SI Module
for
DeConvEELS
(Software Monochromator)

DigitalMicrograph Plugin
for
Electron Energy Loss Spectrum Deconvolution

User's Guide

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1. Introduction

The SI Module for DeConvEELS is an extension module for DeConvEELS to deconvolute a 3D Spectrum Image (SI) efficiently using Maximum Entropy Method (MEM) or Richardson-Lucy Algorithm (RLA). The principles and practices of processing are the same as used in DeConvEELS. Thus, this Guide assumes the user is familiar with DeConvEELS.

1.1 Features

1.1.1 Advanced deconvolution algorithms

The SI Module uses a Maximum Entropy Method (MEM) or the Richardson-Lucy Algorithm (RLA) to deconvolute an EELS Spectrum Image (SI) data. Due to optimized implementation and multi-CPU support an ideal result will be obtained within a reasonably short processing time.

1.1.2 Easy-to-Use User Interface

Like DeConvEELS software the SI Module 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 **Image points and spectra length of *any size* can be handled (not necessary to be a power of two)**.

The spectrum size of a kernel (low-loss spectrum) and data to be processed should be of equal length.

A kernel may be a single spectrum or a SI data (DualEELS data). If the kernel is a single spectrum, the same kernel will be used for all the spectrum of the SI data. If the data set is a DealEELS, the corresponding kernel is used for each spectrum to be processed.

2. SI Module

The SI Module for DeConvEELS consists of a suite of menu commands and a dynamic link library.

2.1 SI Module Commands

The SI Module commands will appear below DeConvEELS commands as shown below.

Figure 2-1 SI Module commands below DeConvEELS commands

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.

TIPS It is highly recommended to process a single spectrum from the SI data, and find good processing conditions, before processing the whole SI data. The conditions used in a previous processing will be transferred to the SI Deconvolution routine.

Most of the usage of the SI Module commands is similar to the corresponding DeConvEELS commands. Thus, this manual focuses on specific features of the SI module.

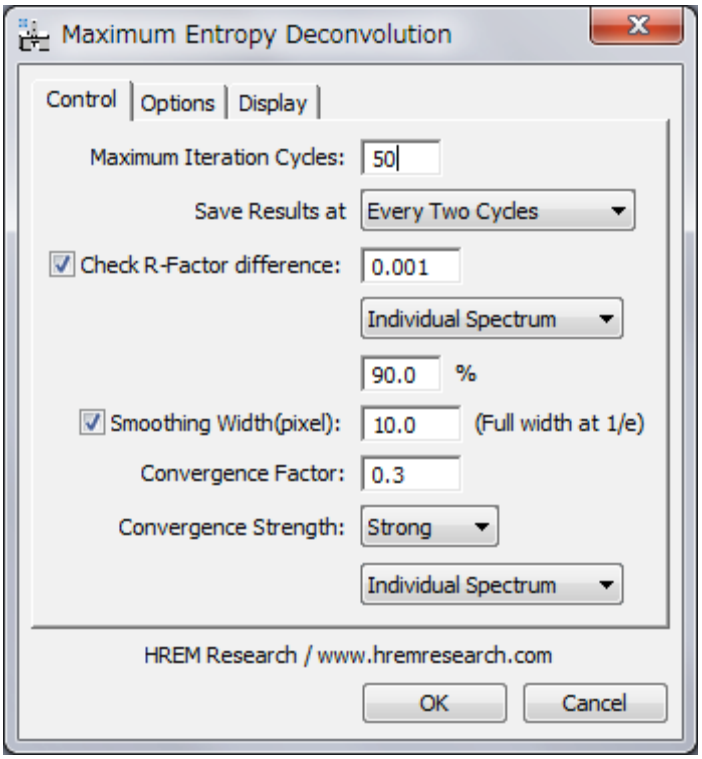
2.2 Maximum Entropy Setup

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 general controls for deconvolution processing.

Figure 2-2 Maximum Entropy Deconvolution (Control Tab)



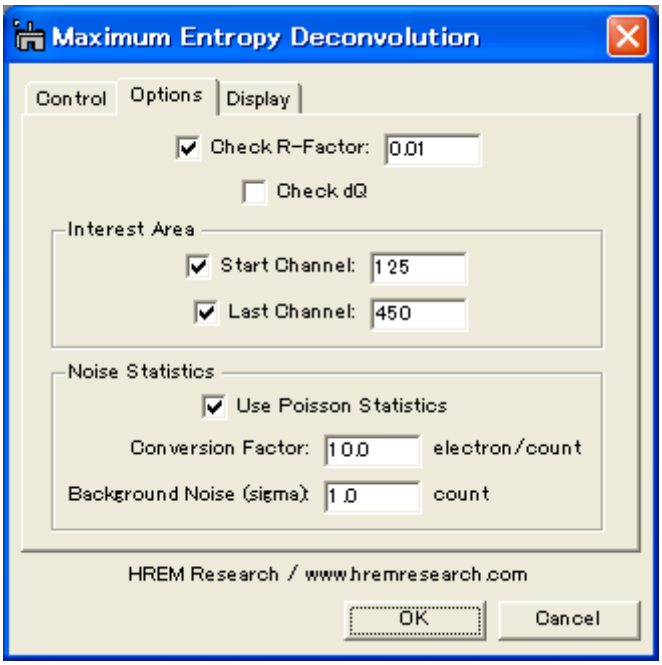
Maximum Iteration Cycles: Maximum number of iteration cycles.
Save Results at: This controls a frequency of saving the results during the progress of deconvolution. Since the result at each cycle is also a SI data, the ResultLog is a kind of 4D data, and its size may become very large. Thus, the result at each specified cycle is saves as an individual SI data in the folder specified in "Display" tab.
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.
*There are two choices to test convergence criteria:
Individual Spectrum: The iteration will stop, when more than the specified percentage of individual spectrum satisfy the criteria.
Whole Spectrum: The iteration will stop, when the SI data as a whole satisfies the criteria.
Smoothing Width (Full width at 1/e): When selected, the raw data will be smoothed out by convoluting a Gaussian with a specified half-width (in pixels).
Convergence Factor: This controls a speed of convergence.
Convergence: There is a selection of convergence between Strong and Weak. The default setting is Strong.
*The convergence mode will be applied to *individual spectrum* or *the whole spectrum*.

TIPS It is highly recommended to process a single spectrum from the SI data, and find good processing conditions, before processing the whole SI data. Then, the same processing conditions will be transferred to the SI Deconvolution routine.

2.2.2 Options tab-panel

The next tab-panel is designed for specifying some optional controls for deconvolution processing. This control tab is identical to the one for DeConvEELS.

Figure 2-3 Maximum Entropy Deconvolution (Options Tab)

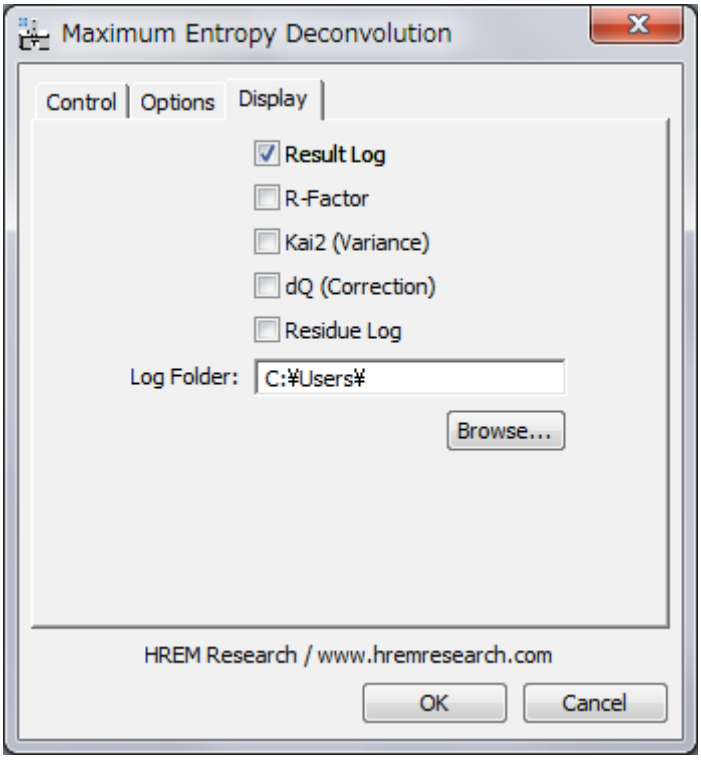


Check R-Factor: When selected, the iteration will stop when R-Factor becomes smaller than the value specified here. It is not recommended to activate this criterion, when you don't know an approximate noise level.
Check dQ: When checked, the iteration will stop when the difference of Q value starts oscillating.
Interest Area: You can specify an interest area (ROI; a region of interest) of your spectrum. This is useful for deconvolution of a low-loss area, since convergence testing will not be affected by the dominant zero-loss area.
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.

2.2.3 Display tab-panel

The last 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 with a name ResultLogxxxx.dm3, where xxxx is a cycle number.
R-Factor: History of R-factor.
χ^2 (Variance): History of squared sum of differences.
dQ (Correction): History of sum of absolute corrections.
Residue Log: All the intermediate residues specified by "Save Results at" will be saved with a name ResidueLogxxxx.dm3, where xxxx is a cycle number.
Log Folder: The result at specified cycle is saves as an individual SI data in the folder specified here. You can choose a folder or create a new folder by browsing the directory tree using "Browse" button.

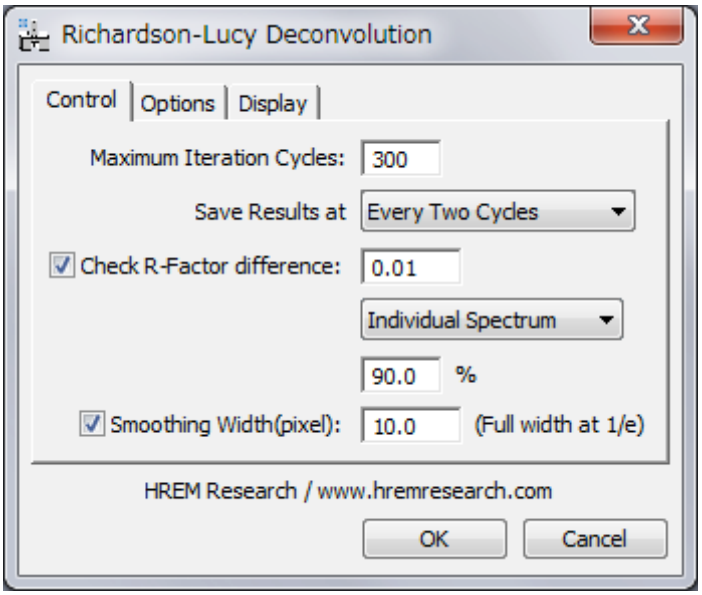
2.3 Richardson-Lucy Setup

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 general controls for deconvolution processing.

Figure 2-5 Richardson-Lucy Deconvolution (Control Tab)



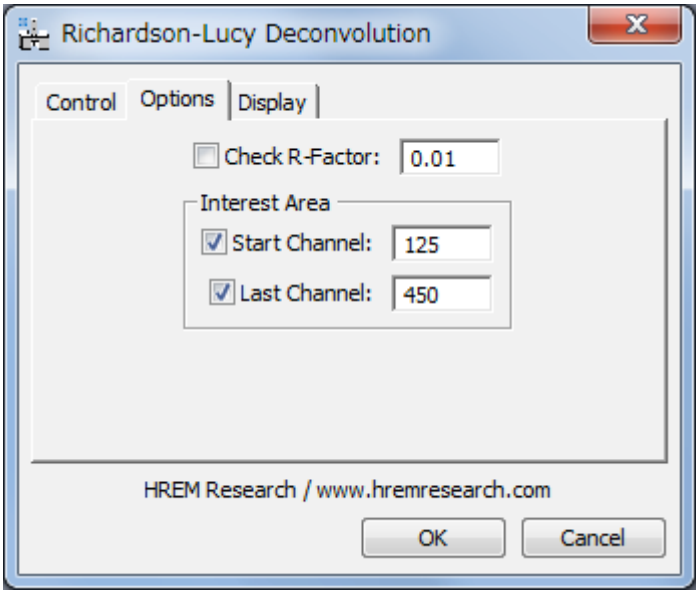
Maximum Iteration Cycles: Maximum number of iteration cycles.
Save Results at: This controls a frequency of saving the results during the progress of deconvolution. Since the result at each cycle is also a SI data, the ResultLog is a kind of 4D data, and its size may become very large. Thus, the result at each specified cycle is saves as an individual SI data in the folder specified in "Display" tab.
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.
There are two choices to test convergence criteria:
Individual Spectrum: The iteration will stop, when more than the specified percentage of individual spectrum satisfy the criteria.
Whole Spectrum: The iteration will stop, when the SI data as a whole satisfies the criteria.
Smoothing Width (Full width at 1/e): When selected, the raw data will be smoothed out by convoluting a Gaussian with a specified half-width (in pixels).

TIPS It is highly recommended to process a single spectrum from the SI data, and find good processing conditions, before processing the whole SI data. Then, the same processing conditions will be transferred to the SI Deconvolution routine.

2.3.2 Options tab-panel

The next tab-panel is designed for specifying some optional controls for deconvolution processing. This control tab is identical to the one for DeConvEELS.

Figure 2-6 Richardson-Lucy Deconvolution (Option Tab)

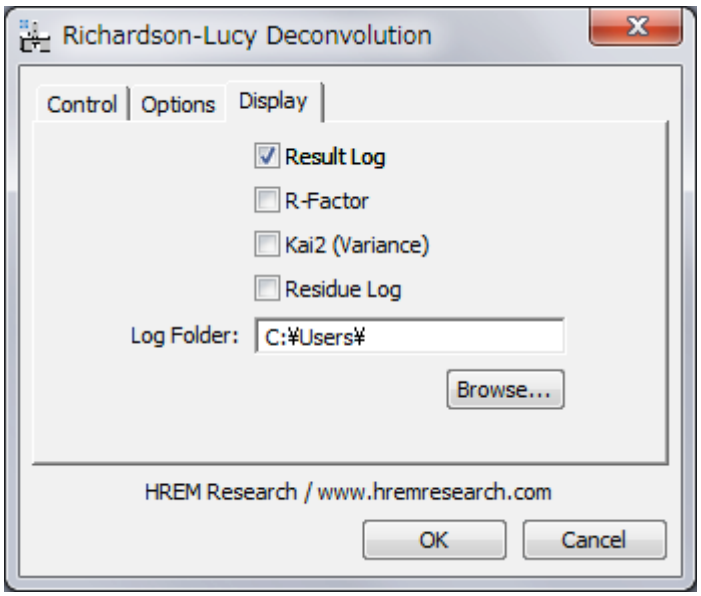


Check R-Factor: When selected, the iteration will stop when R-Factor becomes smaller than the value specified here. It is not recommended to activate this criterion, when you don't know an approximate noise level.
Interest Area: You can specify an interest area (ROI; a region of interest) of your spectrum. This is useful for deconvolution of a low-loss area, since convergence testing will not be affected by the dominant zero-loss area.

2.3.3 Display tab-panel

The last 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 specified by "Save Results at" will be saved with a name ResultLogxxxx.dm3, where xxxx is a cycle number.
R-Factor: History of R-factor.
χ^2 (Variance): History of squared sum of differences.
Residue Log: All the intermediate residues specified by "Save Results at" will be saved with a name ResidueLogxxxx.dm3, where xxxx is a cycle number.
Log Folder: The result at specified cycle is saves as an individual SI data in the folder specified here. You can choose a folder or create a new folder by browsing the directory tree using "Browse" button.

3. Installation

This chapter describes hardware and software requirements to run the SI Module for DeConvEELS software and an installation procedure.

3.1 Requirements

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

3.1.1 Hardware requirement

Since the SI Module for DeConvEELS handles a Spectrum Image (SI) dada, it requires an enough memory to store the SI data itself and its deconvoluted result. It is recommended to use a PC with a multi-CPU (Core), since SI processing is number crunching.

3.1.2 Software requirement

The SI Module for DeConvEELS requires DeConvEELS:

3.2 Software Installation

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

- **DeConvEELS_SI.gtk**
- **DeConvEELS_SI.dll**

Menu commands for SI processing will be appeared below DeConvEELS, when the DigitalMicrograph is launched after placing the plug-ins the PlugIns folder.

4. Getting Started…

This chapter briefly explains typical steps of Spectrum Image (SI) deconvolution. Before doing this section, you have to install the SI Modules for DeConvEELS.

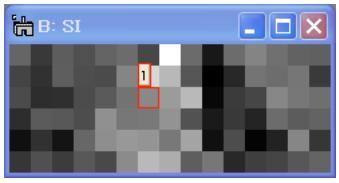
4.1 Deconvolution

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

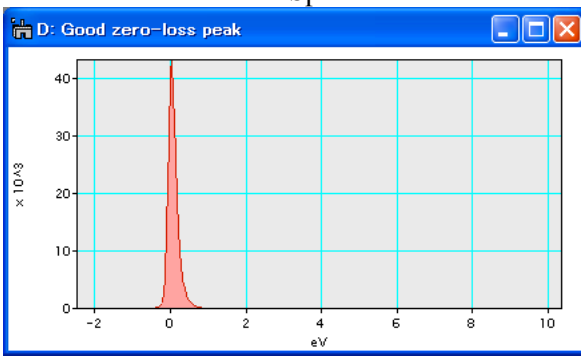
4.1.1 Open Spectrum

The deconvolution routine will work on open images. Therefore, you must open an SI data to be restored and a low-loss spectrum as a kernel function.

SI Data

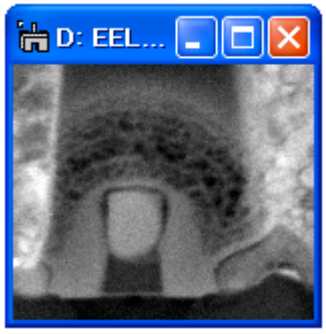


Low-loss Spectrum

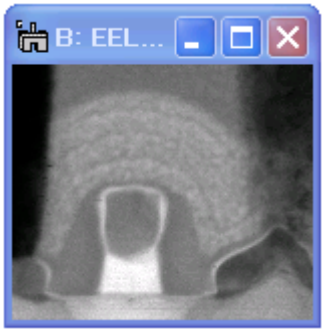


You can also process an opened DualEELS data pair as shown below:

High-loss (Core-loss) SI data



Low-loss (Core-loss) SI data



4.1.2 Establish Deconvolution Conditions

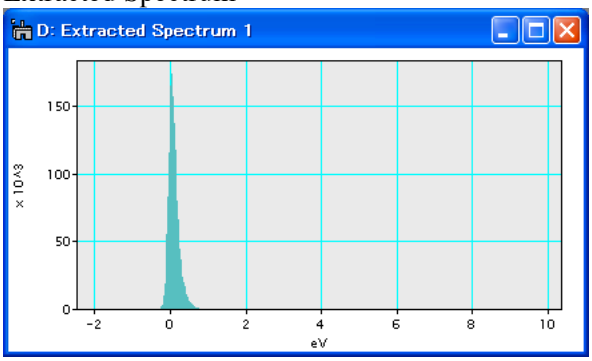
Before doing deconvolution of the whole SI data/DualEELS data, it is recommended to establish deconvolution conditions using a single spectrum. Then, the same conditions will be transferred to the SI Deconvolution routine.

SI Data

A spectrum to be processed can be extracted from the SI data by using "Spectrum Picker Tool."

A single spectrum to be processed can also be extracted from the SI data by using the HREM mouse tool and then using "Get Single Spectrum" of Utility Command.

Extracted Spectrum



This extracted spectrum can be processed with the low-loss spectrum with DeConvEELS to establish the deconvolution conditions.

DualEELS Data

A pair of high-loss and low-loss spectrum to be processed can be extracted from the DualEELS data by using "Spectrum Picker Tool" and then using "Mirror Extract ROI(s)" command of the EELS plug-in.

A pair of high-loss and low-loss spectrum to be processed can also be extracted from the DualEELS data by using the HREM mouse tool and then using "Get Single Spectrum" of Utility Command.

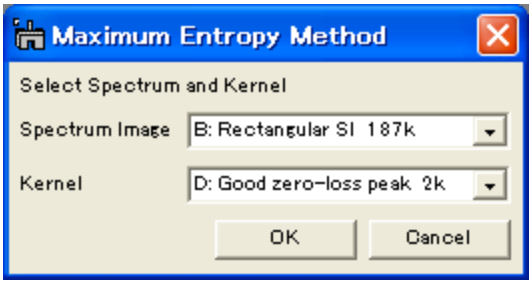
A pair of extracted high-loss and low-loss spectrum can be processed with DeConvEELS to establish the deconvolution conditions.

4.1.3 Launch SI Deconvolution

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

4.1.4 Select Spectrum

Select Spectrum and Kernel from the image list, and click OK to continue processing, or click Cancel to stop the procedure.



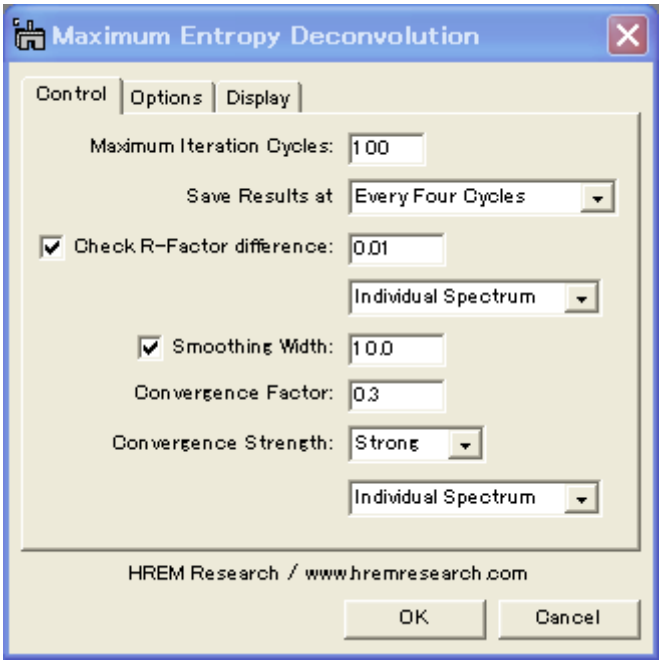
4.1.5 Setup Deconvolution Parameters

You can setup Deconvolution parameters using the dialog below. However, it is advisable to establish the deconvolution conditions based on a single spectrum by using DeConvEELS routine.

4.1.5.1 Control Tab

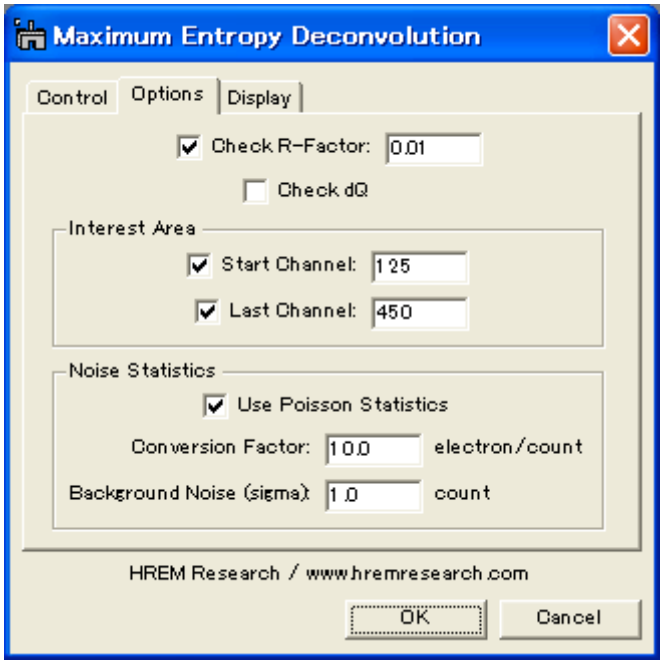
There are two additional parameters specific to the SI deconvolution. Namely, Convergence crireria and the "Convergence Strength" can be applied to each spectrum or the SI data as a whole.

Since the size of result of the SI deconvolution is large, you can change the cycle to save the Results. However, if you want, you can save all the intermediate Results, since the Result will be saved on the hard disk.



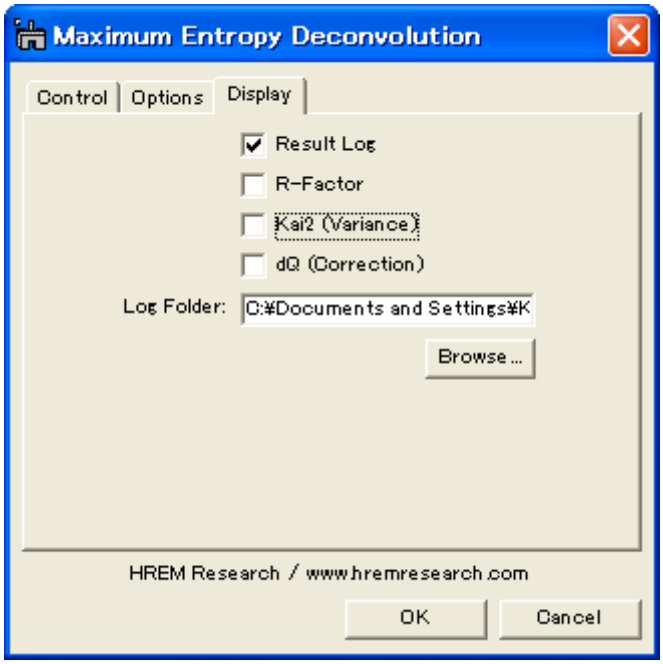
4.1.5.2 Options Tab

There is no additional parameter specific to the SI deconvolution.



4.1.5.3 Display Tab

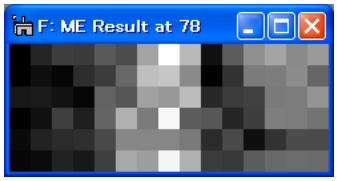
There is one additional parameter specific to the SI deconvolution. You can choose a folder or create a new folder to save the ResultLog(s).



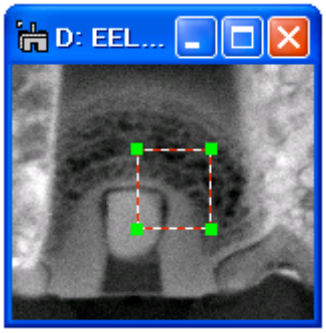
4.1.6 Start Deconvolution

After setting conditions, you can start deconvolution by clicking OK button, or stop the procedure by clicking Cancel button at the bottom of the setup dialog.

The result of restored spectrum will be displayed at each cycle as shown below. Since the result is also an SI image, namely a 3D image, the intermediate results at specified cycles will be saved in the selected folder, if you select "Result Log" check box in the setup dialog.



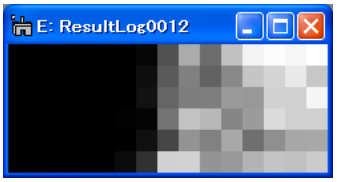
TIPS You can use a ROI as show below to select the points to be processed.



4.1.7 Survey Results

The final result is displayed in the restored spectrum 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, then, you can open one of the ResultLog file, and survey it as a regular SI data.

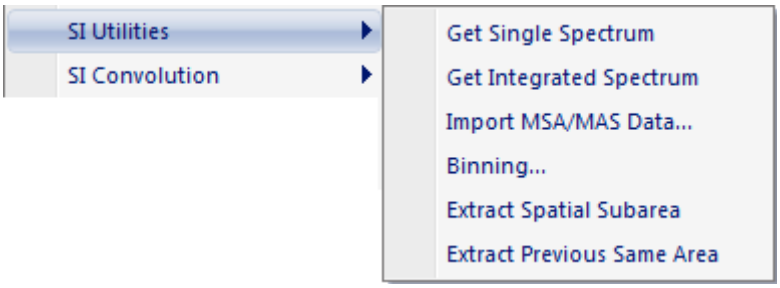


4.2 Utilities

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

4.2.1 Utilities Menu

The following shows the ”Utilities” sub-menu.



4.2.2 Get Single Spectrum

Using this command you can extract a single spectrum from a SI data, or a pair of single high-loss and low-loss spectrum from the DualEELS data at the point selected with the HREM mouse tool.

If you select more than one point, a set of spectrum will be extracted from the points selected with the HREM mouse tool. The extracted spectra will be discriminated by the serial number after the data name.

4.2.3 Get Integrated Spectrum

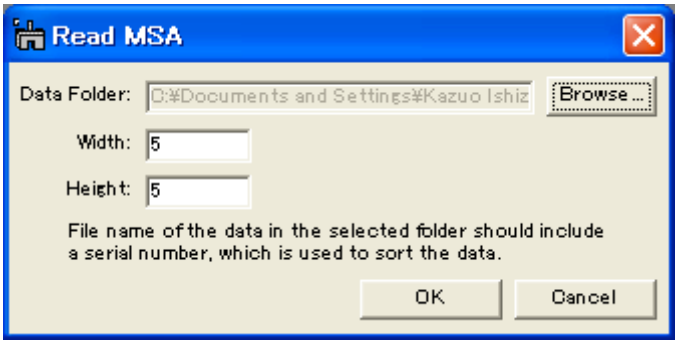
Using this command you can integrate spectra within the area defined by a ROI into a single spectrum. In the case of DualEELS data you can integrate spectra within the same area of high-loss and low-loss spectrum into a pair of the spectra, respectively.

Here, the integrated area for a line-scan data is defined by the top and bottom of a Line ROI or a Rectangular ROI. In the case of 2D scan data the integrated area is obviously inside of a Rectangular ROI.

4.2.4 Import MSA/MAS Data…

Using this command you can convert a set of MSA/MAS data to an SI data, which can be processed with the SI Module for DeConvEELS.

When you select this command, the following dialog will open:

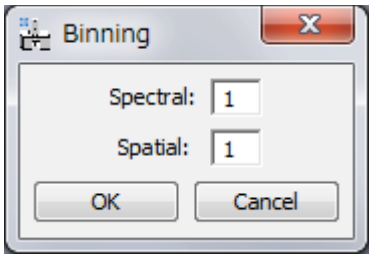


Here, you can select the folder that stores a set of MSA/MAS data, and the numbers of columns (width) and rows (height) of the data. Please note that all the spectra in the folder will be read, and thus the number of spectra in the folder should be equal to (width) x (height). Furthermore, the file names should include a serial number that is used to sort the data.

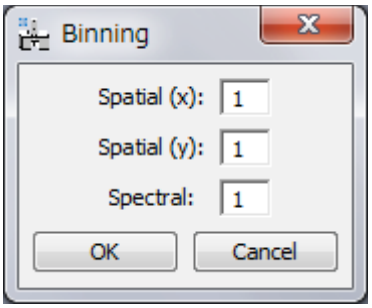
The serial number may be a set of figures, or two sets of figures separated by non-number character(s). In the latter case, the two sets of figures may correspond to the column and row numbers. The possible file name will be: sample9999, sample_9999, sample999_999, sample_999_999, column999row999, column999_row999, where "9" indicates a figure (digit), and you can use any non-number character(s) for a separator.

4.2.5 Binning…

Using this command you can bin an SI data spectrally and spatially. In the case of a DualEELS data both high-loss and low-loss spectrum data will be binned in the same way.



Line-scan data



2D scan data

4.2.6 Extract Spatial Subarea

Using this command you can extract a spatial subarea defined by a ROI. In the case of DualEELS data a pair of spatial subareas will be extracted from high-loss and low-loss spectrum, respectively.

Here, for a line-scan data the spatial subarea is defined by the top and bottom of a Line ROI or a Rectangular ROI. In the case of 2D scan data the spatial subarea is obviously inside of a Rectangular ROI.

4.2.7 Extract Previous Same Area

Using this command you can extract the same spatial subarea defined by previous Extract Spatial Subarea command.

This command will be especially useful for Spatially Resolved (SR) EELS, where a set of high-loss and low-loss spectrum data is acquired from a narrow sample area perpendicular to the energy dispersion. Thus, a SR EELS spectrum is similar to a line-scan SI data.

4.3 Convolution

Two convolution routines are provided for your convenience.

4.3.1 Convolution Menu

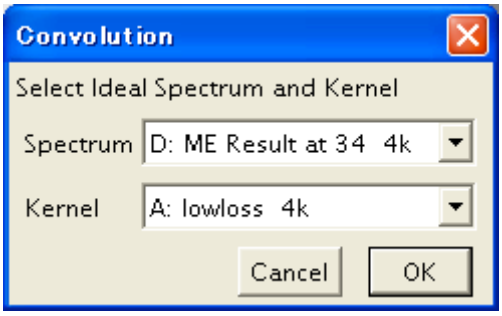
The following shows the ”Convolution” sub-menu.

4.3.2 Kernel

You may check your result by convoluting the restored spectrum and the kernel function (low-loss spectrum) with the same way as used for DeConvEELS. The convolution should be close to the observed spectrum for a good deconvolution.

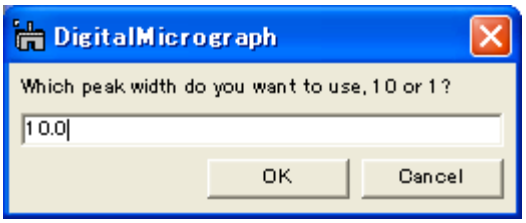
When you want to get a convolution for a final result or an intermediate result (ResultLog), just select these SI data, and next choose this command. Then, a result of convolution will be displayed. This is because the final result keeps information of the Kernel function.

When you want to get a convolution for other than the final or intermediate result, you have to specify a kernel image. In this case, the following windows to select images will appear, when you select the “Convolution” -> “Kernel” command. You have to open the images to be convoluted beforehand.



4.3.3 Smoothing Gaussian

Using this command you can check a smoothed spectrum 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.



4.4 Check Residue

You can check residue for a result of deconvolution with the same way as used for DeConvEELS. The residue should be a random noise for a good deconvolution.

When you want to check a residue for a final result or an intermediate result (ResultLog), just select these SI data, and next choose this command. Then, a residue will be displayed. This is because the final result keeps information of the original observed spectrum and the Kernel function.

5. Tips and Troubleshooting