

DeConvHAADF

(Software Cs-Corrector)

DigitalMicrograph Plugin
for
STEM-HAADF Deconvolution

User's Guide

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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 3.4, or later, both for Windows and Macintosh platforms.

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 or Macintosh 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. 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 **The image (image) size should be a power of two.** If your image size is not a power of two, you have to resample the image, or cut out a portion of the image, or pad out with a constant.

Some utilities routines are provided for your convenience. Using a command in the "Utilities" sub-menu you can make the size of your data to a power of two (See **section 4.3**). Alternatively, you can use a selected area that is 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 (Command + C)
3. Use a modified Paste short cut: Ctrl + Alt + V (Command + Option + 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 in 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.

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

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

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

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

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

1.2.3 Richardson-Lucy Algorithm

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

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

This algorithm is explained as follows by using formulas in statistics. We know an 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 a R-factor itself. The Likelihood (χ^2) is always decreases at each cycle, the constrained entropy Q will oscillate at certain point of cycle. Therefore, dQ may be another useful criterion for the case of MEM processing.

2. DeConvHAADF

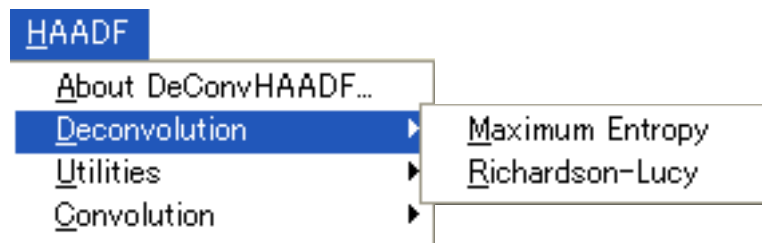
The DeConvHAADF software is a plugin for the Gatan's DigitalMicrograph, and thus only works under the DigitalMicrograph. The DeConvHAADF consists of a suite of menu commands and a dynamic link library.

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 (Option-key) down, you can bypass these setup dialogs and use previously setup parameters.

2.2 Maximum Entropy Setup

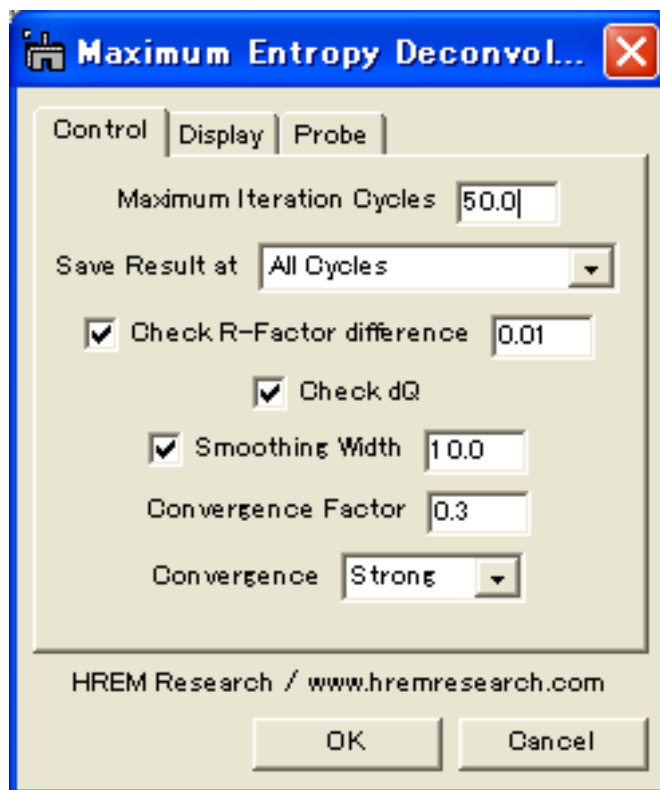
The Maximum Entropy command will open a dialog to control the processing and display the results.

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 control a requirement of memory by selecting a cycle of saving.

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

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 half-width (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.

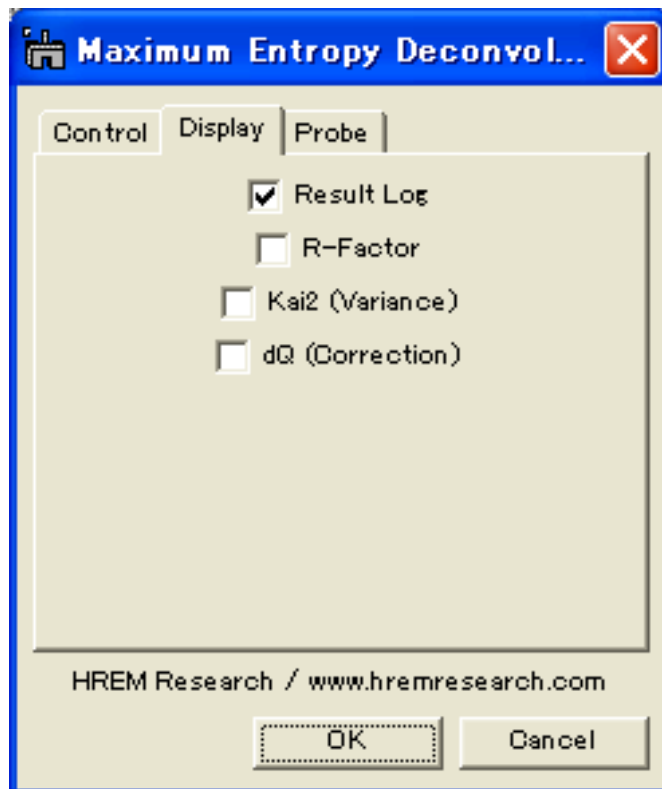
Convergence: There is a selection of convergence between “Strong” and “Weak.” The default setting is “Strong.”

2.2.2 Display tab-panel

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

Figure 2-3

Maximum Entropy Deconvolution (Display Tab)



Result Log: All the intermediate results will be saved at every cycle.

R-Factor: History of R-factor.

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

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

2.2.3 Probe tab-panel

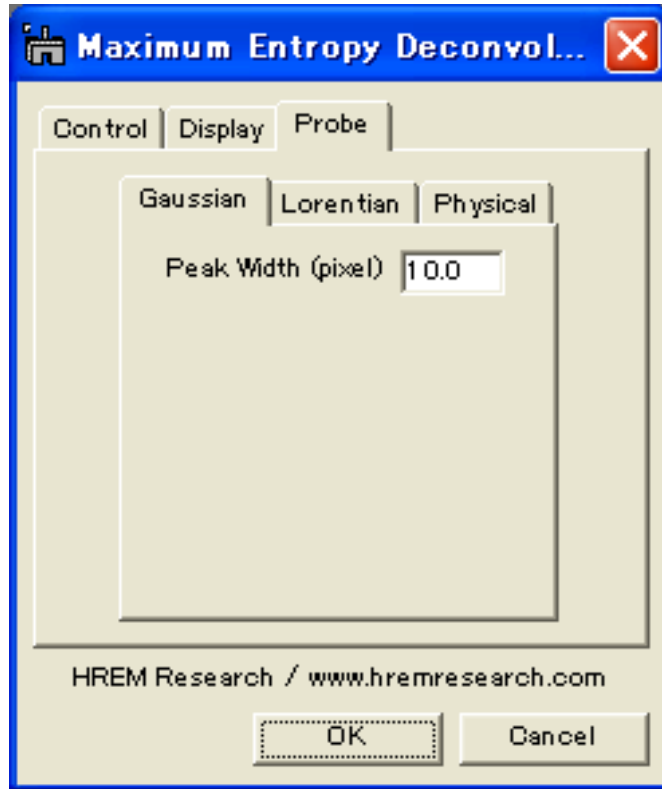
The next tab-panel is designed for selecting the probe used as a point spread function for deconvolution. There are three probe models corresponding to three tabs. The selected probe model will be used in deconvolution.

2.2.3.1 Gaussian or Lorentian Probe

Gaussian or Lorentian 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 2-4

Gaussian Probe (Probe Tab)



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

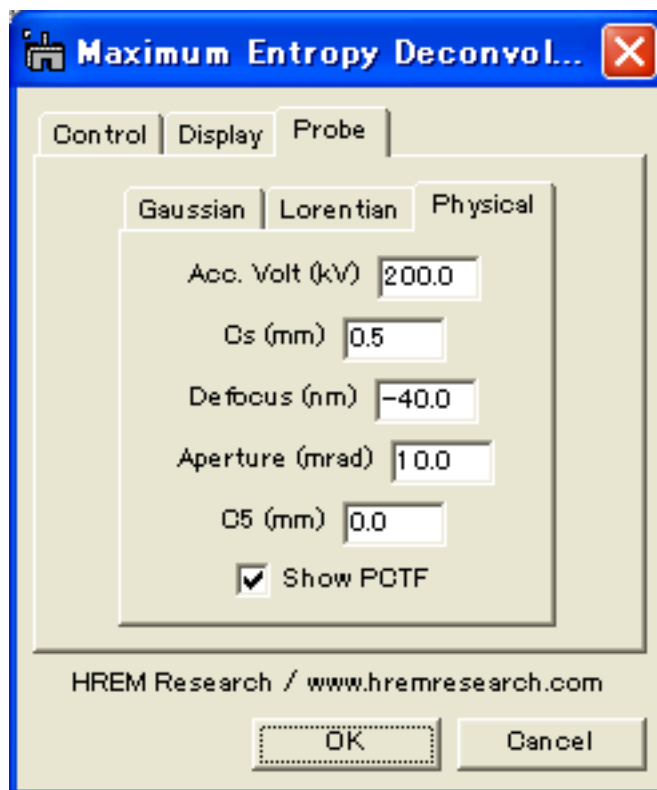
NOTE Lorentian Probe. The function decreases to $1/2$ at the Pear Width.

2.2.3.2 Physical Probe

This is a probe determined by lens aberrations, which are specified in this tag..

Figure 2-5

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.

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

2.3 Richardson-Lucy Setup

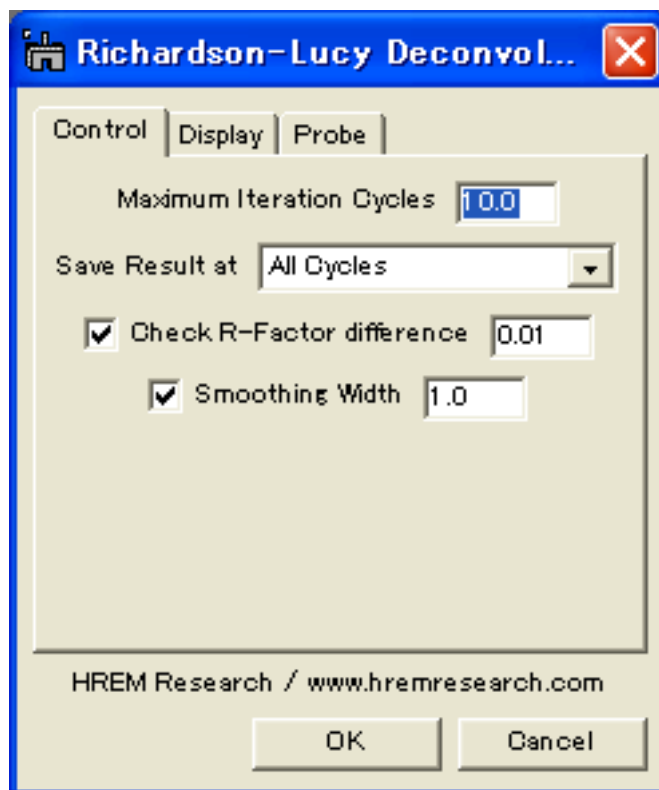
The Richardson-Lucy command will open a dialog to control the processing and display the results.

2.3.1 Control tab-panel

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

Figure 2-6

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 control a requirement of memory by selecting a cycle of saving.

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

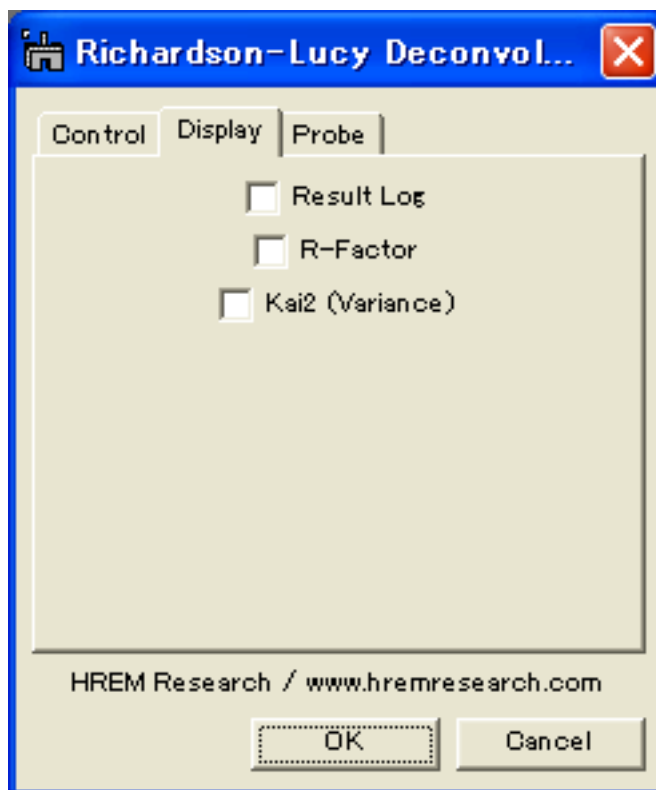
Smoothing Width: When selected, the raw data will be smoothed out by convoluting a Gaussian with a specified half-width (in pixels). This is especially effective for a noisy image

2.3.2 Display tab-panel

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

Figure 2-7

Richardson-Lucy Deconvolution (Display Tab)



Result Log: All the intermediate results will be saved at every cycle.

R-Factor: History of R-factor.

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

2.3.3 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.

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 for Windows (version 3.6 or later) or for Macintosh (version 3.4).**
- **User Key Driver** (supplied with your user key)

3.2 Software Installation

The following plug-ins should be placed in the folder “PlugIns (Packages)” on the same level of the DigitalMicrograph:

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

The PlugIns (Packages) 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 (Packages) folder.

3.3 User Key Installation

Windows

Installing User Key Driver

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

Installing User Key Driver

1. Execute 'hdd32.exe' within HASP4Driver Folder.
2. Continue installation by selecting 'Typical' from Setup type.

A driver corresponding to your Operation System will be installed.

Installing User Key

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

Macintosh

Installing User Key Driver

Installing User Key Driver

1. Copy MacHaspUsbDD within 'MacHASP V4.0 Device Drivers' into System Extensions.
2. Restart your computer.

Installing User Key

Plug in your USB key into an USB port.

4. Getting Started...

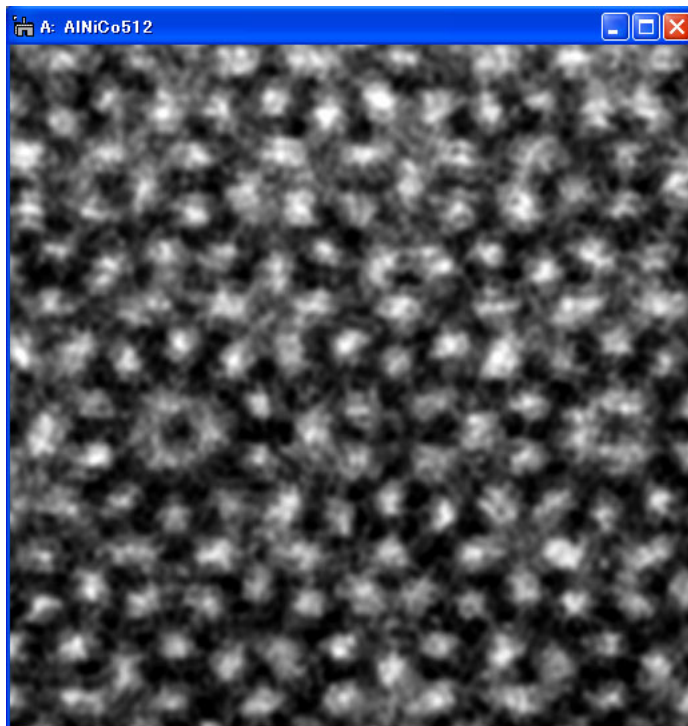
This chapter briefly explains typical steps of the DeConvHAADF. Before doing this section, you have to install the DeConvHAADF plug-ins as well as the driver for your user key, and insert your user key.

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 restored 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.)

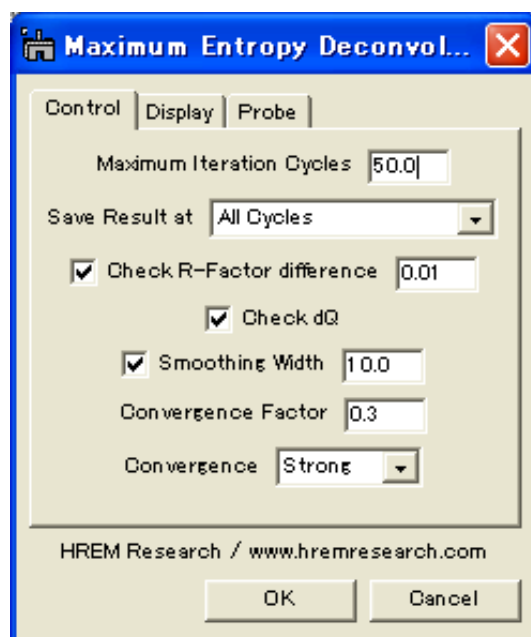
4.1.2 Launch Deconvolution

Select “Maximum Entropy” or “Richardson-Lucy” command from the Deconvolution menu as shown below. Here, we use the MEM as an example.



4.1.3 Setup Deconvolution Parameters

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



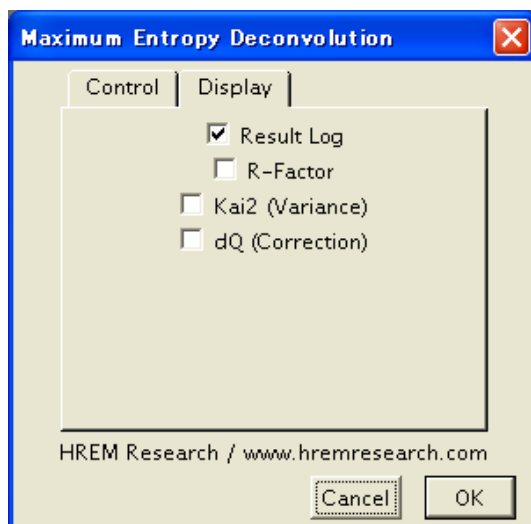
However, if your image quality is too bad (noisy), or extremely good (high signal-to-noise ratio), you may change a R-factor difference to a larger or a smaller value rather than the default value 0.01.

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.

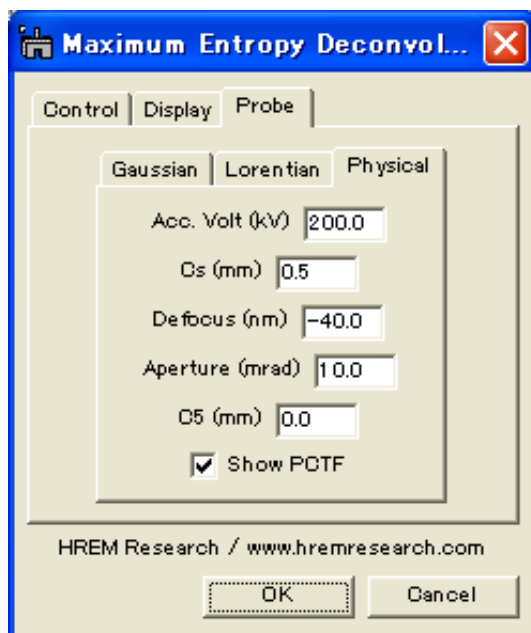
4.1.4 Select Results to Display

The final result after deconvolution will be always shown. If you check “Result Log” box, you can save all the intermediate results at each cycle of deconvolution process, and check the result at each cycle by using a Line-Profile tool or a Slice tool. By selecting other three check boxes, you can see their histories.



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;

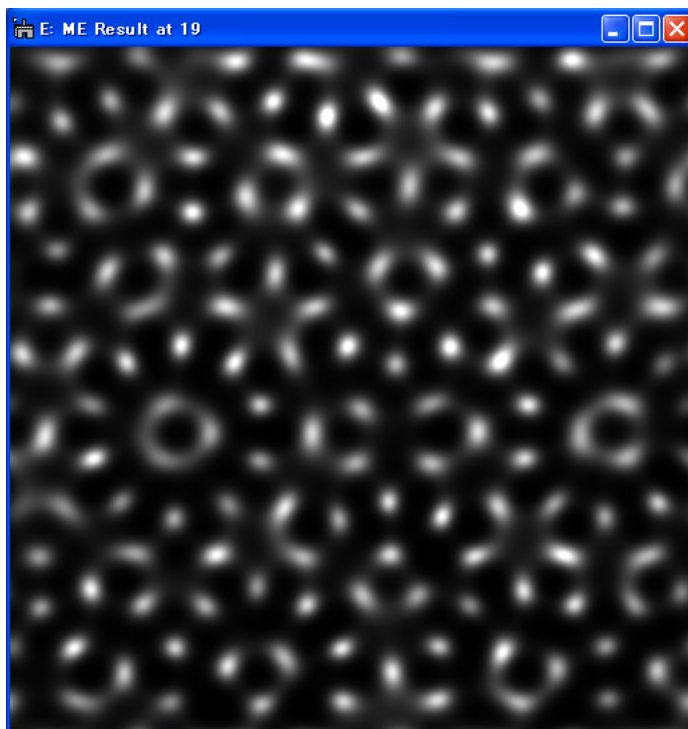


It is recommended to check the probe size and shape by using “Setup Probe” command under the “Utilities” sub-menu as explained later.

4.1.6 Start Deconvolution

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

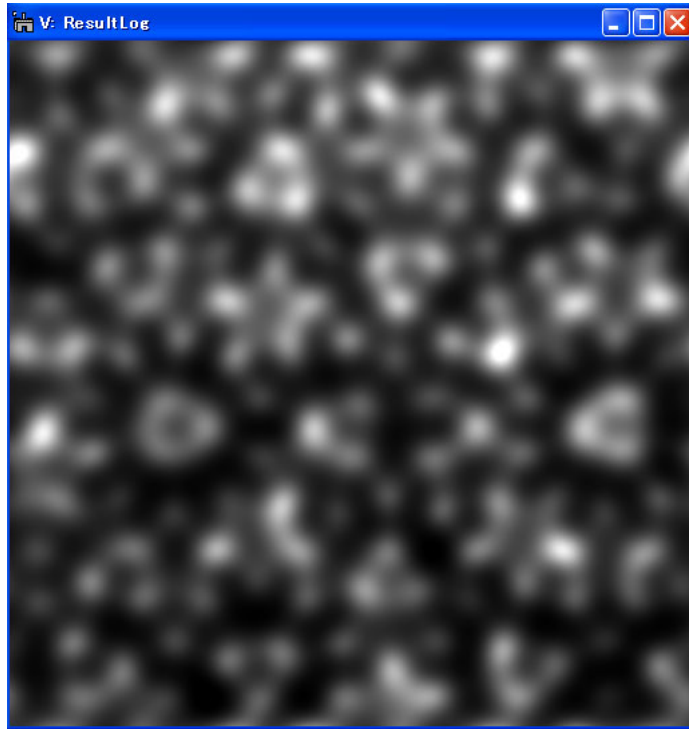
Then, you will see a progress of deconvolution in the restored image window as shown below:



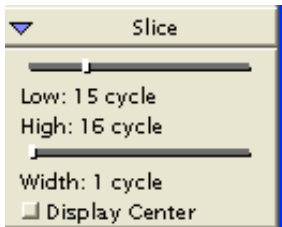
4.1.7 Survey Results

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.



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 image as shown below, you can easily 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..

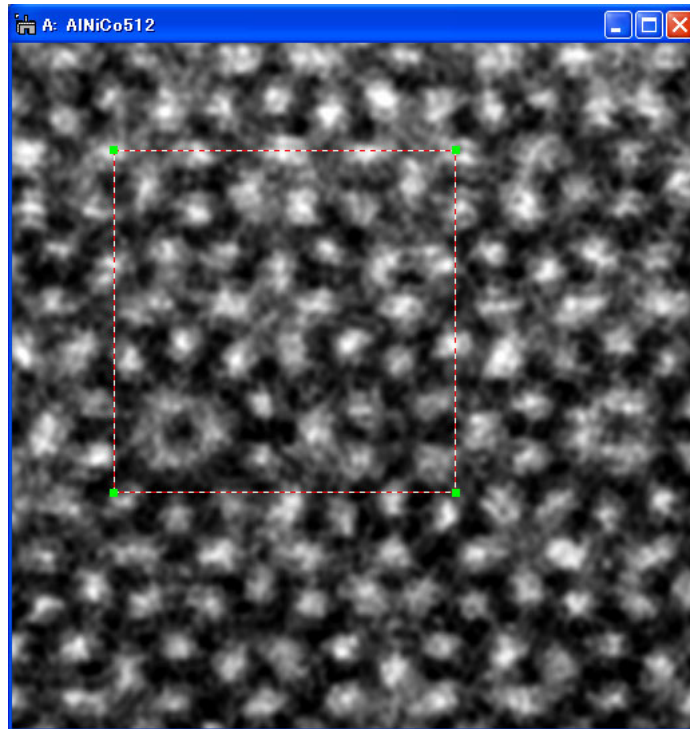
4.2 Selection

4.2.1 Selection of Image

Both deconvolution procedures work on a selection of image, if its size is a power of two. If your original image is not a power of two, the processing of the selection may be used effectively.

A selection is created by using a ROI tool, and its size is made a power of two by clicking the Alt (Option) 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.

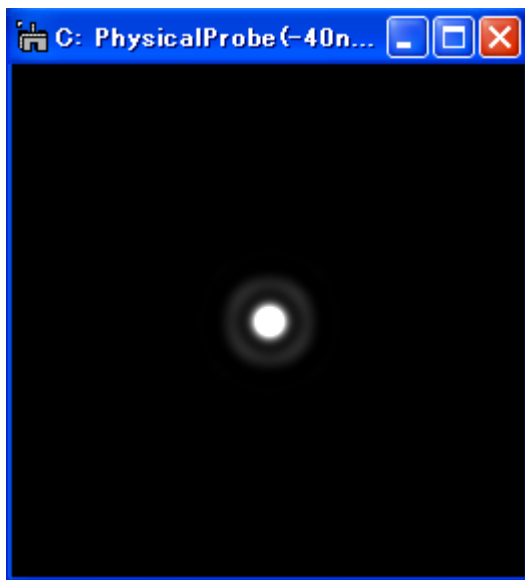
4.3.1 Utilities Menu

The following shows the "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 setting Tabs for each probe model, the Gaussian probe and the Lorential probe does not required 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 pixels of the monitor.

4.3.3 Adjust to Power of Two

Using this command you can adjust the size of your 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.

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

4.3.4 Extract Slice

Using this command you can extract a 2D image (a slice) from the ResultLog (a 3D image). You may be asked to specify a slice number to be extracted.

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

4.3.4 Show as Movie

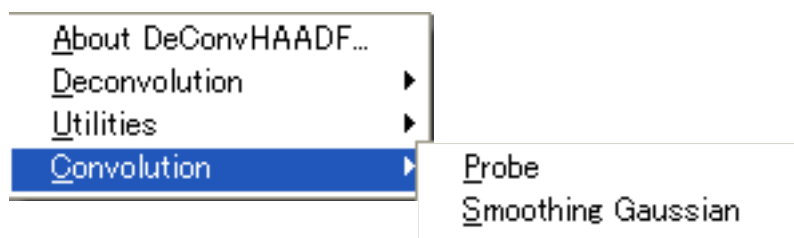
Using this command you can survey through the ResultLog image like a movie. To use this command, you have to select the ResultLog image before launching this command. You can change an interval between the frames using the Left/Right Arrow keys, and change a direction using the Up/Down Arrow keys. You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

4.4 Convolution

Two convolution routines are provided for your convenience.

4.3.1 Convolution Menu

The following shows the "Convolution" sub-menu.



4.3.2 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. Then, the probe you setup lastly will be used.

4.3.3 Smoothing Gaussian

Using this command you can check a smoothed image that will be used at deconvolution when you choose the Gaussian smoothing. When the smoothing widths specified for the MEM and RLA are different, you may be asked the value you want to use. To use this command, you have to select a image before launching this command.



5. Tips and Troubleshooting
