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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 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.

1.2 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 using a custom-made setup dialogs.

NOTE A kernel may be a single spectrum or a SI data (DualEELS SI data). If the kernel is a single spectrum, the same kernel will be used for all the spectrum of the SI data.

Technical Support

General enquiries on the HREM-Filters should be sent to:

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Web: www.hremresearch.com

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2. Installation

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

2.1 Requirements

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

2.1.1 Hardware requirement

Since the SI Module for DeConvEELS handles a Spectrum Image (SI) data, 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.

2.1.2 Software requirement

The SI Module for DeConvEELS requires DeConvEELS plug-in.

2.2 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.

3. 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.

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

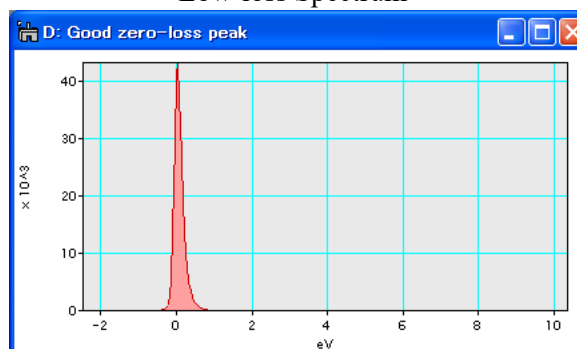
3.1 Open Spectrum

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.

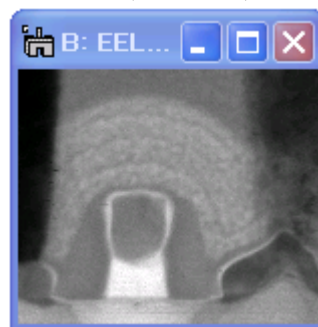
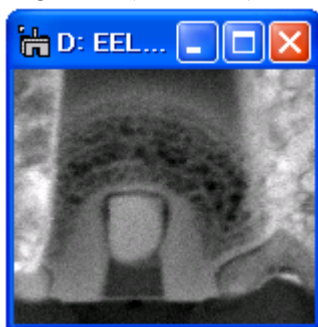
SI Data



Low-loss Spectrum



You can also process an opened DualEELS data pair as shown below:
High-loss (Core-loss) SI data Low-loss (Zero-loss) SI data



3.2 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

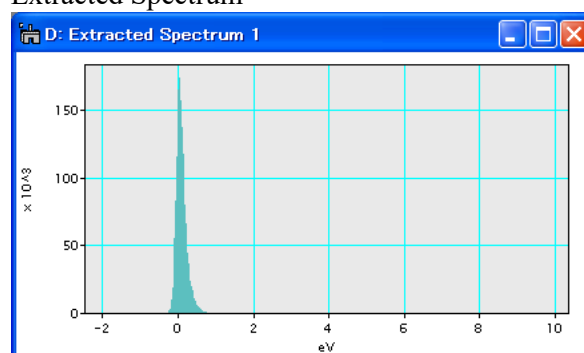


A spectrum to be processed can be extracted from the SI data by using “Spectrum Picker Tool.”



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.

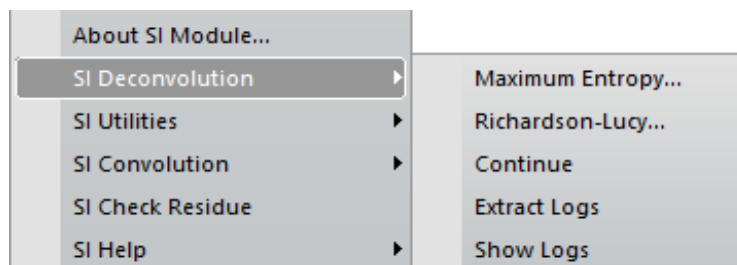


A pair of high-loss and low-loss spectrum to be processed can also be extracted from the DualEELS data by using the HREM mouse tool and then using “Get Single Spectrum” of Utility Command.

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

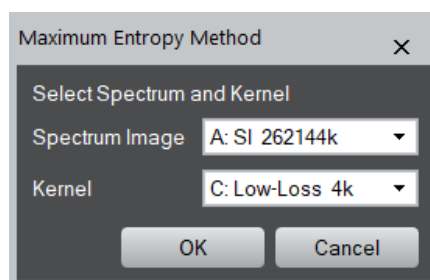
3.3 Launch SI Deconvolution

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



Select Spectrum

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



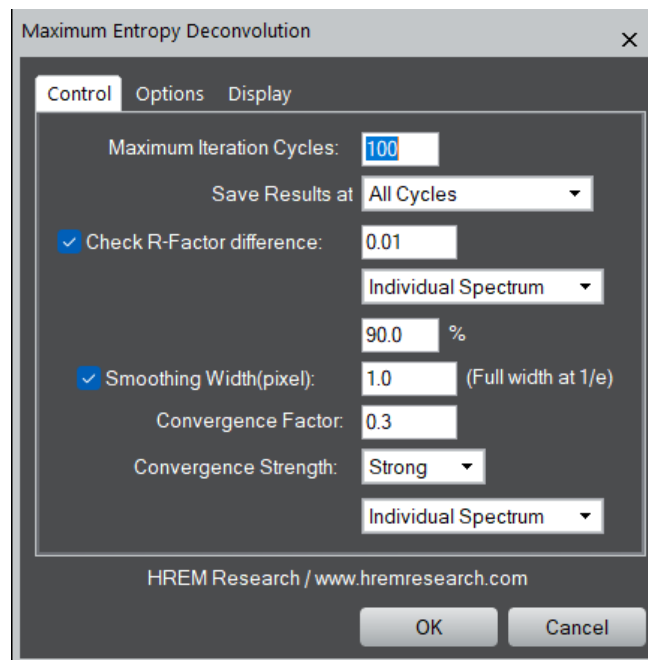
3.4 Setup Deconvolution Parameters

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.

3.4.1 Control Tab

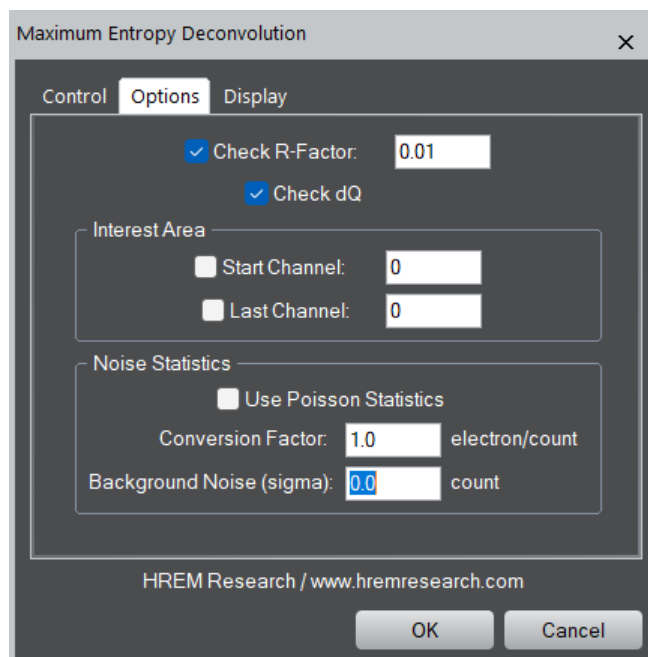
There are two additional parameters specific to the SI deconvolution. Namely, Convergence criteria and the “Convergence Strength” can be applied to each spectrum or the SI data as a whole.

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 external storage specified in Display tab.



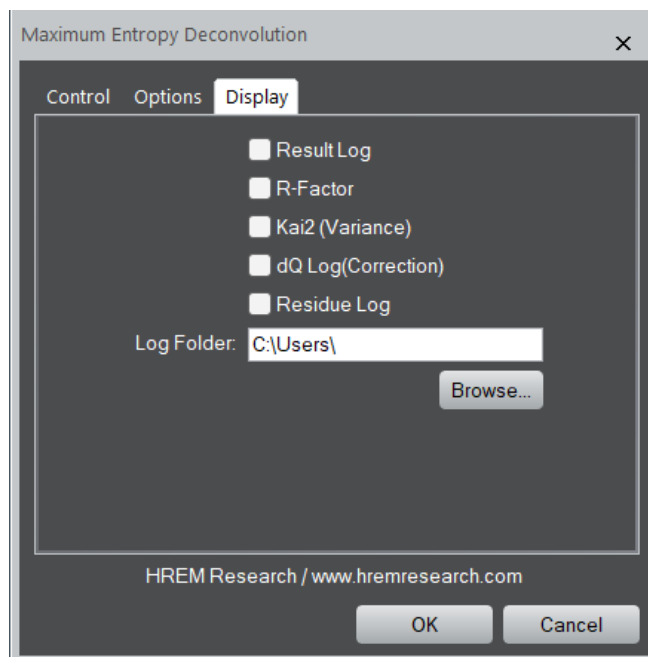
3.4.2 Options Tab

There is no additional parameter specific to the SI deconvolution in addition to DeConvEELS.



3.4.3 Display Tab

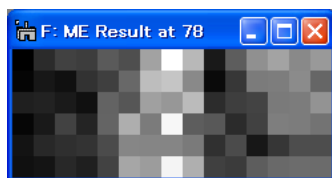
There is one additional parameter specific to the SI deconvolution. You can choose a folder or create a new folder to save the Result Log and other logs.



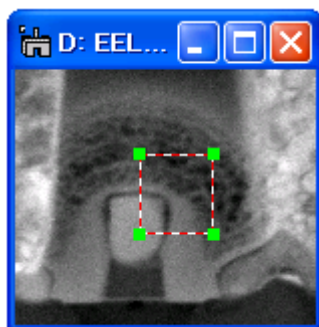
3.5 Start Deconvolution

After setting up the 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 display tab of the setup dialog.



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



3.6 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.

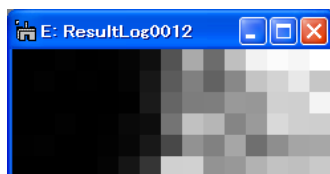
The intermediate results of deconvolution of the whole SI data are saved as Result Log at specified cycles, when "Result Log" box is checked in the display tab of the setup dialog. However, it is not easy to monitor the progress of deconvolution at a specific point.

3.6.1 Check progress of Deconvolution at a specific point

When the intermediate results of deconvolution are saved as Result Log, you can easily check the progress of deconvolution at selected point(s) using Extract Log command (see 4.1.4). The output is equivalent to the ResultLog obtained with DeConvEELS for a selected single spectrum. In the same way, you can display ResidueLog of a selected single spectrum.

3.6.2 Inspect intermediate Results

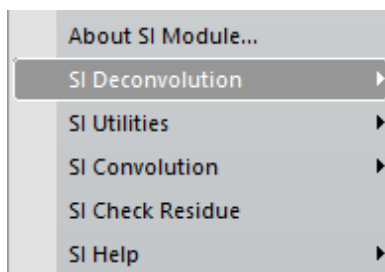
If "Result Log" check box is selected in the display tab of the setup dialog, you can open one of the intermediate results using Windows' explorer (see Show Log command on 4.1.5). Then, you can inspect it as a regular SI data.



4. Command Reference

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

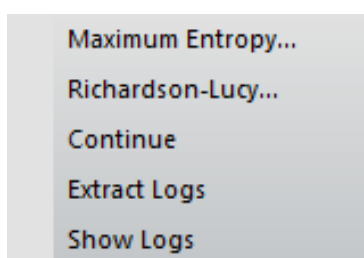
SI Module commands beneath DeConvEELS commands



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.

4.1 Deconvolution

Deconvolution sub-menu 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. When the command is launched with the ALT-key down, you can bypass these setup dialogs and use previous setup parameters.

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.

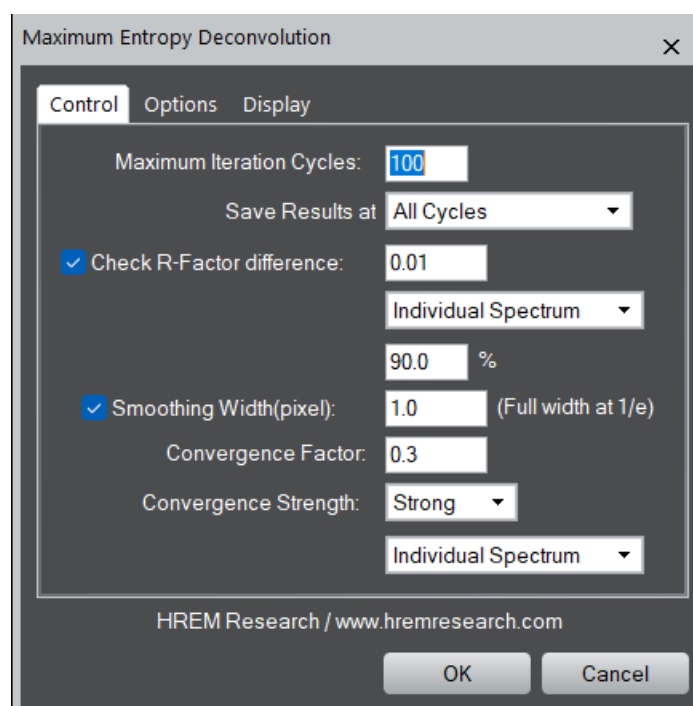
4.1.1 Maximum Entropy

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

Control tab-panel

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

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

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.

Maximum Entropy Deconvolution (Options Tab)

The screenshot shows a software window titled "Maximum Entropy Deconvolution" with a close button (X) in the top right corner. Inside the window, there are three tabs: "Control", "Options" (which is selected), and "Display". The "Options" tab contains several settings:

- ☒ Check R-Factor: 0.01
- ☒ Check dQ
- Interest Area**
 - ☐ Start Channel: 0
 - ☐ Last Channel: 0
- Noise Statistics**
 - ☐ Use Poisson Statistics
 - Conversion Factor: 1.0 electron/count
 - Background Noise (sigma): 0.0 count

At the bottom of the window, there is a text label "HREM Research / www.hremresearch.com" and two buttons: "OK" and "Cancel".

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:-This is useful for deconvolution of a low-loss area, since convergence testing will not be affected by the dominant zero-loss area. When a selected single spectrum has been deconvoluted in advance to test the deconvolution parameters, the same interest area will be shown in the dialog.

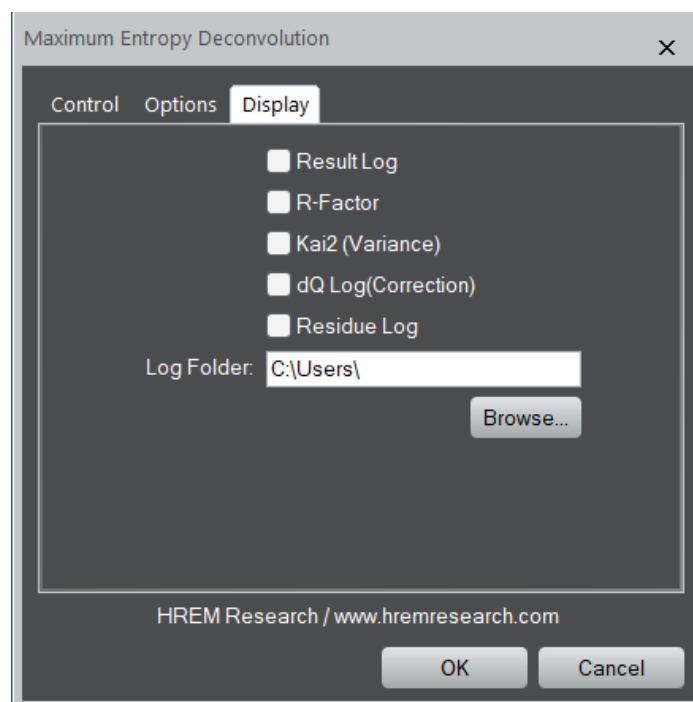
Noise Statistics: You can explicitly use Poisson Statistics for noise distribution. In this case you have to specify **Conversion Factor** in order to convert a signal count to a number of electrons. You can specify also a constant **Background Noise (Gaussian)** such as a read-out noise.

Display tab-panel

In the case of SI deconvolution, contrary to a single spectrum deconvolution, it is not practical to save intermediate results to the final deconvoluted spectrum. Therefore, Result Log and other logs will be saved to an external storage, while R-factor and Kai2 will be stored in the final deconvoluted spectrum. Thus, the selection of the display tab determines the items to be saved in the final spectrum or an external storage.

When R-factor and Kai2 are selected in the display tab, they will be displayed at the end of processing. However, Result Log and other logs will not be displayed, even when they are selected in the display tab. Nevertheless, these logs can be checked later at any time using Extract Log command (see 4.1.4) or Sow Log command (see 4.1.5).

Maximum Entropy Deconvolution (Display Tab)



Result Log: The intermediate result will be saved at the cycle specified by “Save Results at” with a name ResultLogxxxx, where xxxx is a cycle number.

R-Factor: History of R-factor.

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

dQ Log (Correction): The intermediate sum of absolute corrections will be saved at the cycle specified by “Save Results at” with a name dQLogxxxx, where xxxx is a cycle number.

Residue Log: The intermediate residue will be saved at the cycle specified by “Save Results at” with a name ResidueLogxxxx, where xxxx is a cycle number.

Log Folder: The result at specified cycle is saved 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.

NOTE R-Factor and Kai2 has the same dimensions as the original SI data, where the direction of spectrum is replaced by the cycle of iterations. Thus, the R-factor and Kai2 will be stored within the final restored SI data, and displayed at the end of processing.

On the other hand, each intermediate result obtained during deconvolution has the same size of the original SI data. Therefore, the Result Log and other logs will be saved into an external storage, and they are not displayed at the end of processing. However, they can be checked using Extract Log command (see 4.1.4) or inspected using Sow Log command (see 4.1.5) at any time later.

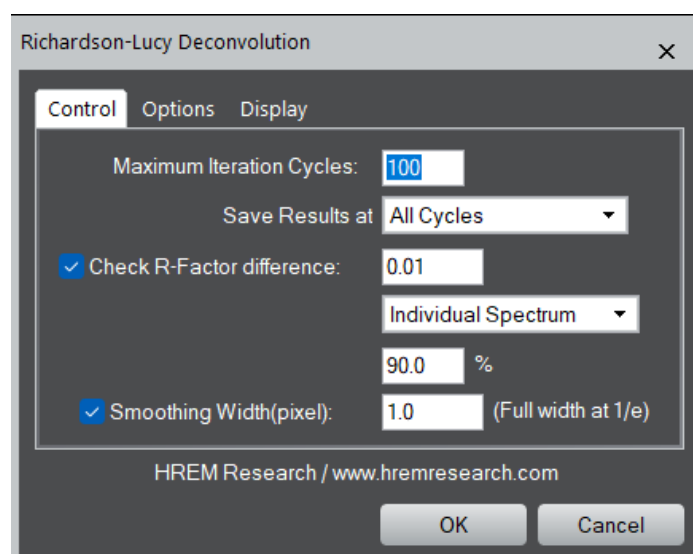
4.1.2 Richardson-Lucy

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

Control tab-panel

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

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 saved 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.

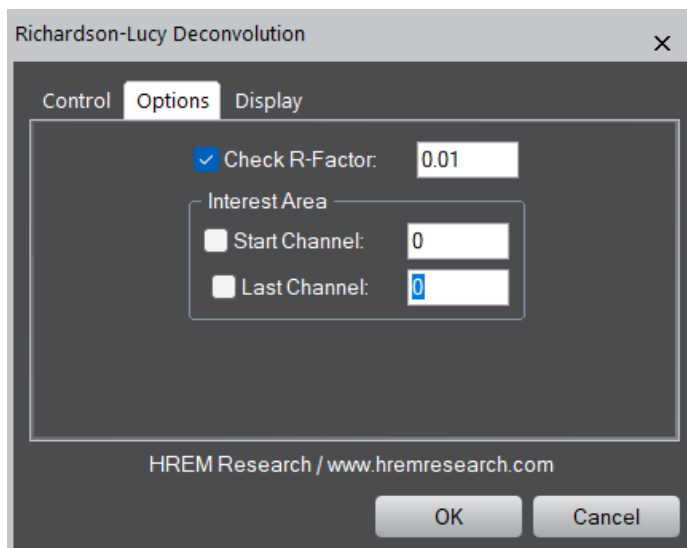
Smoothing Width (Full width at 1/e): When selected, the raw data will be smoothed out by convoluting a Gaussian with a specified half-width (in pixels).

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.

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.

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.

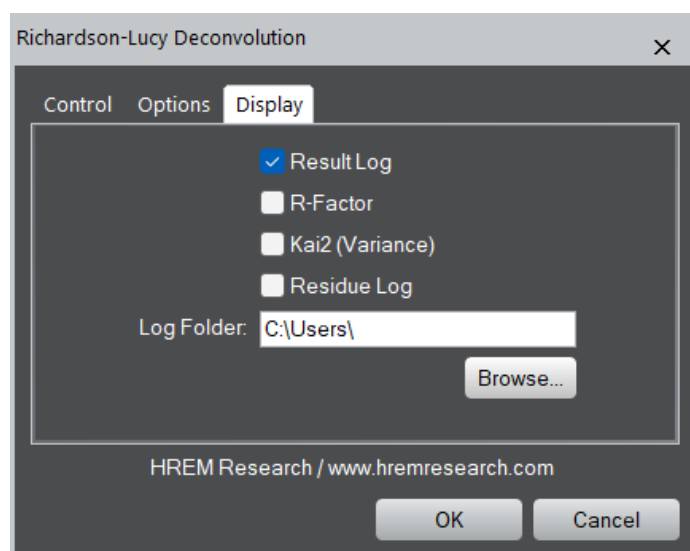
Interest Area: You can define a region of interest (ROI) within the spectrum by holding down and dragging the mouse. This is useful for deconvolution of a low-loss area, since convergence testing will not be affected by the dominant zero-loss area.

Display tab-panel

In the case of SI deconvolution, contrary to a single spectrum deconvolution, it is not practical to save intermediate results to the final deconvoluted spectrum. Therefore, Result Log and Residue Log will be saved to an external storage, while R-factor and Kai2 will be stored in the final deconvoluted spectrum. Thus, the selection of the display tab determines the items to be saved in the final spectrum or an external storage.

When R-factor and Kai2 are selected in the display tab, they will be displayed at the end of processing. However, Result Log and Residue Log will not be displayed, even when they are selected in the display tab. Nevertheless, these logs can be checked later at any time using Extract Log command (see 4.1.4) or Sow Log command (see 4.1.5).

Richardson-Lucy Deconvolution (Display Tab)



Result Log: The intermediate result will be saved at the cycle specified by “Save Results at” with a name ResultLogxxxx, where xxxx is a cycle number.

R-Factor: History of R-factor.

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

Residue Log: The intermediate residue will be saved at the cycle specified by “Save Results at” with a name ResidueLogxxxx, where xxxx is a cycle number.

Log Folder: The result at specified cycle is saved 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.

NOTE R-Factor and Kai2 has the same dimensions as the original SI data, where the direction of spectrum is replaced by the cycle of iterations. Thus, the R-factor and Kai2 will be stored within the final restored SI data, and displayed at the end of processing.

On the other hand, each intermediate result obtained during deconvolution has

the same size of the original SI data. Therefore, the Result Log and Residue Log will be saved into an external storage, and they not displayed at the end of processing. However, they can be checked using Extract Log command (see 4.1.4) or inspected using Show Log command (see 4.1.5) at any time later.

4.1.3 Continue

This command resumes the deconvolution iteration that has been terminated by convergence criteria or Maximum Iteration Cycles.

Execute this command after the deconvoluted spectrum is set to front-most. Settings other than the convergence criteria and the maximum iteration cycle will be inherited from the previous settings for deconvolution.

Control and Option Tabs

Settings inherited from the previous settings for deconvolution will be grayed-out in the Control and Option tabs.

Maximum Iteration cycles is not the total number of iterations, but the maximum number of additional iterations. Thus, any number of additional iterations can be specified for Maximum Iteration cycles.

Contrary, when the deconvolution iteration has stopped due to one of the convergence criteria, its condition should be made stronger than before in order to continue deconvolution processing.

Display Tabs

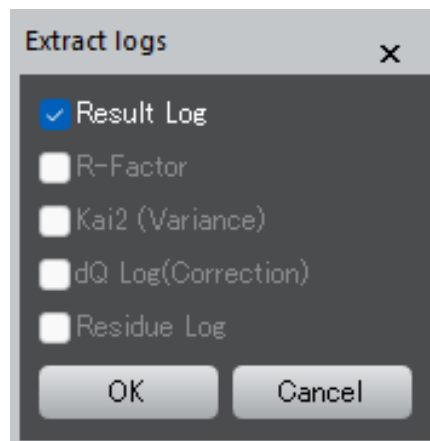
If the selected data has been saved at the previous deconvolution iteration, the result will be concatenated to the previous one. If not, the obtained result during the continued deconvolution will be newly saved.

The data saved in the deconvoluted spectrum can be checked or displayed later at any time using Extract Log or Show Log command.

4.1.4 Extract Log

R-factor and/or Kai2 will be stored in the deconvoluted spectrum, and Result Log and other logs will be saved into an external storage. Therefore, you can display them at any time you want using this command.

After placing one or more Point ROI(s) on the final restored spectrum, launch this command. Then, the dialog shown below will be opened, where the grayed-out item corresponds to the output data that is not saved.

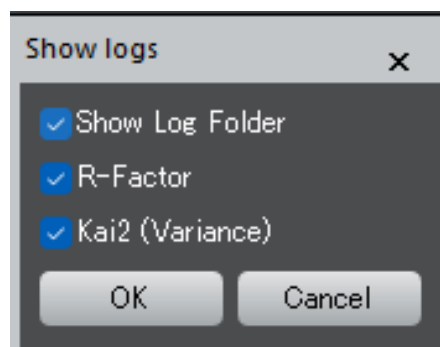


When clicking **OK**, the extracted data at the specified point(s) will appear in a minute.

4.1.5 Show Log

Using this command, you can open the data that is stored within the final restored SI or saved into an external storage. Then, you can process these data as you want.

After placing the final restored SI to the front-most, launch this command. Then the dialog shown below will open.



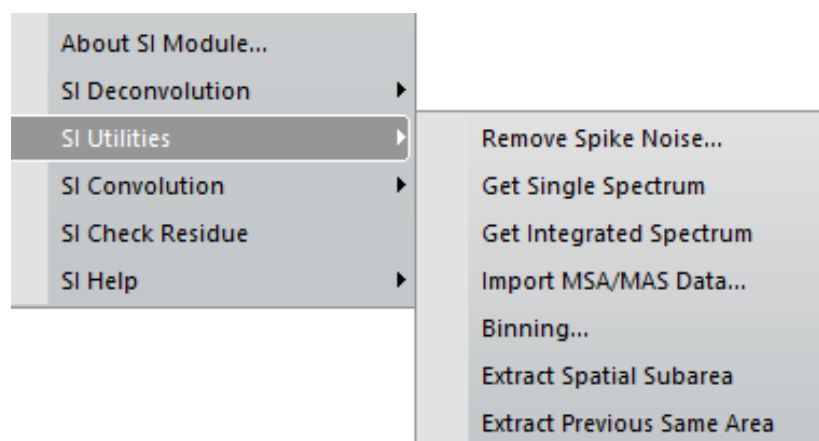
When you select **Show Log Folder**, Windows Explorer will open the sub-folder that has saved all the logs corresponding to the selected restored SI. Then, you can drag-and-drop a file to DigitalMicrograph workspace.

On the other hand, when **R-Factor** and **Kai2** are selected, they will be simply open in DigitalMicrograph workspace, since they are stored in the selected restored SI.

4.2 Utilities

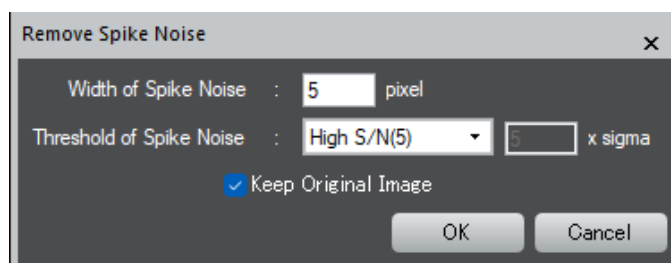
Some useful commands to pre-process or post-process a spectrum are provided for your convenience.

Utilities Sub-menu Commands



4.2.1 Remove Spike Noise

Using this command, you can remove a spike noise(s) from a SI data. A spike noise is defined as the data point that shows an abnormal value. Such a point is created, for example, by cosmic rays. The dialog below appears to set processing parameters.



The spike noise is searched within a specified range of pixels (Width of Spike Noise). The data point that exceeds the specified noise level (Threshold of Spike Noise) is recognized as the spike noise, and replace by the local average.

The number of the removed spike noise will be shown in the dialog, and displayed in the Results (Output) window.

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 spectra 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

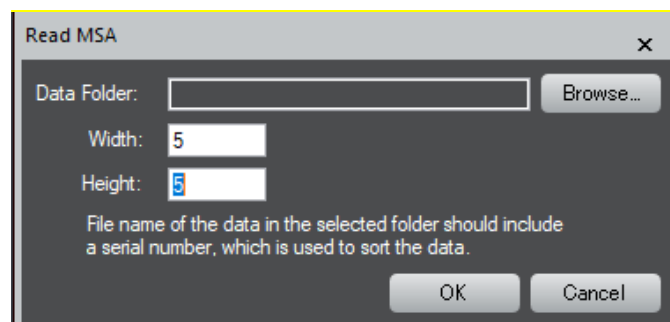
Using this command, you can integrate spectra within the area defined by a ROI into a single spectrum. In the case of DualEELS data you can integrate spectra within the same area of high-loss and low-loss spectrum into a pair of the spectra, respectively.

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:

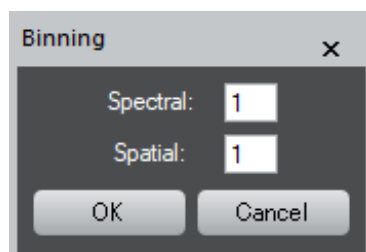


Here, you can select the folder that stores a set of MSA/MAS data, and the numbers of columns (width) and rows (height) of the data. Please note that all the spectra in the folder will be read, and thus the number of spectra in the folder should be equal to (width) x (height). Furthermore, the file names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

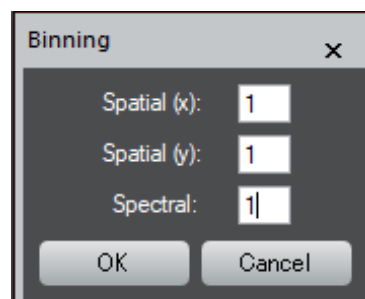
The serial number may be a set of figures, or two sets of figures separated by non-number character(s). In the latter case, the two sets of figures may correspond to the column and row numbers. The possible file name will be: sample9999, sample_9999, sample999_999, sample_999_999, column999row999, column999_row999, 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.

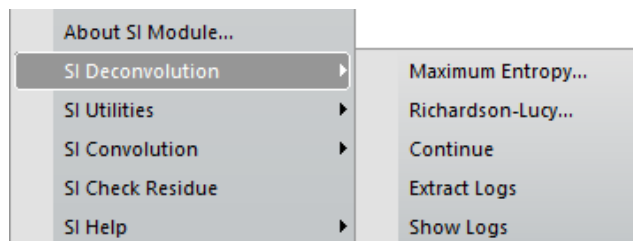
4.2.7 Extract Previous Same Area

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

Convolution Sub-menu Commands



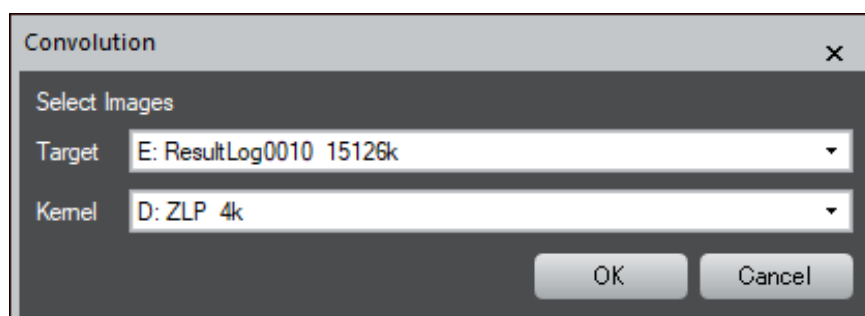
Two convolution routines are provided for your convenience.

4.3.1 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 of the final restored spectrum with the kernel, firstly select these SI data, and next choose this command. Then, a result of convolution will be displayed, since the final result keeps information of the Kernel function.

When the front image is an intermediate result opened from ResultLog, the dialog below will appear by choosing this command. Here, you can select the kernel to be convoluted.

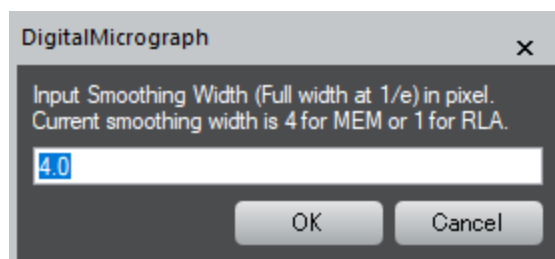


When clicking OK, a convoluted spectrum will appear in a minute.

4.3.2 Smoothing Gaussian

Using this command, you can check a smoothed spectrum that will be used at deconvolution when you choose the Gaussian smoothing.

To get a smoothed spectrum, firstly select a spectrum to be smoothed, and next select this command. Then, the dialog below will appear, where the smoothing width (full-width at 1/e of the Gaussian) can be specified.



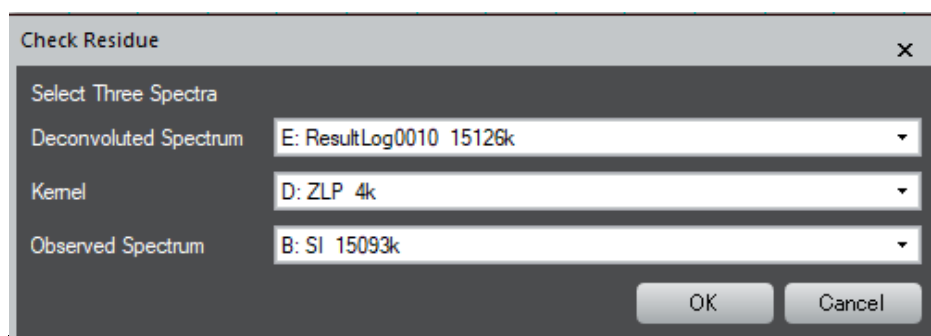
In the dialog, the Gaussian smoothing widths specified for MEM and RLA are shown for your reference.

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. You can manually calculate the residue by subtracting the result obtained by the previous Convolution command from the observed spectrum. However, this is a handy command to calculate the residue.

If you want to get a residue for a final restored spectrum, firstly select the spectrum and choose this command. Then, a residue will be displayed, since the restored spectrum keeps the original observed spectrum and the Kernel function.

When the front image is an intermediate result saved as ResultLog, the dialog below will appear by choosing this command. Here, you can select a kernel and an observed spectrum.



When clicking OK, a residue spectrum will appear in a minute.

5. Tips and Troubleshooting

5.1 Improving SI EELS data with MSA

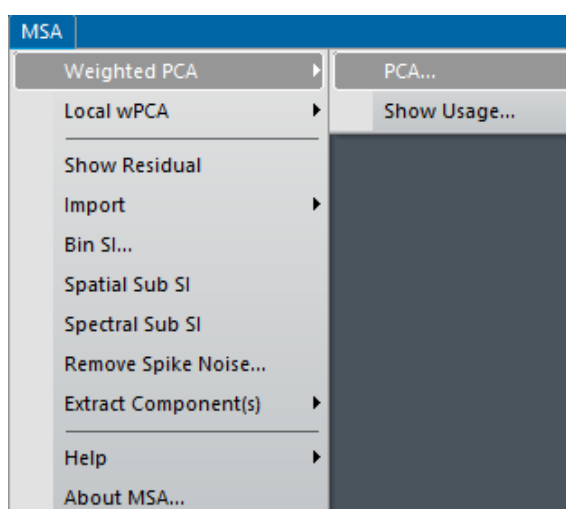
5.1.1 Introduction

The multivariate statistical analysis (MSA) performs principal component analysis (PCA) to 2D or 3D spectrum image (SI) of such as EDX and EELS. This is a very powerful technique to improve the signal to noise ratio in SI data. In PCA the SI data is decomposed into linearly independent components. We select small number of the principal components, and distinguish them from other large number of components that we regard as noise. When we reconstruct the data using the selected small number of the components, the noise is reduced substantially.

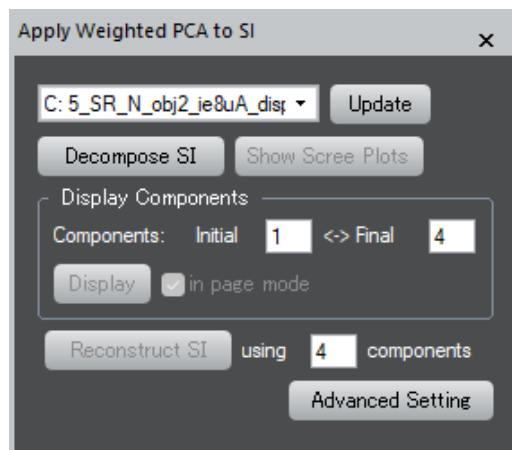
MSA is released from HREM research Inc. as a plug-in of DigitalMicrograph. Please, consult the user's guide of MSA on details of how it works and how to use the MSA program.

5.1.2 MSA Processing

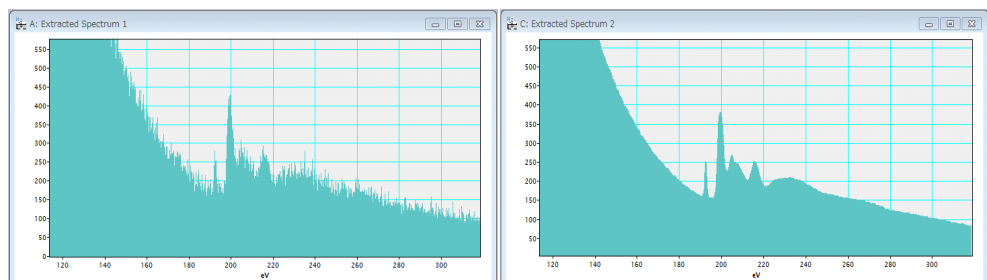
If you have installed MSA plug-in, the MSA menu should appear on the menu bar of DigitalMicrograph. Figure below shows the menu commands of "MSA".



Under "MSA" menu, choose "Weighted PCA" and then select "PCA...". Then, the following dialog for weighted PCA will appear.



By following the procedure described in the user's manual for “MSA”, we can reconstruct the SR-EELS data with improved signal to noise ratio. Figures below shows a single EELS spectrum of Boron K-edge without (left) and with (right) the MSA process, respectively. The MSA is effective as a pre-process for deconvolution.



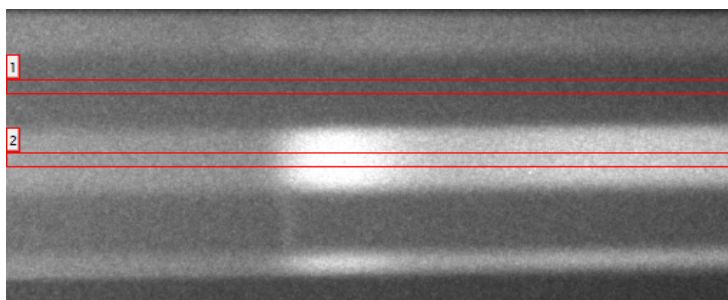
5.2 SR-EELS

This section describes how to analyze the Spatially Resolved (SR)-EELS data using SI-module for DeConvEELS.

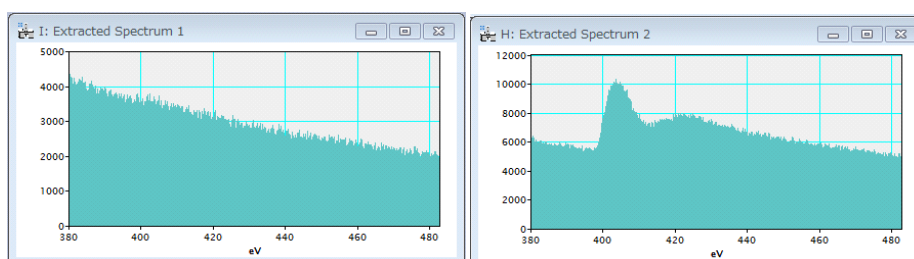
5.2.1 Introduction

Spatially resolved (SR) EELS is a technique to obtain a set of EELS data along a line of the sample in a TEM. An SR-EELS data is similar to the one-dimensional SI EELS data which can be obtained by STEM by scanning the beam along the line on the sample. Typical SR-EELS data is shown below. Here, the horizontal axis of SR-EELS data corresponds to energy dispersion direction of energy loss spectrometer, while the vertical axis corresponds to specimen positions along the line. SR-EELS data can be obtained using a selected area aperture with a narrow slit using line focus mode of the EELS spectrometer.

The figure below shows typical SR-EELS data obtained from the sample of a layered structure that includes nitrogen at some positions.



The images shown below left and right correspond to the EELS respectively integrated over the regions 1 and 2 above. The right spectrum corresponds to Nitrogen K-edge.



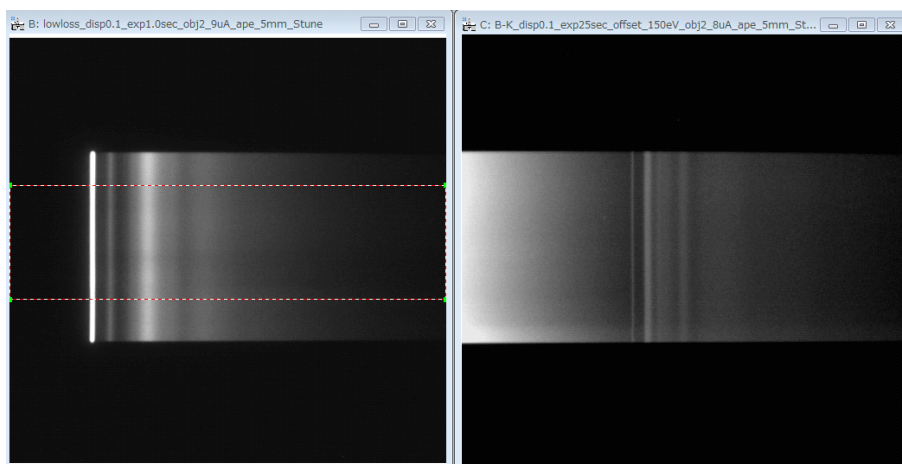
Details of experimental procedure and applications of this technique are described in some articles, see for example Ref [1]. SR-EELS technique is useful to investigate EELS data along the direction perpendicular to interfaces, grain boundary, layered structures, etc. In the following subsection we describe how to process SR-EELS data using the SI module.

Reference

[1] K Kimoto, S Isakozawa, T Aoyama and Y Matsui; *J Electron Microscopy* **50** 523-528 (2001).

5.2.2 Extraction of SR-EELS data

Figures below show raw SR-EELS of low-loss (left) and that of Boron K-edge (right) from a uniform BN crystal, respectively. The regions above and below the area where no spectrum is observed should be removed before deconvolution. When we extract the same regions from experimental raw SR-EELS, the extracted data can be processed using the SI module.



Let's extract an interesting area from these raw data. At first, specify the interest area as shown in the low-loss image using the rectangular ROI tool of DigitalMicrograph. Next, select "*Extract Spatial Subarea*" sub-menu of SI Utilities (see 4.2.6 of the Utilities commands). Then, SR-EELS shown below left will be extracted.



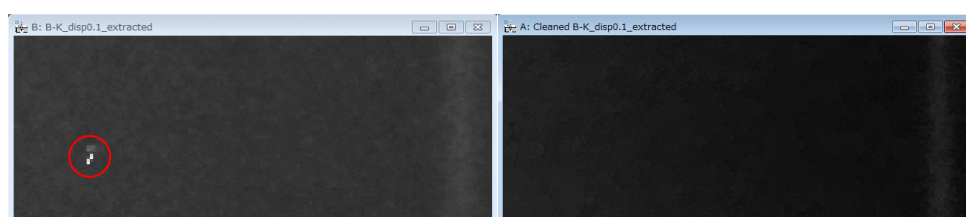
Next, let's extract the same region of SR-EELS from the raw Boron-K-edge data. Firstly, bring the Boron K-edge raw SR-EELS to front-most. Next, select "*Extract Previous Same Area*" sub-menu of SI Utilities (see 4.2.7 of the Utilities commands). Then, the SR-EELS extracted from raw Boron K-edge will appear as shown above right.

Now the extracted data shown above can be processed by using the SI module for DeConvEELS.

5.2.3 Removing Spike Noise with HREM-Filters

Spike noises in experimentally obtained SR-EELS data may be eliminated by using HREM-Filters Pro/Lite, a plug-in for Gatan DigitalMicrograph. Please consult the user's guide for HREM-Filters Pro/Lite. In this subsection we show some applications of the HREM-Filter for SR-EELS data.

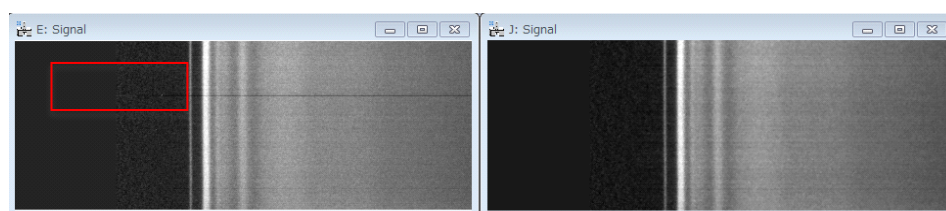
The left image below shows an enlarged part of the SR-EELS data from Born K-edge, where a sudden intensity variation (spike noise) can be seen in the bottom left. This sharp intensity variation is caused by bad pixels of a camera or uncontrollable x-ray or cosmic ray, and reduces the quality of data obtained by post-processing, such as deconvolution. Therefore, it is recommended to remove the spike noise before deconvolution.



Since spike noise of SR-EELS is a sudden change in intensity in the data acquired using a camera, it can be removed by using the "Replace Dud Pixels" command in the HREM-Filters plug-in. You can define the appropriate size of the spike noise in pixels in the dialog of this command.

Using this command, a new SR-EELS data will be obtained as shown by the right image above, where the strong contrast due to spike noise has disappeared.

Note that the enlarged part of the SR-EELS above corresponds to the red rectangle on the figure below left. Therefore, this spike noise will affect background estimation over the signal region. Then, SI-deconvolution without applying the "Replace Dud Pixels" results in the dark horizontal line due to the spike noise.



After applying "Replace Dud Pixels", SI-deconvolution gives the results shown on right, where the dark line is no longer visible.