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DeConvHAADF

(Software Cs-Corrector)

DigitalMicrograph Plugin
for
STEM-HAADF Deconvolution

User's Guide

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Table of Contents

1. Introduction
2. DeConvHAADF
3. Installation
4. Getting Started...
5. Tips and Troubleshooting

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1. Introduction

DeConvHAADF is the software for rectifying High-Angle Annular Dark-Field image taken by using STEM (STEM-HAADF) by deconvoluting it with a probe function. This is thus a software Cs-corrector, if we use a simulated probe function with a given spherical aberration coefficient. The DeConvHAADF software consists of a suite of scripts and a Plug-In for use in Gatan's DigitalMicrograph.

This DeConvHAADF User's Guide is written to provide information on the basic functions of the DeConvHAADF software, a procedure for installation of the Plug-In, some general tips on operation and troubleshooting. This Guide assumes the user is familiar with image manipulation within DigitalMicrograph as well as Windows operating system.

1.1 Features

1.1.1 Advanced deconvolution algorithms

The DeConvHAADF software uses a Maximum Entropy Method (MEM) or the Richardson-Lucy Algorithm (RLA) for a image deconvolution. Both procedures will work on two-dimensional image data obtained by using a CCD camera or by using a serial image acquisition system. The DeConvHAADF software gives an ideal result for a good signal-to-noise data within a reasonable processing time.

1.1.2 Easy-to-Use User Interface

The DeConvHAADF software is easy to use and normally works with default setups. However, the user can change its setups easily within a custom-made setup dialog (See **sections 2.2 and 2.3**).

NOTE An image of *any size* can be handled (not necessary to be a power of two).

TIPS Create a new image of power of two from a selection. You can easily create a new image of power of two using a ROI selection as follows:

1. Select an area of power of two using a ROI tool.
2. Use a regular Copy short cut: Ctrl + C.
3. Use a modified Paste short cut: Ctrl + Alt + V.

1.2 Deconvolution Overview

1.2.1 Observed Image and Deconvolution

An observed image $h(x)$ is given by a convolution of an ideal image $f(x)$ and a probe (a point spread function) $g(x)$:

$$h(x) = g * f(x) = \int g(x-t)f(t)dt.$$

This convolution integral is written as a product in the Fourier space as

$$H(\xi) = G(\xi) \cdot F(\xi).$$

Therefore, if we can ignore a noise, the ideal image is easily restored by taking an inverse Fourier transform of $H(\xi)/G(\xi)$, the observed image's Fourier transform divided by the probe's Fourier transform. However, this Fourier deconvolution does not work for a real image, since we cannot ignore the noise.

1.2.2 Maximum-Entropy Method

Maximum Entropy Method (MEM) tries to find a solution by using a concept of entropy.

$$S(f) = -\sum_i f_i \log(f_i), \text{ where } \sum_i f_i = 1, f_i \geq 0$$

Here, the following constrained entropy is minimized

$$Q(f) = \alpha S(f) - L(f)$$

where $L(f)$ is called a Likelihood defined by

$$L(f) = \frac{\chi^2(f)}{2} = \frac{1}{2} \sum_i \frac{(h_i - (g * f)_i)^2}{\sigma_i^2}$$

There are several ways to minimize the constrained entropy. We choose Collins' iterative procedure, where the following Shannon-Jaynes entropy is employed

$$S(f) = -\sum_i f_i \log(f_i/m_i), \text{ where } \sum_i m_i = 1, m_i \geq 0 \text{ (measure)}$$

Here, we use a previous solution as the measure. Therefore, we have the following iterative formula

$$Q(f^k) = -\sum_i f_i^k \log\left(\frac{f_i^k}{f_i^{k-1}}\right) - \lambda \sum_i \frac{(h_i - (g * f^k)_i)^2}{\sigma_i^2}, \text{ where } f_i^0 = \text{const.}$$

1.2.3 Richardson-Lucy Algorithm

Richardson-Lucy Algorithm (RLA) tries to find a solution by the following iterative formula:

$$\psi^{k+1}(\xi) = \psi^k(\xi) \int \frac{P(x, \xi)\phi(x)}{\int P(x, \xi)\psi^k(\xi)d\xi} dx \quad \text{using } \psi^0(\xi) = \text{const.}$$

This algorithm is explained as follows by using formulas in statistics. We know a kernel function $P(x)$ and observe a data $\phi(x)$, and the data is given by the following convolution integral with an unknown function $\psi(x)$:

$$\phi(x) = \int P(x - \xi)\psi(\xi)d\xi = \int P(x, \xi)\psi(\xi)d\xi$$

If we can find an inverse-kernel function $Q(x)$, we can estimate the unknown function $\psi(x)$ by using the given data $\phi(x)$

$$\psi(\xi) = \int Q(\xi - x)\phi(x)dx = \int Q(\xi, x)\phi(x)dx$$

In the Richardson-Lucy algorithm the inverse-kernel function is iteratively estimated by a previous solution by using the Bayes' theorem as follows:

$$Q^k(\xi, x) = \frac{P(x, \xi)\psi^k(\xi)}{\int P(x, \xi)\psi^k(\xi)d\xi}$$

Thus, we have the Richardson-Lucy formula given above.

1.2.4 Convergence Criteria

For the iteration processes, it is very important to use a useful convergence criterion. The following shows some criteria used in the DeConvHAADF:

$$\text{R-factor: } R = \sum |\phi_{cal}(i) - \phi_{obs}(i)| / \sum \phi_{obs}(i)$$

$$\text{Variance } (\chi^2): \chi^2 = \sum (\phi_{cal} - \phi_{obs})^2 / N$$

$$dQ: dQ = Q(f^k) - Q(f^{k-1}) \text{ (applicable to MEM only)}$$

The useful convergence criterion may be a difference of R-factor at each cycle, not the R-factor itself. The Likelihood (χ^2) is always decreases at each cycle, while the constrained entropy Q will oscillate at certain point of cycle. Thus, dQ may become negative, when a selected convergence factor is too large. Therefore, when iteration is stopped by dQ criteria, you may have to recalculate using a smaller convergence factor. In this way dQ is another useful criterion for the case of MEM processing.

Note Please note that dQ is not a criterion to stop iteration but a measure to check an *inappropriate* convergence speed (convergence factor).

1.2.5 Important Note

Theoretically, a constant background will not affect the result of deconvolution, since a convolution between a constant value and any kernel is a constant. On the other hand, both techniques of deconvolution used in this plug-in always give a positive result all over the region, and guarantee a non-negative result. However, they are apt to give an overshoot around a strong peak. Even though this overshoot will not become negative, but gives a deep valley if there is an appreciable background. Therefore, it is advisable to subtract an unnecessary constant background before performing deconvolution.

2. DeConvHAADF

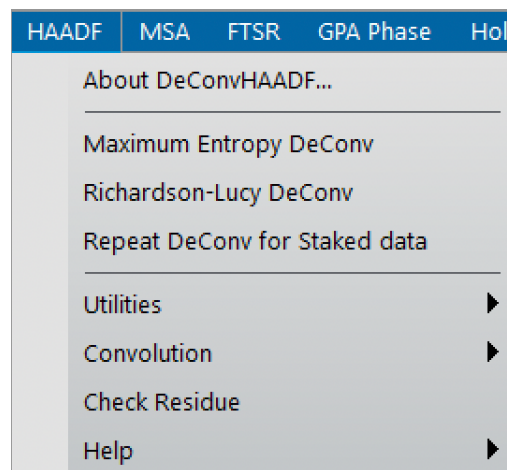
The DeConvHAADF software is a plugin for the Gatan's DigitalMicrograph, and thus only works under the DigitalMicrograph. The DeConvHAADF consists of a suite of menu commands and a dynamic link library.

2.1 DeConvHAADF Commands

The DeConvHAADF commands will appear under the HAADF menu as shown below.

Figure 2-1

DeConvHAADF commands under the HAADF menu



Various control parameters for Maximum Entropy or Richardson-Lucy deconvolution processing will be specified through a dialog that will be opened by selecting a corresponding command. When the command is launched with the ALT-key down, you can bypass these setup dialogs and use previous setup parameters.

2.2 Maximum Entropy Deconvolution

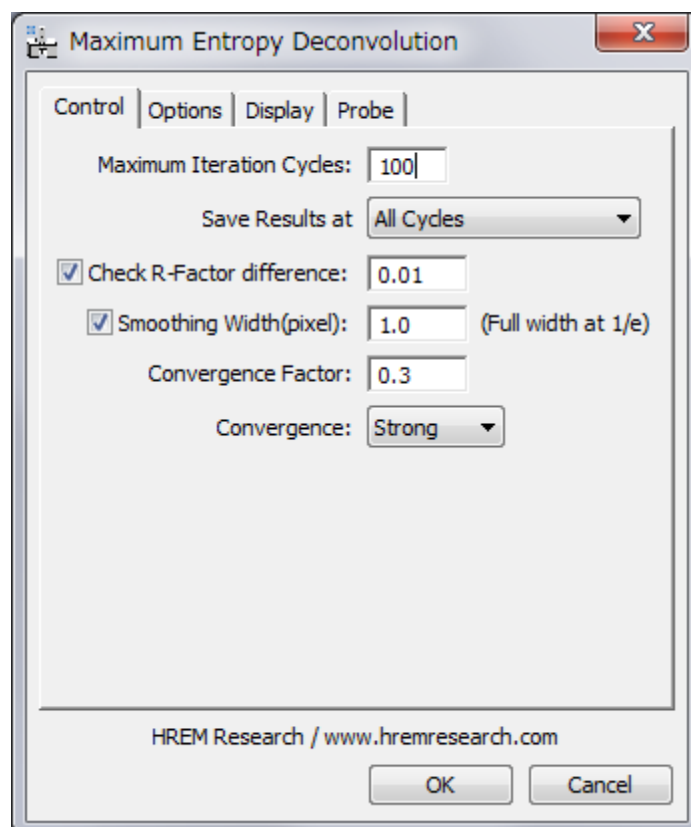
The Maximum Entropy command will open a dialog to control the processing and display the results.

2.2.1 Control tab-panel

The front most tab-panel has some controls for deconvolution processing.

Figure 2-2

Maximum Entropy Deconvolution (Control Tab)



Maximum Iteration Cycles: Maximum number of iteration cycles.

Save Result at: This controls a frequency of saving the results during the progress of deconvolution. A two-dimensional deconvolution usually requires a plenty of memory to save all the intermediate results. You can select from All Cycles, Every Two/Four/Eight Cycles, and R-Factor (1/3, 1, 3).

Check R-Factor difference: When selected, the iteration will stop when the difference of R-Factor divided by the R-Factor itself becomes smaller than the value specified here.

$$\Delta R = (R_{\text{previous cycle}} - R) / R$$

Check dQ: When checked, the iteration will stop when the difference of Q value starts oscillating.

Smoothing Width: When selected, the raw data will be smoothed out by convoluting a Gaussian with a specified full-width at 1/e value (in pixels). This is especially effective for a noisy image

Convergence Factor: This controls a speed of convergence. The default value is 0.3. A smaller value results in a slower convergence.

Convergence: There is a selection of convergence between **Strong** and **Weak**. The default setting is **Strong**.

NOTE: All the convergence criteria will be used logical “OR,” so iteration will stop when one of the criteria is satisfied.

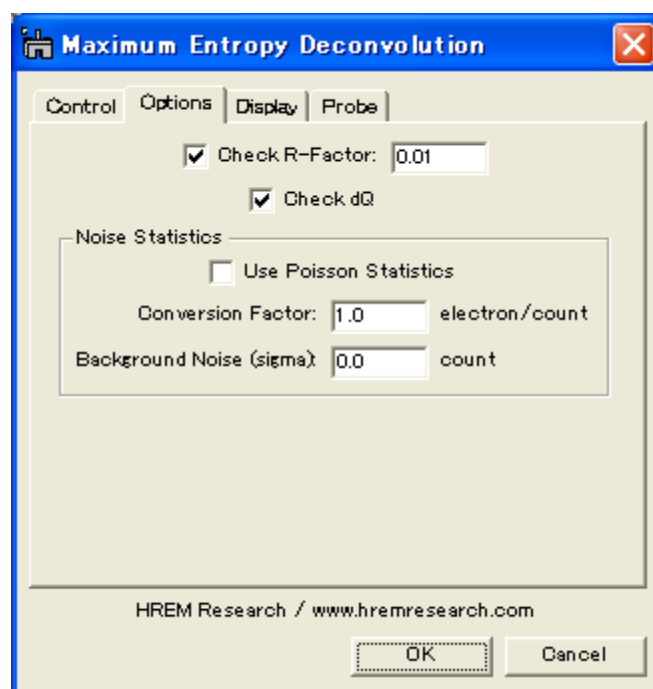
Weak convergence changes the convergence factor automatically, when the difference of Q value starts oscillating. Therefore, dQ criteria in the Options tab has no effect for the **Weak** convergence.

2.2.2 Options tab-panel

The next tab-panel is designed for specifying some optional controls for deconvolution processing.

Figure 2-3

Maximum Entropy Deconvolution (Options Tab)



Check R-Factor: When selected, the iteration will stop when R-Factor becomes smaller than the value specified here. It is not recommended to activate this criterion, when you don’t know an approximate noise level.

Check dQ: When checked, the iteration will stop when the difference of Q value starts oscillating.

Noise Statistics: You can explicitly use **Poisson Statistics** for noise distribution. In this case you have to specify **Conversion Factor** in order to convert a signal count to a number of electrons. You can specify also a constant **Background Noise (Gaussian)** such as a read-out noise.

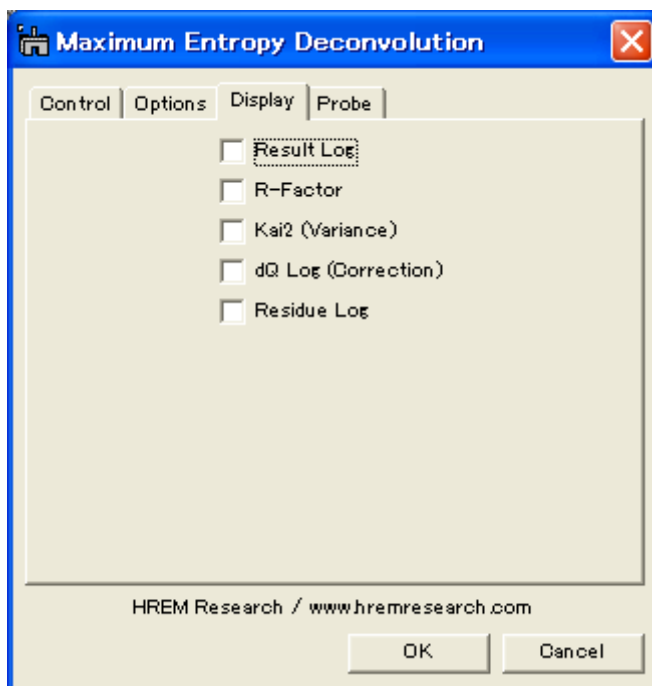
Note When “Use Poisson Statistics” is deselected, a constant noise model is used. Although this is not a real noise model for electron signal, it seems to work very well for a HAADF image.

2.2.3 Display tab-panel

The next tab-panel is designed for selecting the various results to be displayed at the end of processing.

Figure 2-4

Maximum Entropy Deconvolution (Display Tab)



Result Log: All the intermediate results specified by “Save Results at” will be saved.

R-Factor: History of R-factor.

Kai2 χ^2 (Variance): History of squared sum of differences.

dQ (Correction): History of sum of absolute corrections.

Residue Log: All the intermediate difference between an observed image and an estimated image (convolution between the probe and deconvolution) will be saved at specified cycles.

2.2.4 Probe tab-panel

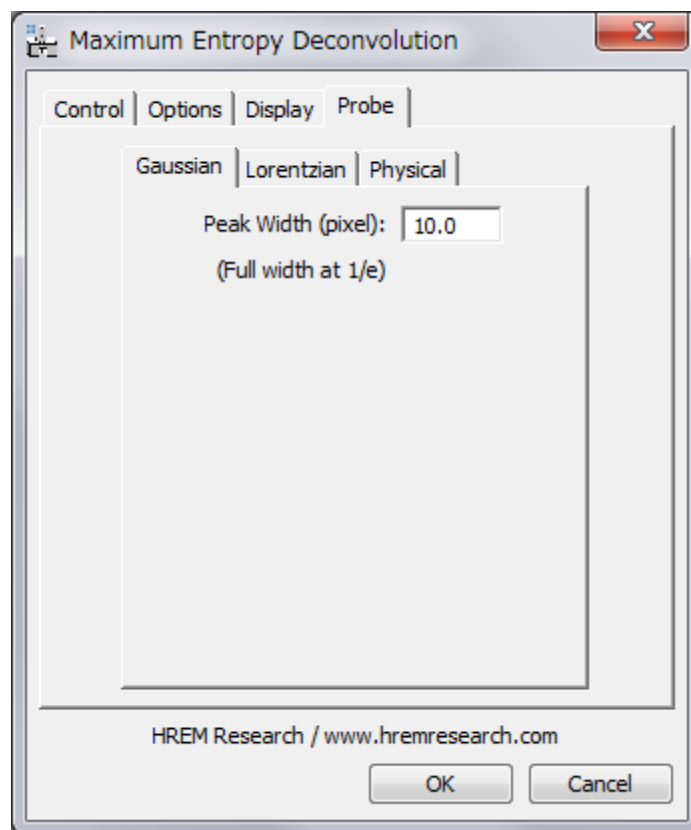
The next tab-panel is designed for selecting the probe used as a point spread function for deconvolution. There are three probe models corresponding to three tabs. The selected probe model will be used in deconvolution.

2.2.4.1 Gaussian or Lorentzian Probe

Gaussian or Lorentzian probe is defined by a single parameter that controls a width of the function. The next dialog shows a case of the Gaussian function.

Figure 2-5

Gaussian Probe (Probe Tab)



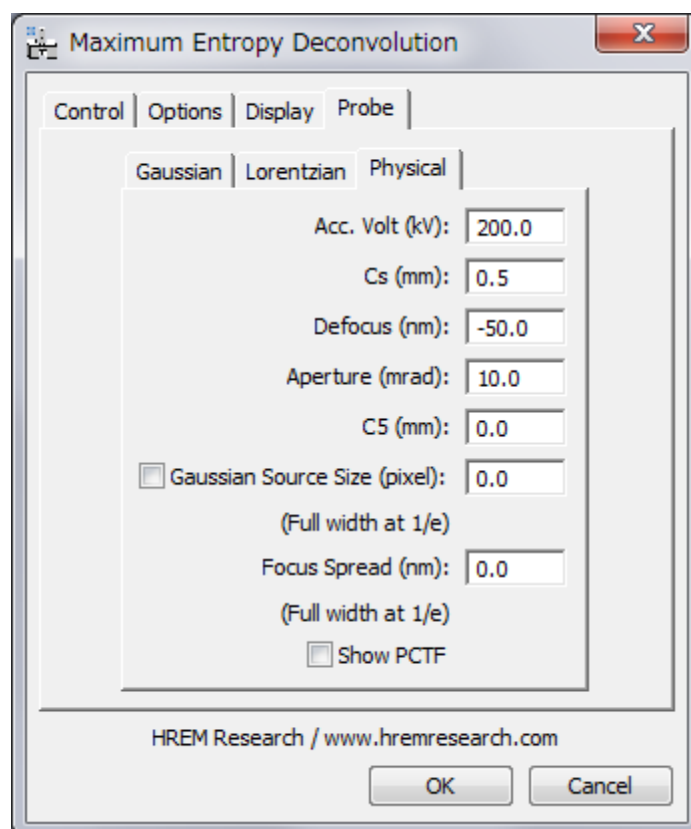
Peak Width: Full-peak width at which the function decreases to $1/e$.

NOTE Lorentzian Probe. The function decreases to $1/2$ at the Peak Width.

2.2.4.2 Physical Probe

This is a probe determined by lens aberrations and probe forming conditions, which are specified in this tab.

Figure 2-6 Physical Probe (Probe Tab)



Acc. Volt (kV): Acceleration voltage specified in kV.

Cs (mm): Spherical aberration coefficient specified in mm.

Defocus (nm): Defocus value specified in nm (a positive value corresponds to an over-focus).

Aperture (mrad): Objective (probe-forming lens) aperture specified in mrad.

C5 (mm): Fifth order spherical aberration coefficient specified in mm. This aberration will affect the probe shape only when the Cs is corrected.

Gaussian Source Size (pixel): Demagnified physical source size at the image plane specified in pixels.

Focus Spread (nm): Defocus spread in nm due to an energy spread of incident electrons and instability of a high-voltage and a objective lens current.

Show PCTF: When checked, the phase contrast transfer function (PCTF) is displayed.

2.3 Richardson-Lucy Deconvolution

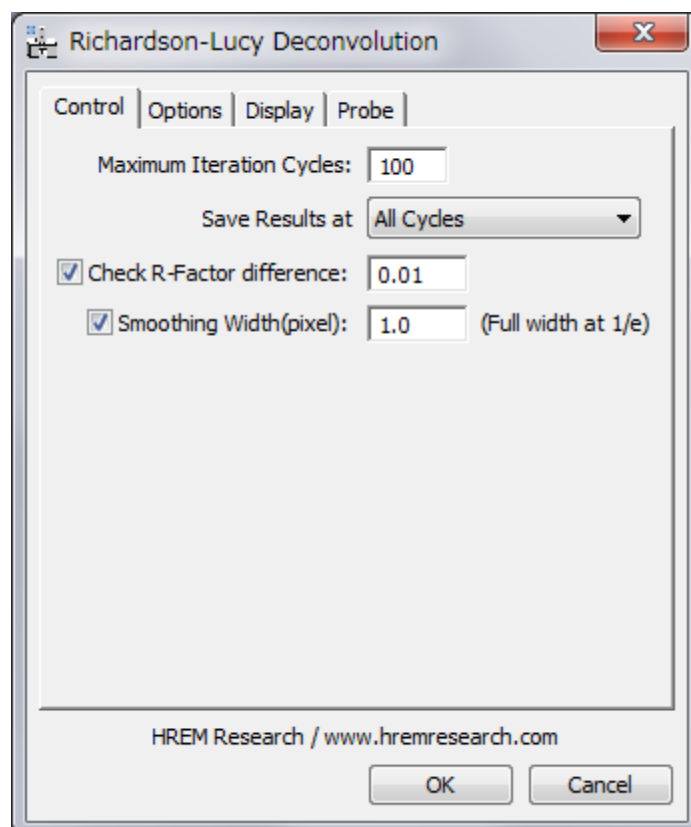
The Richardson-Lucy command will open a dialog to control the processing and display the results.

2.3.1 Control tab-panel

The front most tab-panel has some controls for deconvolution processing.

Figure 2-7

Richardson-Lucy Deconvolution (Control Tab)



Maximum Iteration Cycles: Maximum number of iteration cycles.

Save Result at This controls a frequency of saving the results during the progress of deconvolution. A two-dimensional deconvolution usually requires a plenty of memory to save all the intermediate results. You can select from All Cycles, Every Two/Four/Eight Cycles, and R-Factor (1/3, 1, 3).

Check R-Factor difference: When selected, the iteration will stop when the difference of R-Factor divided by the R-Factor itself becomes smaller than the value specified here.

$$\Delta R = (R_{\text{previous cycle}} - R) / R$$

Smoothing Width: When selected, the raw data will be smoothed out by convoluting a Gaussian with a specified full-width at 1/e value (in pixels). This is especially effective for a noisy image

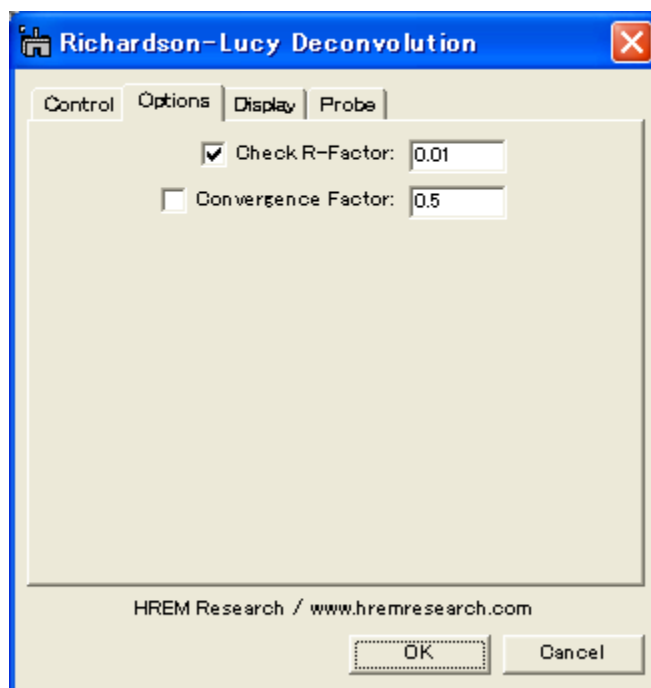
NOTE: All the convergence criteria will be used logical "OR," so iteration will stop when one of the criteria is satisfied.

2.3.2 Options tab-panel

The next tab-panel is designed for specifying optional parameters.

Figure 2-8

Richardson-Lucy Deconvolution (Option Tab)



Check R-Factor: When selected, the iteration will stop when R-Factor becomes smaller than the value specified here. It is not recommended to activate this criterion, when you don't know an approximate noise level.

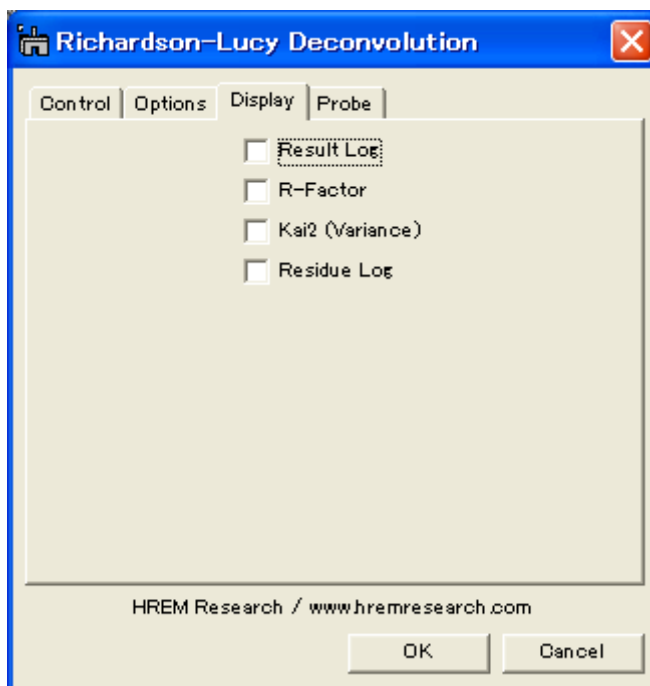
Convergence Factor: Actual modification of each cycle is an estimated change multiplied by this factor. Default value is one (1).

2.3.3 Display tab-panel

The next tab-panel is designed for selecting the various results to be displayed at the end of processing.

Figure 2-9

Richardson-Lucy Deconvolution (Display Tab)



Result Log: All the intermediate results specified by “Save Results at” will be saved.

R-Factor: History of R-factor.

Kai2 χ^2 (Variance): History of squared sum of differences.

Residue Log: All the intermediate difference between an observed image and an estimated image (convolution between the probe and deconvolution) will be saved at specified cycles.

2.3.4 Probe tab-panel

The settings for three probes are shared with the Maximum-Entropy routine. Please refer to the section of Probe for the Maximum-Entropy routine.

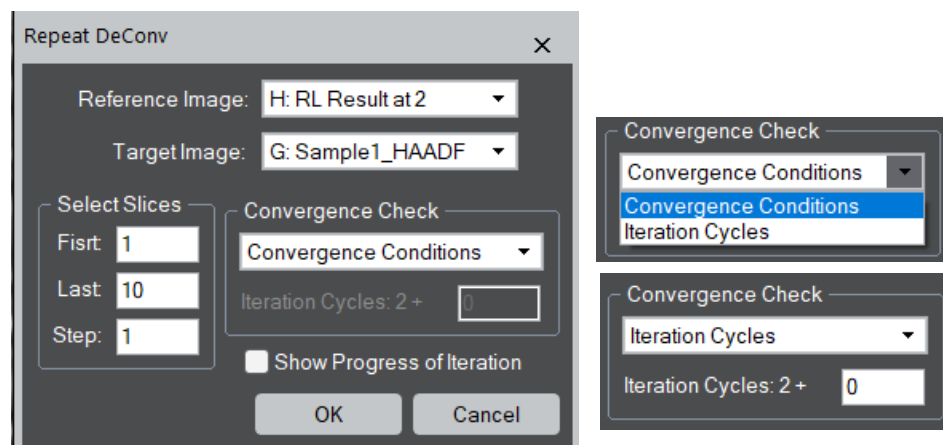
2.4 Repeat Deconvolution for Stacked data

The deconvolution on a stacked data can be performed by either Maximum Entropy or Richardson-Lucy with the same settings used to deconvolute a 2D HAADF. Here, the kernel should be identical over the staked image, and thus the stacked data should be acquired at the same conditions, including defocus.

2.4.1 Repeat Deconv dialog

When this command is selected, the dialog shown below will open where you can select a 2D HAADF image (Reference Image) that is already deconvoluted and a 3D DAADH stack image (Target Image) to be deconvoluted with the same settings. Of course, the same deconvolution method will be applied.

Repeat Deconvolution dialog



Select Slices: You can select the slices of the stacked data to be deconvoluted. Namely, a range (First and Last slice) and an interval (Step) of the slices can be specified.

Convergence Check: The condition of convergence for each slice can be selected from Convergence Conditions and Iteration Cycles.

Convergence Conditions: the same convergence conditions used to process the Reference Image will be applied for each slice.

Iteration Cycles: the maximum iteration cycle of each slice is defined by the sum of the iteration cycle of the Reference Image (here 2), and a specified number of cycles (here 0). **NOTE:** You can specify a negative number.

Show Progress of Iteration: When checked, a window to show the progress of processing will appear. **NOTE:** Updating the image will slow down an overall process time.

3. Installation

This chapter describes hardware and software requirements to run the DeConvHAADF software and an installation procedure of the DeConvHAADF plugin.

3.1 Requirements

The DeConvHAADF runs under DigitalMicrograph environment, and the software and hardware requirements are similar to those for DigitalMicrograph.

3.1.1 Hardware requirement

The DeConvHAADF requires a user key properly installed at a USB port. Therefore, you have to install a driver for the user key. Moreover, if you will to process a two-dimensional image, you need an enough memory to store the ResultLog.

3.1.2 Software requirement

The following is a list of the software requirements necessary to run DeConvHAADF:

- **DigitalMicrograph (GMS 2.x or later)**
- **User Key Driver** (downloadable from the HREM web site)
- **IPU Plug-in** (downloadable from the HREM web site)

3.2 Software Installation

The following plug-ins should be placed in the folder “Gatan/PlugIns” of ProgramData (hidden folder):

- **DeConvBasicLib.gtk (DeConvBasicLib)**
- **DeConvHAADF.gtk (DeConvHAADF)**
- **DeConvHAADF.dll (DeConvHAADF.lib)**

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

DeConvHAADF menu commands will be appeared under the HAADF menu, when the DigitalMicrograph is launched after placing the plug-ins the PlugIns folder.

Note **IPU plug-in should be installed to use DeConvHAADF (see 3.4)**

3.3 User Key Installation

Installing User Key Driver

NOTE: follow the procedure *without* inserting the USB key into an USB port.

Installing User Key Driver

1. Execute the user key installer.
2. Continue installation by selecting 'Typical' from Setup type.

Installing User Key

Simply plug your user key into an USB port. Your computer needs not to be restarted.

3.4 IPU Installation

Please download the IPU (Image Processing Utility) plug-in from the HREM web site and install it according to the ReadMe.txt file.

4. Getting Started...

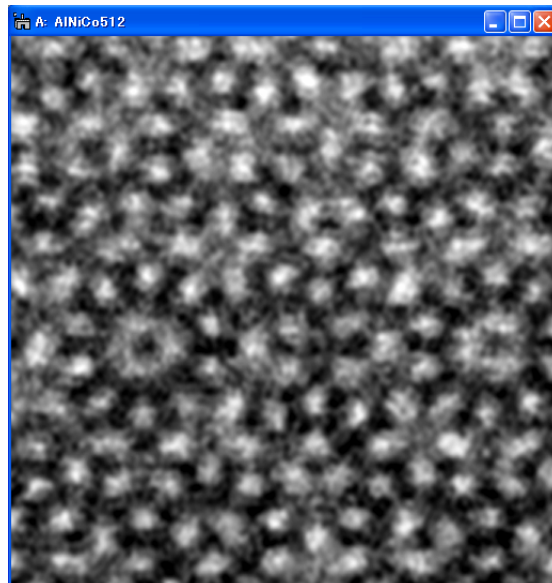
This chapter briefly explains typical steps of the DeConvHAADF. Before doing this section, you have to install the DeConvHAADF plug-ins as well as the driver for your user key, and insert your user key.

4.1 Deconvolution

This section briefly describes steps of image deconvolution using the Maximum Entropy method. Deconvolution using the Richardson-Lucy algorithm follows the same steps.

4.1.1 Open and Select Image

The deconvolution routine will work on open images. Therefore, you must open an image to be processed and select it before launching the deconvolution routine.

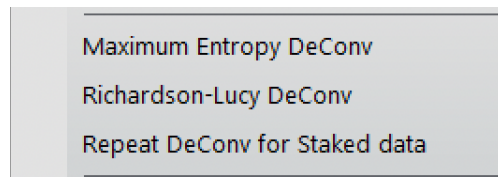


The above image shows a sample data to be processed here, which has been taken from a quasicrystal AlNiCo on JEOL 2010F. (Abe, Pennycook, Tsai: Nature, VOL421 (2003) 347. This image is kindly supplied by Dr. E. Abe for testing the procedure.)

Note You can process a selected area using a rectangular ROI (see 4.2).

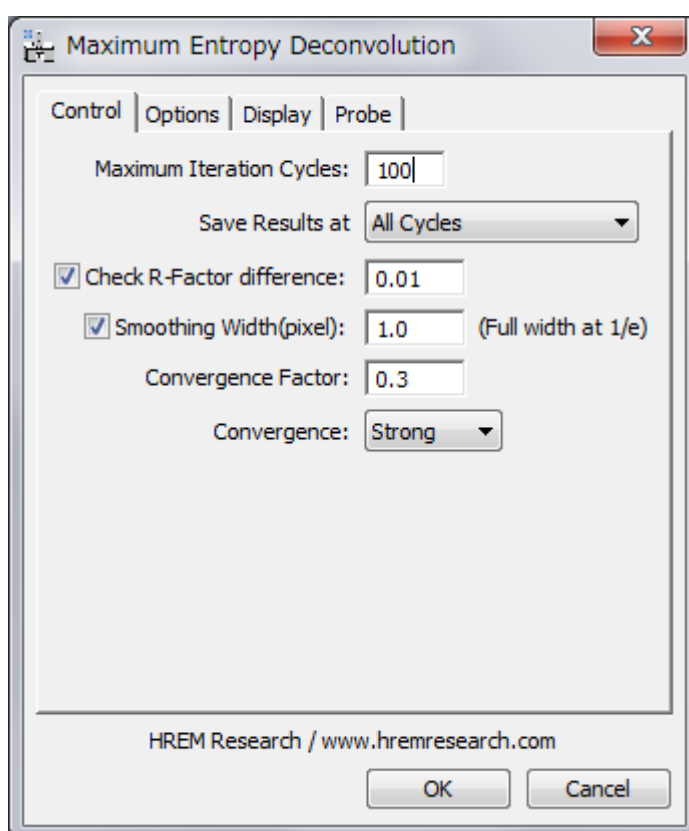
4.1.2 Launch Deconvolution

Select “Maximum Entropy DeConv” command from the menu as shown below.



4.1.3 Setup Deconvolution Parameters

The deconvolution routine will work normally with defaults parameters as shown here.



However, if your image quality is too bad (noisy), or extremely good (high signal-to-noise ratio), you may change a R-factor difference to a larger or a smaller value rather than the default value 0.05.

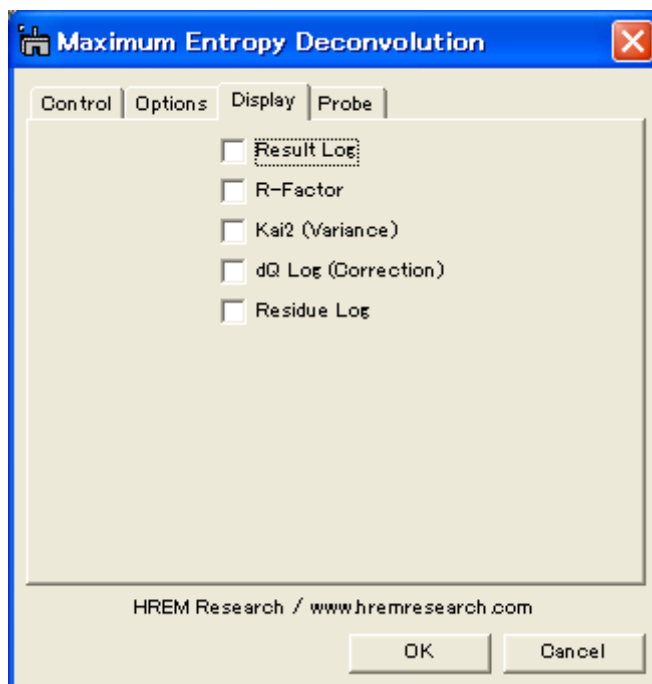
The default Convergence Factor is 0.3. If an iteration stops with the dQ criterion, you may use a smaller value.

Usually, a HAADF image is rather noisy. Therefore, smoothing with a Gaussian function generally gives in a better result. The width close to the probe width may be employed.

If you are short in core memory (RAM), you may want to save results at every two, four or eight cycles. You may also save the final three results corresponding to three R-factor differences of 3, 1 and 1/3 of the specified R-factor difference in this dialog.

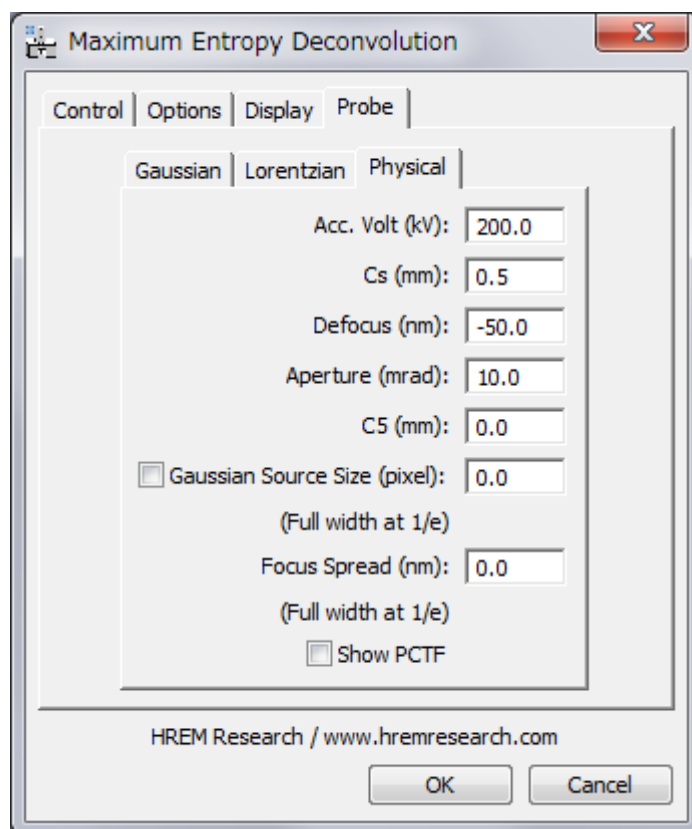
4.1.4 Select Results to Display

The final result after deconvolution will be always shown. If you check “Result Log” box, you can save all the intermediate results at specified cycles of deconvolution process, and check the results later by using a Slice tool. You can see the change of R-factor or Kai2 value as a function of the cycle, when you check the corresponding box. You can also save the Residue and dQ at specified cycles, if you check the corresponding box.



4.1.5 Setup Probe Function

The final step to setup processing condition is a probe selection. Here, we use a physical probe as follows;

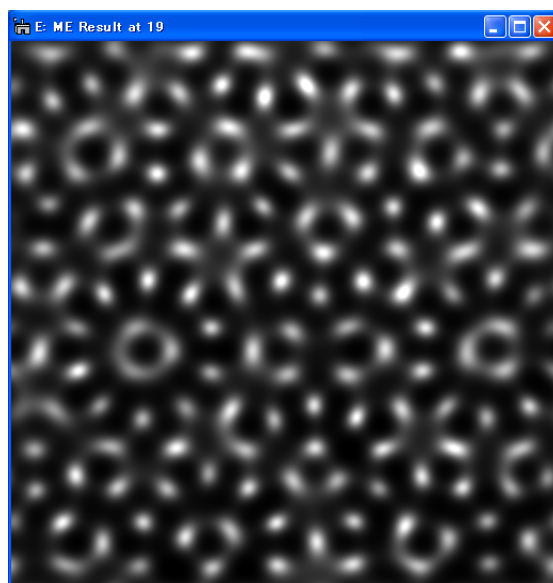


It is recommended to check the probe size and shape by using “Setup Probe” command under the “Utilities” menu as explained later.

4.1.6 Start Deconvolution

After checking all conditions, you can start deconvolution by clicking OK, or stop the procedure by clicking Cancel below the tab panels in the setup dialog.

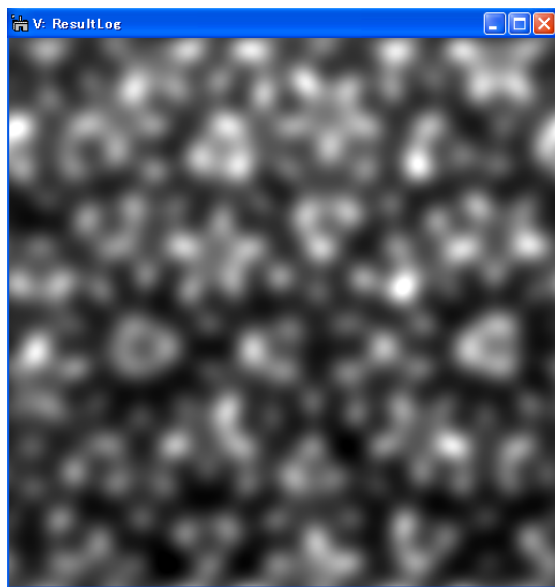
Then, you will see a progress of deconvolution in the restored image window as shown below:



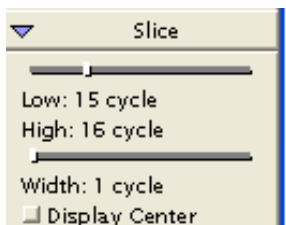
4.1.7 Survey Results

The final result is displayed in the restored image window as shown above. Some information on the progress of deconvolution will be shown in the DigitalMicrograph's Results Window.

If you select "Result Log" check box in the setup dialog, you can save the intermediate results at specified cycles in the ResultLog image.



The ResultLog of a 2D image deconvolution is a 3D image, and easily surveyed by using a utility "Show as Movie" as explained later in the Utility section.



By using a Slice tool as shown here, you can manually survey through the ResultLog image.

You can also check a deconvoluted image at a selected cycle by extracting a slice (section) from the 3D image using "Extract Slice" command in the "Utilities" sub-menu.

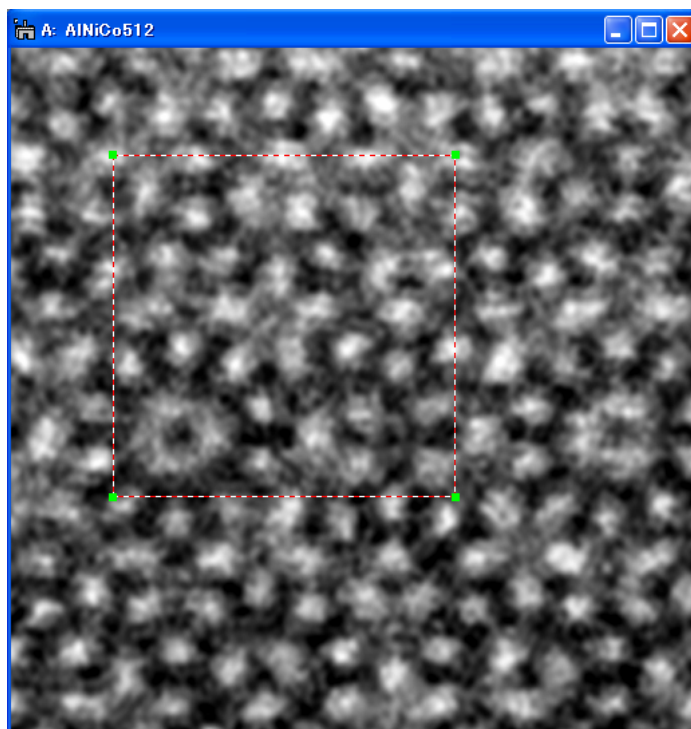
4.2 Selection

4.2.1 Selection of Image

Both deconvolution procedures work on a selection of spectrum of any size (not necessary to be a power of two).

A selection is created by using a ROI tool (and its size is made a power of two by clicking the ALT-key when you drag a mouse).

Selection on the Image

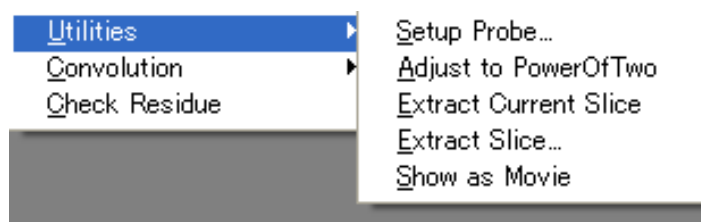


4.3 Utilities

Some useful commands to pre-process or post-process a image are provided for your convenience.

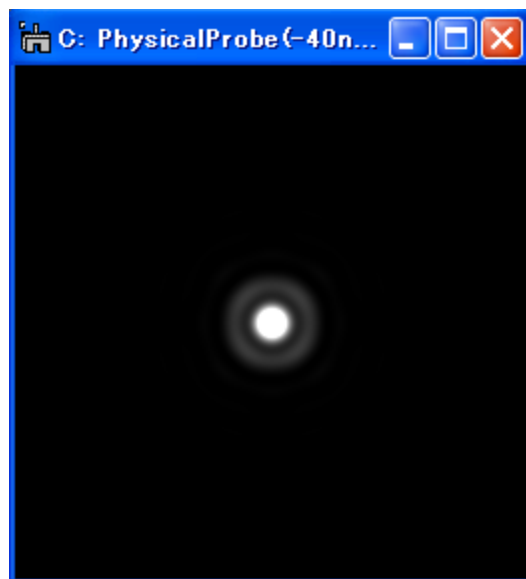
4.3.1 Utilities Menu

The following shows "Utilities" sub-menu.



4.3.2 Setup Probe

You can check the size and shape of the probe by using this command. Launching this command will open the dialog, which shows the Probe Tab explained before. When you click "OK" button of the dialog, you will get a window showing the probe as shown below:



As you see from the Probe setting tab for each probe model, the Gaussian probe and the Lorentzian probe does not require an image to be calibrated beforehand, since their peak size are defined in pixels. Due to this simplification, the image to be deconvoluted should have a square pixel.

Contrary to this, the Physical Probe requires a calibrated image. However, if the image is calibrated, its pixel size needs not to be square. You can use non-square pixel image, if you use the Physical Probe. In this case, you may note that the probe will be displayed as an oval, since a non-square image pixel is displayed by a square pixel of the monitor.

4.3.3 Adjust to Power of Two

Using this command, you can adjust the size of your image or a selection of the image to a power of two, which is required by the deconvolution routines. The size is adjusted to a next larger number that is a power of two in order not to reduce resolution of the original image.

To use this command, you have to select an image before launching the command.

4.3.4 Extract Current Slice / Extract Slice...

Using this command, you can extract a 2D image (a slice) from the ResultLog that is a 3D image. Using **Extract Current Slice** command, you can extract the slice that is currently displayed. On the other hand, you will be asked to specify a slice number to be extracted, when you use **Extract Slice...**command.

To use this command, you have to select the ResultLog image before launching the command.

4.3.4 Show as Movie

Using this command, you can survey through the ResultLog image like a movie. To use this command, you have to select the ResultLog image before launching this command. You can change an interval between the frames using the Left/Right Arrow keys, and change a direction (Forward/Backward) using the Up/Down Arrow keys. You can stop the movie by pressing the Space bar.

4.4 Convolution

Two convolution routines are provided for your convenience.

4.4.1 Convolution Menu

The following shows "Convolution" sub-menu.



4.4.2 Probe

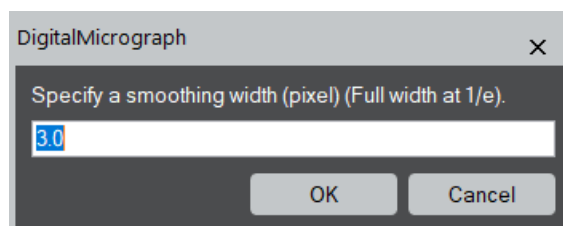
You may check your result by convoluting the restored image and a probe function (a point spread function). The convolution should be close to the observed image.

To use this command, you have to select the original image before launching this command. You can change a probe function, when the probe setup dialog appears.

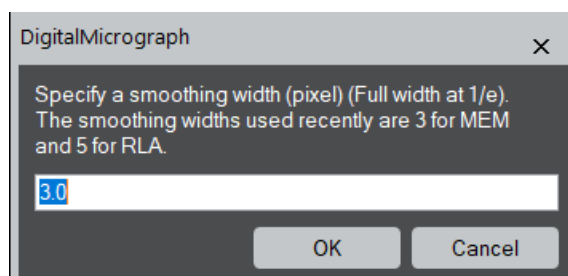
4.4.3 Smoothing Gaussian

Using this command, you can check a smoothed image that will be used at deconvolution when you choose the Gaussian smoothing. To use this command, you have to select an image first.

The dialog that shows the smoothing width used before will be open. If you want, you can change the number here.



When the smoothing widths used for the MEM and RLA are different, the dialog that shows the two smoothing widths appears as shown below. You can choose one of these values, or change the value here, if you want.



4.5 Check Residue

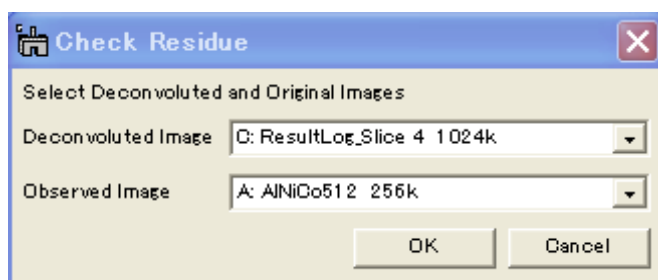
You can check residue for a result of deconvolution. Here, the residue means a difference between the observed image and a convolution between the probe and a deconvoluted image. You can manually calculate the residue by subtracting a result obtained by the previous **Convolution** command from the observed image. However, this is a handy command to calculate the residue.

When you want to get a residue for a final result, just select the final result and choose this command. The probe setup dialog appears, where you can change the probe shape, if you want. Then, a residue will be displayed. This is because the final result keeps information of the original observed image.

When you want to get a result for *other than the final result*, you have to specify an observed image. In this case the steps will be as follows:

1. Choose Check Residue from HAADF menu.

Then, the probe setup dialog appears, where you can change the probe shape, if you want. After this dialog the following windows will appear to select images. You have to open the images to be used beforehand.



2. Choose **Deconvoluted Image** and **Observed Image** from opened images, and then click **OK** to continue the process or click **Cancel** to stop the procedure.

A stack of residue images will appear in a minute.

5. Tips and Troubleshooting
