SPECTROview User Manual

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1. Introduction

Spectroscopy techniques such as Raman Spectroscopy and Photoluminescence (PL) 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 inferface 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 3.8 and 3.12) 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
```

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.

Users can download these files to practice using the tool.

3.1 Spectroscopic data (.txt)

SPECTROview supports spectroscopic data (text format) from Renishaw (WiRE) or Horiba (LabSpec 6) tools. The files must consist of two columns:

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

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) from Horiba (LabSpec 6) and Semilab tools. The data is arranged as follow:

		R_1	R_2	R_3	…	R_{n-1}	R_n
X1	Y1	Intensity1	Intensity1	Intensity1	…	Intensity1	Intensity1
X2	Y2	Intensity2	Intensity2	Intensity2	…	Intensity2	Intensity2
…	…	…	…	…	…	…	…
Xn	Yn	Intensityn	Intensityn	Intensityn	…	Intensityn	Intensityn

- The first row (R1 → Rn) is the Raman shift (cm^{-1}) of all spectrum
- Two first columns list ting the X and Y coordinate of the spectrum within the maps.
- Then the corresponding intensity of each spectrum (Intensity1 → Intensityn) is added from row 2^{nd} to row n.

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.

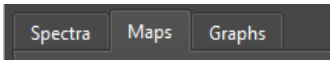
3.4 Formats saved by SPECTROview application

epending 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.

A **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 utility 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 *_converted* (4.4).

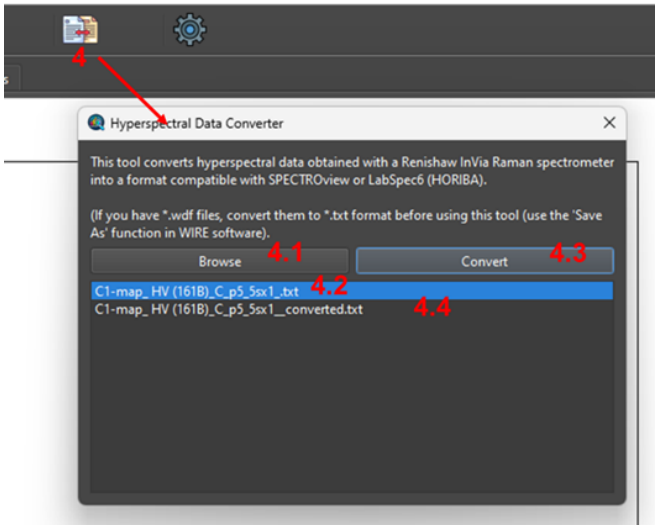
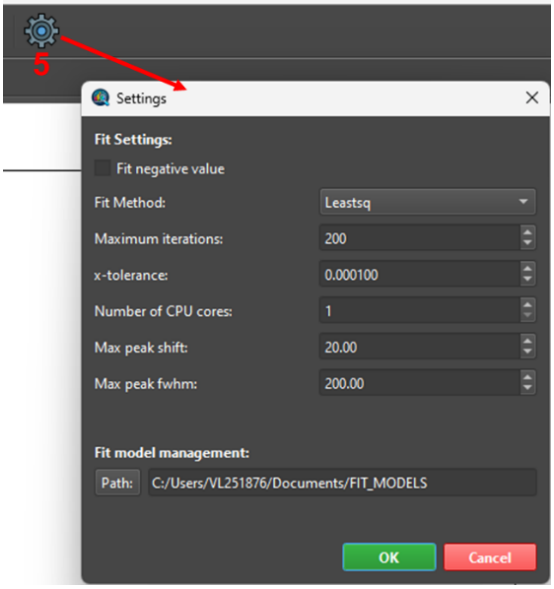


Figure 1: Interface of “Hyperspectral Data Converter”

	**“Settings”:** Opens the **Settings Panel** to adjust fitting parameters and define the storage folder for user-defined fitting models	 Figure 2: Setting Panel
	Theme Toggle: Switches the application GUI between Dark and Light modes.	
	To Open this User Manual document.	
	To displays version information and details about the application..	

5. Spectra and Maps workspaces

The Maps and Spectra 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.

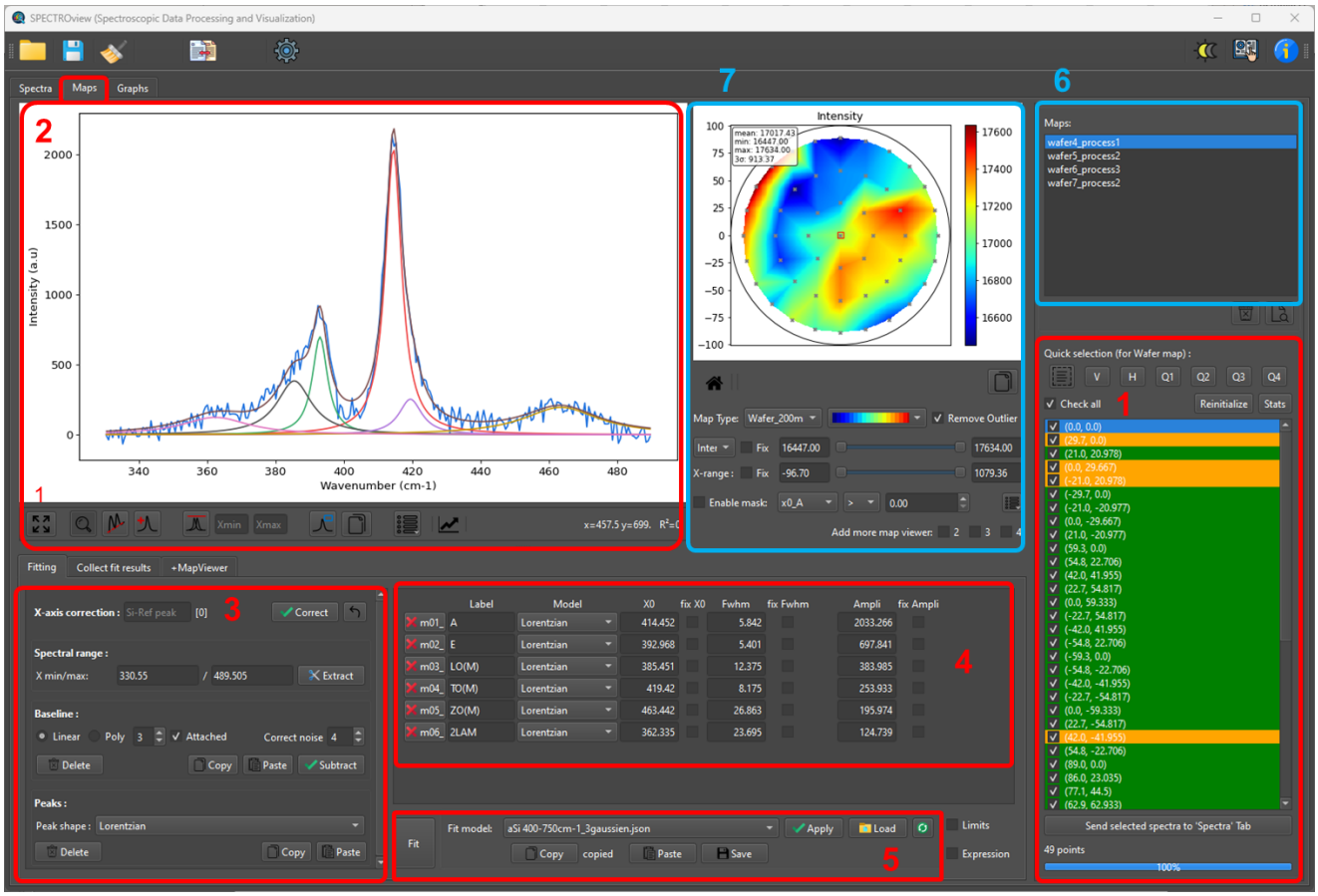


Figure 3: Interface overview of Spectra and Maps workspaces. The interface is divided into different sections, called widgets (1 to 5). Widgets 1 to 5 are identical in both workspaces, whereas widgets 6 and 7 are dedicated specifically to the Maps workspace.

- Widget 1: Spectra List
- Widget 2: Spectra Viewer
- Widget 3: Fit Model Builder
- Widget 4: Peak Table
- Widget 5: Fit Model Control
- Widget 6: Map List
- Widget 7: Map Viewer

5.1 Spectra List

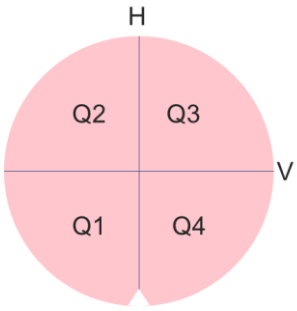
Spectra List widget displays all loaded spectra. The user can select one or several spectra to work with.

Once selected, the spectra will be plotted in Widget Spectra Viewer (see below).

Button functions:

1 : To select all loaded spectra

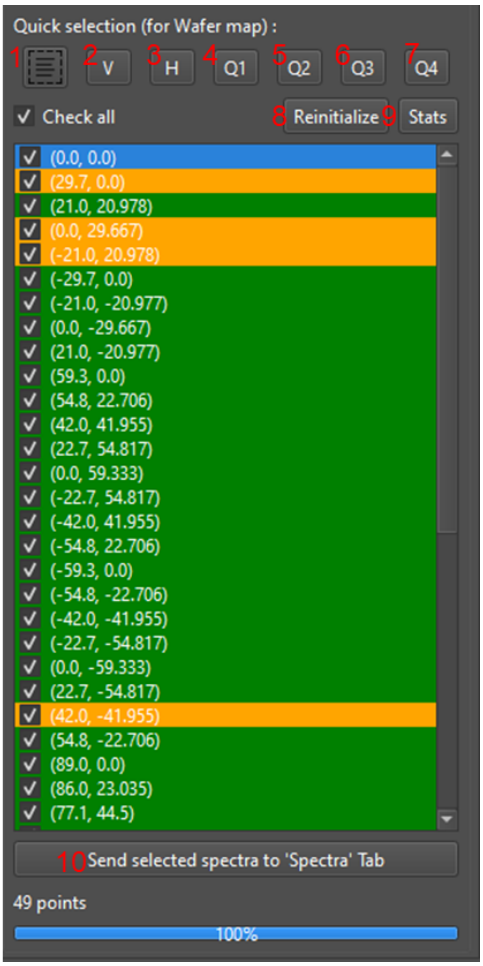
2 → 7 : used for wafer_maps to quickly select a region of interest (vertically, horizontally, or by the 4 different quadrants of the wafer), as illustrated in the figure below:



8 : Reinitilize to the RAW spectrum

9 : Show the fit report and statistics for the selected data (available only for fitted spectra).

10 : Send selected spectra to the Spectra workspace. This is useful for comparing different spectra from different 2D maps or wafer maps.



5.2 Spectra Viewer

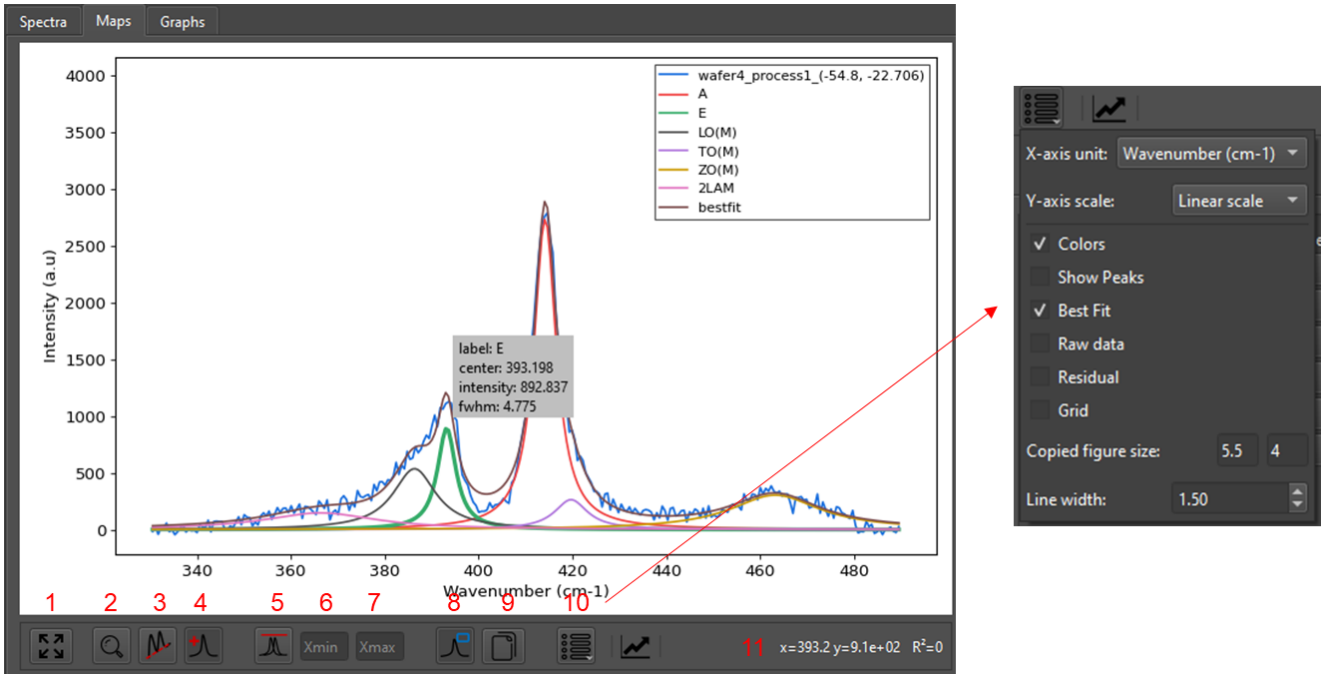
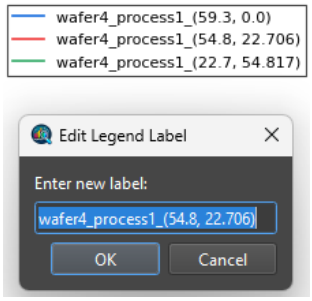
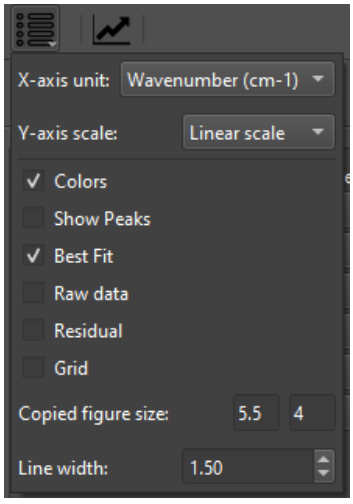


Figure 4: Spectra Viewer (left) widget and View Options Menu (right).

	Rescale: o 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 boxe 'min' and 'max'.
	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). Note: This feature only works when the Zoom button is deactivated. 
	Copy: - Click : copies the spectra plot to the clipbroad as an image. The user can then paste it into other applications (PowerPoint, Excel, etc.). - Ctril + Click (or Cmd + click on macOS): Copies the numerical data of the spectra (including RAW data and best-fit curves) to the clipboard.
	More options: Opens a pop-up window with several view options (as shown figure on the right). The user can adjust these options (figure size, line width, etc.) before clicking Button 9 to Copy. Other menu options: - "Show peaks": Displays peak labels on the plot - "Best Fit":Toggles the visibility of the fitted peaks. - "Raw data" : Toggles the visibility of the raw data. - "Residual": Displays the residual (Raw Data – Best Fit Curve). 

Other Features:

- Show Peak Parameters: Hovering the mouse cursor over a peak displays a pop-up with the peak parameters (label, intensity, FWHM, position), as shown in Figure 4.

- Add/Remove Peaks: Right-click to remove the current peak, or left-click to add a new peak (ensure the Peak button  is active).
- Quick Scale: Use the mouse wheel to quickly adjust the Y-axis (intensity scale).).

5.3 Fit Model builder

This widget contains 4 sections corresponding to the 4 main steps for fitting any spectrum.

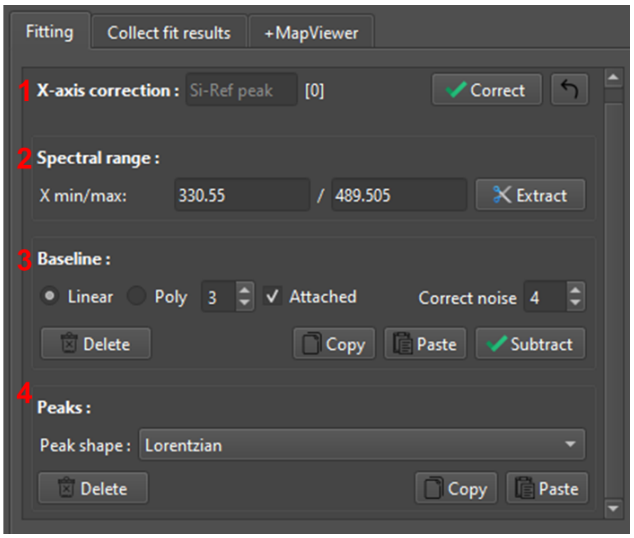


Figure 5: Fit model builder

Step 1: X-axis Correction (Optional) Used when the user wants to perform an X-range correction using a well-known reference sample. In SPECTROview, this feature is designed to work with a Silicon reference sample, which has a theoretical peak position at 520.7 cm^{-1}.

Procedure:

- Record the Si-Ref sample in the same experimental session as the other samples, using the same measurement parameters.
- Fit the Si-REF spectrum to determine the measured Silicon peak position.
- Type the measured position into the text box
- Select spectrum or spectra to be correct → x range correction is done based on the difference between the measured position and the theoretical value (520.7 cm^{-1})

Step 2: Define the X-axis range to use for the fitting process.

Step 3: Baseline:

- Baseline points are defined by the user in the spectra plot (Spectra Viewer widget) by left-clicking. The Baseline button  must be active (cf. section 5.2).
- Attached checkbox : When checked, the baseline points remain attached to the spectrum curve.
- Correct noise: Calculates the baseline point based on the average of the specified number of nearby points, ensuring it sits in the center of the noise level.
- Other properties of baseline: The baseline type (e.g., Linear, Polynomial) can be adjusted as needed.

Step 4: Peak(s) definition:

- Users can define peaks directly on the spectra via the Spectra Viewer by left-clicking. The Peak button  must be active (cf. section 5.2).
- Any peak added to the fit model will be displayed in the Peak Table widget (see below).

5.4 Peak Table

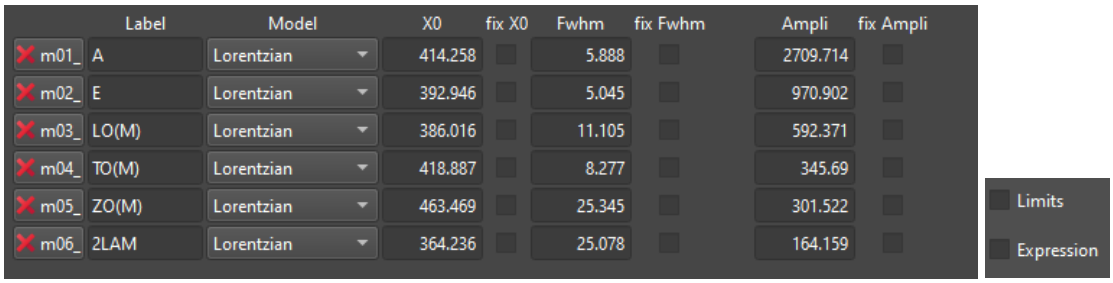


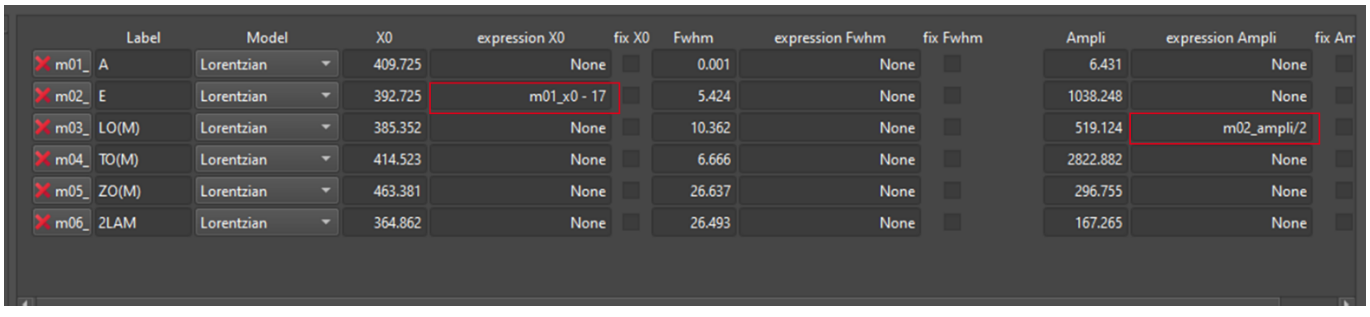
Figure 6: PeakTable widget

The properties of all peaks added in the previous steps (*label*, *model*, *position*, *FWHM*, *intensity*) are dynamically updated in this table. Users can remove peaks or adjust their properties here. Peak labels are optional.

Constraints: Users can fix one or several parameters for each peak by checking the corresponding box next to the parameter. For advanced constraints, two checkboxes options appear below the PeakTable:

- **Limits**: When checked, this displays *Max* and *Min* value columns for each parameter. This allows the user to define a specific range within which the peak parameters can vary (unlike the "Fix" option, which holds the value constant).

- Expression : used to link the variation of different peaks or parameters.
  - Example 1: To constrain the position of peak `m02_` to be 17 units less than `m01_`, type: `m01_x0 - 17`.
  - Example 2: To constrain the intensity of peak `m03_` to be half that of `m02_`, type: *`m02_ampli / 2`*



5.5 Fit Model Control

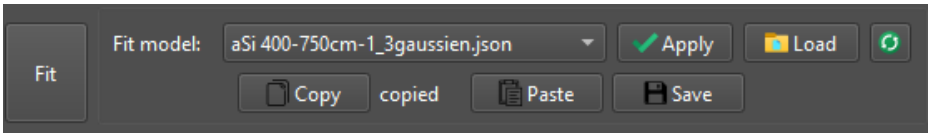
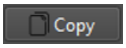


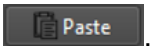
Figure 7: Interface of Fit Model Control

Once the desired "Fit Model" is defined (as shown in the Peak Table), click the Fit button to start the fitting process.

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

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

- Select the fitted spectrum and click **Copy** 

.
- Select one or multiple target spectra and click **Paste** 

.

Saving Fit Models: Users can save the fit model for later use by clicking Save 

. It is recommended to save all models in a predefined folder. This folder can be defined in the Settings Panel (Figure 2). Once saved, models can be quickly accessed via the "Fit Model" dropdown menu.

5.6 Maps List & Map Viewer

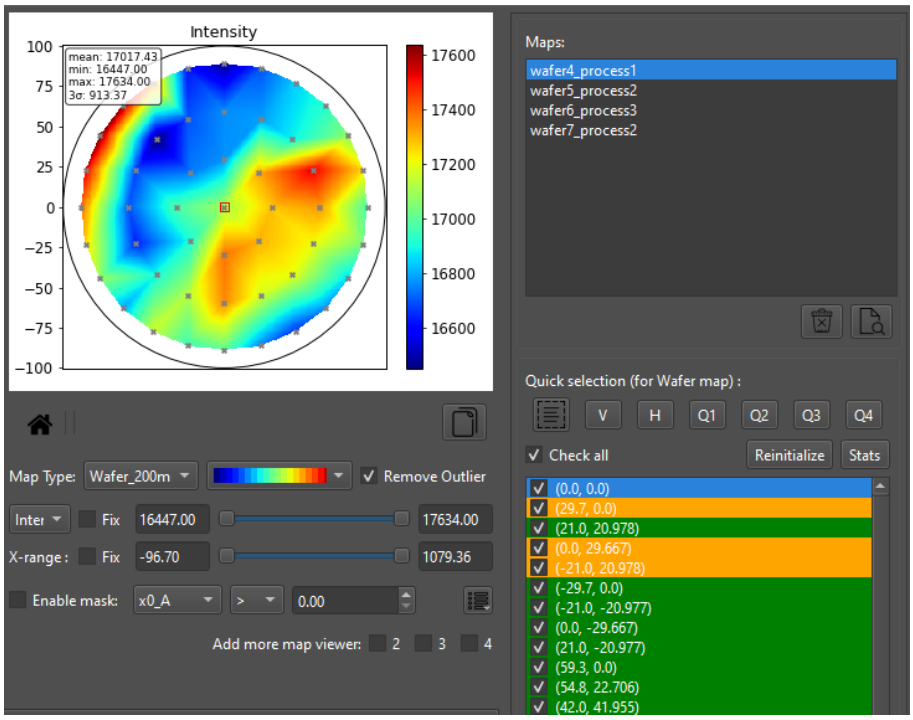


Figure 8: MapsList and MapViewer widgets are specific to the Maps workspace.

- MapList: Allows navigation between loaded 2D maps or wafer maps. Selecting a map automatically updates the SpectraList to show the all spectra of that dataset.

MapViewer: Displays a heatmap of the selected data. This heatmap is synchronized with the SpectraList to highlight selected spectra. A Control Panel below the heatmap contain several GUI elements for quick data processing:

- *Map Type*: Select between Wafer Map (300, 200, 100mm) or 2D Map.
- *Color Palette*: Select the color scheme for the heat map.
- *Remove Outlier*: Removes outlier points (top/bottom 3%) from the visualization.
- *Parameters*: Select which parameter to plot (e.g., "Area", "Max Intensity"). Once the data is fitted, best-fit parameters will also appear here.
- *Parameter/X-Range*: Define the calculation range for Area and Max Intensity using the sliders or text boxes.
- *Mask*: Acts as a filter for the heatmap plot

- Example: Plot the heat map of Parameter A, but only where Parameter B is lower/higher than a specific value.

- *Add More Map Viewers*: Enables viewing 2, 3, or 4 maps simultaneously for comparison..

5.7 Collect and Save Fit Results

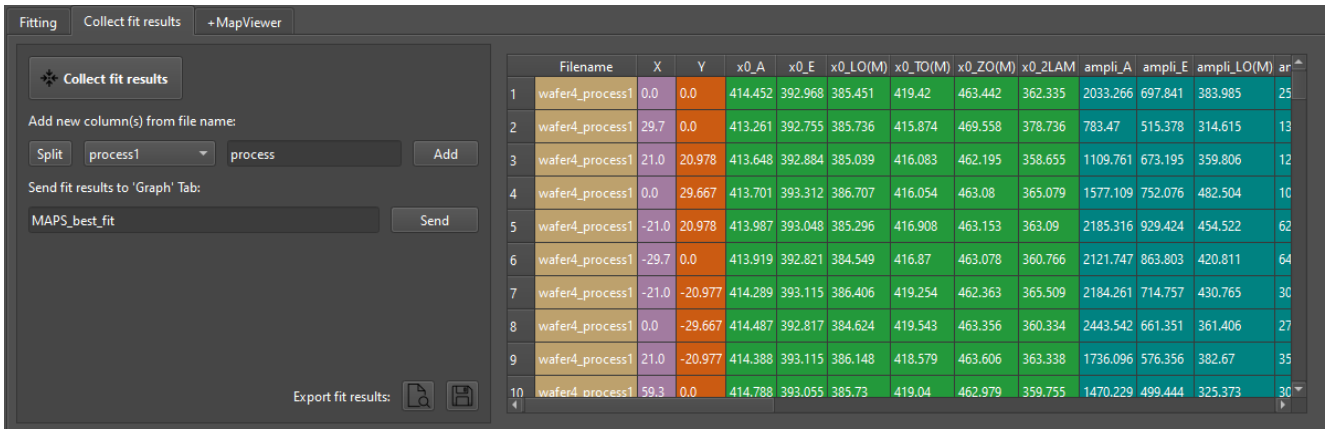
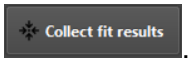


Figure 9: Collect fit results panel

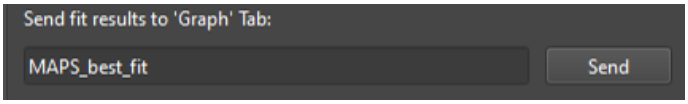
SPECTROview is designed for effortless data access and export. To collect best-fit data from all spectra or maps:

- Switch to the Collect Fit Results.
- Click to the Collect button 

.
- Results are then aggregated into a table and displayed in the GUI (Figure 9).

From here, the user can :

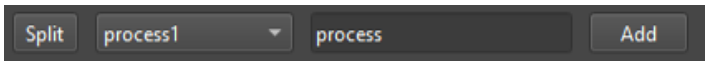
- Name the data table and send it to the Graphs workspace for plotting (cf. Section 6) :



- Export the results as an Excel file .

Split feature: This feature extracts information from filenames and adds it to the data 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"..



5.8 +MapViewer Panel

This panel becomes active when the "Add more map viewer" checkboxes are selected (Figure 8). It allows the user to visualize heat maps of multiple parameters simultaneously, facilitating easy comparison and assessment, as shown in Figure 10.

The functionality of each MapViewer are identifical with main MapViewer as presented in Section 5.6.

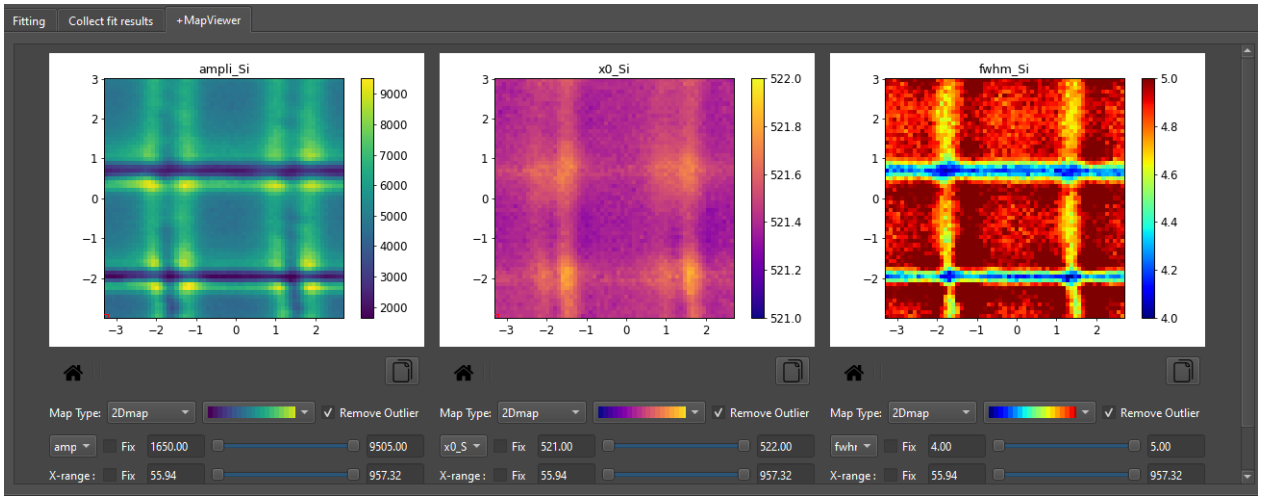


Figure 10: More MapViewer.

5.9 Save workspace.

To save the current workspace, click the Save button 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

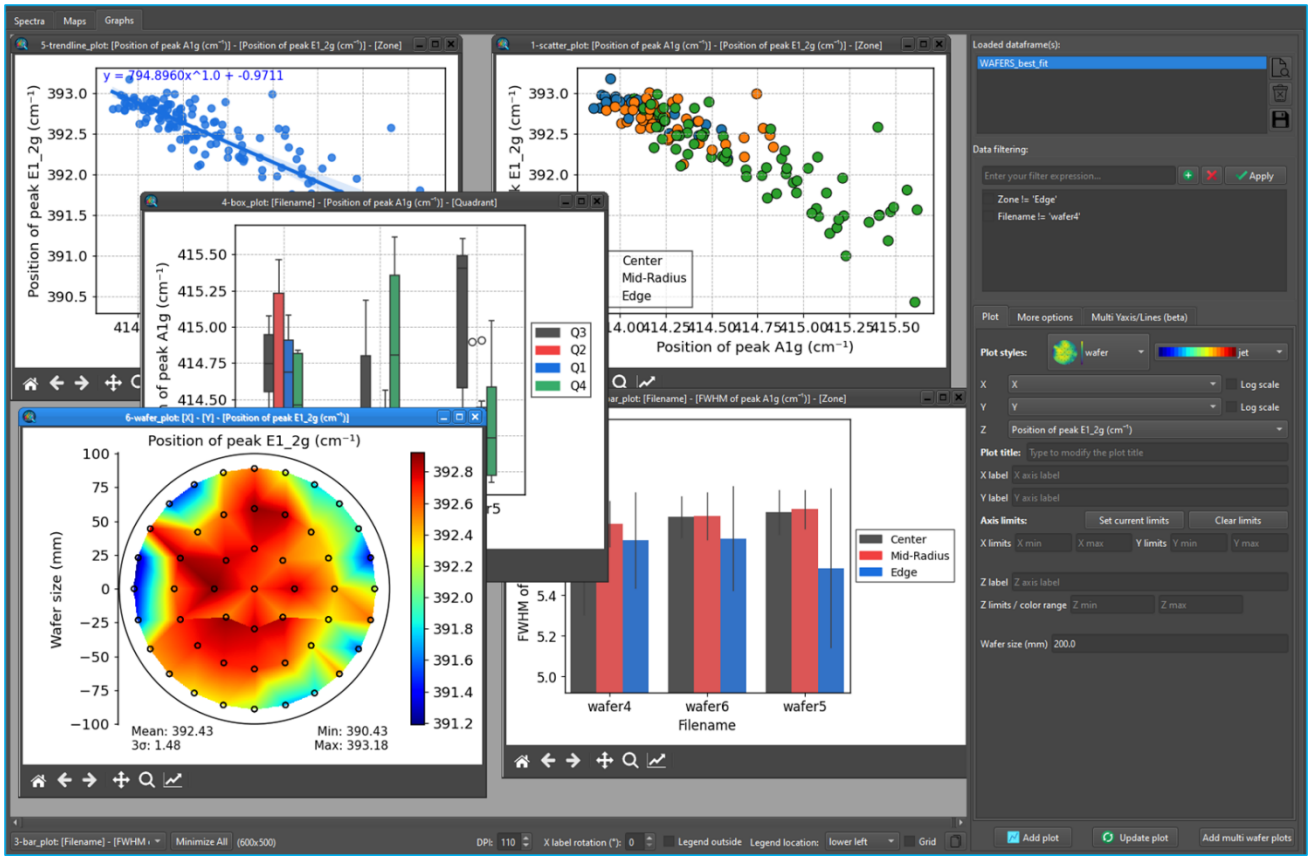


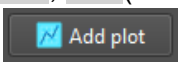
Figure 11: Interface of Graph workspace: one the right i the Control Panel is on the right side and the Graph Viewer is on the left side.

6.1 Loading data

Data can be loaded from an excel file, or sent directly from the “Spectra” or “Maps” workspace.

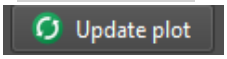
One datasheet or multiple datasheets can be loaded in the same time. Each datasheets are listed in the listbox. User can be selected one to work with.

6.2 Add a New Plot

- Selected datasheet among the loaded datasheets via the Listbox → X, Y, Z dropdown menu will be update with the columns avaibale in the selected datasheet.
- 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 x limit range (for the heatmap type only) (optional).
- Define the wafer size: 100, 200, 300 (mm) (for wafer plot only).
- Click to the Add plot button 

6.3 Update plot

To update the properties or data of an existing plot:

- Select to the plot to update
- Make change(s)/modification(s) via the Control Panel on the right side
- Click Update button to update the plot 

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**, query() method is integrated and can be used via GUI by typing as following:

(`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 cloumns whose headers are : `Confocal, Thickness, a3_LOM, Laser Power` and other columns….

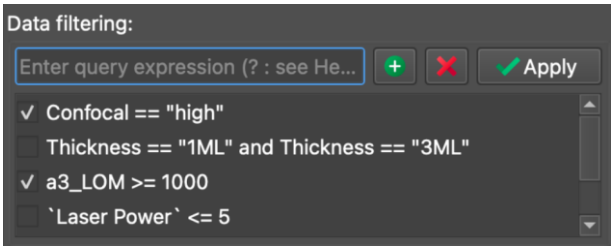


Figure 12: Example of the use of filters for dataframe within SPECTROview

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

6.5 Plot Customization

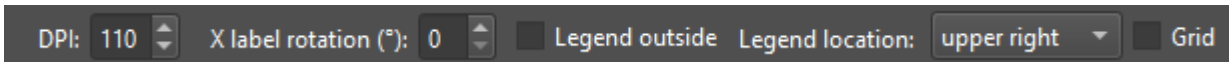


Figure 13: Some customization options to adjust the policy size (DPI), rotate the label of the x axis, place the legend outside of the plot, modify the location of legend box, toogle the grid plot …

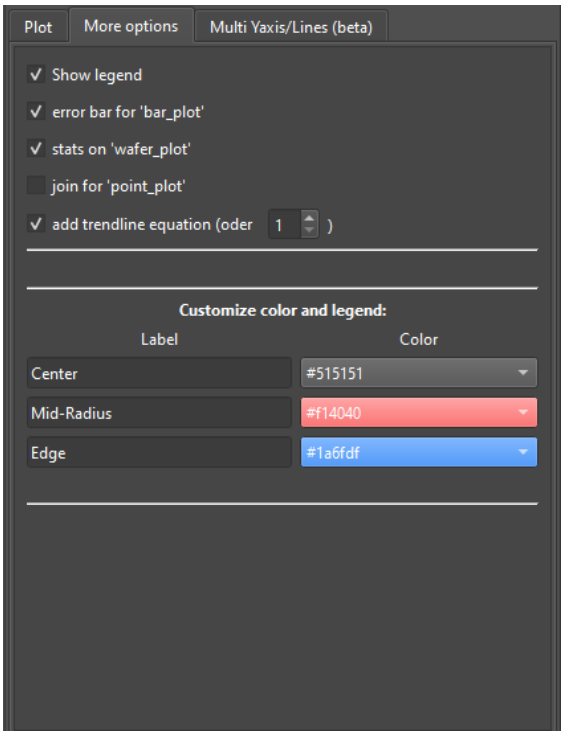


Figure 14: MoreOptions Panel to customized label and color for the legends of the selected plot.