



SPECTROview User Manual

(version 15/01/2026)

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1. Introduction

Spectroscopy techniques (such as Raman, Photoluminescences, XRD, XPS...) are widely used in various fields, including materials science, chemistry, biology, and geology. In recent years, these techniques have increasingly found their place in cleanroom environments, particularly within the microelectronics industry, where they serve as critical metrology tools for wafer-scale measurements. The data collected from these in-line measurements (wafer data) require specific processing, but existing software solutions are often not optimized for this type of data and typically lack advanced plotting and visualization capabilities. Additionally, the licensing requirements of these software solutions can restrict access for a broader community of users.

SPECTROview addresses these gaps by offering free, open-source software that is compatible with both in-line data (wafer-map) as well as standard spectroscopic data (discrete spectra, 2D maps). It also features a built-in visualization tool, enabling users to streamline both data processing and visualization in a single application, making the workflow more efficient.

More details regarding the latest updates and features of the SPECTROview can be found in the Github repository : <https://github.com/CEA-MetroCarac/SPECTROview>

Dont forget to cite the tool when it is used for your data processing , data visualization on your publication:

Le, V.-H., & Quémésré, P. (2025). SPECTROview : A Tool for Spectroscopic Data Processing and Visualization. Zenodo. <https://doi.org/10.5281/zenodo.14147172>

Highlighted features:

- Cross-platform compatibility (Windows, macOS, Linux).
- Supports processing of spectral data (1D) and hyperspectral data (2D maps or wafer maps).
- Ability to fit multiple spectra or 2Dmaps using predefined custom fit models.
- Collect all best-fit results with one click.
- Optimized user interface for easy and quick inspection and comparison of spectra.
- Dedicated module for effortless, fast, and easy data visualization.
- Each module will be described in detail in the following sections.

2. Installation

Ensure that Python (version between v3.8 and v3.12) is already installed on your PC.

The installation of SPECTROview can be performed via the command line (CMD):

```
pip install spectroview
```

You can also install directly via the GitHub repository by copy and paste following line in CMD:

```
pip install git+https://github.com/CEA-MetroCarac/SPECTROview.git
```

To open SPECTROview, Open CMD then type:

```
spectroview
```

To update SPECTROview to the newest version:

```
pip install --upgrade spectroview
```

To update SPECTROview to the specific version:

```
pip install --upgrade spectroview==num-of-version
```

Example: `pip install --upgrade spectroview==26.3.1`



3. Supported data by SPECTROview

Examples of all supported data types can be found in the `/examples` folder within the [GitHub repository](https://github.com/CEA-MetroCarac/SPECTROview/tree/main/examples):

<https://github.com/CEA-MetroCarac/SPECTROview/tree/main/examples>.

Users can download these files to understand the supported files format and data structures; practice using the SPECTROview application with real examples.

3.1 Spectroscopic data (.txt, .csv)

SPECTROview supports spectroscopic data (TXT or CSV format). The files must consist of two columns, separated by *semicolon* or *space*, or *tab*. Data files can contain or not column headers:

- **Column 1:** Raman shift (cm^{-1})
- **Column 2:** Corresponding Raman intensity (a.u.)

header	header
R_1	Intensity
R_2	Intensity
...	...
R_{n-1}	Intensity
R_n	Intensity

3.2 Hyperspectral data (.txt, .csv)

SPECTROview supports hyperspectral data (2D maps or wafer maps) in TXT or CSV format, with the data structure arranged as follows:

		R_1	R_2	R_3	...	R_{n-1}	R_n
X_1	Y_1	I_1	I_1	I_1	...	I_1	I_1
X_2	Y_2	I_2	I_2	I_2	...	I_2	I_2
...
X_n	Y_n	I_n	I_n	I_n	...	I_n	I_n

- The first row ($R_1 \rightarrow R_n$) is the **Raman shift (cm^{-1})** of all spectrum
- Two first columns listing the **X** and **Y** coordinate of the spectrum within the maps.
- The remaining columns contain the corresponding **intensity** values for each spectrum ($I_1 \rightarrow I_n$), from the second row to the last.

Note: 2D map formats from Renishaw tools must be converted before they can be used in SPECTROview. An integrated conversion tool is provided in SPECTROview application for this purpose (see Section 4, File Convert Tool)

3.3 Datasheet (Excel files)

Excel files (.xlsx, .xls) containing one or multiple sheets can be directly loaded into SPECTROview.



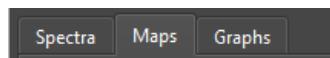
3.4 Formats saved by SPECTROview application

Depending on the active workspace, SPECTROview saves files with specific extensions so work can be resumed later:

- Maps workspace → .maps
- Spectra workspace → .spectra
- Graphs workspace → .graphs

4. User Interface Overview

The SPECTROview application is designed for the efficient processing of spectroscopic data and the easy visualization of fitted results. The interface features three main workspaces, each developed for a specific purpose:



- Spectra: For processing one or multiple discrete spectra.
- Maps: For processing one or multiple hyperspectral datasets, including wafer data and 2D maps.
- Graphs : For plotting and visualizing data.

Tooltip: Most GUI elements in SPECTROview (buttons, text boxes, dropdowns, etc.) feature tooltips.
→ To see a brief explanation of its function : hover the mouse cursor over an element for 1second.

Toolbar : a horizontal toolbar is located at the top edge of the application containing the following buttons:

	Loads all supported data types as listed in section 3. The application will automatically switch to the appropriate workspace based on the loaded file type.
	Saves the current active workspace to a file, allowing the user to reopen it later and resumes the work. As detailed in Section 3.4, the file extension will be .maps, .spectra, or .graphs depending on the active workspace.
	Clears the current active workspace to start a new session. All loaded data will be removed.
	Opens the File Convert Tool to convert hyperspectral data (2D maps) from the Renishaw WiRE format into a format supported by SPECTROview: <u>How to use (see Figure 1):</u> Load the file(s) to convert → Selected file(s) to convert from the list (4.2) → Click button “Convert” (4.3) → The new file is created in the same folder with the suffix <u>_converted</u> (4.4).

Figure 1: Interface of “Hyperspectral Data Converter”



	<p>“Settings”: Opens the Settings Panel to adjust fitting parameters and define the storage folder for user-defined fitting models</p>	
	<p>Theme Toggle: Switches the application GUI between Dark and Light modes.</p>	
	<p>To Open this User Manual document.</p>	
	<p>To displays version information and details about the application..</p>	

5. Spectra and Maps workspaces

The **Spectra** and **Maps** workspaces are very similar. They share many common features, with the **Maps** workspace containing additional specific features designed to handle multiple hyperspectral datasets (2D maps or wafer maps). The following section details the GUI of the **Maps** workspace.

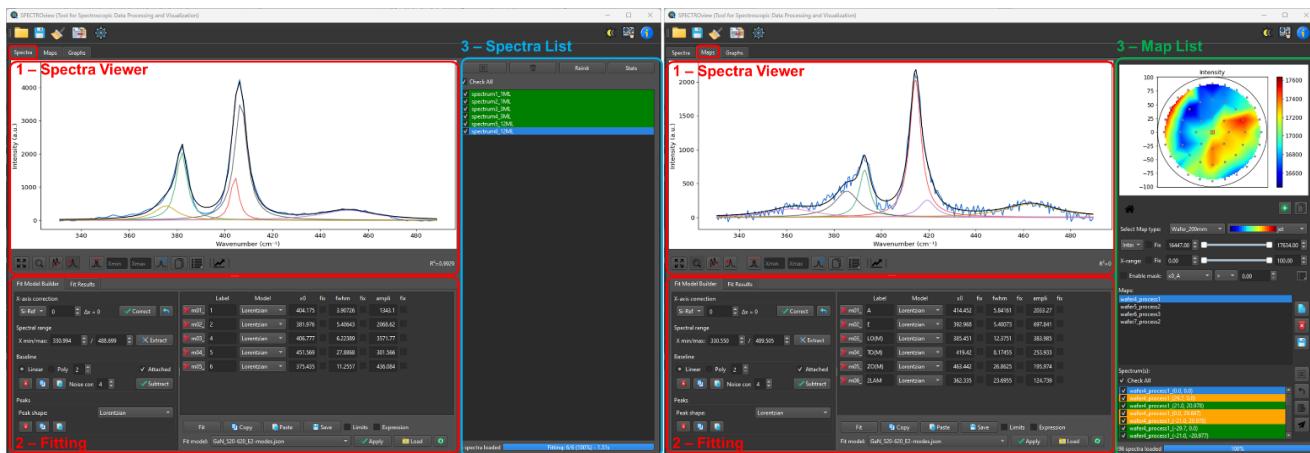


Figure 3: Interface overview of **Spectra** (left) and **Maps** (right) workspaces. The interface is divided into three main sections. Section **1-SpectraViewer**) and **2-FittingPanel** are identical in both workspaces, whereas section **3-SpectraList** (in Spectra workspace) or **3-MapList** (in Maps Workspace) are different.



5.1 SpectraList and MapList

As showed in Figure 3, the SpectraList and MapList sections are designed differently for Spectra and Map workspaces in order to efficiently navigate between spectral or hyperspectral (maps) data.

In the following, the MapList section of the Maps workspace (which also contains also a SpectraList module) is described in detail (Figure 4).

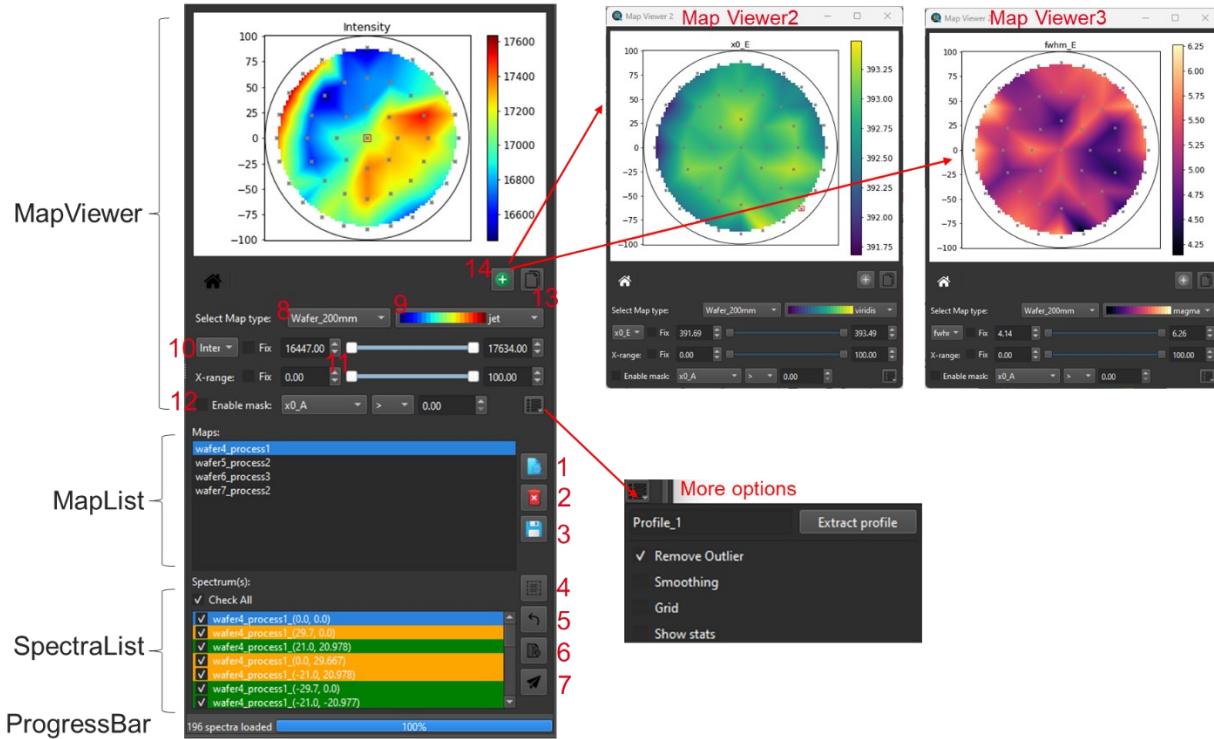


Figure 4: (Left) MapList section within the Maps workspace. On the right: (top) additional MapViewer module(s) can be added as floating window(s); (bottom) More Options to adjust and customize the heatmap display.

MapList: The MapList displays all loaded map files, including wafer maps and 2D map types. Three buttons located on the right side of the MapList allow the user to (1) view the selected map data, (2) delete the selected map, or (3) save the selected map to an Excel file (see Figure 4).

SpectraList: all loaded spectra in the Spectra workspace, or all spectra associated with the map selected in the MapList (in the Maps workspace). Users can select one or multiple spectra simultaneously. The selected spectra are displayed in the SpectraViewer (cf. section 5.2). Four buttons associated with the SpectraList allow the user to (4) Selected all available spectra in the list, (5) reset (reinit) the selected spectra, (6) display the fit statistic report or (7) send the selected spectra to the Spectra workspace (see Figure 4).

MapViewers: displays the heatmap of the selected map (wafer or 2D map type) chosen from the MapList. Several options are available to customize the heatmap:

- (8) **Map type:** 2D map or wafer map with different diameters.
- (9) **Color palette** selection for the heatmap.
- (10) **Displayed parameter:** maximum intensity, area, or any fitted parameter.
- (11) **Range sliders:** two sliders are available to adjust the X-axis range and the color bar limits.
- (12) **Mask feature:** allows the user to define specific regions of the heatmap based on user-defined filters.
- (13) **Copy button:** copies the heatmap to the clipboard, allowing it to be pasted elsewhere.



- **(14) Multiple MapViewers:** users can add additional MapViewer windows as floating windows, enabling comparison between different fitted parameters of the same map (see Figure 4) (see Figure 4).

ProgressBar: placed under the SpectraList (see Figure 5) displays the number of spectra available in the SpectraList, and the progress of the fitting process (number of fitted spectra / total spectra, percentage (%), and elapsed time (s)). The Stop button allow to stop the fitting process at anytime.

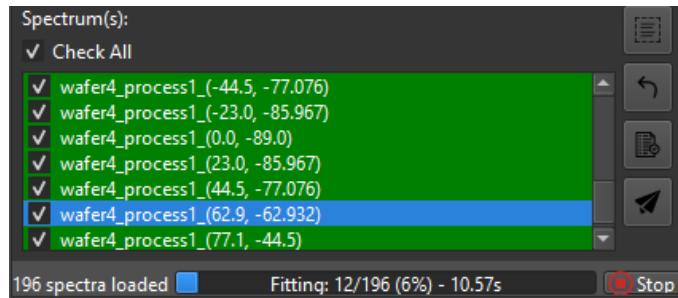


Figure 5: SpectraList and ProgressBar

5.2 Spectra Viewer

SpectraViewer plot all spectra (and its best fit curves) selected via the SpectraList (cf. section 5.1)

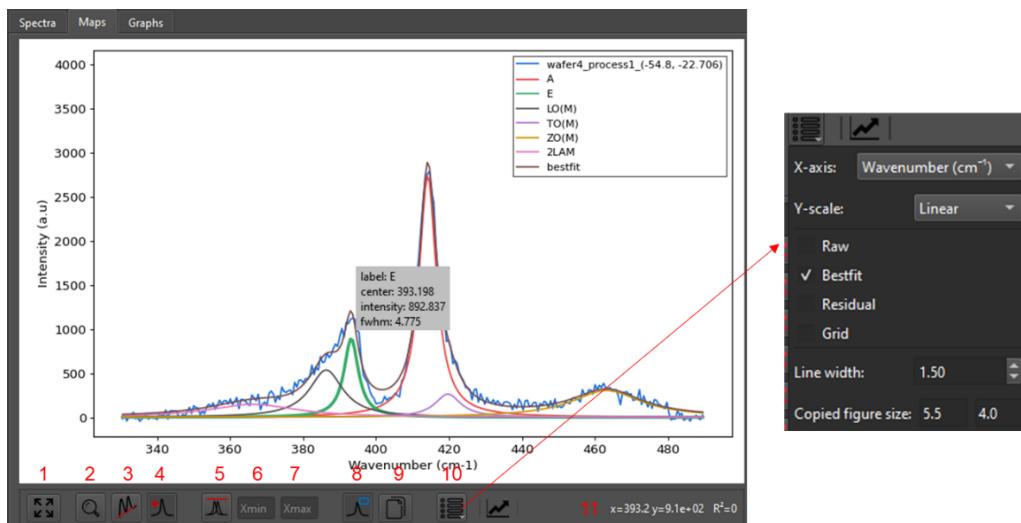


Figure 6: Spectra Viewer (left) widget and View Options Menu (right).

	Rescale: to rescale the spectra plot. Shortcut: Ctrl + R
	Zoom: when active, enables the "zoom" feature of spectra plot using the left mouse click & drag
	Baseline: when active, allows the user to define baseline point(s) using the left mouse click.
	Peaks: when active, allows the user to define peak(s) on the spectra using the left mouse click.
	Normalization: when clicked, displays all selected spectra normalized to the maximum peak intensity. If the user wants to normalize to a specific spectra range or specific peak → type the corresponding spectral range into text boxes 'min' and 'max' (see Figure 7).

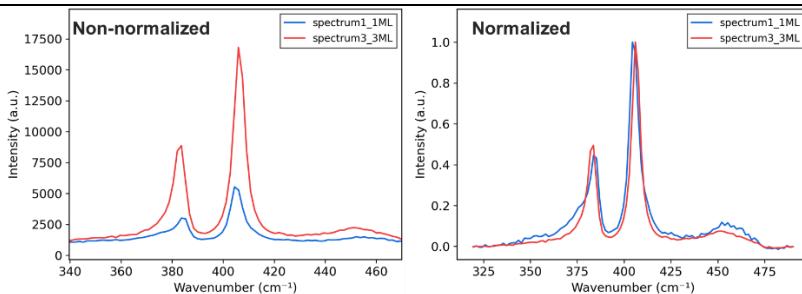
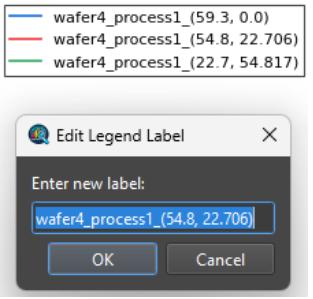
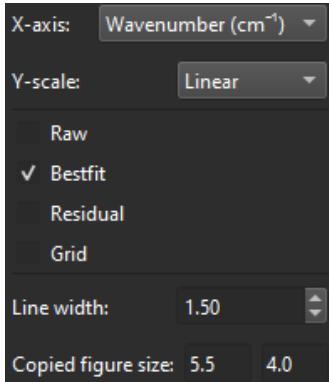


Figure 7: Example of Raw spectra (left) and spectra normalized to the maximum intensity within the 400-420 cm⁻¹ range (right) to facilitate the inspection of peak shifts.

	<p>Legend: displays the legend for all selected spectra. Once the legend is shown, the user can click directly on the legend box to change the color or labels (see figure on the right).</p> <p>Note: This feature only works when the Zoom button is disabled (by selecting Baseline or Peak button).</p>	
	<p>Copy: copies the spectra plot to the clipboard as an image. The user can then paste it into other applications (PowerPoint, Excel, etc.).</p> <ul style="list-style-type: none"> - Ctrl + Click (or Cmd + click on macOS): Copies the numerical data of the spectra (including RAW data and best-fit curves) to the clipboard. 	
	<p>More options: opens a pop-up window with several view options (cf. figure on the right).</p> <ul style="list-style-type: none"> - X-axis unit : available option (Wave number (cm⁻¹), wavelength (nm), Emission energy (eV), binding energy (eV), Frequency (Hz), 2Theta (degree)). - Y axis-scale: Linear or log scale. - Raw : Toggles the visibility of the raw data. - Bestfit: Toggles the visibility of the fitted peaks. - Residual: Displays the residual (Raw - bestfit). - Grid: adding grids on the plot. - Line width: to adjust the line width of the spectra plot. - Figure size: to adjust the ratio (high-width) of copied figure. 	

Other features of SpectraViewer:

- **Show Peak Parameters** on the spectra plot: by hovering the mouse cursor over a peak displays a pop-up with the peak parameters (peak label, intensity, FWHM, position), as shown in Figure 6.
- **Add/Remove Peaks:** Right-click to remove the current peak, or left-click to add a new peak (ensure the Peak button  is active).
- **Adjust peak by dragging.**
- **Quick re-scale** of the y axis: Use the mouse wheel to quickly adjust the Y-axis (intensity scale).



5.3 Fit Model Builder

The FitModelBuilder Tab widget contains three main panel : Fitting, PeakTable Panel, FitModelControl Panels (Figure 8).

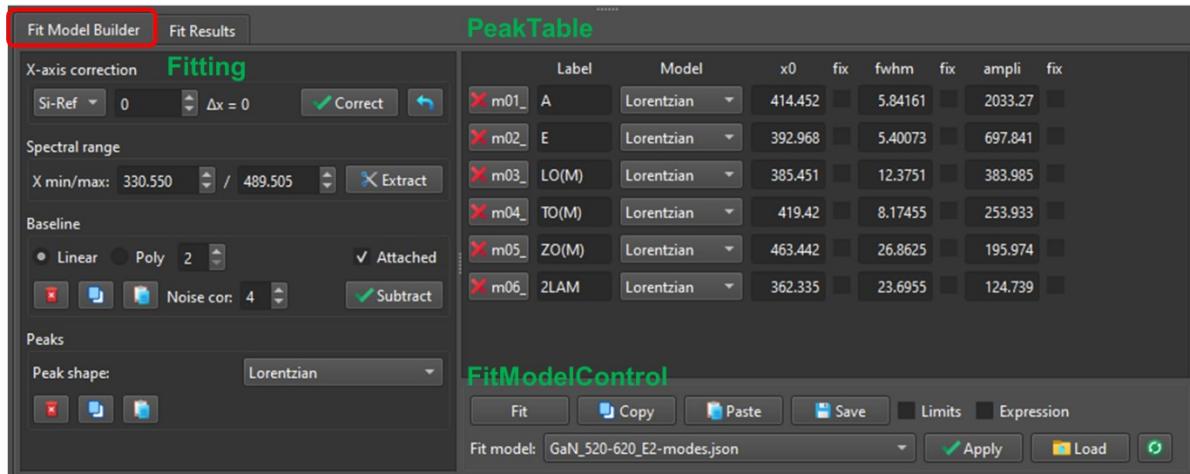


Figure 8: FitModelBuilder tab widget containg three main panels: (1) Fitting, (2) PeakTable and (3) FitModelControl.

5.3.1 Fitting Panel

The FittingPanel (left panel of Figure 8) is divided four small sections, each corresponding to the key steps in the fitting process or in the construction of the fit model.

Step 1: x-axis Correction (optional) : This step is used to perform an x-axis correction based on measurements from a well-known reference sample. In SPECTROview, this feature is currently implemented for a [silicon reference sample](#), which has a theoretical Raman peak position at 520.7 cm^{-1} . Support for additional reference samples will be added in future versions.

Procedure:

- Record the silicon reference spectrum during the same experimental session as the other samples, using identical measurement parameters.
- Fit the Si-Ref spectrum to determine the measured silicon peak position.
- Enter the measured position into the text box.
- Select one or more spectra to correct → the x-axis correction is applied based on the difference between the measured position and the theoretical value (520.7 cm^{-1}).

Step 2: Define the fitting range : to define the x-axis range to be used for the fitting process.

Step 3: Baseline definition:

- **Baseline points** are defined directly in the spectra plot (SpectraViewer widget) by left-clicking. The Baseline button must be active (cf. section 0).
- **Attached checkbox** : When checked, the baseline points remain attached to the spectrum curve.
- **Correct noise**: Calculates each baseline point as the average of the specified number of neighboring data points, ensuring it sits in the center of the noise level.
- **Baseline properties**: The baseline type (e.g., linear, polynomial) can be adjusted as needed.

Step 4: Peak(s) definition:



- Peaks can be defined directly on the spectra using the Spectra Viewer by left-clicking. The Peak button must be active (cf. section 0).
- Any peak added to the fit model is automatically displayed in the PeakTable panel (see below). User can then modify/adjust directly in the PeakTable panel.

5.3.2 PeakTable Panel

The PeakTable displays all available peaks defined of the selected spectrum.

Peak properties (*label*, *model*, *position*, *FWHM*, *intensity*) are dynamically updated as user modifying via SpectraViewer plot (with mouse *click* or *dragging*). Users can also remove peak(s) or manually adjust their parameters directly via PeakTable.

Label	Model	X0	fix X0	Fwhm	fix Fwhm	Ampli	fix Ampli
m01_A	Lorentzian	414.258	<input type="checkbox"/>	5.888	<input type="checkbox"/>	2709.714	<input type="checkbox"/>
m02_E	Lorentzian	392.946	<input type="checkbox"/>	5.045	<input type="checkbox"/>	970.902	<input type="checkbox"/>
m03_LO(M)	Lorentzian	386.016	<input type="checkbox"/>	11.105	<input type="checkbox"/>	592.371	<input type="checkbox"/>
m04_TO(M)	Lorentzian	418.887	<input type="checkbox"/>	8.277	<input type="checkbox"/>	345.69	<input type="checkbox"/>
m05_ZO(M)	Lorentzian	463.469	<input type="checkbox"/>	25.345	<input type="checkbox"/>	301.522	<input type="checkbox"/>
m06_2LAM	Lorentzian	364.236	<input type="checkbox"/>	25.078	<input type="checkbox"/>	164.159	<input type="checkbox"/>

Figure 9: PeakTable panel

Constraints: For each peak, one or more parameters can be fixed by selecting the corresponding checkbox. For more advanced constraints, two additional options (via checkboxes **Limit** or **Expression**) are proposed:

- **Limits** checkbox: When enabled, **min** and **max** value columns are displayed for each parameter, allowing the user to restrict parameter variations within a defined range (as opposed to the **Fix** option, which keeps the value constant).

Label	Model	min X0	X0	max X0	fix X0	min Fwhm	Fwhm	max Fwhm	fix Fwhm
m01_A	Lorentzian	393.68	414.258	433.68	<input type="checkbox"/>	0	5.888	200	<input type="checkbox"/>
m02_E	Lorentzian	369.29	392.946	409.29	<input type="checkbox"/>	0	5.045	200	<input type="checkbox"/>
m03_LO(M)	Lorentzian	360.17	386.016	400.17	<input type="checkbox"/>	0	11.105	200	<input type="checkbox"/>
m04_TO(M)	Lorentzian	398.61	418.887	438.61	<input type="checkbox"/>	0	8.277	200	<input type="checkbox"/>
m05_ZO(M)	Lorentzian	437.78	463.469	477.78	<input type="checkbox"/>	0	25.345	200	<input type="checkbox"/>
m06_2LAM	Lorentzian	338.74	364.236	378.74	<input type="checkbox"/>	0	25.078	200	<input type="checkbox"/>

- **Expression** checkbox: when enabled, **expression** column it allows parameters from different peaks to be linked through mathematical expressions.
 - o Example 1: To constrain the position of peak m02_ to be 17 units less than m01_ → type: `m01_x0 - 17`.
 - o Example 2: To constrain the intensity of peak m03_ to be half that of m02_ → type: `m02_ampli / 2`



Label	Model	X0	expression X0	fix X0	Fwhm	expression Fwhm	fix Fwhm	Ampli	expression Ampli	fix Am
m01_A	Lorentzian	409.725	None	0.001	None	None	None	6.431	None	None
m02_E	Lorentzian	392.725	m01_x0 - 17	5.424	None	None	None	1038.248	None	None
m03_LO(M)	Lorentzian	385.352	None	10.362	None	None	None	519.124	m02_ampli/2	None
m04_TO(M)	Lorentzian	414.523	None	6.666	None	None	None	2822.882	None	None
m05_ZO(M)	Lorentzian	463.381	None	26.637	None	None	None	296.755	None	None
m06_2LAM	Lorentzian	364.862	None	26.493	None	None	None	167.265	None	None

5.3.3 FitModelControl Panel

Once the desired fit model has been defined (as shown in the PeakTable panel), click the button **Fit** to start the fitting process (Figure 10).

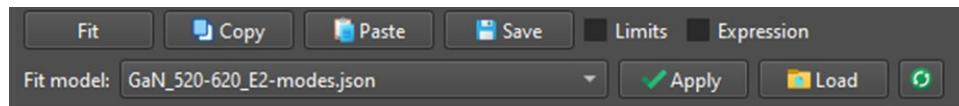


Figure 10: Interface of FitModelControl

If the result is unsatisfactory, adjust the parameters (via PeakTable or SpectraViewer) and click **Fit** again.

Copy / Paste Fit Models: The entire fit model (including spectral range, baseline, and peaks) can be copied and pasted between spectra:

- Select the fitted spectrum and click .
- Select one or multiple target spectra and click .

Saving Fit Models: Users can save the fit model for later use by clicking . It is recommended to store all models in a predefined folder, which can be specified in the Settings Panel (Figure 2). Saved models can then be quickly accessed using the "Fit Model" dropdown menu.

To using a pre-defind fit model :

- Select the fit model via the drop-down list. Then click to the button to perform the fitting for selected spectra.
- Use can also load a fit model store anywhere in the PC via button.

5.4 Collect and Save Fit Results

SPECTROview provides simple and efficient access to fitted data. To collect best-fit results from all fitted spectra or maps. To save bestfit data:

- Switch to the **Fi Results** tab.
- Click to the Collect button .
- Results are then aggregated into a table and displayed in the GUI (Figure 11).



Fit Model Builder																																																																																																													
Fit Results																																																																																																													
Collect Fit Results																																																																																																													
Split the filename of spectra:																																																																																																													
<input type="button" value="Split"/> <input type="button" value="Column name"/> <input type="button" value="Add"/>																																																																																																													
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Figure 11: Collect fit results panel

From here, the user can :

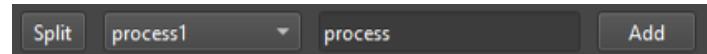
- Name the bestfit dataset and click “send” it to the Graphs workspace for plotting (cf. Section 6) :

Send fit results to 'Graph' Tab:
MAPS_best_fit
<input type="button" value="Send"/>

- Or, export the results as an Excel file

Split feature: allows extracting information from filenames and adds it as new columns in the results table.

- Recommendation: Name files wisely using underscores to separate information/parameters (e.g., **Sample1_ProcessA_Temp25**).
- Example: In the figure below, the process type (process1, process2) is extracted from file name of each spectra; and added as a new column named "Process"..



5.5 Save workspace.

To save the current active workspace, click the **Save** button (2) in the toolbar.



Depending on the active workspace, the file will be saved with a different extension :

(Maps workspace → .maps; Spectra workspace → .spectra; Graphs workspace → .graphs).

6. « Graphs » workspace

The **Graphs Workspace** is dedicated to data visualization, with an emphasis on simplicity and speed. The graphical user interface (GUI) of this workspace is shown in Figure 12:

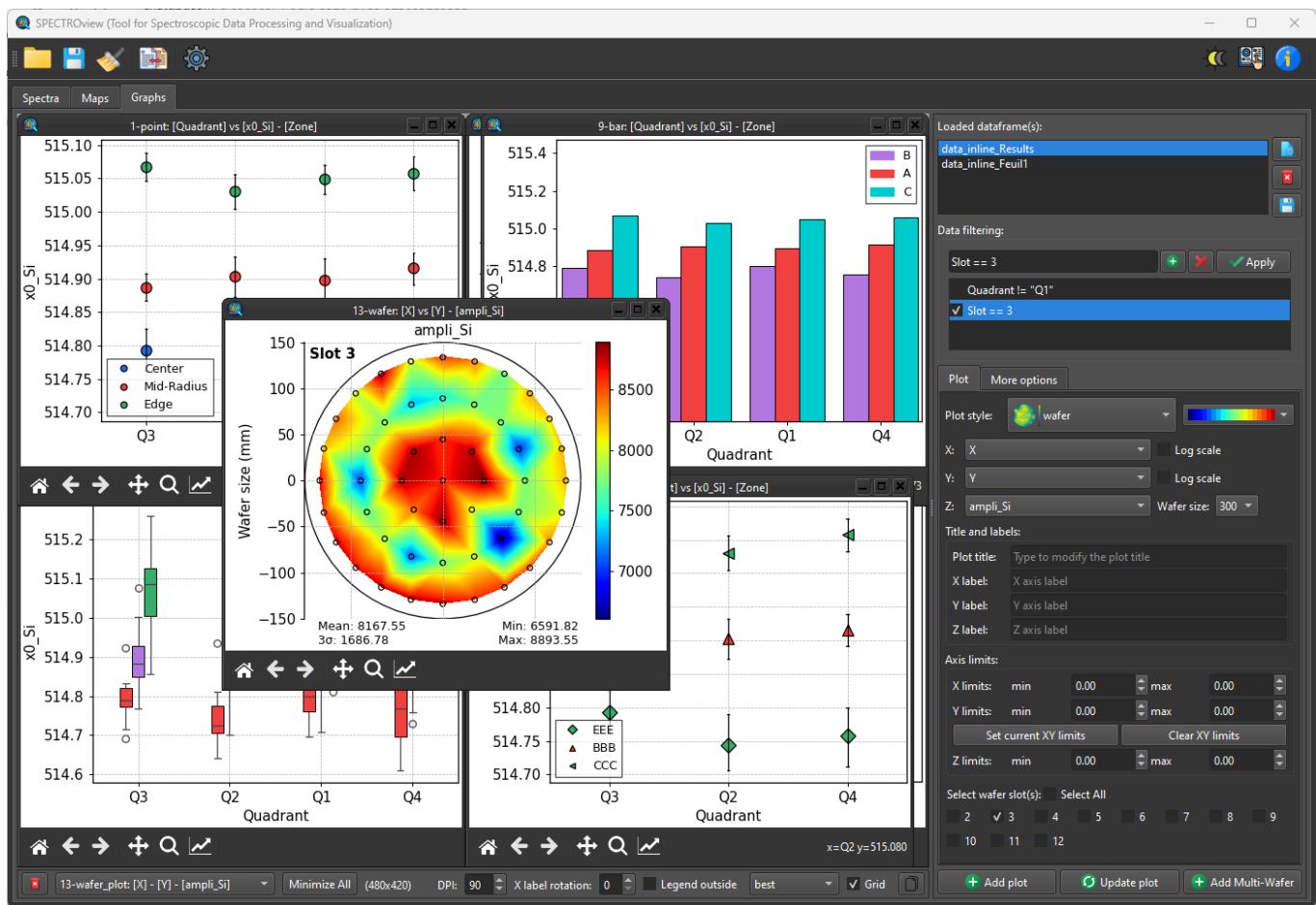


Figure 12: Graphs Workspace interface. The Control Panel is located on the right side, while the Graph Viewer is displayed on the left side.

6.1 Loading data

Datasets (dataframes) can be sent directly from other workspaces (Spectra or Maps) or loaded from Excel files. Excel files may contain one or multiple worksheets; each worksheet is loaded into the Graphs Workspace as an independent dataset. Multiple datasets can be loaded simultaneously.

All loaded datasets are displayed in a list widget (cf. top section of the right control panel within Figure 12), from which the user can select the dataset to work with.

6.2 Add a new plot

- Selected datasheet among the loaded dataset via the Listbox → X, Y, Z dropdown menu will be populated with all columns available in the selected dataset.
- Select the plot styles : scatter, point, bar, box, line, 2Dmap, wafer
- Specify the label of the x and y axis, as well as the title of the plot (optional).
- Set the limits of the x and y axis (optional)
- Define the label as well as the z limit range (for the heatmap type only) (optional).
- For wafer plot type: → define the wafer size: 100, 200, 300 (mm).
- Click to the Add plot button

6.3 Update/Modify existing plot

To update/modify or adjusting the any properties an existing plot:



- Select to the plot to be updated/modified.
- Make change(s)/modification(s) via the ControlPanel on the right side, such as: plot type, axis labels, axis limits, text size (DPI), axis label rotations, legend box location, grid...



- Click Update button to apply the changes/modifications to the selected plot
- Click to the Copy button to copy the select figure into Clipboard.

6.4 Data filtering feature

The **pandas.DataFrame.query()** method allows you to filter rows from a DataFrame based on a boolean expression. It's a powerful and flexible way to subset your DataFrame to include only the rows that meet specific conditions.

In **SPECTROview**, User can work with the entire dataset or a part of the dataset by using **filtering feature** (Figure 13). The selected dataset can be filtered by typing as following syntax:

`(column_name) (operator) (value):`

- `(column_name)`: is the exact header of the column containing the data to be filtered. When the column header contain 'space', you need to enclose them in single or double quotes (see example below).
- `(operator)`: it could be comparison operators (e.g., `==`, `<`, `>`, `<=`, `>=`, `!=`) and logical operators (e.g., `and`, `or`, `not`) to build complex and multiples conditions.
- `(value)`: it could be numeric or string values. String value must be enclosed in double quotes (cf. example below)

Examples of using Filter features: Assuming that the datasheet containing several columns, including the columns whose headers are : Confocal, Thickness, a3_LOM, Laser Power and other columns....

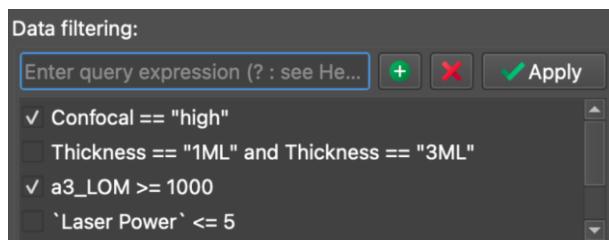


Figure 13: Example of the use of filters for dataframe within SPECTROview

Confocal <code>!=</code> "high"	→ selected all values within column “Confocal” that is different to “high”
Thickness <code>==</code> "1ML" <code>or</code> Thickness <code>==</code> "3ML"	→ selected all values within column “Thickness” that is equal to 1ML OR 3ML
a3_LOM <code>>=</code> 1000	→ selected all values within column “a3_LOM” that is superier to 1000
`Laser Power` <code><=</code> 5	→ selected all values within column “Laser Power” that is superier or equal to 5.

6.5 Other plot customization

Additional view and customization options are available in the **MoreOptions** tab (Figure 14).

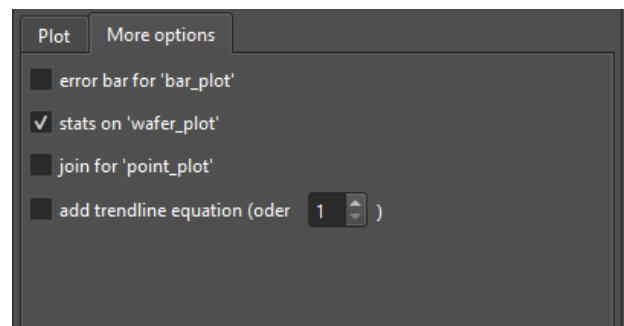


Figure 14: MoreOptions Panel

Users can also customize the legend box (labels, colors, and/or markers) for each curve directly from the plot by clicking on the legend box (Figure 15).

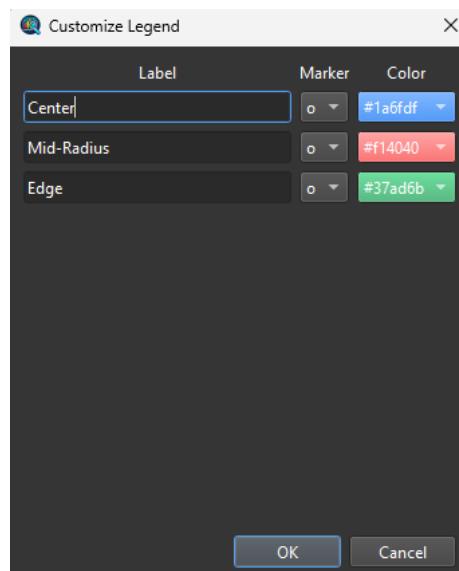


Figure 15: Customize Legend panel displayed when clicking on the plot legend.