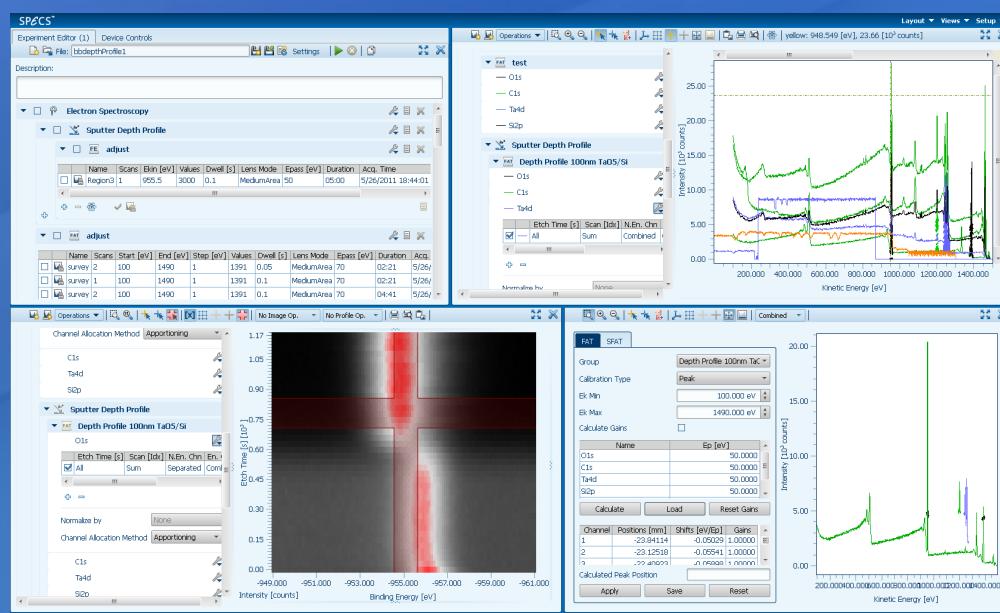


# SpecsLab Prodigy

Data Acquisition and Experiment Control Software Package



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## SPECS User Manual

**SpecsLab Prodigy**—Data Acquisition and Experiment Control Software Package  
SpecsLab Prodigy Version 4.12.0r49869

March 31, 2015

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## Index

## Chapter 1 – Introduction

Welcome to the user manual for the SPECS SpecsLab Prodigy. This is a software package for controlling SPECS equipment, acquiring data and performing basic analysis.

SpecsLab Prodigy has a modular design and is therefore extremely extensible. Some details concerning your instrumentation will therefore not be available. Information that is typically not included in this manual includes:

- Instrument-specific details. Please refer to the instrument manual for instructions on how to control the instrument using SpecsLab Prodigy. Such information is included in the Online Help.
- Advanced configuration operations that cannot be performed in the GUI.
- Support of third-party equipment such as synchrotron beamlines.
- Programming details, such as integrating SpecsLab Prodigy into other software architectures.

However, because of the licensing system that determines which features are available in the software, this manual describes features that you may not be able to access. If you read about a feature that you cannot find in the software, but you would nevertheless like to use, please contact SPECS for licensing information.

Further documentation is available in the *doc* folder of your SpecsLab Prodigy installation directory. If you need further assistance, please contact SPECS support.

This manual was prepared using SpecsLab Prodigy version 4.12.0r49869.

### 1.1 Installation

SpecsLab Prodigy is pre-installed on delivery. It is configured for your equipment and requires no further changes.

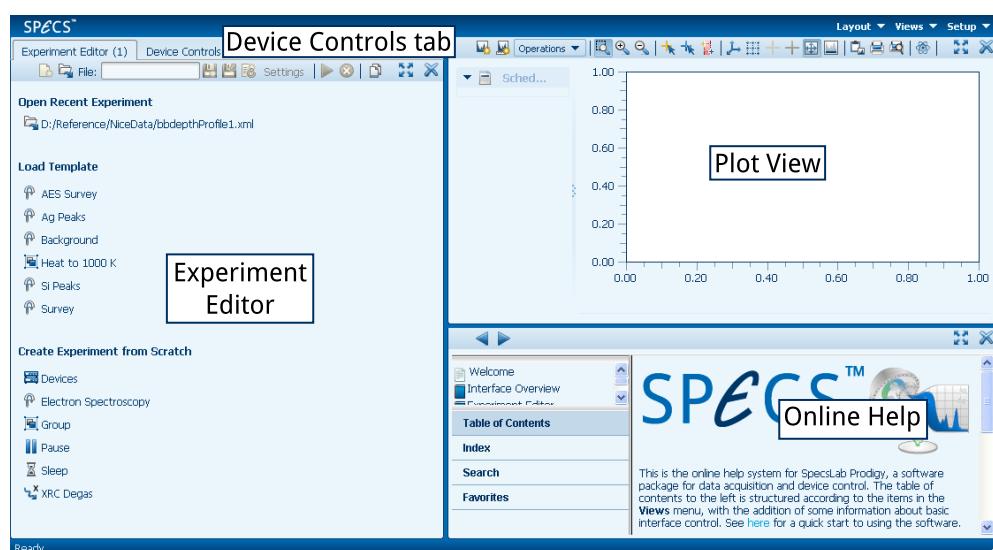
The Quick Guide contains details about installing the software as well as configuring licenses and equipment.

### 1.2 Starting SpecsLab Prodigy

To start SpecsLab Prodigy

1. Switch on the HSA 3500plus. This power supply is controlled by SpecsLab Prodigy to provide all necessary voltages for the analyzer.
2. Select **Start/ SPECS/ Prodigy**. SpecsLab Prodigy will start.

When it starts, the initial window of SpecsLab Prodigy is divided into three panes, as shown in the screenshot below. You can select items from the **Views** menu for further functionality. This manual is divided according to the available views. Major areas, such as the Experiment Editor, have more than one chapter to cover all their features and workflows.



### 1.3 Information

SpecsLab Prodigy is a modular program. This manual covers the core functionality as well as a few specific applications involving other equipment. In addition to the analyzer, SpecsLab Prodigy can control a variety of other equipment. You should therefore consult the SPECS user manuals for other manuals for details of how to control specific instruments using SpecsLab Prodigy.

The Quick Guide contains installation and configuration instructions as well as the basic procedures for acquiring and analyzing data.

The Online Help contains the information in this manual as well as instrument specific instructions.

Selecting **Start/ SPECS/ Documentation** opens a folder containing a set of documents related to SpecsLab Prodigy.

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

Tel. +49 30 46 78 24-0

email: [support@specs.com](mailto:support@specs.com)

## Chapter 2 – Interface Overview

SpecsLab Prodigy uses an intuitive graphical user interface for controlling instruments, designing experiments and viewing data. The following sections describe some of the basic interface tools for managing the appearance of the program:

- Features on the [menu bar](#).
- Managing [views](#).
- Opening a [second window](#).
- [Scrollbar markings](#) to help you find features in various views.

### 2.1 Menu Bar

The menu bar at the top of the window contains three items:

- Layout—Allows you to [save and select pre-saved](#) view layouts.
- Views—Contains entries for opening different views. These views are described elsewhere:
  - Device Controls: See "[Device Controls](#)" on page 183.
  - Experiment Editor: See "[Experiment Editor I: Basic Use](#)" on page 7, "[Experiment Editor II: Schedule Options](#)" on page 21 and "[Experiment Editor III: Reference Information](#)" on page 51.
  - Image View: See "[Image View](#)" on page 135.
  - Plot View: See "[Plot View I: Features](#)" on page 71 and "[Plot View II: Data Operations](#)" on page 85.
- Setup—for opening a [second window](#), using [Expert Mode](#) and exiting SpecsLab Prodigy.

The menu bar also contains a "panic button" icon  which switches off all connected instruments. When instruments are connected, their icons are displayed here, with their [operational status](#) indicated by their color. As with many other features in SpecsLab Prodigy, hovering the mouse over the features produces a tooltip with more information.

### 2.2 Managing Views

SpecsLab Prodigy offers a number of methods for arranging the different views. These are described in the sections below.

#### Moving views

To move a view and dock it in a new position:

1. Click and hold the mouse pointer on the  icon in the control bar of the view you want to move.
2. Drag the view to a new position. The other views will slide to make room for the view.
3. Release the view in its new position.

## Tabbing views

Views can occupy the same area in the window. Tabs at the top of the view allow you to switch between the views:

1. Click and hold the mouse on the control bar of the view you want to move.
2. Drag the view onto a second view. The whole view will be highlighted.
3. Release the view. The old view will appear as a tab at the top of the view.

## Closing, maximizing and minimizing views

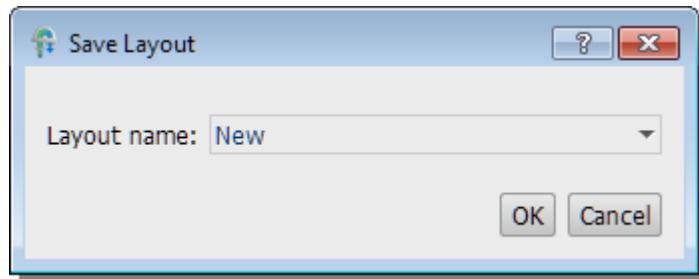
Clicking the  icon at the top right of each view will close the view. You will be prompted to confirm before the window is closed, because all settings in the view are lost on closing.

The  icon can expand the view to the full size of the window. In this case, it is replaced with the  icon, which will return the view to its original size.

## Saving and loading view layouts

You can save the current view layout for future sessions:

1. Select **Layout/ Save Current Layout**. A dialog will open.
2. Enter a new name to save the layout, or select an existing layout from the drop-down list to overwrite the selected layout.



3. Click **OK** to save the layout.

You can easily restore the layout to a previous setting:

Click **Layout** in the menu bar and select the name of a layout.

## 2.3 Opening a Second Window

You can open a second window in SpecsLab Prodigy. This is ideal if you have a second monitor. A typical example is to have the experimental setup in one window with the data display in the second.

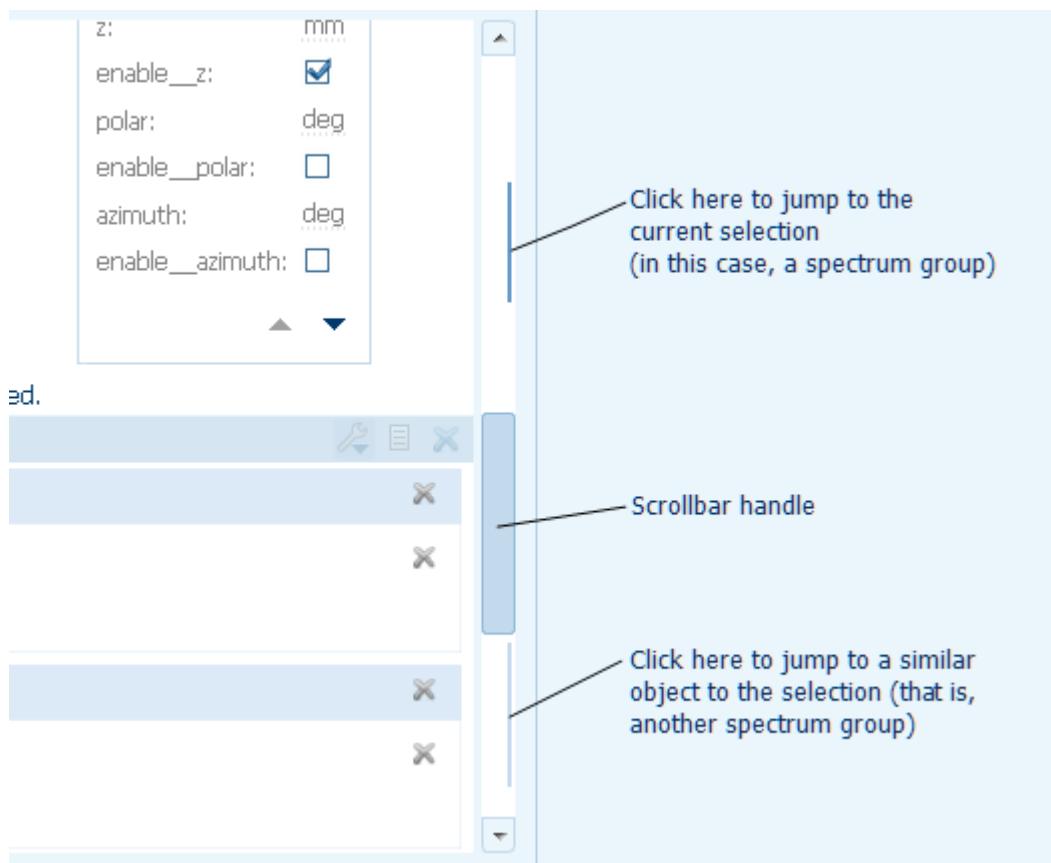
To open a second window:

1. Select **Setup/ Second Window** from the menu bar.
2. Drag a view from the original window into the second.

## 2.4 Scrollbar Navigation Markers

For more complex experiments, the schedule can be very long; there may also be a large number of results in the data browser. To help you navigate, the scrollbars have additional marks that act as anchors:

- The dark blue line shows the position of the current selection in the schedule. Clicking the mark takes you directly to the selection.
- The light blue lines show similar objects to the selection. For example, if a spectrum group is selected, other spectrum groups are marked in light blue. Again, clicking these marks takes you to the corresponding part of the schedule.



The currently active part of the schedule is colored green. The currently acquired spectrum in the data browser is also shown in green. A green bar appears in the schedule so you can easily find which part of the experiment is running.

Spectrum Group											
	Name	Scans	Start	End	Step	Values	Dwell	Lens	Epass	Duration	
<input checked="" type="checkbox"/>	 Spectrum	1	280	330	1	51	0.1	MA	10	00:33	

## Chapter 3 – Experiment Editor I: Basic Use

One of the most important uses of SpecsLab Prodigy is to acquire data in spectroscopy experiments. This chapter guides you through the basic procedure for data acquisition. SpecsLab Prodigy has an intuitive design—once you understand the basic operation, you should be able to adapt it to your workflow and requirements.

The information in this chapter is essential for all users. It covers the following aspects:

- [Measuring](#) a spectrum.
- [Scheduling](#) tasks in the experiment.
- Creating and using [templates](#).
- Using [expert](#) and standard modes.

A description of all options in the Experiment Editor is presented in "[Experiment Editor II: Schedule Options](#)" on page 21. Background information that is likely to be of interest to the majority of users is provided in "[Experiment Editor III: Reference Information](#)" on page 51.

### 3.1 Measuring a Spectrum

The Experiment Editor is used to define and run experiments. On opening, it contains a set of recently performed experiments. If you select one of these links, the experiment, including all parameters and data, is loaded. This allows you to review your results or modify the experiment and take a new set of results.

To create a new experiment

1. Under **Create Experiment from Scratch**, click **XPS**. The Experiment Editor will show the details for an XPS experiment. Instead of XPS, you can also select options for UPS, AES and ISS experiments. The difference is the sources that are available for the experiment. The
2. Edit the experiment file name as necessary. The default is *Experiment*, followed by a date and time stamp.
3. Enter some text in the **Description** field. This is recorded with the data. It is valid for the entire experiment. Typical information would be details of the surface, adsorbate, etc.

#### 3.1.1 Adding a Source

You need to define the properties of the excitation source. For the purposes of this description, we will use a "dummy" X-ray source. Other SPECS sources, as well as instruments such as beamline monochromators, can be controlled directly from SpecsLab Prodigy.

To add a dummy X-ray source to the experiment:

1. Click **XR50 Dummy: Operate**. A new XR50 Dummy entry box will appear in the Experiment Editor.

#### Note

If there is only one source available, it is automatically added to the experiment.



2. Select the desired excitation energy from the **Anode** drop-down list. This information is used to calculate binding energies. It is also stored with the data with other experimental information.
3. If desired, check the **Notify to set up device** box. Before data acquisition starts, a dialog will pop up instructing you to switch on the X-ray source with the correct parameters.
4. For further source parameters, click the ▼ button.



5. Enter desired values for the source power and high voltage as necessary.

### 3.1.2 Adding an Analyzer and Other Devices

An analyzer is essential for all measurements. If you only have one analyzer, this is automatically included in the experiment. If you have additional analyzers and detectors, you can choose which one to use for the experiment.

In addition to the analyzer, you may be able to select other devices for use in the experiment. You can then set the operating parameters to be used in the experiment. Typical devices include:

- Flood gun, to be activated during a measurement.

- Manipulator, to move the sample to the measurement position.

To add an analyzer:

- Click the desired analyzer in the list of devices in the Experiment Editor. The analyzer will be activated when you start the experiment.



In addition to the analyzer, you may be able to select other devices for use in the experiment. You can then set the operating parameters to be used in the experiment. Typical devices include a flood gun, manipulator or sample heater.

Some modules are dependent on a device being defined at this point. If you have the [Profiling](#) and/ or [Ramping](#) modules, you need to add the device in order to be able to access the parameters in the module.

External devices may also be available. These allow you to record a parameter while the experiment is running. A typical example is to measure the sample current for normalizing the signal. The data from the external device can be viewed in the [data browser](#); this also offers the facility to use the data for [normalizing](#) the signal.

#### Note

After the end of the experiment, the all devices are put into a safe status. The exact details of this final status are device dependent.

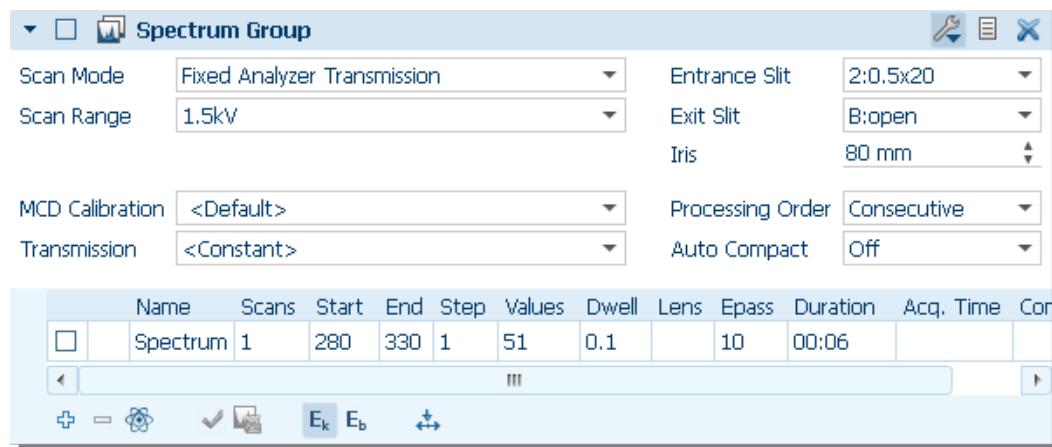
### 3.1.3 Creating a Spectrum Group

Spectrum Groups contain one or more spectra. Each spectrum is recorded using the same analyzer settings, but with different energy settings and lens modes. Within a single experimental run, you can therefore measure a number of regions in the energy range.

To create a new Spectrum Group:

1. Click the icon next to **Add to Electron Spectroscopy**. A new Spectrum Group will be added. If a menu appears, select **Spectrum Group**.
2. Click the name ("Spectrum Group") and enter a name for the group.
3. Click the **Scan Mode** drop-down list. There will be a delay while the software connects to the HSA power supply.

4. Select **Fixed Analyzer Transmission** from the **Scan Mode** drop-down list. For a description of the other scan modes (which may also change the other setup parameters), please refer to "[Scan Modes](#)" on page 51.
5. Select **1.5 kV** from the **Lens Voltage** drop-down list. For the most accurate measurements, you should select the lowest available voltage for the energy range you want to measure. The HSA power supply manual contains more information about the available energy ranges.
6. Select a [calibration file](#) suitable for your detector from the **MCD Calibration** drop-down list. This corrects energy shifts between different measurement channels.
7. Select **Consecutive** from the **Processing Order** drop-down list. There are two options:
  - **Consecutive**—all spectra in the group will be measured consecutively.
  - **Cyclic**—depends on the number of scans defined. All energy regions are measured once consecutively. SpecsLab Prodigy then returns to the start of the group and goes through the group, as defined for each individual spectrum. This cycles until all scans are performed.
8. Select a [transmission function](#) from the **Transmission** drop-down. Transmission functions are dependent on the slit settings.
9. Set **Auto Compact** to **Off**. Auto compacting allows you to reduce file size by discarding the information in separate channels (for multichannel detectors) or summing the data from a number of scans.
10. Set the **Entrance Slit** and **Exit Slit** entries according to the slits selected on the analyzer.
11. Set the **Iris** according to the setting on the analyzer.



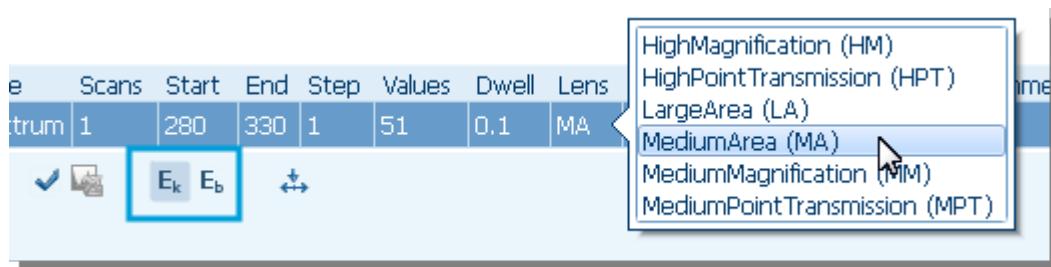
The main settings for the Spectrum Group are now complete. You are ready to define a spectrum. By clicking the icon in the Spectrum Group, you can hide the settings you have just defined and concentrate on the details of the spectrum.

### 3.1.4 Setting Up a Spectrum

Individual spectra are defined in the table below the experiment settings. The entries in the table depend on the scan mode selected.

The spectrum parameters are described in detail for all modes in ["Scan Modes" on page 51](#).

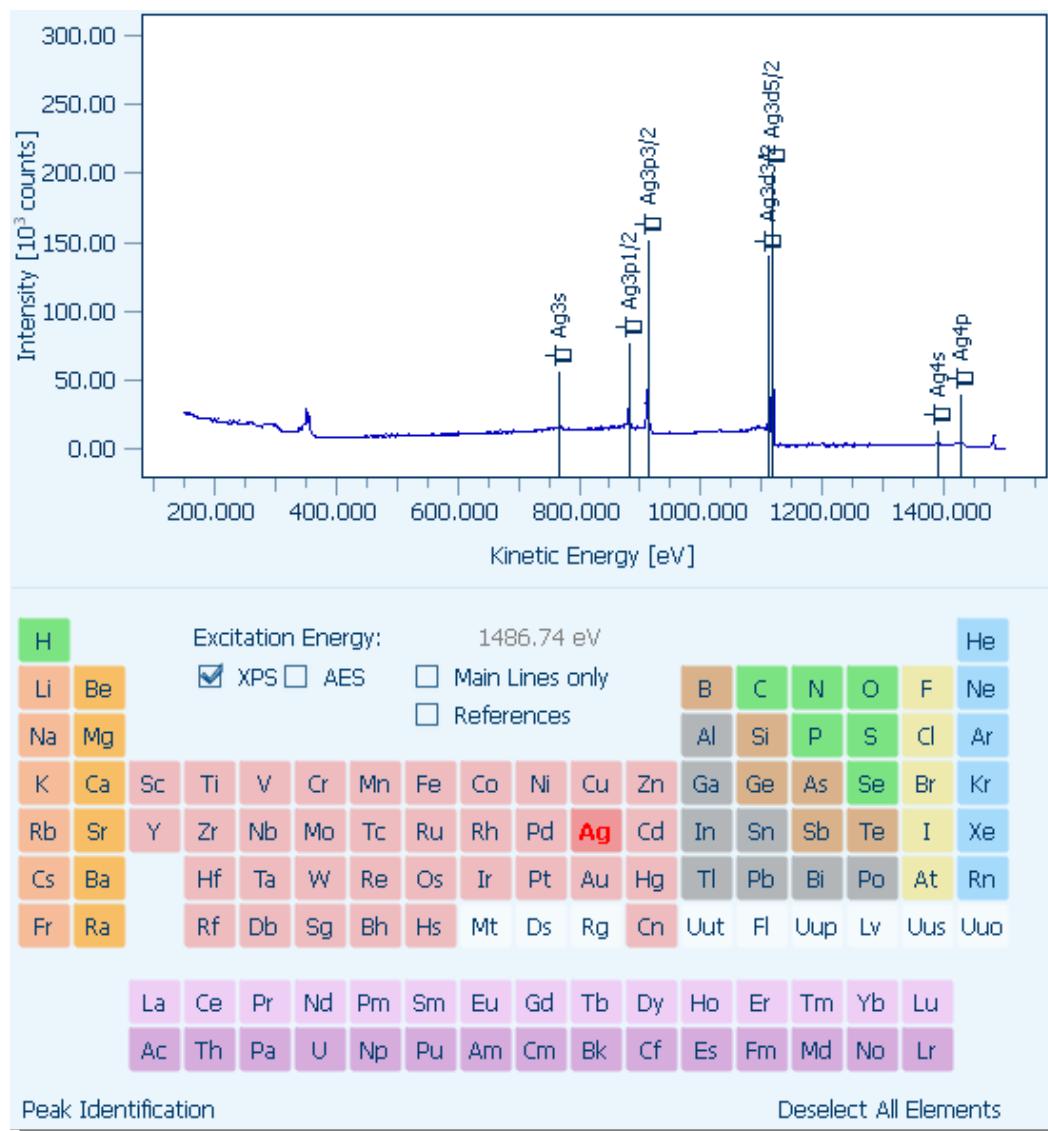
The **Lens Mode** opens a list that contains all available lens modes for your analyzer. This is specific to your analyzer—the modes are described in the analyzer manual.



You can select kinetic energy or binding energy for the display by clicking the E<sub>k</sub> and E<sub>b</sub> button respectively. The binding energy is calculated from the source energy.

A particularly easy method of setting up spectra is to use the periodic table button:

- Click the icon below the spectrum group table and click an element. A menu will appear with a list of peaks that you can select. The spectrum will be set up with suggested parameters for scanning the peak. Remember to set a lens mode for the spectrum!



Further configuration options:

- Click the button to add another spectrum to the group. This duplicates the selected spectrum, or the last spectrum if none is selected. A new line is added to the table with the parameters for the spectrum. To remove a spectrum, first select the row in the table, then click the button. You can move a spectrum to a different position in the group using drag and drop.
- Add a [data operation](#) to the spectrum in the Plot View. The data operation is automatically performed after the spectrum is acquired.
- Add additional spectrum groups or spectroscopy experiments to the Experiment Editor in order to run many measurements in one sequence.

- Add other instruments or [operations](#) to the schedule.

### 3.1.5 Starting a Measurement

SpecsLab Prodigy performs a validation check on the experimental settings before starting acquisition. In general, small inconsistencies in the settings are automatically corrected. If there is a more serious problem in the configuration, an [error message](#) appears which tells you how to fix the problem.

To acquire specified spectra:

1. Use one of the following methods:
  - Check the box in the leftmost cell for the spectrum you want to acquire. This action validates the spectrum. If you have defined additional spectra, you can also check these as you wish. Only spectra which have been selected will be acquired.
  - Select a number of spectra by holding down SHIFT (to select a range of items) or CTRL (to add the selected item) and click the spectra you want to acquire, then click  under the spectrum group.
2. Click the  button in the main toolbar. The selected spectra will be acquired.

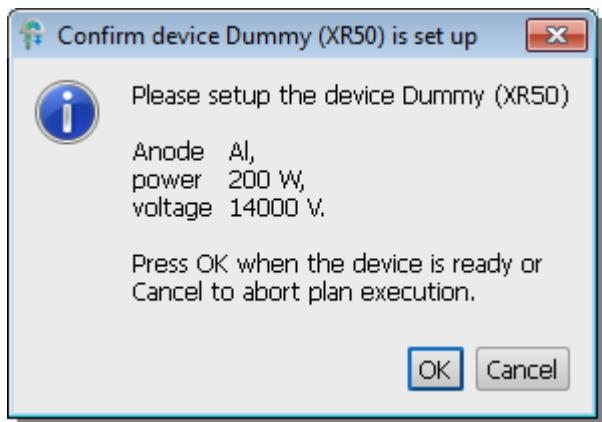
To acquire all spectra:

1. Click the  button in the main toolbar. A dialog will appear, asking if you want to run the entire schedule.
2. Click **Yes**. All spectra will be acquired.

If you selected **Notify to set up device** when adding the source, a dialog will now appear to prompt you to switch the source on with the correct settings.

#### Note

Devices controlled by SpecsLab Prodigy will be automatically switched on without requiring a prompt. The [status](#) of each device is shown in the menu bar.



You can pause acquisition by clicking the icon or abort the scan with the icon. There is also the "panic button" in the menu bar which allows you to switch off all connected instruments.

The Plot View displays data as it is being acquired. For more information about viewing data, please refer to:

- ["Plot View I: Features" on page 71](#), for display options in the Plot View.
- ["Plot View II: Data Operations" on page 85](#), for operations that you can perform on the data.

You can also view 2D data in the Image View—see ["Image View" on page 135](#).

After data acquisition, the spectrum is locked, as indicated by a icon. To unlock spectra:

1. Select the spectrum in the spectrum group. You can select a number of spectra by holding down the SHIFT or CTRL keys, as described above.
2. Click . There is a warning that all data will be deleted from the selected spectra. Confirm this to unlock the spectra. You can now edit the spectrum as necessary and reacquire.

### 3.1.6 Saving Data

SpecsLab Prodigy has an Autosave feature. This saves data during and at the end of acquisition. In the event of a program crash or similar interruption, you can reload the file in order to restore the settings and data. Clicking the Save icon next to the name will also save the current status of the experiment.

Clicking the arrow next to the Save icon produces a menu with the following options:

- Save the experiment.

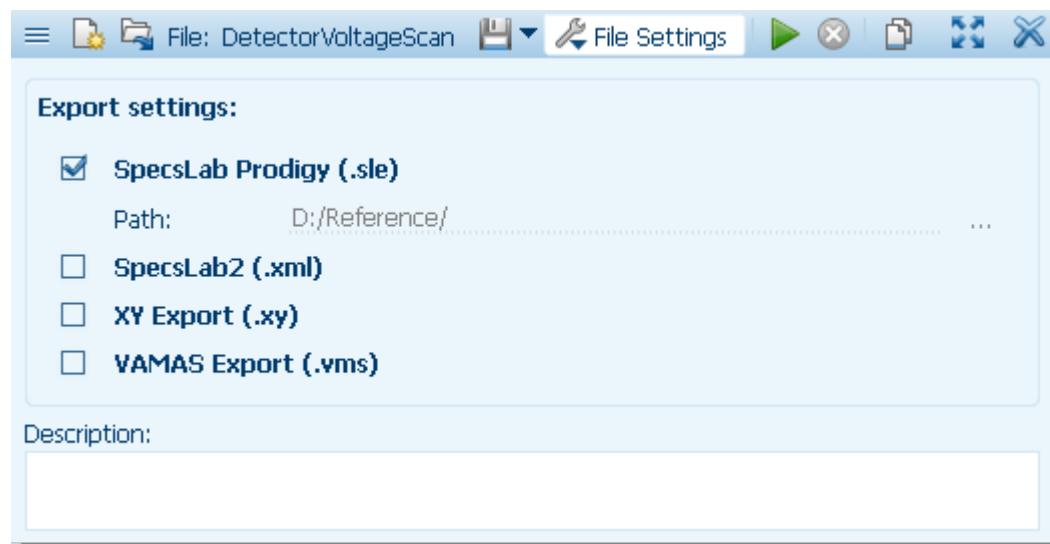
- Save As, which opens a dialog allowing you to specify a new name and location for the experiment file.
- Duplicate the experiment, with the experiment being saved under a new automatically generated name.
- Export to various formats.

Note the following points about files:

- You can set the location by clicking **Settings** and entering a path in the field provided. Clicking the ellipsis button opens a file browser so you can select a folder.
- The default name of the file is the experiment type (e.g. Electron Spectroscopy) with a date and time stamp.
- SpecsLab Prodigy uses a binary format that contains all data and experimental details. You can export data to different formats.

#### Note

As you can see from the screenshot below, SpecsLab Prodigy is able to export to the VAMAS format. Importing from this format is also possible, but not all information in the experiment will be saved for future use.



## 3.2 Scheduling Tasks

The Experiment Editor allows you to run a sequence of experiments. This is a very flexible system that allows you to automate various tasks. Note the following points about the schedule:

- The schedule runs from top to bottom, completing each task before starting the next.
- By adding new spectroscopy experiments, you can define different excitation sources.
- You can set up a sequence of different experiments.

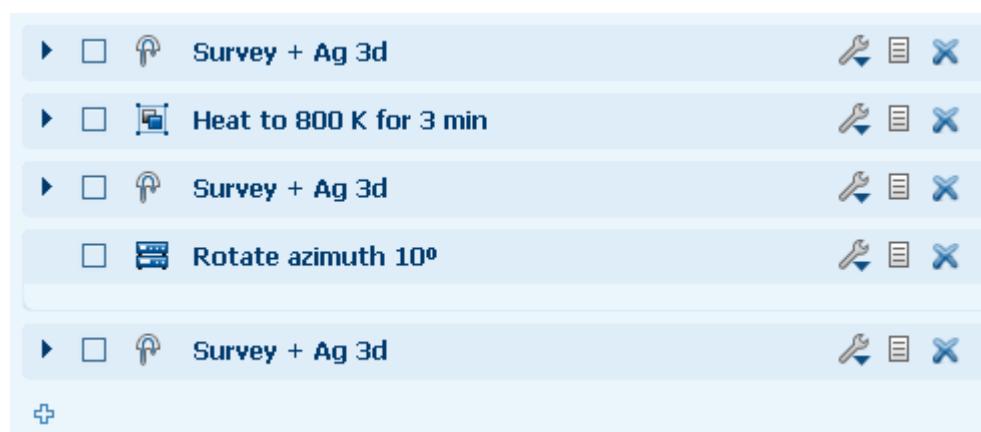
- If you only want to change the analyzer settings, it is best to add new spectrum groups to an existing experiment—this provides a logical order and makes complex procedures easier to follow.
- You can drag and drop items in the schedule to rearrange the order of their execution.

### 3.2.1 Building Schedules

The fastest way to build up a complex experiment is to add a number of predefined [templates](#) in a sequence. The screenshot below shows an example of an experiment built out of several [operations](#). The Survey + Ag 3d item is a template that is added repeatedly without the need for further definition.

#### Note

Groups can also be saved as templates so that complex routines can also be added. See [Using Groups](#) for more information.



The experiment can be started, as usual, by clicking ➤. This will check and validate all parts of the schedule and then sequentially run through the items.

### 3.2.2 Reusing the Schedule

A useful feature for quickly defining new experiments is the repeat function. This copies the existing experiment, complete with all configuration details, to a new file. The copy does not contain any data, and can therefore be immediately started without any further modifications. This is a useful feature for semi-automated procedures, for example if identical measurements are run on different samples.

To duplicate an experiment:

- Click the  icon in the Experiment Editor toolbar. A duplicate will be created. You will see that the timestamp in the filename has been updated.

### 3.2.3 Saving a Schedule

If the schedule represents a commonly executed procedure, you can save it for reuse:

- Click the icon. A **Save** dialog will open.
- Select **Prodigy Template (\*.slt)** from the **File Type** drop-down list.
- Enter a name (including the *.slt* extension) and location for the schedule and click **Save**.

The schedule will be available in the Experiment Editor as one of the quick links.

## 3.3 Templates

Templates are reusable experimental configurations. You can save items in the Experiment Editor together with their configurations for later use. This saves time when performing a series of similar measurements, while reducing errors caused by incorrect configuration.

### Note

You can also save an entire experiment as a template.

After creating a template, you can use it in other experiments. A template manager allows you to remove unused templates.

Typical uses of templates include:

- Defining an electron spectroscopy experiment with spectrum group(s) for commonly used scans.
- Setting up a number of devices.
- Defining a group of actions (or other templates) to perform a complex sequence.

If you are using standard mode (not expert mode), templates are the normal way of operating SpecsLab Prodigy.

### Note

You can also save configurations in devices and recall them for use in experiments or standalone device controls.

### 3.3.1 Creating Templates

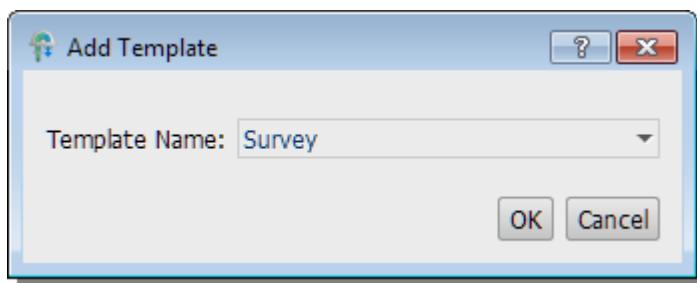
To create a template:

- Add an item (e.g. Electron Spectroscopy, Device, etc) to the Experiment Editor.
- Set up the item so that it is suitable for running in an experiment

## Note

You can run an item in an experiment, then save it as a template when the experiment is finished.

3. Click  and select **Save as Template**. A dialog will open.



4. Type a name for your template and click **OK**. Clicking the arrow reveals a list of other templates of this type.

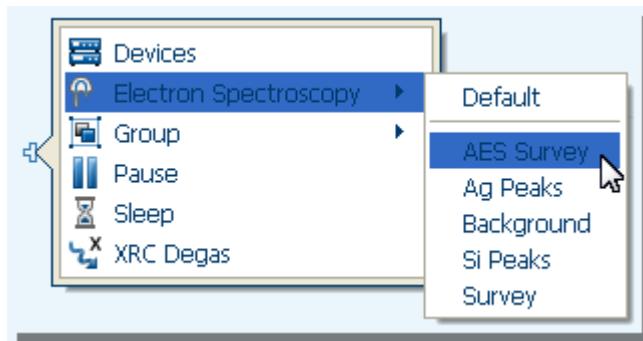
## Note

Templates are stored in the *settings\ExperimentEditor\Templates* folder of the SpecsLab Prodigy installation directory.

### 3.3.2 Adding Templates to Experiments

To add a template to an experiment:

- Click  If the entry in the menu has templates, there is an arrow on the right side. Moving the mouse to the control unit will show all available templates for this type of control item. Selecting a template will add it to the experiment.



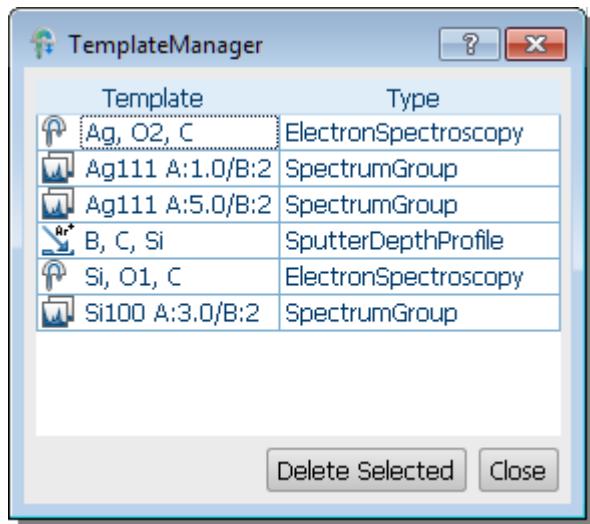
## Note

Selecting **Default** will add the item with no preset values.

### 3.3.3 Managing Templates

All templates you create are always available when you start SpecsLab Prodigy. You can remove outdated templates using the template manager:

1. Click the icon in the Experiment Editor toolbar. The **Template Manager** dialog will open.



2. Select a template that you want to remove and click **Delete Selected**.

#### Note

Deleted templates cannot be recovered.

#### Note

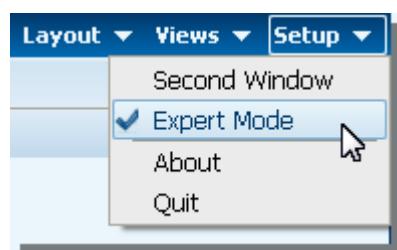
To change a template name, load it, then save it with a new name. You can then delete the original.

## 3.4 Expert Mode

Expert mode allows full access to all features in the software. This is necessary for configuring and optimizing experiments. For regular data acquisition, many of the features are not altered. You can leave Expert Mode. This hides a number of parameters and options, leaving only those which are actually used for running experiments. Building and running experiments involves selecting tried and tested templates which are less prone to error and do not require such a high level of expertise for operation.

To toggle Expert Mode:

- Select **Setup/ Expert Mode** at the top right of the window. A tick indicates when SpecsLab Prodigy is in Expert Mode.



## Chapter 4 – Experiment Editor II: Schedule Options

The schedule consists of a set of instructions and operations that make up an experiment. For an introduction to preparing schedules, please see:

- [Creating a New Experiment](#)
- [Building Schedules](#)

Beyond the basics of setting up a scan, there are a number of additional options that you can use. These are shown in the menu when you add an item to the Experiment Editor or to an Electron Spectroscopy experiment.

Some of these options may not be present in your version of SpecsLab Prodigy as they are included in your configuration. The table below provides a short description of all possible features.

If you would like to add an option to your configuration, please contact SPECS for details about licensing.

Option	Description
<a href="#">Auto Flood Gun Adjustment</a> (optional)	Varies the emission current of a flood gun while recording test spectra. Selects an optimum emission current based on the minimum peak width.
<a href="#">Auto Sample Height Adjustment</a> (optional)	Moves the sample position while measuring signal intensity. Locates the optimum position for maximum intensity.
<a href="#">Device</a> (standard)	Adds a device (e.g. heater, manipulator, etc) to the schedule, allowing you to perform an action with the equipment.
<a href="#">Electron Spectroscopy</a> (standard)	Sets up a source and analyzer.
<a href="#">Group</a> (standard)	Allows you to group other actions together to form logical groups, adding structure to the schedule.
<a href="#">Pause</a> (standard)	Pops up a message prompting user action during a schedule.
<a href="#">Profiling</a> (optional)	Steps through a set of parameter values (e.g. manipulator positions), taking spectra at each point.
<a href="#">Sleep</a> (standard)	Stops the schedule for a user-defined period.
<a href="#">Spectrum Group</a> (standard)	Defines settings for scanning data.
<a href="#">Sputter Depth Profiling</a> (optional)	Controls an ion gun for automating depth-profile experiments.

## 4.1 Electron Spectroscopy

The electron spectroscopy experiment allows you to set up an analyzer and source ready for data acquisition. You can add and configure other devices. These will be activated before the experiment continues.

### Note

See also [Creating a New Experiment](#) for a description of how to set up a standard electron spectroscopy experiment.

An electron spectroscopy experiment must contain the following items:

- Analyzer
- Source

If you only have one analyzer or source, it will be added automatically. Otherwise, you will be offered a choice of all available devices.

To add an electron spectroscopy experiment:

- Click  in the Experiment Editor and select **Electron Spectroscopy**. You can only add electron spectroscopy items directly to the Experiment Editor—they cannot be added to any other item.

After setting up the experiment, you can add items to define the data acquisition procedure.

The most common item is a [spectrum group](#).

## 4.2 Spectrum Group

A spectrum group contains analyzer settings and the parameters for one or more scans. The workflow for [creating](#) and [editing](#) spectrum groups is described elsewhere. The following sections provide reference information about the features in a spectrum group:

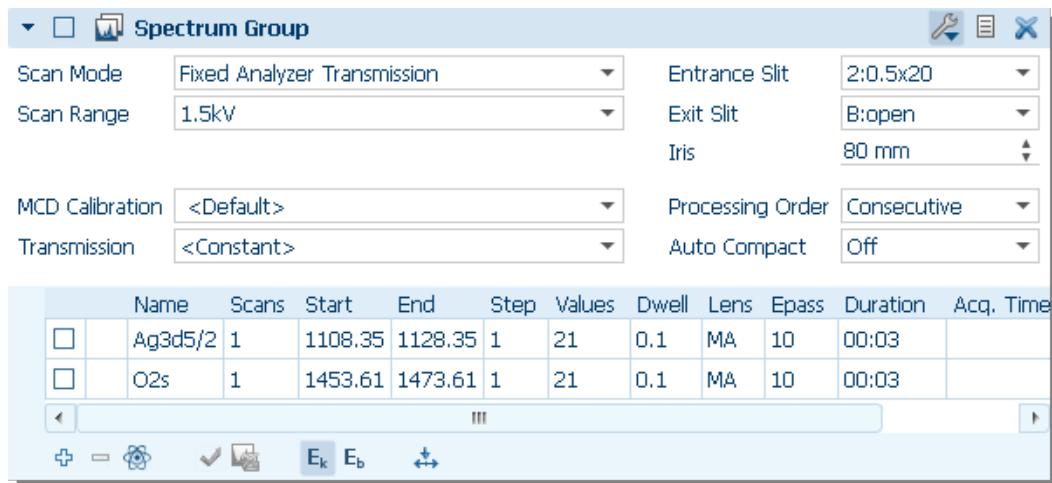
- [Analyzer configuration](#).
- [Menus](#) and context menus.
- [Spectrum definition](#).
- [Icons](#) below the spectrum definitions.

To add a spectrum group:

- In an electron spectroscopy experiment, click  and select **Spectrum Group**.

### Note

The  icon in the main toolbar contains the usual controls for creating templates and unlocking the contents of the group. In addition, it contains the same items as the context menu and allows a convenient way to [export](#) all spectra in the spectrum group.



#### 4.2.1 Spectrum Definition

The spectrum group contains a table which contains a set of definitions for spectra. You can move a spectrum to a different position in the group or to another spectrum group using drag and drop.

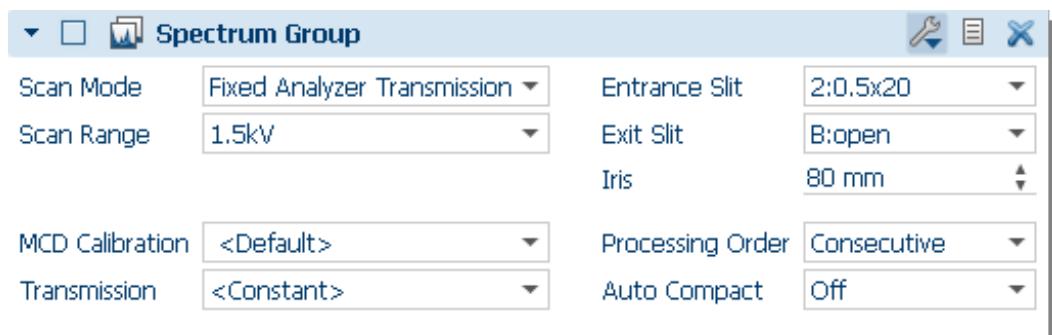
Which items are displayed in the manual depends on other settings. Please refer to the following:

- [Scan mode](#)
- [Context menu](#)

In addition, the analyzer manual has details of which lens modes are available.

#### 4.2.2 Analyzer Configuration

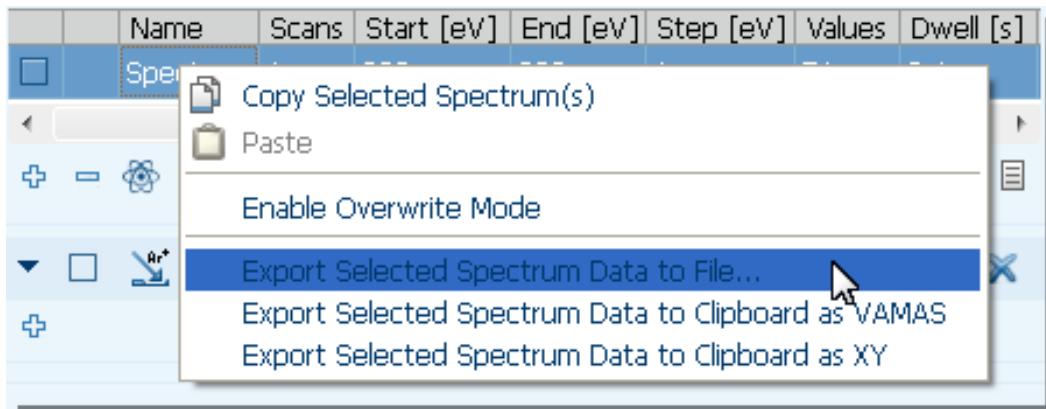
There are a number of settings for the analyzer. These apply to all spectra in the group. The table below lists the function of each setting.



Setting	Description
Scan Mode	See <a href="#">Scan Modes</a> for a description of all available scan modes.
Scan Range	Sets the range of the HSA 3500plus power supply. You should select the lowest possible for your experiment, as the power supply is more accurate in the lower ranges.
<u>MCD Calibration</u>	Corrects energy shifts and intensity differences between different measurement channels
Processing Order	Determines the order that spectra are measured: <ul style="list-style-type: none"> <li>• <b>Consecutive</b>—all spectra in the group will be measured consecutively.</li> <li>• <b>Cyclic</b>—depends on the number of scans defined. All energy regions are measured once consecutively, then the scan returns to the start of the group and goes through the group, as defined for each individual spectrum. This cycles until all scans are performed.</li> </ul>
Transmission	Selects a transmission function for your experiment.
Entrance Slit	Notes the slit settings on the analyzer. You need to set these manually on the analyzer. The transmission function is dependent on the slit settings.
Exit Slit	SpecsLab Prodigy will check that the transmission function is suitable for the selected slits.
Iris	The iris setting of the analyzer. As with the slit settings, this is set manually on the analyzer and the value is recorded with the experiment. The default value for the iris setting is the maximum, as defined in the configuration tool.
Compact Data	<p>There are three options:</p> <ul style="list-style-type: none"> <li>• Off—the data is not compacted.</li> <li>• Combine Channels—the signals from individual channels in a multichannel detector are summed to a single value.</li> <li>• Sum Scans—when measuring a spectrum with several scans, the intensities from the scans are summed into a single value.</li> </ul> <p>Compacting data can significantly reduce file size. However, measurements of individual channels or scans are lost.</p>

#### 4.2.3 Context Menu

Right-clicking on the spectrum definition table shows a context menu. The options in this menu are listed in the table below.



Menu item	Description
Copy Selected Spectrum(s)	Copy and paste the selected spectrum(s). This allows you to quickly create duplicates of definitions in the spectrum group.
Paste	
Enable Overwriting Mode	On selecting this item, the spectrum is marked red in the table. When you run the experiment, spectra are acquired normally until reaching the red spectrum. The red spectrum is then repeated in a loop, with each acquisition overwriting the previous results. This loop will continue until you unselect overwriting mode—data acquisition will then continue through the rest of the spectrum group. Canceling acquisition will also break the loop.  This mode is useful for setting up or optimizing experiments.
Export Spectrum to file, VAMAS or XY	Allows you to export the selected spectrum to VAMAS or XY format. See <a href="#">"Exporting Data" on page 61</a> for more details.  These items are also available in the main toolbar, which allows all spectra to be exported and in the <a href="#">icon</a> below the table, which allows all selected spectra to be exported.

#### 4.2.4 Menus

The icon in the main toolbar brings up a menu which contains the items shown in the table below.

Menu item	Description
Unlock and Clear All Data	Unlocks all spectra in the group, allowing you to modify the definition after running the measurement. This will delete all measured data in the group.

Menu item	Description
Save as Template	Saves the group configuration as a <a href="#">template</a> for future use.
Copy	Copies the configuration. When you add an item to the Experiment Editor (e.g. a Spectrum Group), you can paste this configuration.
Use Start/ End	These two options determine the way you set up the energy range for the experiment. The values are also dependent on whether binding or kinetic energy is selected.
Use Center/ Width	Start/ End directly sets the minimum and maximum settings for the spectrum range. Center/ Width allows you to pick a central energy (e.g. a peak position) and the total width of the spectrum. Although useful for setting up spectra which examine a known peak position, this is especially useful for the snapshot scan mode, where the analyzer is not scanned.

#### 4.2.5 Tools

There are a set of icons below the list of spectrum definitions which add, remove or perform actions on spectrum definitions. The table below lists function of each icon.

You can select multiple spectra as follows:

- Hold SHIFT and click a spectrum to select a range.
- Hold CTRL and click a spectrum to add it to the selection.

Icon	Description
	Adds a spectrum definition to the group. The values in the spectrum are based on the currently selected spectrum or, if no spectrum is selected, on the last spectrum in the table.
	Deletes the selected spectra.
	Shows the periodic table, if available. Selecting an element and excitation in the table adds a suitable energy range to the spectrum definition.
	Validates the selected spectra.
	Uses the electron kinetic energy to define the spectrum.
	Sets the energy settings for the spectrum definition to binding energy, as calculated from the source energy.
	Unlocks selected spectra, allowing you to modify the definition after measurement. This will delete the data in the spectra.
	Displays a menu with the same entries as the <a href="#">context menu</a> .

#### 4.3 Devices

You can add a device to your experiment and operate it. The devices available depend on the configuration of your system.

In general, the settings for devices are intuitive. For a full description, please refer to the manual of the instrument. The device control for the instrument usually has a similar method of operation.

Note the following points about devices:

- If you simply want to control the device, i.e. not operate it as part of an experiment, use the device control.
- A device in an experiment is normally part of the [schedule](#) and often in a [group](#).
- The settings for the device will remain as you set them until the experiment finishes, or until you apply new settings. Thus, if you switch on a flood gun, it will stay on for the rest of the experiment unless you include another device section to switch it off.

#### Note

You can add devices to Electron Spectroscopy experiments. Any parameters you set are valid for the duration of the scan.

To add a device:

1. Click and select **Devices**. A new devices control item will be added.
2. Click a device. Controls for the device will appear.
3. Set the parameters for the device as desired. Clicking will reveal more parameters.
4. Add and configure other devices as necessary.

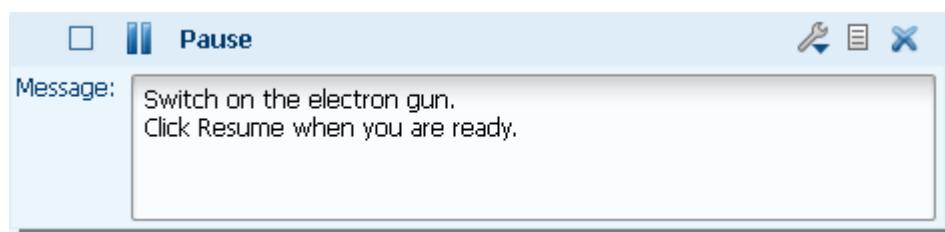
The settings for the device will be applied when you run the experiment and SpecsLab Prodigy reaches the item in the schedule.

#### 4.4 Pausing to Prompt User Action

The Pause action allows you to display a message during an experiment. The schedule is interrupted until the message is accepted by the user.

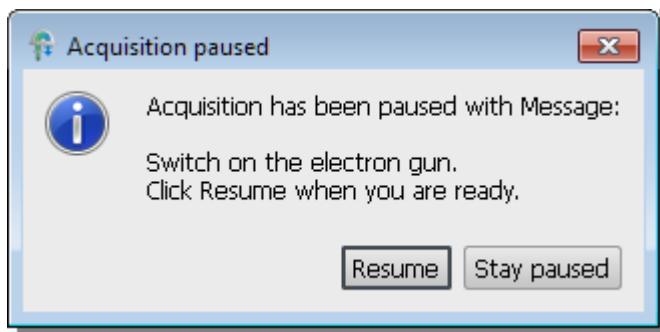
To add a Pause to the schedule:

1. Click  and select **Pause** from the menu.
2. Type a message into the field provided. This text will appear in the prompt



You can now add further items to the schedule. When running the experiment, the Pause item will be executed as part of the schedule. SpecsLab Prodigy displays a dialog with the user instructions:

- **Resume**—Continues the experiment.
- **Stay Paused**—Closes the dialog and pauses the schedule. You can make adjustments to the rest of the schedule as necessary, then click ►. The schedule will restart after the Pause item.



## 4.5 Adding Sleep Intervals

The Sleep item adds an interval to the schedule in which no actions are performed. Typical uses of the Sleep feature are:

- Adding a short break so that a device can initialize and come to stable operation.
- Adding longer breaks so that the sample can cool down or the pressure can recover.

To add a Sleep item to the schedule:

1. Click + and select **Sleep** to add a pause to the schedule.
2. Set the **Sleep** duration.



You can now add further items to the schedule. When running the experiment, the Sleep item will be executed as part of the schedule. The menu bar shows the status of the Sleep as it is running.



## 4.6 Using Groups

As experiments increase in length and complexity, the schedule can quickly become long and unreadable. Groups allow you to apply a hierarchy to the schedule, adding structure and grouping items into logical units.

To add a group to the schedule:

- Click  and select **Group**.

Groups are particularly well-suited to be saved as templates. You can create a common task that uses a number of devices and save this as a template. Each time you need to perform this task, you can insert the group template in the schedule.

### Example

The following example shows how to create a group that contains commands for heating the sample. It performs the following actions:

- Uses the manipulator to move the sample to a "safe" position. This may be in the preparation chamber, or simply away from the analyzer.
- Heats the sample to a specified temperature for a specified time.

To define the group:

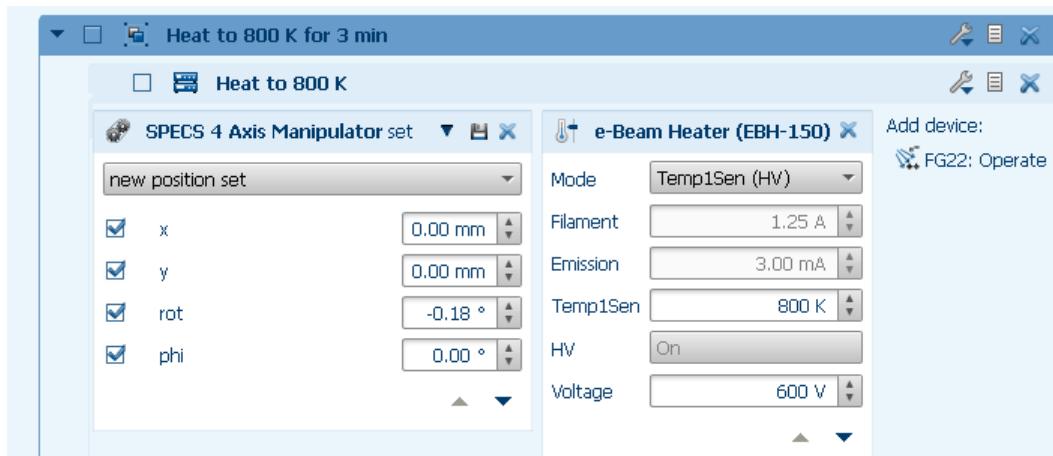
1. Click  and select **Group**.
2. Click  inside the group and select **Devices**. A list of all devices on your system will be shown.

### Note

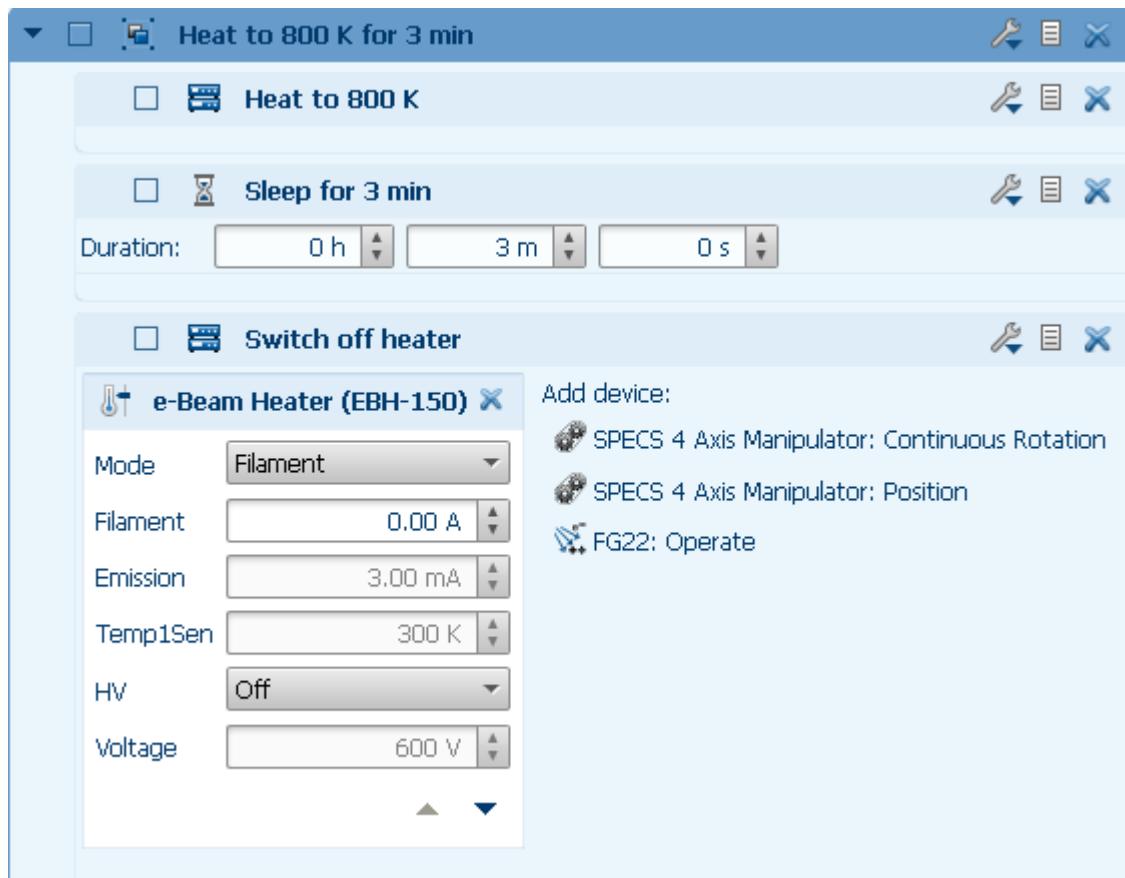
If you accidentally add an item outside the group, you can drag and drop it into the correct position.

3. Click **SPECS 4 Axis Manipulator: Position**. The controls for the manipulator will be shown.
4. Click the drop-down list in the manipulator settings and select a position for the manipulator.
5. Click **EBH 300** and configure the electron beam heater so that it heats the sample to the desired temperature.

**Note** It is a good idea to give items suitable names as you add them so you can easily identify the functions of the group and its components.



6. Click **⊕** inside the group and select **Sleep**.
7. Set a time for the sleep interval. The sample will be held at the temperature for this time.
8. Click **⊕** inside the group and select **Devices**. Another devices section will be added to the group.
9. Add an electron beam heater group to switch off the heating.



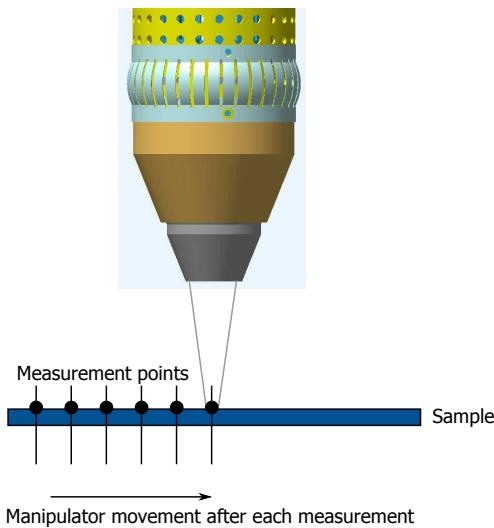
You can save the group as a template for future use:

- Click in the main toolbar of the group (labeled "Heat to 800 K for 3 min" in this example) and select **Save as Template**. A dialog will open allowing you to specify the name of the template

## 4.7 Dimension Profiling

Dimension profiling allows you to change device parameters, running a spectrum group after each change. A typical example would be to move a manipulator a fixed distance between scans in order to build up a spatial chemical map of the surface.

As an example, the following procedure shows you how to use a [manipulator](#) to scan a [series of points](#) on the sample to obtain spatial mapping of the surface.



To continue the example, and thereby demonstrate the flexibility of the software, the experiment will then [ramp the temperature](#) while performing the spatial mapping. Finally, there are instructions on how to [acquire and display data](#).

In principle, you can add dimensions for any item of equipment with adjustable operating parameters. For example, you can run a series of measurements using different HV settings in the X-ray source in order to measure as a function of X-ray power. This makes the procedure extremely powerful and flexible. Moreover, you can add many dimensions to the profile. However, this can quickly lead to long measurements—measuring a grid of points  $5 \times 5$  in size leads to 25 scans. Adding a third dimension can quickly lead to hundreds of measurements in the experiment.

#### 4.7.1 Setting Up Devices

As usual, the first step in defining a new experiment is to set up the [sources](#) and [analyzer](#). In addition, you also need to add the equipment that is used in the profile.

For a position profile, a manipulator is required.

To set up the devices for a position profile:

1. Click **Electron Spectroscopy** in the Experiment Editor to start a new experiment.
2. Add a source and analyzer and define their properties.
3. Add the **Manipulator: Position** device to the experiment.
4. Select a preset position for the manipulator.

User-defined preset



#### Note

You can define presets in the manipulator Device Control. Set the desired position for the axes, then click Add Position. You can then save the settings to a position file. This file will then appear in the preset menu.

#### 4.7.2 Defining the Profile

When defining a profile, you first need to select a parameter that will be varied during the experiment. You then define the range of the parameter and the number of iterations for the scan—the steps are equally spaced. You can also determine whether the settings in the profile are absolute or relative:

- Check **Relative** box—settings in the profile are relative to the settings defined when you added the device to the experiment.
- Uncheck **Relative** box—defined device settings are ignored and the absolute values defined in the profile are used for controlling the equipment.

To define the profile:

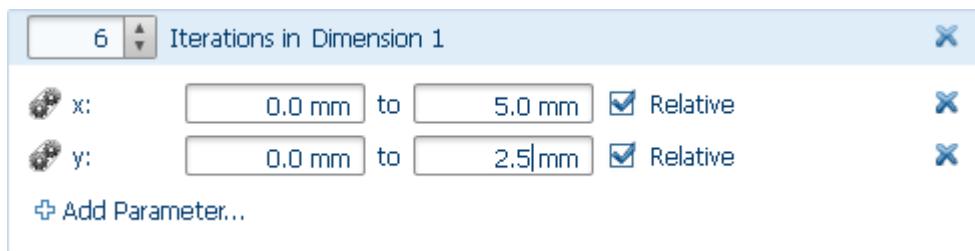
1. Click the  icon to add a profile.
2. Click **Add New Dimension** and select **Manipulator X** from the list. The manipulator will move in the X direction between scans.
3. Set the following values (modify for your own requirements):
  - x: 0.0 mm
  - to 5.0 mm
  - Iterations in dimension 1: 6
  - Check **Relative**.

If we were to define a scan now, the following would occur:

- The spectrum group would be scanned with the manipulator in its present position.
- The manipulator would move 1 mm in the X direction.
- The spectrum group would be scanned again.
- The move/ scan procedure would continue, with the manipulator moving in 1 mm steps until it had moved 5 mm from its initial position.

As an aside, you can add another parameter to this dimension. For example:

- Click **Add Parameter** and select **Manipulator Y** from the list. A new line appears that allows you to define movement of the Y axis. Both X and Y movements are performed together, so the scan would follow a diagonal line (in the X-Y plane) on the sample surface.



### Note

Clicking the icon will remove a dimension without affecting any other part of the configuration.

#### 4.7.3 Adding a Second Dimension

The [previous section](#) showed you how to define a profile for one dimension. You can add as many dimensions as you like to an experiment—the limiting factor is the required measurement time. After measuring points in the X direction, a natural step might be to add a dimension in the Y direction, in order to build up a 2D spatial map of the surface.

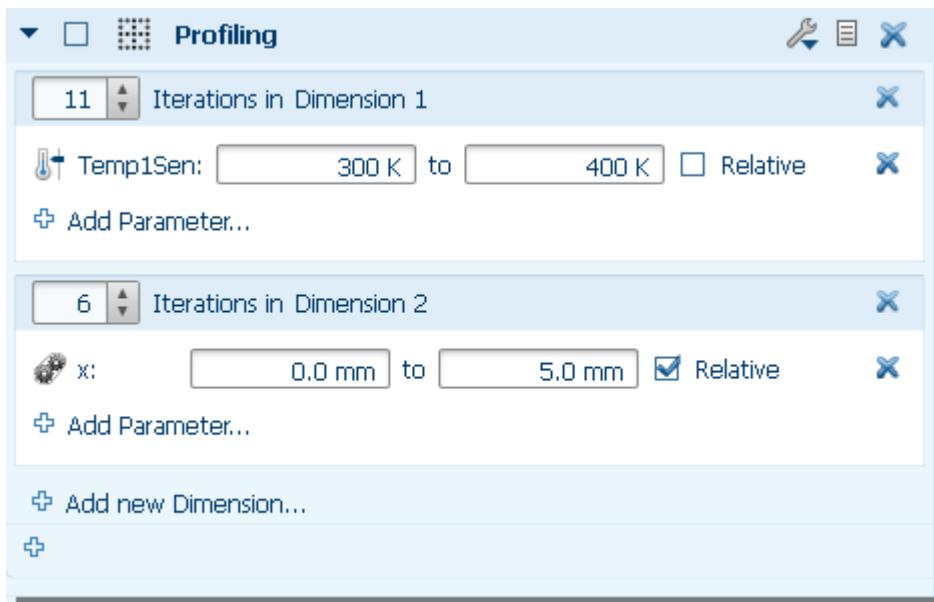
As an alternative, this section shows you how to use two dimensions with a sample heater and manipulator. The sample will be heated to a set temperature, then measured along a set of positions, then the temperature changed before measuring again.

### Note

It is not necessary to add all devices to the experiment before adding the profile. It is sufficient to add the device before you want to add the dimension.

To add a temperature dimension to the profile:

1. Add the device **E-Beam Heater EBH 150**.
2. Select **Temperature IR** from the **Mode** drop-down list.
3. Click **Add New Dimension** and select **E-Beam Heater (EBH 150): Temperature** from the list. The new dimension is added.
4. Set the values for the temperature settings, e.g. such as those in the screenshot below.



5. Add a new dimension for the X axis of the manipulator and define this for a series of positions.

If we were to define a scan now, the following would occur:

- The sample would be warmed up to 300 K and the spectrum group once again recorded over all X positions.
- The spectrum group would be scanned at positions 0 mm to 5 mm in 1 mm steps.
- The sample would be warmed up to 310 K and scanned at each position.
- Scanning would continue until all positions have been recorded at all temperatures up to 400 K.

#### 4.7.4 Running the Profile

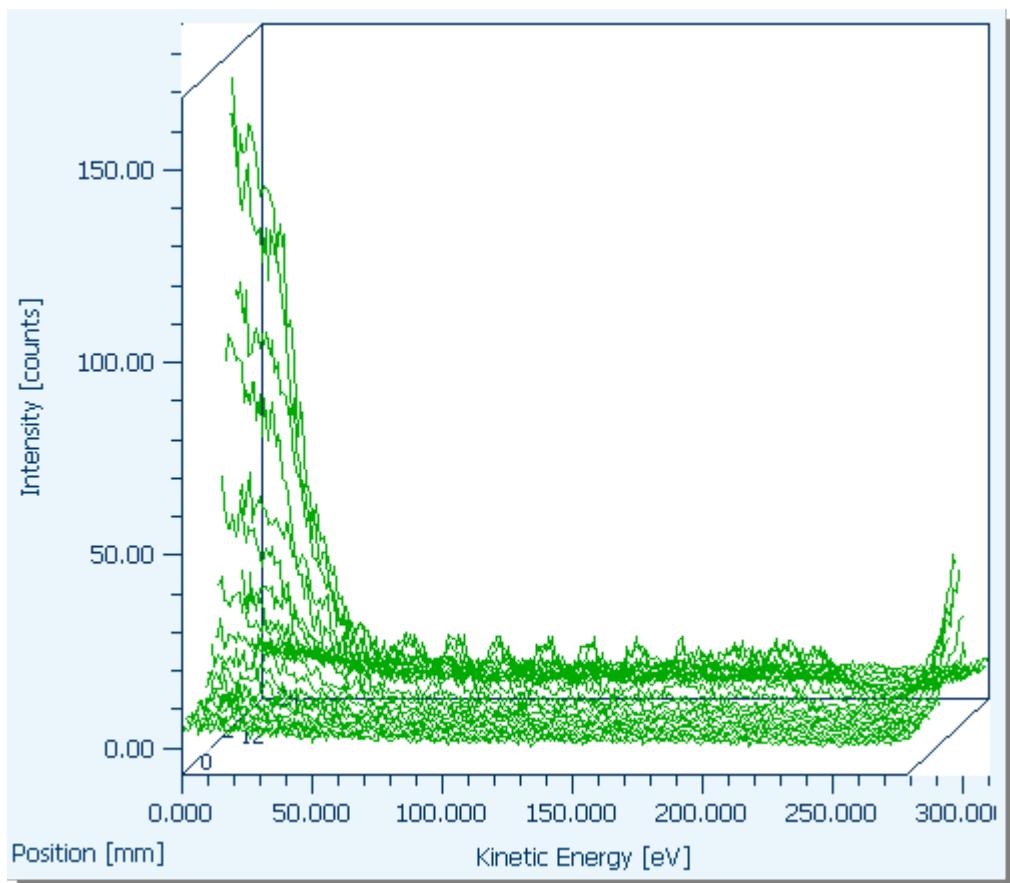
After defining all the desired dimensions in the profile, you can add a spectrum group. As there may be a large number of iterations in the profile, you should try to keep the scan duration as short as possible:

- Scan peaks of interest, rather than survey or other wide-range spectra.
- Use larger energy step times and shorter dwell times.
- Try to use snapshot mode to capture a small energy region without needing to scan.

To acquire spectra with the profile:

1. Click the  icon to add a spectrum group to the profile.
2. Define the spectrum group in the normal way.
3. Click  to validate the scan and start data acquisition.

The tool bar will show the progress of the profile as it runs. Data is shown in the Plot View. For a better view of the scans, you can click to display the [Z axis](#), then [select Position](#) for the Z axis. You can also open the data in the [Image View](#) for an alternative visualization.



## 4.8 Depth Profiling

Depth profiling with an ion gun involves removing the surface layer(s) with ions, then measuring the chemical composition of the newly exposed surface. In this way, you can measure the bulk chemical composition of the sample.

The following sections guide you through the procedure for setting up [sputter cycles](#), the [ion gun](#) and [other equipment](#), then [running](#) a depth profiling experiment in SpecsLab Prodigy.

### 4.8.1 Defining the Sputter Cycles

Depth profiling experiments involve measure-sputter-measure cycles. You need to specify the length of each sputter cycle and the number of cycles. For ease of setup, you can specify a number of iterations for a given duration.

If you want to measure the sample before sputtering, set the duration of the first cycle to zero.

To define the sputter cycles

1. Click the  icon to add a Sputter Depth Profile to the experiment.
2. Click the  icon to add a new entry to the Sputter Cycles.
3. Edit the settings for the sputter cycles:
  - **Duration** sets the time that the ion gun is switched on.
  - **#Iterations** sets the number of times the sputter cycle is performed.
4. Add and define further entries as necessary.

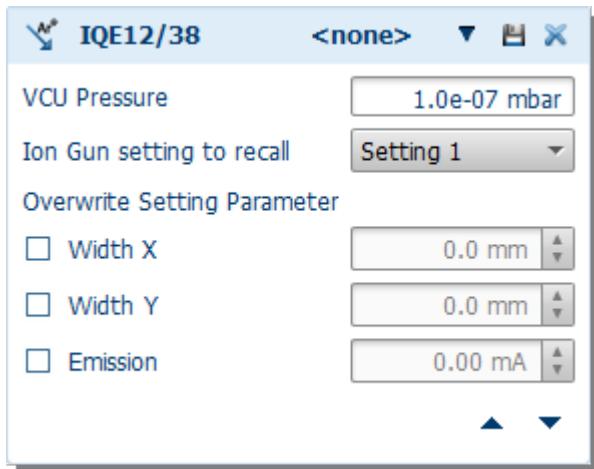
Sputter Cycles	
Duration [s]	#Iterations
10	1
5	2
	

#### 4.8.2 Adding an Ion Source for Sputtering

The SPECS IQE 12/38 has a number of predefined settings. The IQE 12/38 manual describes how to adjust these settings. You can recall one of these settings for the depth profiling experiment. If you do not have a SPECS IQE 12/38, you can define a dummy. This records the settings with the experimental data, while you operate the ion source manually.

To add an ion source to the depth profile configuration:

1. Click **IQE 12/38: Operate** in the **Sputter Device** section. A new field containing settings for the sputter gun will be added.
2. Click the  button to show more settings.



3. Edit the settings for the ion source:

- VCU pressure is the regulating pressure to be set by the VCU 1000 valve control unit. This is not displayed if the VCU 1000 is not installed.
- Select one of the pre-programmed settings for the IQE 12/38. These are defined in the power supply for the IQE 12/38—please see the manual for further details.
- If desired, define new settings for the spot X and Y width settings and emission current. These settings will override those in the pre-programmed setting.

**Note**

The settings for a dummy source are similar to those for the "real" IQE 12/38. As with other dummy sources, you have the option to ask for a prompt to control the device.

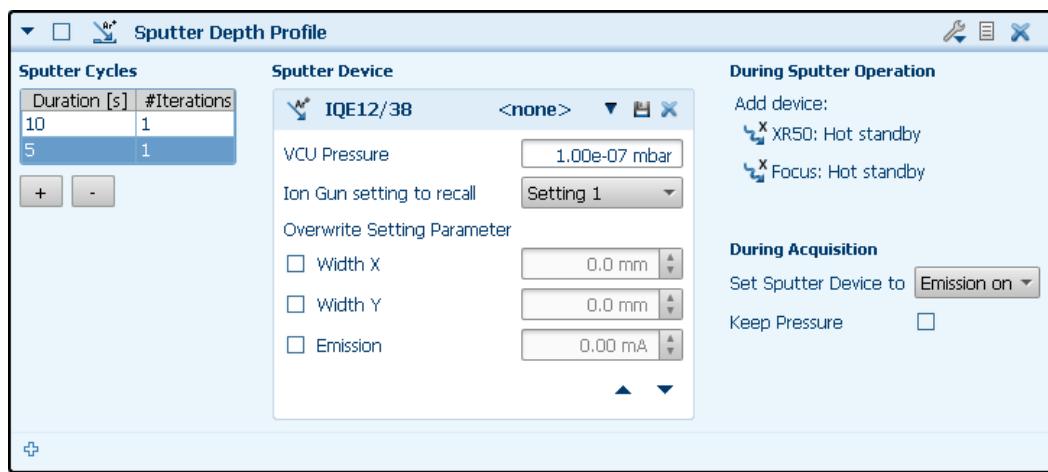
#### 4.8.3 Completing the Sputter Cycle

There are some additional options that may be useful for your sputter experiment. You can set these as you wish before defining the spectrum group.

To finish configuring the sputter cycle:

1. Add additional devices as necessary:
  - **XR50 Hot standby**—Used in conjunction with the XR50 source defined in the experiment. Leaves the source in standby mode when not in use, rather than switching off.
  - **Manipulator Constant Rotation**—Allows you to set the manipulator to rotate at a constant user-defined rate.
2. Set the behavior of the sputter device during data acquisition::
  - You can set the ion gun to standby (HV off, filament at standby level) or Emission On (HV off, filament reduced to allow a small amount of emission). The latter setting allows the ion gun to achieve stability more quickly when it is switched back on for the next sputter cycle.

- You can maintain the gas pressure during the measurement cycle. Only available if you have a VCU 1000 installed.



#### 4.8.4 Running the Depth Profile

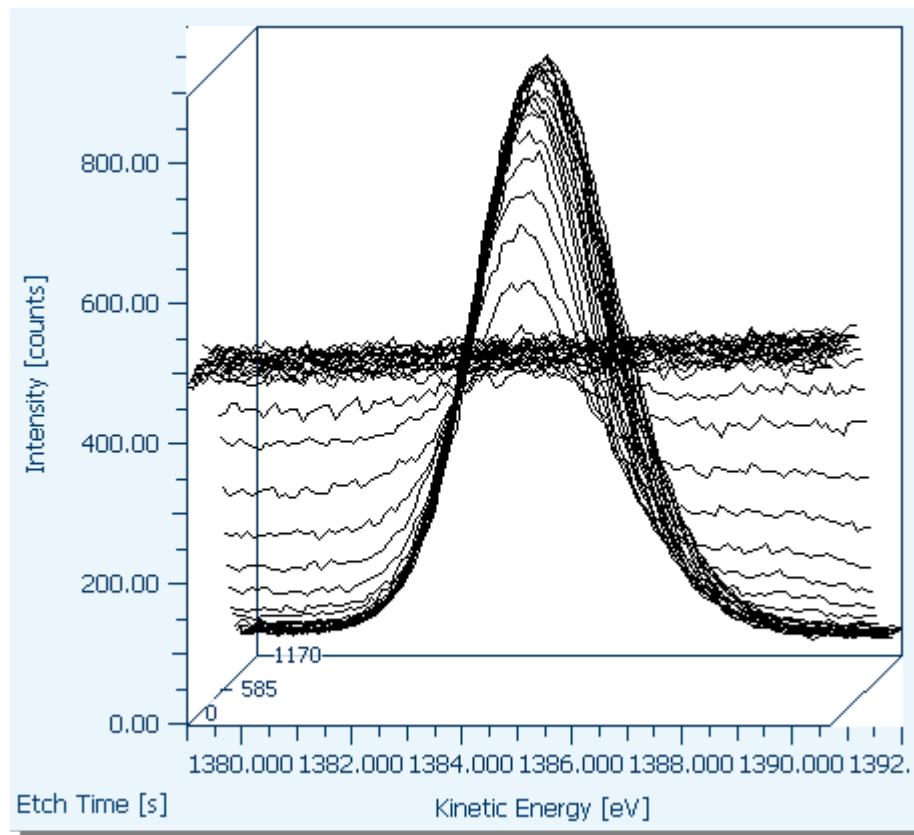
Defining spectra for the depth profile experiment is the same procedure as for a normal scan.

To run the depth profile:

1. Click the icon to add a spectrum group to the depth profile.
2. Define the spectrum group in the normal way.
3. Click to validate the scan and start data acquisition.

Data is shown in the Plot View. For a better view of the scans, you can click to display the Z axis, then select **Etch Time** for the Z axis. You can also view the data in the Image View. For more information, please refer to:

- ["Changing the Axis Labels" on page 83.](#)
- ["Displaying Spectrum Components" on page 72.](#)
- ["Opening Data in the Image View" on page 136.](#)



## 4.9 Auto Adjustment of Flood Gun

The auto adjustment of flood gun procedure assists you in automating experiments on insulating surfaces. These surfaces charge up when exposed to X-rays as a result of photoemission. This prevents reliable measurements of the surface, or even any measurement at all.

In order to compensate for charging, a low energy electron source can irradiate the surface. However, this damages the sample in many cases. The trade-off is peak quality against flood gun emission current.

SpecsLab Prodigy optionally offers a means to automatically measure the full width at half maximum (FWHM) of a peak as a function of flood gun emission current. Following a series of scans, it evaluates the data and finds the emission current with the smallest peak FWHM. SpecsLab Prodigy then sets the flood gun to this emission current and continues to run the experiment.

### 4.9.1 Configuring Auto Flood Gun

You need to include and configure the following items in the Electron Spectroscopy experiment:

- Analyzer.
- Source.
- Flood Gun. The auto flood gun adjustment routine starts with the emission current set for this device. The emission current must be greater than zero.

#### Note

After producing a suitable configuration, you can save it as a template. You can then load this for future experiments without needing to follow the whole procedure described here.

To configure the auto adjustment of flood gun procedure:

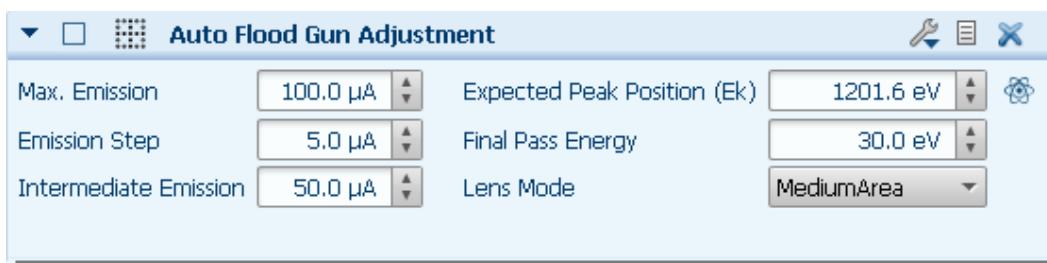
1. Click  and select **Sleep** to add a pause to the schedule.
2. Set the **Sleep** duration to 1 minute. This will allow the flood gun to stabilize before the optimization routine starts.



3. Click  and select **Auto Adjustment of Flood Gun** to the schedule. This should appear directly after the **Sleep** item.
4. Edit the settings. The table below describes each item. The screenshot shows typical settings with a carbon 1s peak selected.

Parameter	Description
Max. Emission	The maximum flood gun emission current. The auto adjustment routine will stop after measuring a spectrum at this flood gun setting.
Emission Step	The increase of emission current in each measurement.
Intermediate Emission	Sets an earlier point for stopping the routine. If the auto adjustment procedure has already located a minimum in the FWHM of the measured peaks, it will stop and use the settings obtained. Otherwise, the emission will be increased up to the limit given in Max Emission.
Expected Peak Position (Ek)	Enter the expected location of the peak (kinetic energy). Ideally, this is the book value of the excitation. Due to charging, it will have moved somewhat, but it will most probably appear somewhere in the scan range. You can click the  icon to display the periodic table and select an excitation.
Final Pass Energy	The initial pass energy of the analyzer is set to 50 eV for an

Parameter	Description
	exploratory scan. This decreases to 30 eV for the second scan. You can define the pass energy for the subsequent scans. For most purposes, 30 eV should be sufficient. If you require very high resolution, you can reduce the pass energy at the cost of count rate.
Lens Mode	Set an appropriate lens mode for your analyzer. Medium Area is suitable for most purposes.



- Set up the analyzer parameters (Scan Mode, etc) in the normal way. If your detector has a suitable number of channels, you can use Snapshot mode; otherwise, you need to use Fixed Analyzer Transmission for a normal XPS scan. The other analyzer parameter should be the same as those for your data acquisition.

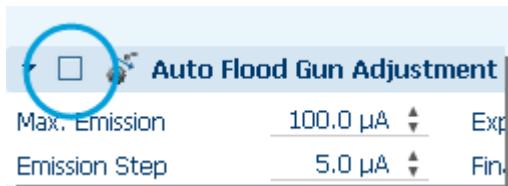
You can now add a spectrum group to the **With Optimized Emission** section below the auto adjustment of flood gun procedure. All items in this section will be executed after the flood gun emission current has been optimized. After running these items, the flood gun emission is returned to the value you defined for the flood gun at the start of the experiment (with the analyzer and source settings).

Note the following points for running spectra in the **With Optimized Emission** section:

- If no optimum emission current can be found, SpecsLab Prodigy will use the emission current you defined for the flood gun at the start of the experiment.
- After running the experiment, you can add new spectra to the **With Optimized Emission** section. These will be run with the optimized emission current found in the previous run. If, however, an optimum emission current has not been found, the optimization routine will run again.

#### 4.9.2 Running Auto Flood Gun

The auto adjustment of flood gun procedure runs as a part of the [schedule](#). You can validate the procedure separately to confirm that it is able to run by checking the validation box:



Otherwise, the procedure will be checked when you validate the whole experiment and will run as scheduled after you click the ➤ icon.

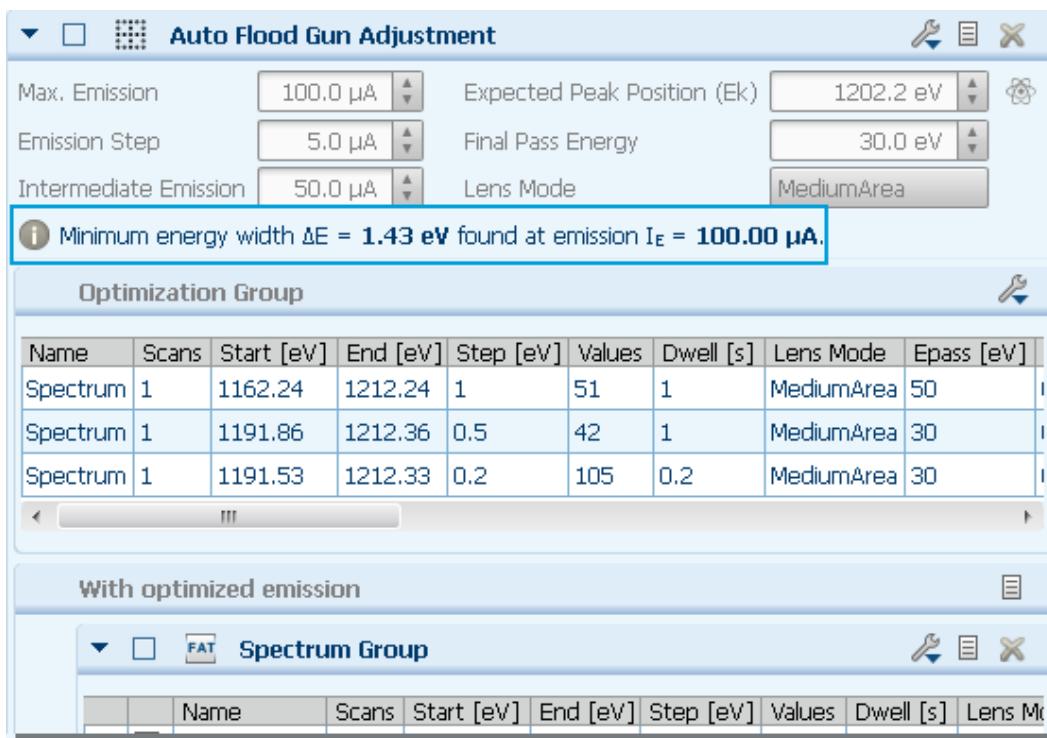
The procedure performs the following steps:

1. Exploratory scan with pass energy of 50 eV and a step size of 1 eV. Although the peak is likely to have shifted from its expected value, it should appear somewhere within this region. SpecsLab Prodigy will locate the peak within this region.
2. Based on the peak found in the previous step, SpecsLab Prodigy will scan a smaller region containing the peak. This is a higher precision scan with a 30 eV pass energy and a smaller step size of 0.5 eV.
3. Having confirmed the position of the peak, a third scan is performed. Again, the step size is smaller at 0.2 eV; the pass energy is a user-defined value. This is used as the basis for all subsequent scans.
4. The emission current of the flood gun increases by a user-defined step and SpecsLab Prodigy runs a scan based on the settings in the previous step. After each scan, SpecsLab Prodigy performs a data operation to determine the FWHM of the peak. This step repeats until the flood gun reaches an intermediate emission current.
5. On reaching the intermediate emission current, SpecsLab Prodigy evaluates the data. It tries to fit a curve to the FWHM vs. Emission Current data set using a Savitsky-Golay curve. If it finds a minimum, it skips to the last item in this list.
6. If no minimum is found in the previous step, the program will continue increasing the emission current and scanning until the maximum emission current is reached.

#### Note

If no obvious minimum is visible even at this point, the algorithm will still attempt to fit the data and continue with the schedule. The results in this case may not be completely reliable.

7. SpecsLab Prodigy will set the emission current of the flood gun to the value obtained from the fit and continue with the schedule. This value is shown in the Experiment Editor, as shown below. The data obtained is displayed in the Plot View.



### 4.9.3 Results of Auto Flood Gun Procedure

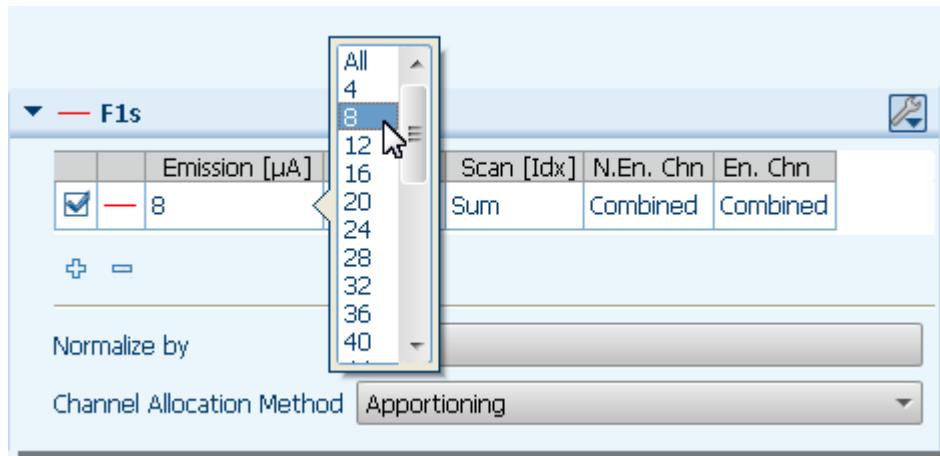
As with other data obtained by SpecsLab Prodigy, you can view results in the Plot View. At first sight, the results from the auto adjustment of the flood gun can appear to be a confusing jumble. This section offers a few tips on using the Plot View to view the results.

#### Note

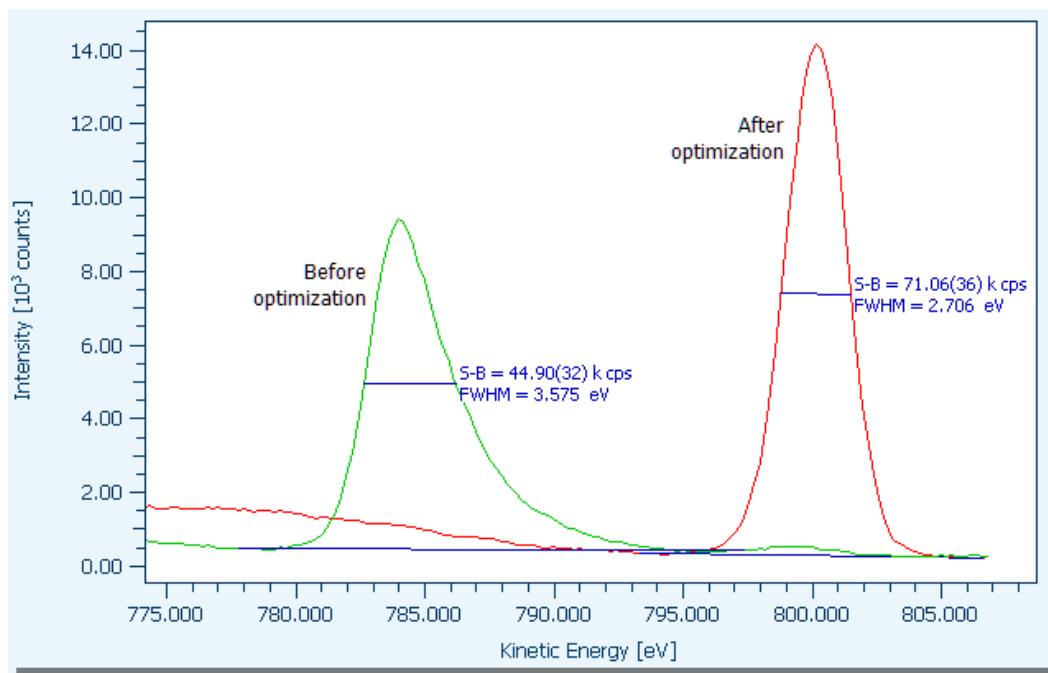
A Savitskz-Golay function fits the data. The minimum of this curve determines the emission current used in the experiment. The parameters of this fit are not displayed in SpecsLab Prodigy—only the results are available in the **Auto Adjustment of Flood Gun** item in the Experiment Editor.

To view data from the auto adjustment of flood gun procedure:

1. Click the icon in the section of the Data Browser that corresponds to the data for the auto adjustment of the flood gun. The section will expand to show the properties of the data.
2. Double click the **Emission** or **Iteration** field. A list will appear.
3. Click an entry in the list. The spectrum corresponding to this entry will be displayed in the Plot View. Moving the scroll wheel on your mouse allows you to browse through the entries.



4. You can create a copy of the spectrum by clicking the and icons. A second line will appear in the table. You can change the settings of this copy to display a second spectrum in the Plot View. The screenshot below shows two spectra displayed in this way. The spectra are fluorine peaks from PTFE, showing the effect of optimization.



#### 4.10 Auto Sample Height Adjustment

The auto sample height adjustment feature changes the sample position until the optimum distance between the sample and analyzer is located.

The lens system on the front of a SPECS electron energy analyzer has a focus which determines the working point. For optimum performance, the sample should be exactly at this point. This is particularly important for small excitation spots, such as from an electron gun or a synchrotron.

SpecsLab Prodigy can control the manipulator while reading the signal intensity to locate the working distance. After obtaining the signal intensity as a function of sample distance, SpecsLab Prodigy evaluates the optimum position and moves the sample accordingly.

Performing auto sample height adjustment typically involves the following steps:

1. [Add an Electron Spectroscopy experiment](#) and define your analyzer, source and other devices as usual.
2. Click  and select **Auto Sample Height Adjustment**.
3. [Configure](#) the auto sample height adjustment routine.
4. Define the rest of your experiment.
5. [Run](#) the experiment with the auto sample height adjustment routine.

When you start the experiment, SpecsLab Prodigy will run the auto sample height adjustment as part of the schedule. Data is saved with the experiment and can be [viewed](#) at any time.

#### 4.10.1 Configuring the Auto Sample Height Adjustment

To add auto sample height adjustment to the experiment:

- Click  at the desired point in the schedule and select **Auto Sample Height Adjustment**.

You need to include and configure the following items in the Electron Spectroscopy experiment:

- Analyzer.
- Source.
- Manipulator: Position. You should set this to a position loaded from a template that you know is near to the measurement position.

#### Note

After producing a suitable configuration, you can save it as a template. You can then load this for future experiments without needing to follow the whole procedure described here.

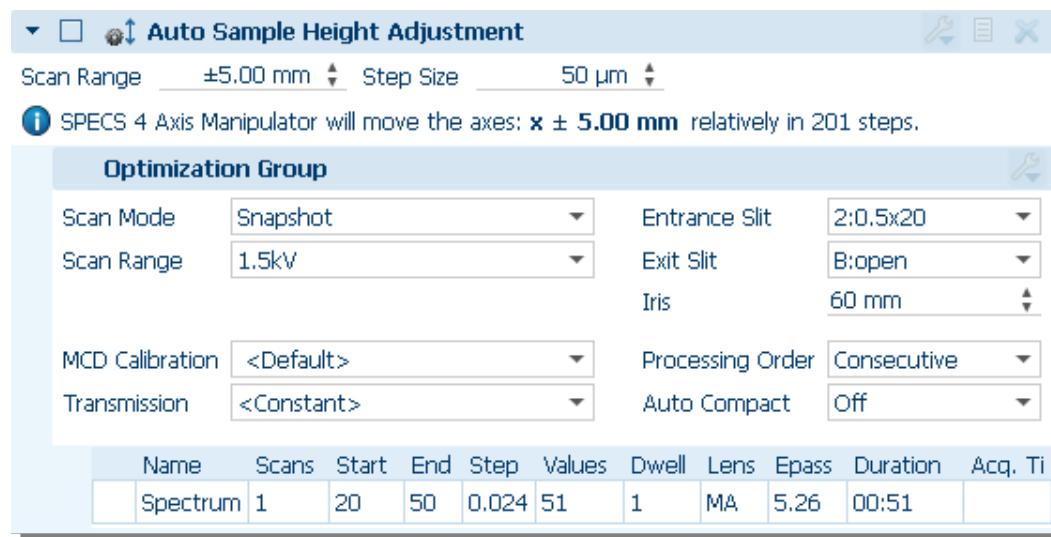
Please note the following points when configuring the auto sample height adjustment routine:

- The sample moves along the lens axis of the analyzer—this involves moving the X and/ or Y axes of the manipulator. The movement of the axes is configured by SPECS. For this reason, SpecsLab Prodigy may indicate different adjustments of X and Y manipulator settings for each step.
- After recording data at each step, SpecsLab Prodigy runs an arithmetic mean data operation. This calculates the mean value of the intensity of all points. As such, it is not

important whether a peak or a secondary electron signal is measured—only an intensity is used.

- **Scan Mode:** Use **Snapshot** mode to quickly measure the signal without needing to scan.
- The other settings for setting up the analyzer (slit settings, configuration file, etc) need to be the same as those for the spectrum group.
- The "spectrum" is set up in the same way as a normal experiment. You can set the energy to look at a peak energy or for secondary electrons.

The screenshot below shows a typical configuration after validation.



Following configuration of the auto sample height adjustment, you can add actions that take place at the optimized position by clicking the icon and selecting an item, e.g. a spectrum group. Please note the following points:

- Only actions within the **At Optimized Position** group will be performed at the sample position obtained by the auto sample height adjustment. After completing actions in the **At Optimized Position** group, the manipulator will move back to the position defined by the **Manipulator: Position** device at the start of the Electron Spectroscopy experiment.
- If you run the experiment again, having already found the optimum sample position, SpecsLab Prodigy assumes that the optimum position has not changed and uses the value already obtained without running the routine again. However, if you close the Experiment Editor and reopen the routine, the optimum position is measured again.
- If you want the auto sample height adjustment to run again, you need to click the icon and select **Unlock and Clear All Data**.

The screenshot below shows a spectrum group correctly nested in the schedule so that the spectrum is scanned at the optimum sample position.

The screenshot displays the SpecsLab Prodigy software interface. At the top, there is a toolbar with various icons. Below the toolbar, the main window shows two levels of a nested experiment schedule:

- Auto Sample Height Adjustment:** This is the top-level dialog. It contains settings for "Scan Range" (±5.00 mm) and "Step Size" (50 µm). A note says "No information about direction of manipulator axes." Below this is a table titled "Optimization Group" with one row:
 

Name	Scans	Start	End	Step	Values	Dwell	Lens	Epass	Duration	Acq. Time
Spectrum	1	20	50	0.024	51	1	MA	5.26	00:51	

 There are also buttons for "E<sub>k</sub>" and "E<sub>b</sub>".
- Spectrum Group:** This is a nested group under the first one. It has its own table:
 

Name	Scans	Start	End	Step	Values	Dwell	Lens	Epass	Duration	Acq. Time
Spectrum	1	280	330	1	51	0.1	MA	10	00:06	

#### 4.10.2 Running Automatic Sample Height Adjustment

Auto sample height adjustment is a part of the [schedule](#). You can validate the procedure separately to confirm that it is able to run by checking the validation box:



Otherwise, the procedure will be checked when you validate the whole experiment and will run as scheduled after you click the ➤ icon.

SpecsLab Prodigy makes a measurement at the current sample position before moving the manipulator. If less than 1 cps per channel is measured, SpecsLab Prodigy will abort the auto sample height adjustment and move to the next item in the schedule. Although this may occur for trivial reasons (e.g. the source is not switched on), it may also be because the manipulator is in the wrong part of the chamber—further movements may be unexpected and dangerous.

After locating the optimum position for the sample, i.e. the position with highest signal intensity, SpecsLab Prodigy fits the data using a Savitsky-Golay curve to locate the maximum. It then moves the sample to this maximum, and makes a final measurement at this new position. The position is reported in the Experiment Editor. SpecsLab Prodigy then executes the next step in the schedule.

**Note**

Only actions in the [At Optimized Position group](#) are performed at this position. After completing these actions, the manipulator moves back to the position set by the Manipulator: Position device.



The data obtained from the auto sample height adjustment is saved in the experiment file with any other data obtained. You can [view this data](#) in the Plot View or—better still—in the [Image View](#).

**Note**

There are occasional outliers in the data which may affect the evaluation of the position. For this reason, you should select an energy that provides an adequate signal and is not unduly affected by noise. [Viewing auto sample height adjustment data](#) allows you to judge the reliability of the procedure.

#### 4.10.3 Viewing Results of Auto Sample Height

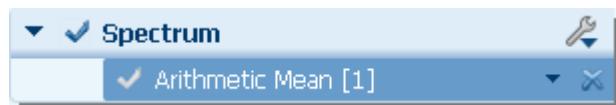
As with other measurements, the Plot View shows data collected as part of the automatic sample height adjustment. It is however better to use the [Image View](#) if you want to understand the data.

**Note**

The Savisky-Golay fit and its parameters are not visible in SpecsLab Prodigy. Only the calculated maximum is shown in the Experiment Editor after the procedure has finished.

To view the data in the Image View:

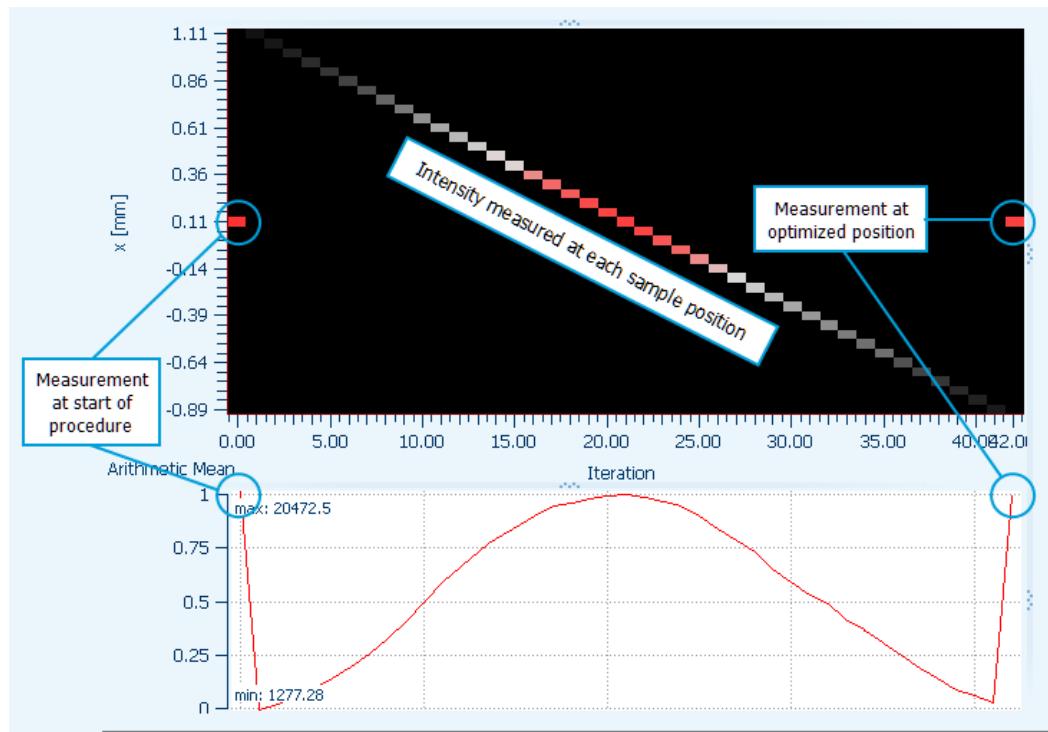
1. Select **Views/ Image View** from the menu bar to open the Image View. No data is displayed in the image because the axes of the image are not yet correctly set up.
2. In the Data Browser, select the spectrum corresponding to the automatic sample height adjustment.
3. Click the icon to expand the spectrum properties. You should see the [Arithmetic Mean](#) data operation.
4. Double click the **Arithmetic Mean** title bar so that a tick appears. This is now the active data set for the image.



5. In the image, select the following axis settings:

- Y axis: x (mm)
- X axis: Iteration

You should now see the data presented in the image. The intensity at each position is represented by the color. You can drag the horizontal profile to see the intensity presented in graphical form.



### Note

The example above uses fewer points than the default settings for reasons of clarity.

## Chapter 5 – Experiment Editor III: Reference Information

This chapter contains useful reference information for using the Experiment Editor. It covers the following topics:

- [Scan modes](#)—their applications and settings.
- [Exporting data](#)—procedures and file formats.
- [Instrument status](#)—indicators and error messages.

### 5.1 Scan Modes

SPECS analyzers can operate in a number of different modes. You set the mode for each spectrum during definition in the [Experiment Editor](#). Each mode has its own characteristics; available parameters and limits also vary between the modes.

The table below summarizes the available scan modes, together with a brief description of their major uses. The following subsections describe the modes in more details.

Scan mode	Description
<a href="#">Fixed analyzer transmission</a>	Normal scanning mode for XPS, UPS, ISS.
<a href="#">Fixed retarding ratio</a>	Normal scanning mode for AES.
<a href="#">Fixed energy</a>	Measures single energy, ideal for analyzer set up and stability checks.
<a href="#">Snapshot</a>	Uses energy resolution of multi-channel detectors for fast peak measurements.
<a href="#">Detector voltage scan</a>	For finding optimum detector operating voltage.
<a href="#">Constant final state</a>	Scans photon energy (synchrotron) and measures fixed kinetic energy. For band structure mapping experiments.
<a href="#">Constant initial state</a>	Scans photon energy (synchrotron) and scans kinetic energy. For band structure mapping experiments.

#### 5.1.1 Fixed Analyzer Transmission

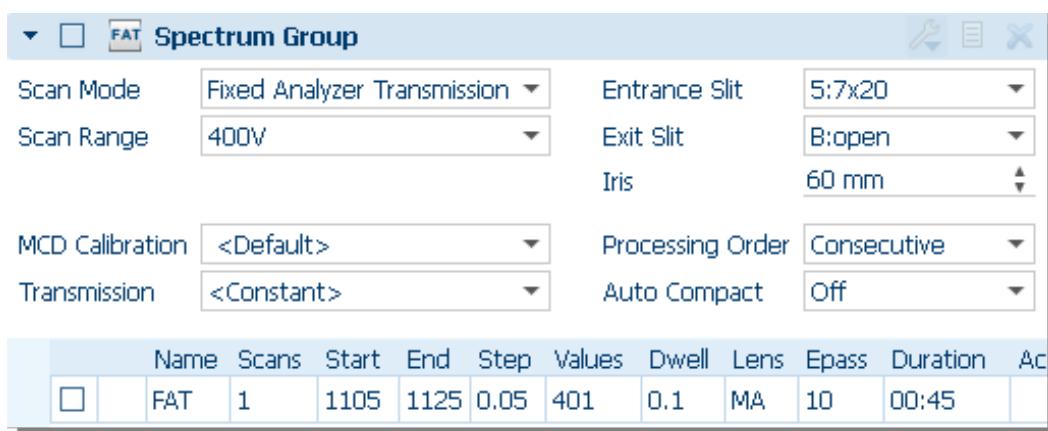
Fixed analyzer transmission (FAT) mode allows you to scan through the kinetic energy while holding the incident excitation energy constant. It is the most commonly used mode for XPS, UPS and ISS.

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

Setting	Dependencies	Description
Name	Free text	Name of the spectrum.
Scans	-	Number of scans performed.
Start	Start < End	Start energy (eV). For binding energy, the initial binding energy.
End	End > Start	Final energy (eV). For binding energy, the final binding energy.
Step	0 < Step < ceil(End – Start) / Step	Energy step between measurement points.
Values	Values = (ceil(End – Start) / Step) + 1	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	See analyzer manual for available lens modes.
Epass	-	Analyzer pass energy.
Duration	Duration = Dwell*Scans*(End – Start) / Step	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the spectrum.



### 5.1.2 Fixed Retarding Ratio

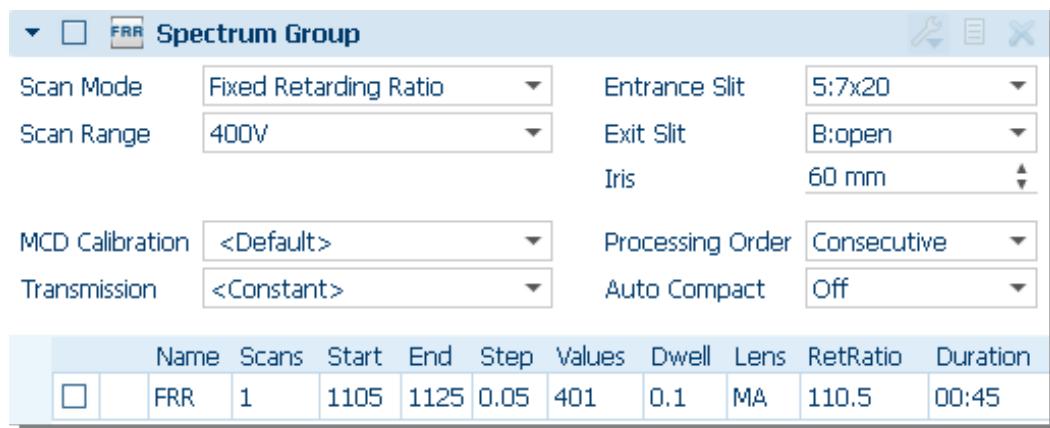
Fixed retarding ratio (FRR) allows you to scan through the kinetic energy while holding the incident excitation energy constant. Unlike [Fixed Analyzer Transmission](#), the pass energy is not

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 photoelectron 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

Setting	Dependencies	Description
Name	Free text	Name of the spectrum.
Scans	-	Number of scans performed.
Start	Start < End	Start energy (eV). For binding energy, the initial binding energy.
End	End > Start	Final energy (eV). For binding energy, the final binding energy.
Step	0 < Step < ceil(End – Start) / Step	Energy step between measurement points.
Values	Values = (ceil(End – Start) / Step) + 1	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	See analyzer manual for available lens modes.
RetRatio	RetRatio = (Ekin – Work function) / Epass	Retarding ratio. The dependency shows its relation to the pass energy. Work function is set in the Device Control.
Duration	Duration = Dwell*Scans*(End – Start) / Step	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the spectrum.



### 5.1.3 Fixed Energies

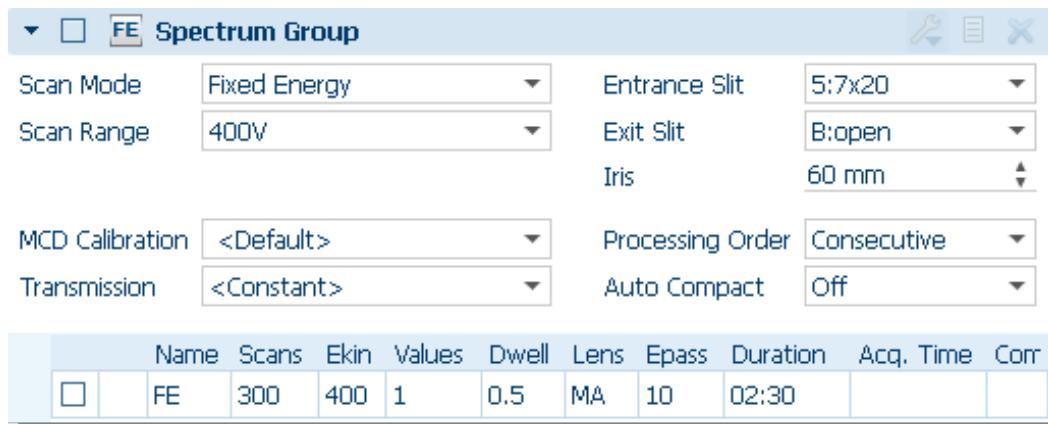
The fixed energy (FE) mode is a simple mode that allows you to monitor a single kinetic energy for a specified time. Particles with a defined kinetic energy pass through the analyzer and are detected. This mode is used when setting up or checking the operation of the analyzer, as well as for investigating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

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

#### Settings

Setting	Dependencies	Description
Name	Free text	Name of the spectrum.
Scans	-	Number of scans performed.
Start	Start < End	Kinetic energy (eV).
Values	Values = (ceil(End - Start) / Step) + 1	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	See analyzer manual for available lens modes.
Epass	-	Analyzer pass energy.
Duration	Duration = Dwell*Values*Scans	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the spectrum.

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



### 5.1.4 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. Snapshot measurements are usually best suited to CCD and DLD detectors, which have hundreds of channels and can show the peak shape. They are also possible with five or nine channel detectors; however, the energy resolution is comparatively poor.

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.

#### Settings

The center/ width configuration mode is particularly useful for snapshot mode:

- Right-click the spectrum settings table and select **Use Center/Width** from the context menu.

Setting	Dependencies	Description
Name	Free text	Name of the spectrum.
Scans	-	Number of scans performed.
Center	-	Kinetic energy/ binding energy at the center channel.
Width		Final energy (eV). For binding energy, the final binding energy.
Step	-	Calculated energy step between measurement points.

Setting	Dependencies	Description
Values	Values/Channel number must be an integer. Validation of scan corrects to nearest integer.	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	See analyzer manual for available lens modes.
Epass	-	Analyzer pass energy.
Duration	Duration = Dwell*Scans*Values	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the spectrum.

### 5.1.5 Detector Voltage Scan

The detector voltage scan (DVS) changes the detector voltage while holding the detected energy constant. Since channel electron multipliers degrade with use, you can use this mode to find the correct operating voltage for the detector.

When examining the results of a DVS, it is best to view the individual channels by selecting **Separated** in the [data browser](#). This allows you to check the performance of the individual channel electron multipliers.

Please also refer to the detector manual for more information.



#### Caution!

You can destroy your detector if you set **Udet End** too high. Refer to the test report for your detector to find suitable operating voltages.

### Settings

Setting	Dependencies	Description
Name	Free text	Name of the scan.
Scans	-	Number of scans performed.
Start	Start < End	Start voltage (V).
End	End > Start	Final voltage (V).
Step	0 < Step < ceil(End – Start) / Step	Voltage step between measurement points.
Values	Values = ceil(End – Start) / Step	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	Use a mode such as large area to allow high transmission of electrons.

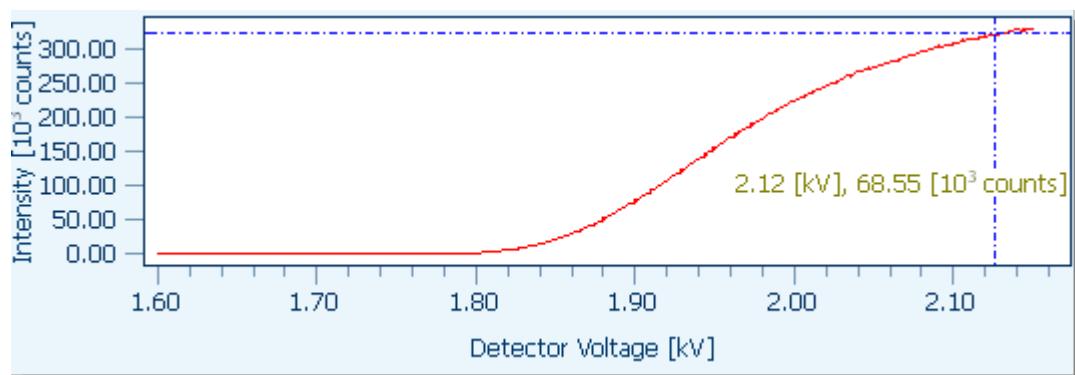
Setting	Dependencies	Description
Ekin	-	Measured kinetic energy. This should be a background level with some signal—not a peak energy!
Epass	-	Analyzer pass energy.
Duration	Duration = Dwell*Scans*(End – Start) / Step	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the scan.

▼   Spectrum Group

Scan Mode	Detector Voltage Scan	Entrance Slit	5:7x20
Scan Range	1.5kV	Exit Slit	B:open
		Iris	60 mm
MCD Calibration	<Default>	Processing Order	Consecutive
Transmission	<Constant>	Auto Compact	Off

	Name	Scans	Start	End	Ekin	Step	Values	Dwell	Lens	Epass	Duration
<input type="checkbox"/>	DVS	1	1000	2300	400	5	261	0.3	MA	10	01:19

The results of a detector voltage scan are displayed in the Plot view. You need to [select](#) **Detector Voltage** in the X axis in order to display the data. You can find the operating voltage with the cursor. The detector voltage is set in the device control for the analyzer.



### 5.1.6 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.

This mode is only available when you select a beamline as your source.

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

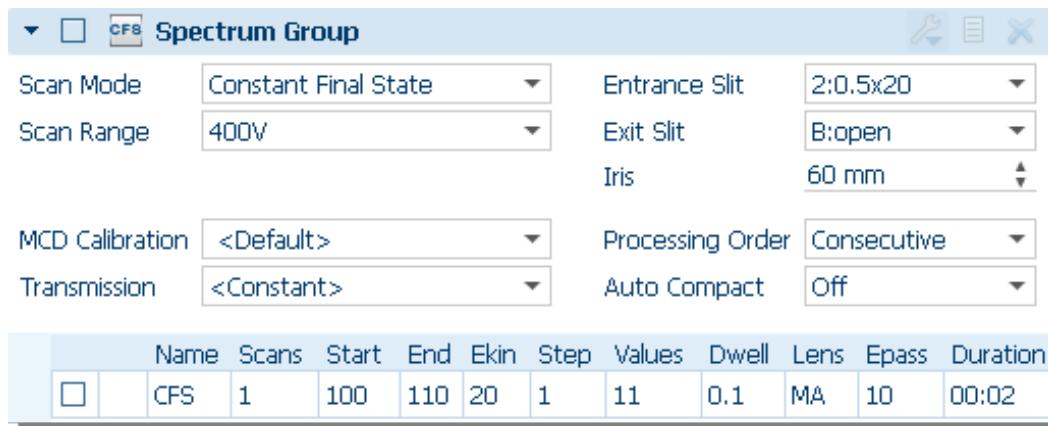
## Settings

Setting	Dependencies	Description
Name	Free text	Name of the spectrum.
Scans	-	Number of scans performed.
Start	Start < End	Source start energy (eV). For binding energy: (Source energy – Kinetic energy).
End	End > Start	Source final energy (eV). For binding energy: (Source energy – Kinetic energy).
Step	0 < Step < ceil(End – Start) / Step	Energy step between measurement points.
Values	Values = ceil(End – Start) / Step	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	See analyzer manual for available lens modes.
Ekin	-	Measured kinetic energy.
Epass	-	Analyzer pass energy.
Duration	Duration = Dwell*Scans*(End – Start) / Step	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the spectrum.

The X-axis in the Plot View shows the difference energy (source energy + kinetic energy). When using binding energy definitions, binding energy is shown.

## Example

The screenshot below shows a spectrum 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.



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.

### 5.1.7 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.

This mode is only available when you select a beamline as your source.

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

### Settings

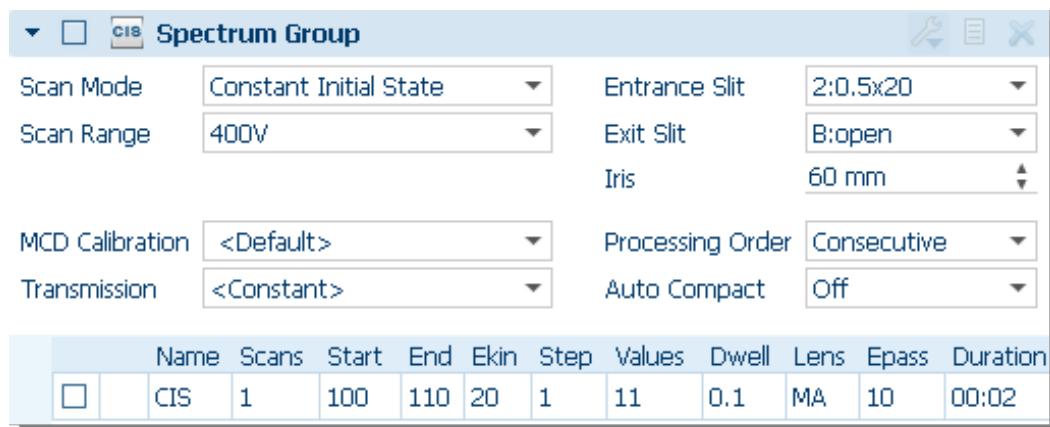
Setting	Dependencies	Description
Name	Free text	Name of the spectrum.
Scans	-	Number of scans performed.
Start	Start < End	Source start energy (eV). For binding energy: (Source energy – Kinetic energy).
End	End > Start	Source final energy (eV). For binding energy: (Source energy – Kinetic

Setting	Dependencies	Description
Step	$0 < \text{Step} < \text{ceil}(\text{End} - \text{Start}) / \text{Step}$	Energy step between measurement points.
Values	$\text{Values} = \text{ceil}(\text{End} - \text{Start}) / \text{Step}$	Total number of values measured.
Dwell	-	Measurement time for each point.
LensMode	-	See analyzer manual for available lens modes.
Ekin	-	Measured kinetic energy.
Epass	-	Analyzer pass energy.
Duration	$\text{Duration} = \text{Dwell} * \text{Scans} * (\text{End} - \text{Start}) / \text{Step}$	Total time taken for measurement (info only).
Comment	Free text	Additional comment about the spectrum.

The X-axis in the Plot View shows the difference energy (source energy + kinetic energy). When using binding energy definitions, binding energy is shown.

### Example

The screenshot below shows a spectrum 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.



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.

## 5.2 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:

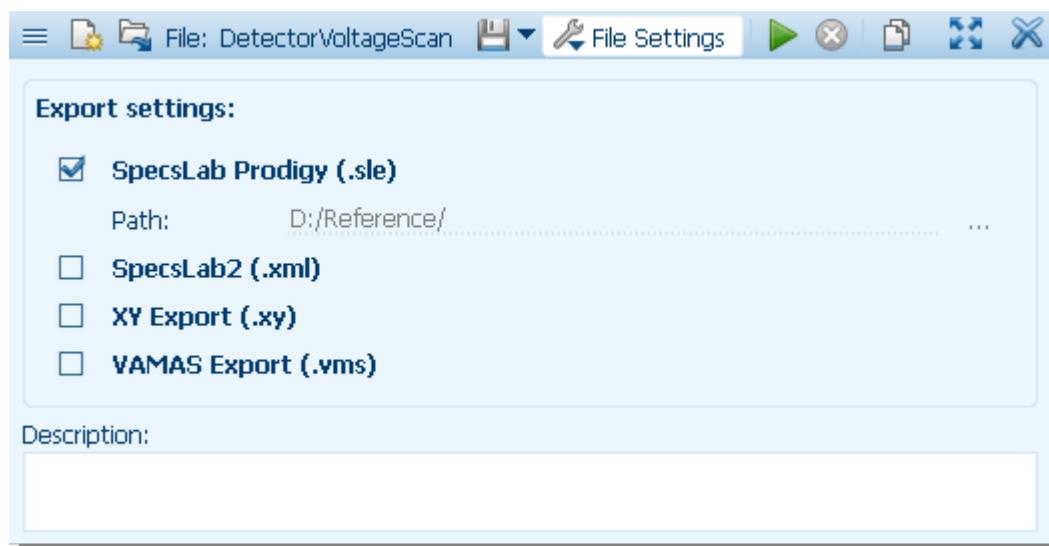
- Prodigy template file—the entire experiment is saved as a [template](#), rather than just part of the configuration.
- [VAMAS](#)—a standard data exchange format.
- [XY](#)—exports the data in space-delimited columns with header information.
- XML—the native file format of SpecsLab2. This allows you to share your data with SpecsLab2 users.

### Note

The [transmission function](#), if included in the spectra, is also exported.

You can automatically export data to any of these formats after acquisition:

1. Click the **File Settings** button in the Experiment Editor toolbar. The export settings will appear.



2. Check the export format that you want to save. After acquisition, the data is automatically saved in the selected format.

You can also export the current experiment:

- Click the arrow next to the icon in the Experiment Editor toolbar. A menu will appear allowing you to export the experiment.

To export data from a single spectrum:

- Right-click the spectrum in the spectrum group and select **Export Spectrum Data** from the context menu. A **Save** dialog will appear, allowing you to select the name, location and file type (XY or VAMAS) for the exported data.

### 5.2.1 VAMAS Files

VAMAS format<sup>1</sup> is a standard that allows interchange of data from SpecsLab Prodigy with other programs such as CASA XPS.

#### Note

SpecsLab Prodigy is able to read VAMAS files and import the data. Importing follows the normal procedure for opening a file.

When exporting a number of spectra, each spectrum is saved in its own VAMAS file.

By default, the export file is saved in a new directory at the same location as the autosaved data file. You can override this setting and specify a different save location.

#### Note

Not all metadata generated by SpecsLab Prodigy is saved in the VAMAS file. This does not affect the import into third-party programs.

For reference, the table below describes the VAMAS format.

Item description	Line	Sample entry	Item description	Line	Sample entry
Format identifier	1	VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4	Source azimuth	43	180
Institution iden-	2	Specs	Analyzer mode	44	FAT

<sup>1</sup>. 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 SPECS conforms to ISO 14976. 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).

Item description	Line	Sample entry	Item description	Line	Sample entry
Identifier					
Instrument model i.d.	3	PHOIBOS HSA3500 DLD 150 R6-WAL[HWType 30:106] DLD	Analyzer resolution characteristic	45	100
Operator i.d.	4	-	Magnification of analyzer	46	1
Experiment i.d.	5	?	Magnification of analyzer	46	1
# Comment lines	6	1	Analyzer work function	47	4.6
Comment lines	7	Created by SpecsLab Prodigy, Version 2.83-r17331	Target sample bias	48	0
Experiment mode	8	NORM	Analysis width x, mu	49	0
Scan mode	9	REGULAR	Analysis width y, mu	50	0
# Regions	10	4	Analyzer axis polar angle	51	0
# Variables	11	1	Analyzer azimuth	52	0
# Parameter exclusion entries	12	Step	Species	53	Silicon
# Manual items	13	d	Transition state	54	Silicon
# Future experiment items	14	0	Charge of analyzed particle	55	-1
# Future block entries	15	0	Abscissa label	56	kinetic energy
# Blocks	16	1	Abscissa units	57	eV
Block i.d.	18	Silicon	Abscissa start	58	1379.31
Sample i.d.	20	Cycle1	Abscissa increment	59	0.05
Year 4 digits	21	2010	# Corresponding variables	60	15
Month	22	06	Corresponding variable label	61	counts_0
Day	23	24	d= none	62	d
Hour	24	14	Signal mode	91	pulse counting
Minute	25	45	Signal collection time/channel	92	1
Second	26	00	# Scans for this block	93	20
# Hours + GMT	27	1	Signal time correction	94	0
# Lines in block	28	6	Sample normal tilt	95	0

Item description	Line	Sample entry	Item description	Line	Sample entry
comment					
Technique	35	XPS	Sample normal azimuth	96	0
source	37	AI	Sample rotation angle	97	0
Source energy	38	1486.6	# Additional params	98	0
Source strength	39	300	# Ordinate values	99	3315
Source width x , mu	40	500	Min y	100	31
Source width y , mu	41	500	Max y	101	10877
Source polar angle	42	54			
Data points					
terminator		end of experiment			

### 5.2.2 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.

Results are saved in a simple space-delimited X Y format. You can specify if individual spectra or channels are to be saved—the file then contains a set of measurements concatenated into one file with a single set of metadata (if specified for export). Each measurement is identified with a title. The export format is readable in a text editor or spreadsheet.

When you check the XY box in the Export Settings, the following settings appear:

- **Location:** By default, the export file is saved in a new directory at the same location as the autosaved data file. You can override this setting and specify a different save location.
- **Output:** This gives you the option of saving the data from spectra in one file or each spectrum in a separate file.
- **Parameters:** Checking the boxes in this table determines the contents of the export file. The metadata contains details of the experimental setup.

Parameter	Value
Comment Prefix	#
Output meta data	<input checked="" type="checkbox"/>
Counts Per Second	<input checked="" type="checkbox"/>
Kinetic Energy Axis	<input checked="" type="checkbox"/>
Separate Scan Data	<input type="checkbox"/>
Separate Channel Data	<input type="checkbox"/>
External Channel Data	<input checked="" type="checkbox"/>
Transmission Function	<input type="checkbox"/>
ErrorBar	<input type="checkbox"/>
Operation Results	<input checked="" type="checkbox"/>

## 5.3 Instrument Status

SpecsLab Prodigy offers two ways of checking the status of an experiment:

- [Status indicators](#) for each device currently being used.
- [Error messages](#) to describe problems in the schedule.

### 5.3.1 Status Indicators

The menu bar of SpecsLab Prodigy shows icons of all devices that are currently connected in the program. The color shows the status of each device, as listed in the table below.



#### Note

Each device has its own icon and is displayed separately in the toolbar. The table below only shows the analyzer icon.

Indicator	Status
	Device inactive.
	Device in operation and working correctly.
	Set up device ready for operation.
	Device error.

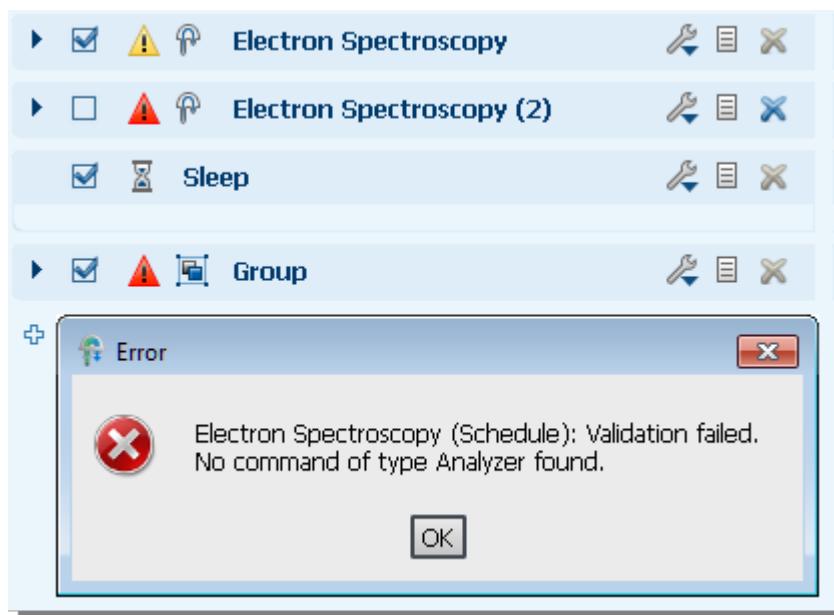
If a device is disconnected in the software, it is not shown in the menu bar.

### 5.3.2 Dealing with Errors

After configuring an experiment, you need to validate, either by checking the box next to items in the schedule, or by pressing  and validating the entire schedule. SpecsLab Prodigy checks that the items can be run. If problems appear, they are indicated by the symbols in the table below.

Error symbol	Comments
	<p>Warning. The instrument may not perform correctly, but operation is possible. On double-clicking the symbol, an error message will appear to explain the cause of the error. After reading and understanding the message:</p> <ul style="list-style-type: none"><li>Click <b>Acknowledge</b> to dismiss the error symbol and continue.</li><li>Click <b>OK</b> to continue, but the error will still be shown.</li></ul>
	<p>Error. The experiment cannot run. An error message will inform you of the reason for the error. Perform the following checks:</p> <ul style="list-style-type: none"><li>The instrument is switched on.</li><li>All electrical connections and interlocks are correct.</li><li>The <u><a href="#">IP address</a></u> is set correctly.</li></ul>

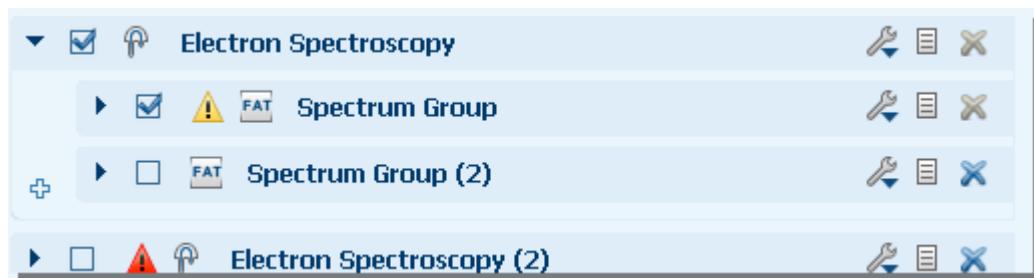
The following example shows some of the features available when errors appear, explaining how you can locate and solve errors. As you can see, there are four items in the schedule: Two Electron Spectroscopy experiments, a Sleep command and a Group which can contain additional items.



The first Electron Spectroscopy group has a warning, while the second Electron Spectroscopy experiment and the Group have errors. An error message provides information about the cause of the errors. Remember that the experiment will still run with a warning, so this is not shown in the error message.

### Warning in Electron Spectroscopy 1

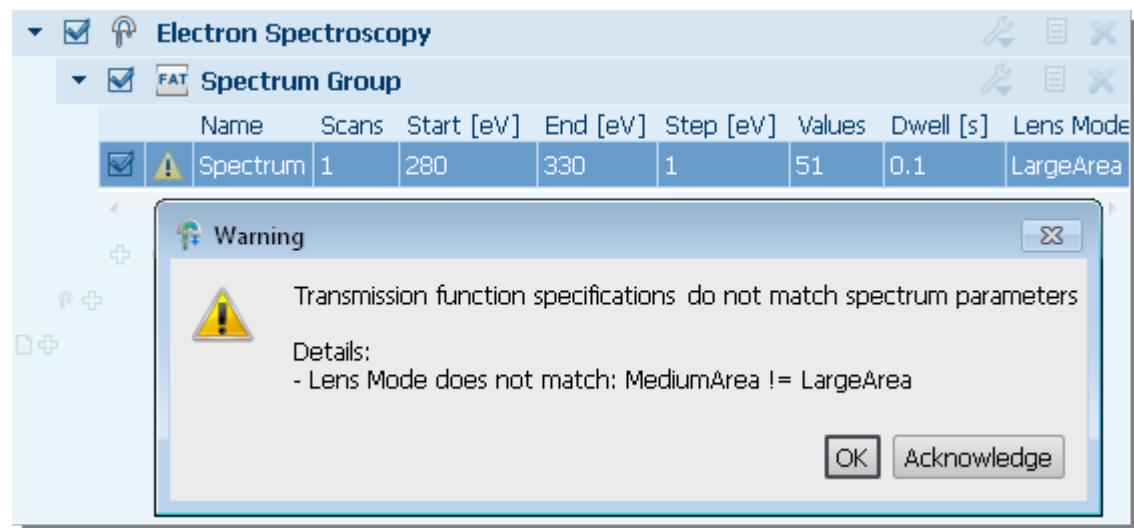
We see that there is a warning in the first Electron Spectroscopy group, so we expand the group by clicking the ▶ button. There are two spectrum groups in this experiment.



Importantly, the warning symbol has moved to show us which spectrum group has the problem. We can therefore focus on this group.

Expanding the spectrum group shows us the spectrum that is causing the problem. Clicking the symbol produces a message that tells us the transmission function is not suitable for the slit set-

tings. We can either acknowledge this (the error will go away) or click **OK** to continue the measurement, but with the error still shown.



### Error in Electron Spectroscopy 2

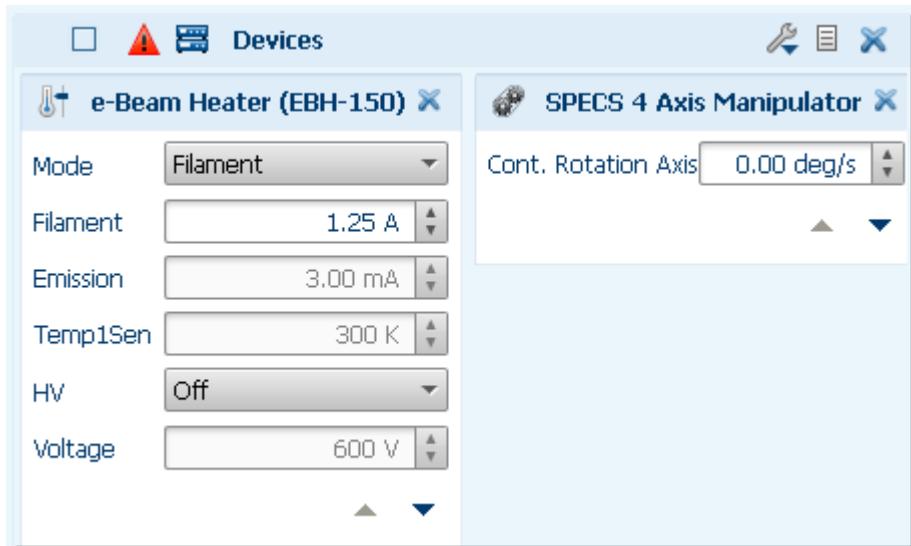
Solving the error for the second Electron Spectroscopy experiment is fairly easy. SpecsLab Prodigy cannot find an analyzer for the experiment, so the analyzer needs to be [defined](#).

### Error in Group

Groups allow you to create hierarchies in the schedule. As with the warning described previously, the error symbol shows you that the failure lies somewhere within this group. On expanding the group, the symbol moves to show the item that is causing the problem.



For hierarchies with many levels, the error symbol will move as you expand the hierarchy until you locate the source of the problem. In this case, SpecsLab Prodigy cannot connect to a sample heater. Looking in the Devices item, we see the heater that is causing the trouble.



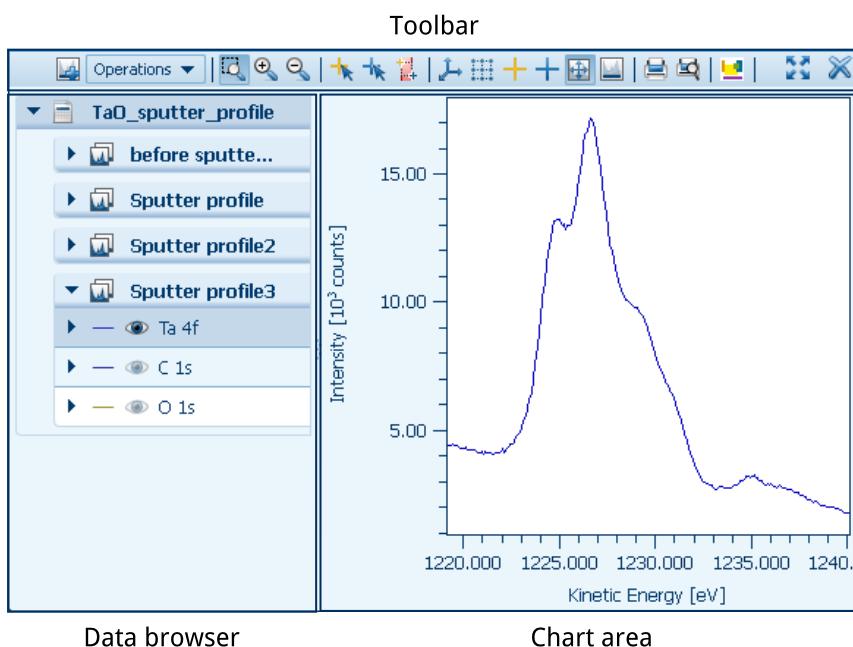
The table above lists the typical reasons for this kind of error so that you can find why SpecsLab Prodigy cannot connect to the device.

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## Chapter 6 – Plot View I: Features

The Plot View 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.

[Chapter 6 –](#) shows the main sections in the Plot View.



The following sections describe the features present in the Plot View. Data operations, which perform calculations on acquired spectra, are described in ["Plot View II: Data Operations" on page 85](#).

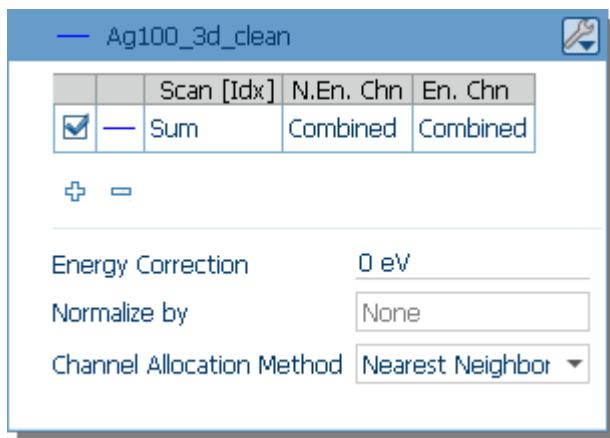
### 6.1 Data Browser

The data browser displays all spectra from the experiment as well as data operations performed on the spectra. You can change the [appearance of the line](#) in the Plot View and [hide spectra](#).

By clicking the icon, you can see more information about the spectrum, including which [spectrum components](#) are displayed and [additional data display settings](#).

**Note**

The columns in the table (e.g. Scan in the screenshot below) depend on what data is available in the scan. For a single-scan, single-channel data set, for example, no column would be shown.



Many of the features have an impact on the display of the spectrum in the Plot View. These features are described in the following sections:

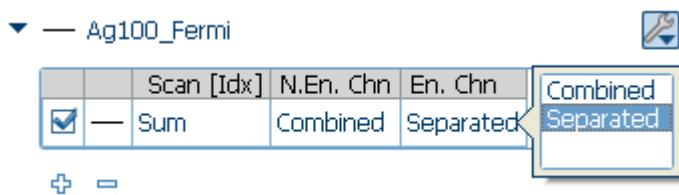
- Displaying components of spectra.
- Changing the appearance of data.
- Showing/ hiding spectra.
- Changing the settings.

### 6.1.1 Displaying Spectrum Components

By default, the total signal intensity is displayed in the Plot View. You can change the display so that individual channels (for multichannel detectors) or individual scans (when multiple passes are scanned in the spectrum) are show. Other scanning options, such as depth profiling, contain additional components that can be selected. Clearly, the options available depend on your configuration and experiment type.

As an example, to display individual channels in a spectrum:

- Double-click the **Combined** button under **En. Chn** and select **Separated** from the drop-down list.



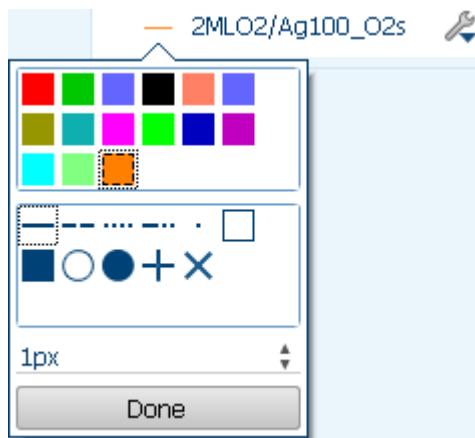
You can show the individual channels on the Z-axis:

1. Click the  icon in the toolbar.
2. Select **Channels** for the Z axis label.

### 6.1.2 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 as follows:

1. Select the line of the spectrum in the legend. The color, linestyle and width are shown.
2. Edit the linestyle accordingly. The plot is updated as soon as you select a setting.
3. Click **Done** or anywhere outside the selection box to close the box.

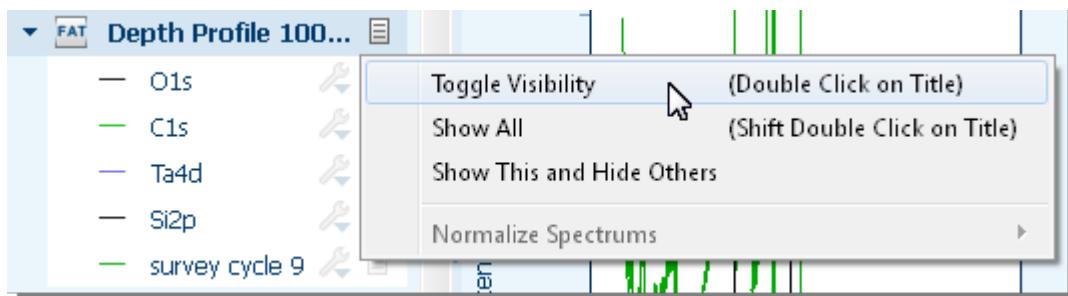


### 6.1.3 Showing and Hiding Spectra

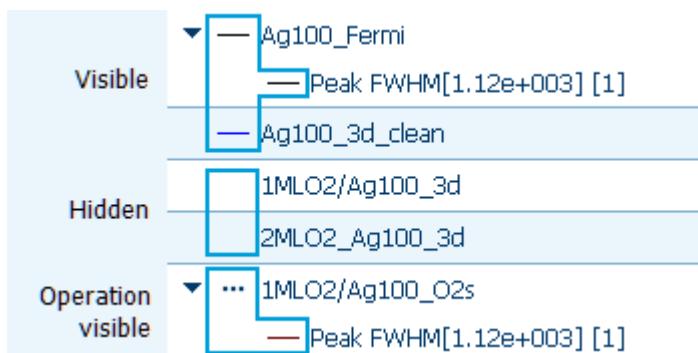
You can toggle the visibility of each spectrum in the Plot View for the purposes of clarity or comparison.

To toggle the visibility of a spectrum in the plot, use one of the following methods:

- Click  next to the spectrum that you want to show or hide and select Toggle Visibility from the menu. You can also use the entries in this menu to toggle all child items in the hierarchy or to hide all others.
- Double click the name of the spectrum or data operation. The axes in the plot are automatically scaled to the displayed spectra.



Visibility of spectra is indicated by a line next to its description. The color of this line is the same as that displayed in the plot.



You can only remove a spectrum completely from the data browser by deleting its data and then removing its from the spectrum group:

1. Select the spectrum (or spectra) in the Experiment Editor and click SpecsLab Prodigy will prompt you before the data is deleted.
2. Click the icon to remove the definition of the spectrum from the group.

#### 6.1.4 Adding New Spectra

You can add new spectra based on existing measurements. These spectra belong to the same spectrum group and have the same settings, except for the selected energy range. After studying or analyzing a spectrum, you can make new measurements based on areas of interest in the data.

There are two options for adding spectra:

- Adding an exact copy of the spectrum, or the range selected in the spectrum.
- Adding a copy of the spectrum or selected area with a 0.1 eV step size.

To add a new spectrum:

1. Select a spectrum in the Data Browser.

2. Click one of the following icons at the bottom of the Data Browser:



Adds an exact copy of the spectrum, or the range selected in the spectrum.



Adds a copy of the spectrum or selected area with a 0.1 eV step size (detailed copy).

The new spectrum will be added to the Spectrum Group in the Experiment Editor. The energy range of the spectrum depends on the following, in order of priority:

1. The area selected in the plot.
2. The zoomed area visible in the plot.
3. The whole spectrum.

You can further edit the configuration in the spectrum group as necessary and start the measurement in the Experiment Editor to acquire the data.

### 6.1.5 Additional Data Display Settings

By clicking the **Settings** button for a spectrum in the legend, you can display and adjust additional settings that affect the appearance of the data in the Plot View. The table below lists the settings.

Setting	Description
Energy correction	Allows you to add an energy shift to the spectrum, e.g. a work function correction. You can enter a value using the keyboard, with the up and down arrows or—on selecting the number in the pop-up—with the mouse wheel. The original data (saved with the experiment) is not affected by this action, but exported data does contain these shifts.
Normalize by	You can acquire other signals (such as sample current) during data acquisition and use this to normalize the signal. This menu allows you to select which data source is used for normalization.
Channel allocation	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", included in the <i>Documents/Additional Information</i> folder of the SpecsLab Prodigy installation directory

## 6.2 Toolbar Controls

The toolbar in the Plot View contains controls to perform the following actions:

- View peak energies with the [periodic table](#) (optional feature).
- Set [cursor positions](#).
- Select a [region of interest](#) in the spectrum.
- Toggle the [grid](#) display.

- Toggle the Z axis display.
- Zoom.

### 6.2.1 Setting the Cursor Position

You can add cursors to the chart in the Plot View. 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.

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.
- You can toggle the operation of each or both of the cursors by selecting the appropriate entry in the cursor menu. Keyboard shortcuts also allow you to toggle the cursors.
- If you display both cursors at the same time in the chart, the toolbar shows the difference between the positions of the two centers.

When setting cursors in the chart:

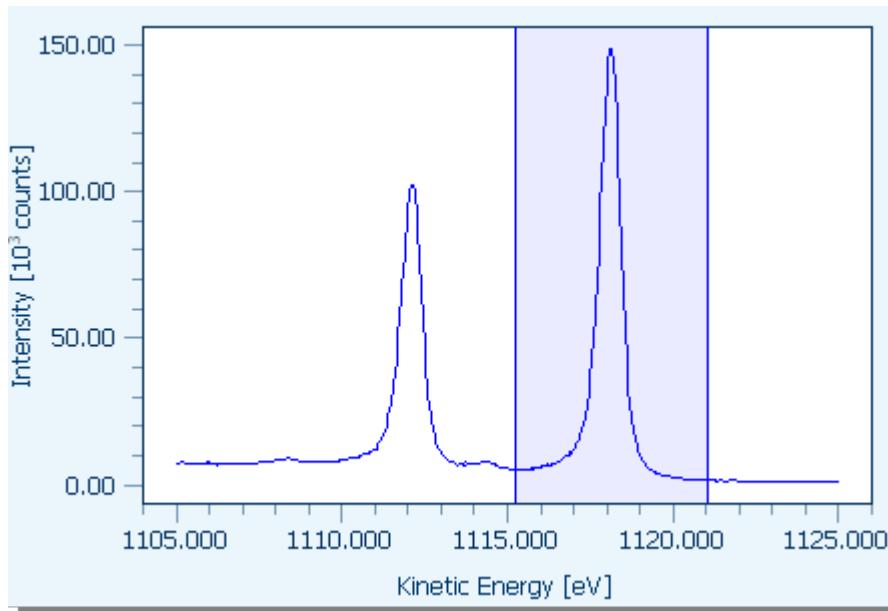
1. Click the  icon in the toolbar or press C to toggle the cursors.
2. Add a cursor:
  - Left-click in the plot to add the yellow cursor.
  - Right-click to add the blue cursor.

### 6.2.2 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.

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. This produces a shaded area. You can perform data operations on this region—see [Performing Data Operations](#) for more information.



### 6.2.3 Displaying the Grid in the Plot View

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 Plot View. 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 77](#).

### 6.2.4 Zooming and Autoscaling in the Data Window

The Data Window automatically zooms to show the selected plot or operation in the data browser. If nothing is selected in the Data Browser, the range is adjusted to show all spectra and operations.

The toolbar contains two icons,  and , which respectively allow you to zoom in and out of the plot in steps.

To display the complete plot again, double click in the plot area. Alternatively, click the  icon in the toolbar. The  button rescales the chart so that Y = 0 is shown.

You can also define an area of the plot 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 Plot View. When you release the mouse button, the plot shows the selected area. Scroll bars on the top and right side of the plot allow you to move to other areas of the plot.

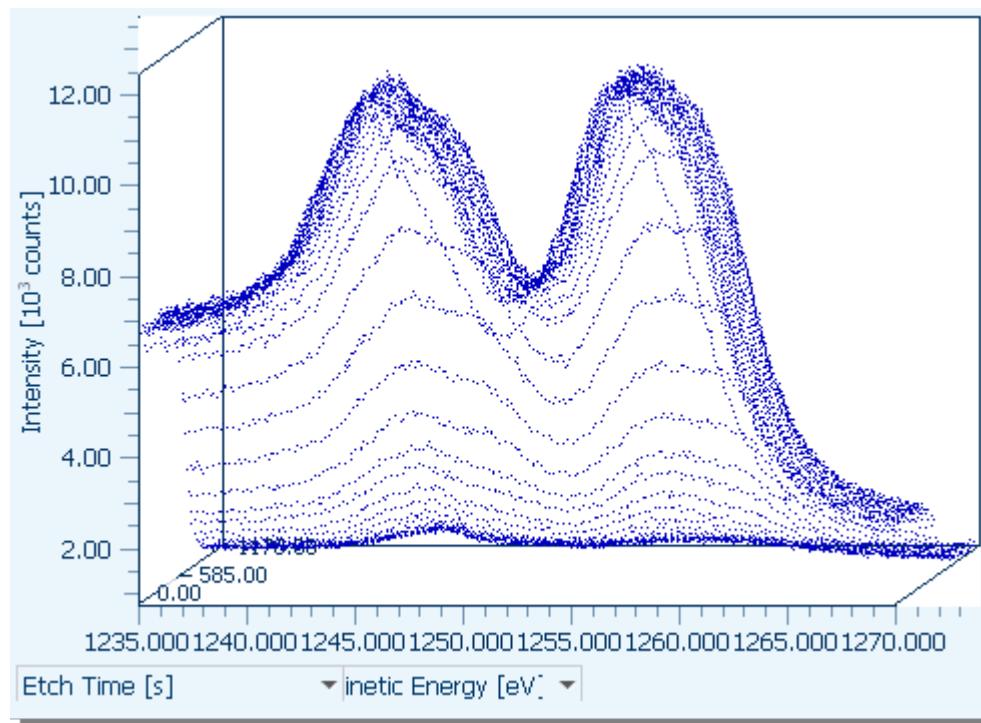
### 6.2.5 Displaying the Z Axis

You can display a Z axis in the Plot View. The scale of the Z axis depends on the type of data in the spectrum, which data components are displayed and the selection of the Z axis label. For more information about these topics, please refer to:

- ["Displaying Spectrum Components" on page 72.](#)
- ["Changing the Axis Labels" on page 83.](#)

To toggle the appearance of the Z axis:

- Click the  icon in the Plot View toolbar.



### 6.2.6 Copying an Image to the Clipboard

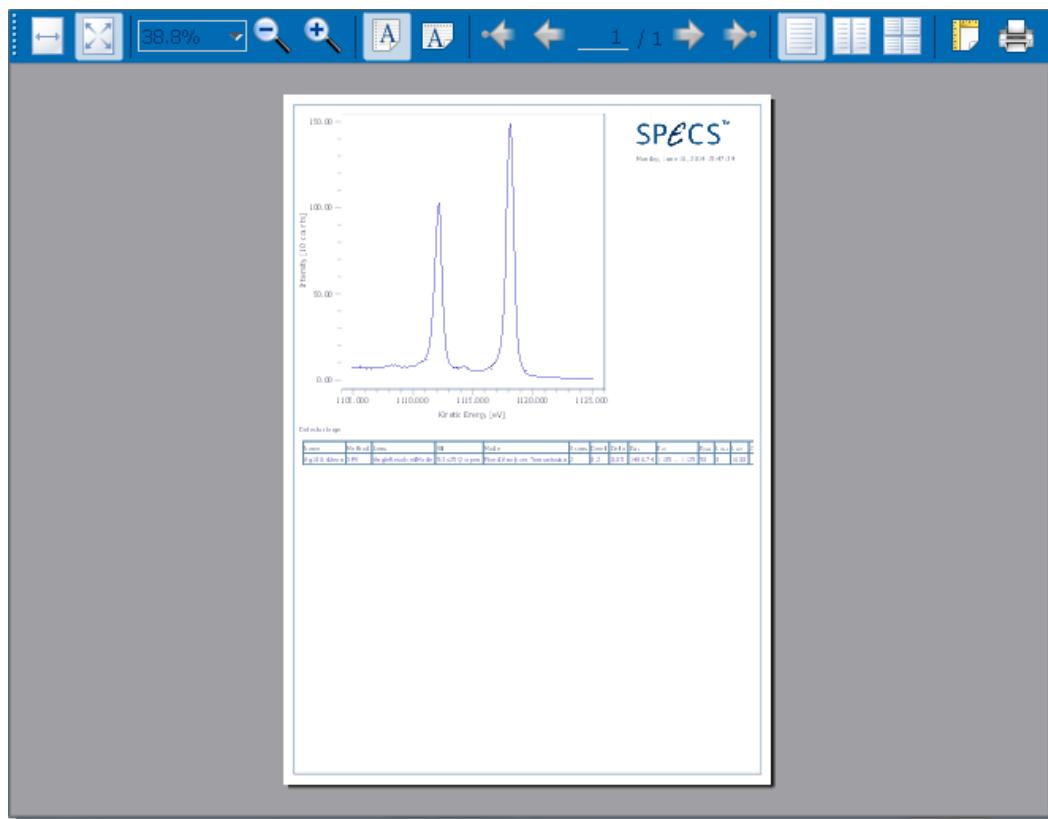
Clicking the  icon will copy the plot (with axes) exactly as it appears in the Plot View. You can paste the bitmap into other applications.

## 6.2.7 Printing the Plot View

The toolbar contains icons for a print preview and for printing the plot. The following information is printed:

- The plot in the Plot View, including all visible spectra and data operations.
- A legend, showing the experimental parameters for each spectrum. The entries in the legend are color coded.

The print preview window allows you to see the page before it is sent to the printer. The toolbar contains a number of controls for changing the orientation and page size, as well as changing the appearance of the preview.



To print the Plot View:

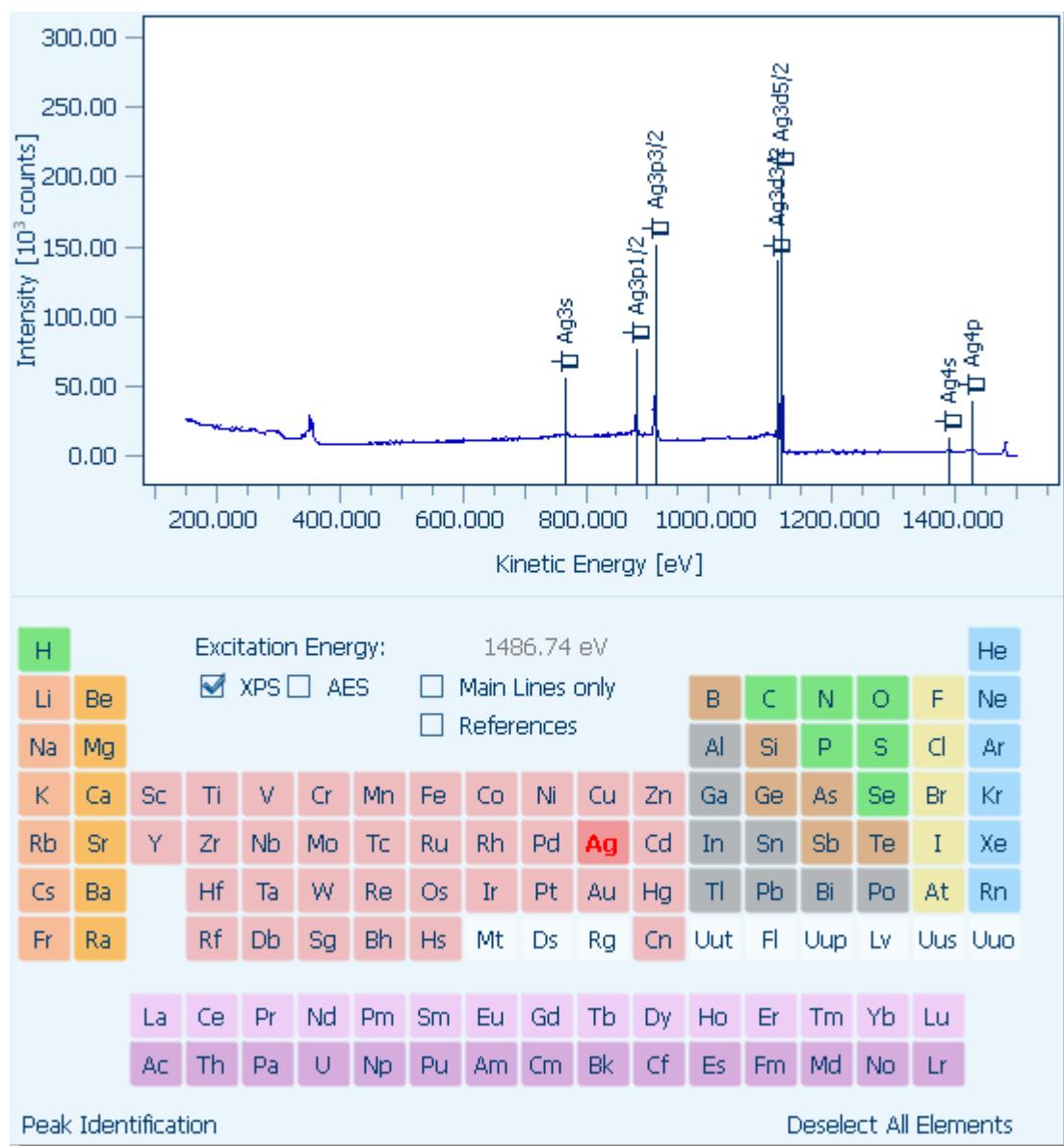
- Click the icon in the Plot View toolbar. The standard MS Windows print dialog will open, allowing you to configure and start the print job.

### 6.3 Periodic Table

The periodic table contains a set of databases for the XPS, UPS and AES transitions of all elements. It allows you to easily [identify peaks](#) in the plot view, as well as providing [additional methods](#) for performing peak operations.

To open the periodic table:

- Click  in the toolbar of the Plot View.



### 6.3.1 Identifying Peaks using the Periodic Table

There are a number of options that you can select to affect the way peak identifications are added to the spectrum. These are listed in the table below.

Feature	Description
Excitation energy	The excitation energy used to measure the data.
XPS	Shows lines for XPS.
AES	Shows lines for AES.
Main lines only	Only shows the most intense lines for the selected element. Hovering the mouse over the line will show all lines of the element.
References	Displays the database reference for each displayed peak.

For identification of peaks in the spectrum, you can use the automatic peak identification feature or manually select peaks. Expand the sections below for more information about these procedures.

#### Automatic peak identification

The automatic peak identification feature can be useful to help you identify unknown peaks in the spectrum. Note the following points:

- Some of the peaks may be included because their energy is close to that of a peak in the spectrum. The identification of a peak does not necessarily mean that the element is present in the sample.
- Artifacts and spikes in the data may be identified as peaks.
- Not all peaks of an element will be shown. This generally applies to weak peaks of the element which are hidden in the noise level of the data.
- Hovering the mouse over the peak identification label in the spectrum or over the identified element in the periodic table will show all peaks for that element in the spectrum.

As a result of these points, checking the Main Lines Only box is a good idea to reduce the number of false identifications.

To use automatic peak identification:

1. Select a spectrum in the Data Browser. The peak identification feature will be run on this spectrum.
2. Click **Peak Identification**. SpecsLab Prodigy will locate all peaks in the spectrum and match them to values in the databases.

Manually selecting peaks for an element

If you expect an element to be present in the spectrum, you can show the database values for the peaks:

- Click the element in the table. All peaks for the element will be displayed in the spectrum.

### Manually selecting peaks for an element

If you expect an element to be present in the spectrum, you can show the database values for the peaks:

- Click the element in the table. All peaks for the element will be displayed in the spectrum.

Right-clicking the element shows a list with the transitions for the element. You can select one of these transitions to add the peak to the **Selected Transitions** pane.

Clicking **Deselect All Elements** will remove all peak identifications from the spectrum. If you have selected any peaks, these will not be removed.

### 6.3.2 Selecting Peaks

You can select peaks of interest. These are highlighted in the Plot View and listed in a table next to the periodic table. You can perform operations on the selected peaks.

There are two ways to select peaks in the spectrum:

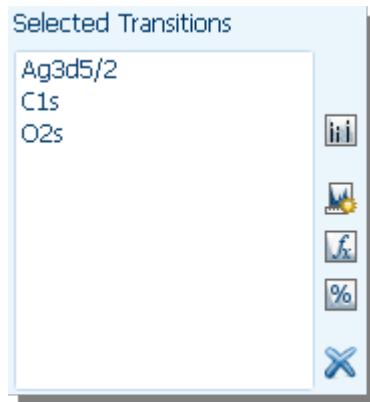
- Click the  icon in the label of the peak. The icon will change to  to show it is pinned.
- Right-click an element in the table and select a peak from the menu.

In both cases, the selected peak will be displayed in a table next to the periodic table. You can select peaks in this table and perform actions on them:

 Shows all peaks for the selected element.

 Adds detailed spectra for all selected peaks.

 Performs an operation on the selected peak(s). The element name and transition is included in the parameters of the operation.



To remove selected peaks:

- Select one or more peaks in the **Selected Peaks** table and click . If no peaks are selected, all will be deleted when you click .

## 6.4 Changing the Axis Labels

You can change the labels of the X, Y and Z axes so that they present different quantities. The options available depend on the axis selected as well as the type of spectrum.

To change the axis label:

1. Move the mouse over the axis label. It will change into a drop-down list.
2. Click the drop-down list and select the desired label.

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## Chapter 7 – Plot View II: Data Operations

SpecsLab Prodigy offers a variety of operations that you can perform on spectra in the Plot View. This chapter describes how to perform data operations and contains descriptions of all operations.

There are essentially two methods of running data operations:

- Setting up the operation before running the experiment. The operation is performed and updated after each scan. Such an approach is ideal as part of a template.
- Running an operation on a region of interest in an acquired spectrum as part of the data analysis.

For all other features in the Plot View, please refer to ["Plot View I: Features" on page 71](#). Data operations in the Image View are covered in ["Performing Operations in the Image View" on page 142](#).

### 7.1 Defining Data Operations before Measurement

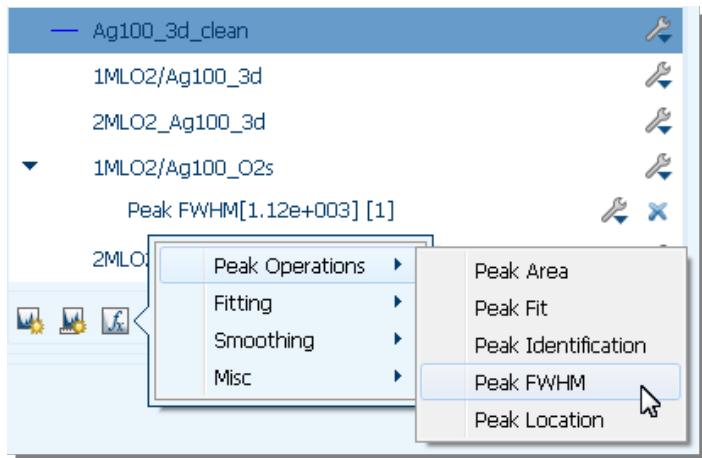
You can define a data operation as part of the experiment configuration. The operation is performed after the experiment runs. In this case, you typically know what form of data analysis is required (for example, FWHM calculation) and want this automatically performed. In particular, if you save the experiment as a template, the definition for the data operation is also saved.

#### Note

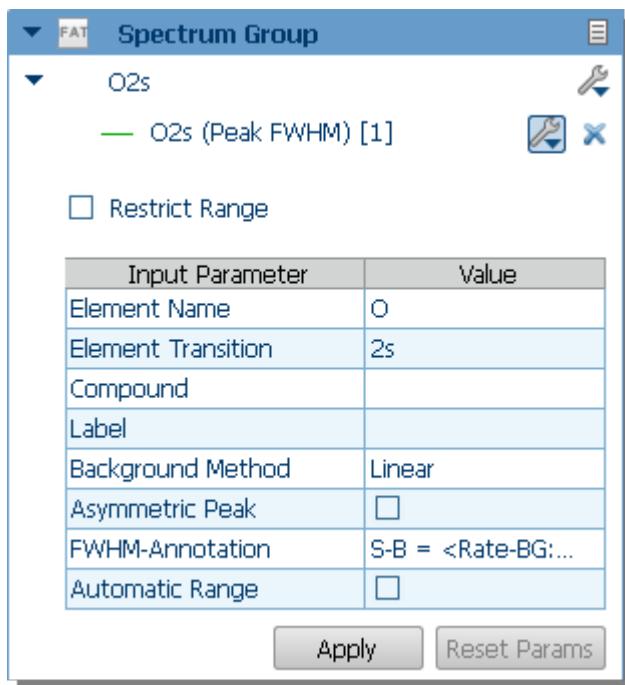
This approach is also useful if you are using overwrite mode (see ). In this case, the spectrum is scanned repeatedly—you can perform an operation after each scan to check current performance.

To define a data operation:

1. Define a spectrum in the Experiment Editor.
2. Select the spectrum in the Experiment Editor or in the legend of the Plot View.
3. Click  and select an operation from the menu, e.g. an FWHM operation as shown in the picture below. The operation will be performed on the selected area and displayed in the data browser below the selected spectrum.



4. Set the color, linestyle and width of the operation. This is the same procedure as for spectrum data—see ["Setting Color and Appearance of Data" on page 73](#).
5. Click the arrow next to the operation to display the settings.
6. If you want to restrict the range over which the calculation is performed, check the **Restrict Range** box and enter the start and end energies for the calculation.



7. Edit the input parameters in the table as necessary and click Apply. See the page for the [data operation](#) for a description of the input parameters.

The data operation is now defined for the spectrum. You can now:

- Run the experiment to take the spectrum. The data operation will be performed at the end of each scan.
- Save the experiment (or spectrum group) as a template. The configuration for the data operation will be saved with the template and will be used every time you use the template.

## 7.2 Performing Operations on Regions of Interest

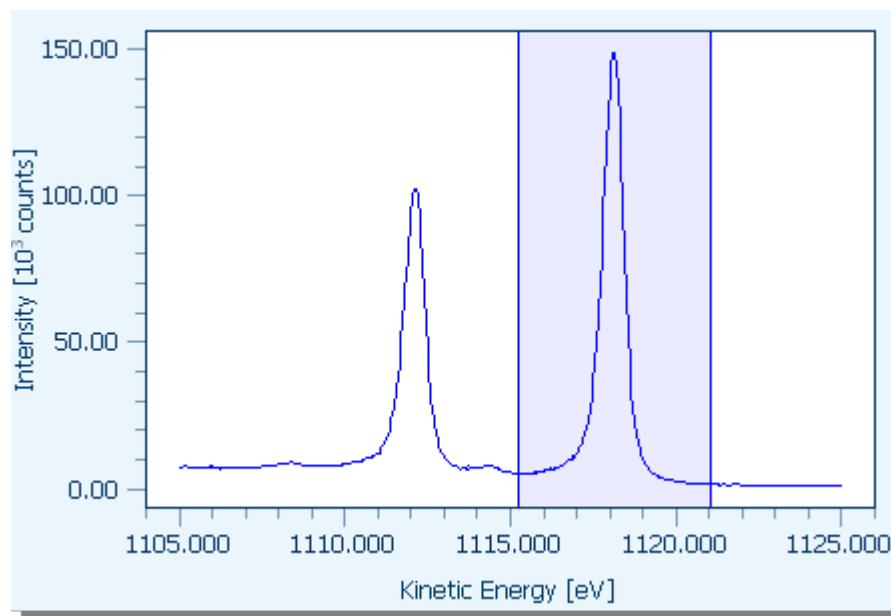
After acquiring a spectrum, you can run data operations on the whole spectrum or a specific region of interest. The operations provide you with some useful tools for analysis.

### Note

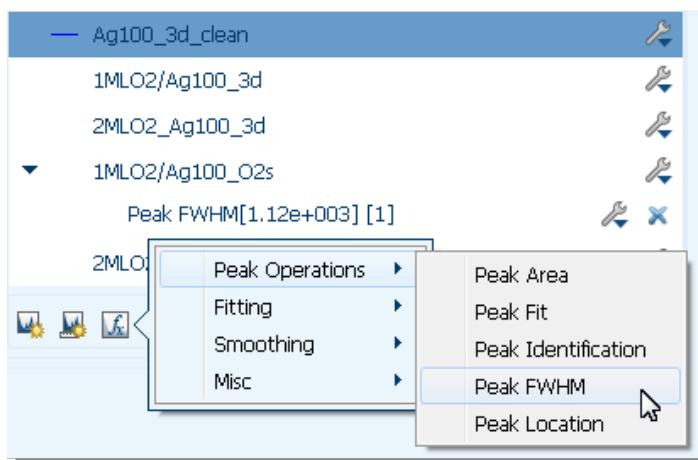
If you do not select a region of interest in the following procedure, the data operation will be performed on the whole spectrum or the zoomed area in the view.

To perform a data operation on a region of interest:

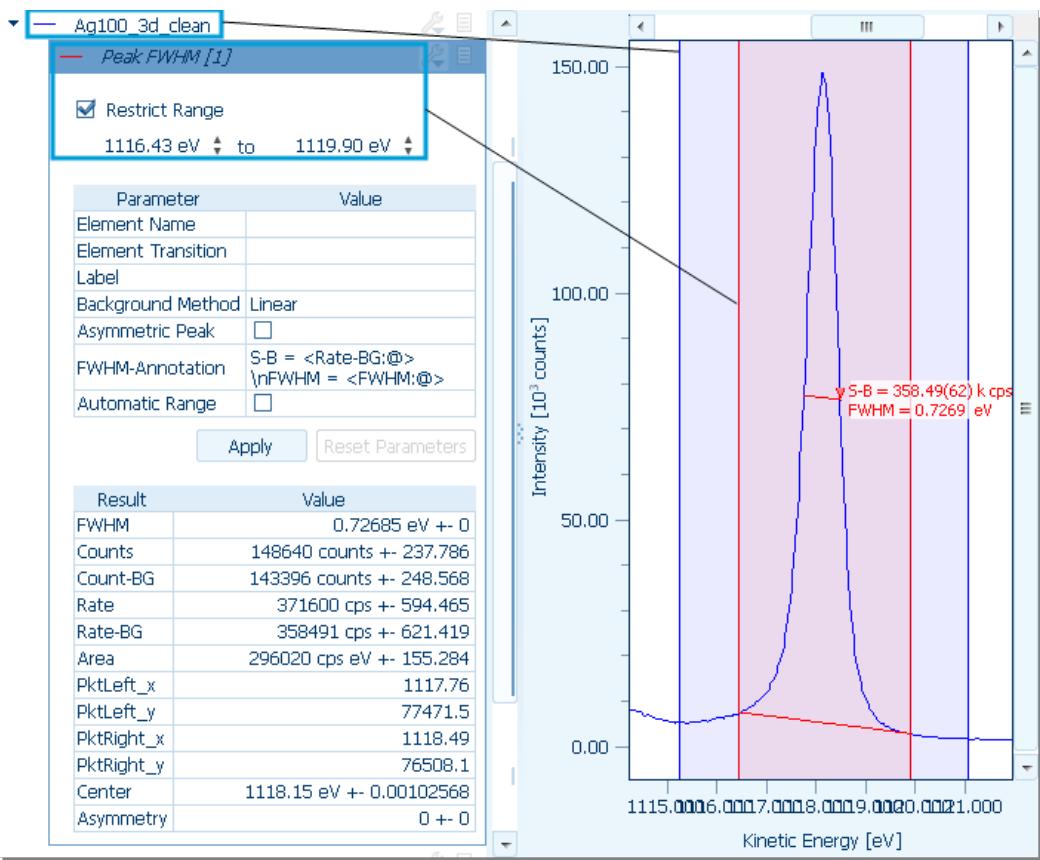
1. Select a spectrum in the Experiment Editor or in the legend of the Plot View. This is the target spectrum for the operation.
2. Click the  icon in the Plot View toolbar.
3. Select a region in the plot. The operation will be performed on the data in this region.



4. Click  and select an operation from the menu, e.g. an FWHM operation as shown in the picture below. The operation will be performed on the selected area and displayed in the data browser below the selected spectrum.



5. Click the arrow next to the operation to display the input and output parameters. You can alter range of the calculation as well as its input parameters. The list of input and output parameters depends on the [operation selected](#) (see the Online Help for more information).



### 7.3 Normalizing Spectrums

You can measure signals from other equipment while taking data. A typical example would be the sample current in order to find the relative source intensity. After measuring this data, you can normalize the acquired data to this signal.

To normalize spectra, perform one of the following:

- Click the icon next to the experiment you want to normalize and select an item from the **Normalize by** list. The normalization will be applied to all spectra in the experiment.
- Click the icon next to the spectrum group you want to normalize and select an item from the **Normalize by** list. The normalization will be applied to all spectra in the group.

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

### Note

Each operation which has an annotation has a pre-defined setting. You can use this as an example 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 is the name shown in the table of output parameters.
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.

### Parameters

All output parameters in the data operation can be used in the annotation.

### 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:

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

### Example

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

Annotation definition	[newline] <u>S-B = &lt;Signal-BG:@&gt;\nFWHM = &lt;FWHM:@&gt;\nArea = &lt;Area:@&gt;</u>	[newline]
Displayed text	S-B = 156 kcounts FWHM = 4.891 eV Area = 11.66 Mcps eV	

**Note**

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

## 7.5 Peak Operations

The peak operations allow you to perform various operations on peaks in spectra for evaluation purposes. The following operations are available:

- Peak area—calculate the area under a peak.
- Peak fit—uses a user-selected algorithm to find the height and width of a peak.
- Peak FWHM—finds the width of a peak.
- Peak identification—matches peaks in a spectrum to values in a database.
- Peak Location—analyzes the points at or near a peak and finds the position of the peak.

### 7.5.1 Peak Area

The peak area operation constructs a series of trapeziums between adjacent data points to the background line, calculates their area and sums the total area.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

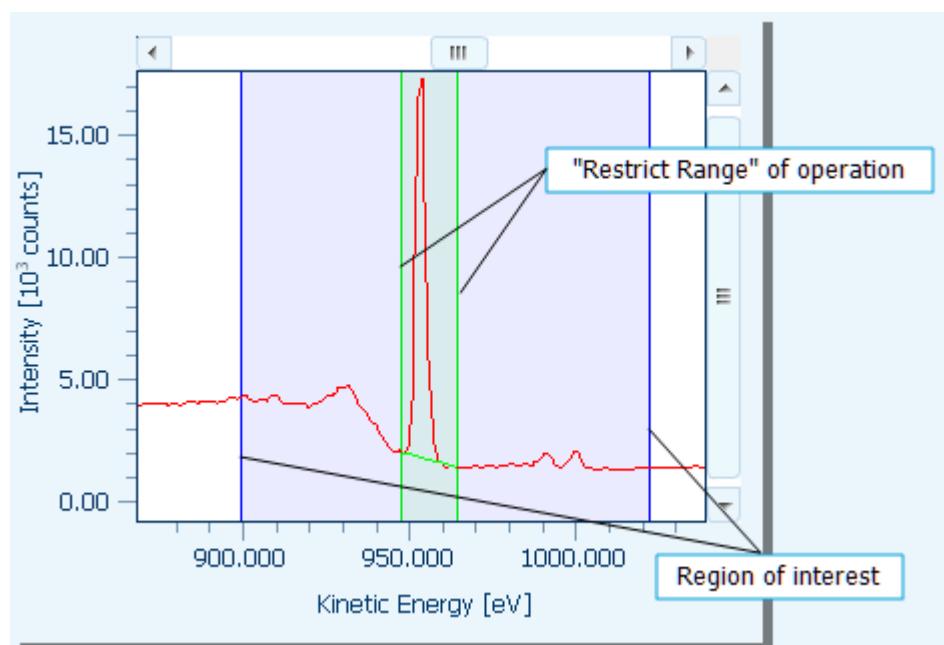
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

**Note**

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

**Input parameters**

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

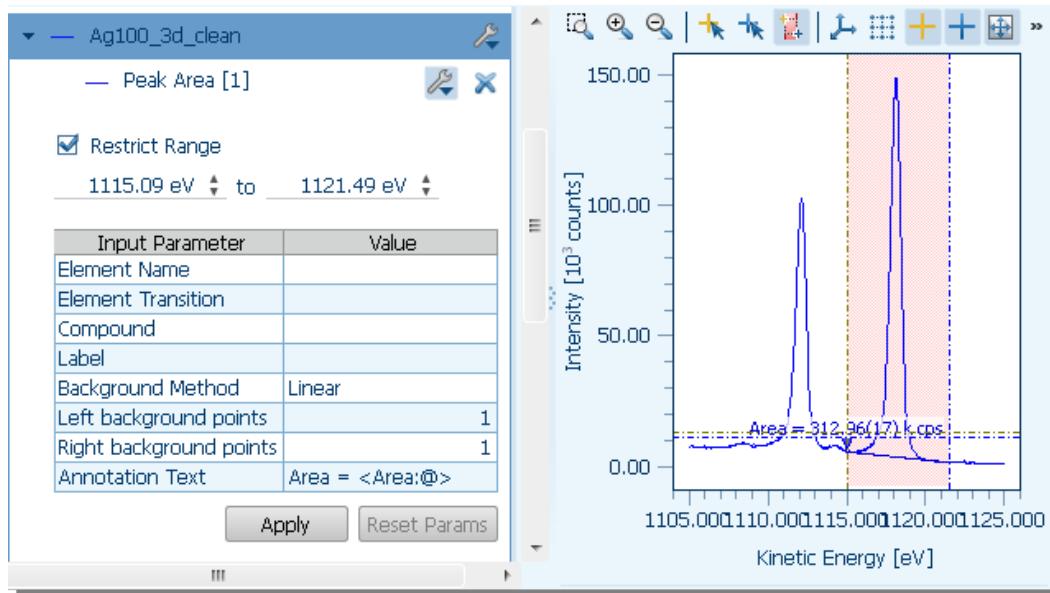
Input parameter	Value
Element name	Optional. Enter an element symbol. This will be sent to the output parameters when you click Apply. This setting is used for further quantitative evaluation of the spectrum area (if available) and can be added to the data in the periodic table (if available).
Element transition	Optional. Enter the name of the transition. See Element name above for more details.
Compound	Optional. Enter the name of the compound in the sample. See Element name above for more details.
Label	Optional. Enter a reference label for the measurement. See Element name above for more details.
Background method	Choose a <u>background subtraction</u> method. The default is

Input parameter	Value
	linear.
Left background points	These values determine how many points in the background are used in the background calculation. Setting the value to zero means that the number will be selected automatically.
Right background points	As Left background points above.
Annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

The **Output Parameters** section contains the results of the operation.



### 7.5.2 Peak Fit

The Peak Fit operation fits a user-selected function to the selected peak.

You can select which background operation is used (see "[Background](#)" on page 105 for a description of all available options) and set the fitting algorithm to operate on asymmetrical peaks, as necessary.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict**

**Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

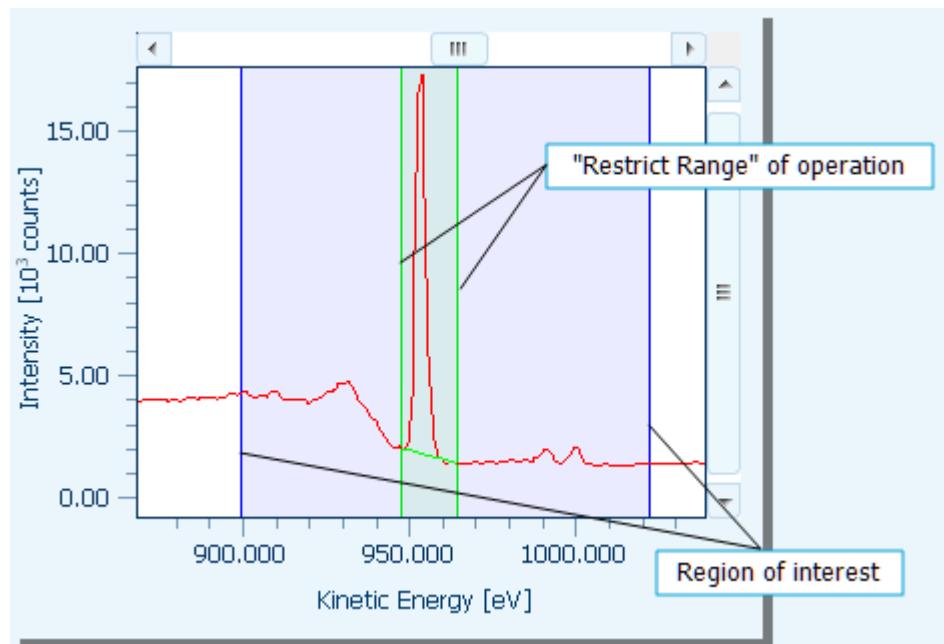
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input

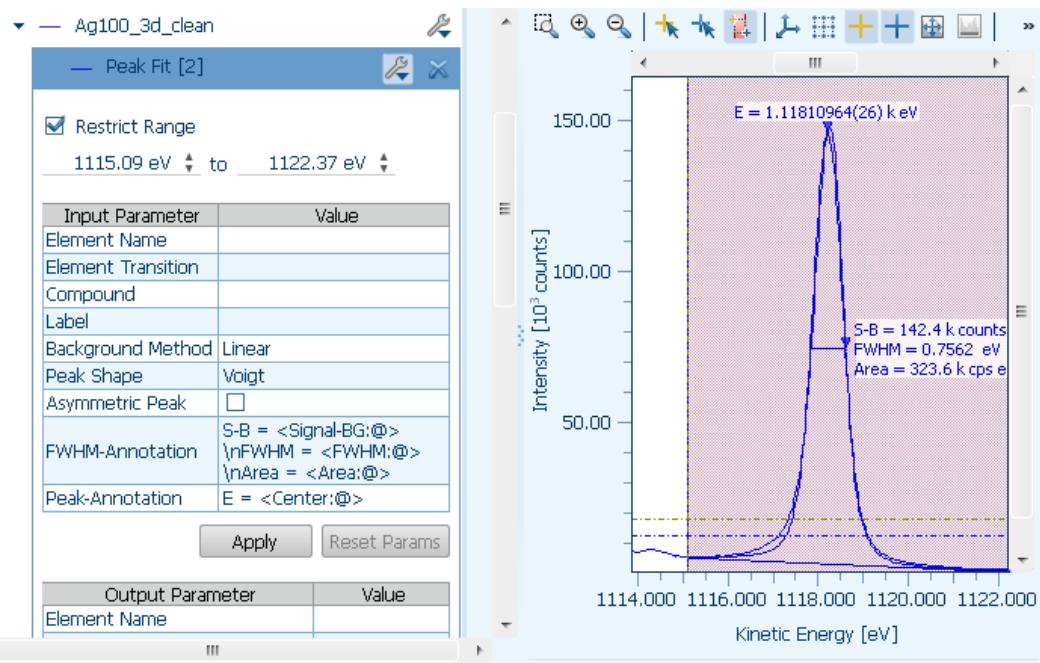
parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Background method	See <a href="#">Background</a> for a description of all available background subtraction methods.
Peak shape	Select the function used to calculate the peak shape. The sections below describe the options.
Asymmetric peak	Check this if the peak shape is asymmetric.
FWHM annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.
Peak annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

The **Output Parameters** section contains the results of the operation.



The following sections describe the different available fitting methods

### DSG—Doniac-Sunjic-Gauss

Theoretical considerations of the energy loss of photoelectrons in metals lead to the asymmetrical Doniac-Sunjic function:

$$DS(x; \alpha, F, E) = \frac{\cos\left(\frac{\pi\alpha}{2} + (1 - \alpha)\arctan\left(\frac{x - e}{f}\right)\right)}{(f^2 + (x - e)^2)^{\frac{1-\alpha}{2}}} \quad (1)$$

where:

- $\alpha$  is the asymmetry parameter—with  $\alpha = 0$ , this is equivalent to a Lorenzian
- $e$  is related to the position of maximum intensity
- $f$  is related to the half-width

In the DSG fit, the Doniac-Sunjic is convoluted with a Gaussian:

$$DSG(x; \alpha, f_{DS}, e_{DS}, f_G, e_G) = DS(x; \alpha, f_{DS}, e_{DS}) * G(x; \alpha, f_G, e_G) \quad (2)$$

where:

- $e_{DS}$  is related to the position of maximum intensity in the D-S function
- $e_G$  is the peak position of the Gaussian
- $f_{DS}$  is related to the half-width in the D-S function
- $f_G$  is the half-width of the Gaussian.

### GLP—Gauss-Lorenz Product

The Gauss-Lorenz product results from multiplying Gaussian and Lorenzian functions together:

$$GLP(x; F, E, m) = \frac{\exp\left(-4\ln 2(1 - m) \cdot \frac{(x - E)^2}{F^2}\right)}{1 - 4m\frac{(x - E)^2}{F^2}} \quad (3)$$

where:

- $E$  is the center of the curve
- $F$  is the half-width
- $m$  is a mix parameter

### GLS—Gauss-Lorenz Sum

The Gauss-Lorenz product results from adding Gaussian and Lorenzian functions together:

$$GLS(x; F, E, m) = (1 - m)\exp\left(-4\ln 2 \frac{(x - E)^2}{F^2}\right) + \frac{m}{1 + 4 \frac{(x - E)^2}{F^2}} \quad (4)$$

where:

- E is the center of the curve
- F is the half-width
- m is a mix parameter

### **Voigt**

In order to obtain a realistic line shape for peaks in a spectrum, a Voigt function is used. This is a convolution of a Gaussian and Lorenzian function:

$$V(x; E, F_G, F_L) = G(x; F_G, E) * L(x; F_L, E) \quad (5)$$

where:

- E is the center of the curve
- $F_G$  is the half-width of the Gaussian
- $F_L$  is the half-width of the Lorenzian

The numerical solution of the convolution integral is very time consuming. For this reason, SpecsLab Prodigy uses an approximation based on the principle of Fourier transformations such that the Fourier transform is equal to the product of the individual Fourier transforms:

$$F(g * f) = F(g) \cdot F(f) \quad (6)$$

### **7.5.3 Peak FWHM**

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

You can select which background operation is used (see "[Background" on page 105](#) for a description of all available options) and set the fitting algorithm to operate on asymmetrical peaks, as necessary. The FWHM annotation defines the text shown in the plot—see "[Annotation Syntax" on page 89](#) for details.

#### **Restrict range**

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

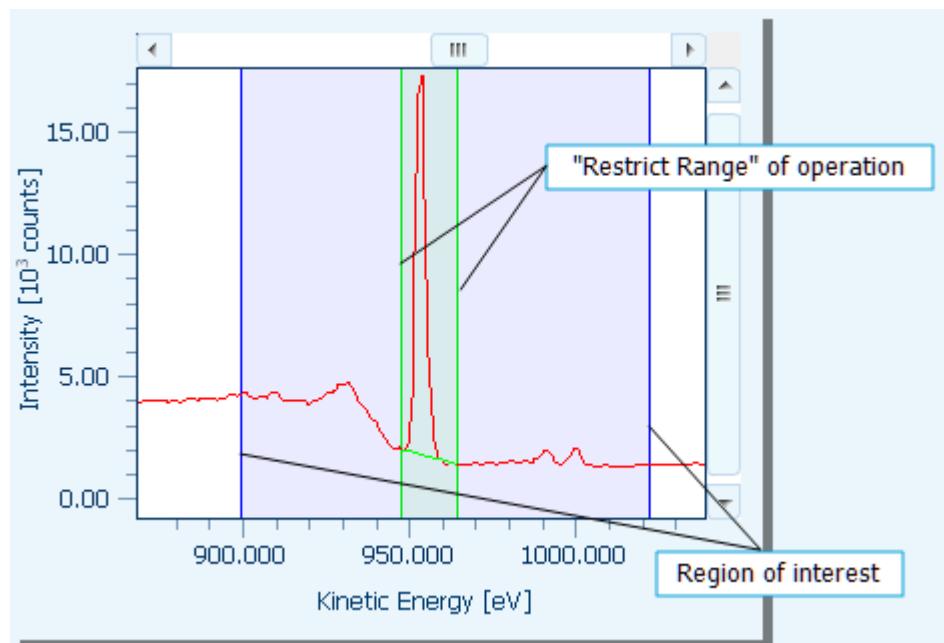
- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

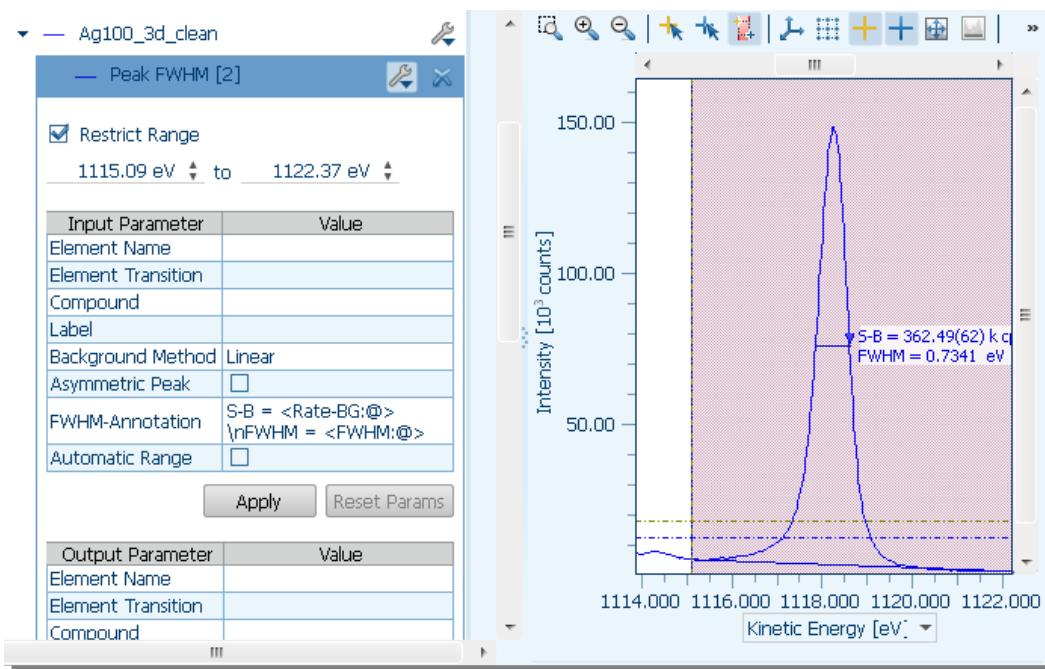
The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Element name	Optional. Enter an element symbol. This will be sent to the output parameters when you click Apply. This setting is used for further quantitative evaluation of the spectrum area (if available) and can be added to the data in the periodic table (if available).
Element transition	Optional. Enter the name of the transition. See Element name above for more details.
Compound	Optional. Enter the name of the compound in the sample. See Element name above for more details.
Label	Optional. Enter a reference label for the measurement. See Element name above for more details.
Background Method	Select a method. See <a href="#">Background</a> for a description of all the options.
Asymmetric Peak	Check this if the peak shape is asymmetric.
FWHM-Annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.
Automatic Range	The operation can select the area to the left and right of the peak in order to optimize the background subtraction.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

The **Output Parameters** section contains the results of the operation.



## 7.6 Peak Identification

The peak identification operation matches peaks in your data to values in a database. It is a convenient way to identify unknown elements in a spectrum.

To run the peak identification operation:

1. Select a spectrum in the Data Browser.
2. If necessary, select a region of interest for the operation.
3. Click the icon and select **Peak Operations/ Peak Identification** from the menu. The operation will run and its parameters and results will be displayed below the selected spectrum. The results will also be shown in the Plot View.

The section below describe the parameters and results.

### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

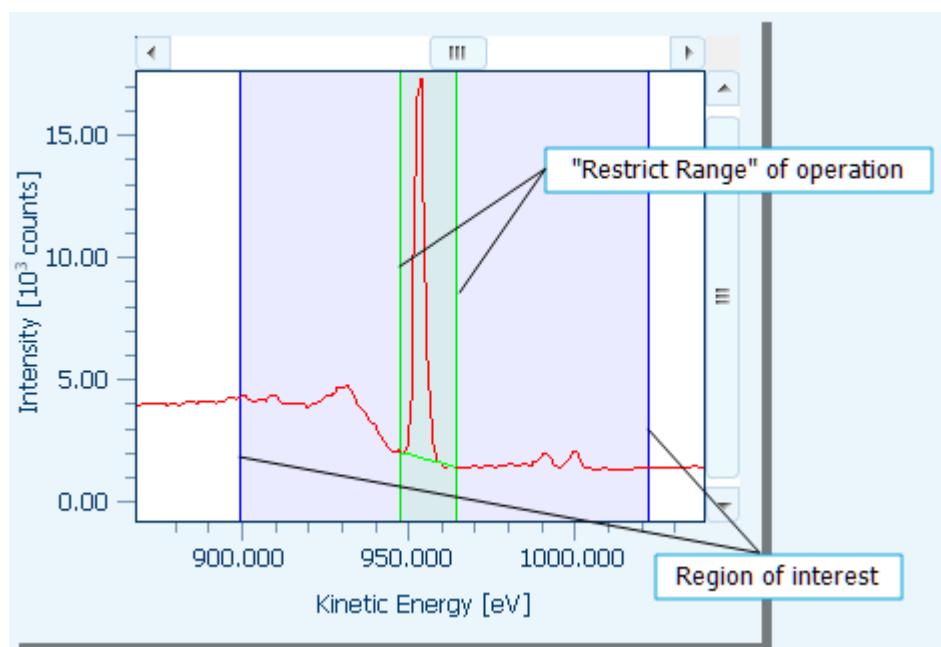
- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

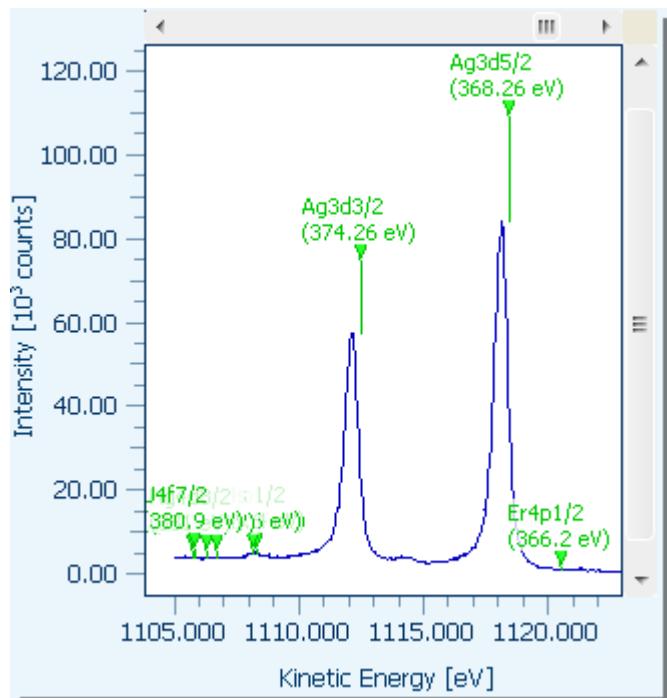
Input parameter	Value
Restrict to specific elements	Enter an element symbol, e.g. Ag (case sensitive).
Energy tolerance to associate	Set the shift allowed from the literature value for the assign-

Input parameter	Value
peaks [eV]	ment.
FWHM threshold	

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters
- **Reset Params**—sets the input parameters to their default values

The **Output Parameters** section contains the results of the operation.



### 7.6.1 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<sup>1</sup>.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

---

<sup>1</sup>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)

You can change the region of interest using one of the following methods:

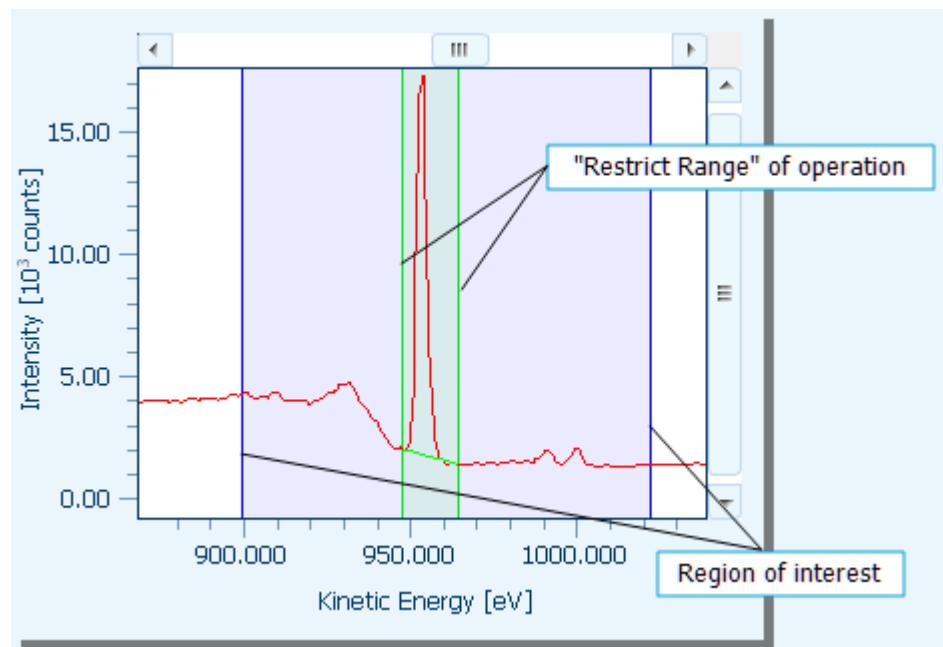
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Left data points	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.
Right data points	As Left data points above.
Asymmetric Peak	Check this if the peak shape is asymmetric.
Background slope	Check this if the background has a slope. You should not use a sloping background when fitting peaks for energy scale calibration. As discussed by Powell <sup>1</sup> , this can introduce systematic errors.
Peak-Annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

[Equation \(7\)](#) shows how the peak location is calculated.

$$I_x = I_c \cdot \exp\left(-4\ln 2 \cdot \left(\frac{x - c}{\text{FWHM}(1 \pm \alpha)}\right)^2\right) + S \cdot (x - c) + B_g \quad (7)$$

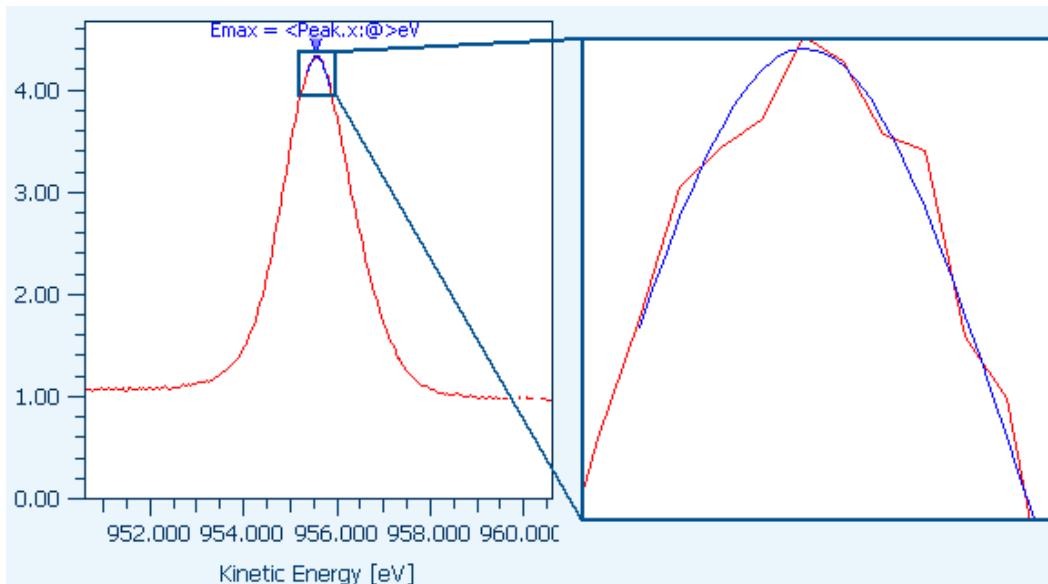
where:

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

The **Output Parameters** section contains the results of the operation.

---

<sup>1</sup>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)



## 7.7 Fitting Operations

The fitting operations menu contains the following items:

- [Fermi Edge](#)—find the position and width of the Fermi edge.
- [Background](#)—various methods of background subtraction. These are also used in [other operations](#) for peak fitting.

### 7.7.1 Background

The background operation allows you to subtract the background of a selected region according to a preset algorithm.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.

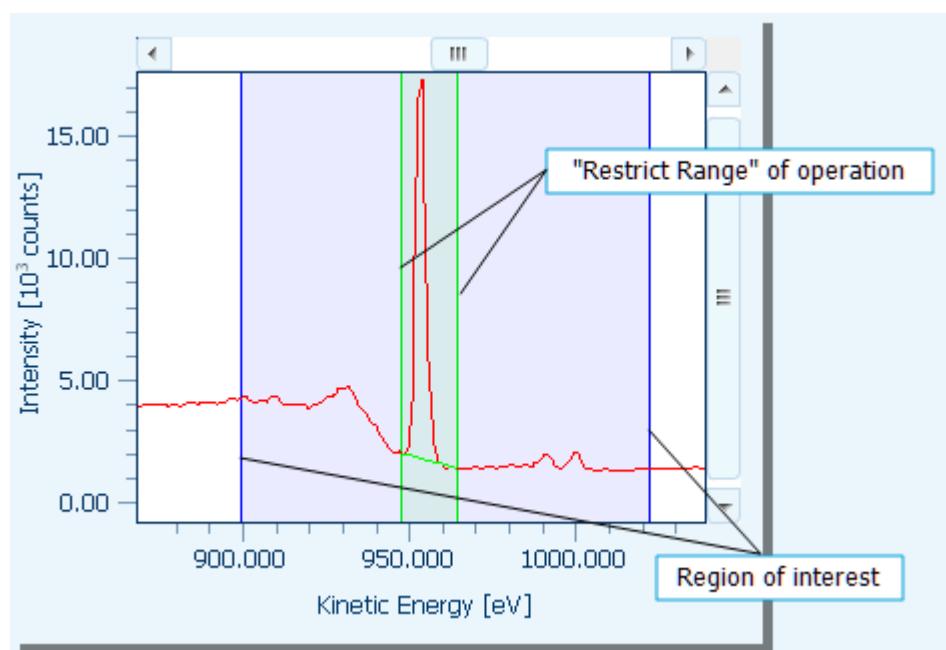
**Restrict Range**

1110.10 eV  to  1115.00 eV

- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Optimize Range	The range of the operation is optimized so that the lowest reasonable background is achieved.
Method	Select a background subtraction method. The various methods available are described below.

There are two buttons below the input parameter table:

- Apply**—runs the operation with the selected input parameters.

- **Reset Params**—sets the input parameters to their default values.

The following background subtraction methods are available:

#### **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.

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. This kind of background does not represent a physical background.

#### **Shirley**

The Shirley background<sup>1</sup> 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 \(8\)](#) shows the calculation method for the Shirley background.

$$b_i = k \sum_{j=i+1}^N p_j \quad (8)$$

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 conditions for the calculations are determined in the same manner as the extreme points for the linear background calculation.

#### **Tougaard**

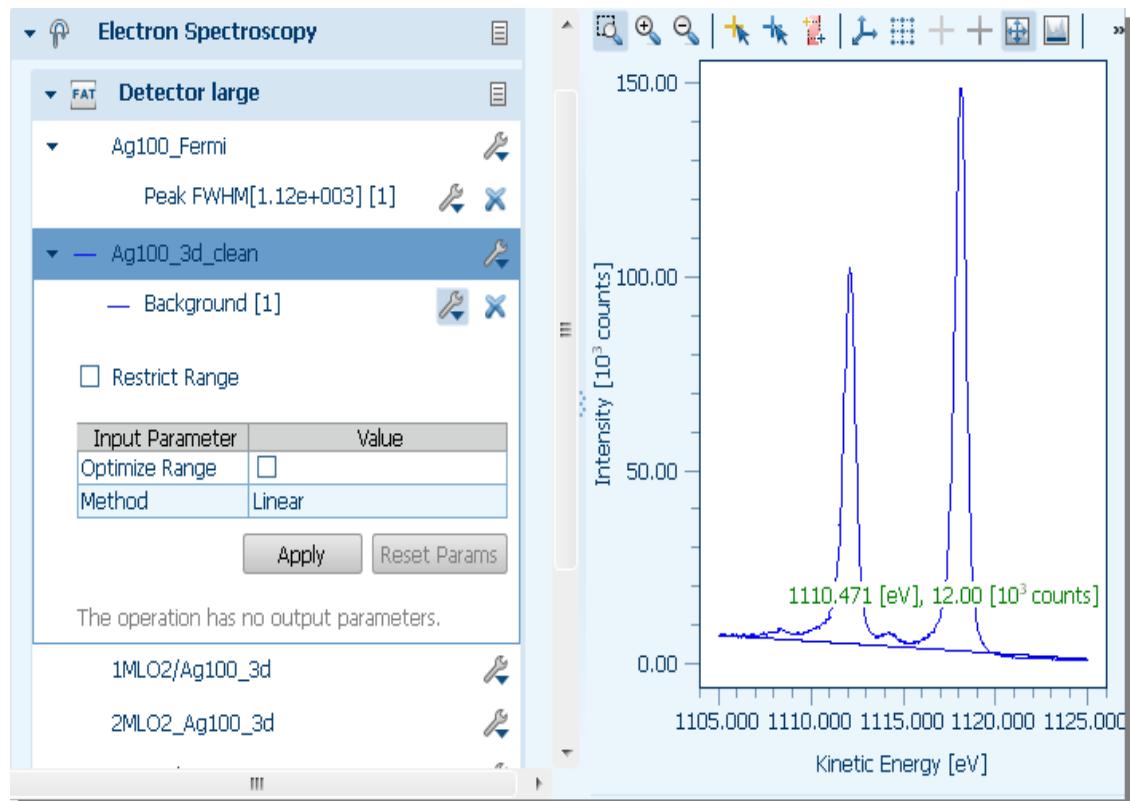
A physical model of the background is based upon the elastic and inelastic loss processes in

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

the solid. Tougaard and Sigmund showed<sup>1</sup> 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:

$$F(E) = j(E) - B \int_{E}^{\infty} \frac{E' - E}{E(C + (E' - E)^2)} \cdot j(E') dE' \quad (9)$$



## 7.7.2 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. The Fermi edge is modeled using an error function:

$$y = \frac{h}{2} \cdot \left( 1 + \operatorname{erf} \left( (x_0 - x) \cdot \frac{2\sqrt{\ln 2}}{\text{FWHM}} \right) \right) \quad (10)$$

<sup>1</sup>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)

where  $h$  is the height of the error function. The rest of the data is fitted with straight lines which can have different gradients, as seen in the figure above. The formula can also be convoluted by another function which adds the peak broadening due to temperature. This convolution is not performed with a set temperature of 0 K.

#### Note

Noisy data or "unexpected" slopes can cause the algorithm to fail.

You can restrict the range over which the operation is applied.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

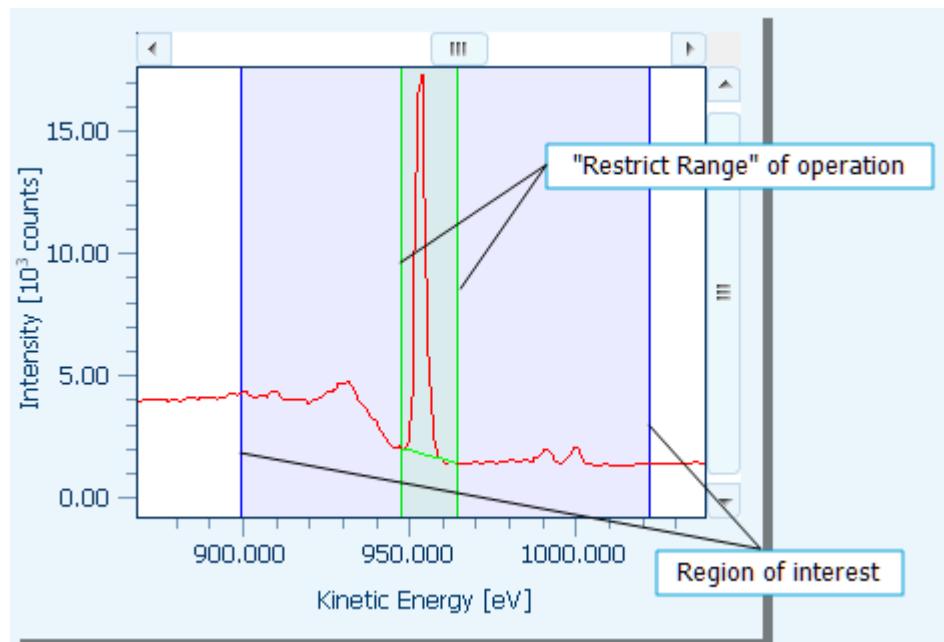
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

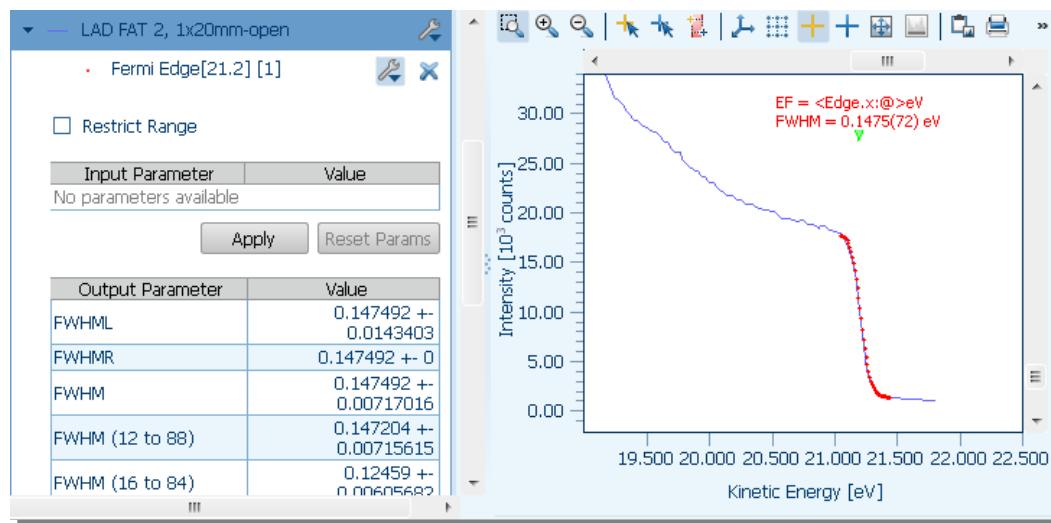
#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

The screenshot below shows a fit with the calculated results.



### Note

Noisy data or "unexpected" slopes can cause the algorithm to fail.

The Fermi edge is modeled using an error function:

$$y = \frac{h}{2} \cdot \left( 1 + \operatorname{erf} \left( (x_0 - x) \cdot \frac{2\sqrt{\ln 2}}{\text{FWHM}} \right) \right) \quad (11)$$

where  $h$  is the height of the error function. The rest of the data is fitted with straight lines which can have different gradients, as seen in the figure above. The formula can also be convoluted by another function which adds the peak broadening due to temperature. This convolution is not performed with a set temperature of 0 K.

## 7.8 Smoothing Operations

The smoothing operations provide a set of methods for processing the appearance of raw data:

- Despiking—removes anomalous spikes from the signal.
- Noise settings—estimates the noise in a signal from a CCD detector.
- Savitsky-Golay smoothing—a method of smoothing that also allows the calculation of derivatives in the data.
- Smoothing spline—fits a spline to the selected data.

### 7.8.1 Despiking

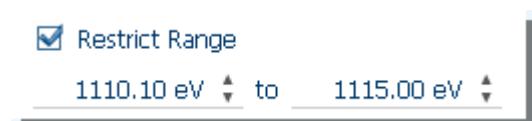
The despiking filter removes spikes from spectra which may occur due to some external event (e.g. sparks) and replaces them with the mean values of the neighbor values by additionally adding some typical noise distribution.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

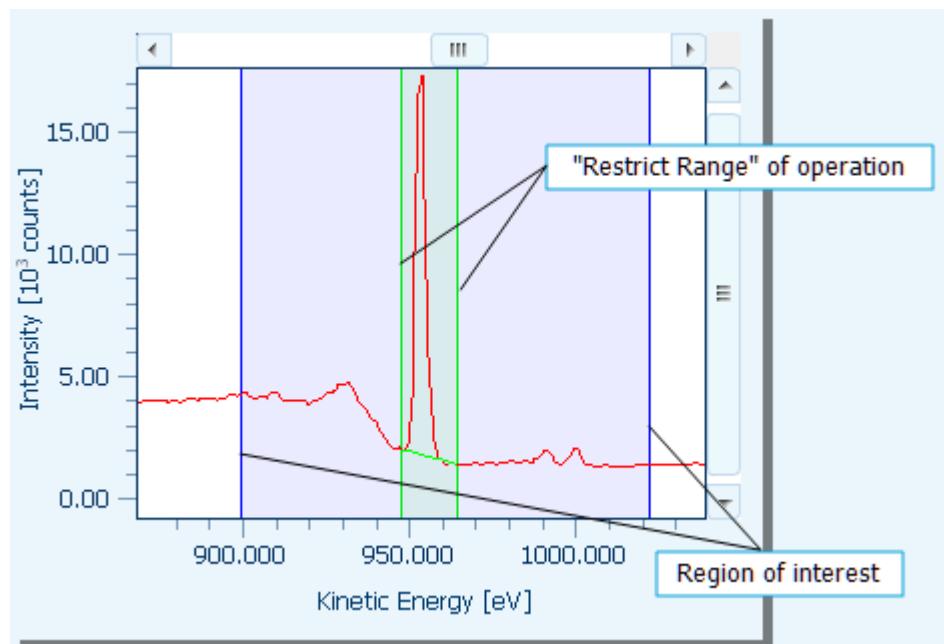
- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

## Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

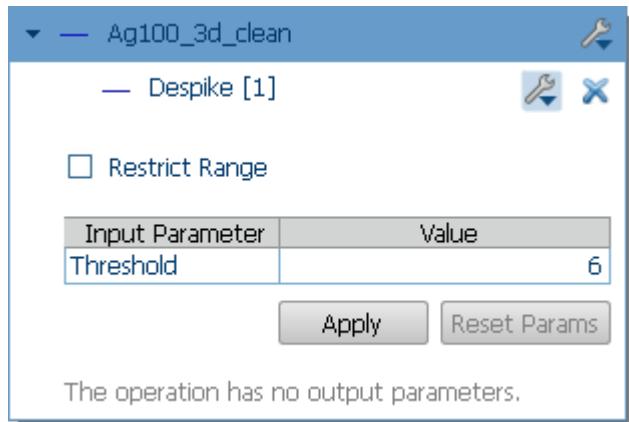
## Input parameter

The input parameter allows you to alter the operation. The table below lists the input parameter for the Despike operation. After setting the parameter, click **Apply** to run the operation with the new settings.

Input parameter	Value
Threshold	A multiple of the expected rms noise threshold.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameter.
- **Reset Params**—sets the input parameter to its default value.



## 7.8.2 Noise Settings

The **Noise** operation estimates the intensity scaling for CCD detector measurements. This calculates a factor for the noise based on the standard deviation from the average signal.

SPECS detectors typically produce a noise factor in the range 0.95–1.05. Consistent noise levels outside this range may indicate a fault with the detector.

### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

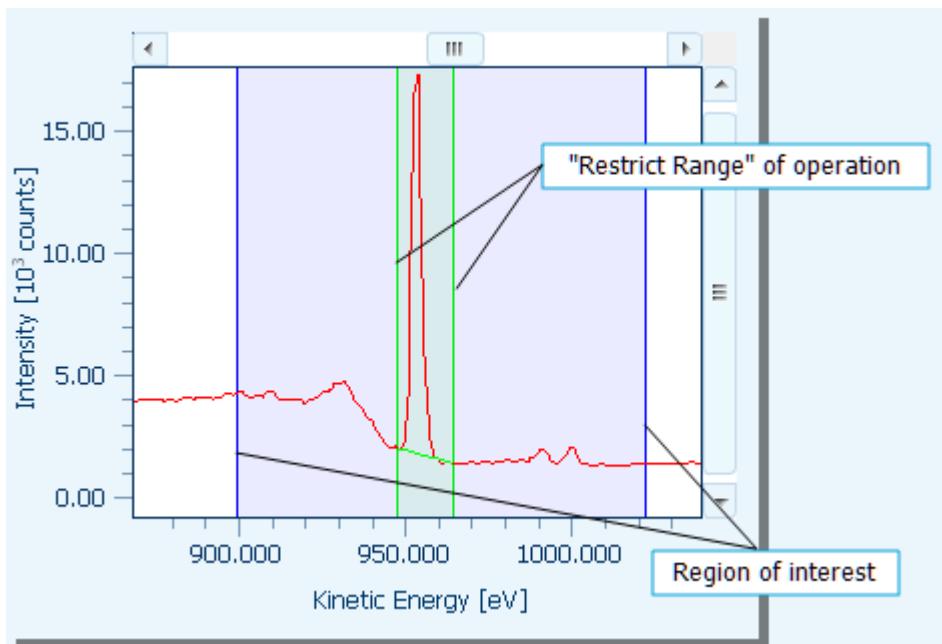
- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

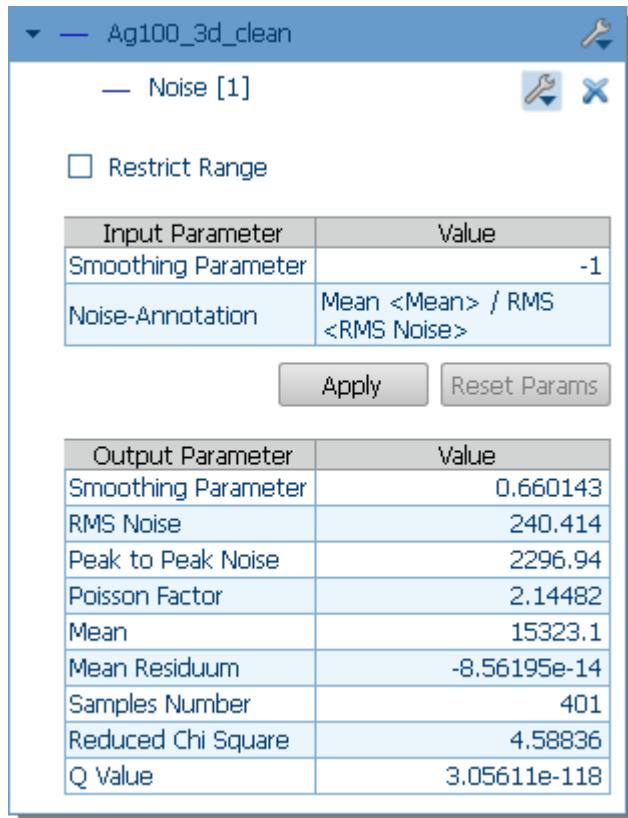
### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Smoothing Parameter	Enter the error variance. The calculation uses this to minimize an unbiased estimate of the true mean square error and thereby determines the degree of smoothing. If the error variance is not known, set this to -1. The routine minimizes the generalized cross validation to determine the degree of smoothing. This approaches the limit of minimizing the true mean square error.
Noise-Annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.



### 7.8.3 Savitzky 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.

SpecsLab Prodigy offers a particular type of low-pass filter, well-adapted for data smoothing, called Savitzky-Golay<sup>1</sup>.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

<sup>1</sup>A. Savitzky and M.J.E. Golay. "Smoothing and differentiation of data by simplified least square procedures", Anal. Chem., 36(8), 1627-1639, 1964

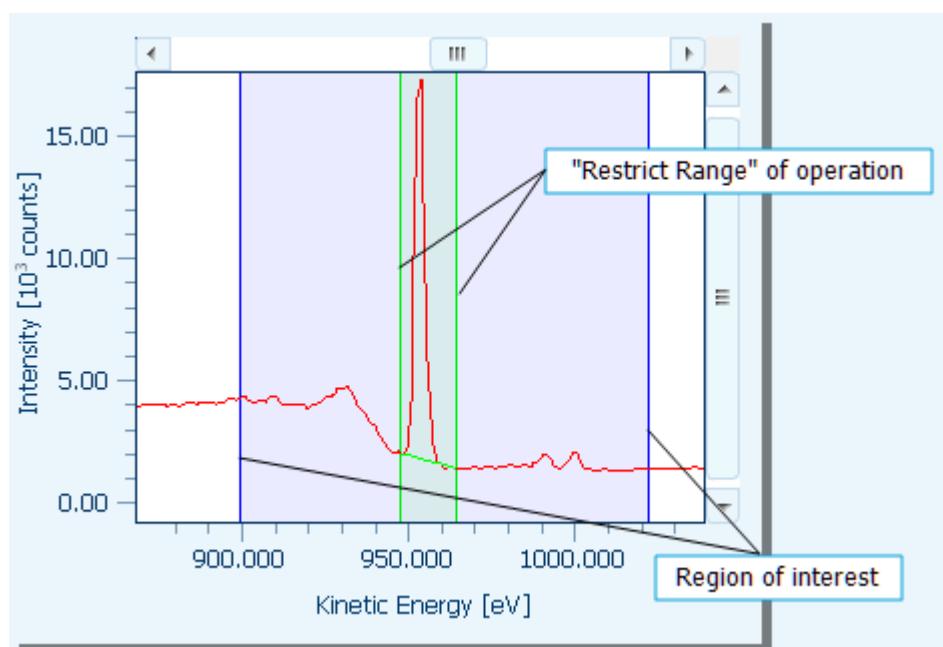
- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

See also the background section below for more information about the input parameters.

Input parameter	Value
Left Data Points	Number of points to the left of the current data point.
Right Data Points	Number of points to the right of the current data point. This is usually set to the same value as the Left Data Points value.
Polynom Order	When using derivatives, you should set this value to 4 or higher.
Derivation Order	Allows you to calculate numerical derivatives. Setting this value to 1 gives a first order derivative.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

### Background theory

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  $\Delta$  and  $i = \dots -2, -1, 0, 1, 2, \dots$ . 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,

$$g_i = \sum_{n=-nL}^{nR} c_n \cdot f_{i+n} \quad (12)$$

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 the equation above with constant:

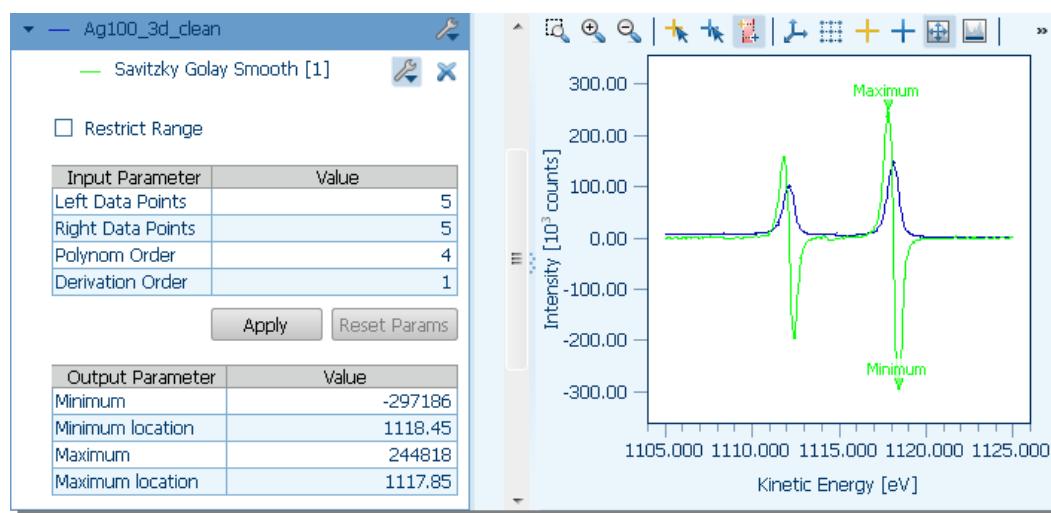
$$c = \frac{1}{nL + nR + 1} \quad (13)$$

If the underlying function is constant, or is changing linearly with time (increasing or decreasing), then no bias is introduced into the result.

The points at the right of the data point in the averaging interval are usually balanced by those at the left. 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  $c_n$  that preserve higher moments. SpecsLab Prodigy fits a polynomial of degree  $M$  in  $i$ , to the values  $f_i - nL \dots f_i + nR$ . For a more detailed description please refer to the paper by Savitzky and Golay.



#### 7.8.4 Smoothing Spline

The smoothing spline operation calculates an interpolating natural cubic spline curve which smooths 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 determine the degree of smoothing.

##### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.

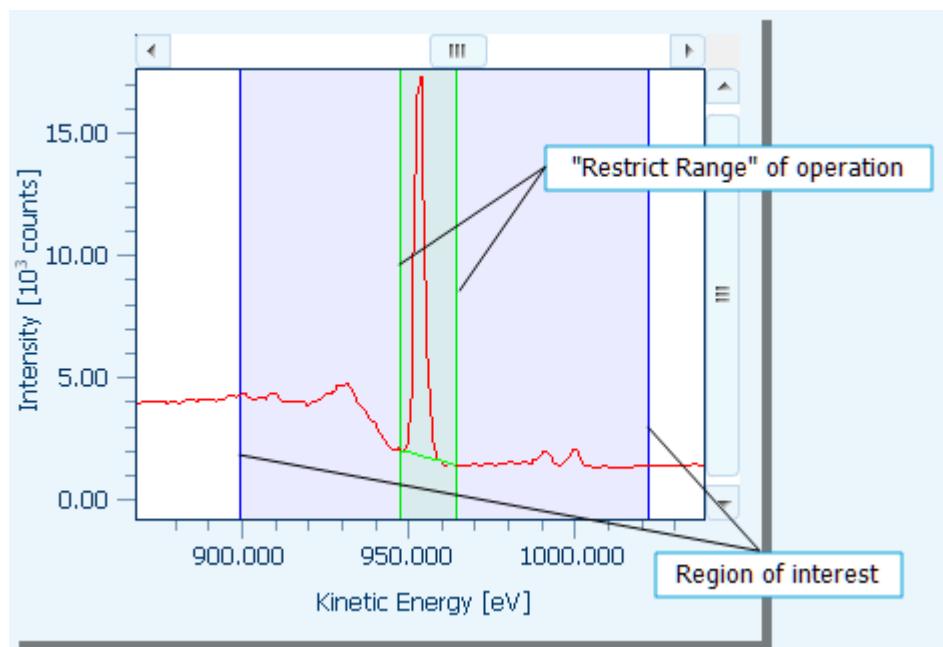
Restrict Range

1110.10 eV  to  1115.00 eV

- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.

### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Smoothing Factor	Enter the error variance. The calculation uses this to minimize an unbiased estimate of the true mean square error and thereby determines the degree of smoothing. If the error variance is not known, set this to -1. The routine minimizes the generalized cross validation to determine the degree of smoothing. This approaches the limit of min-

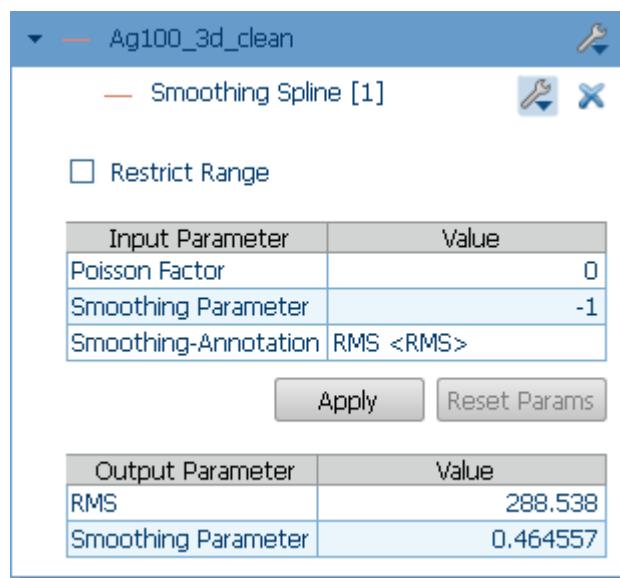
Input parameter	Value
	imizing the true mean square error.
Smoothing-Annotation	Defines the text shown in the plot—see " <a href="#">Annotation Syntax</a> " on page 89.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

The **Output Parameters** section contains the results of the operation:

- RMS—the root mean square of the signal.
- Poisson factor—The RMS value divided by the square root of the signal. For an ideal Poisson distribution, this will be exactly 1. Significant deviations from 1 (e.g. 1.5) may indicate errors in the way the detector counts the signal.



## 7.9 Miscellaneous Operations

The miscellaneous operations are a collection of other functions that do not fit in with other operations. Operations available are:

- [Arithmetic mean](#)—calculate the average value of points in a selected region.
- [Dead time correction](#)—compensate for the dead time in detector acquisition.
- [Least squares gradient](#)—calculates the gradient at each point in the spectrum using a first order least squares fit.
- [Linear operations](#)—add offsets and scaling factors to data.

- [Spin Asymmetry for VLEED](#)—calculate the spin component of a signal from a spin-resolved detector.

### 7.9.1 Arithmetic Mean

The arithmetic mean function sums the intensity of all data points and divides this figure by the number of data points. The result is the mean intensity of the data collected. You can restrict the range over which the mean is calculated.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

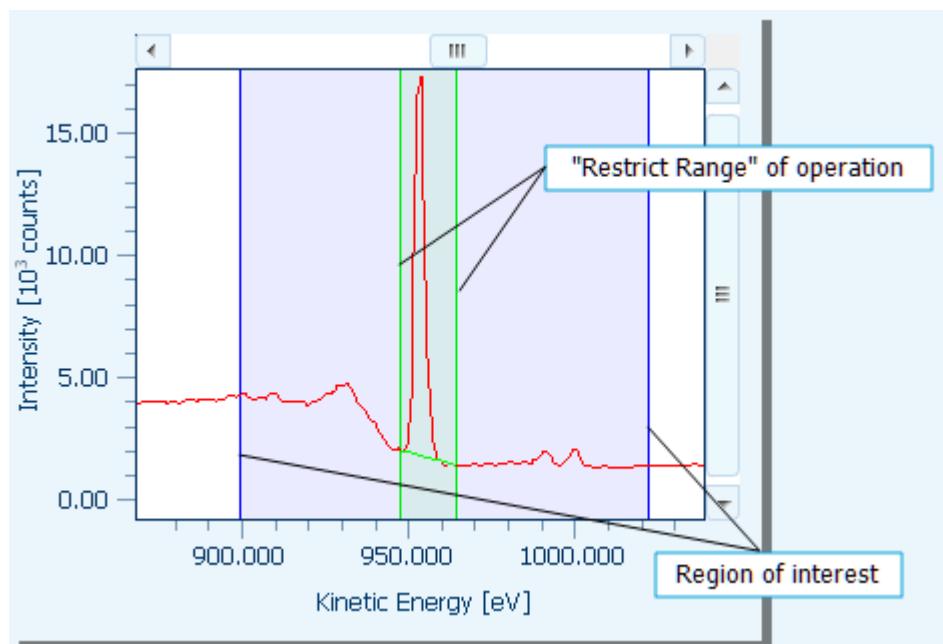
- Check the **Restrict Range** option box and enter start and end values in the fields provided. The operation will run again automatically in the specified range.



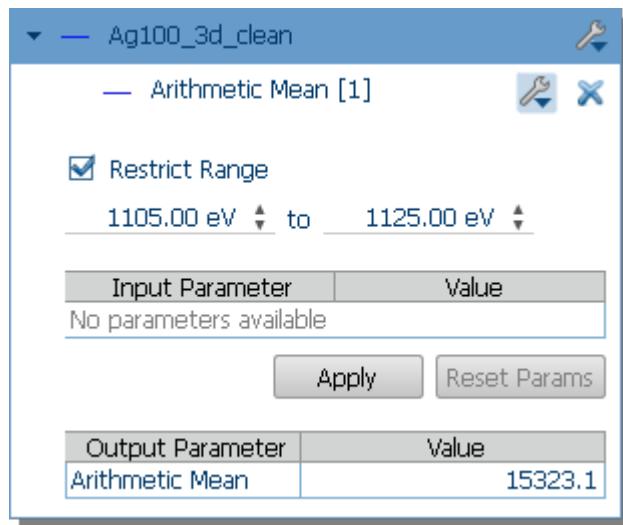
- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.



### 7.9.2 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

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

(14)

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Please see your detector manual for more information about dead time factors. The SPECS technical note "CEM Dynamic Range" also contains some details about the dead time.

You can restrict the range over which the operation is applied.

### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

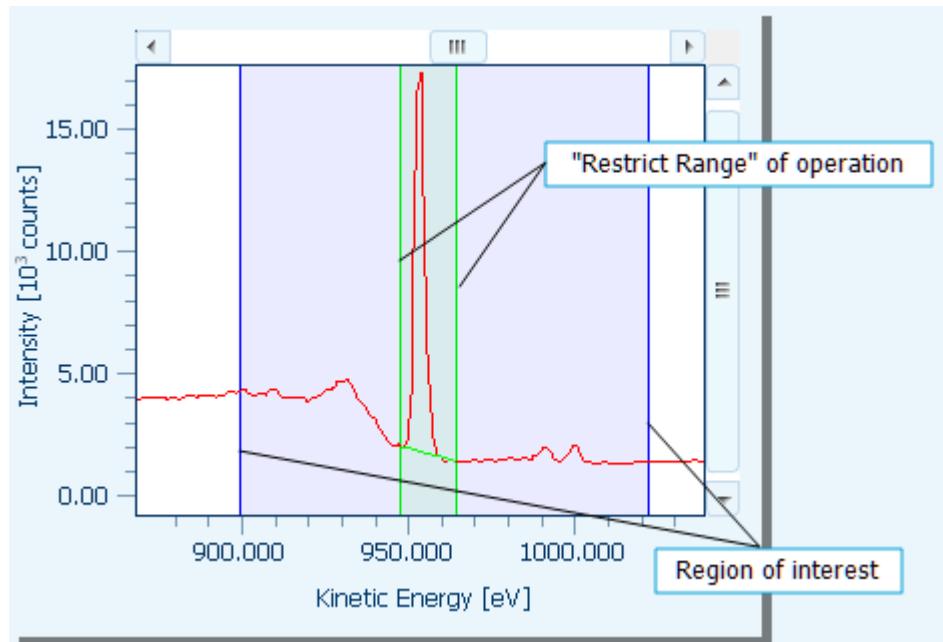
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



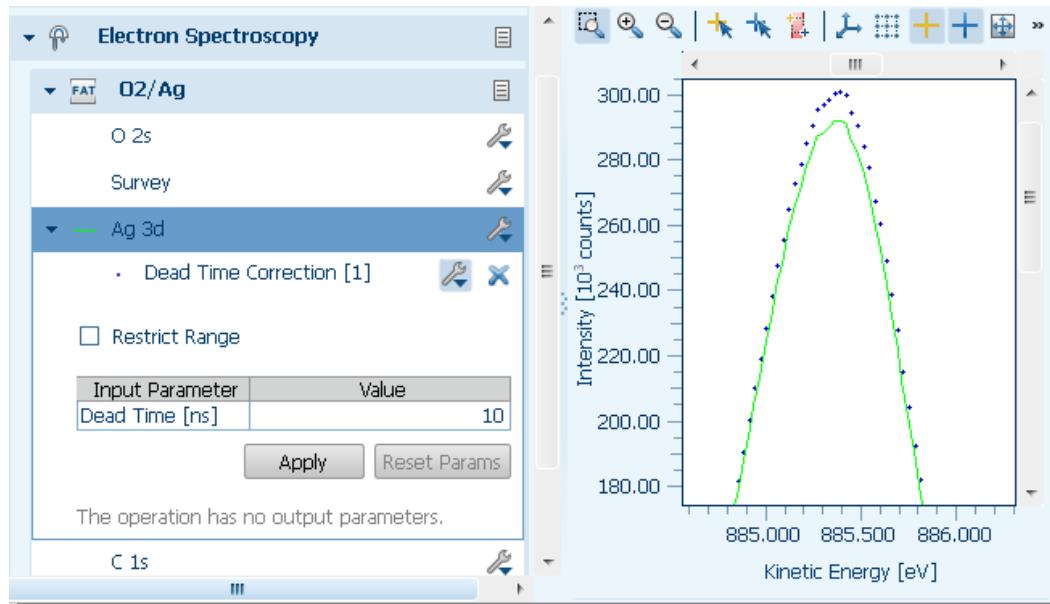
- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.



### 7.9.3 Least Squares Gradient

The least squares gradient function calculates the gradient of the spectrum at each point, based on a user-defined window size. The result is a derivative of the spectrum. This reduces

the noise level in the signal. Peak positions are then located at the zero point in the derivative curve.

### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

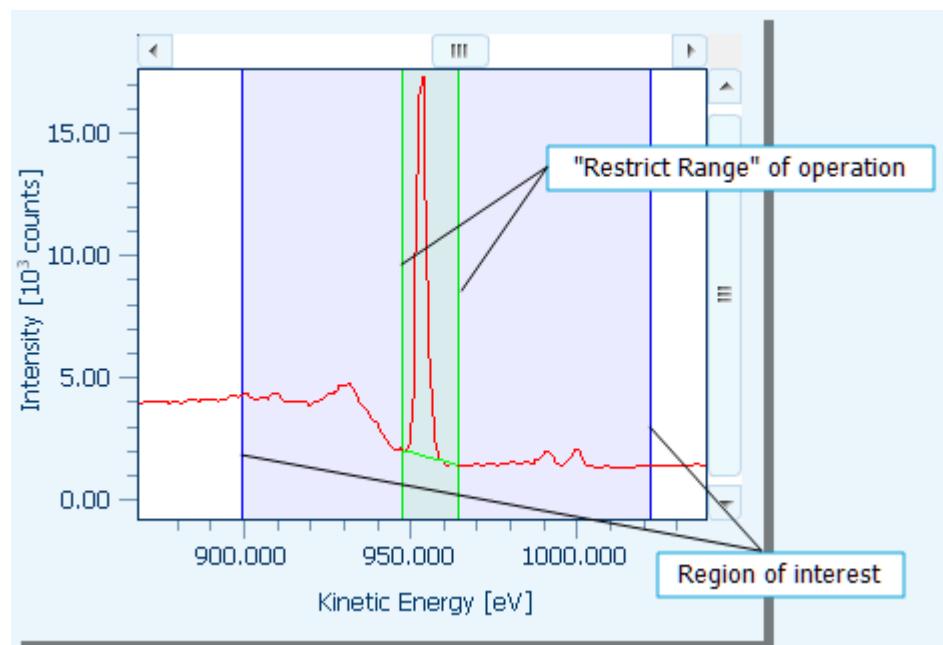
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and selecting a new color.



Unchecking this box will set the range to the whole spectrum.

### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Half Window Size	Half width of the sampling region in eV. See below for more information.

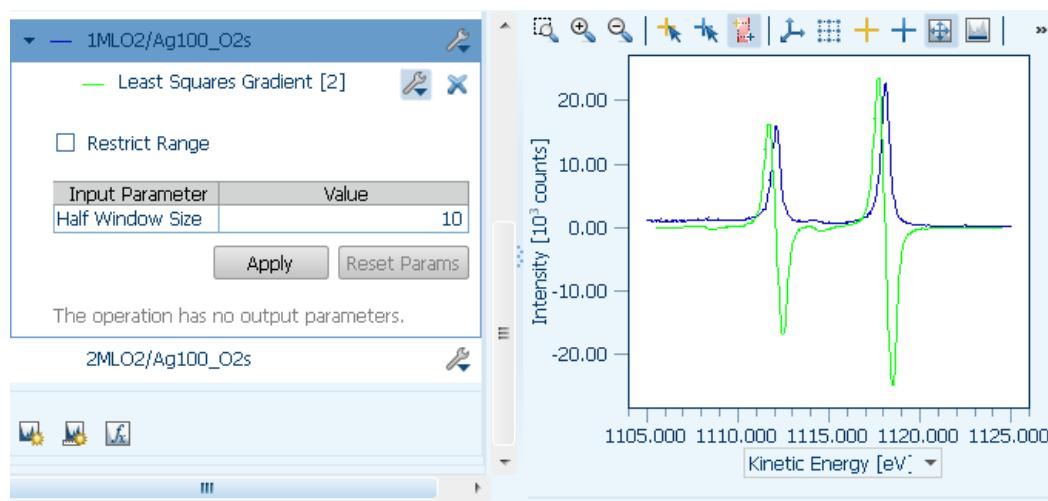
There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

The half window size determines the energy range used for the calculation:

$$\Delta E = E_i \pm \text{Half Window Size}$$

Where  $E_i$  is the current data point used in the calculation. A first order least squares fit is calculated using the data points in this energy region.



### 7.9.4 Linear Operations

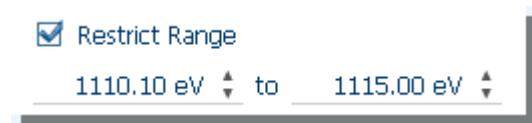
Using linear operations, you can scale and shift your data on the X and Y axes.

#### Restrict range

The operation runs with the selected region of interest. This region is shown in the **Restrict Range** section. If no region is selected, the operation runs on the whole spectrum.

You can change the region of interest using one of the following methods:

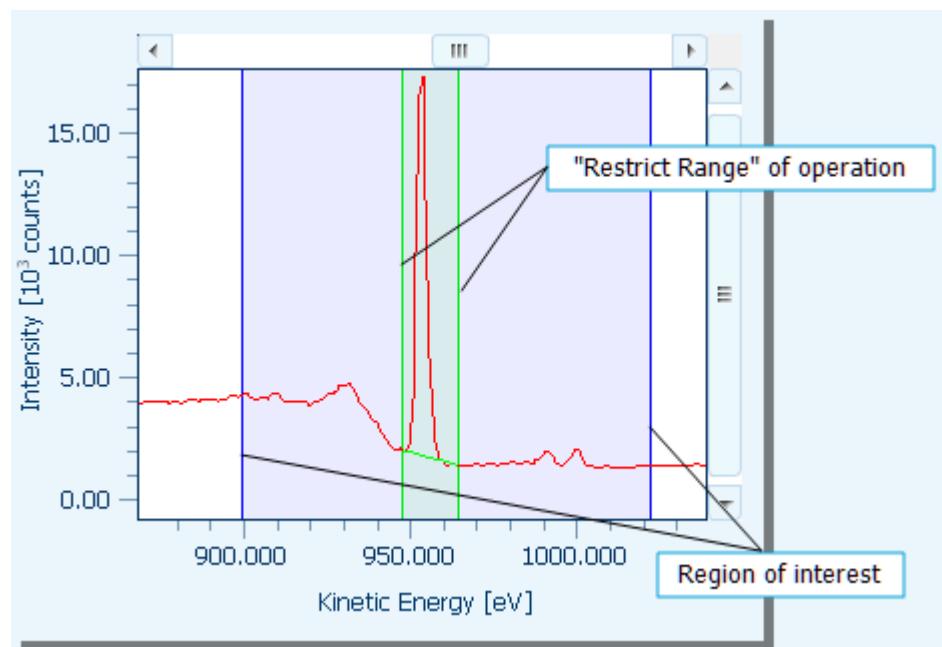
- Check the **Restrict Range** option box and enter start and end values in the fields provided.  
The operation will run again automatically in the specified range.



- Select the operation in the data browser, then drag the bars at the edge of the operation region. The screenshot below shows a range selected for a background subtraction operation.

#### Note

The shaded area has the same color as the operation. You can change this by clicking the line of the operation and [selecting a new color](#).



Unchecking this box will set the range to the whole spectrum.

#### Input parameters

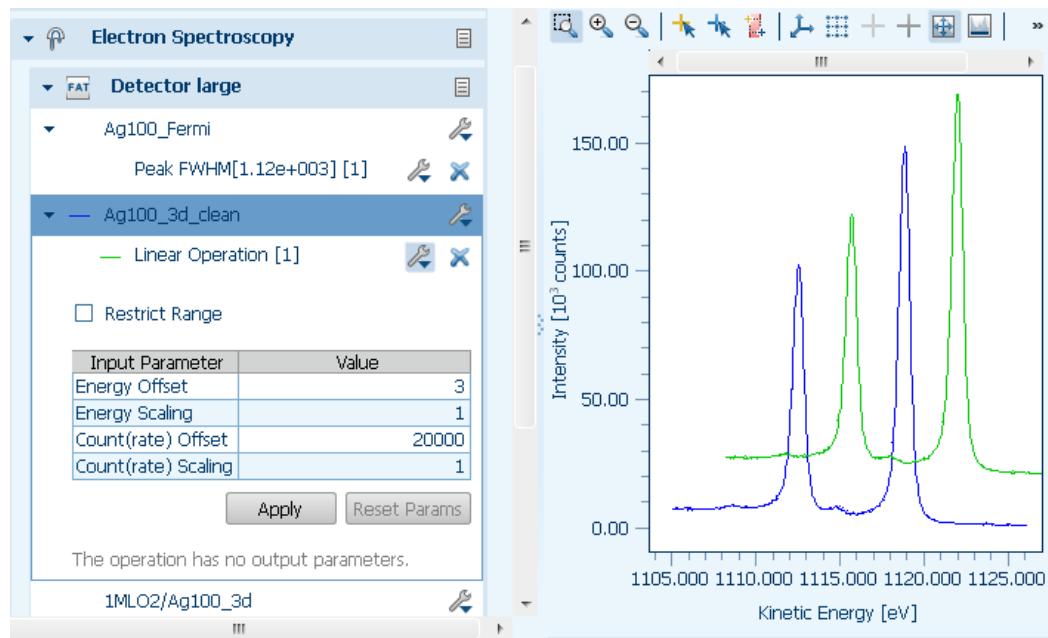
The input parameters allow you to alter the operation. The table below lists all the input parameters for the Peak Identification operation. After setting the parameters, click **Apply** to run the operation with the new settings.

Input parameter	Value
Energy Offset	Moves the spectrum (or the selected region) by the offset in eV, i.e. along the X axis.
Energy Scaling	Scales the spectrum (or the selected region) by the given factor in the horizontal direction.
Count(rate) Offset	Moves the spectrum (or the selected region) by the offset in counts or count rate, i.e. along the Y axis.
Count(rate) Scaling	Scales the spectrum (or the selected region) by the given factor in the vertical direction.

There are two buttons below the input parameter table:

- **Apply**—runs the operation with the selected input parameters.
- **Reset Params**—sets the input parameters to their default values.

There are no output parameters for this operation—the results are shown in the Plot View. The screenshot below shows a data set shifted in intensity and energy.



### 7.9.5 Spin Asymmetry for VLEED

The asymmetry operation evaluates the asymmetry of spin-resolved spectra and can only be used with spin detectors. If you have two spectra which are recorded with opposing spin directions (for example with different magnetizations or opposing collection geometry), you can derive the asymmetry function from the two signals according to the following relation:

$$A_1 = \frac{S_1 - S_2}{S_1 + S_2} \quad (15)$$

#### Schedule setup

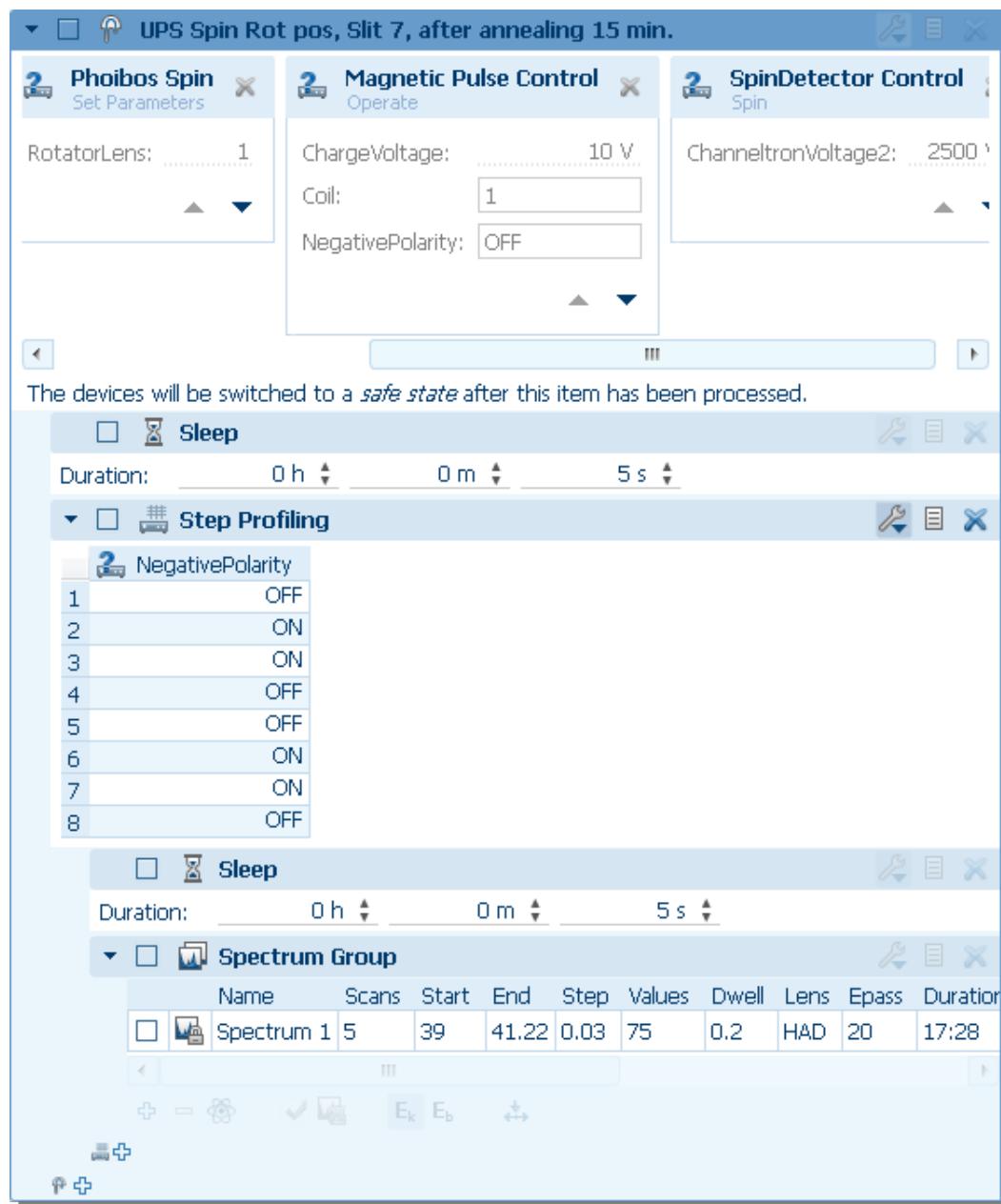
As well as requiring a special detector, the schedule setup is different from the standard data acquisition. This is necessary in order to allow for the magnetization cycles between measurements.

The screenshot below shows a typical schedule for acquiring spin resolved data. Note the following points:

- Devices: In addition to the analyzer and source, you need to include devices for the spin detector controller and the magnetic pulse control.
- Sleep: Provides a pause while the magnetic pulse control charges and magnetizes the spin target.
- Step Profile: Changes the target magnetization, with a spectrum measured at each setting.
- Sleep: Once again, this allows the magnetization to take place before the measurement starts.
- Spectrum Group: The normal definition for the spectrum.

#### Note

You can also include a Loop before the step profile to perform a number of iterations of the experiment.



### Input parameters

The input parameters allow you to alter the operation. The table below lists all the input parameters for the Spin Asymmetry for VLEED operation. After setting the parameters, click **Apply** to run the operation with the new settings.

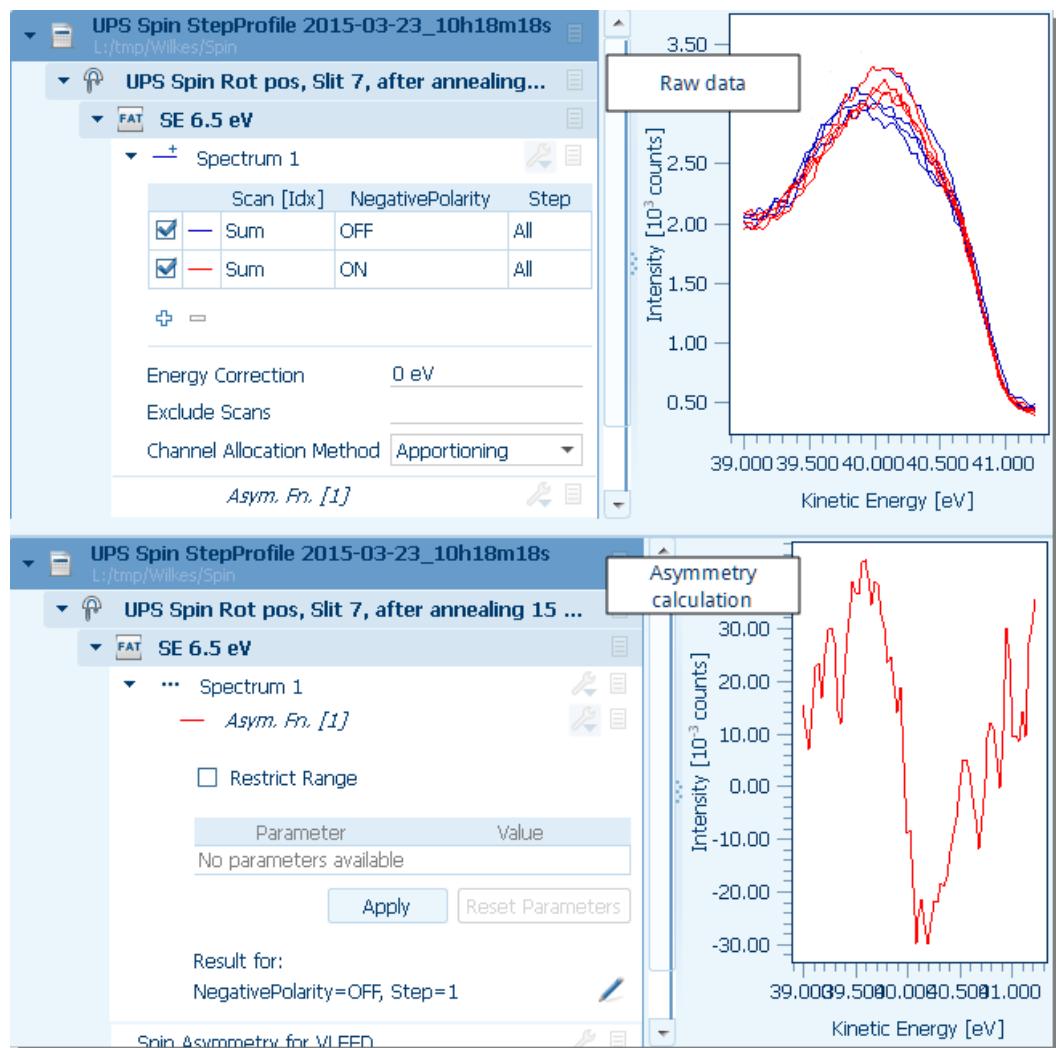
Input parameter	Value
Asymmetry Cycle	The name of the step profile used for the magnetization of

Input parameter	Value
	the target. This is the same as the name shown in the Experiment Editor.
Summation Cycle	You can leave this setting as "Loop". If a loop is used for a number of iterations of the experiment, this is taken into account. In the case of no loop being used, this section is ignored.
Asymmetry Cycles Size	This should be the number of cycles in the magnetization step profile that is included in the Experiment Editor.
Asymmetry Forward Direction	This parameter, together with Asymmetry Backward Direction, determines which scan measures positive spin and which negative. One parameter must be OFF, the other ON. If you change these values, the result of the calculation will be reflected around the horizontal axis.
Asymmetry Backward Direction	See Asymmetry Forward Direction above.

#### Output parameter

There is only one output parameter:

- **Use Summation Cycle**—This box is checked if a loop is used in the calculation.



## Chapter 7 – Chemical Databases

SpecsLab Prodigy has several databases which contain information about excitation levels of elements and compounds, AES excitations, electron mean free path values, etc. These are used for features such as peak identification. The Chemical Databases view allows you to [view](#) the information in the databases and also to [add your own](#) databases.

To open the Chemical Databases view:

- Select **Views/ Chemical Databases** from the menu bar.

### 7.10 Viewing Pre-Installed Databases

Pre-installed databases are supplied by SPECS and can be viewed. The table below provides an overview of the controls that are active for viewing databases.

Feature	Description
Database Type	A drop-down list showing all the databases available. This includes user-defined databases.
Filter	Filters the displayed entries according to the entered criterion. All fields in the displayed databases are used for matching.
Reload all Databases	Reloads all the databases.
Priorities	This pane shows all databases that contain data for the selected database type. You can order them by drag and drop or by using the ▲ and ▼ arrows. The order determines the priority of the database. Lower databases are only used if the value is not present in any higher databases.
	Toggles the availability of the database. Databases with a line through them are not used.
Table	The main area of the view, showing the entries in the database. You can sort the entries in the database by clicking the header of a column.
Export	Opens a dialog so that you can export the database as a csv file.
	Allows you to <a href="#">create a new database</a> .

The grayed out buttons below the table are used for [editing user databases](#) and cannot be used for the pre-installed databases.

	Atomic Symbol	Atomic Level	Atomic Number	BindingEnergy	Reference
1	Li	1s	3	55.6 eV	
2	Be	1s	4	111.8 eV	
3	B	1s	5	189.4 eV	
4	C	1s	6	284.5 eV	
5	N	1s	7	398.1 eV	
6	O	1s	8	531 eV	
7	O	2s	8	23 eV	
8	F	1s	9	684.9 eV	
9	F	2s	9	30 eV	
10	Ne	1s	10	863.1 eV	
11	Ne	2s	10	41 eV	

## 7.11 Creating and Editing User Databases

In order to protect the values in the pre-installed databases, they cannot be edited. However, you may need to supplement the databases with additional values or with corrections. You can create a database and edit its values. Note the following points:

- A database is in CSV format. Although it is not possible to import a database into SpecsLab Prodigy, you can create a new database and then edit its CSV file in a spreadsheet program.
- If you are correcting values in other databases, you should move your new database to the top of the priority list.

To create a new database:

1. Click . A dialog will appear for you to enter the name of your new database. The new database is added at the top of the **Priority** pane (that is, it has top priority—you can move it down if you wish).
2. Select the database in the **Priority** pane. The main area will be empty except for the name of the database and its location
3. Click **Edit Database**. The databases in the **Priority** pane will be grayed out.
4. Click . A new row is added to the table.
5. Enter values in the fields.
6. Click **Save**. Your values will be saved to the database.

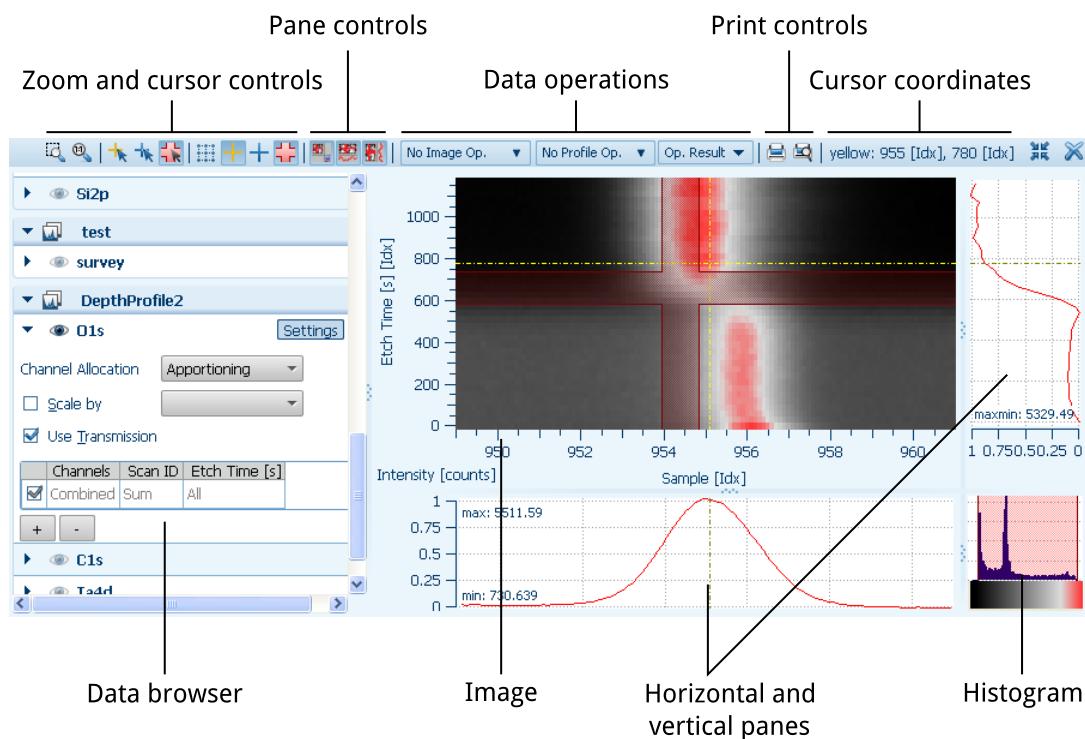
There are other controls below the table that are useful:

- removes the currently selected row.
- **Discard** removes all changes to the database and reverts to the last saved version.
- **Export** opens a dialog allowing you to save the contents of the database in csv format.

## Chapter 8 – Image View

The Image View displays two dimensional data. Frequently, this will be the energy and non-energy axes from a CCD camera or delayline detector. However, you can use the Y axis to display other information, such as etching time in a depth profile experiment.

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.



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](#).

## 8.1 Opening Data in the Image View

To open the Image View:

- Select **Views/ Image View** from the menu bar. The Image View will open, showing the currently selected spectrum. All other spectra will be shown in the legend—you can select a spectrum to view it individually.

The Image View can display data in two dimensions. If the spectrum contains more than two dimensions, the view requires user input to determine how the data is to be displayed. You can change the axis settings or change the data settings in the legend. Using a combination of the following two methods will allow you to display the data in exactly the way you want.

### Note

By comparison with the Plot View, multi-dimensional data is condensed into simple intensity vs energy. In that case, if you want to display additional dimensions on the Z axis, you first have to select which dimension is to be displayed.

### Data browser settings

The data browser is described in detail in "[Additional Data Display Settings](#)" on page 75—all information there also applies to the legend in the Image View. For the present purpose, it is worth focusing on the spectrum components, as shown in the figure below.

	Channels	Scan ID	Etch Time [s]
	Combined	Sum	All

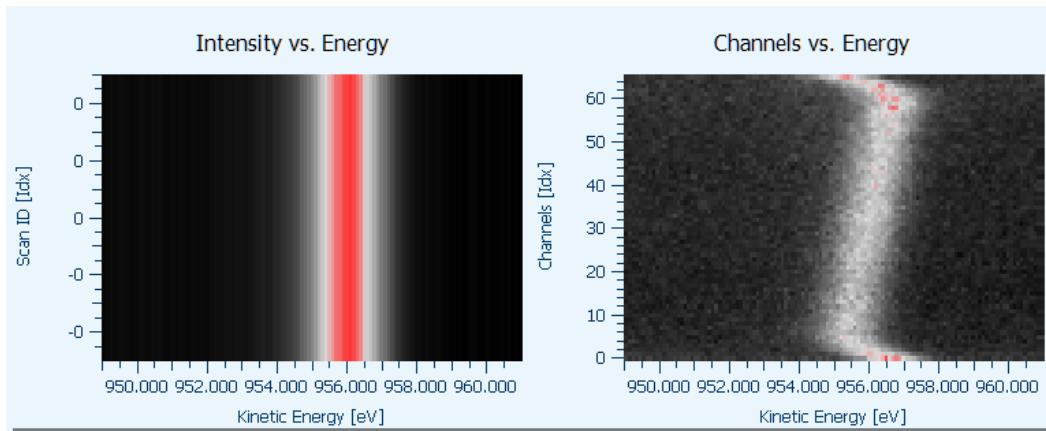
This example shows a depth profile experiment, where etch time can be used as an axis. To reduce the number of dimensions so that the spectrum can be displayed:

- Select an individual etch time from the drop-down list. The spectrum will then display intensity on the Y axis against energy on the X axis.

You can change the Y axis by selecting different spectrum components:

- Selecting **Separated** for **Channels** will put the channel number on the Y axis.
- Selecting **All** (or an individual scan number) for **Scan** will put the scan number on the Y axis.

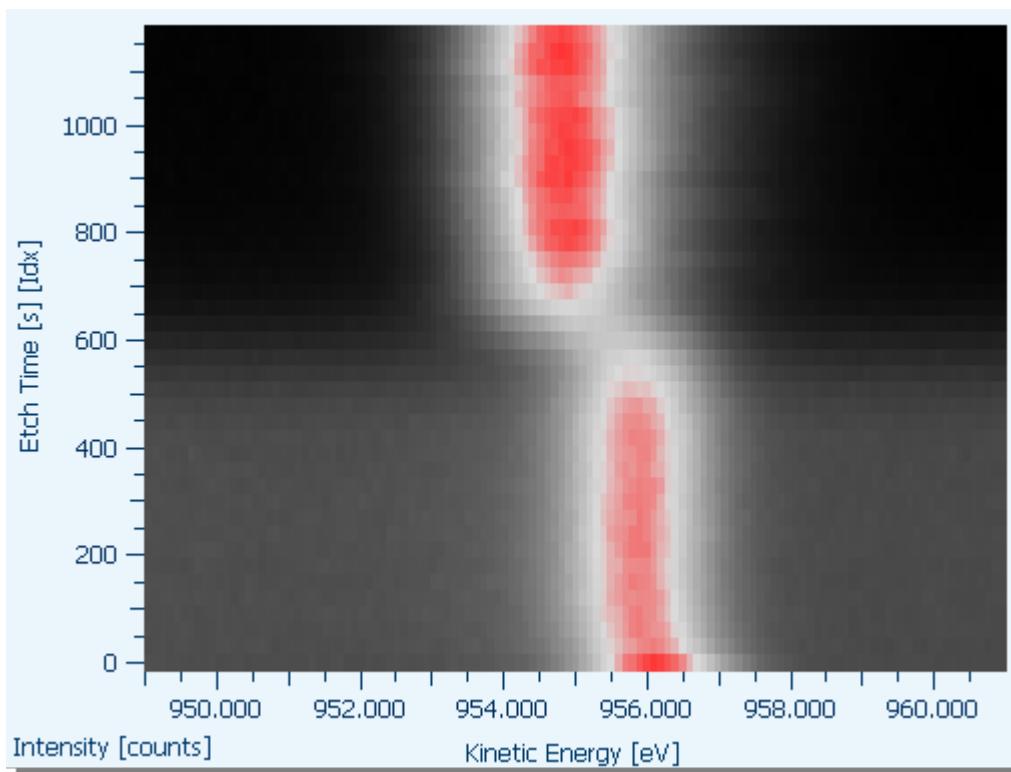
The images below show a comparison of different displays of the same data.



### Y axis label

The axis labels contain all available dimensions. You can therefore change the axis label to tell SpecsLab Prodigy how it should display data. For the above example, using a depth profile scan:

- Hover the mouse pointer over the Y axis label and select Etch Time from the drop-down list. The data will be displayed with the etch time on the Y axis.



## X axis label

The X axis always contains the options for showing kinetic energy and binding energy. Some types of experiment may also give you the option for changing the X axis setting. For example, in slab imaging scans, the X axis will give you the option of Focus Displacement so that you can show one of the profiling parameters on the X axis.

## 8.2 Image Pane

The main part of the Image view 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.

## 8.3 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).



There are handles on the edge of the pane bordering on the image. These allows you to resize the 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:

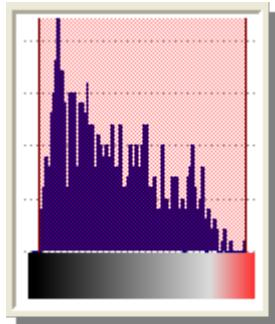
- Click the icon in the toolbar. The vertical profile pane and the histogram will be hidden.  
Click the icon again to show them.

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.

## 8.4 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.



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:

- 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.
- 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.

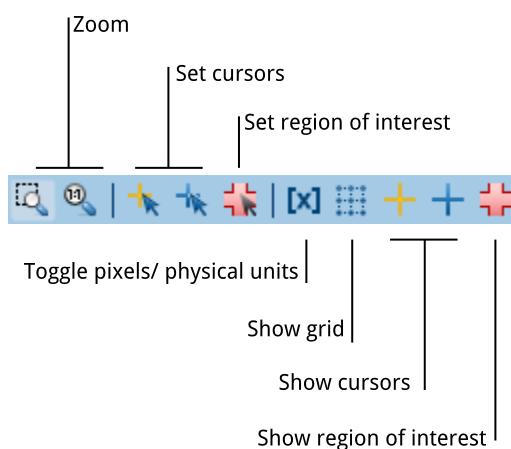
Right-clicking the histogram produces a context menu. The table below describes the actions available in the context menu.

Item	Description
<b>Copy Profile Data</b>	Copies the data in the histogram to the clipboard. The data depends on the <b>Intensities</b> setting in the <b>Histogram Ranges</b> dialog—using this setting, you can restrict the amount of data copied to the clipboard.
<b>Histogram Ranges</b>	Opens the <b>Histogram Ranges</b> dialog. In this dialog, you can: <ul style="list-style-type: none"><li>Set which intensities are displayed in the histogram. With user defined values, the histogram is redrawn so that only the intensities</li></ul>

Item	Description
	selected are displayed. This does not affect the appearance of the data in the main view. <ul style="list-style-type: none"> <li>Set the sampling rate for the intensities. A lower number of samples increases the peak height in the histogram, while also increasing the granularity.</li> </ul>
<b>Color Transformation Range</b>	The sub context menu contains the following items: <ul style="list-style-type: none"> <li><b>Autoscale</b>—Cancels any range selected in the histogram so that all colors are displayed in the viewer.</li> <li><b>User Defined</b>—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.</li> </ul>
<b>Change Colormap</b>	The sub context menu contains a number of different color schemes that you can select to view the data.
<b>Use Zoomed Area</b>	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.
<b>Enable Histogram</b>	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.

## 8.5 Cursor and Zoom Controls

You can change the zoom and cursor settings, as well as toggling the grid. The picture below has an overview of the controls available. Each of these are described in their own section.



### 8.5.1 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.

### 8.5.2 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.

### 8.5.3 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.

#### 8.5.4 Toggling between Pixels and Physical Units

Clicking the  in the toolbar of the Image View toggles the units of the display:

- Camera pixels.
- Physical units, e.g. mm or degrees, depending on the mode of acquisition.

#### 8.5.5 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.

### 8.6 Performing Operations in the Image View

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.



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

#### Image operations

Operation	Description
<b>No Operation</b>	None of the calculations in the drop-down list are performed.
<b>Center/ Integral</b>	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.
<b>X Line Fit</b>	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.

Operation	Description
<b>Y Line Fit</b>	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.

### Profile operations

Operation	Description
<b>No Operation</b>	None of the calculations in the drop-down list are performed.
<b>Gauss</b>	Fits a Gaussian profile to the selected region in the horizontal and vertical profile panes. The calculation reports the center position 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 <b>Show Physical Units</b> from the image context menu for meaningful results
<b>Fermi Edge</b>	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 <b>Show Physical Units</b> from the image context menu for meaningful results

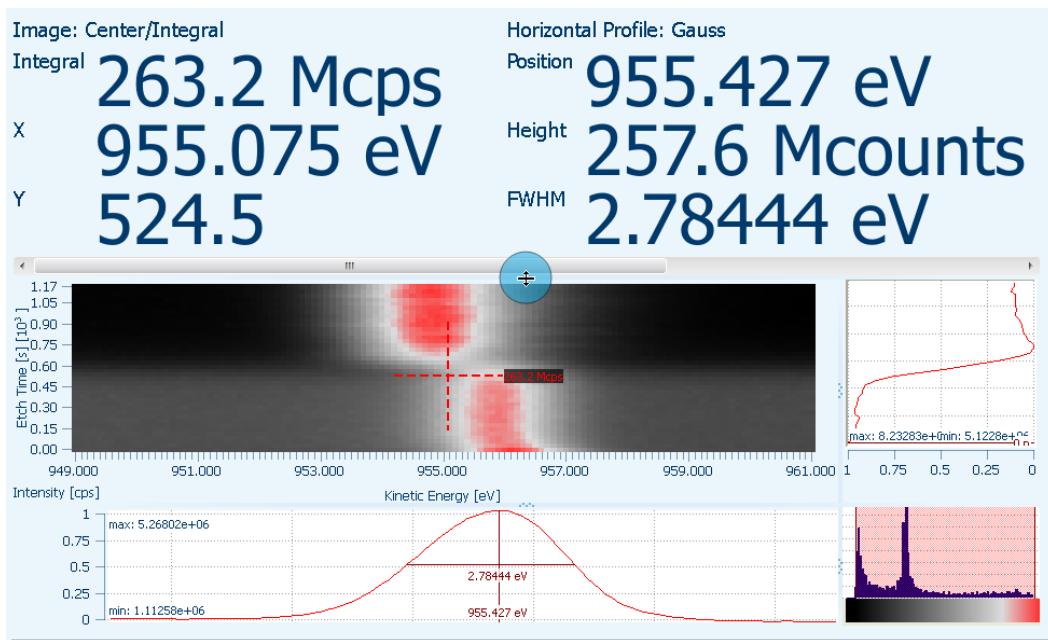
### Displaying operation results

You can display the results in large text, so they can be seen at a distance. Results from all operations are shown:

- Grab the horizontal split bar at the top of the image and drag it down.

### Note

If the view is not wide enough to see all results, a scroll bar is included.



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## Chapter 9 – Live View

The Live View allows you to view the signal received by the detector in real time. This is primarily of interest for 2D detectors which record an image. The Live View is generally used for the following purposes:

- Viewing a 2D image while setting up the analyzer, e.g. for angular dependence calibration.
- Checking the mapping area of the detector.
- Viewing the image during data acquisition.

The Live View also allows you to check for [hot pixels](#) in the camera.

This chapter is divided into the following topics:

- [Viewing an image](#) in the Live View.
- [Available features](#) in the Live View.
- [Active area and channels](#).

### 9.1 Opening the Live View

The Live View displays regular updates of the data whenever the detector is in operation. This means that you can watch live images during regular data acquisition by simply opening the Live View from the **Views** menu.

A common use for the Live View is to see the image as you change analyzer parameters. In this case, you can use the Live View in conjunction with the analyzer Device Control, as described below.

#### Note

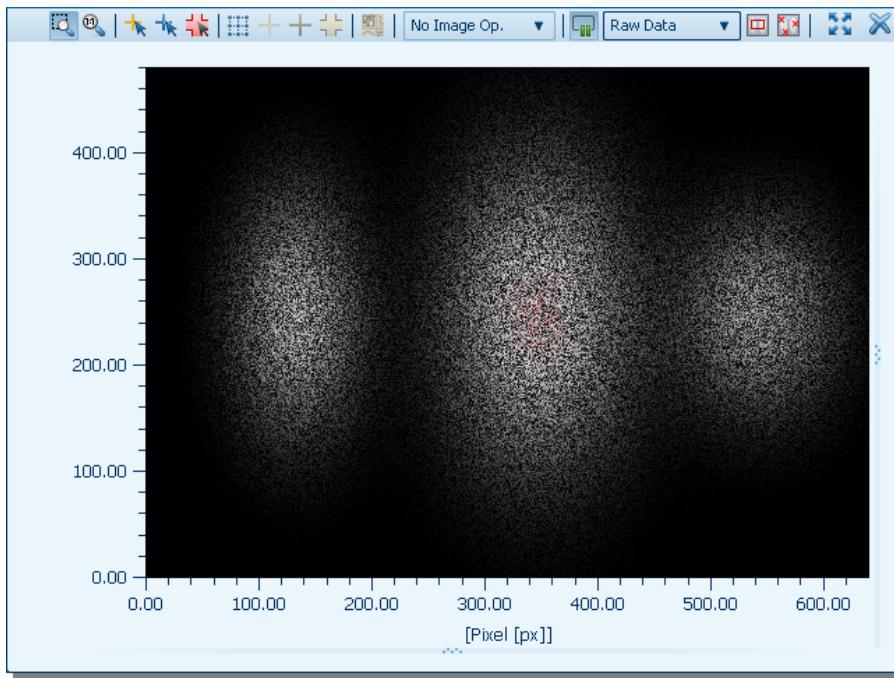
The refresh rate of the image in the Live View is 1 s.

To obtain an image in the Live View:

1. Locate the analyzer control in the Device Control View.
2. Click **Control** to connect to the analyzer. If you have already been using the analyzer for experiments, it will already be connected.
3. Edit the analyzer settings as required. For setting up the analyzer, it is normal to set the kinetic energy and pass energy to the same value.



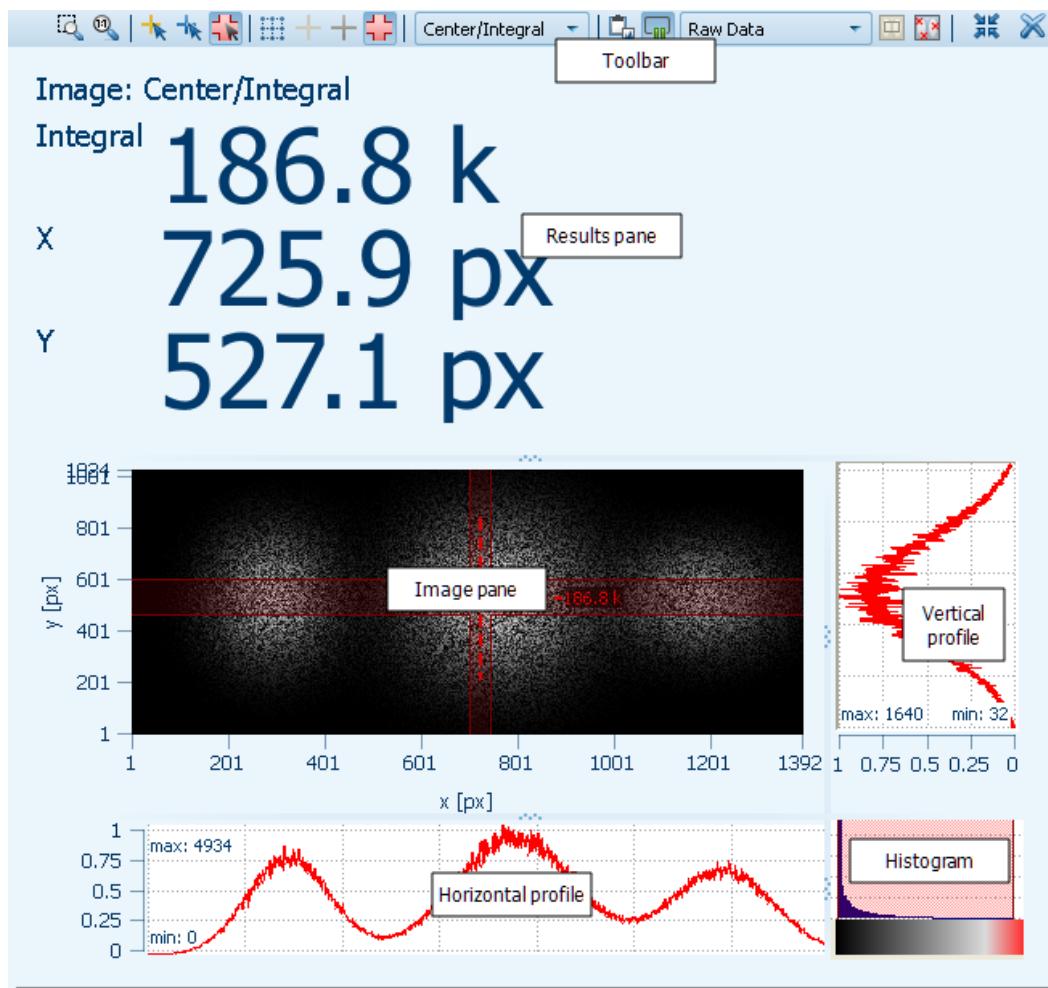
4. Click **Activate** to send the operating values to the analyzer.
5. Select **Views/ Live View** from the menu bar to open the Live View
6. Click in the toolbar to start viewing the image.



## 9.2 Features and Options in the Live View

Visually, the Live View is very similar to the Image View and it shares a lot of functionality. The table below lists the features and explains their operation.

You can hide or display the various panes in the view by grabbing the horizontal and vertical split bars and dragging them.



Feature	Description
	Zoom controls. See " <a href="#">Zooming in the 2D Viewer</a> " on page 141
	Cursor controls. See " <a href="#">Setting Cursor Positions</a> " on page 141
	Grid. See " <a href="#">Displaying the Grid in the 2D Viewer</a> " on page 142
	Region of interest controls. See " <a href="#">Selecting a Region of Interest (ROI)</a> " on page 141.
	Toggle display of traces in horizontal and vertical profiles.
Operation menu (default: No Image Op.)	Drop-down list for image operations. See " <a href="#">Performing Operations in the Image View</a> " on page 142.
	Start/ stop live image view.
Raw Data	Allows you to select between raw data and channel data views. Described fully in " <a href="#">Active Area and Channels</a> " on page 148.

Feature	Description
	Toggles the display of the active area.
	Opens the Calculate Hot Pixel dialog. See <a href="#">"Removing Hot Pixels" on page 150</a> .
Results pane	Shows the results of the operation in large text for easy reading at a distance. See also <a href="#">Performing Operations in the 2D Viewer</a> .
Image pane	Displays the live image. Right-clicking this area opens a context menu—see <a href="#">"Image Pane" on page 138</a> for a description.
Horizontal/ vertical profiles	Shows a cross section of the data signal when a region of interest is selected. See <a href="#">"Horizontal and Vertical Profiles" on page 138</a> .
Histogram	Shows the color distribution in the image. See <a href="#">"Histogram" on page 139</a> .

### 9.3 Active Area and Channels

The active area is the area of the image recorded during data acquisition. In order to maximize the signal from the detector, you should set the active area as large as possible. However, the image is circular, so you need to set the largest area within the circle, so that all channels have equal weight.

Data is recorded in channels rather than as raw pixels. The number of pixels is divided exactly by the number of channels defined, and the signal summed over these pixels. Although this reduces the resolution of the image, the noise is also reduced.

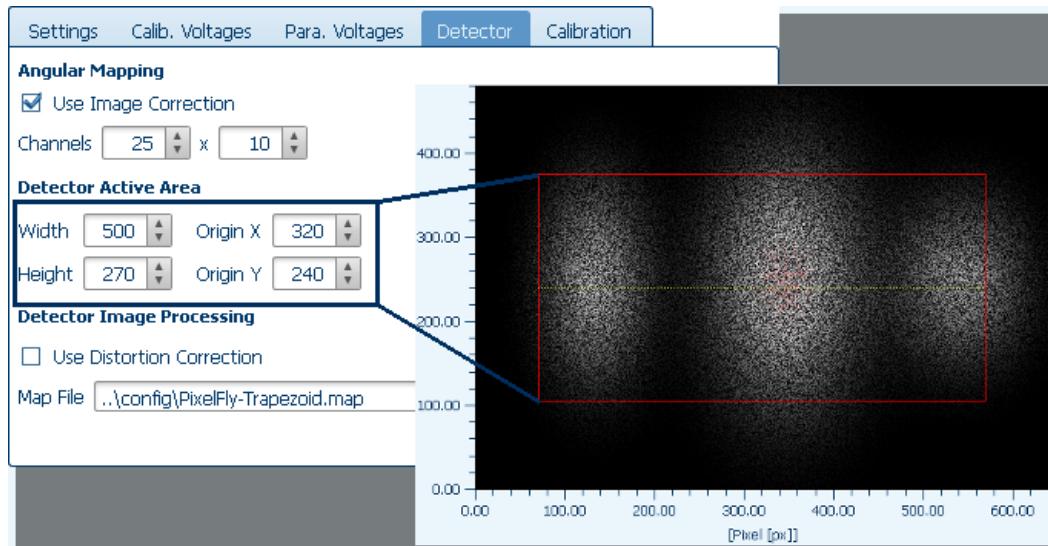
#### Viewing the active area

To view the active area:

- Click the icon in the Live View. The active area is shown in the image.

The active area is set in the Device Control:

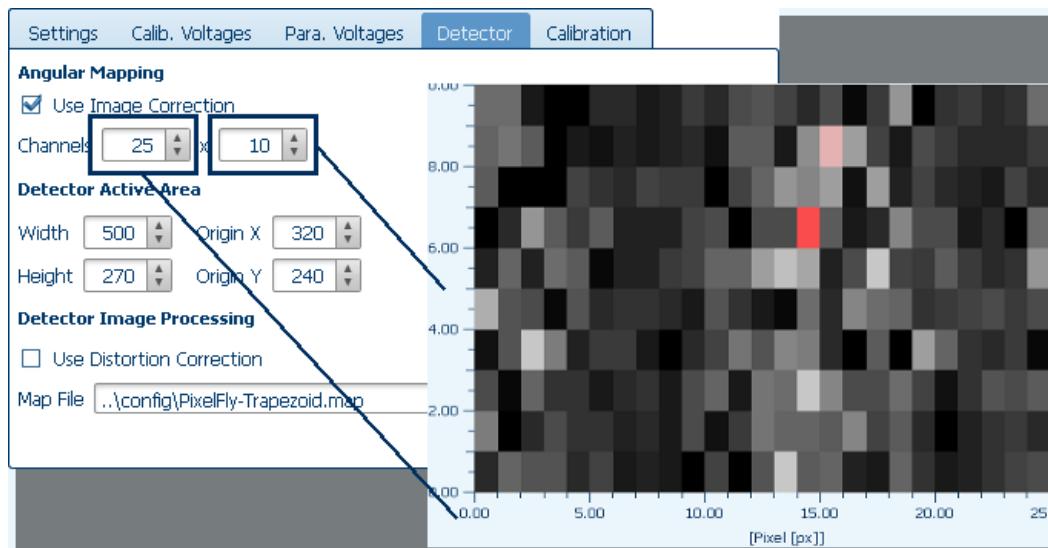
- Click the ▼ arrow in the analyzer device control to show more settings, then select the Detector tab. The picture below shows how the settings relate to the image.



### Viewing channels

To view the channels:

- Click the **Raw Data** button and select **Channel Data**. The image then shows the image within the active area. The pixels in the raw data view are summed together into channels, as shown in the picture below.



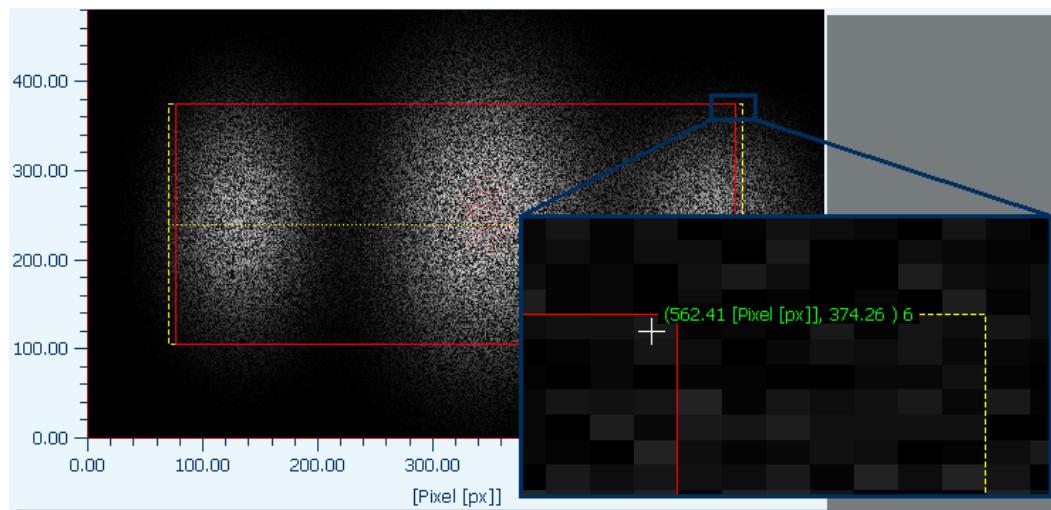
### Incorrect channel settings and pixel coordinates

The number of channels must divide exactly into the number of pixels. If not, pixels at the edge of the image will not be measured because there are not enough to form a complete channel.

If you set a channel number that does not divide exactly into the pixel number, a warning message will appear. By showing the active area, you can see the discrepancy caused by an incorrect channel number:

- The red area is the active area. All data within this area is recorded.
- The dotted yellow area is the area defined by the channel number. These channels are not recorded during data acquisition.

By zooming into the area, you can see the pixel coordinates (with current intensity).



### Changing detector settings

You cannot change detector settings while it is in operation. To change settings:

1. Click **Stop** to switch off the detector.
2. Make the desired changes.
3. Click **Apply and Save**.

You need to disconnect and reconnect the analyzer Device Control to see the effect of the changes.

#### Note

See also the PHOIBOS Device Control for more information about detector settings.

## 9.4 Removing Hot Pixels

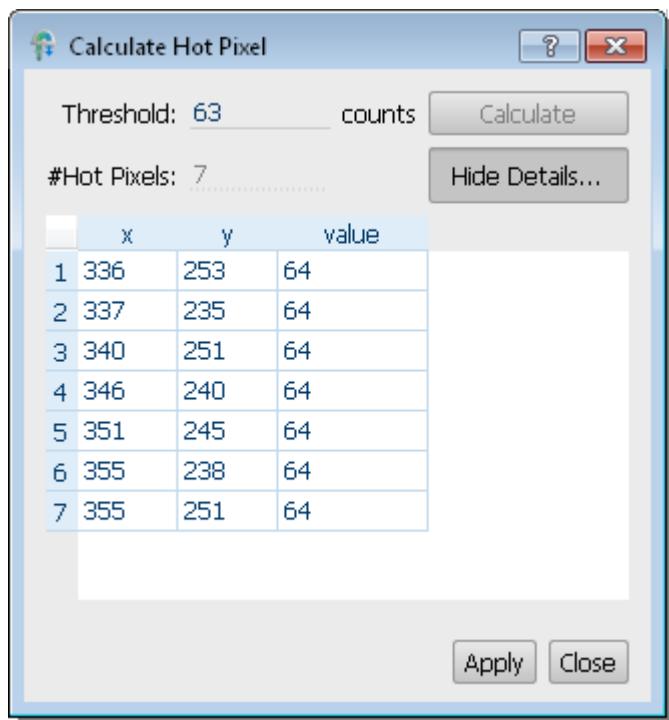
Hot pixels are individual pixels on the CCD with higher intensity than their surrounding area. They can appear as small pixel sized bright points of light on longer exposures. You can configure SpecsLab Prodigy to ignore hot pixels—the pixels are not displayed or recorded.

**Note**

This procedure involves manually editing the MS Windows 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. Click the  icon in the toolbar of the Live View.. 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.



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\Wow6432Node\SPECS\SpecsLab Prodigy\Devices\PhoibosND\Configuration\Detector\ImageProcessing*.

9. Double-click the *HotPixelList* key.
10. 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),...

11. Click **OK** and close the registry editor. The hot pixels will now be ignored by SpecsLab Prodigy when acquiring data.
12. Restart the PHOIBOS Device Control (disconnect the analyzer in the Device Control, then click **Control** to reestablish the connection) to make sure the changes are accepted.

## Chapter 10 – Live Parameter View

The Live Parameter View displays the current value of user-specified device parameters. Most operating parameters of installed equipment are available and you can select which ones to view depending on your current activity.

### Note

Detector and analyzer parameters (e.g. data signal) cannot be observed using the Live Data View. The Live View and data acquisition procedures are intended for use with detectors and analyzers.

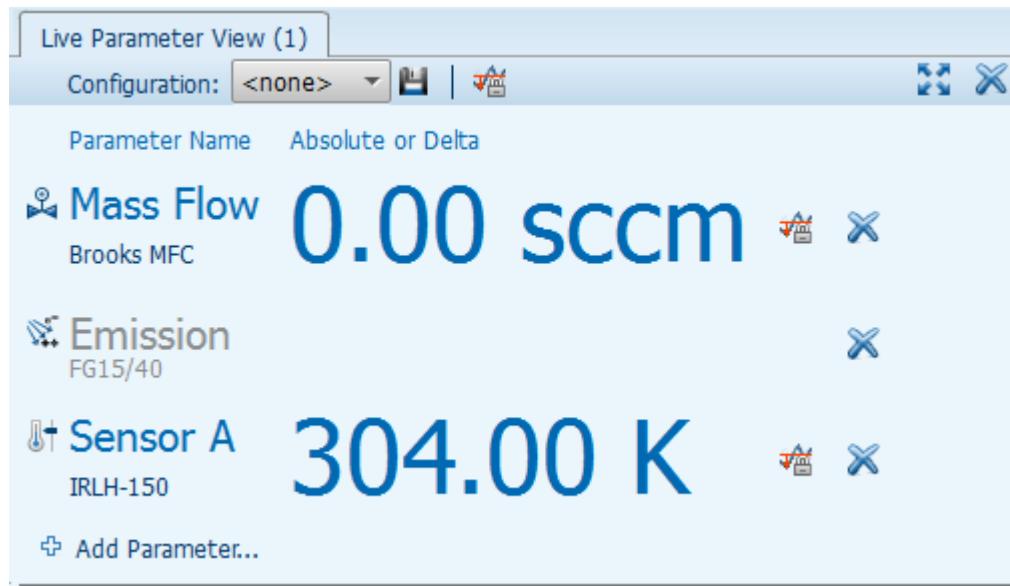
Parameter values are displayed in a large font, allowing you to read them from a distance. You can therefore make adjustments on the chamber while reading the current instrument parameters on the computer screen.

To open the Live Parameter Data View:

- Select **Views/ Live Parameter View** from the toolbar. The view will open at the bottom of the main window. You can move this to a [new position](#) as desired.

The following procedures and features are available:

- [Selecting parameters](#) for display.
- Changing the [mode of display](#).



## 10.1 Selecting Parameters

No parameters are selected when you open the Live Parameter View. You can add parameters individually or by loading a configuration. You can also remove any parameters from the view.

### Note

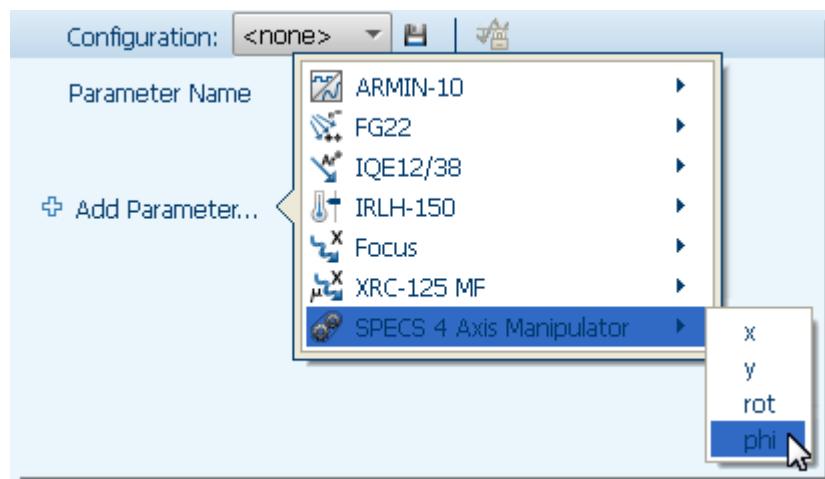
Parameters are grayed out if the device is not connected. In this case, go to the Device Control for the instrument and connect it.

### Adding parameters to the Live Parameter View

To add parameters:

1. Click the **Add Parameter** button. A menu showing all installed equipment will appear.
2. Move the mouse pointer to an item of equipment. A submenu will appear showing all available operating parameters for the equipment.
3. Select a parameter. The parameter will now be listed in the left side of the view. This is regularly updated.

You can select a number of parameters, each of which will be shown separately.



### Saving configurations

You can save the configuration (i.e. which parameters are selected for display, not their values). This allows you to easily display a group of parameters for a particular purpose.

To save a configuration:

1. Click the icon next to the drop-down menu. A **Save** dialog will open.



2. Enter a name for your configuration. This will be saved with a .cfg extension in the *settings\ParameterLiveView* directory of the installation folder.

### Loading configurations

You can recall a saved configuration:

- Click the drop-down menu and select a configuration from the list.



### Removing parameters

You can remove parameters from the Live Data View:

- Click the icon next to the parameter. The parameter is removed from the view.

## 10.2 Viewing Live Parameters

The Live Parameter View shows the current value of selected parameters in a large, easy to read font. The default setting for parameters is to show the absolute value. For each or all parameters, you can display a reference value and the delta (difference) from the reference:

1. Set the parameter to a base value that is to be used for comparison.
2. Click . The reference value will be "frozen" in the left column. The right column will now show the delta (difference) from the reference.

To set all parameters to reference and delta values:

- Click in the toolbar.

When one or more reference value is selected, two columns of numbers are displayed. The number in the right column changes as you make adjustments. Since there may be a mixture of absolute and delta values, you need to know how to identify the type of value:

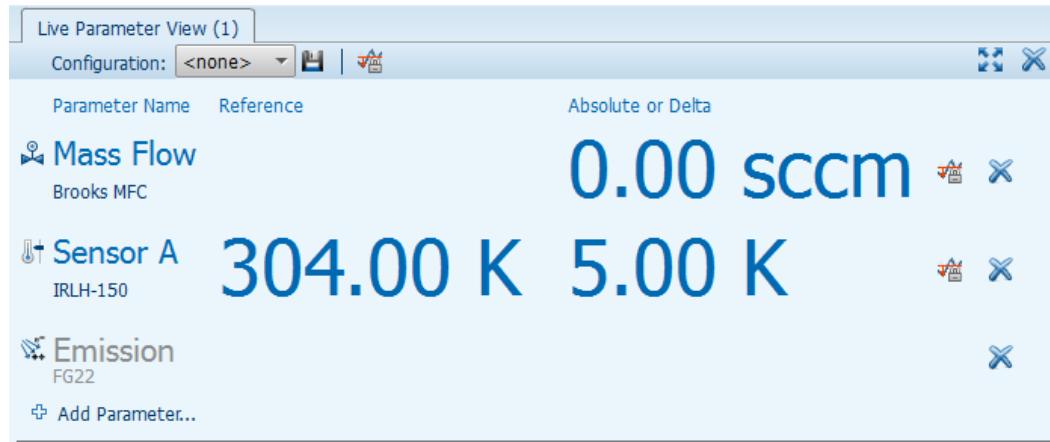
- If only one value is shown, it is the absolute value.
- If two values are shown, the left value is the reference value; the right is the delta.

### Example

The screenshot below shows three parameters:

- Mass Flow: Only one value is shown, so this is the absolute value.
- Sensor A: Two values are shown. The left is the reference, the right is the delta from the reference.

- Emission: This is grayed out and no values are shown. The device (FG 22 flood gun) is not connected.



---

## Chapter 11 – Live Data View

The Live Data View displays the variation of [selected parameters](#) over time. You can [save](#) the data for later examination in the [Data History View](#). Most operating parameters of installed equipment are available, although some of these parameters are not of interest for data recording.

### Note

Detector and analyzer parameters (e.g. data signal) cannot be observed using the Live Data View. The Live View and data acquisition procedures are intended for use with detectors and analyzers.

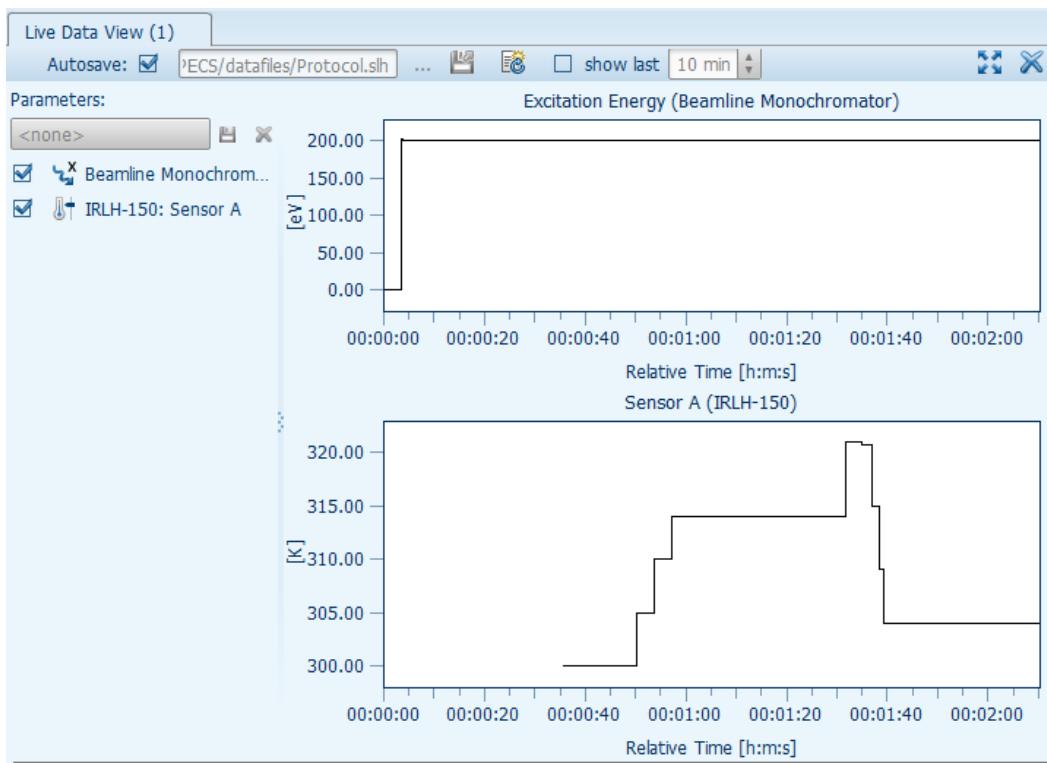
You can adapt the selection of parameters and according to your experimental requirements, e.g. monitoring the pressure during bakeout, producing a record of automated processes or recording equipment parameters during measurements.

To open the Live Data View:

- Select **Views/ Live Data View** from the toolbar. The view will open at the bottom of the main window. You can move this to a [new position](#) as desired.

The following procedures and features are available:

- [Selecting parameters.](#)
- [Viewing options.](#)
- [Saving data.](#)
- [Clearing data.](#)



## 11.1 Selecting Parameters

No parameters are selected when you open the Live Data View. You can add parameters individually or by loading a configuration from a template. You can also remove any parameters from the view.

### Note

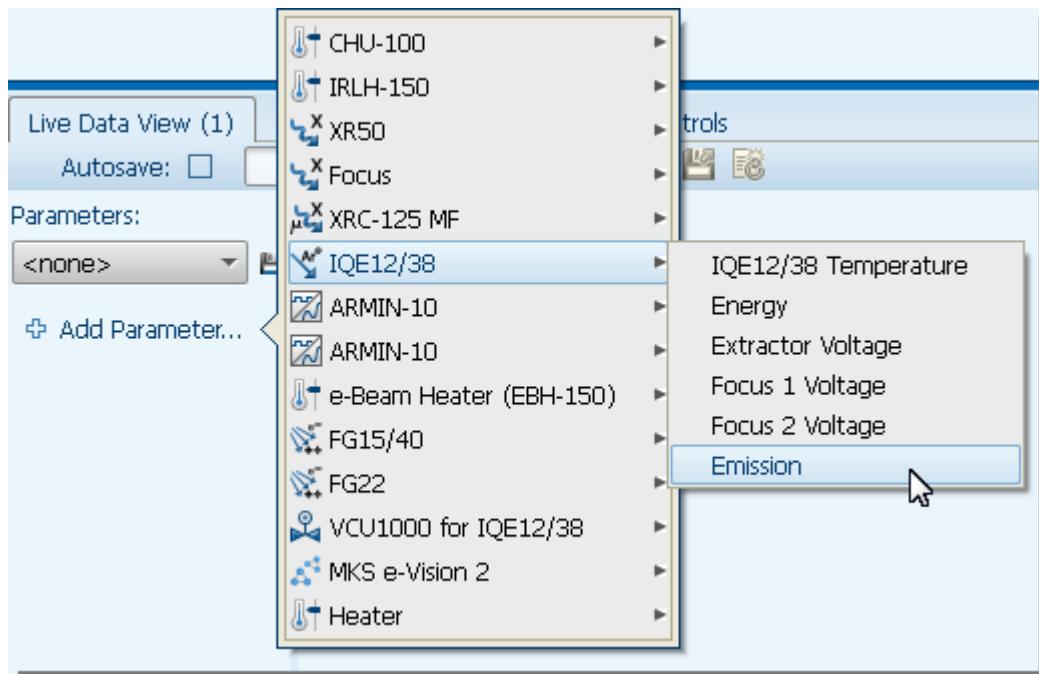
If no data is displayed after selecting a parameter, the device is probably not connected. In this case, go to the Device Control for the instrument and connect it.

### Adding parameters to the Live Data View

To add parameters:

1. Click the **Add Parameter** button. A menu showing all installed equipment will appear.
2. Move the mouse pointer to an item of equipment. A submenu will appear showing all available operating parameters for the equipment.
3. Select a parameter. The parameter will now be listed. A plot will also appear in the view showing the status of the parameter. This is regularly updated.

You can select a number of parameters, each of which will be shown in its own plot.



### Saving configurations

You can save the configuration (i.e. which parameters are selected for display, not their values):

1. Click the icon next to the drop-down menu. A **Save** dialog will open.

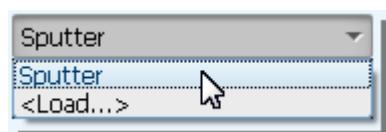


2. Enter a name for your configuration. This will be saved with a .cfg extension in the *settings\LiveData* directory of the installation folder.

### Loading configurations

You can recall a saved configuration:

- Click the drop-down menu and select a configuration from the list. Live updates for all parameters in the configuration will start.



### Removing parameters

You can remove parameters from the Live Data View:

- Click the  icon next to the parameter. The parameter is removed from the list and its data window closed. Updating for this parameter will stop and no more data will be logged.

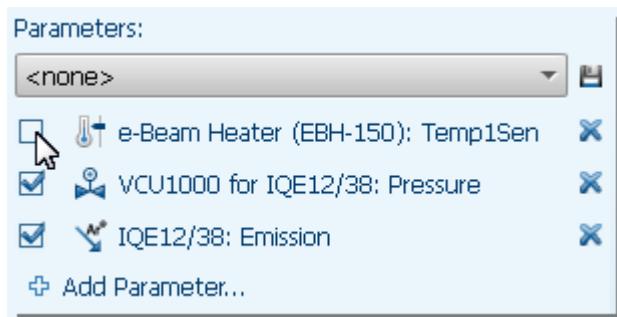
## 11.2 Viewing Live Data

The data for each parameter is shown in its own data window.

### Toggle parameter visibility

When you select a parameter, a data window is automatically displayed. You can toggle the visibility of each parameter:

- Click the check box next to the parameter. When ticked, a data window showing the live data is shown. When empty, the data window is not displayed, but the data is still updated for the parameter and written to a log file, if Autosave is selected.



### Changing the time axis setting

By clicking the time axis label, you can change the way the time is displayed:

- **Relative time:** Time relative to the start of reading data in the Live Data View, i.e. after the first parameter was selected or after data was cleared.
- **Universal Time:** The system clock time in UTC.
- **Local time:** The system clock time with local settings.

### Displaying most recent data

You can restrict the time axis so that it only displays recent data:

1. Check the show last box. The time axes of all data windows will be set to show a 10 min (default setting) time period.
2. Enter a new time in minutes or use the up/ down arrows to adjust the time range.



### Zoom

You can zoom into areas in the data windows:

- Click and drag the mouse to form a rectangle in one of the data windows. When you release the mouse button, the plot shows the selected area. Note the following points:
  - The X axis is the same for all data windows. Moving the scroll bar on the X axis will move the X scroll bars for all data windows. Thus, the same time frame is shown for all data sets.
  - The Y axis is rescaled for the selected data window—other data windows are not affected. If necessary, a scroll bar will appear on the Y axis.
  - Although the Live Data View is still continuously updated, the time axis is not updated—the zoomed area is always shown. The Y axis in the zoomed window is also not updated.

To remove the zoom from a window:

- Double-click in any data window. All data windows will be restored to their full extent.

### **Cursor**

You can place a cursor in a data window:

- Right-click a point in the data window. The cursor will appear with its center at the mouse pointer.

The position of the cursor stays constant. Due to data updating, this means it will appear to move to the left (if you have not used zoom), as it continues to show the selected time.

### **11.3 Saving Live Data**

You can save the data in the Live Data View for later examination in the [Data History View](#).

There is also an autosave feature which saves the data in 60 s intervals.

Data is saved in a binary format with the *.slh* extension.

To save the current contents of the Live Data View:

1. Click the  icon in the toolbar. A **Save** dialog will open.
2. Select a location and name for the file and click **Save**.

If autosave is activated, it will save data to this file.

To activate autosave:

1. Set the parameters that you want to record.
2. Check the **Autosave** box in the toolbar of the Live Data View. Autosave will then start.

If a file is not already listed in the field, a **Save** dialog will open so that you can specify a file for the data. Alternatively, you can click the icon to create a new file, then click **Autosave**.

## 11.4 Clearing the Live Data View

You can clear the data from the Live Data View:

- Click  This removes all data from all parameters in the Live Data View. Live data acquisition will restart.

## Chapter 12 – Data History View

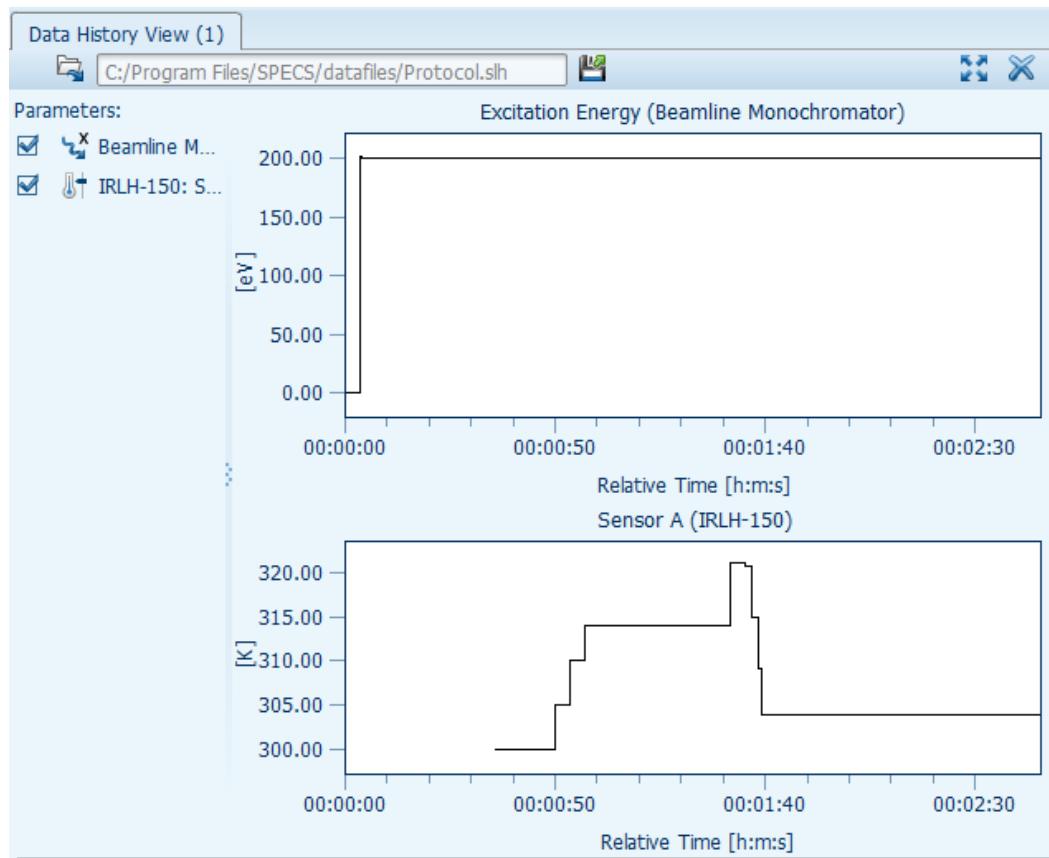
The Data History View is the counterpart to the [Live Data View](#). It allows you to load and view data [saved](#) in the Live Data View. This arrangement allows you to view live data and old data logs simultaneously.

To open the Data History View:

- Select **Views/ Data History View** from the toolbar. The view will open at the bottom of the main window. You can move this to a [new position](#) as desired.

You can perform the following actions in the Data History View:

- [Open data](#).
- [View data](#).
- [Save copies](#) of the data.



## 12.1 Opening Data History

The Data History View can display data [saved](#) in the [Live Data View](#). The data is saved in *.slh* SpecsLab history format.

To open data history:

1. Click  A file browser will open.
2. Select a *.slh* file and click **Open**. The data will be loaded. Each parameter will be displayed in its own data window.

There are a number of options for [viewing the data](#).

## 12.2 Viewing Data History

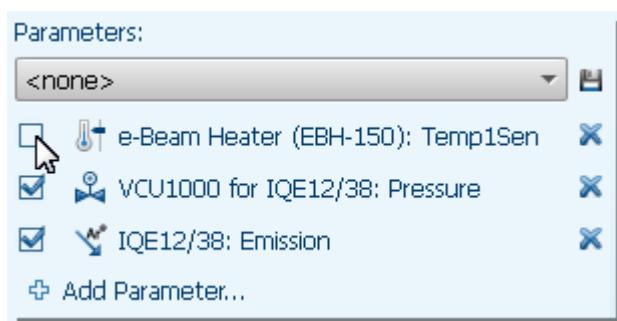
The data for each parameter is shown in its own data window.

### Toggle parameter visibility

On loading a data history file, data windows are automatically displayed for each parameter.

You can toggle the visibility of each parameter:

- Click the check box next to the parameter. When ticked, a data window showing the data history is shown.



### Changing the time axis setting

By clicking the time axis label, you can change the way the time is displayed:

- **Relative time:** Time relative to the start of reading data in the Live Data View, i.e. after the first parameter was selected or after data was cleared.
- **Universal Time:** The system clock time in UTC.
- **Local time:** The system clock time with local settings.

### Zoom

You can zoom into areas in the data windows:

- Click and drag the mouse to form a rectangle in one of the data windows. When you release the mouse button, the plot shows the selected area. Note the following points:

- The X axis is the same for all data windows. Moving the scroll bar on the X axis will move the X scroll bars for all data windows. Thus, the same time frame is shown for all data sets.
- The Y axis is rescaled for the selected data window—other data windows are not affected. If necessary, a scroll bar will appear on the Y axis.

To remove the zoom from a window:

- Double-click in any data window. All data windows will be restored to their full extent.

### **Cursor**

You can place a cursor in a data window:

- Right-click a point in the data window. The cursor will appear with its center at the mouse pointer.

### **12.3 Saving Data History**

You can make a copy of the data history:

- Click . A **Save** dialog will open, allowing you to select a new name and location for the file.

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## Chapter 13 – 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.

### 13.1 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  $E_p$ ,  $\Delta E_{an}$ , is given by:

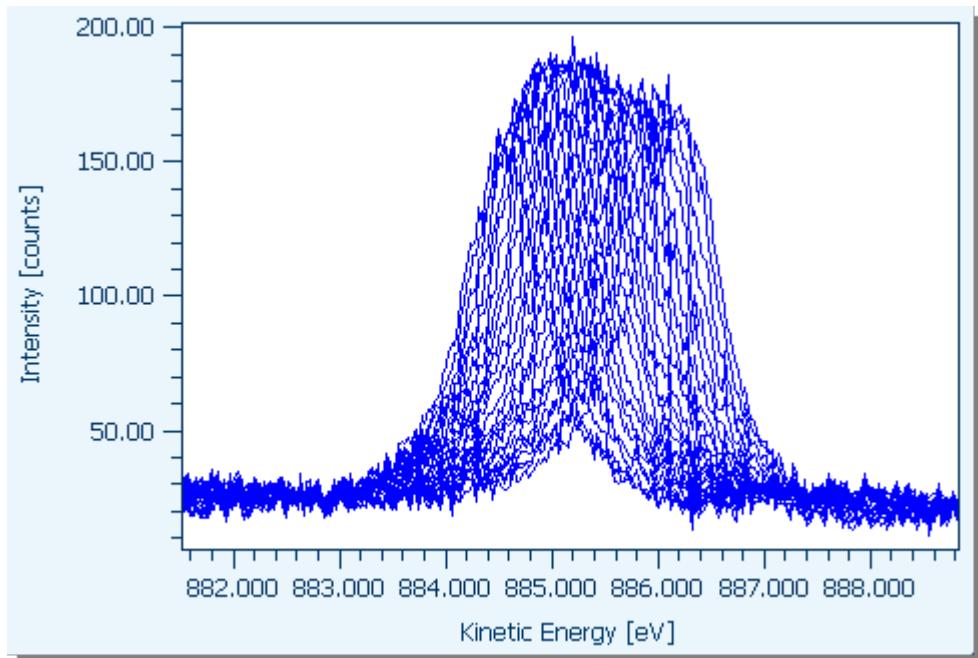
$$\frac{\Delta E_{an}}{E_{pass}} = \frac{W}{2R_0} - \frac{\alpha^2}{4} \quad (16)$$

where:

- $W = (W_1 + W_2)/2$  is the average of the widths of the electron beam at the entrance and exit slits in the energy direction.
- $\alpha$  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 SpecsLab Prodigy 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.

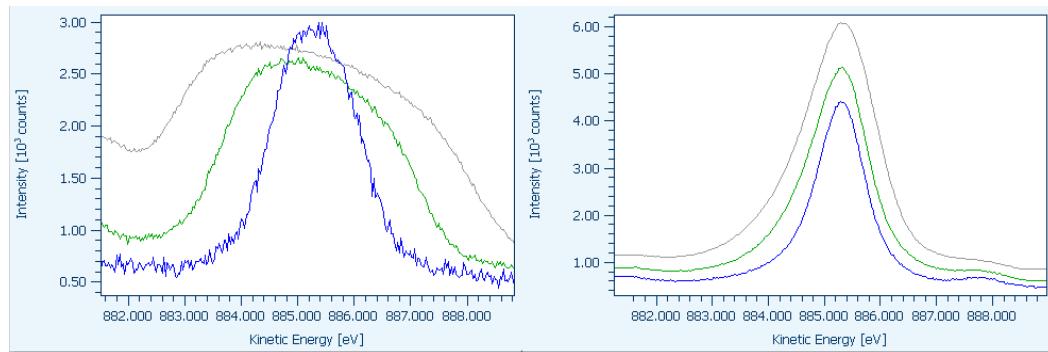
The figure below shows the individual channels measured in a scan using a CCD detector. As you can see, the peak position is different in each channel. This produces a broadening of the summed peak which needs to be corrected. It is also possible that the peak position shifts as a function of pass energy. You can see this by recording a series of spectra at different pass energies and observing the peak positions in the Plot View.



The Detector Calibration View allows you to calibrate 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.

The screenshot below shows the difference between uncalibrated data (left) with calibrated data (right).



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

- Fixed analyzer transmission (FAT) mode, to calculate the energy shifts of the channels.

- Snapshot mode, to calculate energy shifts and gains of the channels.
- Replace, to replace the calibration used in a data set to that in another calibration file.

These are described in the following sections.

### 13.1.1 Calibrating Fixed Analyzer Transmission Groups

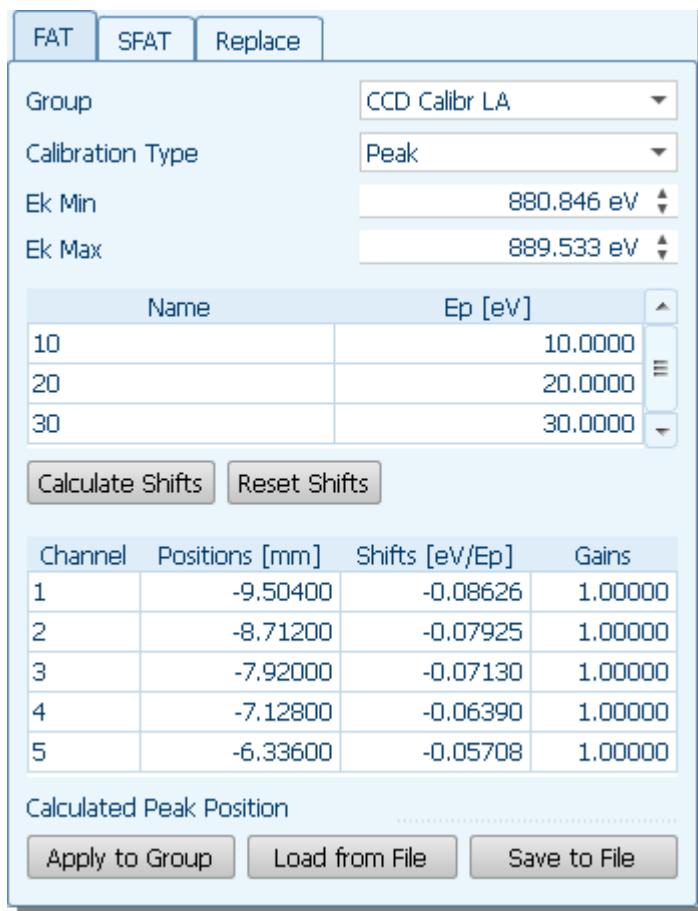
In fixed analyzer transmission mode, the analyzer scans the kinetic energy of the incident particles at a fixed pass energy. You can scan in this mode by selecting the analysis mode **FixedAnalyzerTransmission** when setting up the spectrum group.

#### Note

If the calibration procedure does not succeed, check that the count rate is high enough. This is a problem for regions with low pass energies. Also, you should ensure that SpecsLab Prodigy can detect the peaks by using **Operations/ Peak Location**. If the peak cannot be detected, calibration will fail. For this reason, you should check that all energy channels show a peak—sometimes, channels at the edge do not show a complete peak.

To perform a calibration for fixed analyzer transmission groups:

1. Create a new spectrum group for the calibration.
2. Scan a number of spectra, each with the same parameters but different pass energies (e.g. 5, 10, 20, 50 eV pass energies). These allow the detector to be calibrated for each pass energy.
3. Select **Views/ Detector Calibration** from the menu bar. The Detector Calibration View will open.



4. Select a spectrum group from the **Group** drop-down list. Calibration is performed on this group.
5. Select an entry from the **Calibration Type** drop-down list:
  - **Peak**—the peak is used as the calibration point.
  - **Fermi Edge**—the Fermi edge will be used as the calibration point rather than a peak.
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 spectra.
7. Click **Calculate Shifts**. The calibration will be performed. The new values will be displayed in the table. You will also see the peaks updated in the view pane after the calibration is performed.

This calculation is only applied to the data in the Detector Calibration View. To apply the results to the spectrum data:

- Click **Apply to Group**. The calculated values are updated in the data file. You can see the results, for example, in the Plot View.

You can reset the results of the calculation:

- Click **Reset Shifts**. This sets Shift = 0 for all channels (it does not return the values to their previous settings). If necessary, you can also update the data to these values by clicking **Apply**.

### 13.1.2 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.

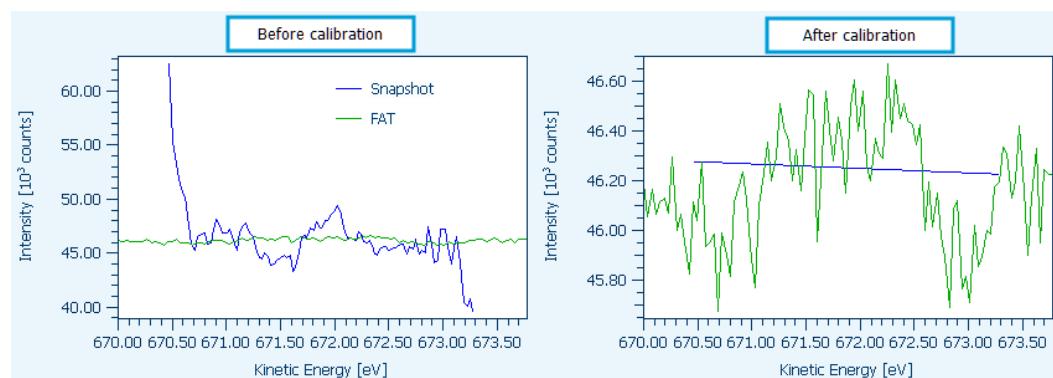
The SFAT detector calibration procedure requires two spectrum groups, recorded with the following scan modes:

- Fixed Analyzer Transmission—to calculate a linear fit over the energy range.
- Snapshot—to record the relative intensities of each channel.

The figure below shows the effect of calibration. The FAT scan is a flat background energy scan. The Snapshot scan shows the different contributions from each channel. Calibration works by fitting a straight line to the spectrum measured in FAT mode. This is used with the values from the snapshot spectrum to calculate the gain factors for each channel. The gain 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.



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

- The SFAT procedure only calibrates gain corrections for the channels. Energy shifts are not calculated.
- Calibration uses a linear fit, so the count rate in the spectrum should be constant, i.e. there should be a flat background signal with no peaks. An example is the 817–812 eV binding energy in the silver spectrum.
- 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  $N \times 0.1$  s for the snapshot mode

To perform a calibration for SFAT spectra:

1. Create two spectrum groups for the calibration. One needs to have the scan type Fixed Analyzer Transmission, the other Snapshot.
2. Record spectra for both spectrum groups using an energy region that shows a flat background signal.
3. Select **Views/ Detector Calibration** from the menu bar. The **Detector Calibration View** will open.
4. Click the **SFAT** tab.

Name	Channels	Scans	Dwell [s]
FAT	100	10	0.10
SFAT	100	100	1.00

Channel	Positions [mm]	Shifts [eV/Ep]	Gains
1	-31.68000	-0.10377	0.74052
2	-31.04000	-0.10131	0.83658
3	-30.40000	-0.09755	0.89365
4	-29.76000	-0.09578	0.91289
5	-29.12000	-0.09353	0.92231
6	-28.48000	-0.09129	0.97336
7	-27.84000	-0.08979	1.01061
8	-27.20000	-0.08757	1.02209
9	-26.56000	-0.08621	0.99612

5. Select a group from the **Group** drop-down list in the **Gains (SFAT)** section.
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 spectra.
7. 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.

This calculation is only applied to the data in the Detector Calibration View. To apply the results to the spectrum data:

- Click **Apply**. The calculated values are updated in the data file. You can see the results, for example, in the Plot View.

You can undo the results of the calculation:

- Click **Reset Gains**. The spectra will be returned to their original values. If necessary, you can also update the data to these values by clicking **Apply**.

### 13.1.3 Replacing a Calibration

When you define an experiment, you can [specify a calibration file](#) which is applied to the results. If necessary, you can replace the calibration file so that the data is corrected with another detector calibration. This procedure allows you to change the calibration file in arbitrary data sets.

To replace a calibration file for a data set:

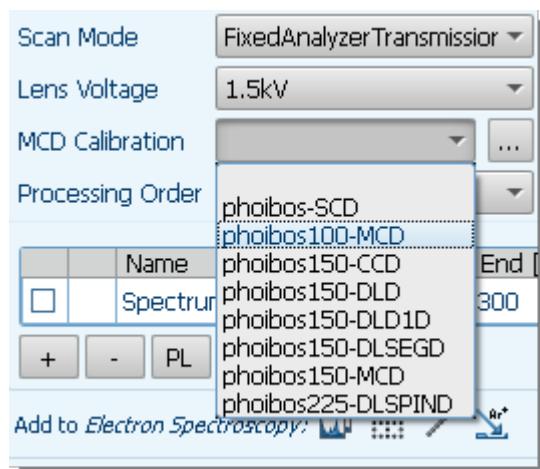
- Select the **Replace** tab in the Detector Calibration view.
- Select a spectrum group from the **Group** drop-down list. The data will be loaded into the table.
- Click **Load**. A file browser dialog will open.
- Select the calibration file that you want to use to calibrate the data in the table.
- Click **Apply to Group**. The calibration file will be applied to the data.

## 13.2 Managing Dataset Files

SpecsLab Prodigy 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 *data-base\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.

### 13.2.1 Saving Calibrations

You can save a calibration for future use. When you save a dataset file, it is available in the Experiment Editor as part of the definition of the spectrum group.



To save a calibration:

1. Perform the calibration as described in the previous sections.
2. Click **Save**. 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.

### 13.2.2 Loading Calibrations

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

To load a dataset file:

1. Select **Views/ Detector Calibration** from the menu bar. The Detector Calibration View will open.
2. Select a spectrum group from the drop-down list in either the **FAT** or **SFAT** tabs.
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. The plot in the Detector Calibration View shows that the calibration has been applied to the spectra.

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## Chapter 14 – Transmission Function

The transmission function is a property of the analyzer that determines the intensity of the measured signal under different experimental conditions.

The transmission function is dependent on the following factors:

- Lens transmission, which is determined by integrating curve intensity as a function of retarding ratio.
- Analyzer transmission, which is proportional to the pass energy.
- Detector transmission, which depends on the conversion voltage.

These quantities are multiplied to give the transmission function. In general, it is necessary to determine the transmission function for

- Each lens mode.
- Each combination of entrance and exit slits.
- Each size of the excitation spot on the sample.

SPECS supplies a set of transmission functions for a few combinations.

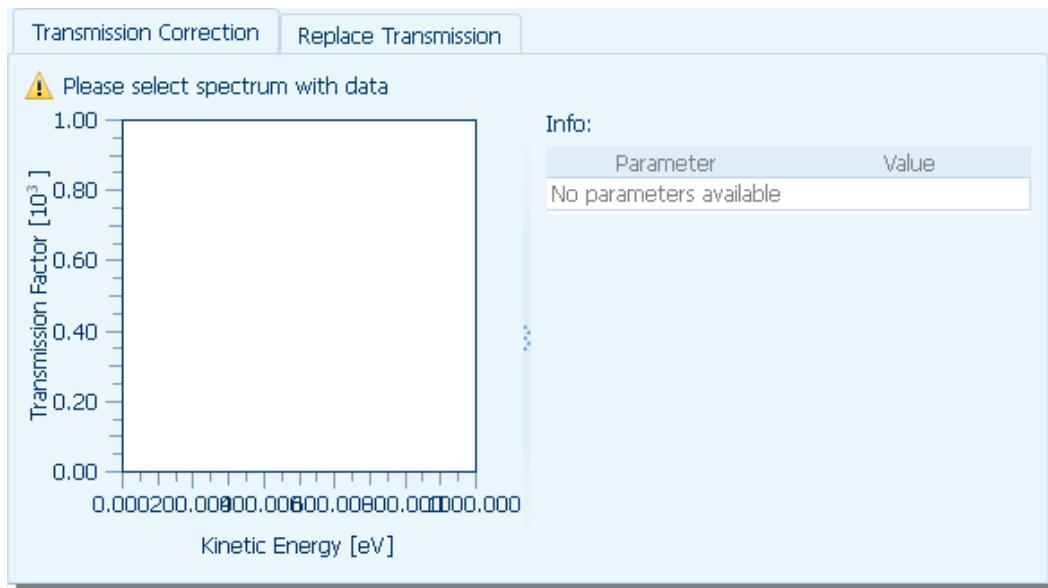
### Note

If a transmission function is not available for your chosen combination, you need to either use a transmission function for a similar combination (this will produce a [warning](#) when you validate the experiment) or measure a new transmission function—please contact SPECS for advice.

For quantitative analysis of data, it is essential to use a transmission function, as this ensures the correct ratios in peak areas. It is important to note that SpecsLab Prodigy does not include the transmission function when displaying or evaluating data. You can however [export](#) spectra with the transmission function in VAMAS or XY format.

The transmission function view allows you to [see the transmission function](#) used with a spectrum and to [change the transmission function](#) if necessary. To open the transmission function view:

- Select **Views/ Transmission Function** from the menu bar. The transmission function view will open.



## 14.1 Viewing the Transmission Function

When you open the transmission function view, the **Transmission Correction** tab is displayed. This shows the following:

- A plot of the transmission function as a function of electron kinetic energy.
- A table containing metadata for the transmission function.

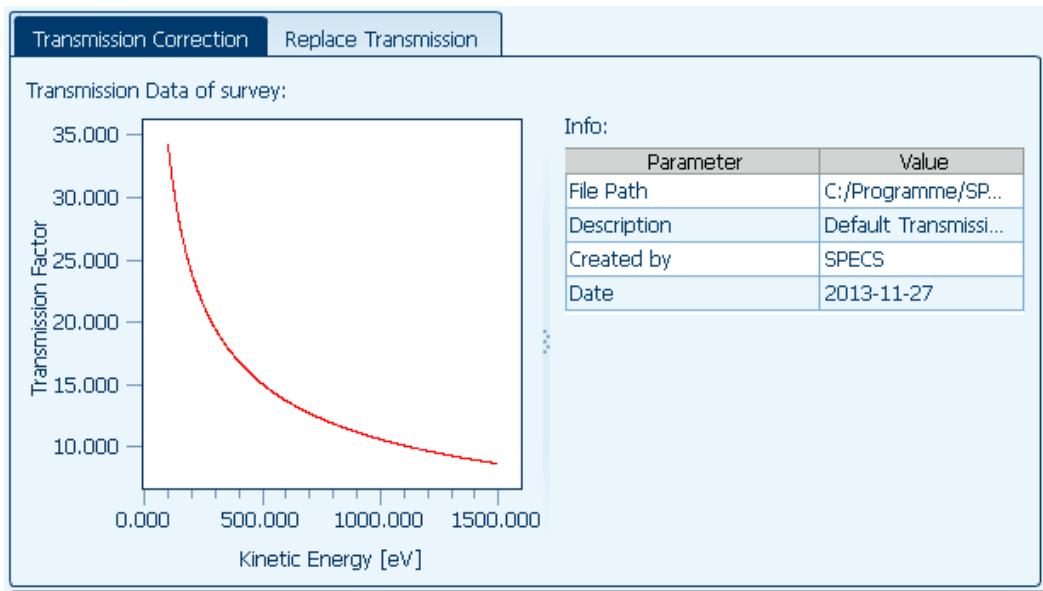
The transmission function shown is for the currently selected spectrum in the experiment editor.

### Note

The numbers in the Y-axis of the plot are arbitrary units. In applying a transmission function, you lose the measured intensities of the peaks, but gain the correct relative intensities.

### Note

Angle-resolved measurements require a transmission function for each angle. In order to use a transmission function for angle-resolved modes, you need to select **Use Image Mapping** in the **Detector** section of the PHOIBOS device control. This only applies to 2D detectors.



## 14.2 Selecting a Transmission Function

You can select a transmission function as part of defining a spectrum group:

- Select an item from the **Transmission** drop-down list in the spectrum group definition. In addition to the transmission functions for specific setups, there is also a default transmission function as well as a constant value, which is equivalent to not applying a transmission function.

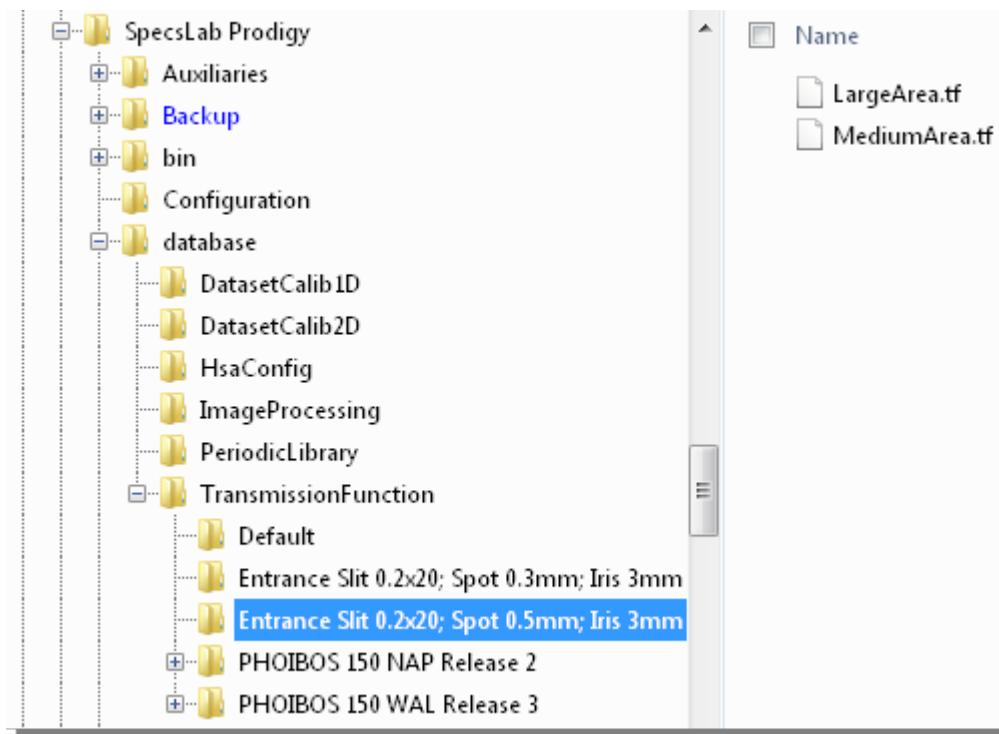
Each spectrum in a spectrum group can use a different lens mode. Since the transmission function is dependent on the lens mode, SpecsLab Prodigy automatically applies the correct transmission function for the lens mode. The picture below shows the file structure of the transmission functions. As you can see, the folders determine the analyzer, detector and slit settings. Each lens mode has its own transmission function file.

### Note

The SpecsLab Prodigy is normally under C:\Program Files (x86)\ .

If a suitable transmission function is not available, a warning will be shown when you validate the experiment. SpecsLab Prodigy deals with missing transmission functions as follows:

- The default transmission function is used.
- If the default is also not available, a constant value is used.



### 14.3 Replacing the Transmission Function

The **Replace Transmission** tab allows you to specify the transmission function in spectra.

To replace the transmission function:

1. Select the **Replace Transmission** tab in the transmission function view.
2. Select a spectrum group in the experiment editor. All spectra in the group will be listed in the transmission function view, along with their transmission function (if any).

#### Note

If you select an element in the experiment editor that contains more than one spectrum group, all spectra in all affected groups will be selected.

3. Select a transmission function from the drop-down list at the bottom left of the transmission function view. Selecting **Load** from this list opens a file browser dialog, allowing you to select a transmission function from the file system.
4. Click **Replace TF Data**. The transmission functions in all spectra listed in the transmission function view will be replaced by the selected transmission function.

The screenshot shows the SPECS SpecsLab Prodigy software interface. At the top, there's a toolbar with icons for file operations like Open, Save, Print, and Settings. The main window has a title bar "File: DepthProfile". Below the title bar is a "Description:" field which is currently empty. The central part of the screen displays a "Sputter Depth Profile" configuration window. This window contains a table titled "Depth Profile 100nm TaO5/Si" with the following data:

	Name	Scans	Start [eV]	End [eV]	Step [eV]	Values	Dwell [s]	Lens M
<input type="checkbox"/>	O1s	1	946.74	962.24	0.1	156	0.1	Mediur
<input type="checkbox"/>	C1s	1	1191.74	1207.74	0.1	161	0.1	Mediur
<input type="checkbox"/>	Ta4d	1	1234.74	1266.74	0.1	321	0.1	Mediur
<input type="checkbox"/>	Si2p	1	1374.74	1393.74	0.1	191	0.2	Mediur
<input type="checkbox"/>	survey cycle 9	1	100	1490	1	1391	0.1	Mediur

Below this table is a "Transmission Correction" dialog box. It contains a warning message: "Selected Spectrum Groups: ! Selection has no analyzers. Using default transmission path." It lists the selected spectrum groups and their corresponding transmission functions:

Name	Transmission Function
File: D:/Reference/NiceData/DepthProfile.sle	C:/Programme/SPECS/SpecsLab2/database/Trans...
Depth Profile 100nm TaO5/Si	
O1s	
C1s	
Ta4d	
Si2p	
survey cycle 9	

At the bottom of the dialog box are buttons for "Replace TF Data" and a dropdown menu labeled "<none>".

This page intentionally left blank.

## Chapter 15 – Device Controls

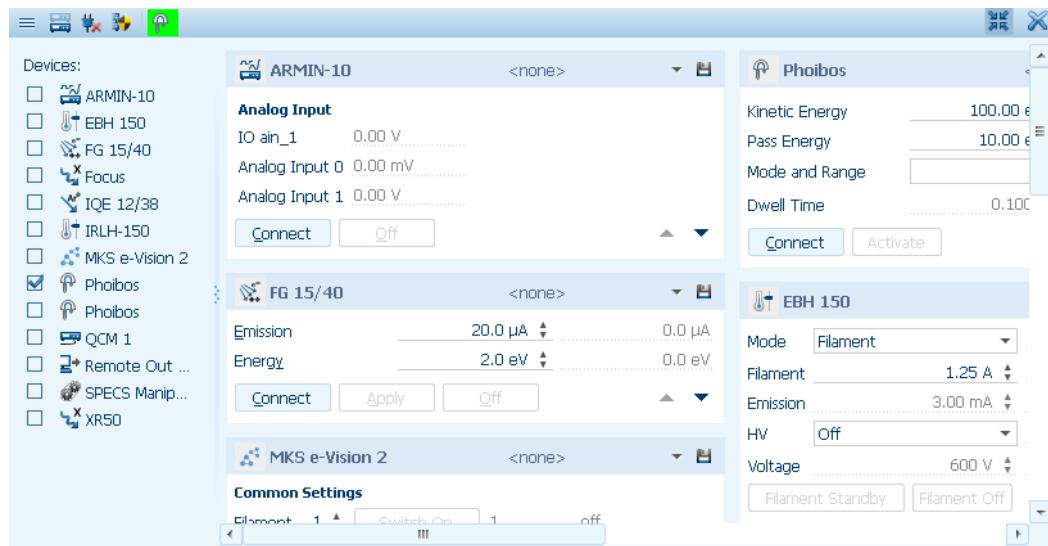
SpecsLab Prodigy is able to control a variety of SPECS equipment. The Device Control view provides an overview of all available SPECS instruments in your system and allows you to set their operating parameters.

The contents of the Device Control view consist of a group of modules which depend on your system configuration. For this reason, the view is not discussed in this manual. Please refer to the manual of the equipment for a description of its Device Control.

In particular, there is a Device Control used to directly control and report the voltages in your analyzer and detector. This is essential when setting up the analyzer, as well as for calibration and test purposes. The Device Control is described in the analyzer manual.

### Note

All modules are documented in the SpecsLab Prodigy Online Help.

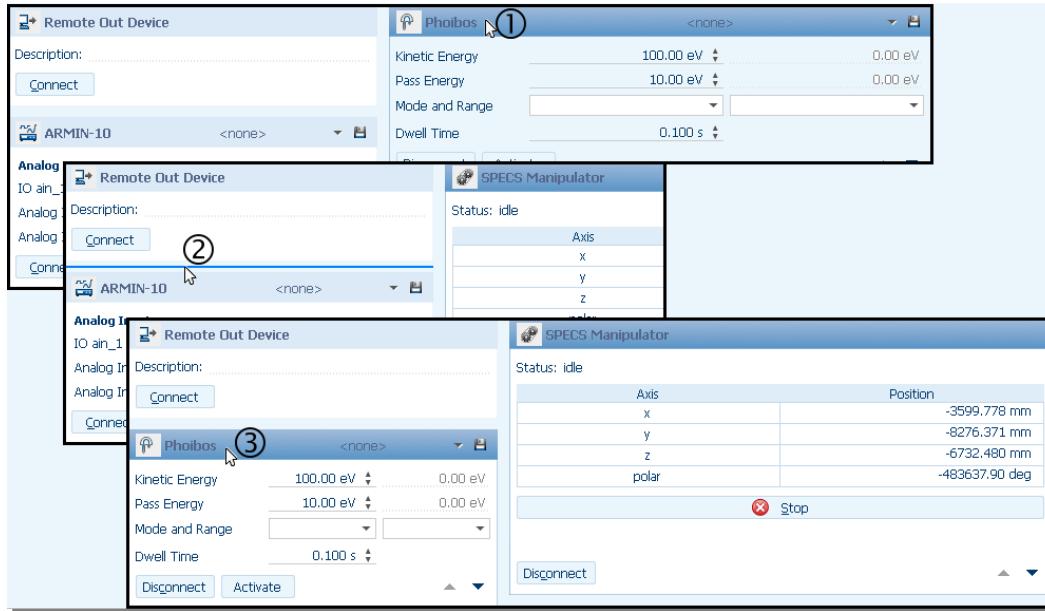


### 15.1 Arranging Devices

You can arrange devices in the Device Control view:

1. Click and hold the title bar of a device.
2. Drag the mouse to a new position in the view. A blue line will appear at the mouse position:
  - Horizontal—the device control will be moved to this position in the column.
  - Vertical—a new column will be created at this position.

3. Release the mouse button. The device control will appear in the new position.



You can save the layout by [selecting Layout/ Save Current Layout](#) from the menu bar.

The **Devices** pane on the left contains an overview of all displayed devices. Clicking a device in this list will jump to the selected device in the main pane.



## 15.2 Device Control Toolbar

There is a toolbar in the Device Control view. The actions of the features in the toolbar affect all devices. It also shows the connected devices and their status.



### Show/ hide inactive devices

Clicking this icon toggles the display of devices in the Device Control view. You can set it so that only connected devices are visible. If you have many devices in your system, this can improve the readability of the view.

All devices are shown in the **Devices** pane on the left side of the view. You can connect to devices by checking the option box in the Devices pane. After connecting, the device control is shown in the main pane.



### Disconnect from all devices

Clicking this icon disconnects all devices.



### Send devices to safe state

On clicking this icon, all connected devices are put into a safe state. The meaning of "safe state" is device dependent.

## Devices

The toolbar also contains icons showing the status of connected devices.

### Note

Each device has its own icon and is displayed separately in the toolbar. The table below only shows the analyzer icon.

Indicator	Status
	Device inactive.
	Device in operation and working correctly.
	Set up device ready for operation.
	Device error.

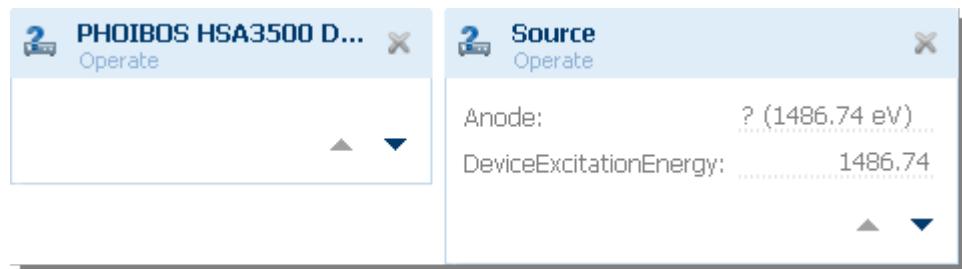
## 15.3 Unknown Devices

Unknown devices are indicated by a question mark icon. This is shown when a file contains details of a device, but the device is not configured in SpecsLab Prodigy. This may occur for the following reasons:

- When data acquired on one installation of SpecsLab Prodigy is opened in another.
- If a device is reconfigured. The configuration in the data file is then different from the current configuration in SpecsLab Prodigy.

Although it is not configured, the data file contains metadata which describes the device. This metadata is shown in SpecsLab Prodigy with the settings used in the experiment. In most cases, this should be sufficient for you to see what equipment was used and the operating parameters.

The screenshot below shows two unknown devices. The analyzer (left) has been correctly identified, while the X-ray source is recognized only as a source with the correct excitation energy.



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