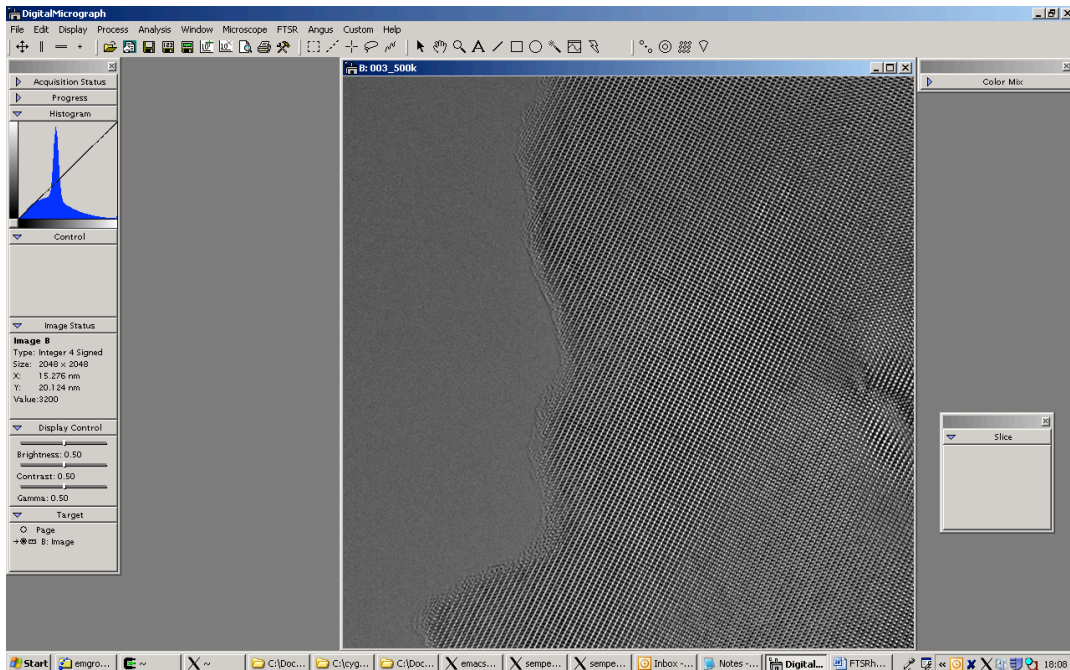Calculate the Fourier transform of the image and measure the distance of a Fourier spot corresponding to a known lattice spacing from the central peak using the Line tool in DigitalMicrograph. This distance (length) will be measured in pixels in the *Control* pane in the Standard Tools (if it is in reciprocal nanometers/Angstrom click on the small ruler icon shown next to the image information in the *Target* pane in the Standard Tools to change the reading to pixels). The sampling interval can then be calculated from the measured distance (length) as follows:

$$\text{Sampling interval (nm)} = \frac{\text{spacing in material (nm)} \times \text{distance in reciprocal space (pixels)}}{\text{total image size (pixels)}}$$

Remember to note the binning of the image (binning the image by 2 or 4 will increase the sampling interval by 2 or 4 times respectively). This process will have to be repeated (not necessarily using the same standard sample) for any magnification at which you wish to restore the exit wavefunction.

Example Calculation
Take an image of a sample with a well characterized lattice spacing, in this example Strontium Titanate in an <011> orientation.

Take the Fourier Transform of the image and measure the number of reciprocal space pixels that separate two of the lattice reflections (make sure that you know the orientation and hence which lattice reflections these spots correspond to) as shown below.
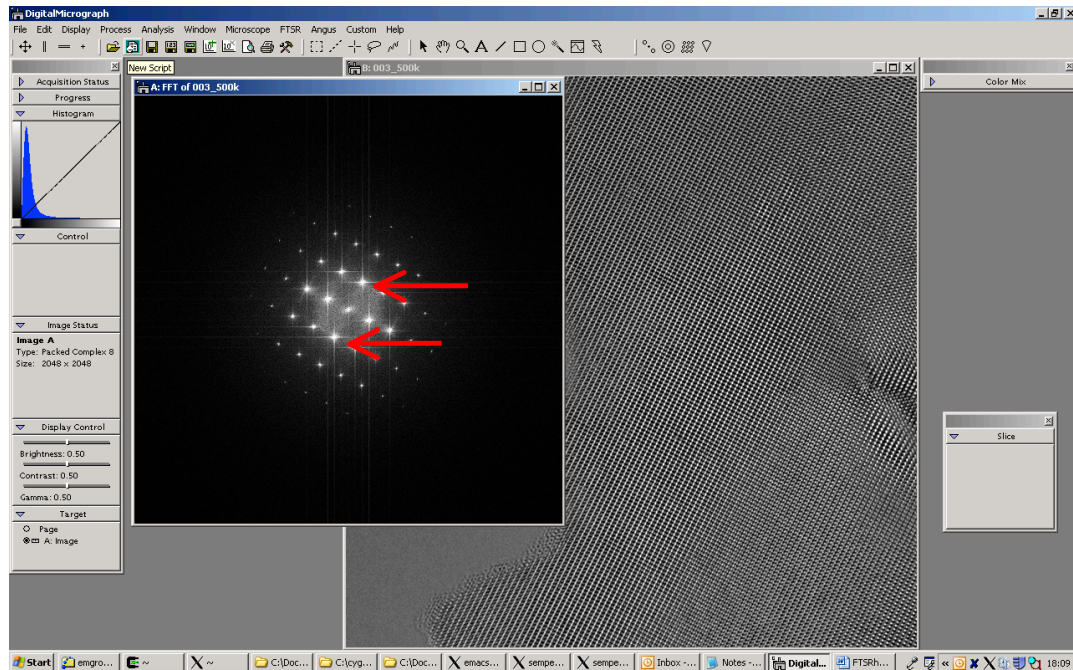
NOTE: If using DigitalMicrograph to do this you can click the ruler icon in the *Target window* in DigitalMicrograph in order to change the *Control windw* to display the length in pixels rather than in reciprocal nm. DigitalMicrograph converts from pixels to nanometers using an internal table of calibration factors that may or may not be sufficiently accurate, depending on how well and when this was last calibrated for your instrument.
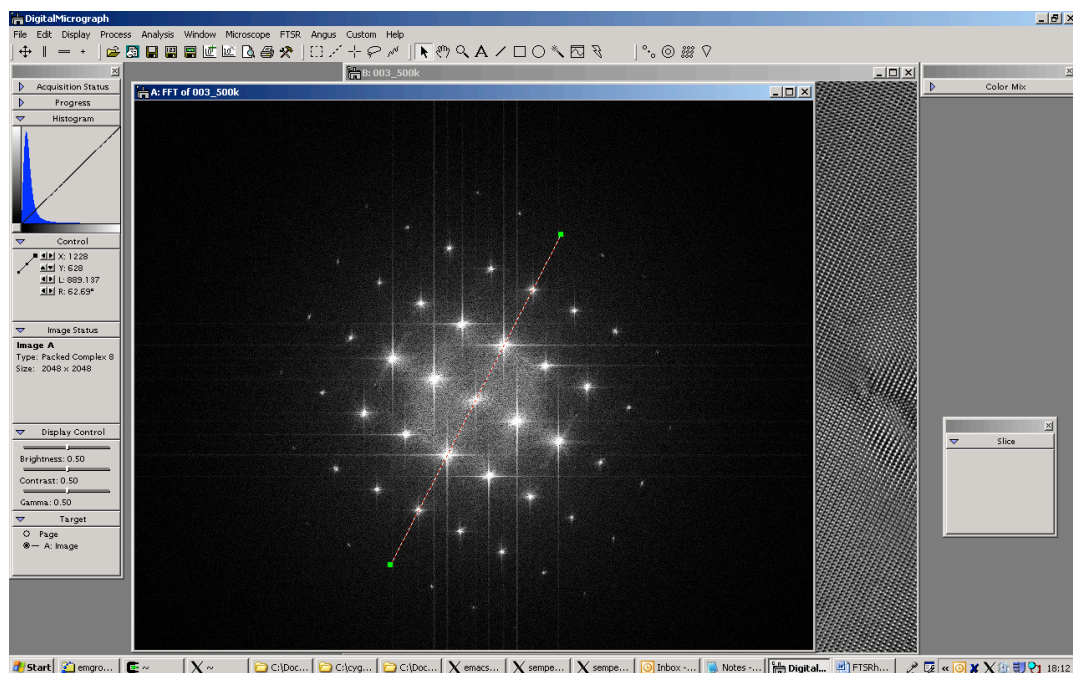
In the example above showing the Fourier transform of a [011] oriented SrTiO$_3$ sample the reciprocal space distance to be measured is the (0,1,-1) reflection. The distance measured for 6 times of this spacing is 889.1 pixels, thus 0.276nm spacing is represented by (889.1)/6 = 148.18 pixels. The image has a total size of 2048x2048. Thus using the equation given previously;

$$\text{Sampling interval (nm)} = \frac{\text{spacing in material (nm)} \times \text{distance in reciprocal space (pixels)}}{\text{total image size (pixels)}}$$

$$\text{Sampling interval (nm)} = \frac{0.2761 \text{ (nm)} \times 148.18 \text{ (pixels)}}{2048 \text{ (pixels)}} = \mathbf{0.0200nm}$$

The accuracy with which the sampling interval is determined can be improved by averaging values found for a number of different measurements and lattice directions.

C: Calculating the MTF/NPS

This example shows how to measure the MTF/NPS for a CCD camera.

The Modulation Transfer Function (MTF) describes how different signal spatial frequencies are transferred by the camera.

The noise power spectrum (NPS) describes how the different spatial frequencies of the noise are transferred by the camera.

To estimate the MTF it is necessary to have an image of a known (deterministic) function containing all the spatial frequencies of interest. A step function (a sharp change from black to white) is ideal for this and can be approximated using either the beam stop or a sharp aperture placed in the back focal plane of the sample.

Step 1) Data Acquisition.

The experimental data that needs to be acquired consists of image data blocks with:

   a) Flat images (bright field images recorded using uniform illumination conditions (Spread the beam so that it covers at least twice the area of the CCD camera).
   b) Dark field images (images taken with no illumination)
   c) Edge images (bright field images including an object approximating to a step function e.g. the beam stop)

The acquisition of this data is automated within FTSR. The practical steps required to obtain the data needed for MTF/NPS measurement are as follows:

   a) Choose a low magnification (20k - 40k) and find an area where there is no specimen present in the field of view.

   b) From the FTSR main menu chose the **Setup** command of **MTF/NPS Data** to display the *MTF/NPS Setup Dialog* below:
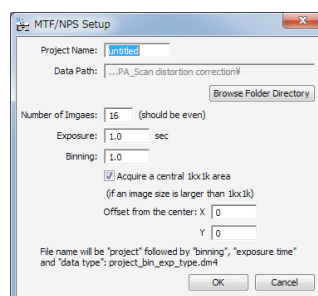
> Give the project a name and select a data path where the images will be stored.
> Set an appropriate *Exposure* so that the number of counts in a bright field image corresponds to the counts used for recording your typical experimental images.
> Set the *Number of Images* to 16.
> Set the *Binning* to the same value used to acquire your experimental data
> If the CCD camera is larger than 1k x 1k pixels (full field) select *Acquire a central 1k x 1k area*.
> If required set the *Offset from the centre* of the1k x 1k area.

c) Acquire the necessary flat and dark images using the **Acquire Dark Images** and **Acquire Flat Images** commands in the **MTF/NPS Data** in the FTSR main menu.

d) Insert the beam stopper and acquire the Edge images using the **Acquire Edge Images** in the **MTF/NPS Data** in the FTSR main menu.

Step 2) Calculating the MTF/NPS

a) Open the 'edge' data block showing the shadow of the beam stopper.

b) Specify two points along the beam stop on the edge image by using the ***HREM Mouse*** 🐭 . Two *red* squares should appear on the beamstop shadow. If you make a mistake you can delete a square by clicking on it using the ***HREM Mouse*** with the ***shift*** key held down.
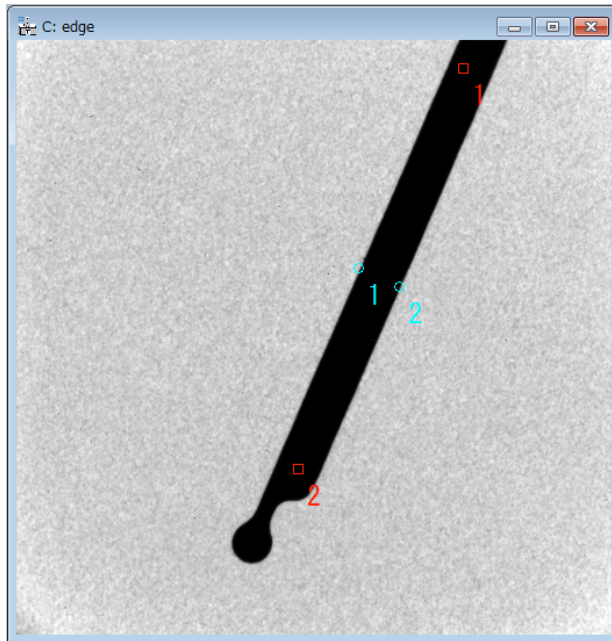
c) Specify two points on both sides of the beam stop on the edge image by using the ***HREM Mouse*** in with <u>the ***alt*** key held down</u>. Two *blue* circles should appear. If you make a mistake you can delete a circle by clicking on it using the ***HREM Mouse*** with the ***shift*** and the ***alt*** key held down.

d) Specify the image area to be used for NPS estimation by using the ***rectangular ROI tool*** on the flat image. Avoid including damaged areas of the CCD or non-uniformly illuminated areas.

e) Choose the **Calculate MTF/NPS** command from the FTSR main menu. Select the appropriate the edge, dark and flat images from the open image list, then click OK.

The MTF and NPS will then be calculated within a few minutes. In both the MTF and NPS the horizontal scale represents pixels in reciprocal space. This data is normalized to a camera size of 1024.

The mtf and nps you calculate should be decaying functions that look like something like this:
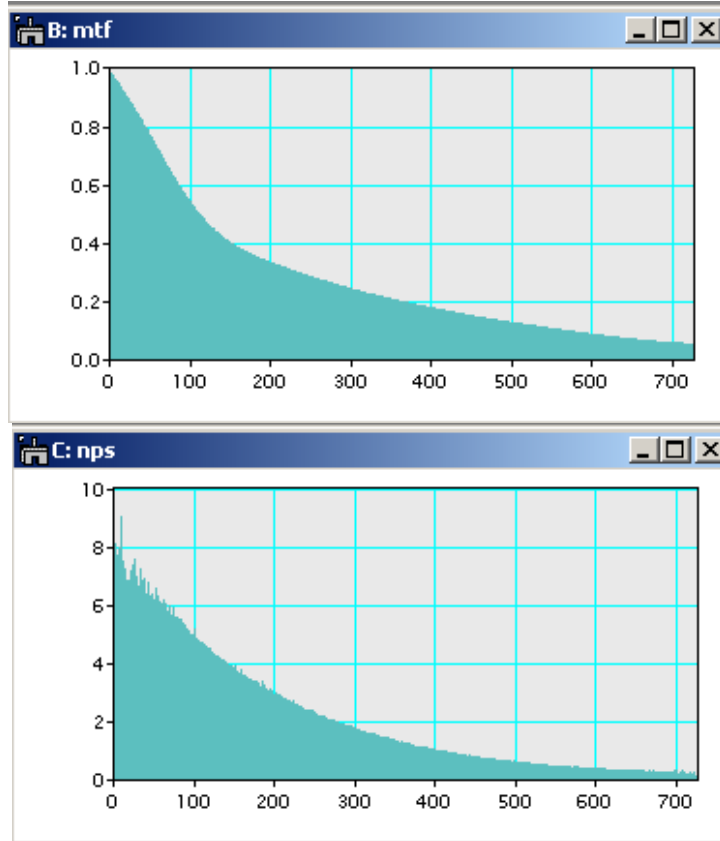
Quick Reference Guide

The FTSR Main Menu

FTSR is controlled from a single main menu within DigitalMicrograph.
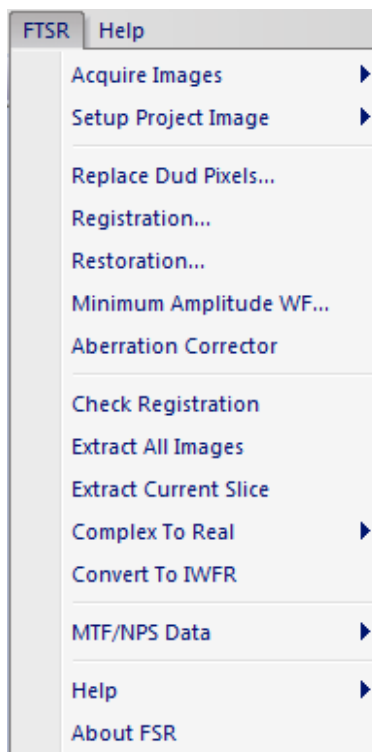
The commands in the FTSR menu are described below.

Command	Description
Acquire Images (see also sub menus)	Acquires an image dataset using a Gatan camera.
Setup Project Image (see also sub menus)	Sets up a new project (stacked image) from a set of previously saved individual images, or an existing image stack.
Replace Dud Pixels…	Bad (defective) pixel values will be replaced by a local mean.
Registration…	Opens a dialog box that controls the parameters used to register the images in the project.
Restoration…	Executes the exit wavefunction restoration.
Minimum Amplitude WF...	Calculates the exit wavefunction with minimum amplitude modulation.
Aberration Corrector	Opens the Software Aberration Corrector that can be used to compensate residual aberrations in the reconstructed exit wavefunction.

Check Registration...	A utility for checking the image registration values calculated during the reconstruction by aligning them into a data stack that can examined using the Gatan Slice Player. Registration vectors can also be forced to specific values.
Extract All Images…	Extracts all component images from within a project using the current registration vectors.
Extract Current Slice	Extracts the current slice from a project to a single image.
Complex to Real (see also sub menus)	Converts Gatan format complex image data into a real image (Phase/Amplitude/Real/Imaginary) that can be displayed, or used to create a complex conjugate image.
Convert to IWFR	Converts image data into a format suitable for use in the IWFR Plugin.
MTF/NPS Data (see also sub menus)	Acquire Dark, Flat Field and Edge Image data, and calculate the detector Modulation Transfer Funciton (MTF) or Noise Power Spectrum (NPS).
Help (see also sub menus)	Opens the FTSR on-line help.
About FTSR	Displays information about the installed version of FTSR.

Acquire Images Menu

Option	Description
FSR...	Opens the FSR Acquisition dialog from where the image acquisition conditions are controlled for focal series acquisition.
TSR...	Opens the TSR Acquisition dialog (if activated) from where the image acquisition conditions are controlled for tilt series acquisition.

NOTE: Before image acquisition it is advisable to check the objective lens hysteresis for the focal range that will be used for data acquisition as this affects the actual defocus value.

For optimum image acquisition it is best to establish a hysteresis loop and collect images along the same direction within the loop.
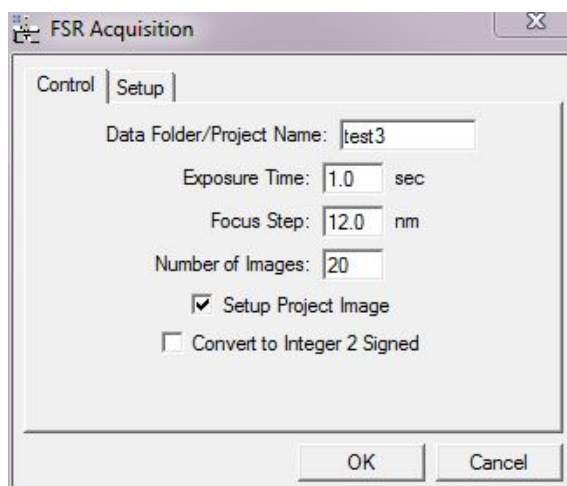
FSR Sub Menu

The FSR Acquisition Dialog

The components of this dialog are described below.

Component	Description
Control Tab	For information about the function of the Control tab see below.
Setup Tab	For information about the function of the Setup tab see below.
OK	Closes the dialog and starts image acquisition using the specified parameters. A series of through-focal images will be acquired at both under- and over-focus with respect to the initial defocus value (plus the Defocus Offset) set prior to image acquisition.
Cancel	Closes the dialog without executing any further functions.

Control Tab

Component	Description
Data Folder/ Project Name	Acquired images will be identified with the name specified together with an additional sequence number corresponding to their position in the acquisition sequence *i.e.* in the above example images will be named "test301, test302… When a project is created after acquisition, the same name is used as the project name.
Exposure Time	Acquisition (exposure time) for each image (s).
Focal Step	Defocus between each image (nm). Underfocus negative.
Number of Images	Total number of images acquired in the focal series (positive number).

Setup Project Image	If checked, a project image will be created using all the acquired images. If unchecked, a project must be created manually using the Setup Images... command after acquisition.
Convert to Integer 2 Signed	If checked converts the data acquired to integer 2 signed data format.

Setup Tab

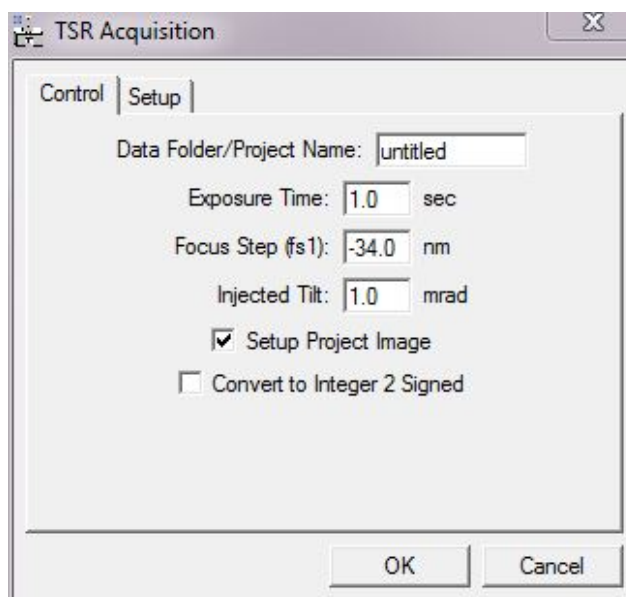| Component	Description
Folder	Sets the destination folder for the FTSR project using a standard Windows Explorer interface to browse the location.
Current Defocus	The estimated current defocus value (nm).
Center Defocus	The required defocus value of the central image in the focal series.
Focus Calibration	Specifies the calibrated focus change (nm) produced by single unit DAC change of the objective lens. This focus value is generally calibrated as part of the microscope installation.
Delay after Focus Change	Settling time after each focus change (s). This should be adjusted to reflect the stability of the objective lens focus change.
Binning	Specifies the camera pixel binning used for data acquisition.

TSR Sub Menu

The TSR Acquisition Dialog

The components of this dialog are described below.

Component	Description
Control Tab	For information about the function of the Control tab see below.
Setup Tab	For information about the function of the Setup tab see below.
OK	Closes the dialog and starts image acquisition using the specified parameters. A 6 member tilt-defocus series of images will be acquired at both under- and over-focus (3 focus values for each tilt) with respect to the initial defocus value at the injected tilt specified.
Cancel	Closes the dialog without executing any further functions.

Control Tab

Component	Description
Data Folder/ Project Name	Acquired images will be identified with this name together with an additional sequence number corresponding to their position in the acquisition sequence *i.e.* in the above example the images will be named untitled01, untitled02… When a project is created after acquisition, the same name is used as the project name.
Exposure Time	Acquisition (exposure time) for each image (s).
Focal Step (fs1)	Defocus between each image (nm). Underfocus negative.

Injected Tilt	Magnitude of injected tilt angle (mrad).
Setup Project Image	If checked, a project image will be created using all the acquired images. If unchecked, a project must be created manually using the Setup Images... command after acquisition.
Convert to Integer 2 Signed	If checked converts the data acquired to integer 2 signed data format.

Setup Tab

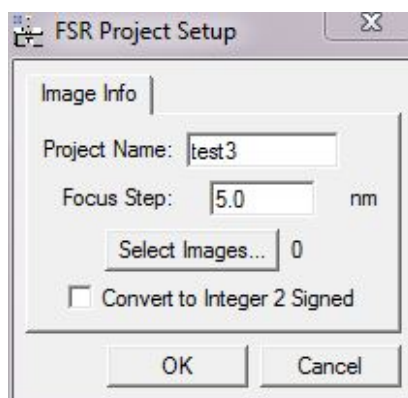| Component	Description
Folder	Sets the destination folder for the FTSR project using a standard Windows Explorer interface to browse the location.
Current Defocus	The estimated current defocus value (nm).
Center Defocus	The required defocus value of the central image in the focal series.
Focus Calibration	Specifies the calibrated focus change (nm) produced by single unit DAC change of the objective lens. This focus value is generally calibrated as part of the microscope installation.
Delay after Focus Change	Settling time after each focus change (s). This should be adjusted to reflect the stability of the objective lens focus change.
Binning	Specifies the camera pixel binning used for data acquisition.
Tilt Calibration	Specifies the calibrated tilt magnitude (mrad) produced by a single DAC change in the beam tilt coils. This value is generally calibrated as part of the microscope installation.

Setup Project Image Menu

FSR Project from Archived Images...

TSR Project from Archived Images...

FSR Project from Image Stack...

Option	Description
FSR From Archived Project Images...	Opens the FSR Project Setup dialog in which you can specify information related to previously saved images. When the OK button is pressed an FSR project is created.
TSR From Archived Project Images...	Opens the TSR Project Setup dialog in which you can specify information related to previously saved images. When the OK button is pressed a TSR project is created.
FSR Project From Image Stack	Opens an alternative FSR Project Setup dialog which Creates an FSR Project from a previously opened image stack. When the OK button is pressed an FSR project is created.

FSR Project Setup Dialog (from Archived Images)

Image Info Tab

FSR Project Setup

Image Info

Project Name: test3

Focus Step: 5.0   nm

Select Images...   0

☐ Convert to Integer 2 Signed

OK   Cancel

Component	Description
Project Name	Name of the project to be created.
Focus step	Defocus step size between images (nm) in the focal series. It is important to ensure that the sign of the focus step is correct, depending on the image order (overfocus to underfocus or vice versa) in which you have acquired the images. A positive value represents the over to underfocus direction.
Select Images...	Opens a standard Windows File Open dialog from which saved images can be selected.
Convert to Integer 2 Signed	If checked converts the data acquired to integer 2 signed data format.

TSR Project Setup Dialog (from Archived Images)

Image Info Tab

Component	Description
Project Name	Name of the project to be created.
Focus step (fs1)	First defocus step size between the images (nm) for the short focal series at each tilt angle.
Focus step (fs2)	Second defocus step size between the images (nm) for the short focal series at each tilt angle. It is important to ensure that the sign of the focus step is correct, depending on the image order (overfocus to underfocus or vice versa) in which you have acquired the images. A positive value represents the over to underfocus direction.
Approximated Injected Tilt	Approximate tilt angle in mrad for each short focal series. This tilt angle will be subsequently refined in the program.
Select Images...	Opens a standard Windows File Open dialog from which saved images can be selected.
Convert to Integer 2 Signed	If checked converts the data acquired to integer 2 signed data format.

NOTE: fs1 and fs2 should not be equal and a good choice is to set these as a Golden mean ratio (see the section on *Dataset Geometries in the main manual*)

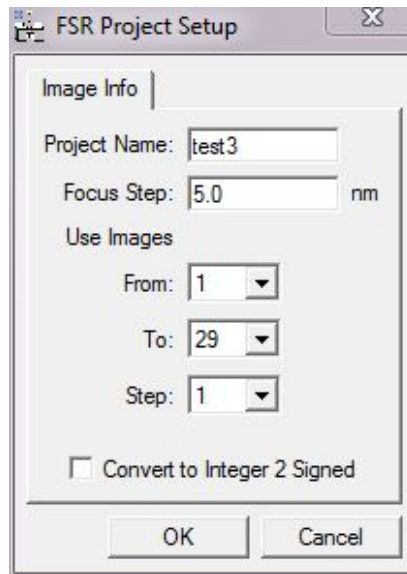## *FSR Project Setup Dialog (from an Image Stack)*

Image Info Tab

Component	Description
Project Name	Name of the project to be created.
Focus step	Defocus step size between images (nm). It is important to ensure that the sign of the focus step is correct, depending on the image order (overfocus to underfocus or vice versa) in which you have acquired the images. A positive value represents the over to underfocus direction.
Use Images	The three controls **FROM**, **TO** and **STEP** select which images are selected from the image stack and converted into an FSR project. This allows exit wave reconstruction from a subset of the acquired images.
Convert to Integer 2 Signed	If checked converts the data acquired to integer 2 signed data format.

Replace Dud Pixels Menu

Bad (defective) pixel values (due to camera blemishes) are replaced by a local mean, and the Results window shows the number of pixels replaced.

The Replace Dud Pixels Dialog
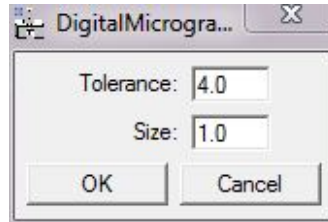
Component	Description
Tolerance	Bad (defective) pixel values that exceed the value of Tolerance (in standard-deviation) will be replaced with a local mean.
Size	Sets the search radius (in pixels) for locating Bad pixels.

Registration Menu

The Registration Menu enables the user to setup and start the image registration process using either a tilt series (TSR) or focal series (FSR).

The FSR or TSR dialog will be open depending on the front image.

NOTE: Before starting the registration process an image area <u>that is a power of 2</u> must be selected with the rectangular ROI tool. The registration will then be performed using this area.

        An area containing either some amorphous material or containing an edge feature is recommended for registration.

FSR Registration Dialog

The components of this dialog are described below.

Component	Description
Control Tab	For information about the components of the Control tab see below.
Setup Tab	For information about the components of the Setup tab see below.
Option	For information about the components of the Display tab see below.
Display	For information about the components of the Display tab see below.
OK	Closes the dialog and starts the image registration process using the parameters specified.
Cancel	Closes the dialog without executing any further functions.

Control Tab

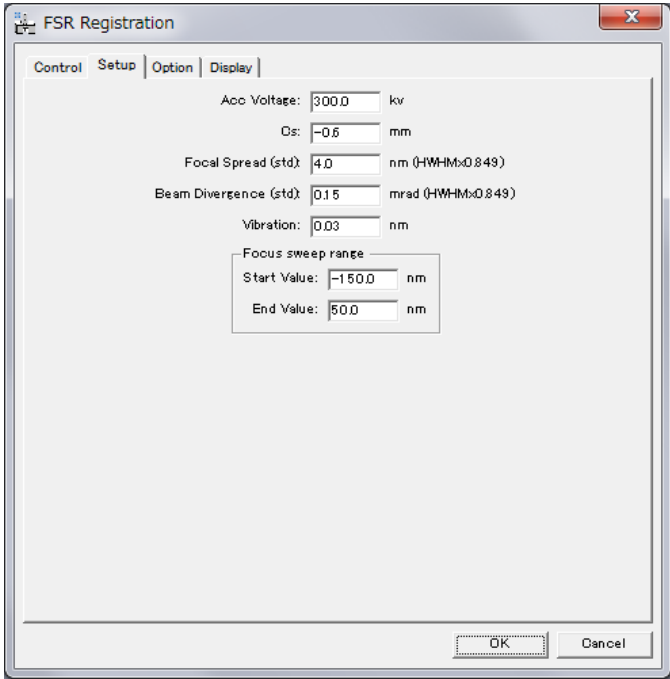| Component	Description
Sampling Interval	Linear size of (square) pixels in object space (nm). This should be calibrated from the microscope magnification or from a known lattice spacing.
Kmax	Resolution of the image (the smallest spatial detail in the image) in reciprocal space (1/nm). This corresponds to the inverse of the highest spatial frequency.
Image Selections	The images in the project data from **First Image** to **Last Image** will be used in the FSR restoration. The image selected as **Reference Image** will be used as the in the image alignment. The default value of the **Reference Image** corresponds to the currently displayed image of the project image. The reference image should be a high contrast image, ideally close to the centre of the image series.
mtf	The MTF (Modulation Transfer Function) file in DigitalMicrograph format to be used for restoration (see later section for a description of how to calculated the MTF file). You can locate a previously saved camera MTF file using the Browse button.
nps	The NPS (Noise Power Spectrum) file in DigitalMicrograph format to be used for restoration (see later section for a description of how to calculate the NPS file). You can locate a previously saved camera NPS file using the Browse button.
Cross Correlation Mode	The Cross Correlation Mode controls the form of the correlation function used for registration as, Phase only (PCF, n=0), Square Root Amplitude (MCF, n=1/2),

	Regular (XCF, n=1) or Arbitrary Amplitude Power (GCF, 0<n<1). See the section on registration in the Main Manual. If the PCF, MCF or XCF are selected the power used in the calculation is automatically set and cannot be adjusted. For the GCF the power can be adjusted to any value.

Setup Tab

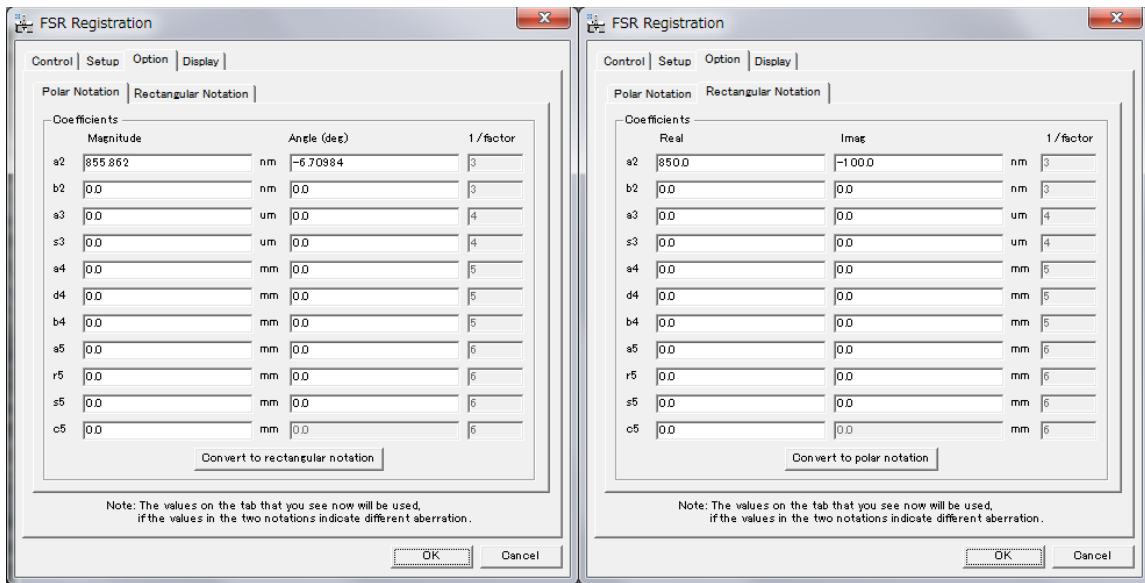| Component	Description
Acc Voltage	Accelerating voltage of the microscope (kV).
Cs	The third order spherical aberration coefficient (mm) of the microscope. For uncorrected instruments this is a fixed positive value and for corrected instruments is output as part of the alignment of the corrector.
Focal Spread	The effective focal spread that defines the partial temporal coherence (HWHM x 0.849) (nm).
Beam Divergence	The beam convergence semi-angle due to a finite source size (HWHM x 0.849) (mrad).
Vibration	Magnitude of the isotropic vibration due to acoustic noise and vibration (nm).
Focus Sweep Range	The **Start Value** and **End Value** (nm) define the overall focus range used to calculate the PCF and PCI functions (see supplementary information).

NOTE: The Focal Spread can be estimated if the values of the energy spread (ΔE), instabilities in the objective lens current, (ΔI) and accelerating voltage, (ΔV) and the chromatic aberration coefficient (C_c) of the objective lens are known as:

$$\Delta = C_c \sqrt{\left\{\left(\frac{\Delta E}{EV}\right)^2 + 2\left(\frac{\Delta I}{I}\right)^2 + \left(\frac{\Delta V}{EV}\right)^2\right\}}$$

A description of how to estimate the convergence semi-angle is given in:

C. Dwyer, R. Erni, J. Etheridge, Ultramicroscopy, 110, 952, (2010)

Option Tab

Component	Description
Coefficients	The input boxes allow the user to set previously measured aberration coefficients (2nd to 5th order) in either Polar (Magnitude and Angle) or Cartesian (Real and Imaginary) notation. You can convert between the two notations using the 'Convert to…' button.

NOTE: The section describing the wave aberration function in the full manual gives details of the Rectangular and Polar Notations used for the wave aberration coefficients.

Display Tab

Component	Description
Registration	Displays the estimated focus values (**Estimated Focus**), the value of the cross correlation coefficient (**Cross Correlation**), and the values of specimen drift in pixels (x,y) (**Specimen Drift**) during the registration process if selected.
Message level	Controls the level of detail in the output messaging reported in the *Digital Micrograph Results Window*. Three levels of increasing detail are available: None/Normal/Detail.

TSR Registration Dialog

The components of this dialog are described below.

Component	Description
Control Tab	For information about the components of the Control tab see below.
Setup Tab	For information about the components of the Setup tab, see below.
Option	For information about the components of the Display tab see below.
Display	For information about the components of the Display tab see below.
OK	Closes the dialog and starts the image registration process using the parameters specified.
Cancel	Closes the dialog without executing any further functions.

Control Tab

Component	Description
Sampling Interval	Linear size of (square) pixels in object space (nm). This should be calibrated from the microscope magnification or from a known lattice spacing.
Kmax	Resolution of the image (the smallest spatial detail in the image) in reciprocal space (1/nm). This corresponds to the inverse of the highest spatial frequency.
mtf	The MTF (Modulation Transfer Function) file in DigitalMicrograph format to be used for restoration (see later section for a description of how to calculated the

	MTF file). You can locate a previously saved camera MTF file using the Browse button.
nps	The NPS (Noise Power Spectrum) file in DigitalMicrograph format to be used for restoration (see later section for a description of how to calculate the NPS file). You can locate a previously saved camera NPS file using the Browse button.
Cross Correlation Mode	The Cross Correlation Mode controls the form of the correlation function used for registration as, Phase only (PCF, n=0), Square Root Amplitude (MCF, n=1/2), Regular (XCF, n=1) or Arbitrary Amplitude Power (GCF, 0<n<1). See the section on registration in the Main Manual. If the PCF, MCF or XCF are selected the power used in the calculation is automatically set and cannot be adjusted. For the GCF the power can be adjusted to any value.

Setup Tab

Component	Description
Acc Voltage	Accelerating voltage of the microscope (kV).
Cs	The third order spherical aberration coefficient (mm) of the microscope. For uncorrected instruments this is a fixed positive value and for corrected instruments is output as part of the alignment of the corrector.
Focal Spread	The effective focal spread that defines the partial temporal coherence (HWHM x 0.849) (nm).
Beam Divergence	The beam convergence semi-angle due to a finite source size (HWHM x 0.849) (mrad).

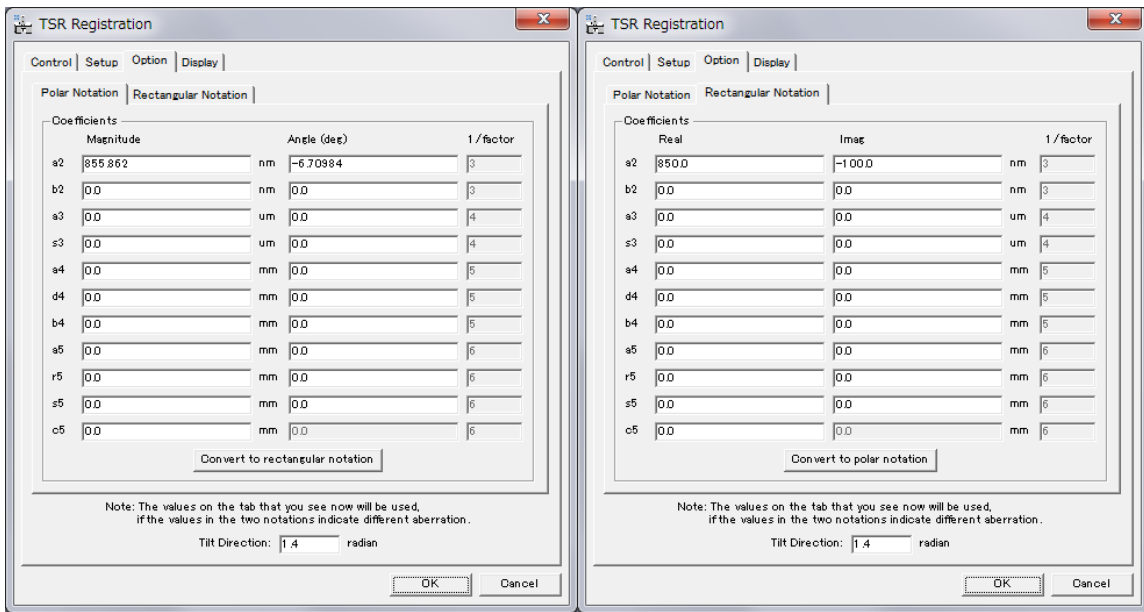| Vibration	Magnitude of the isotropic vibration (nm) due to acoustic noise and vibration.
Focus Sweep Range	The **START** and **END** values (nm) define the overall focus range used to calculate the PCF and PCI functions (see supplementary information).

NOTE: The Focal Spread can be estimated if the values of the energy spread (ΔE), instabilities in the objective lens, (ΔI) and accelerating voltage, (ΔV) and the chromatic aberration coefficient (Cc) are known as:

$$\Delta = C_c \sqrt{\left\{ \left(\frac{\Delta E}{EV}\right)^2 + 2\left(\frac{\Delta I}{I}\right)^2 + \left(\frac{\Delta V}{EV}\right)^2 \right\}}$$

A description of how to estimate the convergence semi angle is given in:

C. Dwyer, R. Erni, J. Etheridge, Ultramicroscopy, 110, 952, (2010)

Option Tab:

Component	Description
Coefficients	The input boxes allow the user to set previously measured aberration coefficients (2nd to 5th order) in either Polar (Magnitude and Angle) or Cartesian (Real and Imaginary) notation. You can convert between the two notations using the 'Convert to…' button.
Tilt Direction	This sets the tilt direction (rad) with respect to the image (camera) axes.

NOTE: The section describing the wave aberration function in the full manual gives details of the Rectangular and Polar Notations used for the wave aberration coefficients.

Display Tab

Component	Description
Registration	Displays the estimated focus values (**Estimated Focus**), the value of the cross correlation coefficient (**Cross Correlation**), and the values of specimen drift in pixels (x,y) (**Specimen Drift**) during the registration process if selected.
Message level	Controls the level of detail in the output messaging reported in the *Digital Micrograph Results Window*. Three levels of increasing detail are available: None/Normal/Detail.

Restoration Menu

The Restoration Menu enables the user to setup the parameters needed for the final exit wave restoration process using previously registered images.

Restoration Dialog

The components of this dialog are described below.

Component	Description
Area Tab	For information about the components of the Area tab, see below.
Use Images Tab	For information about the components of the Setup tab, see below.
OK	Closes the dialog and starts the image restoration process using the parameters specified.
Cancel	Closes the dialog without executing any further functions.

Area Tab
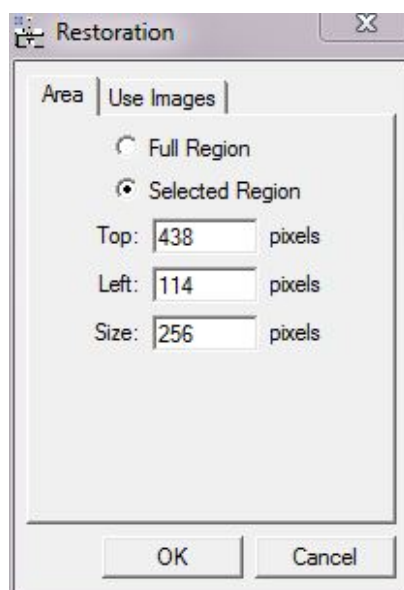
Component	Description
Full / Selected Region	Allows the user to select an image area for restoration either from the **Full Region** or a **Selected Region**. In the case of the Selected Region, the user can modify the position (**Top** and **Left**) and the **Size** of the area (The selected **Size** must be a power of 2.)

Use Images Tab

Restoration — Area | Use Images

- ☑ 0:-19.625 ☑ 13:13.875 ☐ 26:-19.625 ☑ 39:130.125
- ☑ 1:-13.625 ☑ 14:15.875 ☐ 27:-19.625 ☑ 40:138.375
- ☑ 2:-11.625 ☑ 15:19.875 ☐ 28:-19.625 ☐ 41:-19.625
- ☑ 3:-7.625   ☑ 16:21.875 ☐ 29:-19.625 ☐ 42:-19.625
- ☑ 4:-5.625   ☑ 17:23.875 ☐ 30:-19.625 ☑ 43:152.375
- ☑ 5:-3.625   ☑ 18:25.875 ☑ 31:85.875   ☐ 44:-19.625
- ☑ 6:-1.625   ☑ 19:27.875 ☐ 32:-19.625 ☐ 45:-19.625
- ☑ 7:0.375   ☑ 20:29.875 ☑ 33:93.875   ☑ 46:172.375
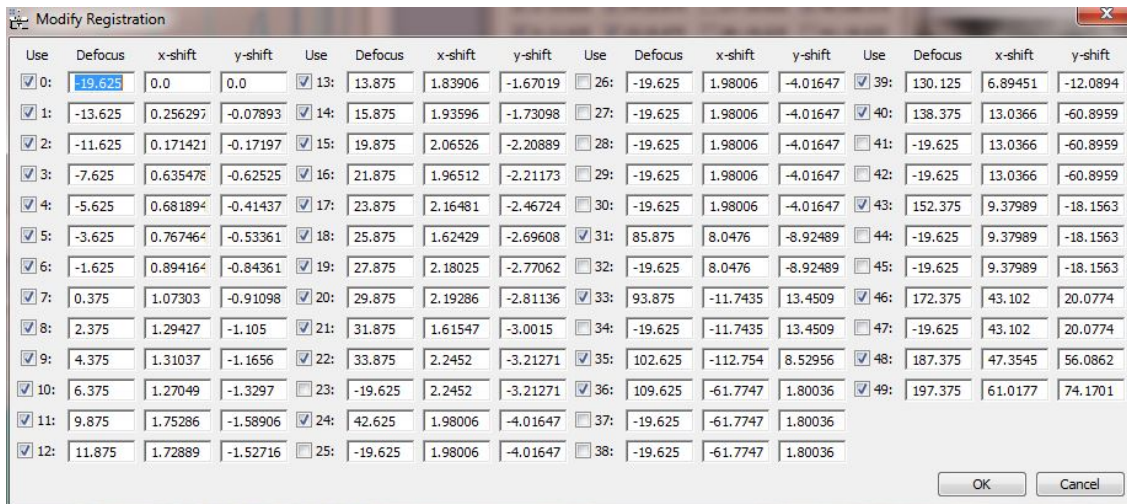- ☑ 8:2.375   ☑ 21:31.875 ☐ 34:-19.625 ☐ 47:-19.625
- ☑ 9:4.375   ☑ 22:33.875 ☑ 35:102.625 ☑ 48:187.375
- ☑ 10:6.375   ☐ 23:-19.625 ☑ 36:109.625 ☑ 49:197.375
- ☑ 11:9.875   ☑ 24:42.625 ☐ 37:-19.625
- ☑ 12:11.875 ☐ 25:-19.625 ☐ 38:-19.625

Modify Registration   OK   Cancel

Component	Description
Use Images	Allows the user to manually select the images used in the restoration. Images with low cross-correlation values determined during the registration process may be unselected. (In the Dialog shown images 23, 25, 30, 32, 34, 37, 38, 44, 45 and 47 are excluded.)
Modify Registration	Opens the Dialog Box below that allows the user to manually set the registration values for each image, e.g. to values calculated outside FTSR.

Modify Registration

Use	Defocus	x-shift	y-shift	Use	Defocus	x-shift	y-shift	Use	Defocus	x-shift	y-shift	Use	Defocus	x-shift	y-shift
☑ 0:	-19.625	0.0	0.0	☑ 13:	13.875	1.83906	-1.67019	☐ 26:	-19.625	1.98006	-4.01647	☑ 39:	130.125	6.89451	-12.0894
☑ 1:	-13.625	0.256297	-0.07893	☑ 14:	15.875	1.93596	-1.73098	☐ 27:	-19.625	1.98006	-4.01647	☑ 40:	138.375	13.0366	-60.8959
☑ 2:	-11.625	0.171421	-0.17197	☑ 15:	19.875	2.06526	-2.20889	☐ 28:	-19.625	1.98006	-4.01647	☐ 41:	-19.625	13.0366	-60.8959
☑ 3:	-7.625	0.635478	-0.62525	☑ 16:	21.875	1.96512	-2.21173	☐ 29:	-19.625	1.98006	-4.01647	☐ 42:	-19.625	13.0366	-60.8959
☑ 4:	-5.625	0.681894	-0.41437	☑ 17:	23.875	2.16481	-2.46724	☐ 30:	-19.625	1.98006	-4.01647	☑ 43:	152.375	9.37989	-18.1563
☑ 5:	-3.625	0.767464	-0.53361	☑ 18:	25.875	1.62429	-2.69608	☑ 31:	85.875	8.0476	-8.92489	☐ 44:	-19.625	9.37989	-18.1563
☑ 6:	-1.625	0.894164	-0.84361	☑ 19:	27.875	2.18025	-2.77062	☐ 32:	-19.625	8.0476	-8.92489	☐ 45:	-19.625	9.37989	-18.1563
☑ 7:	0.375	1.07303	-0.91098	☑ 20:	29.875	2.19286	-2.81136	☑ 33:	93.875	-11.7435	13.4509	☑ 46:	172.375	43.102	20.0774
☑ 8:	2.375	1.29427	-1.105	☑ 21:	31.875	1.61547	-3.0015	☐ 34:	-19.625	-11.7435	13.4509	☐ 47:	-19.625	43.102	20.0774
☑ 9:	4.375	1.31037	-1.1656	☑ 22:	33.875	2.2452	-3.21271	☑ 35:	102.625	-112.754	8.52956	☑ 48:	187.375	47.3545	56.0862
☑ 10:	6.375	1.27049	-1.3297	☐ 23:	-19.625	2.2452	-3.21271	☑ 36:	109.625	-61.7747	1.80036	☑ 49:	197.375	61.0177	74.1701
☑ 11:	9.875	1.75286	-1.58906	☑ 24:	42.625	1.98006	-4.01647	☐ 37:	-19.625	-61.7747	1.80036				
☑ 12:	11.875	1.72889	-1.52716	☐ 25:	-19.625	1.98006	-4.01647	☐ 38:	-19.625	-61.7747	1.80036				

OK   Cancel

NOTE: In practice it is often advisable to exclude images where there is a significant focal shift, where the images have very low contrast (close to the Gaussian focus) or where the image registration is otherwise unreliable (low cross correlation values).

Minimum Amplitude WF Menu

This command locates the wavefunction with minimum amplitude modulation, which under certain conditions corresponds to the wavefunction at the exit specimen plane of a phase object.

NOTE: A rectangular ROI should be defined on the restored wavefunction before using this command.

Minimum Amplitude WF dialog

The components of this dialog are described below.

Component	Description
Control Tab	For information about the components of the Control tab see below.
Display Tab	For information about the components of the Display tab see below.
OK	Closes the dialog and calculates the minimum amplitude image using the specified parameters.
Cancel	Closes the dialog without executing any further functions.

Control Tab
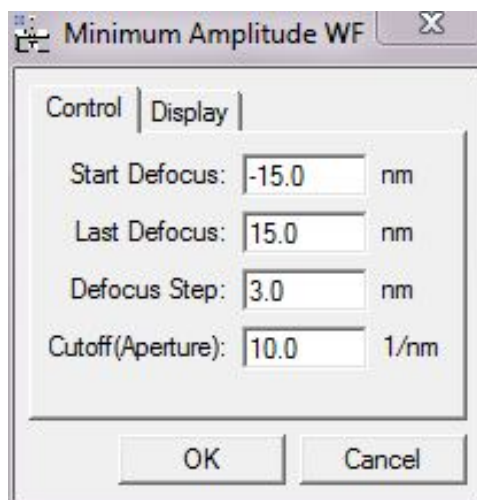
Component	Description
Start Defocus	Sets the start value (nm) for the defocus range over which a minimum amplitude wavefunction is searched for. Underfocus is defined as negative in the FTSR software.
Last Defocus	Sets the end defocus (nm) for the defocus range over which a minimum amplitude wavefunction is searched for. Underfocus is defined as negative in the FTSR software.

Defocus Step	Sets the defocus step (nm) within the defocus range over which a minimum amplitude in the wavefunction is searched for.
Cutoff (Aperture)	Applies a sharp edged computational aperture function (specified in reciprocal nm) which is applied to limit the resolution of the restored exit wavefunction.

Display Tab
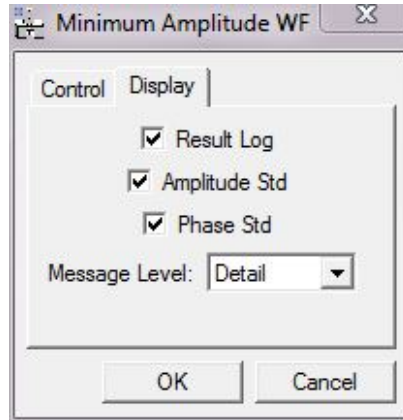
Component	Description
Result Log	If selected displays all wavefunctions as a set of stacked images.
Amplitude Std	If selected displays the standard deviation in the amplitude of the wavefunction from the mean value.
Phase Std	If selected displays the standard deviation in the phase of the wavefunction from 0.0.
Message level	Controls the level of detail in the output messaging reported in the *Digital Micrograph Results Window*. Three levels of increasing detail are available: None/Normal/Detail.

Aberration Corrector Menu

The aberration Corrector is an interactive tool that allows the user to adjust the coefficients of the wave aberration function (see Table 1) as applied to a previously recovered exit wavefunction. This enables any residual uncorrected aberrations to be compensated.

NOTE: The Aberration Corrector tool becomes active only after a rectangular ROI is placed on a complex image (exit wavefunction).

The Aberration Corrector Dialog

The components of this dialog are described below.

| Component	Description
Aberration Tab (Rotation/Basic/3rd/4th/5th)	All coefficients can be adjusted, in user selectable steps, by Modulus and Angle except for the rotationally symmetric coefficients where only modulus adjustment is possible.
Display	Selects the display mode of the aberration corrected region of interest (ROI) of the *complex* image as either Phase/Modulus/Log of Modulus or Real/Imaginary.
Show aberration	When pressed, the Show Aberration Figure Dialog is displayed .
Apply	When pressed, the whole image area will be corrected using the present values of the aberration coefficients.

The Aberration Corrector Tabs
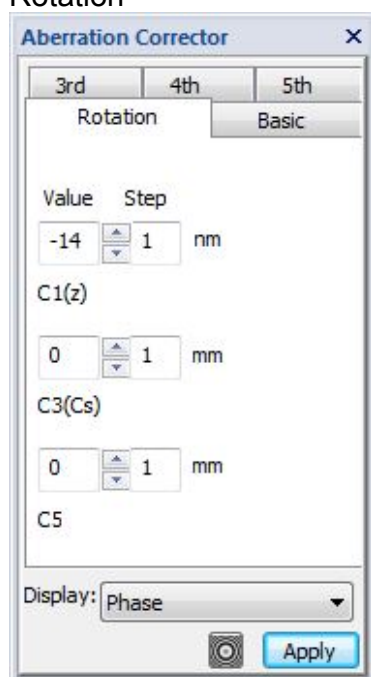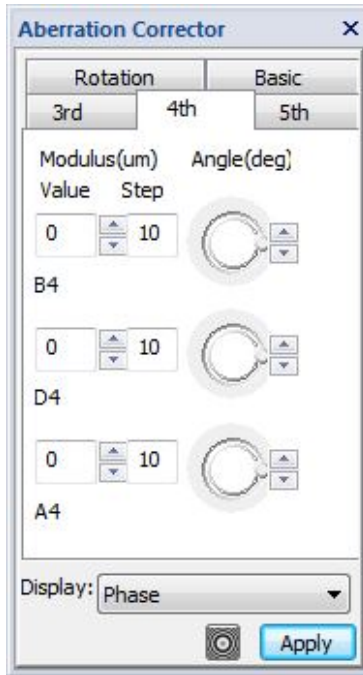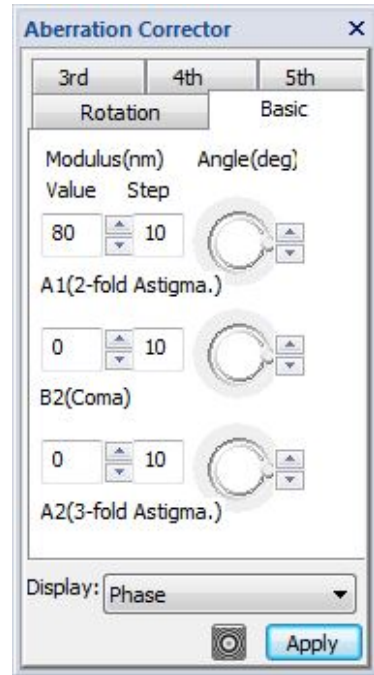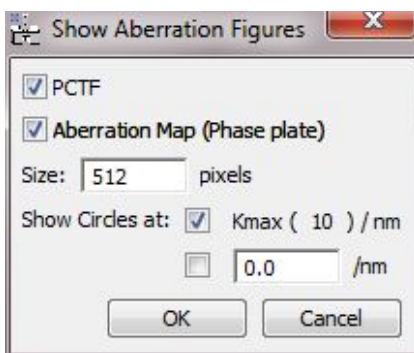
Rotation   Basic
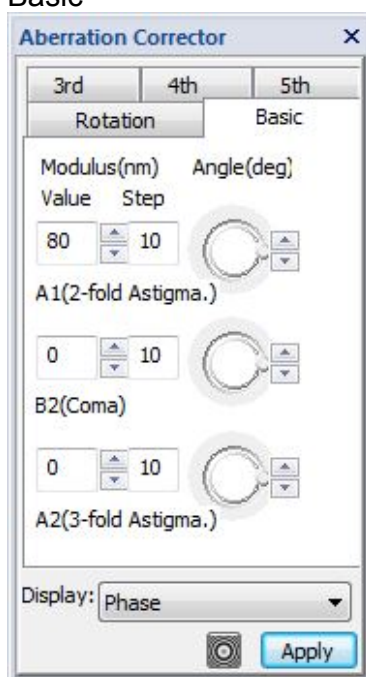
3rd
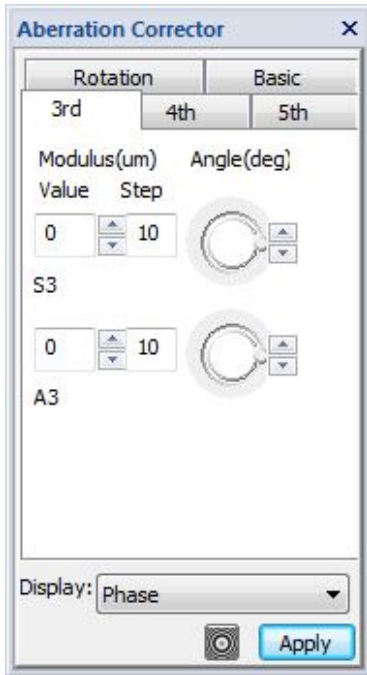
4th

5th

NOTE: The Aberration Corrector tabs use the Typke notation described in Table 1 of the theoretical summary of the wave aberration function and the pre-factors used are the same as defined in the Option tab of *Registration*.

The Show Aberration Figures Dialog

The dialog below will appear when the Show Aberration Button is pressed.

The components of this dialog are described below.

Component	Description
PCTF	When checked displays the 2D Phase Contrast Transfer Function corresponding to the current values of the aberration coefficients.
Aberration Map	When checked displays the 2D Phase Plate

	corresponding to the current values of the aberration coefficients. Resolution Limits corresponding to kmax, 10/nm and a user selectable limit can be superimposed on the PCTF and Phase
Size	Specifies the image size of the PCTF and Aberration map.
Show Circles at	
Kmax (value) /nm	When selected a circle corresponding to a resolution limit Kmax is superimposed on the PCTF and Aberration Map. The Kmax value is displayed in parentheses.
[Edit box] /nm	When selected a circle corresponding to the resolution limit specified in the edit box is superimposed on the PCTF and Aberration Map.
OK	Closes the dialog and displays the PCTF and/ or Aberration Map.
Cancel	Closes the dialog without executing any further functions.

Check Registration Menu

The Check Registration Menu allows the user to confirm the calculated registration values from the automated registration process.

This option operates on an open image stack and displays all the images in the stack aligned using their calculated registration vectors.

The DigitalMicrograph slice player tool can then be used to assess the quality of the registration by "playing through" the image stack and visually assessing any movement between the images. In this way images that have not been registered correctly can be identified and removed from the final restoration.

Convert to IWFR Menu

This Menu option converts the output from FTSR to a format suitable for use with the IWFR DigitalMicrograph plugin available separately.

The Convert to IWFR Dialog
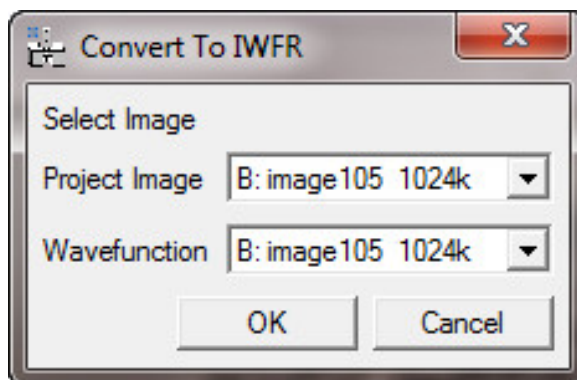
Component	Description
Project Image	Selects a Project Image.
Wavefunction	Selects an open Wavefunction.
OK	Closes the dialog and converts the FTSR project to an IWFR project.
Cancel	Closes the dialog without executing any further functions.

MTF/NPS Data Menu

Setup...
Acquire Dark Images
Acquire Flat Images
Acquire Edge Images
Calculate MTF/NPS
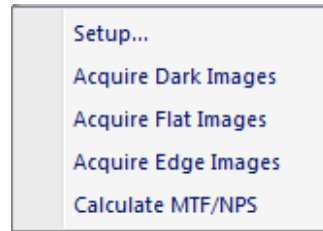
The MTF/NPS Data Menu enables the automated acquisition of the image data required for measuring the MTF and NPS of a camera, with four options as described below.

NOTE: It is necessary to repeat the calculation of both MTF and NPS for all camera pixel-binning values used.

Option	Description
Setup…	Opens the Acquire MTF/NPS Setup dialog in which the information required to acquire the data for MTF and NPS calculation as described below can be specified. When the OK button is the current input data is saved.
Acquire Dark Images…	Starts Dark Image Data acquisition with no illumination.
Acquire Flat Images…	Starts Flat Field (uniform illumination) Image Data acquisition. The illumination should be adjusted to give approximately 66% (2/3) of the CCD saturation count value.
Acquire Edge Images…	Starts Edge Image Data acquisition (uniform illumination with a sharp edge such as a beam stop). The illumination should be adjusted to give approximately 66% (2/3) of the CCD saturation count value.
Calculate MTF/NPS…	Calculates the MTF / NPS from previously acquired Dark, Flat and Edge images.

MTF/NPS Setup Dialog

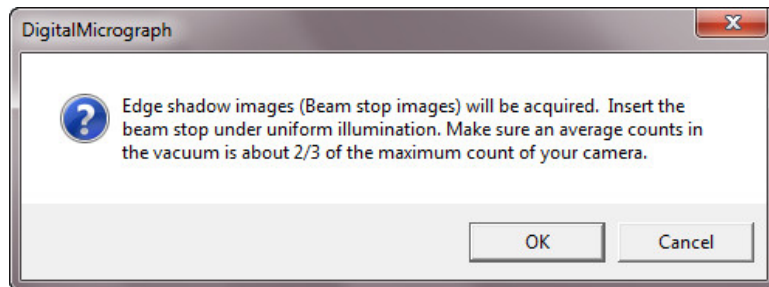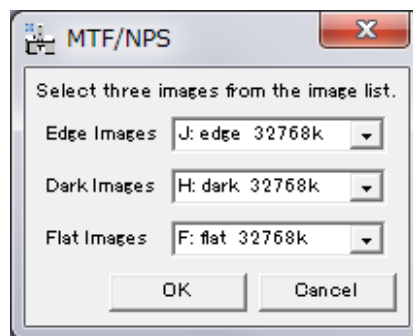| Component	Description
Project Name	Name of the project to be created that will contain the MTF and NPS files.
Data Path	The Directory Location where the MTF and NPS Data will be stored.
Number of Images	Total number of Images used in Dark, Edge and Flat Field Image Data acquisition.
Exposure	Exposure time in sec for each Image.
Binning	CCD Camera pixel Binning.
Acquire a Central 1k Area	If this option is checked then the MTF and NPS Data is acquired using only a 1k x 1k region of the CCD camera. The position of this area can be set using the Offset X and Offset Y variables.
OK	Closes the dialog and saves all parameters.
Cancel	Closes the dialog without executing any further functions.

Acquire Dark Images Dialog
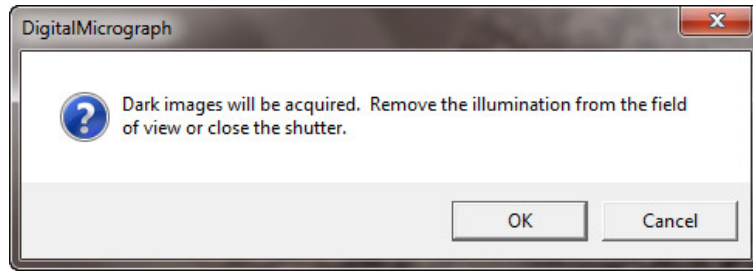
Acquire Flat Images Dialog
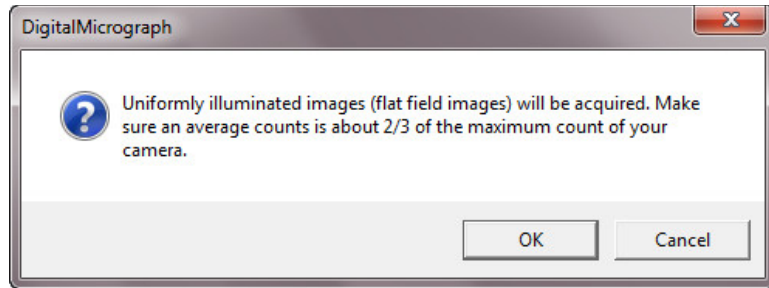
Acquire Edge Images Dialog

Calculate MTF/NPS Dialog

Component	Description
Edge Images	Selects an open Edge Image.
Dark Image	Selects an open Dark Image.
Flat Images	Selects an open Flat Image.