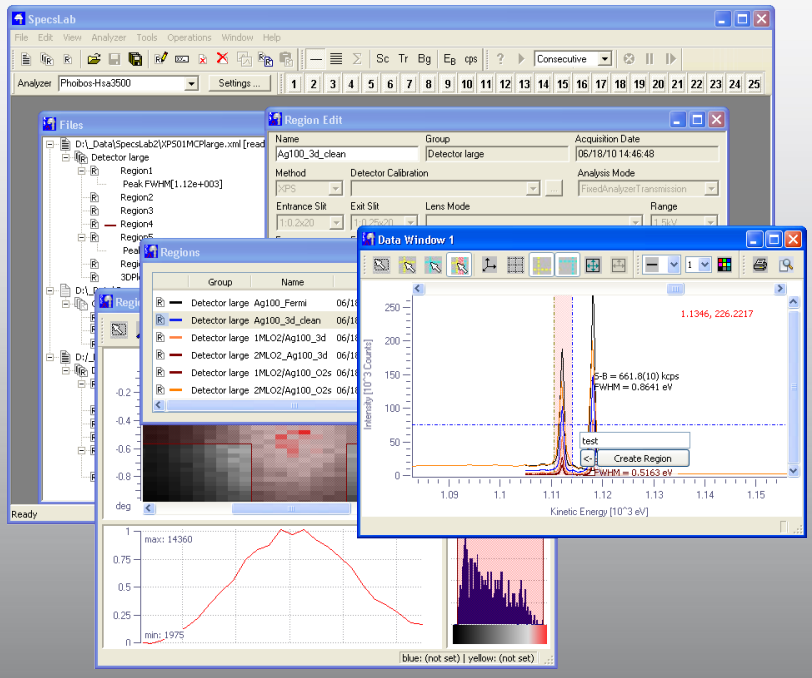
SpecsLab2

Data Acquisition Software



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ISO 9001 Certificate

SPECS User Manual
SpecsLab2—Data Acquisition Software, Version 3.2

June 07, 2011

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Chapter 1
Introduction

Welcome to the user manual for SpecsLab2. This software controls SPECS analyzers and other equipment for data acquisition and basic analysis.

This chapter explains briefly how to use the manual and points you toward further sources of information.

This manual was prepared using SpecsLab2 version 2.71r20938.

1.1 About

This manual is intended for users of SpecsLab2 who use the software for scientific data acquisition and data analysis.

The manual is divided into the following chapters:

Chapter 2 describes installation procedures that you may need to perform.
Chapter 3 covers the configuration of the software so that it can interface with hardware.
Chapter 4 contains the procedures and background information required for acquiring data.
Chapter 5 deals with file management in SpecsLab2.
Chapter 6 explains the data analysis methods available in SpecsLab2.
Chapter 7 shows you how to change the appearance of data in the Data window and 2D viewer.
Chapter 8 looks at postprocessing, i.e. printing and exporting data to other programs.

There are also appendices:

Appendix A is a general reference, providing an overview of all features, menus, windows and toolbars.
Appendix B describes the calibration procedure.

1.2 Information

This manual describes the functionality of SpecsLab2. You can find more information about a number of subjects concerning spectroscopy and computer control in the doc folder of your SpecsLab2 installation directory.

You should read the manuals supplied with the analyzer and detector before starting to make any measurements. These provide information about available operational modes as well as advice on best practice.

An online help, containing much of the information in this manual, is available from within the program by selecting Help/ Online Manual from the menu bar.

For further advice and assistance, please also contact SPECS support:

Tel. +49 30 46 78 24-0
email: support@specs.com

Chapter 2
Installation

SpecsLab2 is preinstalled on a computer when your analyzer is delivered. Under normal circumstances therefore, you do not need to install the program.

There are a few cases where you will need to perform an installation or change the existing installation:

- Performing updates of the software.
- Changing the installation so that the program can control additional equipment.
- Installing a demo version so that you can process data files away from the measurement computer.

An uninstaller is also provided for removing the software from your computer.

2.1 Installing an Update

SPECS releases new versions of SpecsLab2 with new features. If you need to take advantage of these new features, you need to install the update.

The update is a full release of SpecsLab2, and has a normal MS Windows installer to guide you through the process. There are a couple of points that you should bear in mind:

- You will be offered the chance to make a backup of your existing installation. It is a good idea to do this so that you can return to your previous installation if necessary.
- You do not need to make any changes to the Choose Components page. The installer automatically selects the correct options based on your existing installation.

2.2 Custom Installations

SpecsLab2 is automatically configured for your hardware on delivery. You may need to change the installation in order to provide support for additional hardware, e.g. for manipulator or synchrotron control.

Note: If you need advice or assistance with custom configurations, please contact SPECS support.

A custom installation involves running the standard SpecsLab2 installer and selecting new options in the Choose Components page. You can expand the nodes in the pane and select the components you want to install.

Note: The installer offers you the opportunity to backup your existing version. You should do this in case you need to revert your custom installation to the original setting.

2.3 Installing a Demo Version

You can install a demo version of SpecsLab2 on any computer. This allows you to open and analyze spectra on computers outside the laboratory.

To install a demo version:

1. Start the SpecsLab2 Installer and follow the instructions.
2. When you reach the Choose Components page, select Demo from the Select the type of install drop-down menu.

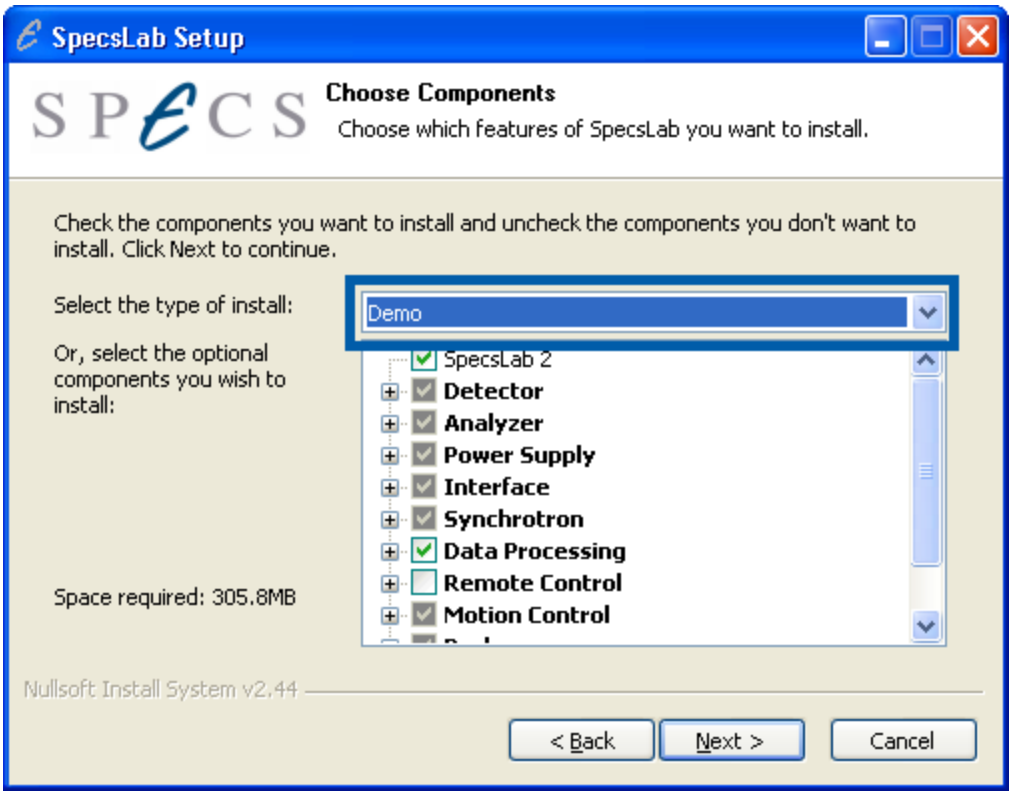


Figure 1: Installing a demo version

3. Continue with the installation as usual. All components required for the demo version will be included.

After installation, you can start SpecsLab2 as normal. All features for viewing and analyzing data work as normal.

Note: The Demo mode also installs a simulator. If you run the simulator, additional features, beyond opening and viewing SpecsLab2 data, are available.

2.4 Uninstalling

SpecsLab2 is provided with an uninstaller.

To uninstall SpecsLab2:

- Select Start/ SPECS/ Uninstall-Recover from the MS Windows task bar. The uninstall wizard will start. Follow the instructions in the wizard to uninstall the program.

Chapter 3
Analyzer Settings

SpecsLab2 is preconfigured for your hardware. If you change computer or add extra hardware, you will need to configure the software so that it can interface with your hardware correctly.

There are three stages of configuration:

- Analyzer—select your analyzer and detector. You can also change the calibration settings for your analyzer.
- Source—the excitation source for your experiments.
- Remotes—optional. Remotes allow you to control additional equipment such as manipulators, as well as enabling more sophisticated techniques such as depth profiling.

All of these stages are configured in the Analyzer Settings dialog. You can open this in the following ways:

- Select Analyzer/ Settings from the menu bar.
- Click the Settings button in the toolbar.

The following sections describe the configuration performed using this dialog.

3.1 Analyzer Server

You need to select an analyzer server. This information ensures that the software communicates correctly with the hardware and configures the software so that you can run experiments appropriate to your hardware. Standard environments usually define one analyzer server. For example, the name PHOIBOS HSA3500 MCD9 corresponds to "analyzer type / analyzer power supply type / analyzer detector type".

To select an analyzer server, use one of the following methods:

- Click the Server drop-down list in the Analyzer section of the Analyzer Settings dialog and select the item that corresponds to your hardware.
- Select an analyzer from the drop-down list in the toolbar.

Further configuration options for the analyzer are dependent on the type of analyzer and detector in your system.The following sections describe the available options.

3.1.1 Changing Analyzer Settings

You may need to change the settings for the analyzer as part of the calibration procedure or to compensate for aging of the detector. Your analyzer manual contains details about settings and procedures specific to your analyzer—you should refer to this before changing any analyzer settings.

To change the settings for your analyzer:

- Click the Settings button in the dialog below the analyzer name. A new dialog will open containing all the operating parameters for your analyzer.

Note: The settings displayed in the dialog depend on your analyzer. The values are measured as part of the calibration of your analyzer.

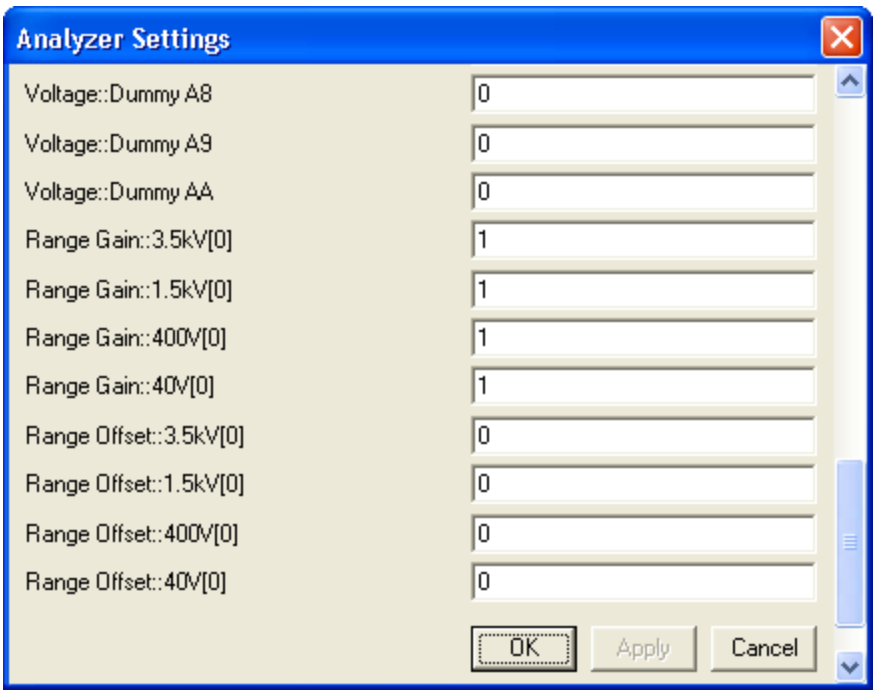


Figure 2: Setting parameters for the analyzer



Caution!
You should only change values in this dialog if you fully understand the consequences. Changing the settings here can affect the calibration of the spectrometer or cause irreversible damage to the detector.

The following points provide an overview of the available settings:

- Voltage Range—change these settings if you want to measure at higher maximum voltages or to achieve the optimal step width for the chosen energy range.
- Default Bias voltages—are optimized for your analyzer and, in general, should not be changed.
- Default Detector Voltage—this value is given in your specification report. If you change this value, do so *very carefully* to prevent damage to the channeltrons. The manual for your detector contains more information about how to

set the channeltron voltage. See "Detector Voltage Scan" on page 36 for information on how to find the plateau for channeltron operation.

- Analyzer Workfunction—applies an energy shift to spectra so that you can account for changes in workfunction. The manual for your spectrometer describes the procedure for correcting the workfunction.
- Gain and Offset—allow you to correct individual voltage modules. You may need to change these values after calibrating your spectrometer. Please see the spectrometer manual for further details of these procedures.

You can save the current settings for the source:

- Click the Save Settings button in the Analyzer section of the dialog. A Save dialog will open to allow you to select a location and filename. The file is saved with a *.ase* extension. You can load the settings at any time by using the Load Settings button.

3.1.2 Detector Mapping

The Detector Mapping dialog contains settings used for CCD cameras or 2D delayline detectors. You can therefore only access this dialog if you have a 2D detector.

To open the Detector Mapping dialog:

- Click the Mapping button in the Analyzer Settings dialog.

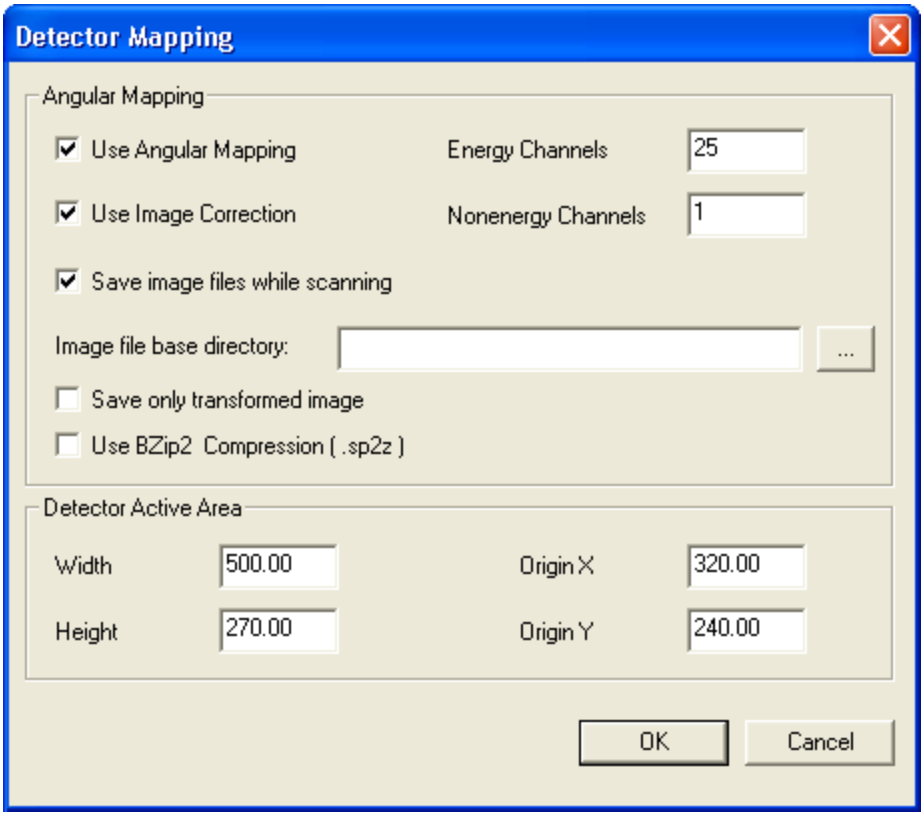


Figure 3: Detector Mapping dialog

The dialog is divided into Angular Mapping and Detector Active Area sections. These are described below.

Angular mapping

The Angular Mapping section contains settings for configuring the number of energy channels and handling images. The table below summarizes each of the options in this section.

Item	Description
Use Angular Mapping	Allows you to measure data in the non-dispersive direction, e.g. the angular direction in the image.
Use Image Correction	This applies the image transformation to correct the image, compensating for the analyzer transmission.
Save image files while scanning	In addition to measuring data in SpecsLab2, image file will also be saved. The images are saved in *.sp2* format—these can be read by CCD Acquire. Using this feature can slow operation considerably. Only active when the Use Image Correction box is checked.
Image file base directory	Sets the location for saving image files. Clicking the ellipsis button opens browser so you can select a location. Only active when the Save image files while scanning box is checked.
Save only transformed image	By default, both corrected and uncorrected images are saved. Checking this box means that only the corrected images are saved, reducing the amount of data saved. Only active when the Save image files while scanning box is checked.
Use BZip2 compression	Compress data files using the BZip2 algorithm. Only active when the Save image files while scanning box is checked.
Energy Channels	Specify the number of energy channels. A higher number offers increased resolution; however, the number of counts in each channel will decrease, which can lead to a noisy signal.
Nonenergy Channels	Specify the number of channels in the non-dispersive direction, e.g. in the angular direction. A higher number offers increased resolution; however, the number of counts in each channel will decrease, which can lead to a noisy signal. Only active when the Use Angular Mapping box is checked.

Table 1: Angular mapping settings

Detector active area

The detector active area is the area that is used for data acquisition. In general, you should select the largest possible area on the image—remember however that the camera image you see in CCD Acquire is circular, so you should aim for the largest square within this circle, so that all channels have the same contribution to the signal.

Energy channels and non-energy channels have a specified width in pixels. You need to be able to fit a whole number of channels into the picture. In order to make best use of the selected area, observe the following points:

- The specified width should be exactly divisible by the number of energy channels.
- The specified height should be exactly divisible by the number of non-energy channels.

If these conditions are not fulfilled, parts of the border of the image will not be read. A warning message will appear if before the values are accepted.

The values are preset for the optimum area, so you do not normally have to change them. The procedure below describes the steps required to obtain and enter new settings, should you wish to change the defaults.

To set the detector active area:

1. Close SpecsLab2.
2. Start CCD Acquire and Juggler.
3. Obtain an image from the camera.
4. Right-click the image in CCD Acquire and make sure that Use Physical Axis Units is not selected (no tick). The axes of the image are displayed in pixels rather than physical units. SpecsLab2 uses the range in pixels.
5. Click the toggle dispersion relation icon so that the transformed view of the image is displayed, i.e. all stripes are horizontal.
6. Mark the top left corner of the image with a crosshair marker. Observe the following points:
   - Do not include the curved areas at the edge of the image. You should try to ensure that all areas have an equal contribution to the signal.
   - Make sure that the signal from the top stripe is completely included.
7. Mark the bottom right corner of the image in a similar way with the other crosshair marker.
8. Note the X and Y coordinates of the two markers in the Cursor1 and Cursor2 sections in the status line at the bottom of the window.
9. Calculate the settings with the following relations:
   - Width = X1 – X2
   - OriginX = (Width/2) + X2
   - Height = Y1 – Y2
   - OriginY = (Height/2) + Y2
10. Close Juggler so that you can run SpecsLab2.
11. Start SpecsLab2 and open the Detector Mapping dialog.
12. Enter the new settings in the Detector Active Area fields.
13. Click OK to accept the settings and close the Detector Mapping dialog.

You need to reload the analyzer server (select none from the Server drop-down list, then select your server again) to make sure the changes are accepted.

3.1.3 Detector Settings

The Detector Settings dialog allows you to define settings for individual or all channeltrons or MCPs in your detector.

To change the detector settings:

1. Select an item from the Detector drop-down list in the Analyzer Settings dialog. The numbers refer to the available channels in your detector; all std selects all the channels.
2. Click the Settings button. The Detector Settings dialog will open.
3. Edit the settings in the Detector Settings dialog. These settings will be applied to the channel(s) you selected in the first step:
   - Threshold—sets the voltage for the operation threshold on the detector. More information about this is provided in the manual for your detector. The optimum value is provided in the specification sheet for your detector—you should only increase this value to compensate for aging.

- Deadtime—the channeltrons need a short time to recover after measuring a signal. This setting allows you to change the dead time for the detector, should this be necessary in your experiment. See also "Dead Time Correction" on page 52.

4. Click OK to accept your changes and close the dialog.

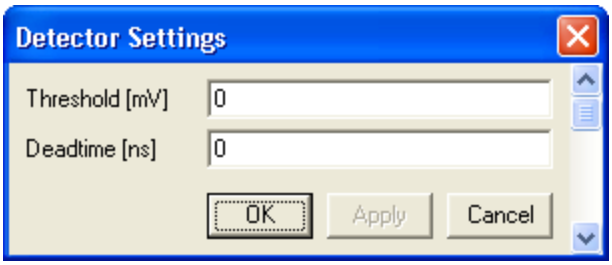


Figure 4: Detector Settings dialog

3.2 Sources

You need to select a source and measurement technique. The selections in this section work together—for example, if you select the method AES, you need to select a server for an electron source. You cannot use an ion source in this case.

When you select a server for a measurement technique, SpecsLab2 remembers the server and its settings and uses it when the measurement technique is selected—this includes selecting the technique while defining a region in the Region Edit window.

Note: If the source is not controlled by the software, this is an optional step. It is however recommended to select a "dummy" source in this case, as you can define experimental properties which are then recorded with the data.

To select a new source:

1. Select Analyzer/ Settings from the menu bar.
2. Check that the Server drop-down list in the Sources section is set to none.
3. Select a measurement technique from the Method drop-down list.
4. Select an item from the Server drop-down list. This must be compatible with the measurement technique, e.g. you need an ion source if you are performing ion scattering. The name of the source will be displayed in the Name field.
5. You can inspect and change the settings for your source by clicking the Settings button in the Sources section. The following sections provide more details about the settings of each server.
6. Click Close to close the dialog.

You can save the current settings for the source:

- Click the Save Settings button in the Sources section. A Save dialog will open to allow you to select a location and filename. The file is saved with a *.sse* extension. You can load the settings at any time by using the Load Settings button.

Note: Do not change the settings for a source unless you understand exactly what will happen. It is a good idea to save the source settings before changing them so that you can restore the original settings if necessary.

3.2.1 Dummy Sources

When you select a source, SpecsLab2 can control it, setting its operational parameters before data acquisition begins. If your source cannot be controlled by SpecsLab2, you can use a dummy source. The information you supply is recorded with the data for future reference.

There are a number of dummy sources, corresponding to different types of experiment:

- XPS—for X-ray photoelectron spectroscopy. You can select a common excitation source from the Anode drop-down list or define your own excitation energy. In this case, you need to enter a value in the E exc field in the Region Edit window while setting up a scan.
- UPS—for ultraviolet photoelectron spectroscopy. You can select the common lines used in UPS for hydrogen, helium, neon and argon. If you choose to define your own energy, you need to enter a value in Energy field.
- AES—for Auger electron spectroscopy.
- ISS—for ion scattering spectroscopy.

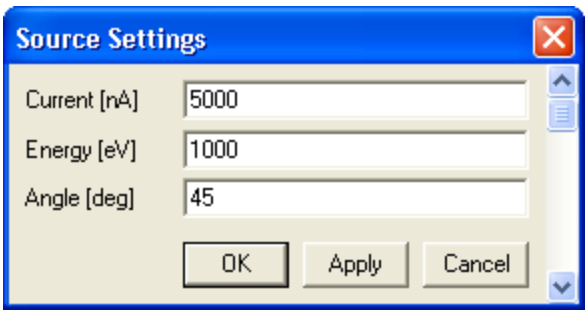


Figure 5: Dummy electron gun settings

3.2.2 X-Ray Sources

There are a number of different servers for X-ray sources. When you specify the source, SpecsLab2 will establish a connection with the device. SpecsLab2 can set the operational status of the source as well as selecting the anode.

You can specify a mode for the X-ray source at the end of the experiement (operate, standby, off). In addition to this setting, you can edit the MS Windows registry to switch the source off completely, including the water cooling. The switch off takes place after a user-defined delay. The delay is counted from the time SpecsLab2 finishes a scan with the X-ray source.

To automatically switch off the X-ray source, start regedit and set the following keys:

- *HKEY_LOCAL_MACHINE\SOFTWARE\SPECS\Sources\XRaySource*—set this to "1" to enable automatic switch off. Set it to "0" to disable automatic switch off.
- *HKEY_LOCAL_MACHINE\SOFTWARE\SPECS\Sources\XRaySource*—set the value to a number. This is the delay in seconds before the X-ray source switches off. Remember that the water cooling is also switched off, so you should allow some time for the source to cool down!

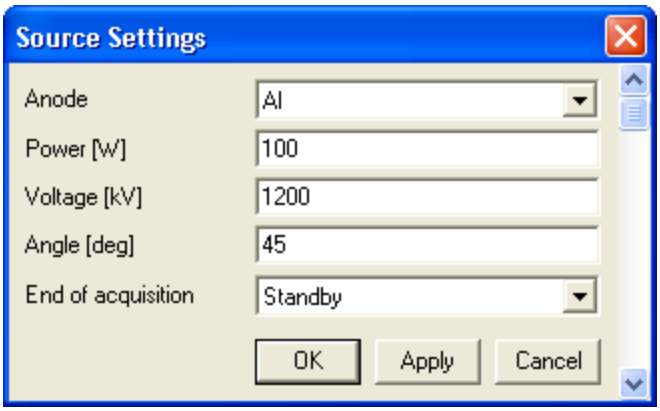


Figure 6: X-ray source settings

You can set the following parameters:

- Anode—switches the X-ray source to the selected anode and uses the energy of this excitation to calculate parameters in the experiment.
- Power—sets the power of the X-ray source.
- Voltage—sets the voltage of the X-ray source.
- Angle—records the angle setting used during the experiment.
- End of acquisition—sets the status of the X-ray source after the scan is completed. There are three options:
  - Standby—the source is put into standby more, with the high voltage off and the filament in a low current mode.
  - Operate—leaves the source on in normal operation.
  - Off—switches off the high voltage and the filament current.

3.2.3 Count Rate Scaling

With the count rate scaling server, you can read an analog signal from an external device and use this to scale the results. A typical example for its use is to normalize the measured results to the sample current.

SpecsLab2 can read the input from the following ADCs:

- ARMIN
- WASCO

SpecsLab2 assumes that the external device has a full scale of 0…10 V. The signal is normalized when scaling so that measured data is multiplied by 1 for the maximum analog signal. The scaled values are shown in the Data window when you click the Sc icon in the main window toolbar.

In the Source Settings dialog for this server, you need to enter the analog input channel so that SpecsLab2 can identify the external device.

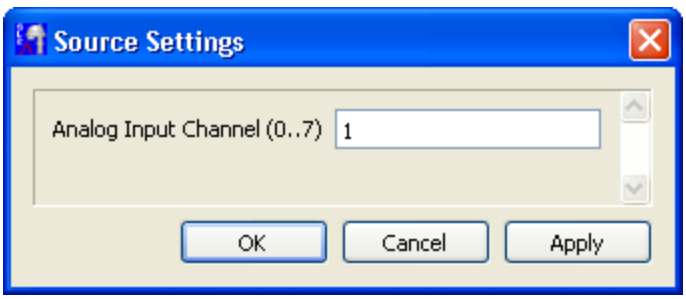


Figure 7: Count rate scaling server settings

The remote server "Remote Input" offers similar functionality; however, the remote only records the external data, without scaling the measured results.

3.2.4 Beamline Monochromator Sources

There is a server that is able to operate monochromators at synchrotron radiation sources. The standard SpecsLab2 installation provides a server that communicates via the AMC (Asynchronous Monochromator Control) protocol. The monochromator control computer is connected via a serial port with the PC which runs SpecsLab2 for spectrometer control. SpecsLab2 sends the appropriate commands to control the monochromator via this link to the AMC program running on the monochromator control computer.

For details about setting up SpecsLab2 to communicate with a beamline, please refer to the document "Beamline Monochromator Control". For further assistance, contact SPECS support.

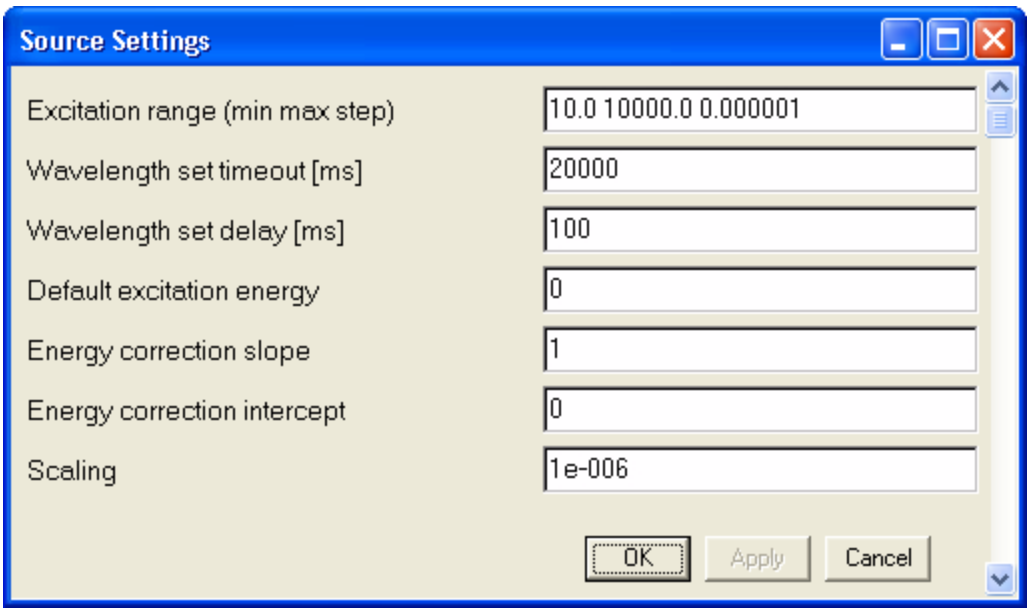


Figure 8: Monochromator server settings

You can set the following parameters using the monochromator server:

- Excitation range (min, max, step)—minimum and maximum available photon energy and the minimum step size increment for changing the energy.
- Wavelength set timeout—time in milliseconds that SpecsLab2 will wait for a feedback of the monochromator after having sent a command. After the time out an error message will appear. A typical value is 10 000 ms.
- Wavelength set delay—time in milliseconds that SpecsLab2 waits after the monochromator has reached the target wavelength. This is evident for older monochromator models. A typical value is 100 ms.
- Default excitation energy—used as a default value if a new region is created. In addition, this field enables the user to set directly the monochromator to a desired energy. If a value is entered in this field and Apply or OK is pressed, the monochromator will drive to this energy.
- Energy correction slope and Energy correction intercept—factors used for the correction of excitation energy. The wavelength that is set is calculated according to the following formula:

$$\lambda = \frac{1239.84244}{E_{excitation} \cdot \text{slope} + \text{intercept}} \quad (1)$$

- Scaling—reference value for calculation of intensity scaling.

3.3 Remotes

Remotes are additional pieces of equipment or services that can be used as part of an experiment. The following remotes are available:

- Delay server—introduces a pause between scans and adds timestamps.
- Timestamp—adds a timestamp at the end of each scan.
- Axis profile—for automating experiments with different sample positions.
- Depth profile—controls a SPECS ion source to sputter between scans.
- Imaging—create a 2D chemical map by moving the manipulator between acquisition points and scans.
- Slab mapping—create a 2D chemical map using deflectors in the analyzer.
- Remote input—reads a signal from other equipment during the experiment.
- AMC monochromator—interface with the AMC monochromator program.

You can add remotes using the SpecsLab2 installer:

- In the Choose Components page of the installation, select one or more items in the Remotes section. When you install the software, the remote will be included and is available in the Remotes section of the Analyzer dialog.

3.3.1 Delay Server

The delay server is a remote server which allows you to introduce a delay between measurements. The measurement is divided into cycles; the delay occurs after each cycle. A timestamp is inserted into the data (before acquiring the region and *after* sleeping) in seconds relative to the acquisition start. This is included on export to a VAMAS or XY file and can be used in other programs. The delay serverworks both for consecutive and cyclic modes—see "Acquiring Data" on page 40 for details about these modes.

Note: Due to hardware timing issues the timestamps are accurate in the region of 1 to 10 seconds.

To use the delay server:

1. In the Remote section of the Analyzer Settings dialog, select Delay Server from the Server drop-down list. There will be a delay as the server is loaded by SpecsLab2.
2. Click the Settings button. The Remote Settings dialog will open.

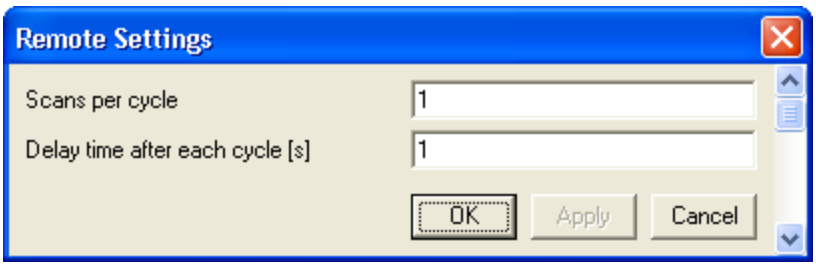


Figure 9: Delay server settings

3. Enter the number of scans per cycle.

Note: This setting has an influence on the Scans field in the Region Edit window. The Scans setting is the total number of scans. The number of cycles (i.e. the number of times the delay server will wait) is [scan number]/[scans per cycle].

4. Enter a number in the Delay time after each cycle field. The system will pause for this length of time after each cycle.
5. Click OK to accept the settings and close the dialog.

Note: You can save and load the remote settings by using the Save Settings and Load Settings buttons.

3.3.2 Timestamp

The timestamp remote allows you to insert a timestamp into the recorded data at regular intervals known as cycles. Each cycle lasts a pre-defined number of scans. The time in ms from the start of data acquisition to the start of the cycle is included in the data file. The data for each cycle is recorded separately.

The timestamp is is included on export to a VAMAS or XY file and can be used in other programs. The remote server-works both for consecutive and cyclic modes—see "Acquiring Data" on page 40 for details about these modes.

A Z value is also recorded with each cycle (Z = 0,1,2…). This allows you to view the cycles in a 3D plot, with the Z axis representing time.

To use the timestamp remote:

1. In the Remote section of the Analyzer Settings dialog, select Timestamp from the Server drop-down list.
2. Click the Settings button. The Remote Settings dialog will open.

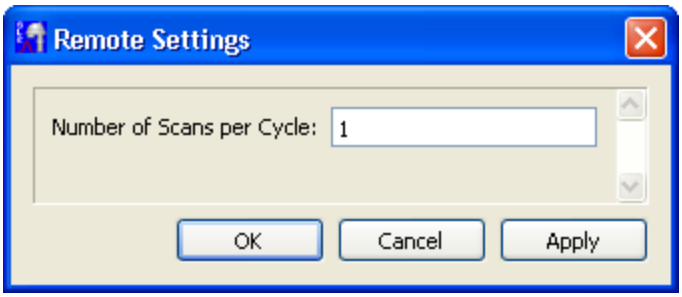


Figure 10: Timestamp settings

3. Enter the number of scans per cycle.
4. Click OK to accept the settings and close the dialog.

3.3.3 Axis Profile

The Axis Profile remote allows you to perform a number of scans with different manipulator settings. There are two versions of this remote:

- Axis Profile—this controls the manipulator and automatically makes the correct movements between scans.
- Axis Profile Manual—this pauses the measurement after each scan and instructs you to manually move the manipulator before continuing the measurement.

Position list file format

If you are using the Axis Profile remote with a motorized manipulator, you can define a list of positions in a file. The Axis Profile remote can read this file and move the manipulator to a new position for each scan.

The following points explain the format of the file:

- Each coordinate is a number.

- Coordinates are separated by commas or newline. These delimiters are treated in the same way by the remote.
- For each scan, you need to specify a coordinate for each manipulator axis. For example, for a manipulator with X, Y, Z axes, you need to specify three points per scan. The number and order of the coordinates is determined by your manipulator configuration.
- If you specify too many coordinates, they will be ignored. If there are too few, an error message will appear before the measurement starts.
- If an axis is not moved, do not include a number, but remember to include a comma or newline.
- Use a # symbol at the start of a line for comments

As an example, the following shows a point list file for 2 scans with an X, Y, Z manipulator:

```
#Comment for example
1.0,2.0,1.5
0.5,2.5,2.0
```

In scan 1, X = 1.0; Y = 2.0; Z = 1.5
In scan 2, X = 0.5; Y = 2.5; Z = 2.0

Using a return at the end of the position for each scan is convenient when reading the file; however, the above example is equivalent to:

```
1.0,2.0,1.5,0.5,2.5,2.0
```

If you do not want to move the Y axis in the second scan, leave out the value:

```
1.0,2.0,1.5
0.5,,2.0
```

Note: Do not put commas at the end of the line (before a newline) as this can be confusing—the ",<newline>" is read in the same way as ",,".

Configuration

To use the Axis Profile remote server:

1. In the Remote section of the Analyzer Settings dialog, select either Axis Profile or Axis Profile Manual from the Server drop-down list. There will be a delay as the server is loaded by SpecsLab2.
2. Click the Settings button. The Remote Settings dialog will open.

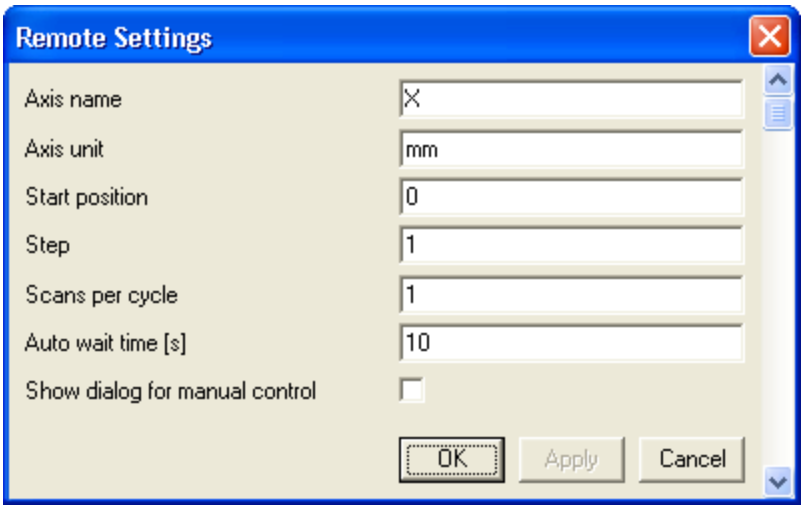


Figure 11: Axis Profile settings

3. Enter the Axis name. For automated versions, this determines the manipulator axis that will be moved. For manual versions, this setting will appear as part of the instruction to move the manipulator.
4. Enter a unit for the axis. This should normally be mm.
5. Enter the start position. For automated versions, this sets the start position for the manipulator. For manual versions, this setting will appear as part of the instruction to move the manipulator.
6. Enter a step. For automated versions, the manipulator will be moved this distance after each cycle. For manual versions, this setting will be used as part of the prompt to move the manipulator to a new position.
7. Enter the number of scans per cycle.

Note: This setting has an influence on the Scans field in the Region Edit window. The Scans setting is the total number of scans. The number of cycles (i.e. the number of times the manipulator will step) is [scan number]/[scans per cycle].

8. Enter an Auto wait time. The system will pause for this length of time while the manipulator moves.
9. Depending whether you are using the manual or motorized version, perform the following:
   - For manual versions, check the Show dialog for manual control box. At the start of each cycle, a message box will appear to tell you to move the manipulator.
   - For motorized versions, you can use a position list. If you wish to do this, check the box and enter the path and filename in the field provided. You can either enter an absolute path or a path relative to the *bin* folder in the SpecsLab2 installation directory.

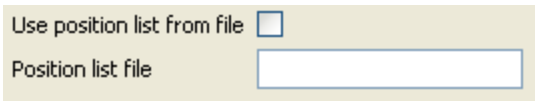


Figure 12: Using a file list

10. Click OK to accept your changes and close the dialog.

3.3.4 Depth Profile

You can perform depth profiling by sputtering (using a SPECS remote-controlled ion source) followed by the data acquisition of the scheduled regions.

This section explains the definition of the depth profiling remote, including a description of how the ion source power supply operates during the depth profiling experiment.

Restrictions for the depth profile Feature:
The depth profile feature generally works only with the following restrictions:

- To measure a depth profile with more than one region the acquisition mode needs to be Cyclic.
- Each region defined in the Region Edit window should have the same scan number. If the Scans per cycle value is set to 1, the number of scans in the Region Edit window is then equal to the number of sputter cycles.
- The measurement time can be only controlled by the dwell time.
- The SpecsLab2 tool IgControl must be switched off, deactivated or set to "local".

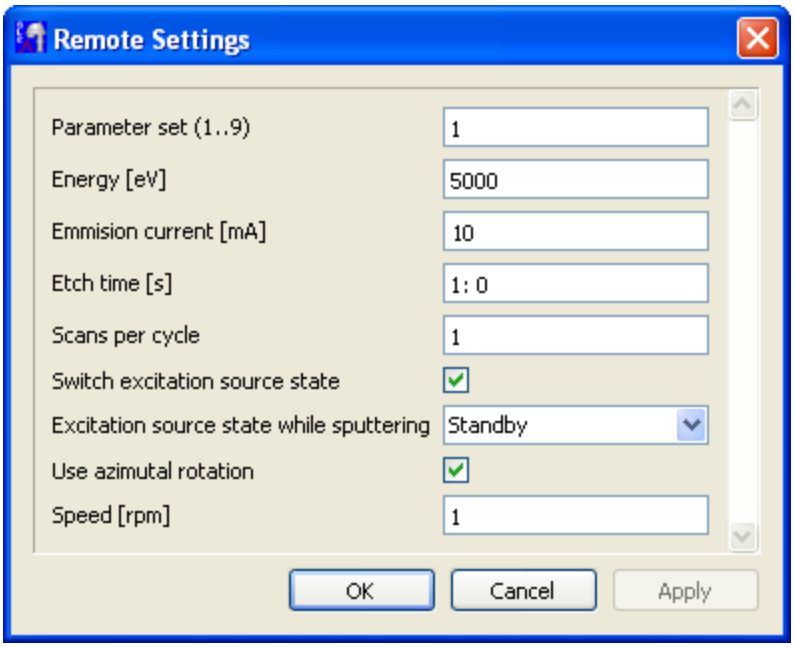


Figure 13: Remote Settings dialog for depth profiling

To define the depth profile remote server:

1. In the Remote section of the Analyzer Settings dialog, select Depth Profile from the Server drop-down list. There will be a delay as the server is loaded by SpecsLab2.
2. Click the Settings button. The Remote Settings dialog will open.
3. Enter a number between 1 and 9 in the Parameter set field. This selects the parameter set stored in the ion source power supply.
4. Enter a value in the Energy field. This sets the PU-IQE energy parameter in addition to the recalled parameter set (0 to 5 kV). It is important that this setting is the same as the energy setting in the parameter set. For parameter set 1, the default value is 5000 V.

Note: In the parameter sets in the PU-IQE, the focus setting is derived from the stored energy value. If the energy set in SpecsLab2 is different to the focus setting in the PU-IQE, the spot is defocused—meaningful results cannot be obtained under these circumstances.

5. Enter a value in the Emission current field. This sets the PU-IQE emission current in addition to the recalled parameter set (0 to 10 mA). In general, you should set this to 10 mA. If the filament is old and cannot reach this emission current, you can set the value a little lower.

6. Enter a value in the Etch time field. The format for defining this setting is described below, with examples provided in Table 2.
7. Enter a number in the Scans per cycle field. This sets the scans per cycle, i.e. scans for each of the regions defined in the Region Edit dialog. The number of cycles is equal to "scans per cycle divided by number of scans". The default is 1, so that the number of scans defined in the Region Edit window is the same as the number of sputter cycles.
8. If desired, check the Switch excitation source state option. This activates the drop-down list, so that you can define the condition of the X-ray source during ion bombardment.
9. If you have checked the Switch excitation source state option, select an item from the Excitation source state while sputtering drop-down list:
   - Off—HV off, Emission Off, Water On
   - Standby—HV on, Emission Off, Water On (default value)
   - Operate—HV on, Emission On, Water On
10. If desired, check the Use Azimuthal Rotation option. This rotates the sample in the azimuthal direction so that the surface is evenly sputtered.
11. If you have checked the Use Azimuthal Rotation option, enter a rotation speed. A typical value lies in the range 1–10 rpm.
12. Click OK to accept your changes and close the dialog.

Defining the etch time

The etch time definition string is written as a list of single etch time entries. Each entry consists of a depth cycle number and an etch time value in seconds, separated by a colon. The list entries are separated by commas. A definition string can contain only one single etch time value and will be interpreted as etch time to be used starting with the second depth cycle.

Table 2 shows some examples of etch time definitions with explanations.

Entered string	Evaluated instructions	Description
45	1:0, 2:45	First depth cycle without sputtering. Second depth cycle and all following with 45 s etch time.
1:10, 2:25, 10:40	1:10, 2:25, 10:40	First depth cycle starts with 10 s etch time and subsequent data acquisition. Depth cycle 2 to 9 with 25 s etch time. Depth cycle 10 and all following with 40 s etch time.
2:25, 15:40, 10:60	1:0, 2:25, 10:60, 15:40	First depth cycle with 0 s etch time. Depth cycle 2 to 9 with 25 s etch time. Depth cycle 10 to 14 with 60 s etch time. Depth cycle 15 and all following with 40 s etch time.
2:0, 3:45	1:0, 3:45	First and second depth cycle without sputtering. Third depth cycle and all following with 45 s etch time.

Table 2: Defining etch times

Preparations before depth profiling starts

Before starting the experiment, you should perform the following steps:

- Position the sample in the ideal position for analyzer acceptance.
- Take care that the X and Y offset positions are corretly adusted on the ion source for the chosen parameter set.
- Adjust theh X and Y scan width on the ion source according your needs.
- Save the changes of the parameter set in the ion source power supply.
- Ensure that the argon gas supply and differential pumping valves are set up correctly.

Ion source operation while depth profiling

Due to the design of ion sources, the emission current needs a few seconds to stabilize, so the emission current is not switched off between data acquisition cycles. This avoids time losses and unstable sputter onset, which would result in non-continuous sputter rates. This is especially relevant for very short sputter periods.

Ion source operation during acquisition

- High voltage is switched off.
- The power supply is in "Operate" mode.
- The emission current remains at the preset value.

Note: After the depth profile finishes, the ion source power supply will remain in this state. To leave this state, the depth profile server should be switched to "none". The ion source power supply status changes to "local" and "standby".

Monitoring depth profiling

The depth profiling is monitored in the Acquisition window under Currently Acquiring.

Aborting depth profiling

You can abort the depth profiling experiment at any time in the usual way by clicking Abort in the Acquisition window. This has the following effects on the ion source:

- High voltage is switched off.
- The power supply is in "Operate" mode.
- The emission current remains at the preset value.

You can therefore restart a new depth profile quickly.

Error handling

In case of error messages, time outs of analyzer and source power supplies as well as other obvious malfunctions, the situation should be diagnosed.

Note: SpecsLab2 does not receive information about the state of the source, data acquisition could continue. In this case, stop data acquisition and save the partly failed results.

If an error occurs:

1. Switch source server and depth profile server to "none".
2. Check the modes of the power supplies, whether they are "local", "enable-local" or "remote".
3. Analyze the situation and put the power supplies into standby mode or re-initialize all devices to regain the start position for a further depth profile.

To start IgControl, the depth profile server should be set to "none" to avoid an error message about failure to open a serial port. In the event that sources need be switched manually from "remote" to "local" or cut off from mains (e.g. in emergency situations), set the servers to "none" before trying a restart.

Depth profile diagram and data evaluation

You can view the results of a depth profile in the Data window. Switch on the Z axis for a pseudo-3D image.

Note: For data processing you can transfer the data to Casa XPS.

3.3.5 Imaging

The imaging remote allows you to obtain a 2D spatially resolved chemical map of the sample using one of the following methods:

- Rastering—the sample is moved in the X and Y directions, with measurements taken at each X,Y coordinate.
- Slab imaging—the sample is moved in one direction; the imaging properties of the detector take care of the other direction.

Figure 14 shows the data collection methods for imaging and slab imaging. In the case of imaging, on the left, a large number of measurements need to be made in a raster. Recording "slabs" of the sample, as shown on the right, is clearly faster since it involves considerably fewer measurements.

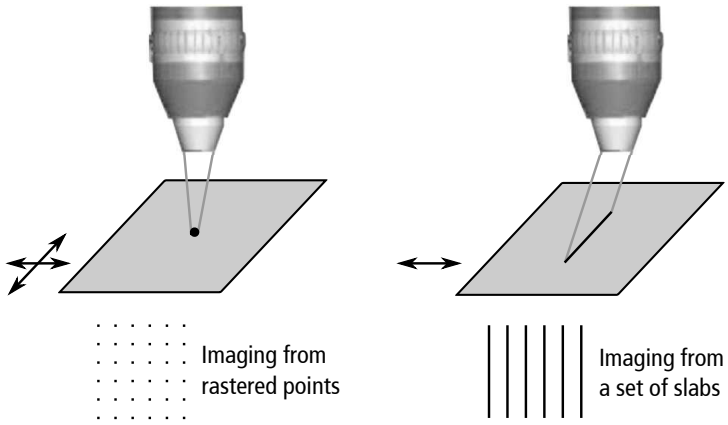


Figure 14: Imaging and slab imaging

When recording a spectrum, the signal collected has a spatial component and a dispersive component. You can record the spatial component and hence use slab imaging with a 2D detector. MCD detectors can also record the spatial component, but with lower resolution.

To use the imaging remote:

1. In the Remote section of the Analyzer Settings dialog, select Imaging from the Server drop-down list.
2. Click the Settings button. The Remote Settings dialog will open.

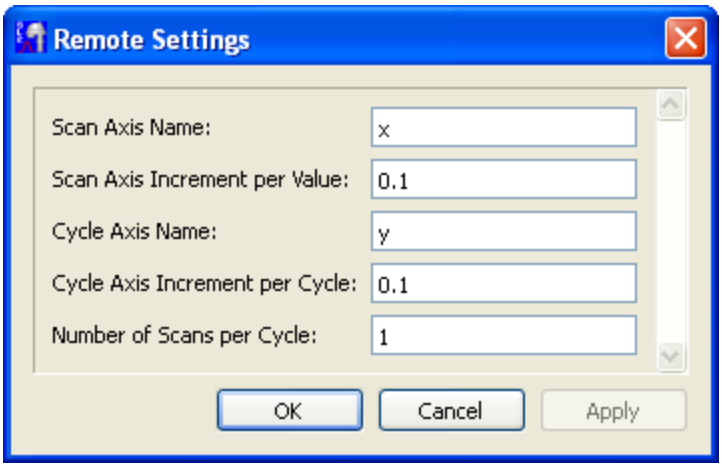


Figure 15: Imaging remote settings

3. Enter the scan axis name.
4. Enter an increment for the scan axis. The manipulator will move this distance after each scan.
5. Enter a name for the cycle axis.
6. Set the cycle axis increment per cycle as follows:
   - If using imaging, enter a cycle axis increment. After completing the scans along the scan axis, the manipulator will move this distance and then start scanning along the scan axis again.
   - If using slab imaging, set this value to zero. If using imaging, setting this to zero will lead to you acquiring a straight line.
7. Enter the number of scans per cycle.
8. Click OK to accept the changes and close the dialog.

The following sections contain important points about using imaging and slab imaging.

Imaging

When setting up a region for imaging, please note the following:

- Set a circular entrance slit, e.g 3 mm, so that you detect a spot on the sample.
- Use a magnification lens mode. For example, using the High Magnification 2 mode offers 10× magnification, leading to a measured spot size of 0.3 mm.
- Use the Fixed Energies analyzer mode to acquire data.
- Set the iris aperture on the analyzer to a value in the range 5–20 mm.

After scanning, the results are presented as follows:

- In the Data window, the X axis shows the scan direction; the Z axis shows the cycle direction.
- In the 2D viewer, the X axis shows the scan direction; the Y axis shows the cycle direction.

Slab imaging

When setting up a region for measurement using image slabs, please note the following:

- Set a rectangular entrance slit, e.g 0.5 × 20 mm, so that you can detect a spatially resolved signal in one dimension (a "slab").
- Use a magnification lens mode. For example, using the High Magnification 2 mode offers 10× magnification, leading to an image width of 2 mm.
- Set the number of scans to the same as that in the Number of Scans per Cycle setting in the Remote Settings dialog. There can only be one cycle for slab imaging.
- Use the Fixed Energies analyzer mode to acquire data.
- Set the iris aperture on the analyzer to around 5 mm.
- Set the non-energy channel in the Detector Mapping dialog to >1. A typical value is 40 for a resolution of ~5 µm. See "Detector Mapping" on page 9 for further details.

After scanning, the results are presented as follows:

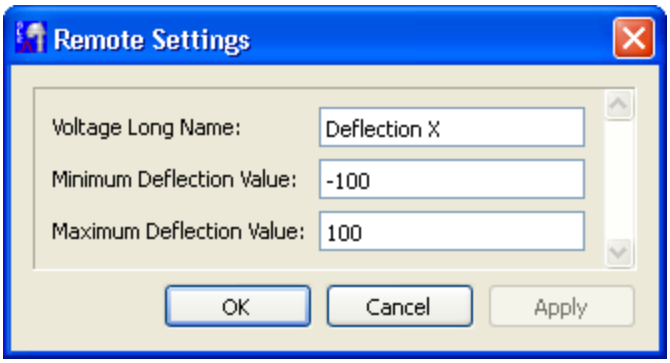
- In the Data window, the X axis shows the scan direction; the Z axis shows the dimension from the spatially resolved component (i.e. the non-dispersive direction of the detector). Make sure that you can view individual channels in the Data window—do not activate the Σ icon in the toolbar.
- In the 2D viewer, the X axis shows the scan direction; the Y axis shows dimension from the spatially resolved component.

3.3.6 Slab Mapping

The slab mapping remote[1] allows you to control the deflectors in the PHOIBOS analyzer in order to obtain a 2D image of the sample. The result is similar to that obtained by the slab imaging technique (see "Imaging" on page 23); however, the procedure is faster because the manipulator is not moved.

Note: This remote can only be used with analyzers that are fitted with the deflector option.

When recording a spectrum, the signal collected has a spatial component and a dispersive component. Due to the spatial component, there is therefore one-dimensional information about the chemical distribution on the sample surface. The deflectors allow you to change the acceptance area of the analyzer in a direction orthogonal to the spatial component of the signal.



Slab mapping imaging builds up a set of spectra with different deflection settings. The result is a chemical map of the surface in two spatial dimensions—one dimension from the acceptance of the analyzer; the other from scanning the deflectors.

To use the mapping remote:

1. In the Remote section of the Analyzer Settings dialog, select Mapping from the Server drop-down list.
2. Click the Settings button. The Remote Settings dialog will open.
3. Enter the voltage long name. This is the full name of the parameter voltage that you can find in the Analyzer Settings dialog, e.g. Deflection X.
4. Enter a minimum and maximum deflection values in the respective fields. Zero means no deflection.
5. Click OK to accept the changes and close the dialog.

When setting up a region with the mapping remote, please note the following:

- Set a rectangular entrance slit, e.g 0.5 × 20 mm, so that you can detect a spatially resolved signal in one dimension (a "slab").
- Use a magnification lens mode. For example, using the High Magnification 2 mode offers 10× magnification, leading to an image width of 2 mm.
- Set the iris aperture on the analyzer to around 5 mm.

[1] This documentation describes the beta version of the slab mapping feature. The deflection values represent the applied voltage to the deflector and have not been calibrated to represent a distance. It is important to remember that the deflection is dependent on kinetic energy. As a rough guide, the maximum deflection voltage of ±400 V leads to a deflection of ±18 mm at 500 eV, and a deflection of ±6 mm at 1500 eV.

- Use the Fixed Energies analyzer mode to acquire data.
- Set the non-energy channel in the Detector Mapping dialog to >1. A typical value is 40 for a resolution of ~5 µm. See "Detector Mapping" on page 9 for further details.

After scanning, the results are presented as follows:

- In the Data window, the X axis shows the scan direction; the Z axis shows the dimension from the spatially resolved component (i.e. the non-dispersive direction of the detector). Make sure that you can view individual channels in the Data window—do not activate the Σ icon in the toolbar.
- In the 2D viewer, the X axis shows the scan direction; the Y axis shows dimension from the spatially resolved component.

3.3.7 Remote Input

Remote Input allows you to monitor a signal while scanning. The measured signal can by used to normalize the intensity of the spectrum.

Note: If you are using a beamline monochromator source and you need a remote input, use the AMC Monochromator remote.

Note: The Count Rate Scaling server can scale the measured data by the signal.

SpecsLab2 can read the input from the following ADCs:

- ARMIN
- WASCO

The signal read has a full scale of 0…10 V. You can enter a scaling factor so that this is converted to the correct measurement units.

To use the depth profile remote server:

1. In the Remote section of the Analyzer Settings dialog, select Remote Input from the Server drop-down list. There will be a delay as the server is loaded by SpecsLab2.
2. Click the Settings button. The Remote Settings dialog will open. The appearance of this dialog will depend on how many channels are available.

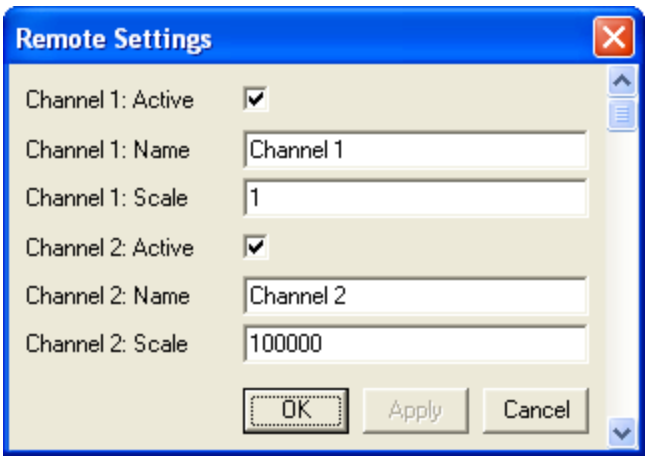


Figure 16: Remote Input settings

3. Check the Active boxes for all of the channels you want to monitor.
4. Enter a name for each selected channel. This name will appear in the data set when you measure spectra.
5. Enter a scaling factor for each selected channel. The acquired signal will be multiplied by this number. This feature is useful for performing a unit conversion.
6. Click OK to accept your changes and close the dialog.

3.3.8 AMC Monochromator

Specs AMC-Monochromator Control is an additional remote server for the SPECS data acquisition and processing software. It implements the Asynchronous Monochromator Control (AMC) protocol defined by BESSY.

Please refer to the document "Beamline-Monochromator Control" for details on how to configure the hardware and software for use with a beamline.

Chapter 4
Performing Scans

The main purpose of SpecsLab2 is to acquire data. This chapter covers the steps involved in using the software to measure data.

The process for acquiring data with SpecsLab2 essentially follows this process:

1. Create a region.
2. Define the scanning parameters in the region.
3. Validate the parameters.
4. Acquire the data.

This chapter covers all of the steps in this process and expands particular aspects as necessary for additional information about the working of SpecsLab2. The following topics are covered:

- Files, groups and regions—how to manage data within SpecsLab2.
- Defining regions—an explanation of all scanning modes and parameters.
- Scanning data—different ways to use the interface and manage data acquisition.
- Changing parameters—editing (or recreating) regions after data acquisition.

4.1 About Files, Groups and Regions

Data in SpecsLab2 is structured in three tiers:

- File—this is the unit that is stored on the hard disk. Generally, a file contains the measurements of an entire experiment.
- Group—a group allows you to structure a large number of spectra. You can use them to collect spectra that belong together for experimental or logical reasons.
- Region—a region is a single spectrum. It contains the scanning parameters and data.

A tree structure of these items is shown in the Files window. To open the Files window:

- Select Windows/ Files from the menu bar. The Files window will open.

As well as viewing all open data, you can copy or move groups and regions within the window by using drag and drop or copy and paste.

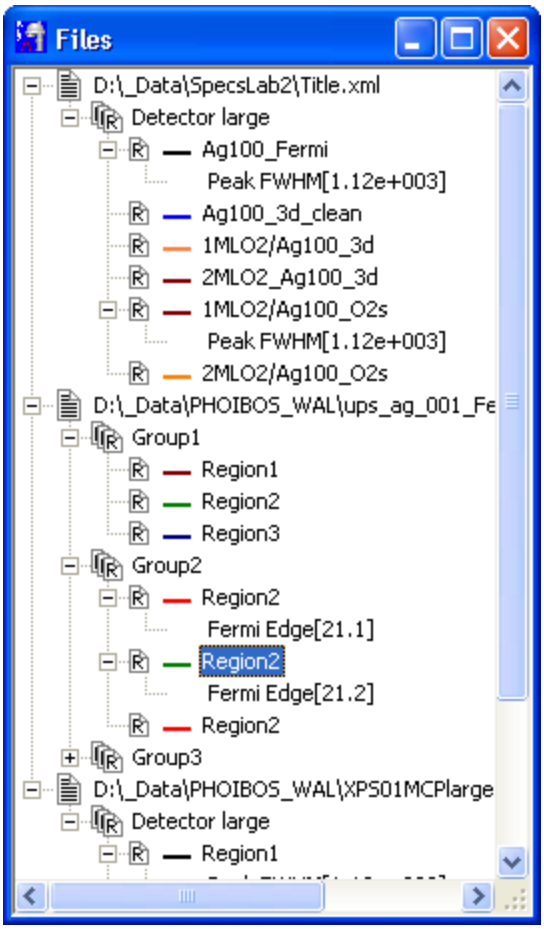


Figure 17: The Files window

4.1.1 Creating Files

Files are the top level holder in the data structure. A file is the unit that is stored on the hard disk. Groups and regions are defined within the file.

Note: The file is in XML format and can therefore be opened in any text editor. You should avoid editing files in this way, however, as SpecsLab2 may be unable to open the file. You can export the file in other format—please see "Exporting Numerical Data" on page 88 for further details.

To create a new file, use one of the following methods:

- Select the new file icon from the main toolbar.
- Select File/ New File from the menu bar.

This adds a new file to the Files window. Nothing is written to disk until you save the file.

4.1.2 Creating Groups

Groups are a useful way of organizing large numbers of regions so that you have a better overview of your data.

The location of newly created groups depends on the context:

- If a file is selected in the Files window, the new group will be created in the file.
- If a file is not selected in the Files window, a new file will be created with the group.

You can create a group using one of the following methods:

- Click the New Group icon in the main toolbar.
- Select File/ New Group from the menu bar.
- Right-click a file in the Files window and select New Group from the context menu.

The new group is created with a default name (Group1, Group2, …). You can change this name:

1. Right-click the group and select Rename from the context menu.
2. Enter a new name for the group.

Note: You can also edit the group name in the Region Edit window when you select the group.

4.1.3 Creating Regions

Regions contain recorded data from a scan as well as the measurement settings. You can view regions as part of the tree structure in the Files window; alternatively, all regions in currently open files are listed in the Regions window.

Regions are indicated in the Files and Regions windows with the following icons:

—New region. The measurement settings have not yet been validated.

—Valid region. The measurement settings have been validated and data can now be acquired for this region.

—Region is currently being measured.

—Measured region. This region contains measured data.

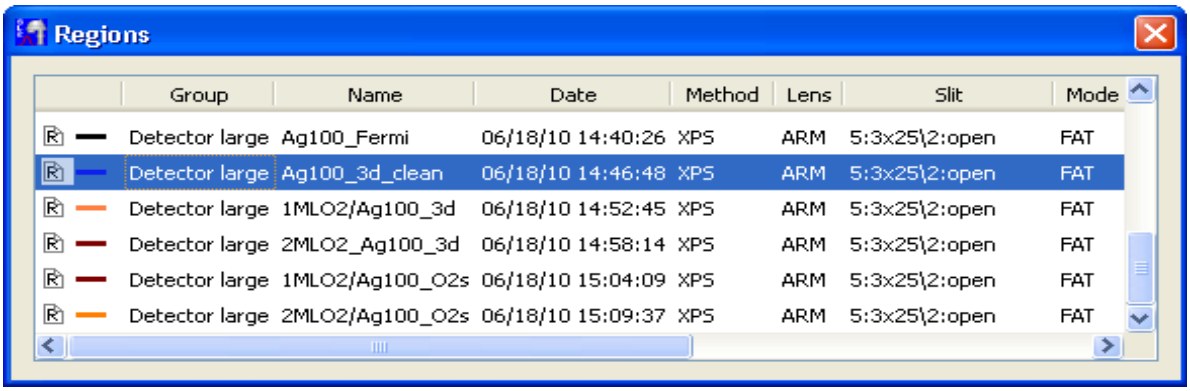


Figure 18: The Regions window

There are a number of ways to create a new region:

- Click the new region icon in the main toolbar. If there is no file or group open, these will be automatically created.
- Select File/ New Region from the menu bar. If there is no file or group open, these will be automatically created.
- Right-click a group in the Files window and select New Region from the context menu.
- Click the New button in the Region Edit window.

When you create a new region, the Region Edit window is automatically opened. If it is already, open, it is moved into focus.

A region is created with a default name (Region1, Region2, …). You can change this name in the following ways:

- Edit the Name field in the Region Edit window as part of the region definition.
- Right-click the region in the Files or Regions window and select Rename from the context menu. You can then enter a new name for the region.

4.1.4 Merging Files

You can merge the contents of a number of files into one single file. The groups in all open files, together with their regions, are added to a new file. You can then save this file.

To merge files:

1. Open the files that you want to merge.
2. Select File/ Merge Open Files from the menu bar. A new file is added to the Files window. The file has the contents of the other open files.
3. Select the new File in the Files window and click the icon in the toolbar. A Save dialog will appear to select a name and location for the file.

4.2 Defining Regions

The Region Edit window allows you to define the properties of the scan. In addition to selecting parameters such as the energy range and step size, you can set the analysis mode and calibration setting of the analyzer.

Note: All scan settings defined in the Region Edit window are saved with the acquired data for future reference.

To open the Region Edit window, perform one of the following actions:

- Select Windows/ Region Edit from the menu bar. The parameters of the currently selected region will be displayed.
- Right-click the region in the Regions or Files window and select Edit from the context menu.

In addition, when you create a new region, the Region Edit window will automatically open to display the properties of the new region.

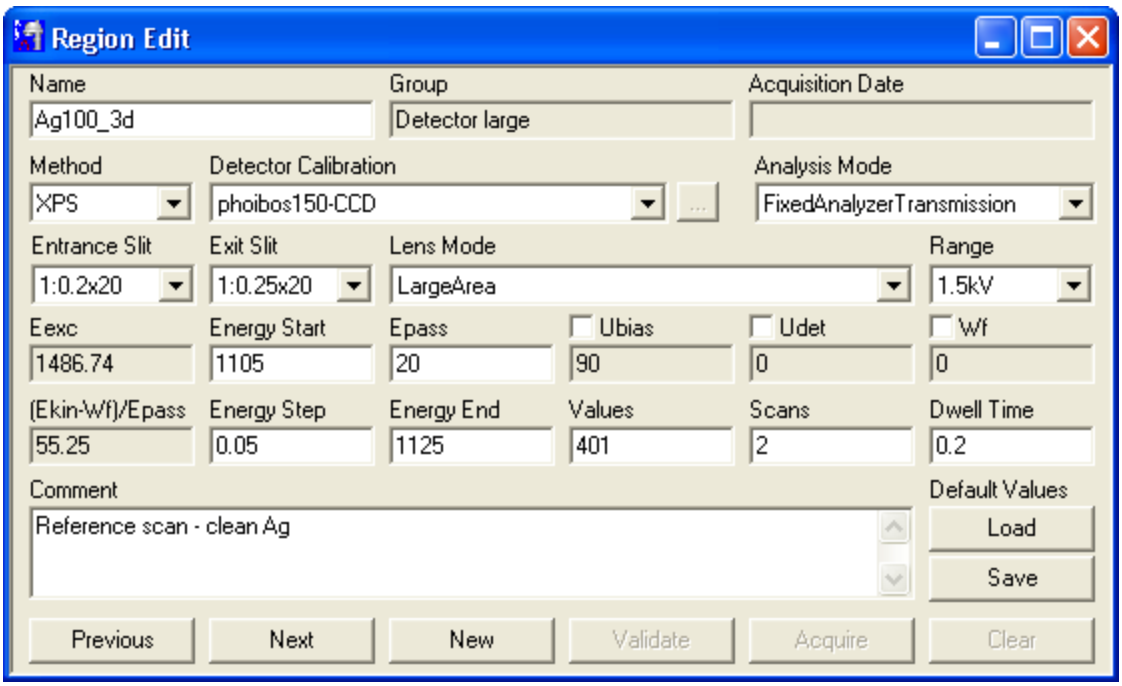


Figure 19: The Region Edit window

The table below describes the meaning of each of the fields. Depending on the analysis mode, some of these settings might be active, while others are grayed out. Some analysis modes cause a name change for some of the fields. In addition, some values have dependencies—this also changes with the analysis mode. The explanations in the table apply to the most commonly used analysis modes.

The analysis modes are described in the following sections, together with the variances from the descriptions in this table. A further section also describes the action of the Detection Calibration in more detail.

Feature	Description
Name	Enter a name for the region here. You can change the name of the region here as well as in the Files and Regions window. If you do not enter a name, a default is used (Region1, Region2 …).
Group	The name of the group that the region belongs to.
Acquisition Date	A date and time stamp. This is filled in at the end of data acquisition.
Method	Select the type of measurement from the drop-down list. This can affect the value of Eexc. The setting is recorded with the data for future reference.
Detector Calibration	Select between different detector calibrations. Please refer to "Applying Calibrations" on page 39 for details of how to use this. The detector calibration procedure is described in "Detector Calibration" on page 109.
Analysis Mode	Select a mode from the drop-down list.
Entrance Slit	Set the entrance slit. You need to set this mechanically on the analyzer. The setting here is recorded with the data for reference. The list of available slits depends on your analyzer—please refer to the analyzer manual for details.
Exit Slit	Set the exit slit. You need to set this mechanically on the analyzer. The setting here is recorded with the data for reference. The list of available slits depends on your analyzer—please refer to the analyzer manual for details.
Lens Mode	Select a lens mode from the drop-down list. This sets a pre-defined set of voltage for the analyzer lens. The options available depend on your analyzer—please refer to the analyzer manual for details.
Range	Voltage range of the high voltage modules in the HSA 3500plus. You should select an appropriate range for your experiment, e.g.: ■ 3.5 kV for AES ■ 1.5 kV for XPS ■ 400 V or 40 V for UPS
Eexc	The energy of the incident photons. This is generally set by in the Sources section of the Analyzer Settings dialog and cannot be changed in this dialog. However, for some measurement techniques (CFS, CIS), you can edit this field.
Energy Start	The starting energy for the scan.
Epass	Pass energy of the spectrometer. This determines the resolution of the analyzer.
Ubias	Acceleration voltage on the channeltrons or channel plates. Check the box to activate the field. In general, you do not need to change this setting. Please refer to "Detector Voltage Scan" on page 36 and observe the warnings there before changing this value.
Udet	High voltage on the channeltrons or channelplates. Check the box to activate the field. In general, you do not need to change this setting. Please refer to "Detector Voltage Scan" on page 36 and observe the warnings there before changing this value.
Wf	A value for the work function. Check the option box to make this field active. If you enter the value here, it overrides the pre-defined work function value and is only used in the measurement for this region.

Feature	Description
	By default, the pre-defined work function value is used in the measurement—see "Analyzer Server" on page 7 for details of how to change this.
(Ekin-Wf)/Epass	The braking ratio.
Energy Step	The step size in the scan.
Energy End	The final energy in the scan.
Values	The number of points recorded in the scan.
Scans	Set the number of scans performed during acquisition.
Dwell Time	Set the duration that each data point is recorded.
Comment	Free text field. You can use this to add information about the experiment.
Default Values Load/ Save	Click the Save button to save all settings in the Region Edit window to the registry. Click the Load button to load the last set of saved settings.
Previous	Selects the previous region, as listed in the Regions window
Next	Selects the next region, as listed in the Regions window.
New	Creates a new region in the current group.
Validate	Checks that the parameters for the scan are
Acquire	Starts the data acquisition.
Clear	Clears all data in the region. A message asks you to confirm the operation before the data is cleared. The other parameters are unchanged. You can edit the region, then validate and acquire.

Table 3: Fields and buttons in the Region Edit window

4.2.1 Fixed Analyzer Transmission

Fixed analyzer transmission (FAT) mode allows you to scan through the kinetic energy while holding the incident excitation energy constant. It is the most commonly used mode for XPS, UPS and ISS.

The pass energy is held constant during the scan, so that the energy resolution of the spectrometer is constant throughout the scan. The retarding potential of the analyzer is varied in order to measure different kinetic energies.

Measurements are normally performed with a fixed excitation energy, e.g. an X-ray gun. You can easily set up measurements defined in terms of the binding energy, as well as kinetic energy.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

The Energy Start and Energy End show the start and final kinetic energies. With Eb active, they show the start and final binding energies.

The Y-axis in the Data window shows the intensity. The X axis shows kinetic energy; with Eb active, it shows binding energy.

The settings have the following dependencies:

- Energy Start < Energy End .
- Energy Start > Energy End (Eb active).
- Energy Start, Energy End, Energy Step and Values are related by the following equation:

$$\text{abs}\left(\frac{E_{End} - E_{Start}}{E_{Step}}\right) = Values = \text{integer}$$

Note: The values are automatically corrected so that this relation is satisfied.

4.2.2 Fixed Retarding Ratio

Fixed retarding ratio (FRR) allows you to scan through the kinetic energy while holding the incident excitation energy constant. Unlike Fixed Analyzer Transmission, the pass energy is not held constant—the ratio of retarding potential to pass energy is constant. This means that the energy resolution is lower at higher kinetic energies.

Although this mode is rarely used for photoelecton spectroscopy because of the non-constant energy resolution, it is the mode best suited to AES. Auger data tables are compiled from results obtained using a cylindrical mirror analyzer (CMA). Using the PHOIBOS analyzer in FRR mode has the same characteristics as a CMA, so you can use the data directly without any further correction.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

There are a few points that you should note about the parameter settings when making AES measurements:

- Eexc is set to 0. Since Auger lines are not dependent on incident energy, this is not set. The properties of the source (from the Analyzer Settings are recorded with the output data).
- The braking ratio, (Ekin – Wf)/Epass can be set. The pass energy is calculated from this value at each kinetic energy.
- Epass Start. The number shown is the pass energy of the first measurement point.

The settings have the following dependencies:

- Energy Start < Energy End .
- Energy Start > Energy End (Eb active).
- Energy Start, Energy End, Energy Step and Values are related by the following equation:

$$\text{abs}\left(\frac{E_{End}-E_{Start}}{E_{Step}}\right) = Values = \text{integer}$$

Note: The values are automatically corrected so that this relation is satisfied.

4.2.3 Fixed Energies

The fixed energy (FE) mode is a simple mode that allows you to monitor a single kinetic energy for a specified time. Particles with a defined kinetic energy pass through the analyzer and are detected. This mode is used when setting up or checking the operation of the analyzer, as well as for investigating the stability of the excitation source.

Since the mode measures intensity as a function of time, signals from multiple channels are not of interest. SpecsLab2 therefore treats all channels as a single detector and sums the signal from all channels.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

There are a few points that you should note about the parameter settings for fixed energymeasurements:

- Energy sets the kinetic energy detected by the analyzer.
- Values is the number of points recorded.

- Step is always 1, since the analyzer does not scan.

Data is displayed in the Data window as intensity vs values. If you set the dwell time to 1 s, the X axis is therefore effectively measured in seconds.

4.2.4 Snapshot

The analyzer is not scanned in snapshot mode. Data is collected from all channels of the detector without performing any averaging. The spectrum shows the energy distribution of the particles that pass through the analyzer with its current settings.

A typical use for snapshot mode is to position the detection energy at the top of a peak and record the signal. This allows faster data acquisition for the limited energy range compared to FAT. For useful measurements, you need a CCD or DLD detector. In general, detectors with five or nine channeltrons are not suitable for snapshot mode, since you can only measure one data point for each channeltron; this is not enough to record a peak with suitable resolution.

If you want to use the analyzer in snapshot mode, you should calibrate the detector so that the signal delivered by each channel is normalized. Please see "Detector Calibration" on page 109 for a description of the calibration procedure.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

There are a few points that you should note about the parameter settings for snapshot measurements:

- Energy Start is the kinetic energy of the middle channel. If Eb is selected, this value is the binding energy.
- Energy End = Energy Start. The analyzer does not scan in this mode.
- Values is the number of points recorded. This needs to be an exact multiple of the number of available channels. Pressing Validate will correct the Values setting to the nearest acceptable value.

4.2.5 Detector Voltage Scan

The detector voltage scan (DVS) changes the channeltron voltage while holding the detected energy constant. It is used for checking the correct operating voltage for channeltrons.

When examining the results of a DVS, it is best to view the individual channels. The Channels toolbar allows you to toggle the display of each channel in the Data window. This allows you to check the performance of the individual channeltrons.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

This analysis mode has a few differences from the standard set of parameters:

- Energy replaces Energy Start. The scan is performed at a constant energy. This energy should be a setting where there is a background signal of electrons.
- Udet Step replaces Energy Step. This is the step size for the increase in detector voltage during the scan.
- Udet End replaces Energy End. This is the final detector voltage in the scan.



Caution!
You can destroy your detector if you set Udet End too high.

Please refer to the detector manual for more information.

4.2.6 Constant Final State

Constant final state (CFS) mode involves scanning the photon energy while detecting a single kinetic energy. The resulting scans show intensity as a function of binding energy. This mode ensures that you only measure occupied states in the sample.

In order to use this mode, SpecsLab2 needs to be able to control the monochromator at the synchrotron. For details about using SpecsLab2 at a synchrotron, please see "AMC Monochromator" on page 27.

Measurements with multiple channels are not suitable with this mode, since you are only examining a single kinetic energy. SpecsLab2 therefore treats all channels as a single detector and sums the signal from all channels.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

Since the mode varies the excitation energy rather than the kinetic energy, this analysis mode has a few differences from the standard set of parameters:

- Energy replaces Energy Start. The detected kinetic energy.
- Eexc Start replaces Eexc. The start energy of the source. If Eb is activated, this parameter is (source start) – (kinetic energy).
- Eexc Step replaces Energy Step. The energy step that the source moves.
- Eexc End replaces Energy End. The final energy of the source. If Eb is activated, this parameter is (source final) – (kinetic energy).

Note: The Y-axis in the Data window shows the difference energy (source energy + kinetic energy). If Eb is activated, binding energy is shown. The X axis shows photon energy.

The settings have the following dependencies:

- Eexc Start < Eexc End.
- Energy < Range setting (corrected by Validate, if necessary).
- 0 < Eexc Step < ceil(Eexc_End – Eexc_Start) / Eexc_Step.
- Values = ceil(Eexc_End – Eexc_Start) / Eexc_Step.

Example

The screenshot below shows the Region Edit window with a set of typical parameters for a measurement with CFS. The data acquired from these parameters represent a binding energy of 80–90 eV.

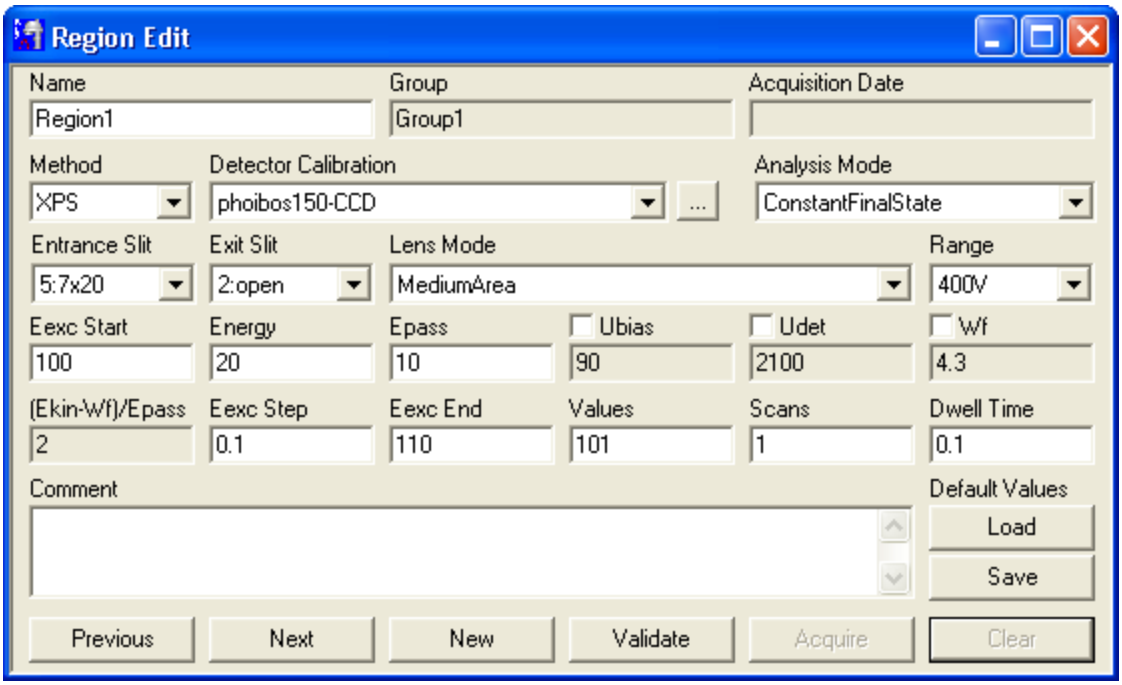


Figure 20: Constant final state parameters

As an explanation, the following steps take place in an experiment with these parameters:

1. Monochromator moves to 100 eV.
2. Analyzer measures electrons with energy 20 eV for 0.1 s dwell time.
3. Monochromator moves to 100.1 eV.
4. Analyzer measures with energy 20 eV, monochromator moves an increment of 0.1 eV. This is repeated until the monochromator reaches 110 eV.

4.2.7 Constant Initial State

Constant initial state (CIS) mode involves scanning the photon energy while simultaneously scanning the detected kinetic energy. When the photon energy is changed, the detected kinetic energy of the analyzer is changed by the same amount. In this way, the same binding energy is always measured. This allows you to measure the density of states in unoccupied states.

In order to use this mode, SpecsLab2 needs to be able to control the monochromator at the synchrotron. For details about using SpecsLab2 at a synchrotron, please see "AMC Monochromator" on page 27.

Measurements with multiple channels are not suitable with this mode, since you are only examining a single kinetic energy. SpecsLab2 therefore treats all channels as a single detector and sums the signal from all channels.

Settings

An overview of the settings in the Region Edit window is provided in "Defining Regions" on page 32.

Since the mode varies the excitation energy, this analysis mode has a few differences from the standard set of parameters:

- Eexc Start replaces Eexc. The start energy of the source. If Eb is activated, this parameter is (source start) – (kinetic energy).
- Eexc Step replaces Energy Step. The energy step that the source moves.

- Eexc End replaces Energy End. The final energy of the source. If Eb is activated, this parameter is (source final) – (kinetic energy).

Note: The Y-axis in the Data window shows the difference energy (source energy + kinetic energy). If Eb is activated, binding energy is shown. The X axis shows photon energy.

The settings have the following dependencies:

- Eexc Start < Eexc End .
- Energy Range setting (corrected by Validate, if necessary).
- 0 < Eexc Step < ceil(Eexc_End – Eexc_Start) / Eexc_Step.
- Values = ceil(Eexc_End – Eexc_Start) / Eexc_Step.

Example

The screenshot below shows the Region Edit window with a set of typical parameters for a measurement with CIS. The data acquired from these parameters represent a kinetic energy of 20–30 eV.

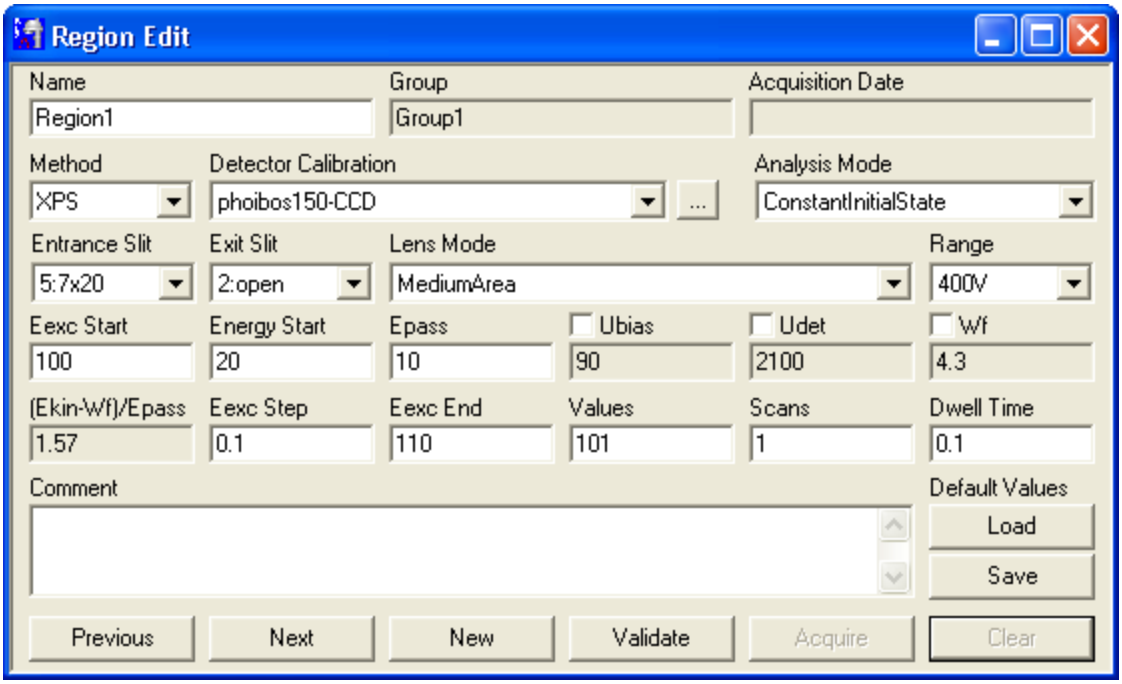


Figure 21: Constant initial state parameters

As an explanation, the following steps take place in an experiment with these parameters:

1. Monochromator moves to 100 eV.
2. Analyzer measures electrons with energy 20 eV for 0.1 s dwell time.
3. Monochromator moves to 100.1 eV.
4. Analyzer measures electrons with energy 20.1 eV for 0.1 s dwell time
5. Monochromator moves an increment of 0.1 eV, analyzer measures an increment of 0.1 eV. This is repeated until the monochromator reaches 110 eV.

4.2.8 Applying Calibrations

You can select a saved dataset file so that its calibration settings are automatically applied to data as it is measured:

- Select a dataset file from the Detector Calibration drop-down list in the Region Edit dialog. When you run the measurement, this calibration will be used.

Note: Clicking the ellipsis button ... next to the drop-down list allows you to select a new directory. All dataset files in the new directory will then be available in the drop-down list.

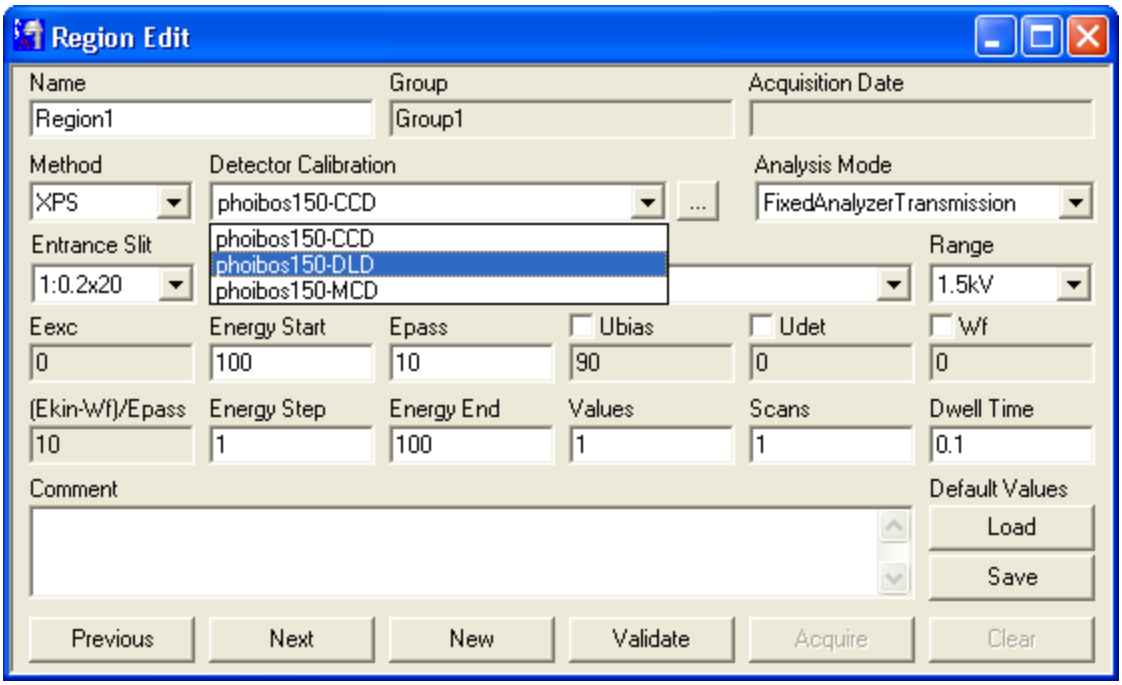


Figure 22: Selecting the dataset file for the region

4.3 Acquiring Data

After defining the parameters for a region, you can start data acquisition. Data is displayed in the Data window or 2D viewer as it is acquired.

Before you can acquire data, you need to validate the region. This checks the parameters in the Region Edit window and makes sure that a scan is physically possible.

The easiest way to start data acquisition is as part of the region definition in the Region Edit window:

1. After defining the scanning parameters, click Validate. The parameters will be grayed out and the Acquire button will become active.
2. Click Acquire. The scan will start.

Note: Pressing the Validate and Acquire buttons perform those actions on all selected regions. You can select a number of regions in the Regions window. If you select a group or file in the Files window, you can select these options from the context menu and apply them to all regions in the group or file.

There are other ways to run data acquisition:

- The Acquisition window
- The analyzer toolbar

These are described in more detail in the following sections.

4.3.1 Using the Acquisition Window

The Acquisition window allows you to manage and run validated regions. You can queue a number of regions so that they will be measured consecutively.

To use the Acquisition window for data acquisition:

1. Select Windows/ Acquisition from the menu bar. The Acquisition window will open. If it is already open, it will be brought into focus.

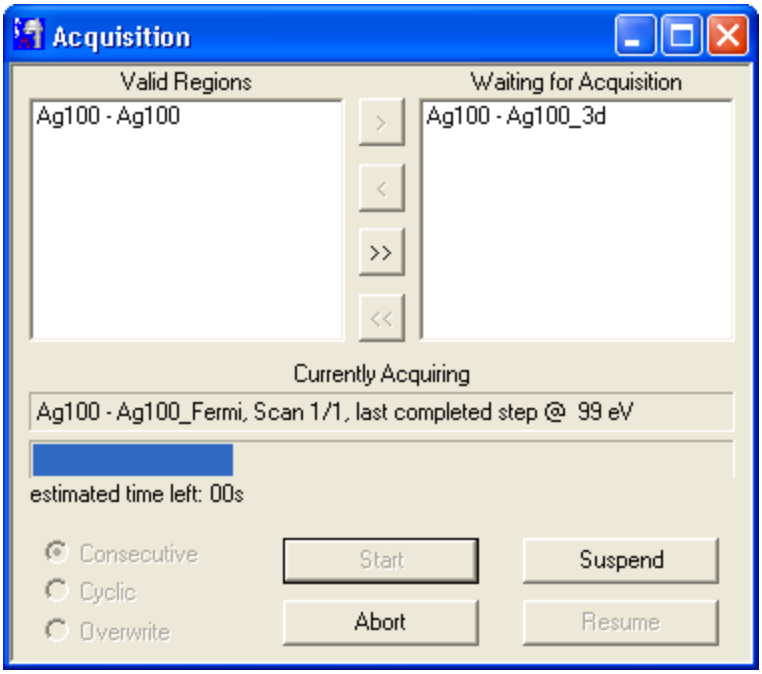


Figure 23: Acquisition window

Note: When you open the Acquisition window, all validated regions are listed in the Valid Regions pane.

2. Select the regions you want to measure and move them to the Waiting for Acquisition pane using the arrow buttons.
3. Select the desired acquisition mode by clicking one of the following options:
   - Consecutive—all selected regions will be measured consecutively, i.e. all scans within the region will be finished before starting the next region in the Waiting for Acquisition pane.
   - Cyclic—after a scan, the next region in the Waiting for Acquisition pane will be active for acquisition. If all waiting regions are measured once, the next scan will start. This procedure will be stopped for each region if the desired scan value is reached and all regions are measured.
   - Overwrite—all selected regions will be measured continuously, i.e. first region one scan, next region one scan, up to the end. After this, the measurement will start again, beginning with the first selected region and the data will be overwritten. This measurement does not stop automatically.
4. Click Start to start data acquisition. The currently measured region is indicated in the window, together with the estimated time for completion. During acquisition, the following buttons are active:
   - Suspend—pauses the measurement. You can continue by clicking Resume.
   - Abort—stops the measurement. You will have the chance to keep or discard data measured up to this point.

4.3.2 Using the Toolbar for Data Acquisition

The analyzer toolbar allows you to validate and acquire regions selected in the File and Regions windows. By selecting a number of regions, you can validate or acquire a number of regions.

Note: You can display the analyzer toolbar by selecting View/ Toolbars/ Analyzer from the menu bar.

To use the toolbar for data acquisition:

1. Open the Regions window by selecting Windows/ Regions from the menu bar.
2. Select the regions you want to measure. You can select a number of regions.
3. If any regions need to be validated, the question mark icon in the analyzer toolbar will be active. Click this icon to validate the regions.
4. Select an acquisition mode from the drop-down list:
   - Consecutive—all selected regions will be measured consecutively, i.e. all scans within the region will be finished before starting the next region in the Waiting for Acquisition pane.
   - Cyclic—after a scan, the next region in the Waiting for Acquisition pane will be active for acquisition. If all waiting regions are measured once, the next scan will start. This procedure will be stopped for each region if the desired scan value is reached and all regions are measured.
   - Overwrite—all selected regions will be measured continuously, i.e. first region one scan, next region one scan, up to the end. After this, the measurement will start again, beginning with the first selected region and the data will be overwritten. This measurement does not stop automatically.
5. Click the acquire icon to start data acquisition. During measurement, the following icons are active:
   - —Suspend. You can resume the scan with the button.
   - —Abort. You will have the chance to keep or discard data measured up to this point.

4.4 Modifying Regions

After you acquire data, the measurement parameters and data in the region cannot be edited. Most fields in the Region Edit window for the region are grayed out: You can only change the region name and add text comments.

If you want to change settings in a region, you first have to clear it in one of the following ways:

- Click Clear in the Region Edit window.
- Right-click the region in the Files or Regions window and select Clear from the context menu.



Caution!
Clearing a region deletes all of the measurement data. You will be asked to confirm the clear before any data is deleted. If you are unsure, you should make a copy of the region and clear the copy, leaving the original unchanged.

After clearing the region, you can edit the measurement settings.

4.5 Compacting Data

SpecsLab2 records the signal from each channel separately. The channel data is preserved when the measurement is saved. In order to reduce the size of the file, you can compact the data. This sums the recorded signal over all channels and saves only the sum. As a result, you keep the data about peak position and intensity, but you lose the individual channel information.

To compact data:

1. Right-click the file, group or region in the Files window or the region in the Regions window and select Compact Data from the context menu.
   - If selecting a file, all regions within the file will be compacted.
   - If selecting a group, all regions within the group will be compacted.
2. A warning message will appear to inform you that you cannot reconstruct the channel information after compacting. Click OK to accept this condition and compact the data.

Chapter 5
Saving and Loading Files

SpecsLab2 stores your data in the following hierarchy:

- Regions—contain the data from individual measurements or the results of fits.
- Groups—contain a set of regions.
- Files—contain a set of groups.

You can see the three tiers in the data architecture in the Files window. SpecsLab2 can only read and write the File tier, so all groups and regions are included when you save and load a file.

Note: A change in software architecture introduced in SpecsLab2 in version 2.55-r18573 led to a modified file format. You can still open files created by previous versions of SpecsLab2; however, earlier versions cannot open files in the new format. When you save old files with version 2.55-r18573 or later, the files are automatically converted to the new format.

Note: You can export individual groups and regions to other formats for analysis with other programs; these cannot however be loaded into SpecsLab2. For further details about exporting, please refer to "Exporting Data" on page 87.

This chapter covers the following topics:

- Setting the Autosave feature.
- Saving files.
- Editing the contents of files.
- Loading files.

5.1 Using Autosave

The Autosave feature saves open files at after a scan. When you next open SpecsLab2, you can restore the autosaved files. This can help protect against data loss.

Note: Autosave can slow performance considerably when large quantities of data are open.

To use Autosave:

1. Select File/ Settings/ Autosave from the menu bar. The Autosave dialog will open.

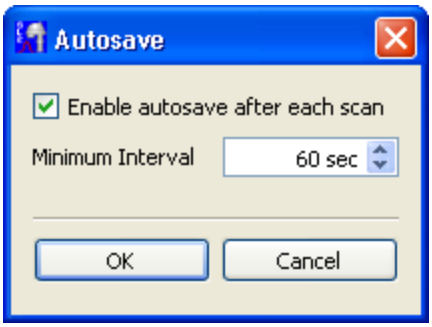


Figure 24: The Autosave dialog

2. To activate Autosave, check the Enable Autosave after each scan option. This is the default setting.
3. Enter a time interval in the field. This is the minimum time that elapses between each Autosave. Remember that Autosave only occurs after a scan. If this time is shorter than the time taken for a scan, the scan will be automatically saved on completion. If it is longer than a scan, SpecsLab2 will wait until the time has elapsed, then save the current scan on completion.
4. Click OK to accept the changes and close the dialog.

If SpecsLab2 has autosaved data, you can access it next time you start SpecsLab2:

- Select File/ Restore Autosave from the menu bar. All files that were open in the previous session will be opened with read-only status.

5.2 Saving Files

You should save the files you are working on at regular intervals.

To save a file:

1. Select the file you want to save in the Files window.
2. Use one of the following methods to save the file:
   - Select File/ Save from the menu bar.
   - Click the Save icon in the Main toolbar.
   - Right-click the file in the Files window and select Save from the context menu.
3. If the file has not yet been saved, a Save dialog will appear so that you can enter a filename and location.

Note: You can also select Save All in a similar way to save the selected file under a new name.

To save all open files:

- Select File/ Save All from the menu bar or click the Save All icon in the Main toolbar. If any files have not yet been saved, a Save dialog will appear for each unsaved file so that you can enter a filename and location.

5.3 Editing the Contents of Files

You can move groups and regions freely within the Files window by using drag and drop. This allows you to transfer regions to different groups or groups to different files.

5.4 Loading Files

You can load previously saved files into SpecsLab2 in order to view the results or to continue your measurements.

To load a file:

- Select File/ Open from the menu bar. Alternatively, you can click the Open icon  in the Main toolbar. A file browser will open to allow you to locate and open a file.

5.5 Closing Files

When you close a file, it is removed from the Files window.

To close a file:

1. Select the file you want to close in the Files window.
2. Use one of the following methods to save the file:
   - Select File/ Close from the menu bar.
   - Right-click the file in the Files window and select Close from the context menu.
3. If the file has not yet been saved, a Save dialog will appear so that you can enter a filename and location.

Chapter 6
Data Operations

After acquiring data, you can perform some analysis operations on the spectra such as background subtraction or peak width determination.

The sections in this chapter describe how to perform data operations and their configuration options. The following data operations are available:

- Background subtraction
- Dead time correction
- Despiking
- Fermi edge determination
- Linear operations to scale and shift peaks
- Noise subtraction
- FWHM of peak determination
- Peak location
- Savitsky Golay smoothing
- Smoothing spline

A further section describes the syntax used for generating labels.

Note: If you have angle-resolved data, operations are performed on the sum of all angle channels.

6.1 Performing Data Operations

When you perform a data operation, a new node is added to the Files window below the corresponding region. This node contains the results of the operation. The original data is left unchanged—you can export the operation data separately along side the measurement data for further processing.

Data operations are performed on selected areas of the data in the Data window. After clicking the  icon in the Data window, you can select an area. Clicking the Perform Operation button allows you to select, configure and run a data operation.

If no area is selected, you can perform an operation on all data in the window by selecting the operation from the Operations menu. This does not always provide satisfactory results—for example, the peak fitting operation can only fit one peak, not everything in a spectrum.

Note: Although you normally perform data operations on regions, you can perform data operations on the results of data operations.

You can see the parameters that were used in calculating the operation:

- Right-click the results node in the Files window and select Parameters from the context menu. A dialog will open showing the parameters.

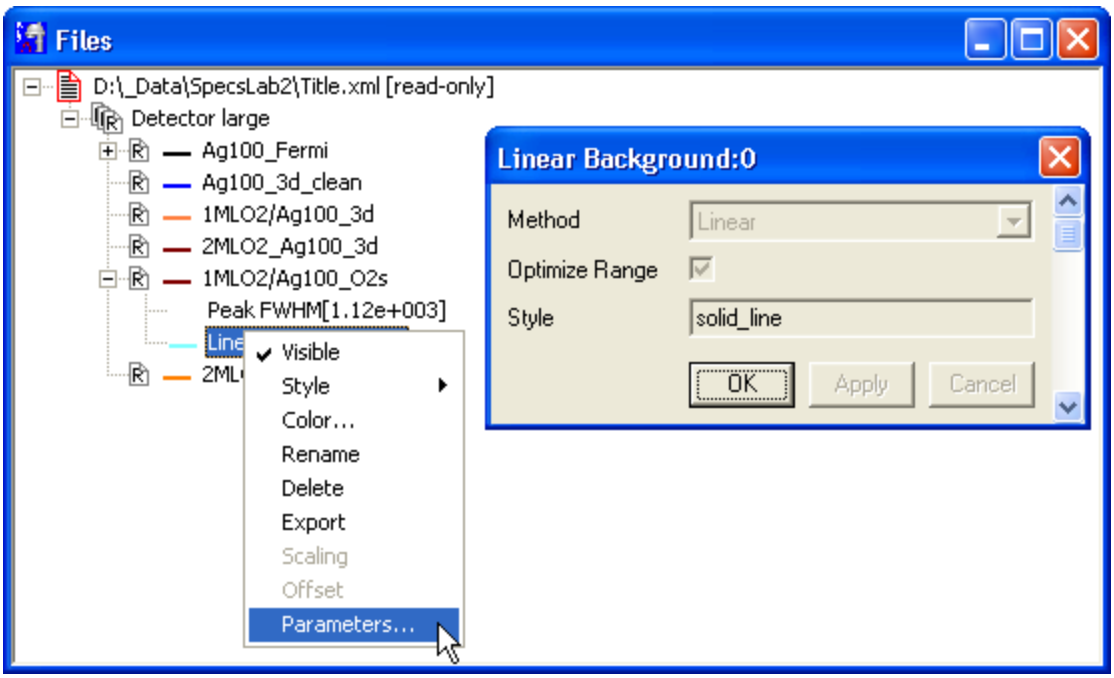


Figure 25: Data operation parameters

6.2 Background

The background setting allows you to subtract the background of a selected region according to a preset algorithm. When you run the background subtraction, the calculation is applied to the currently selected regions. Only the data selected in the Data window is used for the calculation—this means that you can select parts of your data for background subtraction.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run the background subtraction:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The background subtraction will be run separately on all selected regions.
2. Click the  icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the background subtraction is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Background from the drop-down list.
6. Click Parameters. The Background Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Background from the menu bar.

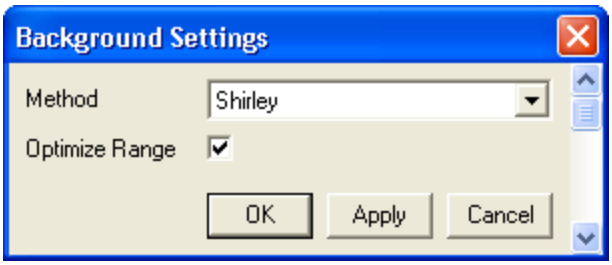


Figure 26: Background subtraction settings

7. Select an algorithm from the Method drop-down list. Further details about the options are provided below.
8. If desired, check the Optimize Range box. The algorithm optimizes the range within the displayed data and performs the subtraction based on this optimization. It reduces the background to the lowest reasonable level.
9. Click OK to accept your changes and close the dialog.
10. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Background from the menu bar.

11. Click the  button to return to the area selection settings.

Note: The background subtraction icon  in the data view toolbar allows you to view the effect of the background subtraction in the Data window..

The following paragraphs describe the available algorithms for background subtraction[1].

None

No algorithm is used. The results from this setting are a straight line at Intensity = 0.

Linear

This is a simple subtraction in which draws a straight line between two suitable points.

[1]You can find more details on this subject in "Practical Surface Analysis", D.Briggs and M.P.Seah, 2nd edition, Volume 1 (1990)

The endpoints are calculated by selecting several points from the extremes within the visible regions along the energy axis and performing a linear least square fit to those points. With the Optimize Range setting enabled, the extremes are picked which achieve the lowest reasonable background.

This kind of background makes no physical background.

Shirley

The Shirley background[1] determines the background intensity at a point by means of an iterative analysis.

The background at a given kinetic energy E(i) is proportional to the intensity area above the background between the given energy and the maximum energy boundary N.

Equation (2) shows the calculation method for the Shirley background.

$$b_i = k \sum_{j=i+1}^{N} p_j \tag{2}$$

This is run iteratively. In the first iteration the background is set to zero. In the i-th channel, the signal s_i is the sum of the background b_i and the peak intensity p_i. The calculation is repeated until the change in results is below the desired error. k is determined to fit the background at the high kinetic energy side.

The method assumes that the energy loss function for electron scattering is constant. As in the case of the linear background, the extremes correspond to the visible region or to the value determined through range optimization. The boundary comditions for the calculations are determined in the same manner as the extreme points for the linear background calculation.

Tougaard

A physical model of the background is based upon the elastic and inelastic loss processes in the solid. Tougaard and Sigmund showed[2] that if j(E) is the measured flux of emitted electrons at energy E from a homogenous solid, the primary excitation spectrum F(E) is given by:

$$F(E) = j(E) - B \int_E^{\infty} \frac{E' - E}{(C + (E' - E)^2)^2} j(E')dE' \tag{3}$$

6.3 Dead Time Correction

This operation corrects the measured data by dead time considerations. After each point is recorded, there is a dead time before the next point can be recorded. For an ideal counter with a non-extended dead time t, the measured count rate N' and the true count rate N is given by

[1] D.A.Shirley, "High-Resolution X-Ray Photoemission Spectrum of the Valence Bands of Gold", Phys. Rev. B, 5, 5, 4709 (1972)

[2] S.Tougaard and I.Sigmund, "Influence of elastic and inelastic scattering on energy spectra of electrons emitted from solids", Phys. Rev. B, 25, 4452 (1982)

$$N' = \frac{N}{1 + Nt} \tag{4}$$

The graph below shows the effect of dead time correction on a typical survey spectrum.

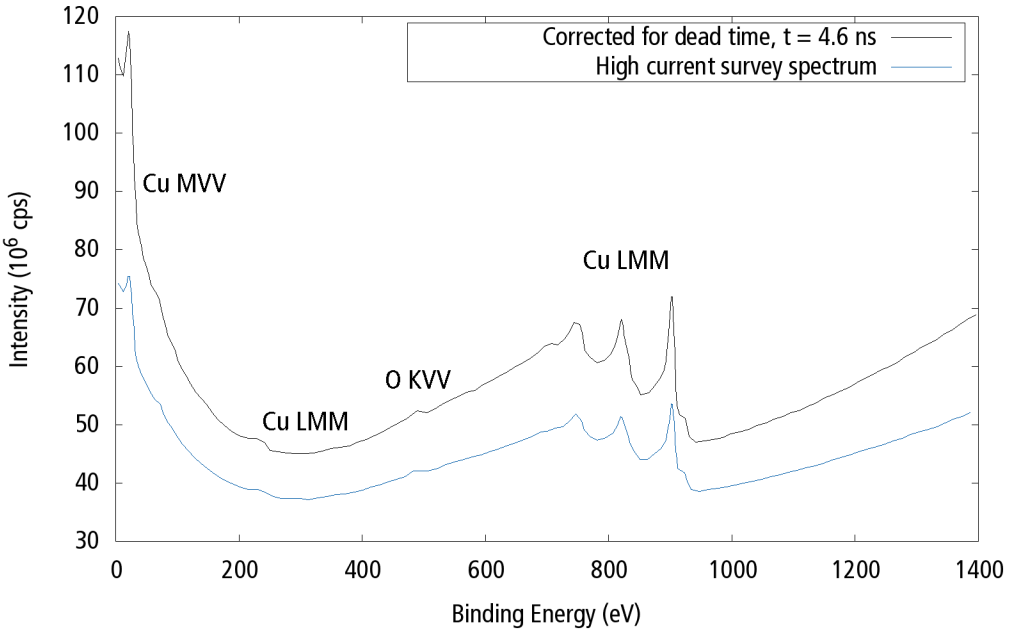


Figure 27: Illustration of dead time correction

To set and run the peak location:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The dead time correction will be run separately on all selected regions.
2. Click the  icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the dead time correction is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

4. Click the Perform Operation button.
5. Select Dead Time Correction from the drop-down list.
6. Click Parameters. The Dead Time Correction Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Dead Time Correction from the menu bar.

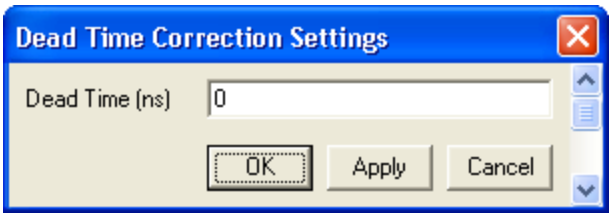


Figure 28: Dead time correction settings

7. Enter a time for the Dead Time in the field provided. This is the value t in the equation above.
8. Click OK to accept your changes and close the dialog.
9. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Dead Time Correction from the menu bar.

10. Click the <- button to return to the area selection settings.

6.4 Despiking

The despike filter removes spikes from spectra which may occur due to some external event (e.g. sparks). By default, the threshold for searching for spikes is six times the expected noise level (root mean square noise). Spikes will be replaced by the mean values of the neighbor values by additionally adding some typical noise distribution.

When you run the despiking operation, the calculation is applied to the currently displayed regions. Only the data selected in the Data window is used for the calculation—this means that you can select parts of your data for background subtraction.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button — selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run the despiking operation:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The despiking will be run separately on all selected regions.
2. Click the icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the despiking is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Despiking from the drop-down list.
6. Click Parameters. The Despiking Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Despiking from the menu bar.

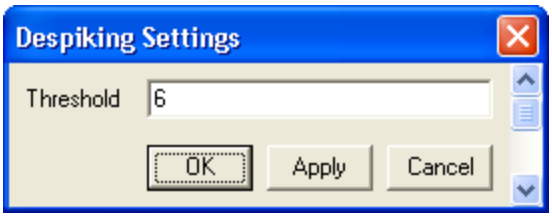


Figure 29: Despiking settings

7. Enter a value in the Threshold field. A higher value makes the algorithm less sensitive to spikes, i.e. the spikes need to be higher compared to the noise level.
8. Click OK to accept your changes and close the dialog.
9. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Despiking from the menu bar.

10. Click the <- button to return to the area selection settings.

6.5 Fermi Edge

The Fermi edge operation calculates a fit to the Fermi edge. As well as finding the position, you can use it for energy scale calibration or for finding the FWHM of the Fermi edge. Figure 30 shows a fit with the calculated results.

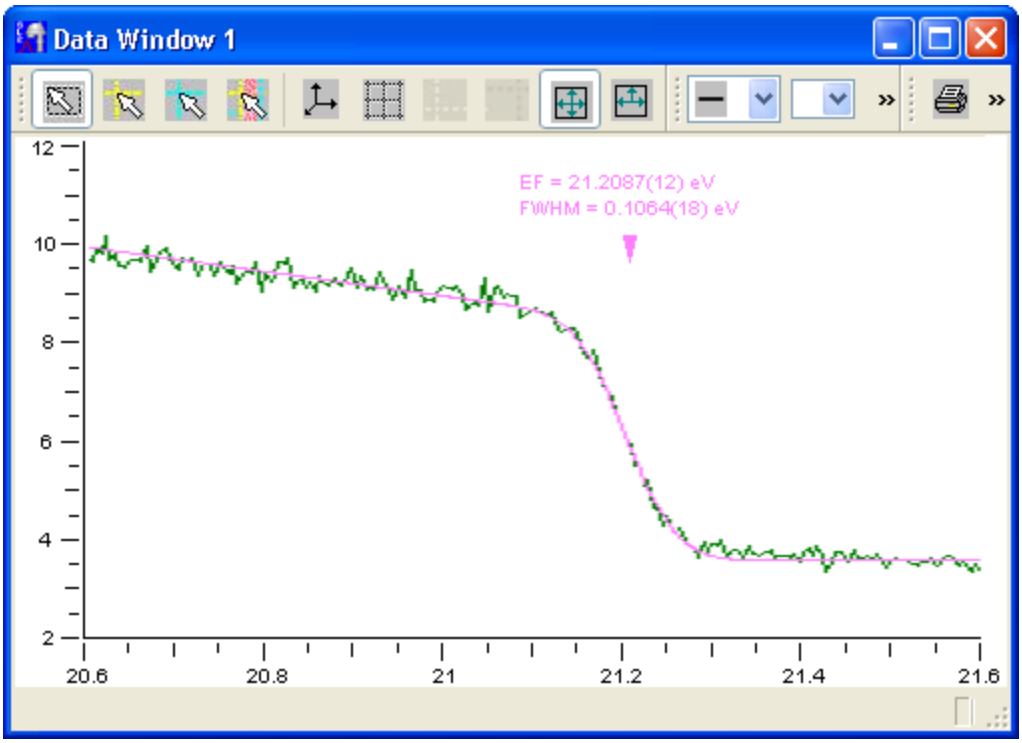


Figure 30: Fermi edge fit

When you run the Fermi edge algorithm, the calculation is applied to the currently displayed regions. Only the data selected in the Data window is used for the calculation. You should therefore make sure that the area containing the Fermi edge is displayed in the Data window before starting the calculation. Noisy data or "unexpected" slopes can cause the algorithm to fail.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run the Fermi edge calculation:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The Fermi edge operation will be run separately on all selected regions.
2. Click the icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the Fermi edge fit is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Fermi Edge from the drop-down list.
6. Click Parameters. The Fermi Edge Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Fermi Edge from the menu bar.

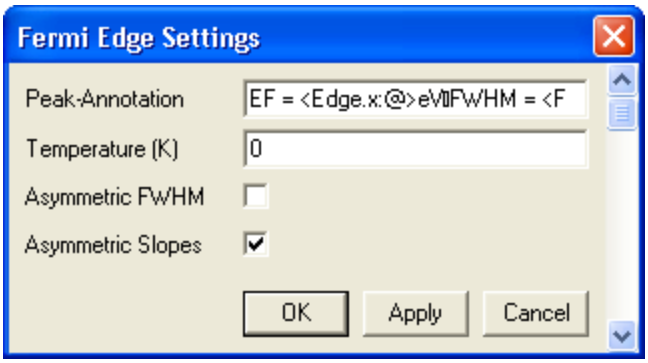


Figure 31: Fermi edge settings

7. Set an expression in the Peak Annotation field. This defines the text and results that will appear in the Data window. You can find details of how to write these expressions in "Annotation Syntax" on page 67.
8. Enter the sample temperature used to obtain the results in the Temperature field.
9. Check the Asymmetric FVWM box to calculate the FWHM of an asymmetric slope. The algorithm will take account of the full width of the slope when determining the FWHM.
10. Check the Asymmetric Slopes box if the slope is asymmetric. The algorithm will calculate the fit assuming that the top and bottom parts of the slope have different shapes.
11. Click OK to accept your changes and close the dialog.
12. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Fermi Edge from the menu bar.

13. Click the <- button to return to the area selection settings.

6.6 Linear Operations

Using linear operations, you can scale and shift your data on the X and Y axes. Figure 32 shows a data set scaled in intensity and shifted in energy.

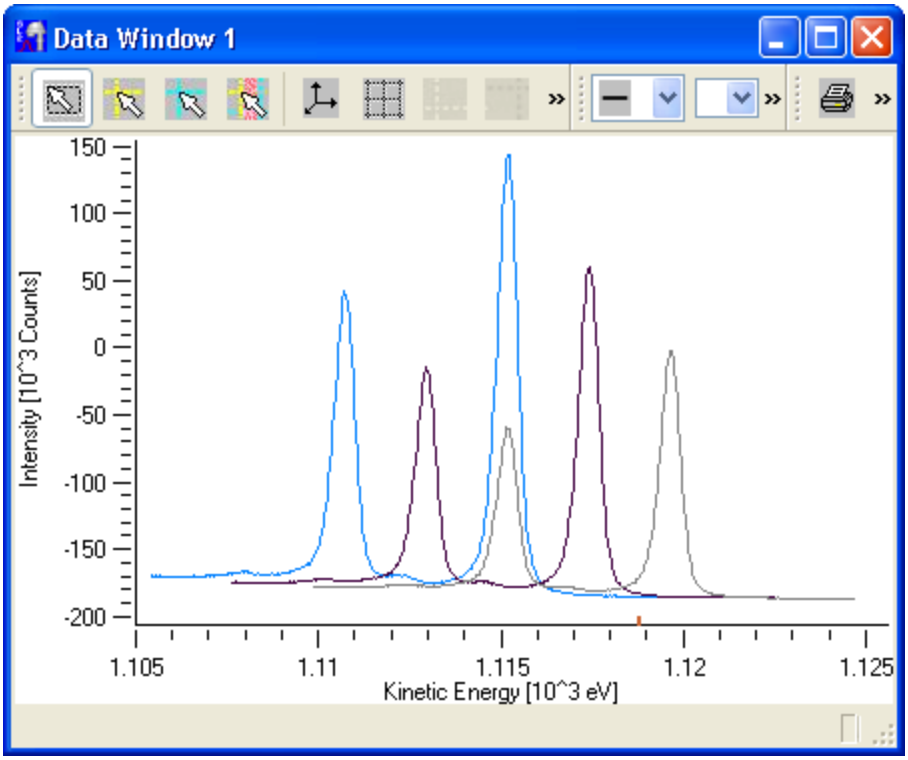


Figure 32: Linear operations

When running linear operations, the calculation is applied to the currently selected regions. Only the data selected in the Data window is used for the calculation—this means that you can perform the scaling and shifting on a selected area of your data.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run a linear operation:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The linear operation will be run separately on all selected regions.
2. Click the icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the linear operations is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.

5. Select Linear Operations from the drop-down list.
6. Click Parameters. The Linear Operations Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Linear Operations from the menu bar.

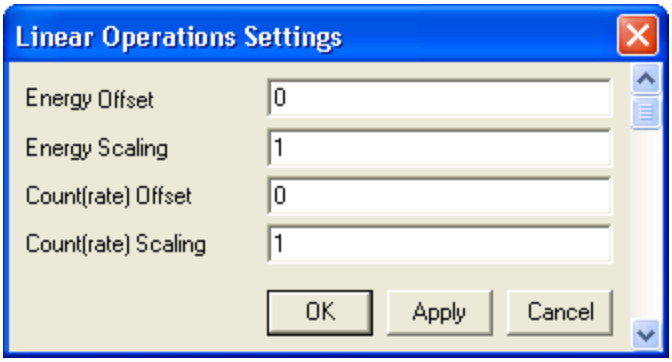


Figure 33: Liner operations settings

7. Enter a value into the Energy Offset field. This moves the data on the X axis. If you set it to 0, no change is made.
8. Enter a value into the Energy Scaling field. This has the effect of making peaks narrower or wider. If you set it to 1, no change is made.
9. Enter a value into the Count(rate) Offset field. This moves the data up and down on the Y axis. If you set it to 0, no change is made.
10. Enter a value into the Count(rate) Scaling field. This has the effect of making peaks higher or lower. If you set it to 1, no change is made.
11. Click OK to accept your changes and close the dialog.
12. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Linear Operations from the menu bar.

13. Click the <- button to return to the area selection settings.

6.7 Noise Settings

The Noise operation estimates the intensity scaling for CCD detector measurements. The product of the current set "Intensity Scale" with the square of the "Poisson Factor" gives an estimation of the correct "Intensity Scale".

When you run the noise operation, the calculation is applied to the currently selected regions. Only the data selected in the Data window is used for the calculation—this means that you can select parts of your data for background subtraction.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button — selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run the Noise operation:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The noise operation will be run separately on all selected regions.
2. Click the  icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the noise operation is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Noise from the drop-down list.
6. Click Parameters. The Noise Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Noise from the menu bar.

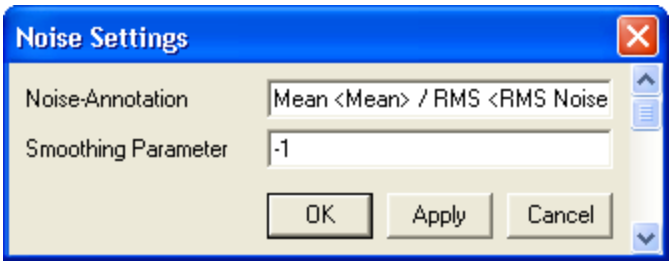


Figure 34: Noise settings

7. Set an expression in the Peak Annotation field. This defines the text and results that will appear in the Data window. You can find details of how to write these expressions in "Annotation Syntax" on page 67.
8. Enter a value in the Smoothing Parameter field.
9. Click OK to accept your changes and close the dialog.
10. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Noise from the menu bar.

11. Click the  button to return to the area selection settings.

6.8 Peak FWHM

The Full Width at Half Maximum operation uses a smoothing spline calculation. It automatically performs a background subtraction before determining the peak height and width.

When you run the Peak FWHM operation, the calculation is applied to the currently selected regions. Only the data selected in the Data window is used for the calculation—this means that you can select parts of your data for background subtraction.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

The results of this operation overwrite previously calculated FWHM data.

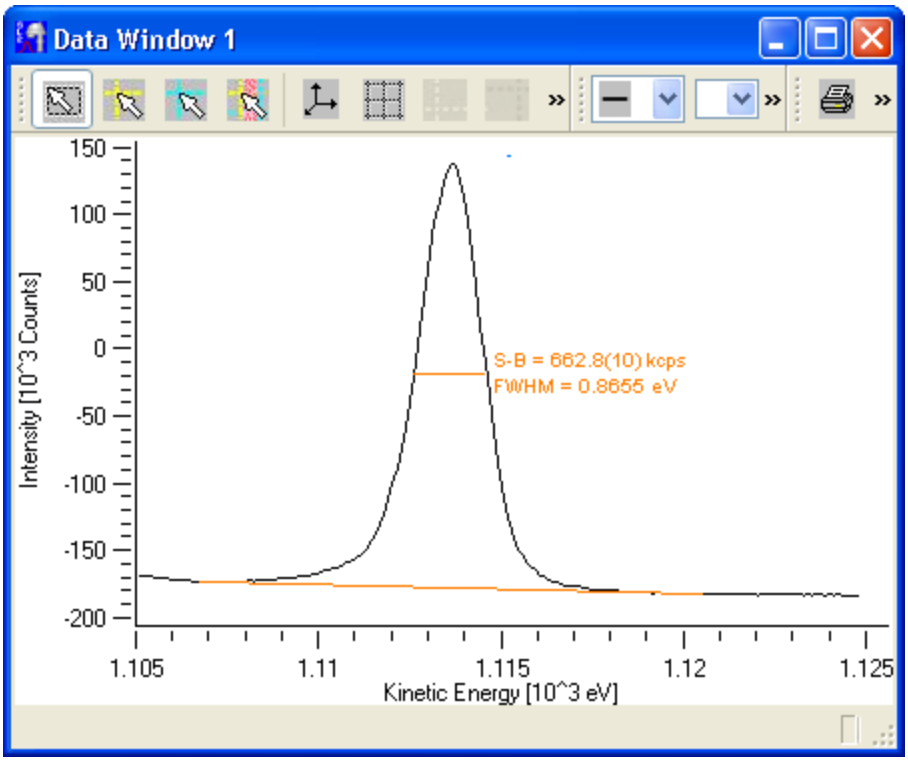


Figure 35: Peak FWHM

Note: The spectrum should be displayed with the Data button selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run the Peak FWHM operation:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The peak FWHM operation will be run separately on all selected regions.
2. Click the icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the peak FWHM operation is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Peak FWHM from the drop-down list.
6. Click Parameters. The Peak FWHM Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Peak FWHM from the menu bar.

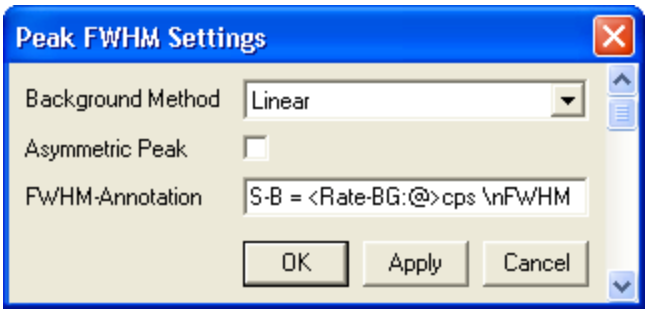


Figure 36: Peak FWHM settings

7. Select an algorithm for background subtraction from the Background Method drop-down menu. The available methods are described in "Background" on page 50.
8. Click the Asymmetric Peak box to take account of an asymmetric peak shape.
9. Set an expression in the FWHM Annotation field. This defines the text and results that will appear in the Data window. You can find details of how to write these expressions in "Annotation Syntax" on page 67.
10. Click OK to accept your changes and close the dialog.
11. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Peak FWHM from the menu bar.

12. Click the <- button to return to the area selection settings.

6.9 Peak Location

The Peak Location operation fits a quadratic function to the topmost region of the peak for calibration purposes (peak location), following the procedure of Anthony and Seah[1].

When you run the peak location, the calculation is applied to the currently selected regions. Only the data displayed in the Data window is used for the calculation.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button — selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

[1] M.T. Anthony and M.P. Seah, "XPS: Energy calibration of electron spectrometers. 1—An absolute, traceable energy calibration and the provision of atomic reference line energies", Surf. Interface Anal . 6, 95 (1984); M.P. Seah, "Measurement: AES and XPS", J. Vac. Sci. Technol. A 3, 1330 (1985)

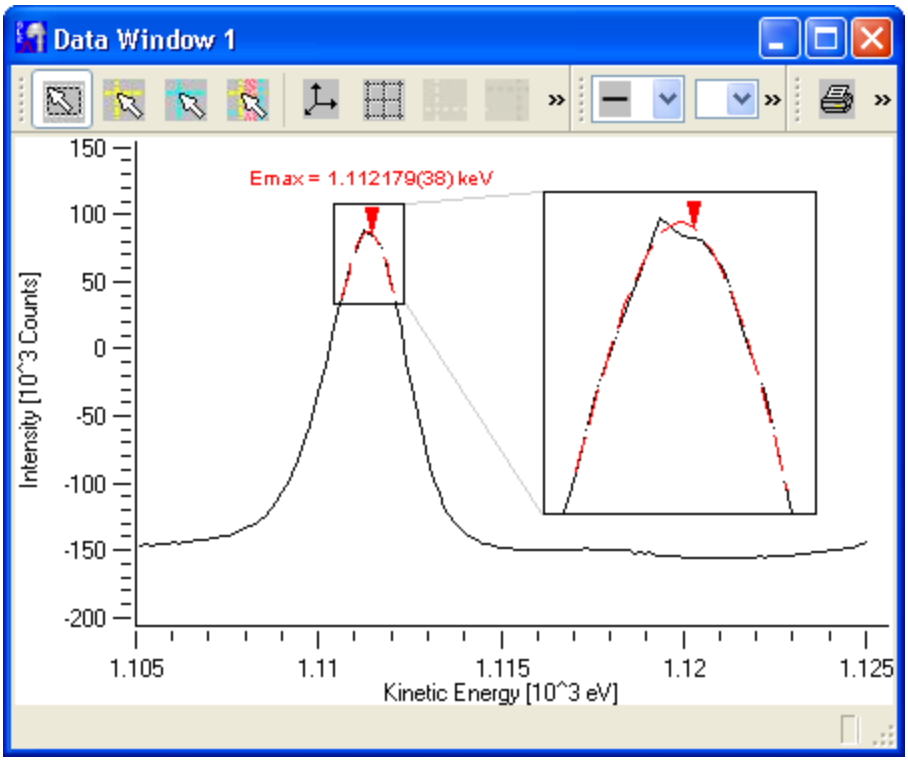


Figure 37: Peak location

Equation (5) shows how the peak location is calculated.

$$I_x = I_c \cdot \exp\left(-4\ln 2 \cdot \left(\frac{x-c}{FWHM(1 \pm \alpha)}\right)^2\right) + S \cdot (x-c) + B_g \quad (5)$$

where:

- I_x is the intensity at x
- I_c is the intensity at the center
- c is the peak maxima value of x
- α is an asymmetric factor
- S is the sloping background value
- B_g is the constant background intensity

Note: You should not use a sloping background when fitting peaks for energy scale calibration. As discussed by Powell[1], this can introduce systematic errors.

To locate the position of peaks in spectra that have multiple components (e.g. for the identification of chemical states), you should include an appropriate background and with appropriate functions to obtain satisfactory results.

To set and run the peak location:

1. Select regions:

[1] C.J. Powell, "Energy Calibration of X-ray Photoelectron Spectrometers. II. Issues in Peak Location and Comparison of Methods", Surf. Interface Anal. 25, 777-787 (1997)

- You can select a single region in the Files window.
- You can select multiple regions in the Regions window. The peak location will be run separately on all selected regions.

2. Click the  icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the peak location is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Peak Location from the drop-down list.
6. Click Parameters. The Peak Location Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Peak Location from the menu bar.

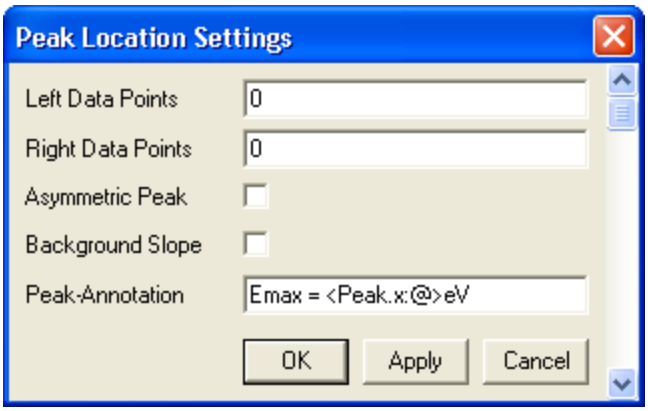


Figure 38: Peak location settings

7. Set values in the Left Data Points and Right Data Points fields. These values determine how many points on each side of the maximum are used in the calculation. Setting the value to zero means that the number will be selected automatically—top 5% of the peak and at least enough points for fit.
8. Check the Asymmetric Peak box to take account of an asymmetric peak shape.
9. Check the Background Slope box if there is a sloping background under the peak.
10. Set an expression in the FWHM Annotation field. This defines the text and results that will appear in the Data window. You can find details of how to write these expressions in "Annotation Syntax" on page 67.
11. Click OK to accept your changes and close the dialog.
12. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Peak Location from the menu bar.

13. Click the  button to return to the area selection settings.

6.10 Savitsky Golay Smooth

The idea behind data smoothing is the signal is slowly varying and also corrupted by noise. Sometimes it can be useful to replace each data point by a local average of surrounding data points. Since nearby points measure very nearly the same underlying signal, averaging can reduce the level of noise without significant change the signal (and the containing information) obtained.

SpecsLab2 offers a particular type of low-pass filter, well-adapted for data smoothing, called Savitzky-Golay[1].

Savitzky-Golay filters were initially (and are still often) used to render visible the relative widths and heights of spectral lines in noisy spectrometric data. A digital filter is applied to a series of equally spaced data values $f_i = f(t_i)$, where $t_i = t_0 + i\,\Delta$ for some constant sample spacing Δ and $i = \ldots -2, -1, 0, 1, 2, \ldots$. The simplest type of digital filter replaces each data value f_i by a linear combination g_i of itself and some number of nearby neighbors,

$$g_i = \sum_{n=-nL}^{nR} c_n \cdot f_{i+n} \tag{6}$$

Here nL is the number of points used to the left of a data point i , i.e., before it, while nR is the number used to the right, i.e., after. As a starting point for understanding Savitzky-Golay filters, consider the simplest possible averaging procedure: For some fixed nL = nR, compute each g i as the average of the data points from $f_i - nL$ to $f_i + nR$. This is sometimes called moving window averaging and corresponds to Equation (6) with constant $c_n = 1 / (nL + nR + 1)$. If the underlying function is constant, or is changing linearly with time (increasing or decreasing), then no bias is introduced into the result.

Higher points at one end of the averaging interval are usually balanced by lower points at the other end. A bias is introduced, however, if the underlying function has a non-zero second derivative. At a local maximum, for example, moving window averaging always reduces the function value. In the spectrometric application, a narrow peak has its height reduced and its width increased. Since these parameter are themselves of physical interest, the bias introduced is distinctly undesirable.

The idea of Savitzky-Golay filtering is to find filter coefficients cn that preserve higher moments. SpecsLab2 fits a polynomial of degree M in i, to the values $f_i - nL \ldots f_i + nR$. For a more detailed description please refer to the paper by Savitzky and Golay.

For another purpose, namely the computation of numerical derivatives, the useful choice is Derivation Order = 1. The filtered first derivative is the convolution divided by the step size. For derivatives, you should usually set a polynomial order of 4 or larger.

[1] A. Savitzky and M.J.E. Golay. "Smoothing and differentiation of data by simplified least square procedures", Anal. Chem., 36(8), 1627–1639, 1964

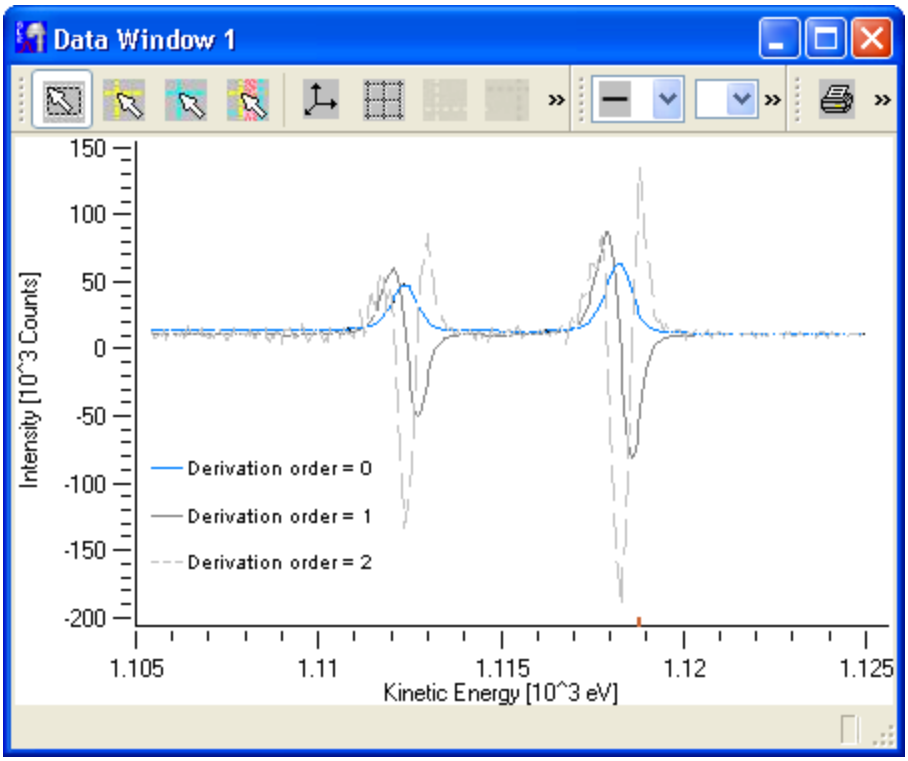


Figure 39: Derivatives of data in Savitzky Golay smoothing

When you run Savitzky Golay smoothing, the calculation is applied to the currently selected regions. Only the data selected in the Data window is used for the calculation.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run theSavitzky Golay smoothing:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The Savitsky Golay smoothing will be run separately on all selected regions.
2. Click the icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the smoothing is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Savitzky Golay Smooth from the drop-down list.
6. Click Parameters. The Savitzky Golay Smooth Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Savitzky Golay Smooth from the menu bar.

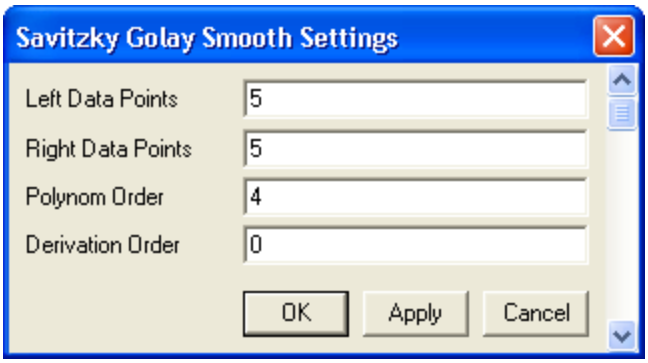


Figure 40: Savitzky Golay smoothing settings

7. Set values in the Left Data Points and Right Data Points fields. These values determine how many points on each side of the maximum are used in the calculation. Setting the value to zero means that the number will be selected automatically—top 5% of the peak and at least enough points for fit.
8. Set a value for the polynomical order. As a guide, low values provide better smoothing on broad features, while higher values preserve height and width of narrow features. You may need to iterate the smoothing to find the best value for your data.
9. Enter a value for the Derivation Order. Setting this to zero smooths the data; an order of 1 applies a first derivative, etc.
10. Click OK to accept your changes and close the dialog.
11. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Savitzky Golay Smooth from the menu bar.

12. Click the <- button to return to the area selection settings.

6.11 Smoothing Spline

The smoothing spline operation calculates a interpolating natural cubic spline curve which smoothes a given set of data points, using statistical considerations to determine the amount of smoothing required. The smoothing factor can be set (0–1) to determines the degree of smoothing.

When you run the smoothing spline operation, the calculation is applied to the currently selected regions. Only the data selected in the Data window is used for the calculation—this means that you can select parts of your data for background subtraction.

Note: If you do not select a region, the data operation will be performed on all data in the Data window.

Note: The spectrum should be displayed with the Data button — selected in the Data View toolbar. This displays the sum of all channels. The operation cannot work with the multiple data sets from individual channels.

To set and run the smoothing spline operation:

1. Select regions:
   - You can select a single region in the Files window.
   - You can select multiple regions in the Regions window. The smooting will be run separately on all selected regions.

2. Click the  icon in the Data window.
3. Use the mouse to select an area in the Data window. The active region for the smoothing is shaded pink. You can fine-tune this region by entering new values in the Start and End fields, or by clicking the up and down arrows in the fields.
4. Click the Perform Operation button.
5. Select Smoothing Spline from the drop-down list.
6. Click Parameters. The Smoothing Spline Settings dialog will open.

Note: Alternatively, you can open the settings dialog by selecting Operations/ Settings/ Smoothing Spline from the menu bar.

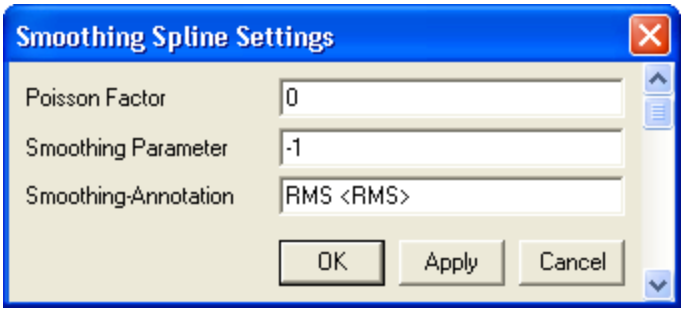


Figure 41: Smoothing spline settings

7. Enter a value in the Poisson Factor field between 0–1.
8. Enter a value in the Smoothing Parameter field. Smaller values match the data better, larger values provide more smoothing.
9. Set an expression in the Smoothing Annotation field. This defines the text and results that will appear in the Data window. You can find details of how to write these expressions in "Annotation Syntax" on page 67.
10. Click OK to accept your changes and close the dialog.
11. Click Perform to run the calculation with your settings.

Note: You can also run the calculation by selecting Operations/ Smoothing Spline from the menu bar.

12. Click the  button to return to the area selection settings.

6.12 Annotation Syntax

Some of the data operations display text on the chart. This is usually a summary of the calculation and some explanatory text. The information displayed is determined by a command string in the settings dialog for the operation. You can modify this string to change the information.

The following data operations produce output that you can change in this way:

- Fermi Edge
- Peak FWHM
- Peak Location
- Smoothing Spline

The syntax used to write annotations is similar to the `printf` command of the C language.

Note: Each of the above operations has a pre-defined setting. You can use these as examples and as a basis for further modification.

Syntax

The annotation syntax is summarized as follows:

```
< x [ . m ] [ *f ] : { @ [ n ] | [n] . g }>
```

Note: Square brackets indicate optional terms; the pipe symbol | indicates OR.

Item	Description
x	Parameter name. This depends on the data operation in use. A summary of all available parameter names is shown in Table 5.
m	[value | error].
*f	Scale factor (useful if kcps instead of cps etc).
@	The @ sign indicates that the default number format is to be used when displaying results.
n	Field width (number of digits, width = digits + sign + separator sign).
g	Fixed-point arithmetic.

Table 4: Syntax of annotations

Property names

To find the available parameter names for a data operation:

1. Right-click the results of the data operation in the Files or Regions window and select Properties from the context menu. A dialog will open.

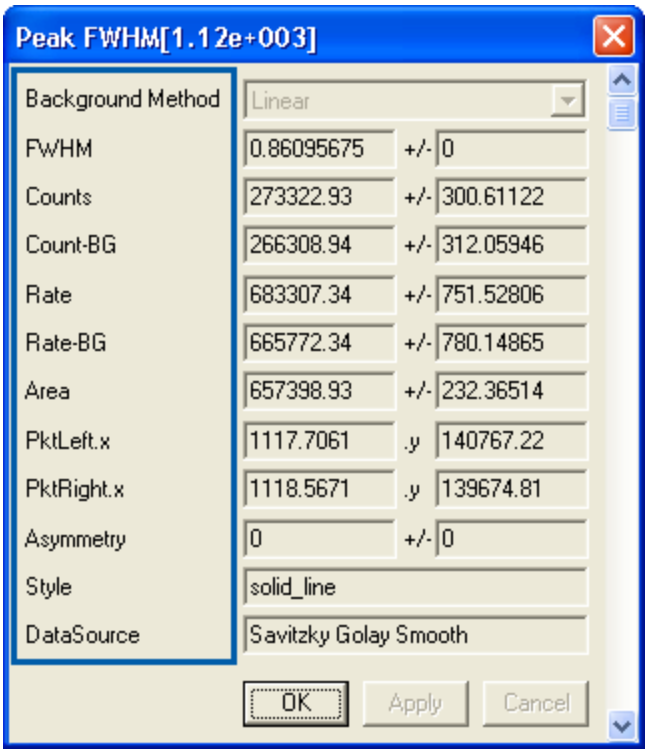


Figure 42: Property names for annotation—Peak FWHM

2. The available parameter names for this operation are listed in the diagram, as shown in Figure 42. A summary of parameters is shown in Table 5.
3. Click OK to close the dialog.

Fermi Edge	Peak FWHM	Peak Location	Smoothing Spline
Edge.x	Background Method	Left Data Points	Poisson Factor
Edge.y	FWHM	Right Data Points	Smoothing Factor
FWHML	Counts	Peak.x	RMS
FWHMR	Counts.BG	Peak.y	Style
FWHM (12 to 88)	Rate	Asymmetry	DataSource
FWHM (16 to 84)	Rate-BG	Background Slope	
FWHM (20 to 80)	Area	Style	
Background	PktLeft.x	DataSource	
Background Slope Left	PktRight.x		
Background Slope Right	Asymmetry		
Height	Style		
Temperature	DataSource		
Q			
Reduced Chi2			
Style			
DataSource			

Table 5: Parameter names in annotations

Default number format

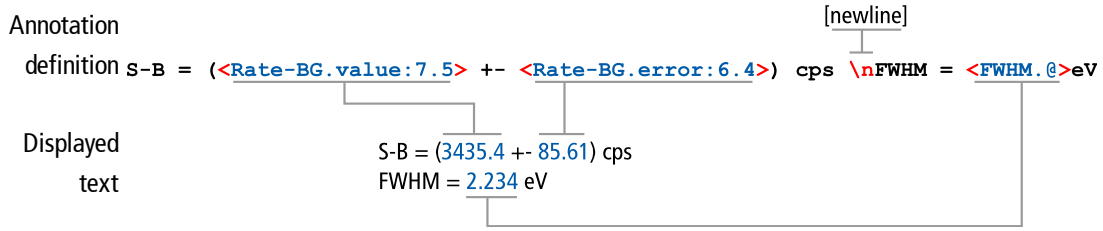
When using the default number format (with the @ symbol), the value is scaled to lie between 1 and 1000 (exclusive) and the prefix used to form decimal multiples and submultiples of the unit is set accordingly. Additionally the standard deviation appears in parenthesis in a standard abbreviated form. This is the rounded two digit integer value of the standard deviation after normalization by the magnitude of the parameter value's last digit.

Some examples of how numbers are displayed in the standard format:

- (3435.3518 ± 85.613096) cps is abbreviated to 3.435(86) kcps
- (881.62159 ± 0.00087205) eV is abbreviated to 881.62159(87) eV
- (11403390.1 ±5130.74971) cps is abbreviated to 11.4034(51) Mcps
- (2.668437 ± 0.00006868) eV is abbreviated to 2.668437(69) eV

Example

The following example shows how a typical definition and how it relates to displayed text.



Note: The default settings in the software for data operation provide further examples.

Chapter 7
Visualization in the Data Window

There are two ways of displaying data in SpecsLab2:

- Data window—2D or 3D charts.
- 2D viewer—images such as those obtained from a CCD detector.

This chapter describes the options for displaying data and how to change the appearance. The section on the 2D viewer also covers the operations you can perform on data, such as fitting a Gaussian.

Note: The more extensive data operations available for the Data window are described in a separate chapter—see "Data Operations" on page 49 for details.

7.1 Data Window

The Data window contains a chart that displays data from selected regions. You can choose which data is shown in the Data window; you can also create additional Data windows in order to compare spectra.

Figure 43 shows the available options for visualization.

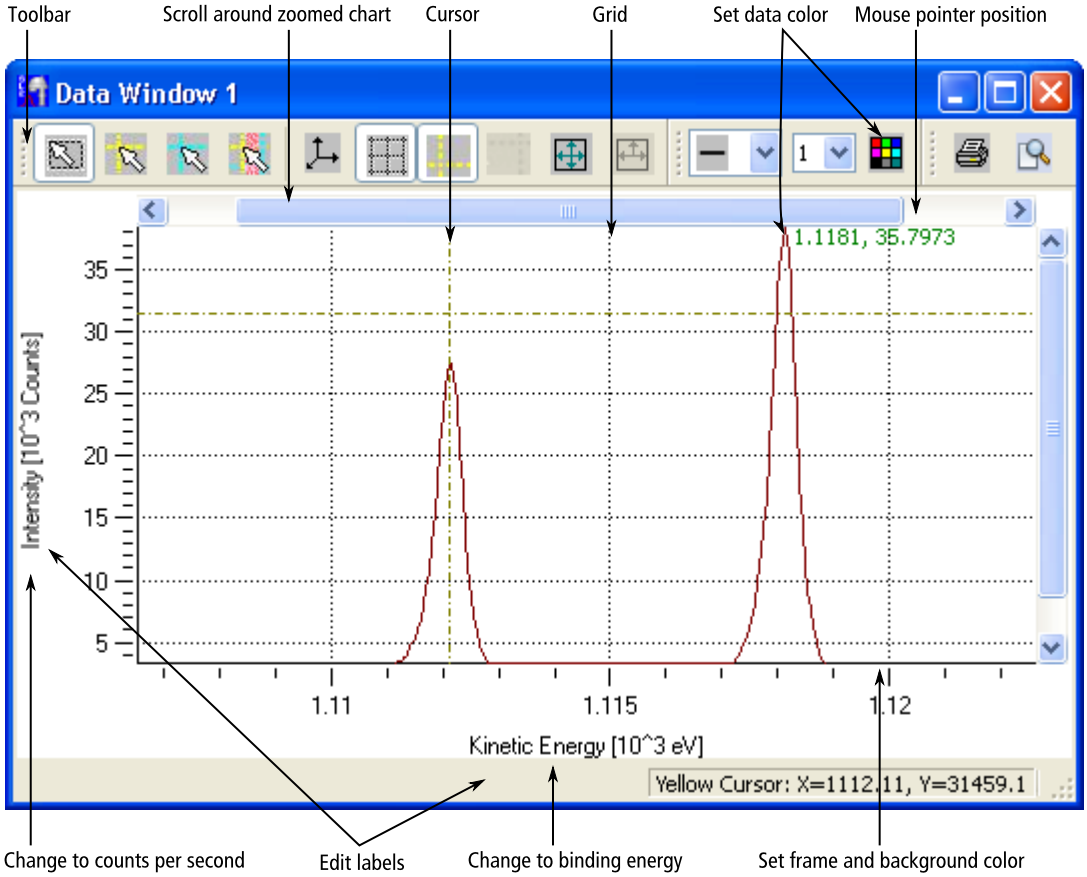


Figure 43: Visualization options in the Data Window

Note: The following sections only describe changes that affect the appearance of the Data window. Operations which involve calculations are presented in "Data Operations" on page 49.

To add a region to a Data Window:

1. Select the Data window. If no window is open, select Window/ New Data Window from the menu bar.
2. In the Files or Regions window, right-click the region you want to display and select Visible from the context menu. Alternatively, you can double-click the region.
3. If necessary, click the icon in the toolbar. This redraws the axes of the chart so that all data can be seen.

7.1.1 Zooming and Autoscaling in the Data Window

You can zoom into an area of the chart in order to inspect items of particular interest:

1. Click the icon to activate zoom mode.
2. Click and drag the mouse to form a rectangle in the Data window. When you release the mouse button, the chart shows the selected area. Scroll bars on the top and right side of the chart allow you to move to other areas of the chart.
3. To display the complete chart again, double click in the chart area. Alternatively, click the icon in the tool-bar.

Note: CTRL + right-click zooms out in steps.

The button rescales the chart so that Y = 0 is shown.

7.1.2 Setting the Cursor Position

You can add cursors to the chart in the Data window. A cursor is a cross that allows you to look at X and Y values. Typically, you can use them for checking peak positions and heights.

There are two cursors that can be set independently. A feature allows you to set both cursors simultaneously—this selects an area of the data.

When setting cursors, note the following points:

- If you select another mouse tool (e.g. the Zoom mode), the cursor is sticky and remains in its position until you reactivate the cursor.
- The  and  icons toggle the display of the cursors in the chart.
- If you display both cursors at the same time in the chart, the status bar shows the difference between the positions of the two centers.

To show a cursor in the chart:

1. Click the  icon or the  icon. These activate the yellow and blue cursors respectively.
2. Click a point in the chart. The cursor will be displayed with the center at the selected point. The status bar at the bottom of the Data window will show the coordinates of the cursor center point.

7.1.3 Selecting an Area

You can set the position of both cursors with one action. In this case, the area between the two X coordinates is also displayed. You can perform various actions on this region, such as data operations and creating a new region based on the selected area.

To select an area with cursors:

1. Click the  icon.
2. Click a point in the chart and drag the mouse to a second point. When you release the mouse button, both cursors are set. You will notice the following points:
   - The X area between the two cursors is shaded pink.
   - Start and End fields appear to show the X coordinates of the two cursors. You can change these values by clicking the up/ down arrows or by entering a new value directly.
   - Click the Perform Operation button to select and run a data operation—see "Performing Data Operations" on page 49 for more details. Click the  button to return to the main options.
   - Click the Create Region button to create a new region based on the data. You can enter a name for the region and click Create Region—the new region is added to the group that contains the currently selected region in the Files window. Click the  button to return to the main options.

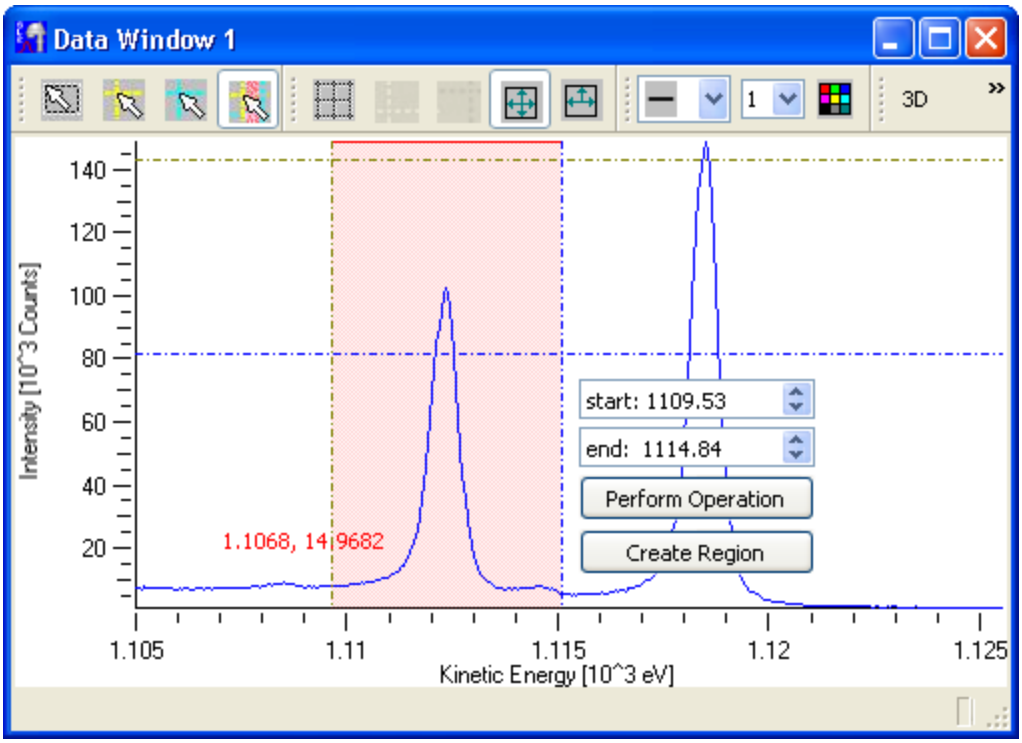


Figure 44: Selecting an area in the Data Window

7.1.4 Changing the Y Axis Display

You can set the Y axis so that it either shows the absolute number of counts or the count rate in counts per second:

- Click the cps icon in the Data View toolbar in the main window. This toggles the Y axis between absolute counts and count rate.

You can change the label on the Y axis in the Diagram Settings dialog—see "Setting Labels" on page 75.

7.1.5 Changing the X Axis Display

You can set the X axis so that it either shows kinetic energy or binding energy:

- Click the E_B icon in the Data View toolbar in the main window. This toggles the X axis between kinetic energy and binding energy. You need to make sure that the excitation energy is correctly set up in the source server (see "Sources" on page 12) so that the binding energy can be calculated.

Please note the following:

- This has a greater effect than simply changing the display of the X axis. The way you define regions is also affected—you need to enter binding energies rather than kinetic energies. See "Defining Regions" on page 32 and the descriptions of each analysis mode for more information.
- You can set the label for the X axis in the Diagram Settings dialog—see "Setting Labels" on page 75.

7.1.6 Setting Color and Appearance of Data

There are a number of different linestyles and data markers that you can use to display your data. You can access these in the following ways:

- By selecting a line or point style from the drop-down list in the Data window toolbar. The style is applied to the currently selected region.
- By right-clicking the region you want to change in the Regions View or Files View and selecting an item from the Style context menu.

A second drop-down list in the Data window toolbar, containing numbers, allows you to set the line thickness or point size. This setting has no effect on the point style "Dots".

Note: You can select a data marker style *or* a linestyle. You cannot select, for example, a dotted line with filled square data points.

An overview of the available linestyles and data markers in the style toolbar is shown below.

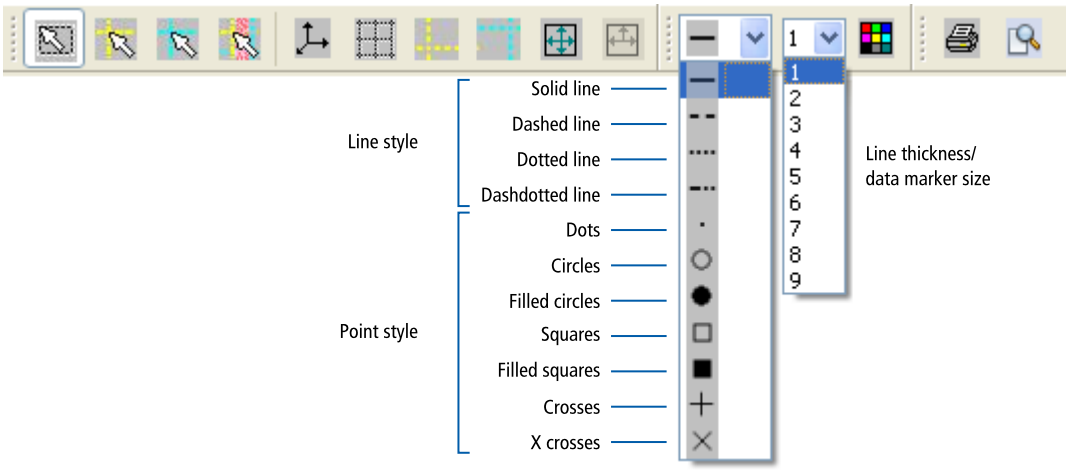


Figure 45: Setting linestyles in the Styles toolbar

You can change the colors for better contrast and appearance. The color palette is a normal MS Windows dialog for selecting or defining colors.

To open the color palette, use one of the following methods:

- Select a region in the Regions View or Files View and click the icon in the toolbar. The color will be applied to the selected region.
- Right-click the desired region in the Regions View or Files View and select Color from the context menu.

7.1.7 Displaying the Grid in the Data Window

You can switch on a grid to help you judge the position and height of peaks in the spectrum:

- Click the grid icon in the toolbar. This button toggles the display of the grid.

The grid lines are shown for major ticks on the axes. The intervals between the major ticks depend on the scaling of the plot—see "Zooming and Autoscaling in the Data Window" on page 72.

7.1.8 Setting Labels

You can change the labels on the X and Y axes and set a title for your chart. The Diagram Settings dialog contains all the information for these labels.

To open the Diagram Settings dialog:

- Select View/ Diagram Settings from the menu bar. The tabs in the Diagram Settings dialog are described below.

Title

The Title tab contains the following settings:

- Title—a title for your chart, displayed above the chart in the center.
- Print Info—a comment that is displayed in the page header when the chart is printed.

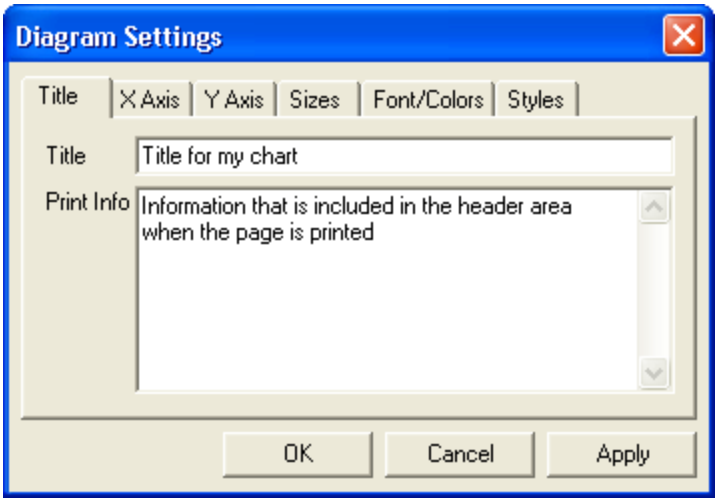


Figure 46: Diagram Settings dialog: Title tab

X Axis

There are a number of measurement modes which can lead to different parameters being set on the X axis. This tab allows you to set all of the possible labels. The text will be displayed when the parameter is plotted on the X axis for a measurement.

Note: The Restore Defaults button returns all settings to pre-defined values.

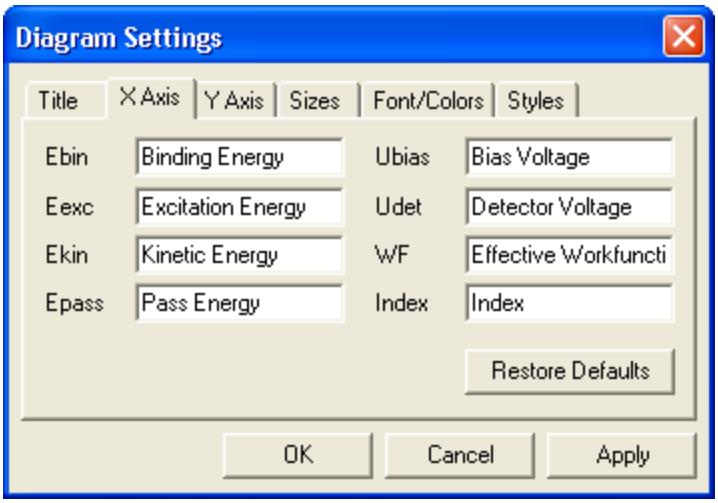


Figure 47: Diagram Settings dialog: X Axis tab

Y Axis

You can switch between displaying absolute counts and counts per second on the Y axis. The fields in this tab allow you to define the name of the Y axis as well as the units that are displayed for each of the two display modes.

Note: The Restore Defaults button returns all settings to pre-defined values.

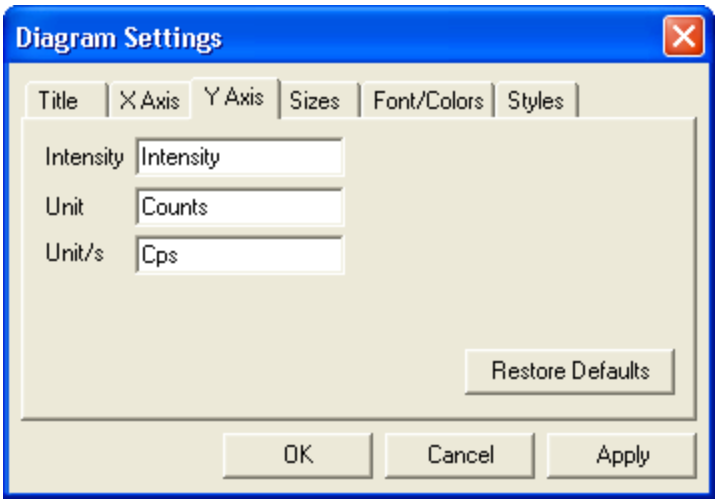


Figure 48: Diagram Settings dialog: Y Axis tab

Sizes

The Sizes tab is used to set the size of the chart for printing. See "Defining Print Settings" on page 90 for further details.

The Minimum Screen Size setting determines the minimum size you can set the window by resizing. Scrollbars appear on the window once this minimum size is achieved. The size is set in mm—this assumes a screen resolution of 72 dpi.

Font/ Colors

You can define the following properties in the Font/ Colors tab:

- Font—the standard MS Windows font selector opens, allowing you to define the font used for all labels in the chart.
- Foreground—the standard MS Windows color palette allows you to select the color properties of the text and chart frame.
- Background—the standard MS Windows color palette allows you to select the background color of the chart.

Note: The Restore Defaults button returns all settings to pre-defined values.

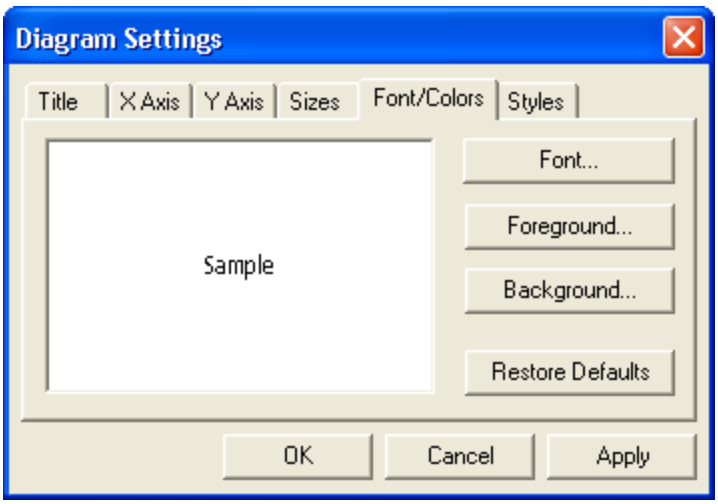


Figure 49: Diagram Settings dialog: Font/ Colors tab

Styles

The Styles tab contains the following settings:

- Ekin descending—sets the X axis so that kinetic energy decreases from left to right.
- Ebin descending—sets the X axis so that binding energy decreases from left to right.
- Show Z axis—displays the Z axis.
- Show grid—displays the grid on the plot.
- Autoscale—switches on autoscale to display all data in the plot.

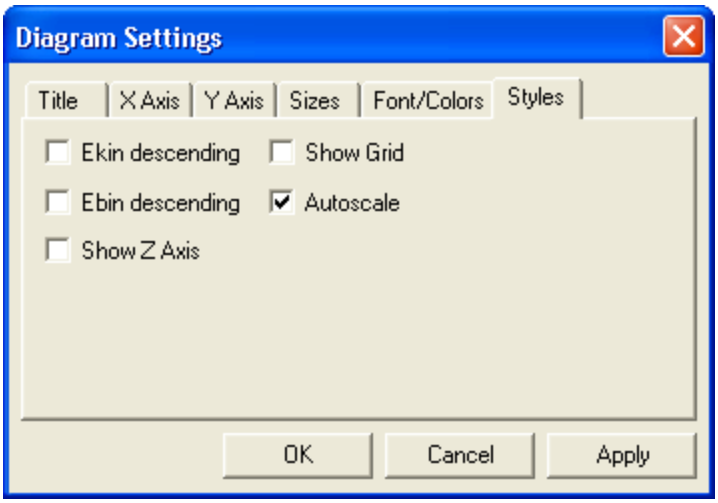


Figure 50: Diagram Settings dialog: Styles tab

7.1.9 Displaying the Z Axis

The Z axis allows you to display a number of scans with a Z component. This is particularly useful for plotting data obtained from depth profiling measurements.

Note: Z values are only recorded for certain server settings, e.g. for CCD detectors.

7.2 2D Viewer

The 2D viewer displays the output from a CCD camera or 2D delayline detector. The X axis of the data shows the energy distribution of the collected electrons; the Y axis is either distance or angle resolved.

The 2D viewer displays the contents of a single region. You can open a number of 2D viewers if you want to view more than one region.

The picture below shows the major features in the 2D viewer. These are described in more detail in the following sections.

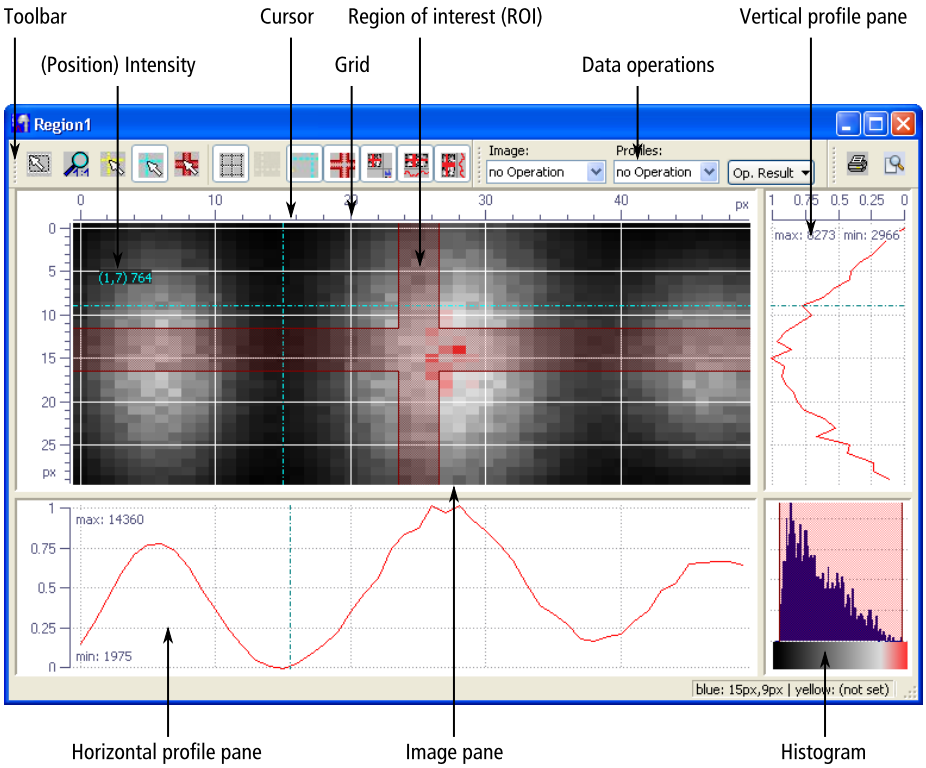


Figure 51: Data visualization in the 2D viewer

In addition to displaying data, the 2D viewer offers features for data analysis as well as configuring the spectrometer with a CCD detector:

- Selecting regions of interest in the data and zooming the image.
- Setting cursors to mark positions in the image.
- Viewing profiles of the data.
- Changing the color coding and display threshold in the image.
- Data operations.
- Hot pixel removal.

To open the 2D viewer:

- Right-click the region you want to view and select Open 2D Viewer from the context menu.
  A 2D viewer window will open for the selected region. You can open a region as it is being acquired—the image is updated during acquisition.

7.2.1 Image Pane

The main part of the 2D viewer is the image pane. This shows the data from the selected region.

When you move the mouse within the image pane, the coordinates and intensity of the indicated pixel is shown next to the pointer.

Right-clicking within the image pane brings up a context menu. The contents of the context menu are described in the table below.

Item	Description
Show Physical Units	Toggles the display of units on the image pane. If unchecked, the numbers on the axes show

Item	Description
	pixels. When selected, the physical units displayed on the axes depend on the analysis mode used for data acquisition.
Hot Pixel List	Opens the Calculate Hot Pixel List dialog. See "Removing Hot Pixels" on page 85 for a description of the procedure for removing hot pixels.
Data View	These items toggle the display of toolbars.
Operations	
Print	

Table 6: Image pane context menu

7.2.2 Zooming in the 2D Viewer

You can zoom into an area of the chart in order to inspect items of particular interest:

1. Click the  icon to activate zoom mode.
2. Click and drag the mouse to form a rectangle in the image pane. When you release the mouse button, the image shows the selected area.
3. To display the complete image again, double click in the image pane. This fits the image to the image pane.

You can also click the  icon to show each data point as a single pixel in the image pane.

7.2.3 Setting Cursor Positions

You can set the position of two cursors in the 2D viewer. These allow you to mark the position of peaks and other features; you can, for example, use them to measure the distance or energy difference between features.

When setting cursors, note the following points:

- If you select another mouse tool (e.g. the Zoom mode), the cursor is sticky and remains in its position until you reactivate the cursor.
- The  and  icons toggle the display of the cursors in the image pane.

To display a cursor in the image pane:

1. Click the  icon or the  icon. These activate the yellow and blue cursors respectively.
2. Click a point in the chart. The cursor will be displayed with the center at the selected point. The status bar at the bottom of the 2D viewer will show the coordinates of the cursor center point.

7.2.4 Displaying the Grid in the 2D Viewer

You can switch on a grid to help you view features in the image pane:

- Click the grid icon  in the toolbar. This button toggles the display of the grid.

7.2.5 Selecting a Region of Interest (ROI)

You can select a region of interest (ROI) of the image. Data operations and analysis will be performed on this ROI, rather than the whole image. The selection is a cross, containing a horizontal and vertical section of the image.

To select an ROI in the image pane for analysis:

1. Click the  icon in the toolbar.
2. Click a point in the image pane. A red cross will be displayed with its center at the selected point. The cross is semi-transparent with bold lines at its edge.

3. Click and drag the horizontal and vertical red lines at the edge of the cross until you achieve the desired area. Alternatively, edit the numbers to change the start and end positions of the X and Y coordinates for the selection (in pixels). You can enter numbers or click the up/ down arrows to change these settings.

To hide the selection:

- Click the  button in the toolbar. This toggles the display of the ROI.

7.2.6 Horizontal and Vertical Profiles

The horizontal and vertical profile panes show one dimensional views of the data from the 2D image. The data in the profiles shows the summed up intensity in the image or region of interest. The profiles also show the results of profile operations (i.e. Gaussian or Fermi edge fits).

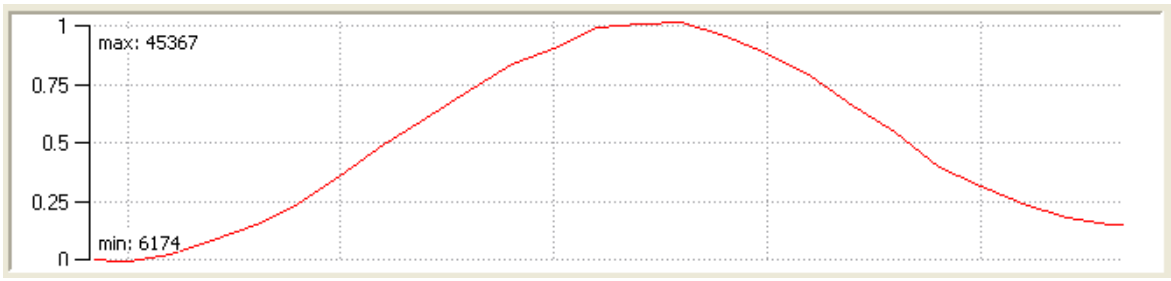


Figure 52: Horizontal profile pane

By default, the data in the profiles is shown. You can hide the data:

- Click the  icon in the toolbar.

To hide the vertical profile pane:

- Click the  icon in the toolbar. The vertical profile pane and the histogram will be hidden. Click the icon again to show them.

To hide the horizontal profile pane:

- Click the  icon in the toolbar. The vertical profile pane and the histogram will be hidden. Click the icon again to show them.

7.2.7 Histogram

The histogram is shown in the bottom right corner of the 2D viewer. It shows a distribution of the colors in the image. The shape of the histogram is produced by counting the number of pixels within a fixed intensity range of a given image.

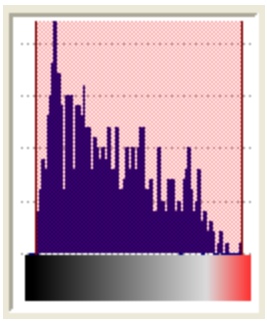


Figure 53: Histogram in the 2D viewer

You can restrict the displayed color range by changing the selected area in the histogram. This is especially useful if you want to suppress noise, which is situated in the left hand part of the histogram. To change the displayed color range:

1. Click the histogram and drag the mouse. Release the mouse when you have selected the desired area. Only pixels with the selected colors are displayed—all others are shown as maximum or minimum intensity.
2. Fine tune the region by entering numbers or clicking the arrows in the fields below the histogram. The numbers represent the minimum and maximum limits to the selected range.

Right-clicking the histogram produces a context menu. The table below describes the actions available in the context menu.

Item	Description
Copy Profile Data	Copies the data in the histogram to the clipboard. The data depends on the Intensities setting in the Histogram Ranges dialog—using this setting, you can restrict the amount of data copied to the clipboard.
Histogram Ranges	Opens the Histogram Ranges dialog. In this dialog, you can: ■ Set which intensities are displayed in the histogram. With user defined values, the histogram is redrawn so that only the intensities selected are displayed. This does not affect the appearance of the data in the main view. ■ Set the sampling rate for the intensities. A lower number of samples increases the peak height in the histogram, while also increasing the granularity.
Color Transformation Range	The sub context menu contains the following items: ■ Autoscale—Cancels any range selected in the histogram so that all colors are displayed in the viewer. ■ User Defined—Adds the limit fields below the histogram so you can define a range. This option is automatically selected when you define a range in the histogram.
Change Colormap	The sub context menu contains a number of different color schemes that you can select to view the data.
Use Zoomed Area	When checked, the histogram is calculated based on the contents of the zoomed area of the image pane. If it is not selected, all data in the region. is used in calculating the histogram.
Enable Histogram	When checked, the histogram is updated following changes to the image pane (e.g. due to zooming or data acquisition). If it is not selected, the histogram is not updated. This can speed up operation if you have performance problems.

Table 7: Histogram context menu

7.2.8 Live Images

When configuring the spectrometer, it is often useful to see a constantly updated view of the camera output. You can thereby see the effect your changes have on the results.

You can achieve this by running a number of fast scans. The procedure below describes how to perform this. You will need to optimize the procedure to suit your own requirements, e.g. scan speed, energy range, etc.

To view "live" images from the camera:

1. Create a new region and open it in the Region Edit window.
2. Configure the region, taking the following points into account:

- The scan speed should be fast so that the refresh rate in the 2D view is high. Select a narrow energy range with a short dwell time. Using the Snapshot mode is a fast way to acquire data.
- Set a large number of scans (e.g. >100).

3. Validate the scan.
4. Select Overwrite from the drop-down list in the Analyzer toolbar. This ensures that the image is refreshed after each scan.
5. Click Acquire to start scanning.
6. Right-click the region as it is being scanned and select Open 2D Viewer from the context menu. The 2D Viewer will open and display the image as it is being scanned.

7.2.9 Performing Operations in the 2D Viewer

There are a number of operations you can perform on an image or a region of interest (ROI) which are useful for instrument calibration or data evaluation. The interface for the operations consists of three drop-down lists:

- Image—operations on the image.
- Profiles—operations on the selected profiles in the horizontal and vertical profile panes.
- Op. Result—display a dialog with large text so you can read operation results at a distance.

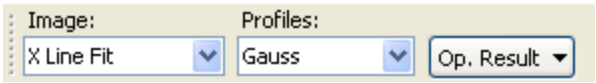


Figure 54: 2D data operations toolbar

The following tables describe the available features in these three lists.

Image operations

Operation	Description
No Operation	None of the calculations in the drop-down list are performed.
Center/ Integral	Calculates the center point of the image (X, Y coordinates) and the total number of counts. If you have selected a range with the profile marker, the point calculated is the center of the profile.
X Line Fit	Fits a line to the data in the X direction. It reports the angle of the line from the horizontal. You need to select an ROI. This feature is useful when setting up the analyzer in conjunction with a test grid, e.g. when determining the angular resolution of the detector.
Y Line Fit	Fits a line to the data in the Y direction. It reports the angle of the line from the vertical. You need to select an ROI. This feature is useful when setting up the analyzer in conjunction with exit slit setting A, e.g. aligning the camera.

Table 8: Image operations

Profile operations

Operation	Description
No Operation	None of the calculations in the drop-down list are performed.
Gauss	Fits a Gaussian profile to the selected region in the horizontal and vertical profile panes. The cal-

Operation	Description
	culation reports the center postion of the fitted peak and its FWHM. If the data are not suitable for a fit, a message appears to say the calculation is impossible. This may be the case in one profile pane; it does not affect the calculation in the other pane. You need to select an ROI in order to run this operation. You should also select Show Physical Units from the image context menu for meaningful results
Fermi Edge	Locates the Fermi edge in the selected region in the horizontal and vertical profile panes. The calculation shows a line fitting the Fermi edge and reports the position and FWHM. If the data are not suitable for a fit, a message appears to say the calculation is impossible. This may be the case in one pane; it does not affect the calculation in the other pane. You need to select an ROI in order to run this operation. You should also select Show Physical Units from the image context menu for meaningful results

Table 9: Profile operations

Displaying operation results

The results of the operations described above are displayed in the 2D viewer. You can also display the results in large text in resizable dialogs. This allows you to work at a distance from the computer, while still being able to see the spectrometer performance.

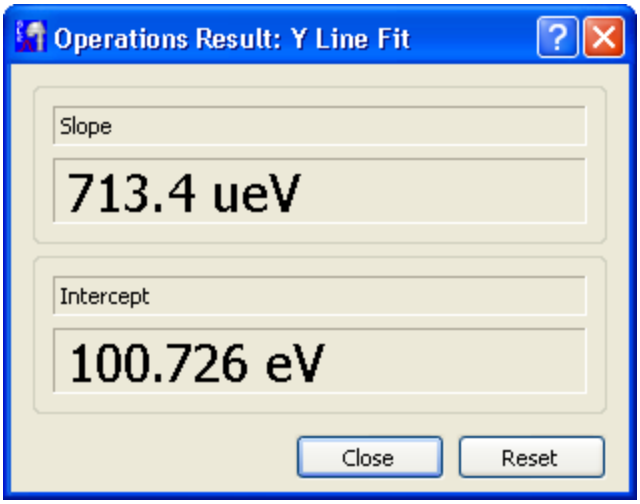


Figure 55: Displaying operation results

These dialogs are opened by clicking the Op Result button and selecting an item from the list.

Operations result	Description
Image	In order to display the results in this dialog, you need to first select an operation from the Image drop-down list. The results shown in the dialog depend on the operation selected: ■ Center/Integral—the X and Y coordinates of the center of the image (or selection) and the total intensity of the image (or selection). ■ X Line Fit—the slope of the fitted line and its Y intercept.

Operations result	Description
	■ Y Line Fit—the slope of the fitted line and its X intercept.
Horizontal	In order to display the results in this dialog, you need to first select an operation from the Profiles menu. The dialog shows the values calculated by the fit in the horizontal profile pane, i.e. the peak center position or Fermi edge position as well as the FWHM.
Vertical	In order to display the results in this dialog, you need to first select an operation from the Profiles menu. The dialog shows the values calculated by the fit in the vertical profile pane, i.e. the peak center position or Fermi edge position as well as the FWHM.

Table 10: Operation results display

7.2.10 Removing Hot Pixels

Hot pixels are individual pixels on the CCD with higher intensity than their surrounding area. They can appear as small pixel sized bright points of light on longer exposures. You can configure SpecsLab2 to ignore hot pixels—the pixels are not displayed or recorded.

Note: This procedure involves manually editing the MS Window registry. This ensures that you know precisely what changes are being made. With an automated process, a simple error would "simulate" a broken camera; the source of the problem might be hard to identify.

To remove hot pixels:

1. Right-click the image pane and select Hot Pixel List from the context menu. The Calculate Hot Pixel dialog will open.
2. Enter a threshold value. When the mouse pointer hovers over a pixel, it shows "(x,y coordinates) intensity". You can therefore find the intensity of the pixel.
3. Click Calculate. All pixels with an intensity above the threshold value are identified as hot pixels. The Hot Pixel field shows the number of hot pixels identified.
4. Click Show Details. A list of hot pixels is shown, showing the coordinates and intensity of each hot pixel.

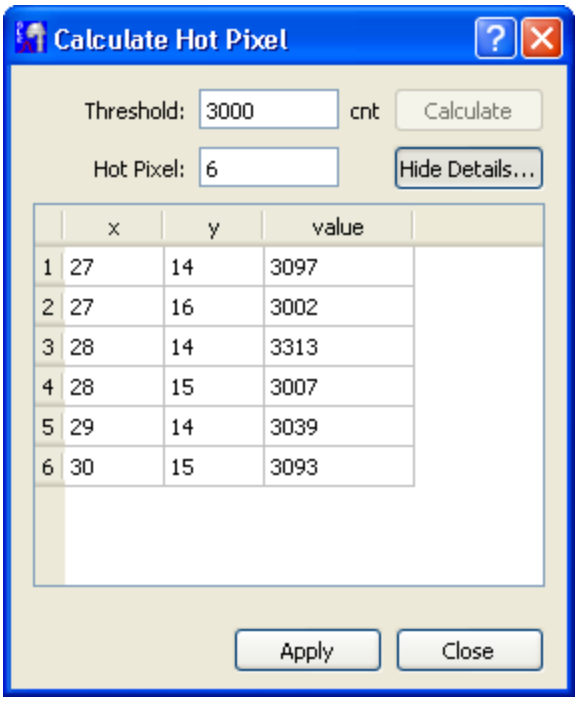


Figure 56: List of hot pixels

5. Check the list carefully to confirm that all identified pixels really are hot pixels.
6. Click Apply. The list of hot pixels is copied to the clipboard.
7. Start the MS Windows registry editor, e.g. by selecting Start/ Run and entering regedit in the Run dialog.
8. Locate the registry entry *HKEY_LOCAL_MACHINE\SOFTWARE\SPECS\CCDDetector*.
9. Read the registry key *CameraType* to identify your camera.
10. Open the folder that corresponds to your camera.
11. Open the *ImageProcessing* folder.
12. Double-click the *HotPixelList* key.
13. Paste the contents of the clipboard into the Value field. You will see a list of coordinates with the format:

```
PointVec: (x1,y1),(x2,y2),...
```

14. Click OK and close the registry editor. The hot pixels will now be ignored by SpecsLab2 when acquiring data.
15. Restart the analyzer server (in the Analyzer Settings dialog, select none from the Server drop-down list, then select your server again) to make sure the changes are accepted.

Chapter 8
Postprocessing

SpecsLab2 enables you to produce printed versions of your measurements. You can also export data for further processing in other programs.

8.1 Exporting Data

There are a number of ways to export data obtained from measurements. These allow you to import the data into other programs for further analysis and processing.

The following export formats are supported:

- VAMAS—a standard data exchange format.
- XY—exports the data in space-delimited columns with header information.
- EXP—a binary format.
- SP2—for opening 2D data in CCD Acquire.
- XML—the native file format of SpecsLab2 is XML; you can export individual regions as XML.

In addition, you can copy image data to the clipboard and paste it into other programs. The following sections provide more details about the available export formats and describe the export procedure.

8.1.1 VAMAS

The Versailles Project on Advanced Materials and Standards (VAMAS) introduced a standard data exchange format specifically designed for the interchange of data for analysis methods such as UPS, XPS, AES and many others. It is capable of storing elemental maps, depth profiles, and data sequences.

The VAMAS format used by SpecsLab2 conforms to ISO 14976[1].

[1]See, for example, "VAMAS Surface chemical analysis standard data transfer format with skeleton decoding programs", W.A. Dench, L.B. Hazell, M.P. Seah, Surf. Int. Anal. 13, p. 63–122 (1988).

Note: The analysis program CASA XPS uses files in VAMAS format.

8.1.2 XY Format

The XY format is a simple format that contains:

- Header information about the measurement and the export details.
- The numerical data from the scan in two space-separated columns.

Note: The header region for the first data set in an XY file is 39 lines long.

You can change the properties of the XY export as follows:

1. Select File/ Settings/ SpecsLab2 XY Data File from the menu bar. The SpecsLab2 XY Data File Settings dialog will open.

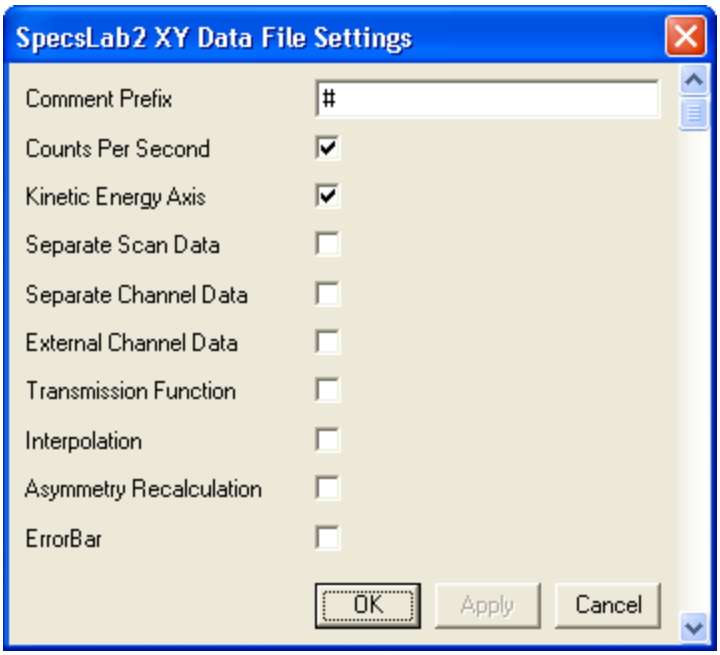


Figure 57: The SpecsLab2 XY Data File Settings dialog

2. If necessary, type a new character into the Comment Prefix field. This character is used to prefix header lines so that the importing program recognizes them as comments and is able to ignore the lines.
3. Check the option boxes as appropriate. The text for each option box is included in the export file. Checking a box includes the label "yes" in the file; unchecked boxes include the label "no". This helps you identify the data after the export.
4. Click OK. These settings will be used the next time you use the XY export.

8.1.3 Exporting Numerical Data

You can export data in the following ways:

- File, with all its groups and regions.
- Group, with all its regions.
- Region, by itself.

If you export a file or group, the regions are concatenated in the file.

Exporting individual groups or regions

To export a single group (and all of its regions) or a single region:

1. Right click the group or region in the Files window and select Export from the context menu. An Export dialog will open.

Note: If you want to export a single region, you can also right-click it in the Regions window.

2. Select a location for your file and type a name into the Filename field.
3. Select an export option from the File Type drop-down list:
   - EXP. This is a binary format that can be read by SpecsLab2, allowing you to save individual regions.
   - SP2. The format for CCD Acquire. You can save 2D data in this format and open the file in CCD Acquire.
   - VAMAS. The file will have the extension .vms.
   - XY. The file will have the extension .xy.
   - XML. Enter a file name with the extension *.xml*. The region will be exported in XML format.
4. Click Save. The data will be exported in the selected format.

Note: There are also options for exporting data to the clipboard in the VAMAS and XY formats. After using these options, you can paste the data into a program.

Exporting a file

This procedure exports all groups and regions to the selected format:

1. Select the file to be exported in the Files window.
2. Start the export procedure with one of the following methods:
   - Select File/ Export from the menu bar.
   - Right-click the file in the Files window and select Export from the context menu.
3. Select a location for your file and type a name into the Filename field.
4. Select an export option from the File Type drop-down list:
   - EXP. This is a binary format that can be read by SpecsLab2.
   - VAMAS. The file will have the extension .vms.
   - XY. The file will have the extension .xy.
5. Click Save. The data will be exported in the selected format.

8.1.4 Exporting Graphical Data

You can export the Data window to the clipboard and then paste the image into another program for presentation or reference purposes.

The size of the exported image depends on the settings in the Sizes tab of the Diagram Settings dialog. See "Defining Print Settings" on page 90 for further details.

To export the contents of the Data window to the clipboard:

1. Make sure the correct Data window is selected, if more than one is open.
2. Select Edit/ Copy Diagram from the menu bar. This copies the image to the clipboard.

8.2 Printing

You can print the contents of the Data window or 2D viewer. When printing the Data window, a summary of parameters for each of the displayed regions is included. The printout of the 2D viewer includes the vertical and horizontal profiles as well as the image.

To print the Data window, use one of the following methods:

- Select File/ Print from the menu bar.
- Click the  icon in the Data window toolbar.

To print the 2D viewer:

- Click the  icon in the 2D viewer toolbar.

8.2.1 Defining Print Settings

You can modify the appearance of the output when printing the Data window in the Diagram Settings dialog. The standard sizes are optimized; however, you may need to change the settings for certain applications or data sets.

When changing the size of the output chart, it is best to use the Print Preview feature to check the results and then iterate the size settings until you get the result you want.

Note: This section only deals with the settings that are only relevant for printing. For details about the other settings, please refer to "Setting Labels" on page 75.

To define the print settings:

1. Select View/ Diagram Settings from the menu bar. The Diagram Settings dialog will open.
2. If desired, type a comment in the Print Info field. This comment will appear as a header in the printed output.
3. Select the Sizes tab.
4. Set the size of the chart using the settings in the Sizes tab. Their meaning is shown in Figure 58 below.

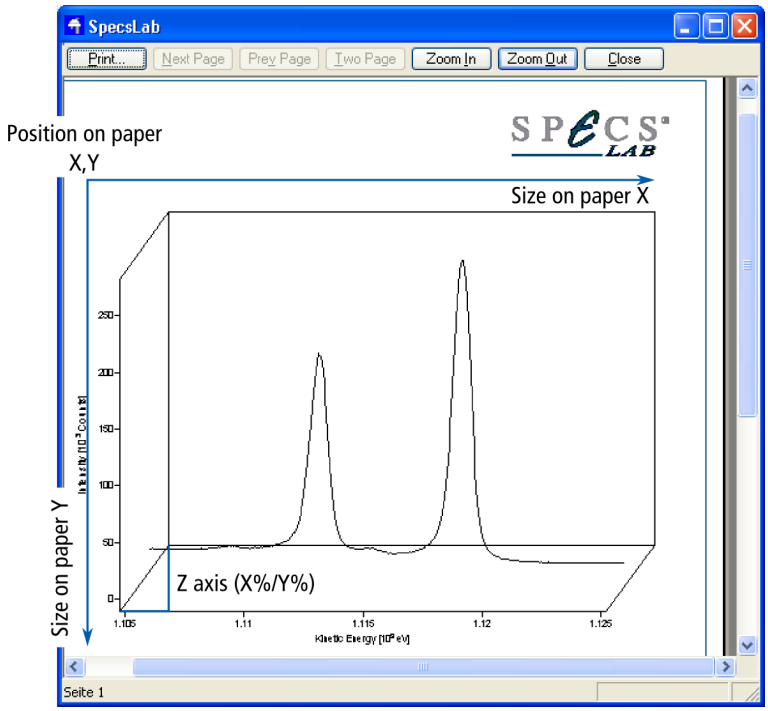


Figure 58: Setting the chart size for printing

Note: The Minimum Screen Size setting is an on-screen setting and has no influence over the print settings.

Note: The Restore Defaults button returns all settings to pre-defined values.

5. Click OK to accept the changes and close the dialog.

8.2.2 Using the Print Preview

The print preview allows you to see the output before sending it to the printer. You can therefore check that the information is correctly presented before sending it to the printer.

To start the print preview, use one of the following methods:

- Select File/ Print Preview from the menu bar.
- Click the icon in the toolbar of the Data window or the 2D viewer.

To close the print preview, use one of the following methods:

- Click Close.
- Click Print. The preview will close and the standard MS Windows printer dialog will appear.

Appendix A
Reference

The following sections contain an overview of the menus and toolbars in SpecsLab2. The descriptions are intended for quick reference—detailed descriptions of most commands are provided elsewhere in this manual.

Note: All commands here are also listed in the index.

A.1 Windows

SpecsLab2 uses windows to manage, acquire and display data. Since they deal with many of the core aspects of operation, these are described in detail in the main body of the manual.

To display a window:

- Select the Windows menu and click one of the windows entries. If it is not already open, the window will be displayed. If the window is open, it will be given the focus. The currently active window is marked with a tick.

The following sections provide a brief overview of the windows for reference purposes:

- 2D viewer
- Acquisition
- Data
- Files
- Regions
- Region Edit

A.1.1 2D Viewer

The 2D viewer displays data images, e.g. data obtained from a CCD camera. It shows the data from a single region. You can open a number of 2D viewers, each displaying a different region.

If you open a region during data acquisition, the 2D viewer is updated as data is collected.

The 2D viewer contains toolbars. You can move the toolbars and dock them to the side of the window or allow them to free float. Right-clicking the image pane reveals a context menu that allows you to hide individual toolbars. The available functions on the toolbars are described in "2D Viewer Toolbar" on page 104.

To open a 2D viewer:

- Right-click a region (e.g. in the Files window) and select Open 2D Viewer from the context menu.

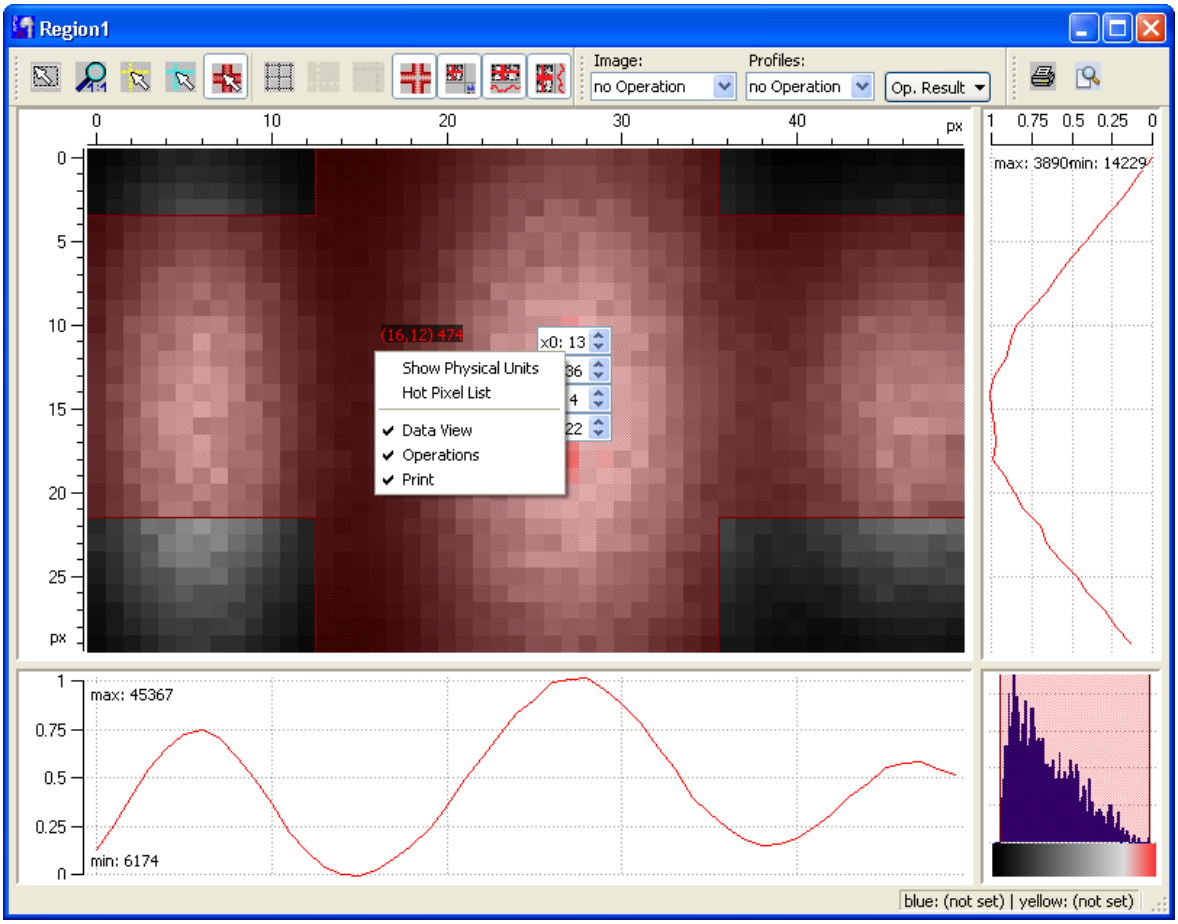


Figure 59: 2D viewer

A.1.2 Acquisition

The Acquisition window shows the current status of data acquisition. You can use this to queue and execute a number of validated regions.

A full description of the Acquisition window is provided in "Using the Acquisition Window" on page 41.

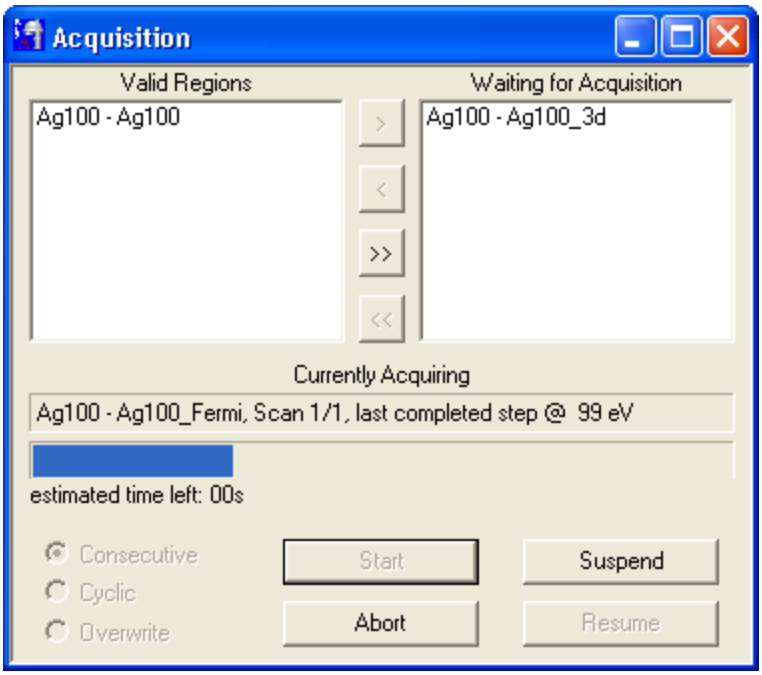


Figure 60: The Acquisition window

A.1.3 Files

The Files window contains a tree view that displays the following hierarchy:

- Files—data containers stored on the hard disk.
- Groups—logical containers for different measurements.
- Regions—data and configuration for individual measurements.
- Operation results—calculated results of data operations on a region.

When you right-click on one of the items in the Files window, a context menu appears. The contents of the context menus are summarized in the tables below.

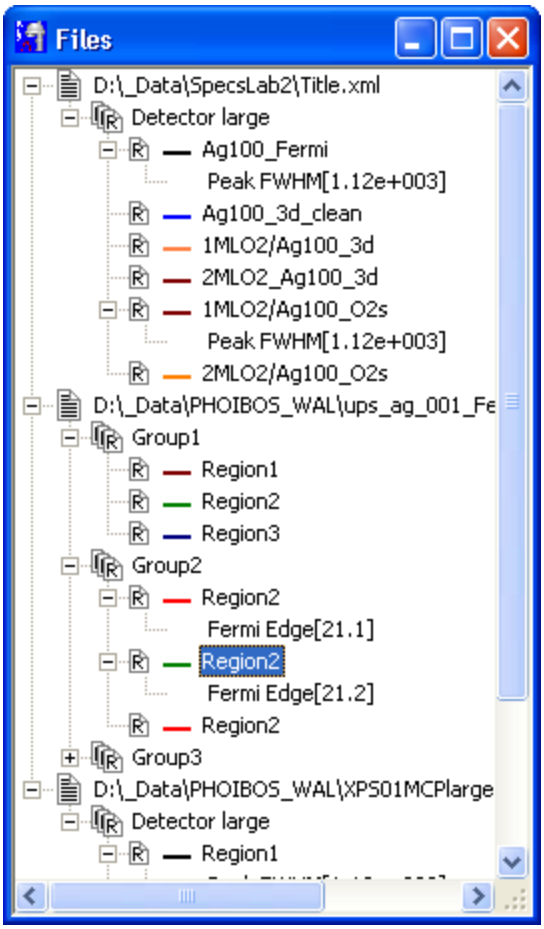


Figure 61: The Files window

File context menu

Item	Description
Visible	Toggles the visibility of the regions in the file.
Copy	Copies the current file to the clipboard.
Paste	Pastes the contents of the clipboard into the Files window. You can paste files, groups and regions. If you are pasting a file, you will be asked if you want to overwrite the current file. Click No to append the contents of the file to the current file.
Validate	Validates all regions in the file.
Acquire	Starts data acquisition in all validated regions in the file.
Close	Closes the currently selected file. You will be given the opportunity to save the file if there are any unsaved changes.
Save	Saves the currently selected file. If is has not yet been saved, a Save dialog will open so you can enter a filename.
Save As	Opens a Save dialog so that you can save the currently selected file under a different name.
Clear	Clears the data in all regions in the file. You will be asked to confirm this action before the data is cleared.
Export	Allows you to export all regions in the currently selected file in VAMAS or XY format.

Item	Description
Export to Clipboard as VAMAS	Exports all regions in the currently selected file to the clipboard in VAMAS format. Please refer to "VAMAS" on page 87 for further details of this format.
Export to Clipboard as XY	Exports all regions in the currently selected file to the clipboard in XY format. Please refer to "XY Format" on page 88 for further details of this format.
New Group	Adds a new group to the currently selected file.
Compact Data	Sums all channels to a single value.

Group context menu

Item	Description
Visible	Toggles the visibility of the regions in the group.
Validate	Validates all regions in the group.
Acquire	Starts data acquisition in all validated regions in the group.
Edit	Opens the Region Edit window so that you can edit the properties of the group. Only the name and comment fields are active.
Rename	Allows you to rename the current group.
Delete	Deletes the current group. You will be asked to confirm this action before the group is deleted.
Clear	Clears the data in all regions in the group. You will be asked to confirm this action before the data is cleared.
Copy	Copies the current group to the clipboard.
Paste	Pastes the contents of the cliphoard. You can paste groups or regions.
Export	Allows you to export all regions in the currently selected group in VAMAS or XY format.
Export to Clipboard as VAMAS	Exports all regions in the currently selected file to the clipboard in VAMAS format. Please refer to "VAMAS" on page 87 for further details of this format.
Export to Clipboard as XY	Exports all regions in the currently selected file to the clipboard in XY format. Please refer to "XY Format" on page 88 for further details of this format.
New Region	Adds a new region to the group
Compact Data	Sums all channels to a single value.

Region context menu

Item	Description
Visible	Toggles the visibility of the data in the the Data window.
View	The sub menu allows you to toggle the visibility of data: ■ Data—toggles the visibility of the sum of all channels. ■ Channels—toggles the visibility of the data channels.
Scaling	Applies the source scaling factor, if set—see the source settings in the Analyzer Setting dialog.
Transmission	Applies the transmission function to the data in the region.
Background	Toggles the display of the spectrum with background subtraction. If you have run a background subtraction calculation, this button shows the spectrum with or without the subtraction.
Channel Allocation Method	You can apply an interpolation to data obtained from multi-channel detectors. Apportioning or nearest neighbor approaches are available. More information about this procedure is provided in the SPECS software note "Acquiring Data with Multi-Channel Systems", inlcuded in the *doc/Additional Information* folder of the SpecsLab2 installation folder.
Style	Allows you to select the linestyle or data point style of the data in the Data window.
Color	Opens a color palette so that you can choose a color for the data in the Data window.

Item	Description
Validate	Validates the region.
Acquire	Starts data acquisition in the region.
Edit	Opens the Region Edit window so that you can view the configuration of the region. If the region has not yet been validated, you can edit the fields in the window. The Name and Comment fields are always available for editing.
Rename	Allows you to rename the region.
Clear	Clears the data in the current region. You will be asked to confirm this action before the data is cleared.
Delete	Deletes the current region. You will be asked to confirm this action before the region is deleted.
Copy	Copies the current region to the clipboard.
Paste	Allows you to paste a copied region.
Export	Allows you to export all regions in the currently selected group in VAMAS or XY format.
Export to Clipboard as VAMAS	Exports the currently selected region to the clipboard in VAMAS format. Please refer to "VAMAS" on page 87 for further details of this format.
Export to Clipboard as XY	Exports the currently selected region to the clipboard in XY format. Please refer to "XY Format" on page 88 for further details of this format.
Open 2D Viewer	Opens the region in a 2D Viewer.
MCD Info	Displays information about the individual channels.
Source Info	Displays the source settings for the data, as defined in the Analyzer Settings dialog.
Compact Data	Sums all channels to a single value.

Operation results context menu

Item	Description
Visible	Toggles the visibility of the calculation in the the Data window.
Style	Allows you to select the linestyle or data point style of the calculation in the Data window.
Color	Opens a color palette so that you can choose a color for the data in the Data window.
Rename	Allows you to rename the current calculation.
Delete	Deletes the current data. You will be asked to confirm this action before the data is deleted.
Export	Opens a color palette so that you can choose a color for the calculation in the Data window.
Scaling	Multiplies the data by a user-defined factor.
Offset	Shifts the data by a user-defined amount.
Parameters	Opens a dialog showing the parameters used in the calculation.

A.1.4 Region Edit

The Region Edit window is used to define the parameters for a measurement. You can also validate the parameters and start data acquisition in this window.

Full details of the fields and options available in this window are described in "Defining Regions" on page 32.

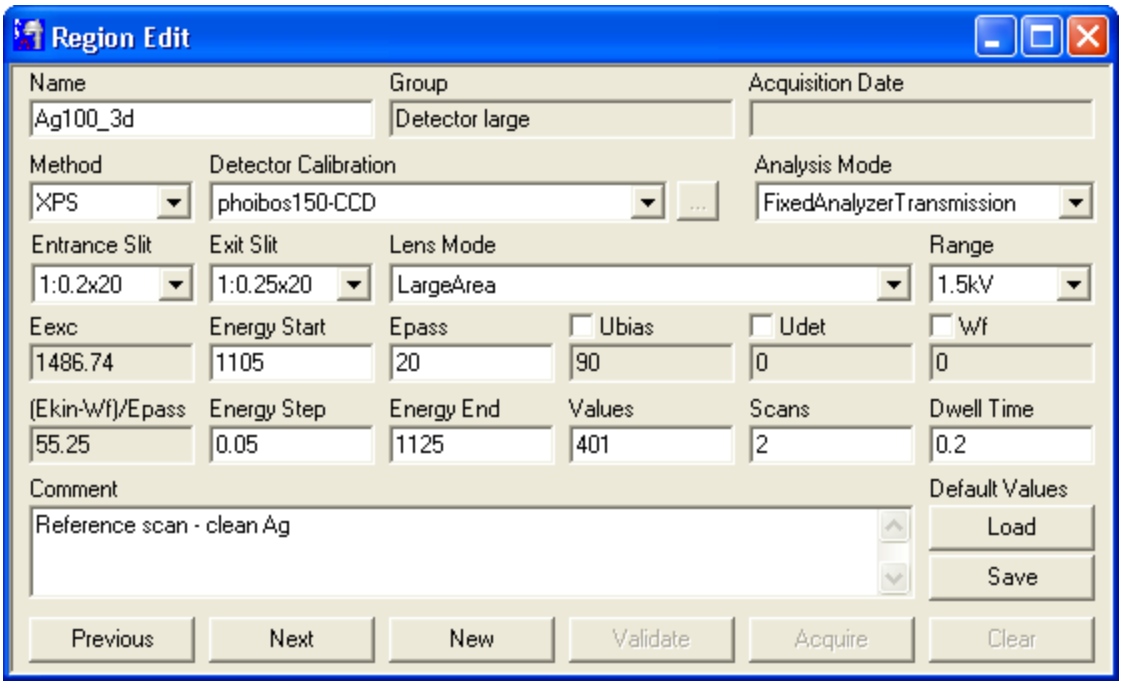


Figure 62: The Region Edit window

A.1.5 Regions

The Regions window contains an overview of the regions available in all currently open files.

When you right-click a region, a context menu appears. There is an overview of the commands in this context menu in "Files" on page 95.

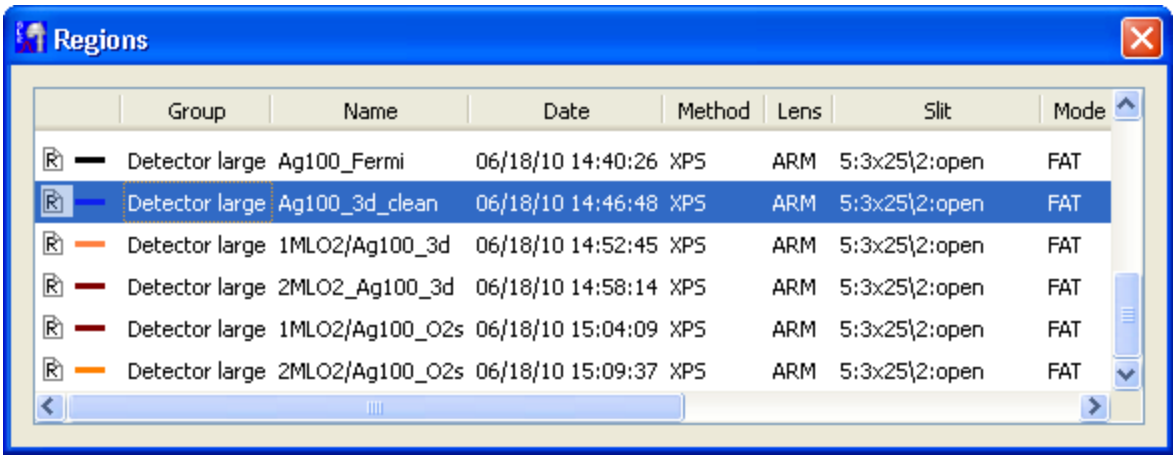


Figure 63: The Regions window

A.1.6 Data

The Data window displays data in chart form.

Data is shown during acquisition. You can also toggle the display of a region by double-clicking it in the Files or Regions window.

The Data window contains toolbars. You can move the toolbars and dock them to the side of the window or allow them to free float. Right-clicking the chart reveals a context menu that allows you to hide individual toolbars. The available functions on the toolbars are described in "Data View Toolbar" on page 106.

You can open additional Data windows:

- Select Windows/ New Data Window from the menu bar. A new, empty, Data window will open.

To display data in the new Data window:

- Double-click a region in the File or Regions window. The data will be displayed in the Data window that was most recently active.

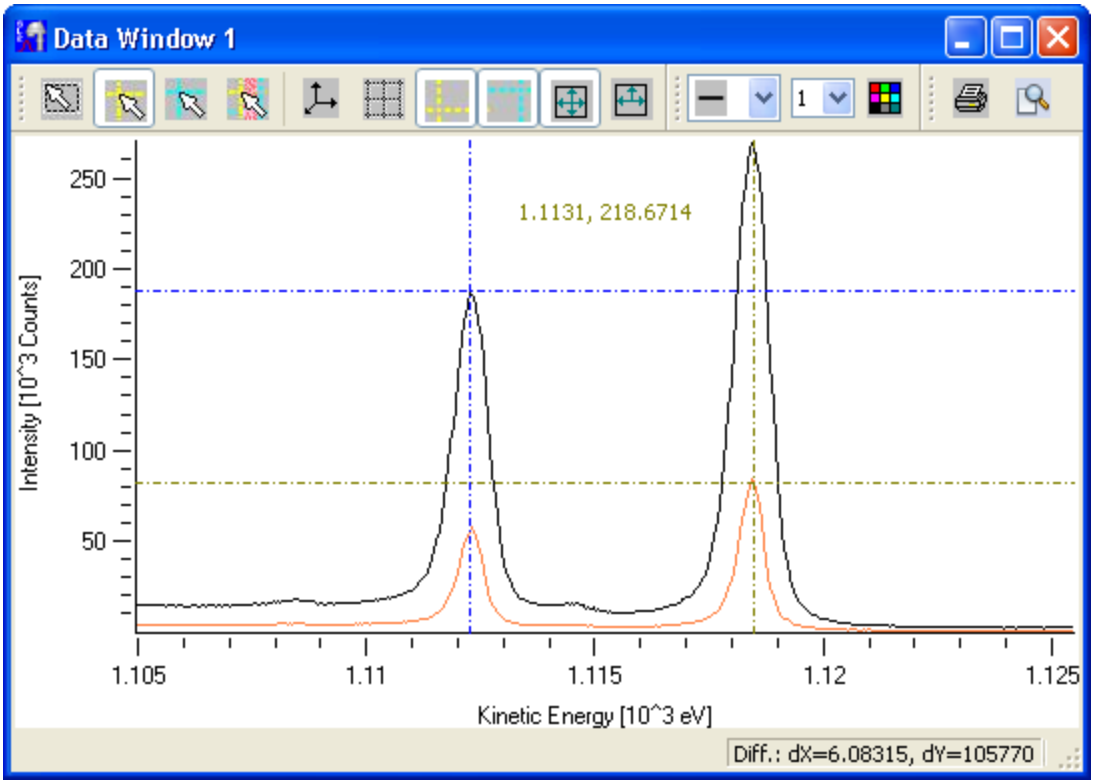


Figure 64: The Data window

A.2 Menus

The menu bar in the main window of the program contains a number of menus. The following sections describe the commands in each menu:

- File
- Edit
- View
- Analyzer
- Operations
- Tools
- Window
- Help

A.2.1 File Menu

The File menu contains a set of commands for loading, saving and exporting files. Printing is also called from this menu.

Item	Description
New File	Adds a new file for the purposes of data collection.
New Group	Adds a new group to the currently selected file.
New Region	Adds a new region to the currently selected group.
Open	A file browser will allow you to load an existing file from the file system. XML files created by SpecsLab2 can be opened.
Close	Closes the currently selected file. You will be given the opportunity to save the file if there are any unsaved changes.
Save	Saves the currently selected file. If is has not yet been saved, a Save dialog will open so you can enter a filename.
Save As	Opens a Save dialog so that you can save the currently selected file under a different name.
Export	Allows you to export the currently selected file in VAMAS or XY format.
Export to Clipboard	Exports the currently selected file to the clipboard.
Merge Open Files	Creates a new file which contains the groups (and regions) of all open files.
Save All	Saves all files.
Settings	A sub-menu containing the following entries: ■ SpecsLab2 XY Data Settings—these settings allow you to specify information included in the XY export files. Please see "XY Format" on page 88. ■ Reset Serializers—SpecsLab2 uses external services known as serializers for various purposes. If one of these services fails, you can reset all serializers to regain the functionality without restarting SpecsLab2. This is a troubleshooting feature. ■ Default Channel Allocation Method—You can apply an interpolation to data obtained from multi-channel detectors. Apportioning or nearest neighbor approaches are available. More information about this procedure is provided in the SPECS software note "Acquiring Data with Multi-Channel Systems", inlcuded in the *doc/Additional Information* folder of the SpecsLab2 installation folder. ■ Autosave—switch autosave on and off; set the time delay for saving.
Restore Autosave	Restores the autosaved files from the last session of SpecsLab2.
Print	Prints the contents of the most recently selected Data window, together with the properties of the plotted data.
Print Preview	Allows you to see what will be printed before it is sent to the printer.
Recent Files	The most recently opened files. Select an entry to open the file.
Exit	Quit SpecsLab2.

A.2.2 Edit Menu

The Edit menu contains commands to perform common MS Windows commands such as Copy and Paste. It also contains related commands that are specific to SpecsLab2.

Item	Description
Copy	Copies the current selection to the clipboard. In addition to text, you can use this to copy regions and groups.
Copy Diagram	Copies the currently displayed chart in the Data window to the clipboard. The size of the image is determined by the Sizes settings in the Diagram Settings dialog.
Paste	Pastes the contents of the clipboard. Note that this is context sensitive, e.g. you can only paste into a text field if there is text in the clipboard.

Item	Description
Clear	Clears the data in the currently selected region.
Delete	Deletes the currently selected region.

A.2.3 View Menu

The View menu contains commands that allow you to change the scaling of the axes in the Data window, as well as setting options for the appearance of the window. You can also toggle the visibility of toolbars in the main window.

Item	Description
Toolbars	Contains a sub-menu that lists all toolbars and the status bar at the bottom of the window. Ticks next to the entries show if the item is displayed.
Binding Energy	Sets the X axis so that binding energy is displayed. If this is not selected (no tick), kinetic energy is displayed.
Counts Per Second	Sets the Y axis so that counts per second are displayed. If this is not selected (no tick), absolute counts are displayed.
Diagram Settings	Opens a dialog that allows you to change various aspects of the diagram. See "Setting Labels" on page 75.

A.2.4 Analyzer Menu

The Analyzer menu allows you to start, stop and pause scans,as well as selecting the scanning mode. You can also open the Analyzer Settings dialog to configure the hardware.

Item	Description
Validate	Validates the settings for the currently selected region(s).
Acquire	Acquires data in the currently selected region(s) (after validation).
Abort Acquisition	Cancels the current data acquisition.
Suspend Acquisition	Pauses a scan.
Resume Acquisition	Resumes a paused scan.
Consecutive Mode	All selected regions will be measured consecutively, i.e. all scans within the region will be finished before start of the next region in the Waiting for Acquisition pane.
Cyclic Mode	After a scan, the next region in the Waiting for Acquisition pane will be active for acquisition. If all waiting regions are measured once, the next scan will start. This procedure will be stopped for each region if the desired scan value is reached and all regions are measured.
Overwrite Mode	All selected regions will be measured continuously, i.e. first region one scan, next region one scan, up to the end. After this, the measurement will start again, beginning with the first selected region and the data will be overwritten. This measurement does not stop automatically.
Settings	Opens the Analyzer Settings dialog. You can set the properties of the analyzer, source and remotes in this dialog. Please see "Analyzer Settings" on page 7 for further details.

A.2.5 Tools Menu

The Tools menu contains additional commands that are not used in the normal workflow of SpecsLab2.

Item	Description
Detector Calibration	Opens a dialog for the detector calibration. See "Detector Calibration" on page 109.

A.2.6 Operations Menu

The Operations menu contains a set of commands that perform specific actions on your data. You can configure each of the commands by selecting the corresponding item in the Settings submenu.

Item	Description
Background	Performs a background subtraction on visible data. Available settings are: ■ None ■ Linear ■ Shirley ■ Tougaard
Dead Time Correction	Corrects measured data by considering the dead time after each point is recorded.
Despiking	Removes data points that lie far out of the noise range.
Fermi Edge	Calculates the Fermi edge in the visible data and displays the results in the Data window.
Linear Operations	You can configure the settings to scale or offset the visible data in the X or Y directions.
Noise	Estimates the noise level in CCD experiments.
Peak FWHM	Calculates the full width at half maximum of the peak in the visible data and displays the width and peak height in the Data window. It automatically performs background subtraction.
Peak Location	Calculates the peak position in the visible data and displays the results in the Data window.
Sasvitsky Golay Smooth	Smoothes the data using the Savitsky-Golay method.
Smoothing Spline	Uses a spline to smooth the data.
Settings	A submenu that allows you to configure all of the above commands.

A.2.7 Window Menu

The Windows menu allows you to display and arrange the control windows used in SpecsLab2.

Item	Description
Layout	Sets all windows to equal size and cascades them.
Next	Selects the next open window. The selection moves upward through the order of windows listed below.
Files	Allows you to select a window. The currently selected window is indicated by a tick.
Region	
Region Edit	
Acquisition	
Data	
New Data Window	Opens a new Data window.

A.2.8 Help Menu

The Help menu allows you to open the online help and check the version number of the software.

Item	Description
About SpecsLab	Opens a dialog containing the version number of SpecsLab2 as well as copyright notices.
Online Manual	Opens the online help in a browser. The help files are stored locally.

A.3 Toolbars

There are a number of toolbars that you can use to perform actions in SpecsLab2. You can set which toolbars are displayed in the program:

- Select View/ Toolbars and then click an entry in the sub-menu. This toggles the display of the toolbar. When a toolbar is visible, it is marked with a tick in the sub-menu.

The following sections describe the features available in each of the toolbars:

- 2D viewer
- Analyzer
- Channels
- Data View
- Data window
- Main

A.3.1 2D Viewer Toolbar

There are three toolbars in the 2D viewer; Data View, Operations and Print. You can toggle their appearance by right-clicking in the image pane and selecting a toolbar name from the context menu.

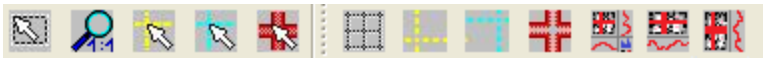


Figure 65: 2D viewer Data View toolbar

Icon	Tooltip	Description
	Zoom	Activates the zoom pointer. Selecting a region in the chart zooms into the selected area.
	Zoom to a 1:1 view	Resets the image so that each pixel in the measured data is represented by a single pixel on the screen.
	Set yellow cursor	Activates the yellow cursor. You can set its position by clicking in the chart.
	Set blue cursor	Activates the blue cursor. You can set its position by clicking in the chart.
	Set red profile marker	Allows you to set the region of interest (ROI) for the profiles and data operations.
	Show a grid on the image view	Toggles the display of the grid.
	Show yellow cursor	Toggles the display of the yellow cursor. The icon is grayed out if the cursor position has not been set. The position of the cursor is stored when the cursor is hidden.
	Show blue cursor	Toggles the display of the blue cursor. The icon is grayed out if the cursor position has not been set. The position of the cursor is stored when the cursor is hidden.
	Show red profile	Toggles the appearance of the region of interest (ROI).
	Show red profile curves	Toggles the appearance of the profile curves in the horizontal and vertical profile panes.
	Show horizontal profile frame	Toggles the appearance of the horizontal profile pane. The histogram is also hidden with the pane.
	Show vertical profile frame	Toggles the appearance of the vertical profile pane. The histogram is also hidden with the pane.
Image dropdown	–	Performs operations on the image or region of interest: ■ Center/ Integral—calculates the center and the total intensity. ■ X Line Fit—best horizontal fit to the data. Result is the angle from horizontal. ■ Y Line Fit—best vertical fit to the data. Result is the angle from vertical. See "Performing Operations in the 2D Viewer" on page 83 for details.
Profiles dropdown	–	Performs operations on the data in the horizontal and vertical profile panes: ■ Gaussian—fits a Gaussian function to both profiles, if possible. Result is peak

Icon	Tooltip	Description
		position and FWHM. ■ Fermit Edge—fits a Fermi edge to both profiles, if possible. Result is peak position and FWHM. See "Performing Operations in the 2D Viewer" on page 83 for details.
Op. Result	–	Selecting an item opens a resizable window containing the results of an image or profile operation. This allows you to see the results at a distance while setting up the analyzer. See "Performing Operations in the 2D Viewer" on page 83 for details.
	Print view	Opens the MS Windows print dialog to print the contents of the 2D viewer.
	Show print preview	Opens a print preview window so you can see what will be sent to the printer.

Table 11: Features in the 2D viewer toolbar

A.3.2 Analyzer Toolbar

The Analyzer toolbar allows you to control scanning. The action performed by each button is shown in the table below.

You can toggle the visibility of the Analyzer toolbar by selecting its entry in the View/ Toolbar menu.



Figure 66: The Analyzer toolbar

Icon	Tooltip	Description
	Validate	Validates the settings for the currently selected region(s).
	Acquire	Acquires data in the currently selected region(s) (after validation).
Drop-down list		The list contains the following entries: ■ Consecutive—all selected regions will be measured consecutively, i.e. all scans within the region will be finished before starting the next region in the Waiting for Acquisition pane. ■ Cyclic—after a scan, the next region in the Waiting for Acquisition pane will be active for acquisition. If all waiting regions are measured once, the next scan will start. This procedure will be stopped for each region if the desired scan value is reached and all regions are measured. ■ Overwrite—all selected regions will be measured continuously, i.e. first region one scan, next region one scan, up to the end. After this, the measurement will start again, beginning with the first selected region and the data will be overwritten. This measurement does not stop automatically.
	Abort	Cancels the current data acquisition.
	Suspend	Pauses a scan.
	Resume	Resumes a paused scan.

Table 12: Buttons in the Analzer toolbar

A.3.3 Channels Toolbar

The Channels toolbar shows you which channels are currently used to display data. You can switch individual channels on and off to see their signal or their contribution to the spectrum.

A.3.4 Data View Toolbar

The Data View toolbar allows you to control the display of data in theData window. The action performed by each button is shown in the table below.

You can toggle the visibility of the Data View toolbar by selecting its entry in the View/ Toolbar

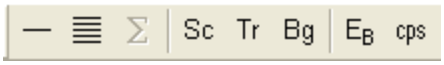


Figure 67: The Data View toolbar

Icon	Tooltip	Description
—	Data	Shows the sum of data from all channels.
≣	Channels	Shows the data taken from individual channels.
Σ	Sum	Shows the sum of data acquired from a CCD camera.
Sc	Scaling	Toggles the display of data with a measured scaling factor. If you are measuring a second signal during data acquisition (e.g. a synchrotron beam current), the data will be scaled using this signal.
Tr	Transmission	Toggles the display of the data with a transmission function.
Bg	Background	Toggles the display of the spectrum with background subtraction. If you have run a background subtraction calculation, this button shows the spectrum with or without the subtraction.
E_B	Binding Energy	Sets the X axis so that binding energy is displayed. If this is not selected (no tick), kinetic energy is displayed.
cps	Counts Per Second	Sets the Y axis so that counts per second are displayed. If this is not selected (no tick), absolute counts are displayed.

Table 13: Buttons in the Data View toolbar

A.3.5 Data Window Toolbars

The Data window contains several toolbars. You can drag the toolbars to new positions and dock them at the sides of the Data window. You can also have free-floating toolbars. Right-clicking the Data window produces a context menu—by selecting the items in the context menu, you can toggle the appearance of the toolbars.



Figure 68: Data window toolbars

Icon	Tooltip	Description
	Zoom	Activates the zoom pointer. Selecting a region in the chart zooms into the selected area.
	Set yellow cursor	Activates the yellow cursor. You can set its position by clicking in the chart.
	Set blue cursor	Activates the blue cursor. You can set its position by clicking in the chart.

Icon	Tooltip	Description
	Set both cursors	Allows you so set the positions of both cursors by selecting a region with the mouse.
	3D	Toggles the display of the Z axis. This is only suitable for certain server settings.
	Show grid	Toggles the display of the grid.
	Show yellow cursor	Toggles the display of the yellow cursor. The icon is grayed out if the cursor position has not been set. The position of the cursor is stored when the cursor is hidden.
	Show blue cursor	Toggles the display of the blue cursor. The icon is grayed out if the cursor position has not been set. The position of the cursor is stored when the cursor is hidden.
	Autoscale	Sizes the axes in the Data window so that data in all selected regions is displayed.
	Preserve zero	When the data is autoscaled, this setting ensures that Y=0 at the baseline of the chart.
	–	Select a linestyle or point style for the data. The setting is applied to the currently selected region.
1	–	Set the thickness of the line or size of the point. This does not apply to dots.
	Color	Opens a color palette to set the line or marker color for the currently selected region.
	Print	Prints the contents of the Data window, together with the properties of the plotted data.
	Preview	Allows you to see what will be printed before it is sent to the printer.

Table 14: Data window toolbar

A.3.6 Main Toolbar

The Main toolbar contains buttons that allow you to manage files, groups and regions. The action performed by each button is shown in the table below.

You can toggle the visibility of the Main toolbar by selecting its entry in the View/ Toolbar menu.



Figure 69: The Main toolbar

Icon	Tooltip	Description
	New File	Adds a new file for the purposes of data collection.
	New Group	Adds a new group to the currently selected file.
	New Region	Adds a new region to the currently selected group.
	Open	A file browser will allow you to load an existing file from the file system. XML files created by SpecsLab2 can be opened.
	Save	Saves the currently selected file. If is has not yet been saved, a Save dialog will open so you can enter a filename.
	Save All	Saves all files.
	Print	Prints the contents of the most recently selected Data window or 2D viewer.
	Edit	Opens the Region Edit dialog for the current region.
	Rename	Allows you to rename the current region in the Files window.
	Clear	Clears the data in the currently selected region.

Icon	Tooltip	Description
	Delete	Deletes the currently selected region.
	Copy Diagram	Copies the currently displayed chart in the Data window to the clipboard. The size of the image is determined by the Sizes settings in the Diagram Settings dialog.
	Copy	Copies the current selection to the clipboard. In addition to text, you can use this to copy regions and groups.
	Paste	Pastes the contents of the clipboard. Note that this is context sensitive, e.g. you can only paste into a text field if there is text in the clipboard.

Table 15: Buttons in the Main toolbar

Appendix B
Detector Calibration

Detector calibration is a procedure that corrects the peak height and position of channels. It does this by comparing measurements to a reference scan and modifying the energy and/ or intensity scales.

B.1 Calibration Procedures

Measured peak positions can shift for different lens modes and slit settings. This is caused by the changing incidence angle of electrons onto the entrance slit. The spread in energy around the pass energy E_p, ΔE_{an}, is given by:

$$\frac{\Delta E_{an}}{E_{pass}} = \frac{W}{2R_0} + \frac{\alpha^2}{4} \quad (7)$$

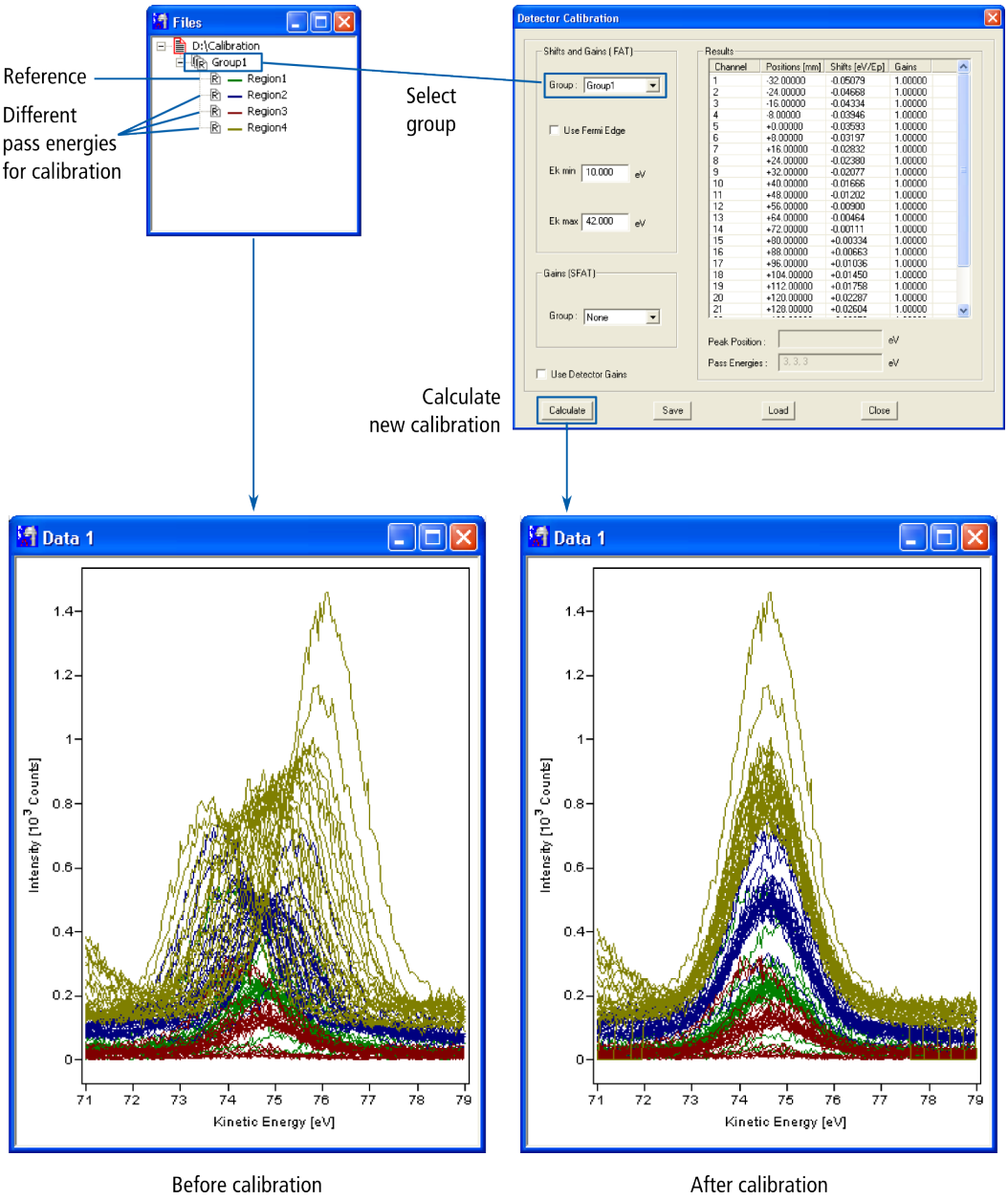
where:

- W = (W1+ W2)/2 is the average of the widths of the electron beam at the entrance and exit slits in the energy direction.
- α is the average angular width of the electron distribution.
- R_0 is the radius of the hemispherical energy filter.

There are calibration settings included in SpecsLab2 that provide a good correction to this effect. However, not all lens/ slit combinations are calibrated and you may find that the approximation for your combination is not sufficient. After performing the detector calibration, you can use it for this lens/ slit combination in future experiments.

You can easily find out if the values are correct or not by observing the following:

- Peak position for each energy channel. The left graph in Figure 70 shows how this can vary.
- Peak position as a function of pass energy. The blue and green peaks in the figure show this effect.



Before calibration

After calibration

Figure 70: Calibrating the detector

SpecsLab2 contains a tool for calibrating the energy position and detector gain settings to compensate for the above effects. The basic procedure for calibration is:

1. Find a suitable reference area.
2. Measure this area at different pass energies. These will be calibrated.
3. Perform the calibration.
4. Save the calibration.

Figure 70 shows an overview of this procedure. You can see a comparison of results before and after calibration.

The following results are displayed after calibration:

- Channel—this is a number that orders the other results.
- Positions—the channel position. This is measured in millimeters; the zero point is approximately the center of the detector (there is a small offset).

- Shifts—the amount the point is shifted when the new peak position is calculated.
- Gains—the correction factor to the gain when comparing the peak to the reference.

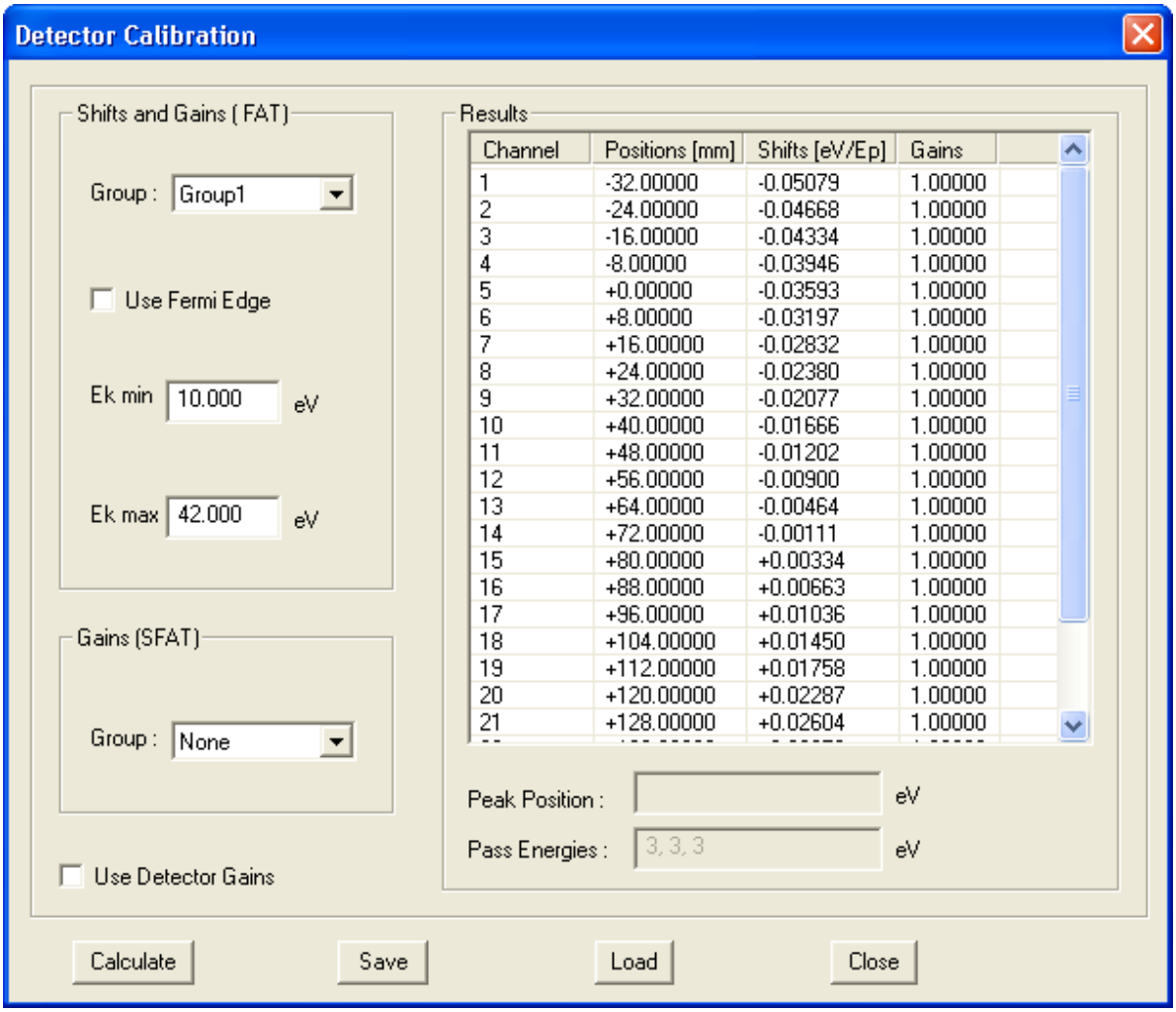


Figure 71: The Detector Calibration dialog

There are two different calibration algorithms, which are applied to these use cases:

- Fixed analyzer transmission (FAT) mode
- Snapshot mode

These are described in the following sections.

B.1.1 Calibrating Fixed Analyzer Transmission Groups

In fixed analyzer transmission mode, the analyzer scan the kinetic energy of the incident particles at a fixed pass energy. You can scan in this mode by selecting the analysis mode FixedAnalyzerTransmission in the Region Edit dialog.

Note: If the calibration procedure does not succeed, check that the count rate is high enough. This is a problem for regions wih low pass energies. Also, you should ensure that SpecsLab2 can detect the peaks by using Operations/ Peak Location. If the peak cannot be detected, calibration will fail.

To perform a calibration for fixed analyzer transmission groups:

1. Create a new group for the calibration.
2. Scan a number of regions using the same set of parameters, but with different pass energies (e.g. for regions with 5, 10, 20, 50 eV pass energies). These allow the detector to be calibrated for each pass energy.
3. Select Tools/ Detector Calibration from the menu bar. The Detector Calibration dialog will open.
4. Select a group from the Group drop-down list in the Shifts and Gains (FAT) section. Calibration is performed on this group.
5. Set the Fermi Edge checkbox:
   - Checked—the Fermi edge will be used as the calibration point rather than a peak.
   - Unchecked—the peak is used as the calibration point.
6. Set values for Ek min and Ek max, if necessary. These settings restrict the range used in the calibration. By default, the values in the Ek min and Ek max fields are the parameters you entered when defining the region.
7. Set the Use Detector Gains checkbox:
   - Checked—gain values will be calculated for each channel.
   - Unchecked—the gain value for each channel is taken as 1.
8. Click Calculate. The calibration will be performed. The new values will be displayed in the table. If the data window is open, you will also see the peaks updated after the calibration is performed.

B.1.2 Calibrating Snapshot Fixed Analyzer Transmission Groups

You can use snapshot mode when acquiring data. In this case, the spectrum is generated by reading out the whole detector array at once—there is no averaging over the channels.

This procedure is a variation of the calibration for fixed analyzer transmission groups, described above. There are some important differences:

- You can only select groups which contain at least one region where the Analysis Mode is Snapshot (FAT).
- Only the gain is calculated for each channel—peak shifts are not calculated.

You should remember the following points when calibrating the snapshot mode:

- Calibration uses a linear fit, so the count rate in the region considered should be constant, i.e. there should be no peaks. An example is the 817–812 eV binding energy in the silver spectrum.
- At least one region in the group is a scan—this is used to obtain the linear fit for the calibration.
- At least one of the other regions is a snapshot—this is used to calculate the calibration factors, together with the linear fit.
- You should ensure that the average number of counts is similar for each measurement by taking into account the number of energy channels N, e.g.
  - 10 scans, dwell time 1 s for the scan mode
  - 100 scans, dwell time N × 0.1 s for the snapshot mode

The algorithm works by fitting a straight line to the spectrum measured in scan mode. This is used with the values from the snapshot spectrum to calculate the calibration factors for each channel. The calibration factors are equal to the inverse of the average number of counts for each channel (energy value) in the snapshot spectrum divided by the value obtained from the linear fit for the corresponding energy value.

Note: The maximum absolute value of the residuals (i.e. the difference between the scan mode intensity and the linear fit for all the energy values measured) should be less than 5% of the energy averaged number of counts. If the residuals are greater, the spectrum is either too noisy or not sufficiently flat. In this case the procedure will fail.

To perform a calibration for snapshot fixed analyzer transmission groups:

1. Create a new group for the calibration.
2. Perform measurements of the same region for a number of different pass energies. Remember to include at least one scan and at least one snapshot in these measurements!
3. Select Tools/ Detector Calibration from the menu bar. The Detector Calibration dialog will open.
4. Select a group from the Group drop-down list in the Gains (SFAT) section.
5. Set the Use Detector Gains checkbox:
   - Checked—gain values will be calculated for each channel.
   - Unchecked—the gain value for each channel is taken as 1.
6. Click Calculate. The calibration will be performed. The new values will be displayed in the table. If the data window is open, you will also see the peaks updated after the calibration is performed.

B.1.3 Calibrating FAT and SFAT Groups

In addition to selecting a group from the Shifts and Gains (FAT) or Gains (SFAT) drop-down lists as described above, it is possible to select groups in both lists and run a calibration based on two groups. In this case, the following are calculated:

- Peak shifts are calculated in the same way as for fixed analyzer transmission groups. This data is not used for calculating the gains.
- Gains are calculated in the same way as for snapshot groups, and use the selected snapshot group for the calibration.

B.2 Managing Dataset Files

SpecsLab2 stores calibration data in text files known as dataset files. There is a text file for each dataset file. After installation, the dataset files are stored in the *database\datasetCalib1d* folder in your *SpecsLab2* installation directory. Calibration files have a *.calib1d* extension. You can open these files in a text editor to view their contents; however, you should not change their contents.

B.2.1 Saving Calibrations

You can save a calibration for future use. When you save a dataset file, it is available in the Region Edit dialog so that it can be applied to scans as they are performed.

To save a calibration:

1. Perform the calibration as described in the previous sections.
2. Click Save in the Detector Calibration dialog. A Save dialog will open.
3. Select a location for the file and enter a filename. The *.calib1d* extension will be added automatically to the name.
4. Click Save. The dataset file will be saved.

This procedure is slightly more involved if no analyzer is connected. When you select an analyzer, the channel positions are automatically read. Without an anaylzer, no position data is available—you see a row of zeroes in the Positions column of the Detector Calibration dialog. When you attempt to save a file without any position data defined, a dialog will appear:

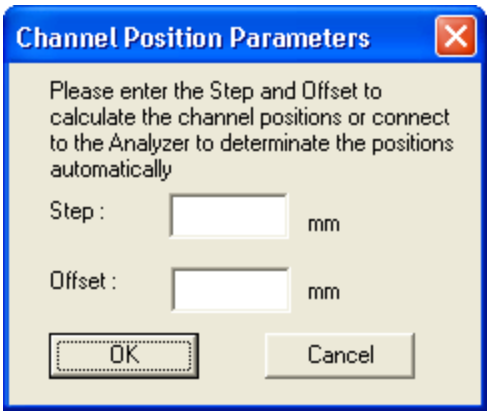


Figure 72: Generating position values for old SpecsLab2 data

You need to fill in the Offset and Step fields with suitable values:

- Step—the distance between each channel position in the table.
- Offset—the difference between the recorded zero position and the detector center.

SpecsLab2 will then generate a list of position values that will be written to the file. After saving the file, it is a good idea to load the file again to check that the position data is realistic.

Note: In general, you will only perform calibrations when the program is attached to an analyzer. This feature allows you to continue working even when not connected to an analyzer.

B.2.2 Loading Calibrations

When you load a dataset file, it is applied to the currently selected group in the Detector Calibration dialog. This allows you to see the effect of a different calibration on existing data.

To load a dataset file:

1. Select Tools/ Detector Calibration from the menu bar. The Detector Calibration dialog will open.
2. Select a group from the drop-down list in either the Shifts and Gains (FAT) or Gains (SFAT) sections. The calibration will be applied to this group. The load button is grayed out until you select a group.
3. Click Load. A file browser will open.
4. Locate the dataset file you want to load. The file must have a *.calib1d* extension.
5. Click Open. The calibration settings are opened and displayed in the table. You can also see in the Region Edit window that the calibration has been applied to the group and its regions.

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