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# *The NCEM Focus*

## *Determination Extension to*

### *Digital Micrograph*

**Roar Kilaas**

## **User Manual**

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This package has been created by Dr. Roar Kilaas at the NCEM at the Lawrence Berkeley National Laboratory.

### *Intended Use*

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The routines were created to facilitate the determination of the defocus of the objective lens from a single HRTEM image containing some amorphous material and to also determine the defocus of each image and the focus step between images in a through-focus series.

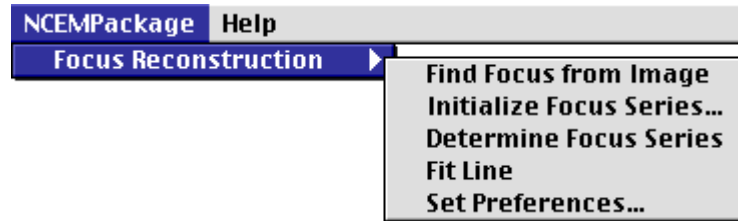
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## The NCEM Focus Menu “Focus Reconstruction”

### The NCEM Focus Menu



The package installs by placing the File “FindDefocus.PPC” in the “Packages” folder that resides in the same location as the Digital Micrograph application. Once the program is started a new menu shows up under the NCEMPackage menu in the menubar. If the package “NCEMPackage” already exists on the computer, the submenu “Focus Reconstruction” appears as the first item together with the routines installed by the “NCEMPackage”. If the “NCEMPackage” is not installed, the menubar of Digital Micrograph will contain a new menu called “NCEMPackage” with “Focus Reconstruction” as the only menu item. The general operation of the various menu commands are described in the following sections.

## Background

### *Background*

The amount of defocus in a HRTEM image can be determined from its power spectrum if sufficient amount of amorphous material is present. Under these conditions it assumed that the weak phase object approximation can be applied to describe the features in the power spectrum that derives from the effect of the objective lens on the scattered electrons passing through a thin amorphous material. Under the weak phase object approximation, the power spectrum for a HRTEM image is proportional to:

$$\sin^2 \chi(\vec{u}, Cs, \lambda, f_0, \Delta f, \alpha)$$

where

$\vec{u}$  = reciprocal lattice vector

$Cs$  = spherical aberration coefficient

$\lambda$  = electron wavelength

$f_0$  = objective lens defocus

$\Delta f$  = spread of focus

$\alpha$  = convergence angle

In the absence of any astigmatism and ignoring the effect of the spread of focus (temporal incoherence) and convergence (spatial incoherence), the intensity in the power spectrum is approximately proportional to

$$\sin^2 \chi(|\vec{u}|, C_s, \lambda, f_0)$$

where

$$\chi = \frac{\pi}{2} (C_s \lambda^3 u^4 - 2\lambda f_0 u^2)$$

This shows that there will be maxima in the power spectrum whenever

$$\chi = \frac{\pi}{2} (C_s \lambda^3 u^4 - 2\lambda f_0 u^2) = n \frac{\pi}{2}$$

for  $n = \text{odd integer}$

Thus if the spherical aberration is known, the focus can be determined by finding the locations of the maxima in the power spectrum, assigning indices ( $n$ ) to the various maxima (rings) and solving for focus ( $f_0$ ).

With several rings in the power spectrum, the value for focus obtained from each ring will vary and the focus is expressed as the average value together with a standard deviation.

## Operating the routines

### Set Preferences... *Set Preferences...*

Before you do anything with these routines, you will need to specify the microscope parameters that are used in the calculation of the focus from the HRTEM image. The parameters that you will need to set are “Microscope Voltage” and “Objective Lens Spherical Aberration Constant”.

In addition, there are a number of parameters used by the program in its search for rings in the image power spectrum and the assignment of ring indices. It is recommended that you first accept the default parameters until a better understanding of the influence of the parameters is gained by use of the program.

<b>Microscope Parameters</b>		<b>Peak Finding Criteria</b>	
Accelerating Voltage [kV]	<input type="text" value="300.0"/>	Minimum distance between peaks [Å <sup>-1</sup> ]	<input type="text" value="0.040"/>
Spherical Aberration Coefficient [mm]	<input type="text" value="0.65"/>	<input checked="" type="checkbox"/> Use center of mass refinement	Center of mass radius [Å <sup>-1</sup> ]
Spread of Defocus (chromatic aberr.) [Å]	<input type="text" value="50"/>	<input type="checkbox"/> Report data on all peaks found and excluded	<input type="text" value="0.020"/>
Electron beam convergence angle [mrad]	<input type="text" value="0.15"/>		
<b>Defocus Determination Criteria</b>		For assisting in the assignment of ring indices, indicate the range of expected defocus [Å]:	
<input checked="" type="checkbox"/> Always exclude inner peak (ring)		Smallest defocus	<input type="text" value="-600"/>
When possible use maximum	<input type="text" value="3"/> peaks (rings)	Largest defocus	<input type="text" value="-2000"/>
		<input type="button" value="Cancel"/> <input type="button" value="OK"/>	

### ***Microscope Parameters***

#### Voltage

This is the accelerating voltage of the microscope in kV. It is used in determining the contrast transfer function for the microscope.

#### Spherical Aberration

This is the spherical aberration coefficient of the objective lens in mm. It is used in determining the contrast transfer function for the microscope.

#### Spread of Defocus

This is the effective spread of defocus which is a due to of the chromatic aberration of the objective lens in conjunction with fluctuations in accelerating voltage, lens current and the energy of the electrons emerging from the filament. It is given in Å and is used in determining the contrast transfer function for the microscope.

#### Convergence Angle

This is the half angle for the cone of incoming electrons onto the specimen in mradians. It is used in determining the contrast transfer function for the microscope.

### ***Peak Finding Criteria***

When search for ring maxima in the power spectrum, the program uses adjustable parameters in order to exclude spurious peaks and to determine the “exact” position of a ring.

#### Minimum distance between peaks

If two peaks are closer than the specified distance in Å<sup>-1</sup>, the smaller of the two are discarded.

Use center of mass (Intensity) within given distance.

If the option is to use center of mass, the peak position will be refined by using the intensities within the given distance in  $\text{\AA}^{-1}$  to obtain a new position for the peak.

#### Report all peaks found

If this option is set, the program outputs data on all the peaks that it finds.

#### *Focus Determination Criteria*

In assigning the ring indices, the first maxima will be assigned the index 1 provided that the first ring gives a focus that lies within the range of acceptable focus values. If it doesn't, the program will move to the next maximum in the power spectrum. Following rings are given indices 3,5,7, etc.. Generally the first ring has a large uncertainty associated with the location of its maximum and the program will not use the focus value obtained from the first ring if that option is set (default).

#### Exclude the first ring

This makes the program not include the focus calculated from the first ring when it finds the average focus value.

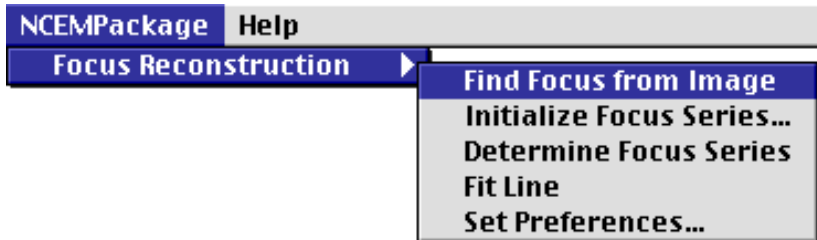
#### Use maximum # rings

The program might find many maxima which increasing uncertainty with respect to whether they should be included in the focus determination. The program will not use any more than the number specified.

#### Focus Range

The program will use this range to help the algorithm determine if certain peaks are spurious and should not be used in assigning ring indices.

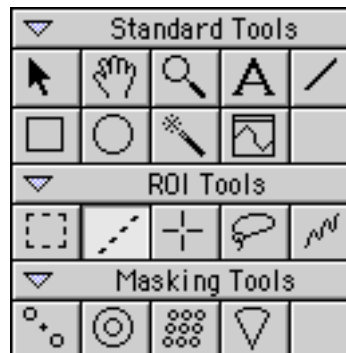
## Find Focus from Image *Find Focus from Image*



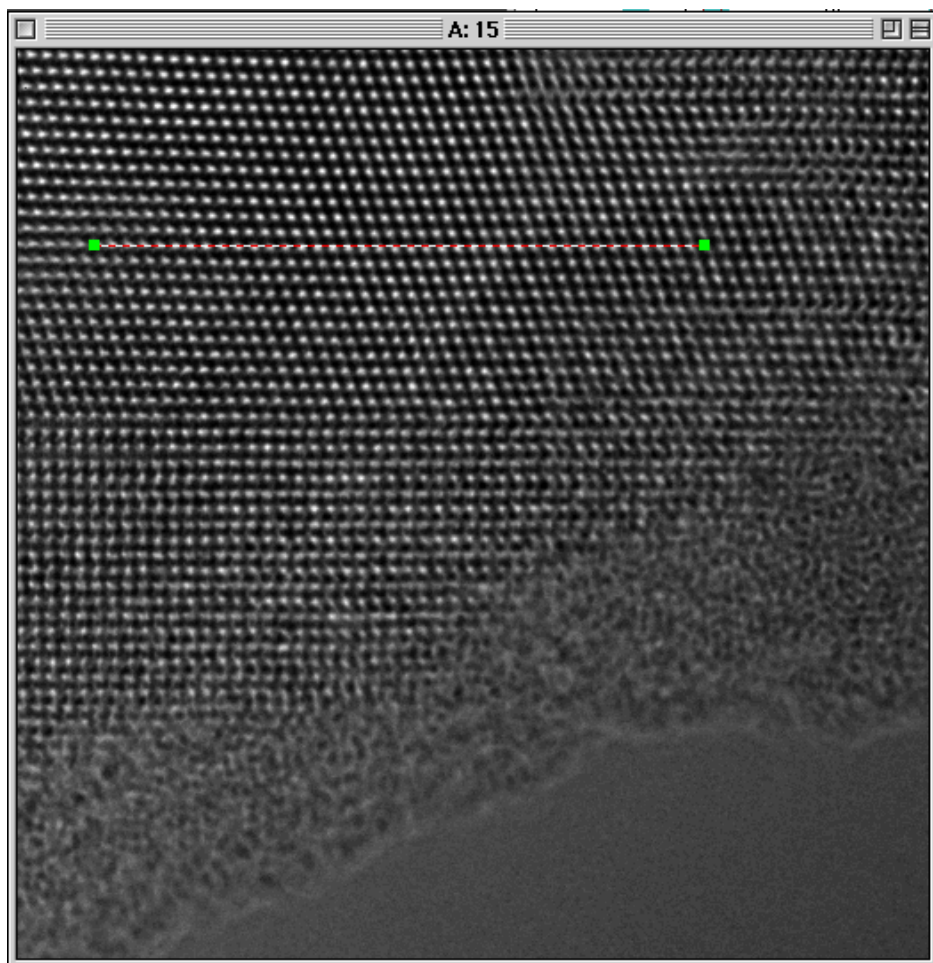
This will attempt to find the focus value from a single HRTEM image. The accuracy to which the focus can be determined depends on many factors; the resolution of the image, the size of the Fourier transformed region (the resolution in reciprocal space), the number of rings in the power spectrum (the value of the focus) and the amount of amorphous material present in the image.

Procedure:

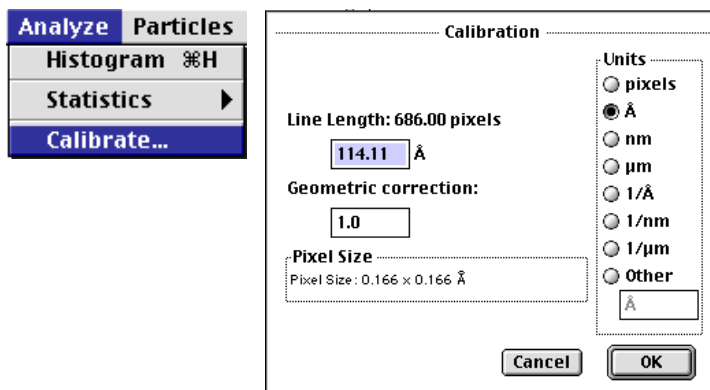
You will first need to calibrate the image you are working on.



Use the line selection tool to create a line of known dimension in the HRTEM image.



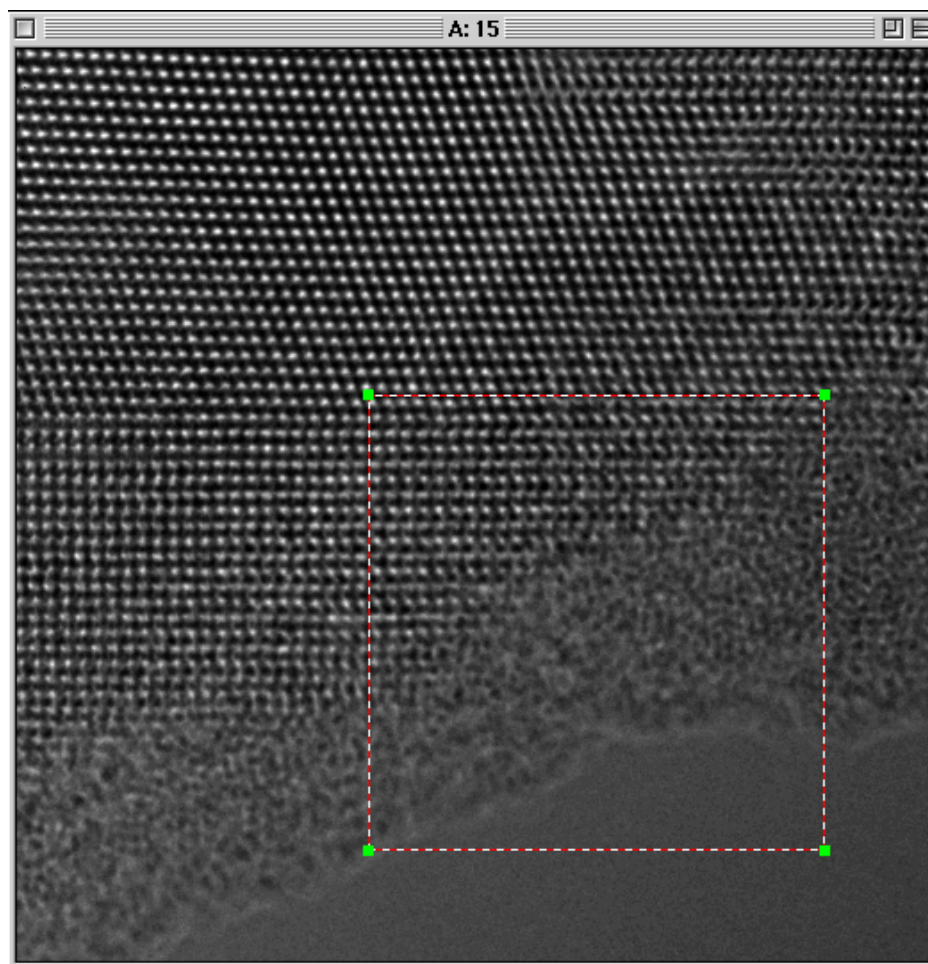
and calibrate the line.





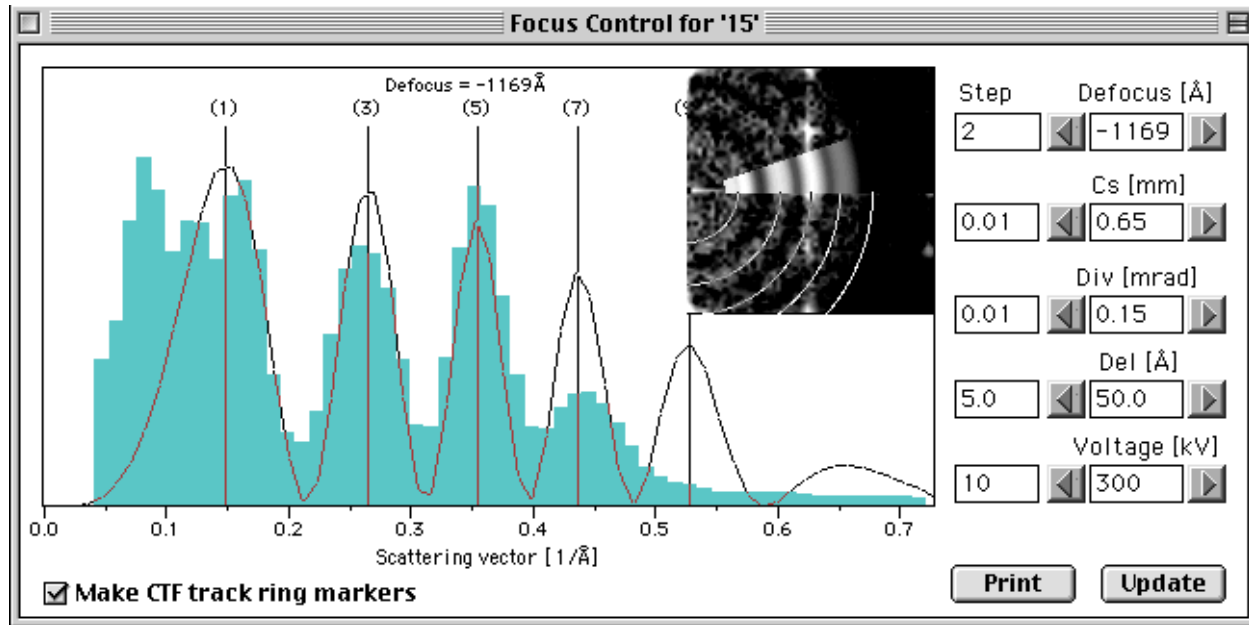
The calibration should be in Å for the routine to work.

Once this is done, select an area that is square with dimensions being powers of 2 (hold down the Option key when you select the area) that contains some amorphous region. In this example, the area is a 512 square region of a 1024 image. If no selection is set, the routine will use the entire image. In this particular example, choosing a 256 square region would give insufficient sampling in reciprocal space to give good results.



Before you execute the command “Find Focus from Image”, make sure that there is only one selection set in the image.

Executing the command brings up the following result window.



The program attempts to calculate the power-spectrum associated with the amorphous content as a function of the radius (reciprocal distance). This is calculated by producing the median value for the magnitude of the power spectrum for each radius. The median is plotted in blue-green and corresponds to the experimental data. The peaks in the one dimensional data set are found and assigned ring indices. The focus is calculated from each ring and the mean value for focus (defocus) is used to calculate the hypothetical Contrast Transfer Function CTF which is plotted as

$$\sin^2 \chi(u, Cs, \lambda, f_0, \Delta f, \alpha)$$

based on the values that are listed.

The maxima for the CTF are shown by their vertical markers which can be dragged by the mouse. Click on a marker, hold down the mouse and the location of the maximum can be changed. All the maxima changes and the corresponding value for focus is shown. As an inset, the experimental power-spectrum is shown with a region showing the average data that the program uses for finding the rings. Superimposed on the experimental data

are the rings corresponding to the current value for the focus. By moving the markers, the rings change position and the user can manually try to obtain the best fit for the value of focus.

## WORKING WITH A FOCUS SERIES

### *WORKING WITH A FOCUS SERIES*

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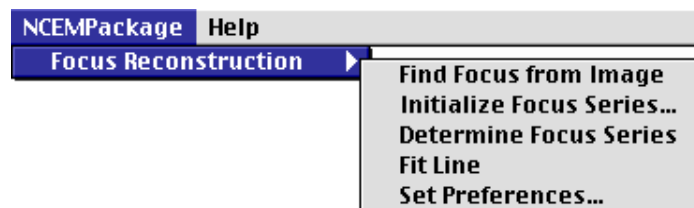
#### **Background:**

These set of routines were written originally to help determining the focus for each image in a series of images taken with a “fixed” increment of focus. Thus the routine finds the mean value and standard deviation for focus from each image and subsequently does a least squares fit to determine the equation for the line that fits the data points. All the set up is done on a first image which is chosen as part of the “Initialize Focus Series” command. These routines only work on data in binary form (typical from data obtained from a CCD camera) and you will need to specify the dimensions of the data, the data type and the number of images in the series. The values for the microscope will need to be set up beforehand as well.

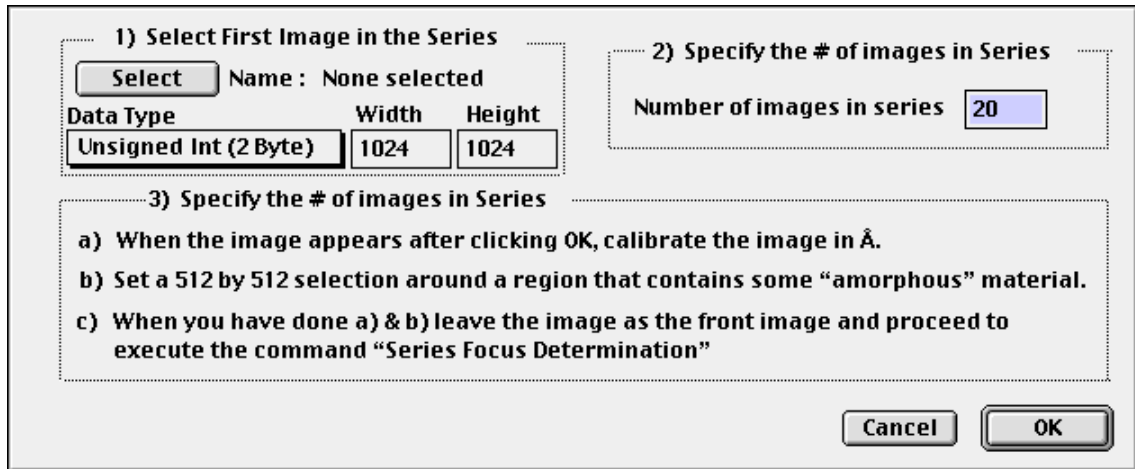
## Initialize Focus Series

### *Initialize Focus Series*

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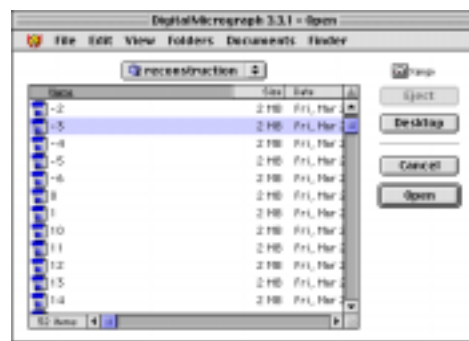


Executing the command brings up the following dialog box.

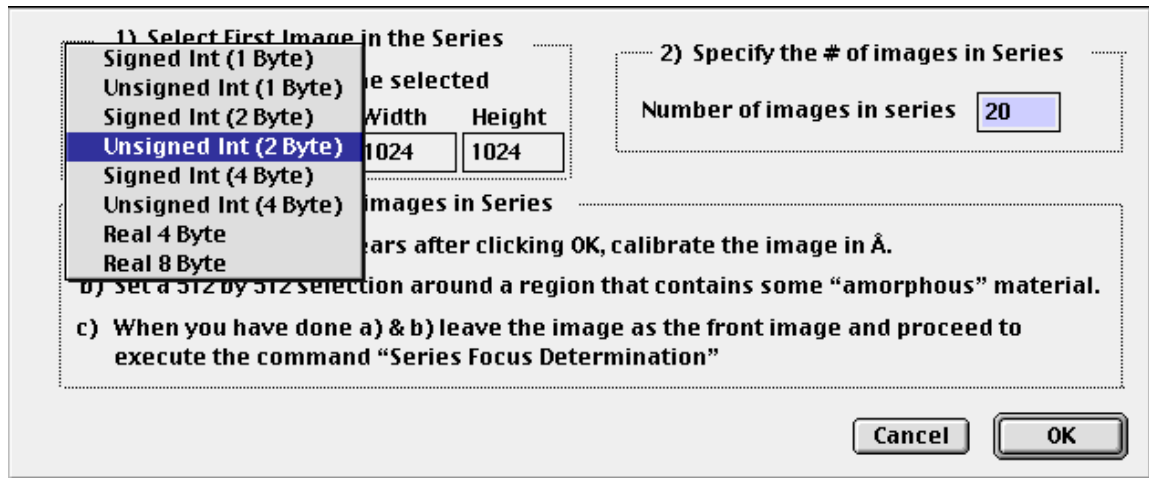


**Usage:**

Select the first file in the image which brings up a Macintosh “Open File” dialog box.



Choose the file name, click okay and select the data type and the dimensions of the image.



Also specify the number of images in the series.

The program depends on a particular naming sequence. There are 2 naming sequences that are allowed:

- a) <characters><#> with a number as in “myimage1” or “xxx12”
- b) <characters>.dat\_# with a number formatted as “myimage\_001.dat” or “xxx\_012.dat”

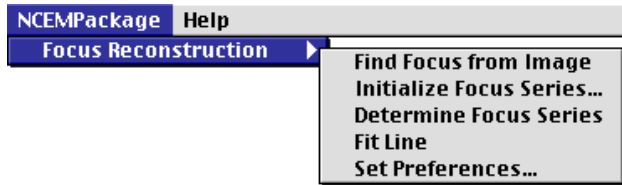
The name is the name of the first image. Each subsequent image name will be formed by adding 1 to the previous image name.

### IMPORTANT

After you have dismissed the “Initialize Focus Series” dialog box, the first image will appear. **You will need to make sure it is calibrated and you must place a selection (unless you want the whole image) around the area of some amorphous material before you go to the next step.** Using a selection around the amorphous material helps the program by minimizing the influence of the crystalline material.

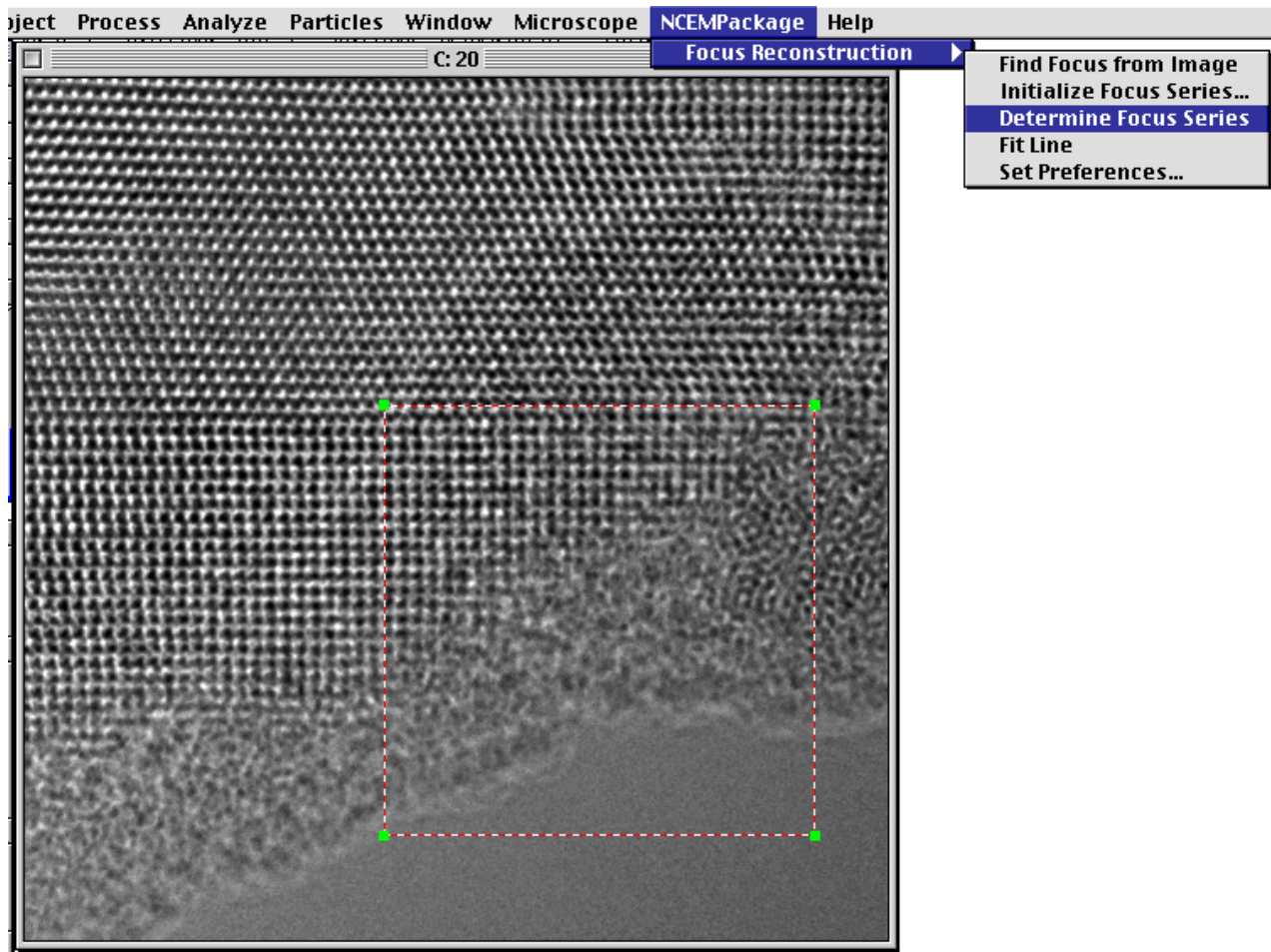
## Determine Focus Series

### *Determine Focus Series*



#### Note:

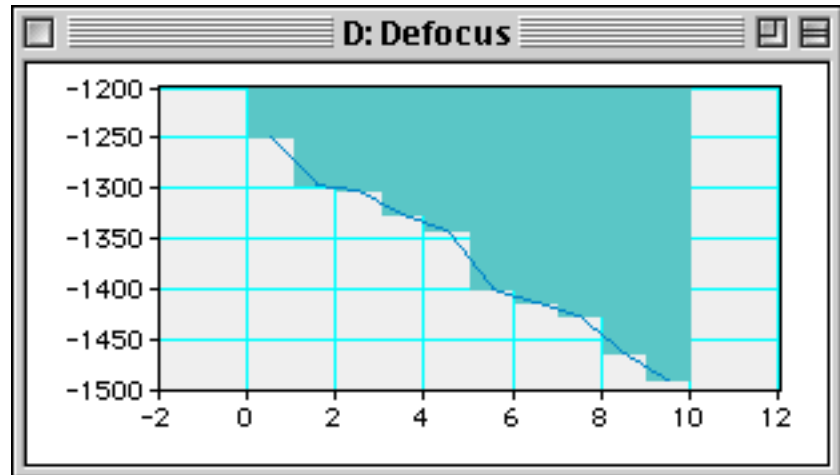
As mentioned above, you must first initialize the focus series before you proceed to this step



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## Fit Line

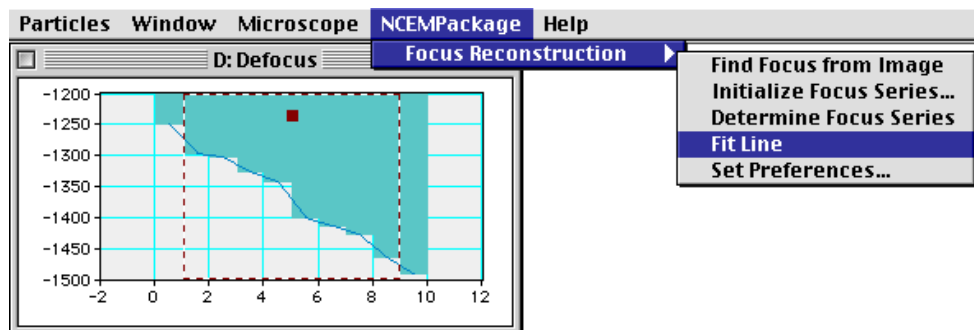
The program calculates the focus from each image and reports the data in the result window. The image is updated as the subsequent images in the series are read in. At the completion of the task, the focus as a function of step is displayed in its own window.



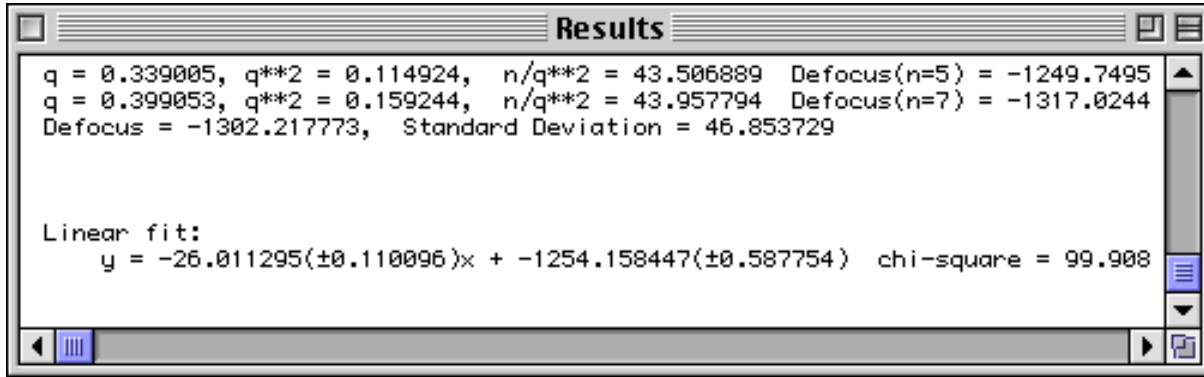
## Fit Line

### *Fit Line*

Sometimes the defocus window will indicate that for various images, the program did not find the correct focus. It also might indicate that something happened during the focus series and that either the whole series should be discarded or that there may be a range of usable images. The final command “Fit Line” works on a 1-dimensional data set or a selection within the data set.



Executing the command with the “Defocus” window being the front window results in the fitting parameters being shown in the “Result” window



By placing a selection around the “good” data, the command will find the linear fit for the selected range.

