LabSpec 5 (LS 5)

Notation

- Names of icons and menu items are denoted in **bold**.
- Names of windows are denoted in *italic*.
- Names of columns, rows or entries in a window are denoted in all CAPITAL.

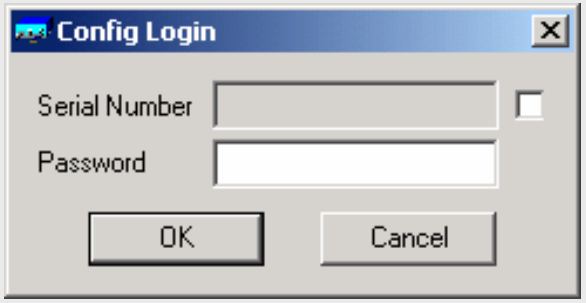
Configuration Utility

Versatility

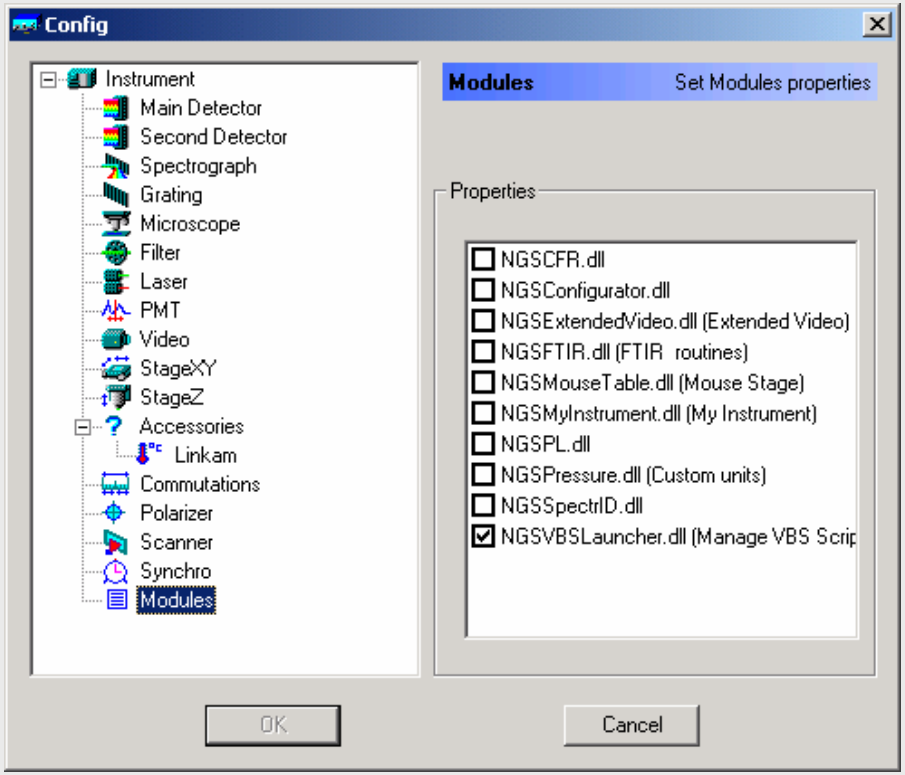
- We provide a wide range of Raman microscope/spectrometer instruments (analytical, research, processing, etc.), which require various configurations to meet the need of the applications specified by customers.
- While we can optimize the system to yield the best results in the target application, the service (maintaining existing systems, adding accessories, upgrading obsolete parts, etc.) could become a daunting task.
- The design goal of LabSpec 5 is to provide a platform that can adapt and control dynamically changing configurations without having to replace the software.
- The task is accomplished mainly through Config utility, where the specific configuration of the instrument is specified.

Accessing Config

- Double clicking **Config** icon opens the *Config Login* window, the operator can access the configuration of the LabSpec 5 in three levels.
  - No password: Clicking **OK** button with no password will prompt a message box that informs that changing configuration will be disabled. Clicking **OK** button of the message box opens the *Config* window in read-only format.



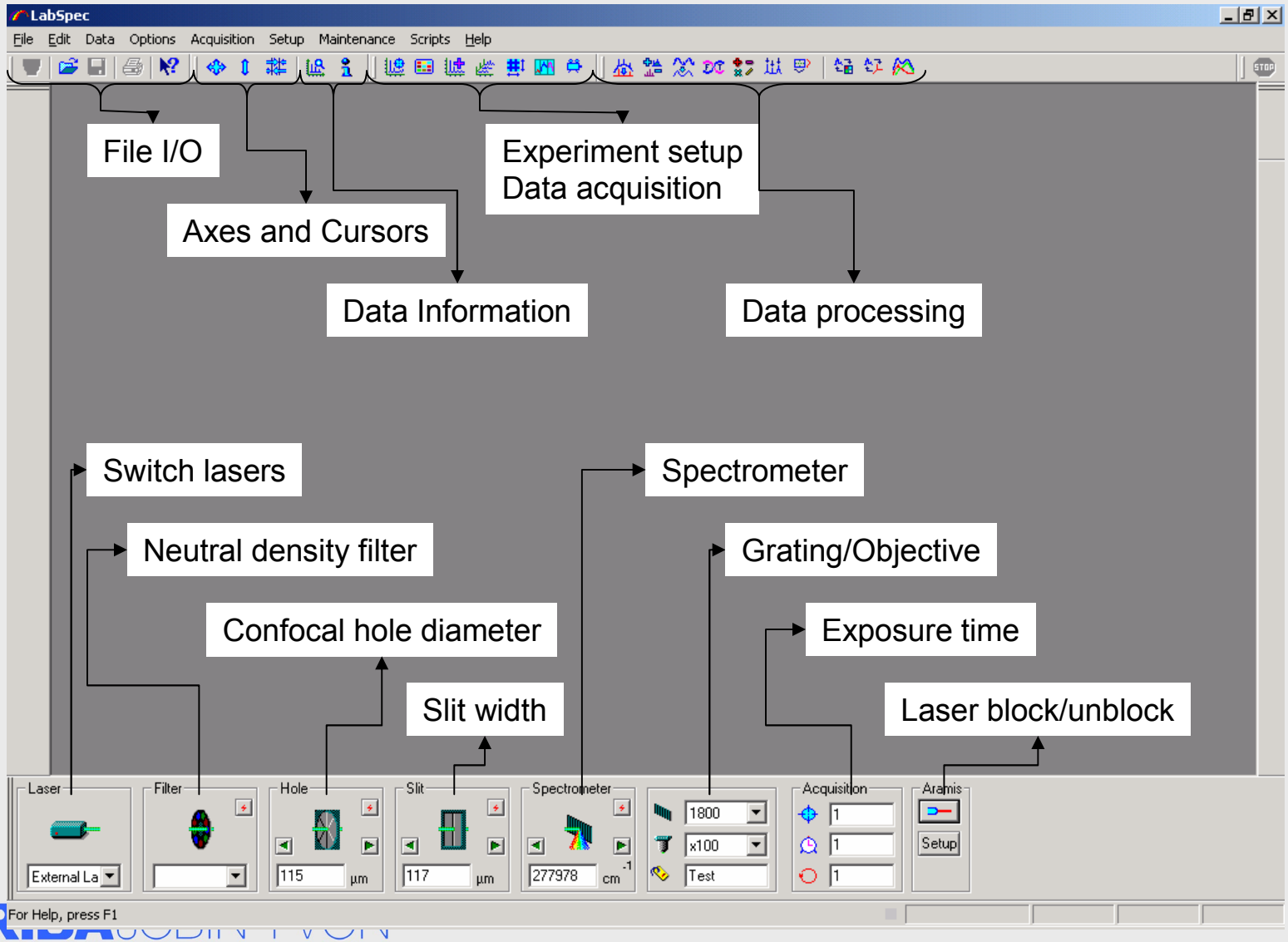
Config



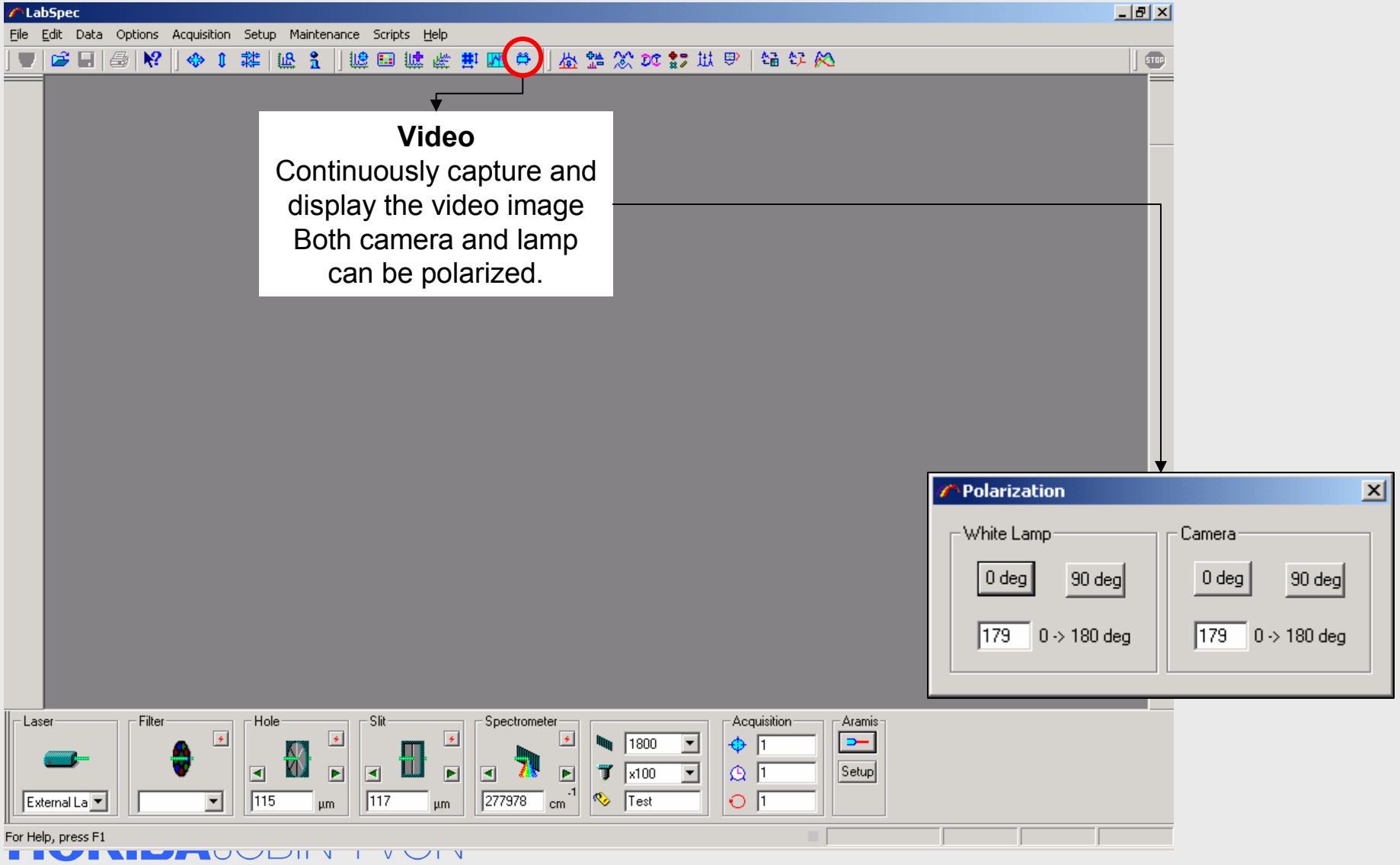
- Each element comes with a list menu, from which the specific component and its configurations can be defined.
- Module option is where customized options are listed. When activated, corresponding icons or controls will become available in LabSpec 5 main window.

Overview

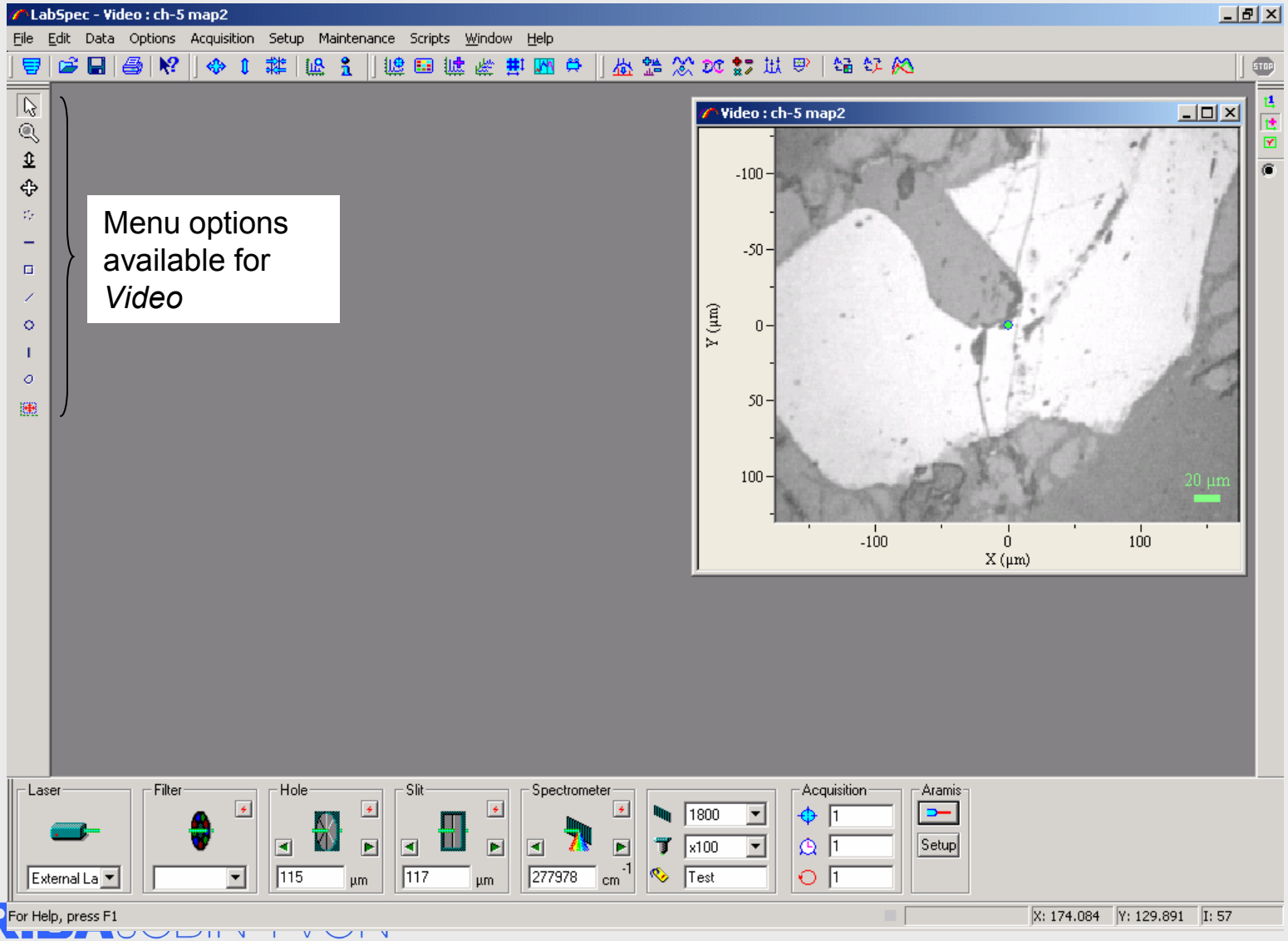
Main Window


LabSpec
File Edit Data Options Acquisition Setup Maintenance Scripts Help
File I/O
Axes and Cursors
Data Information
Experiment setup
Data acquisition
Data processing
Switch lasers
Neutral density filter
Confocal hole diameter
Slit width
Spectrometer
Grating/Objective
Exposure time
Laser block/unblock
Laser
Filter
Hole
Slit
Spectrometer
Acquisition
Aramis
External La
115 µm
117 µm
277978 cm-1
1800
x100
Test
Setup
For Help, press F1

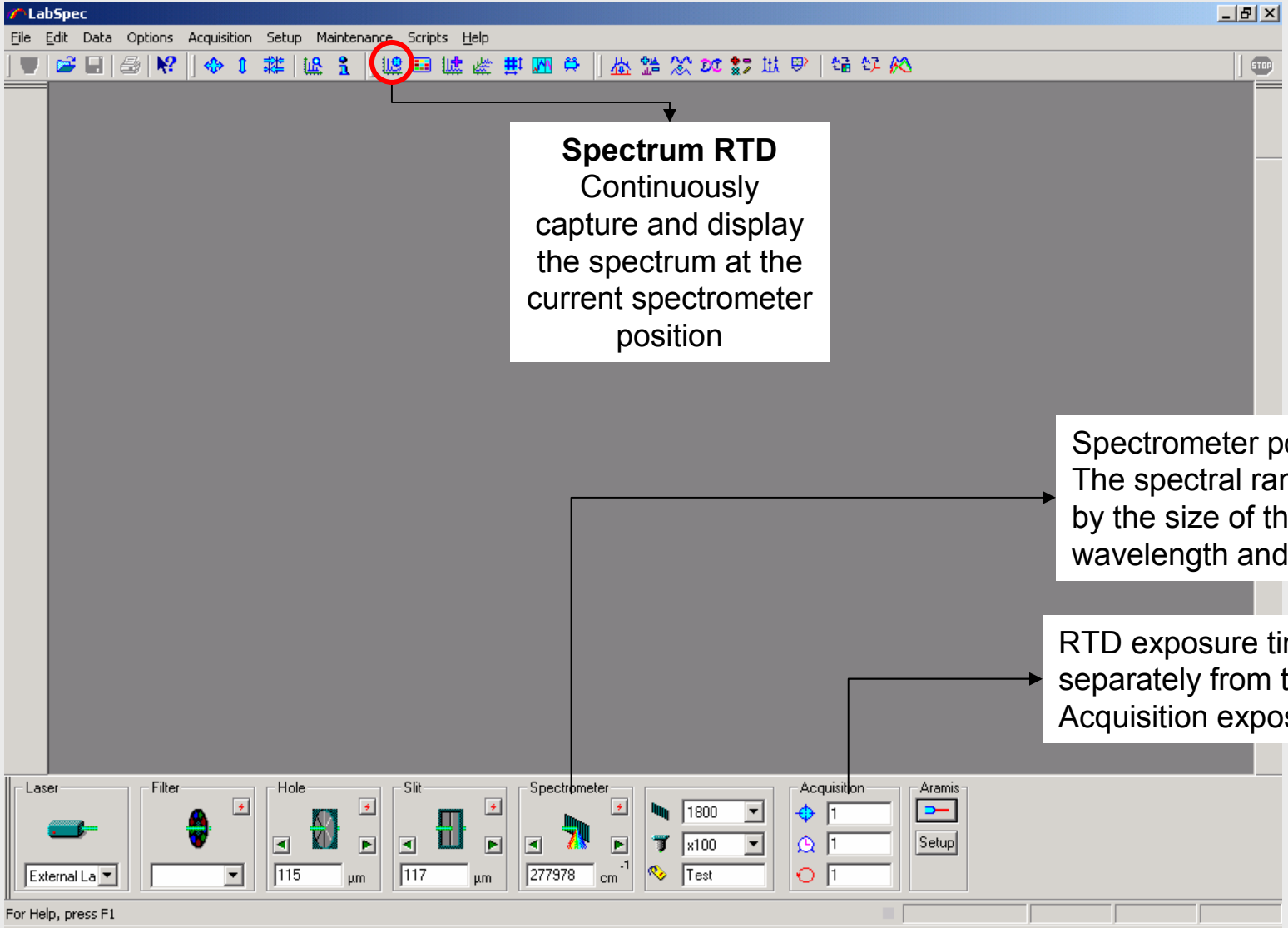
Video Acquisition



Video


LabSpec - Video : ch-5 map2
File Edit Data Options Acquisition Setup Maintenance Scripts Window Help
Menu options available for *Video*
Video : ch-5 map2
-100
-50
0
50
100
Y (µm)
-100
0
100
X (µm)
20 µm
Laser
External La
Filter
Hole
115 µm
Slit
117 µm
Spectrometer
277978 cm-1
1800
x100
Test
Acquisition
1
1
1
Aramis
Setup
For Help, press F1
X: 174.084
Y: 129.891
I: 57

Spectrum RTD (Real Time Display)

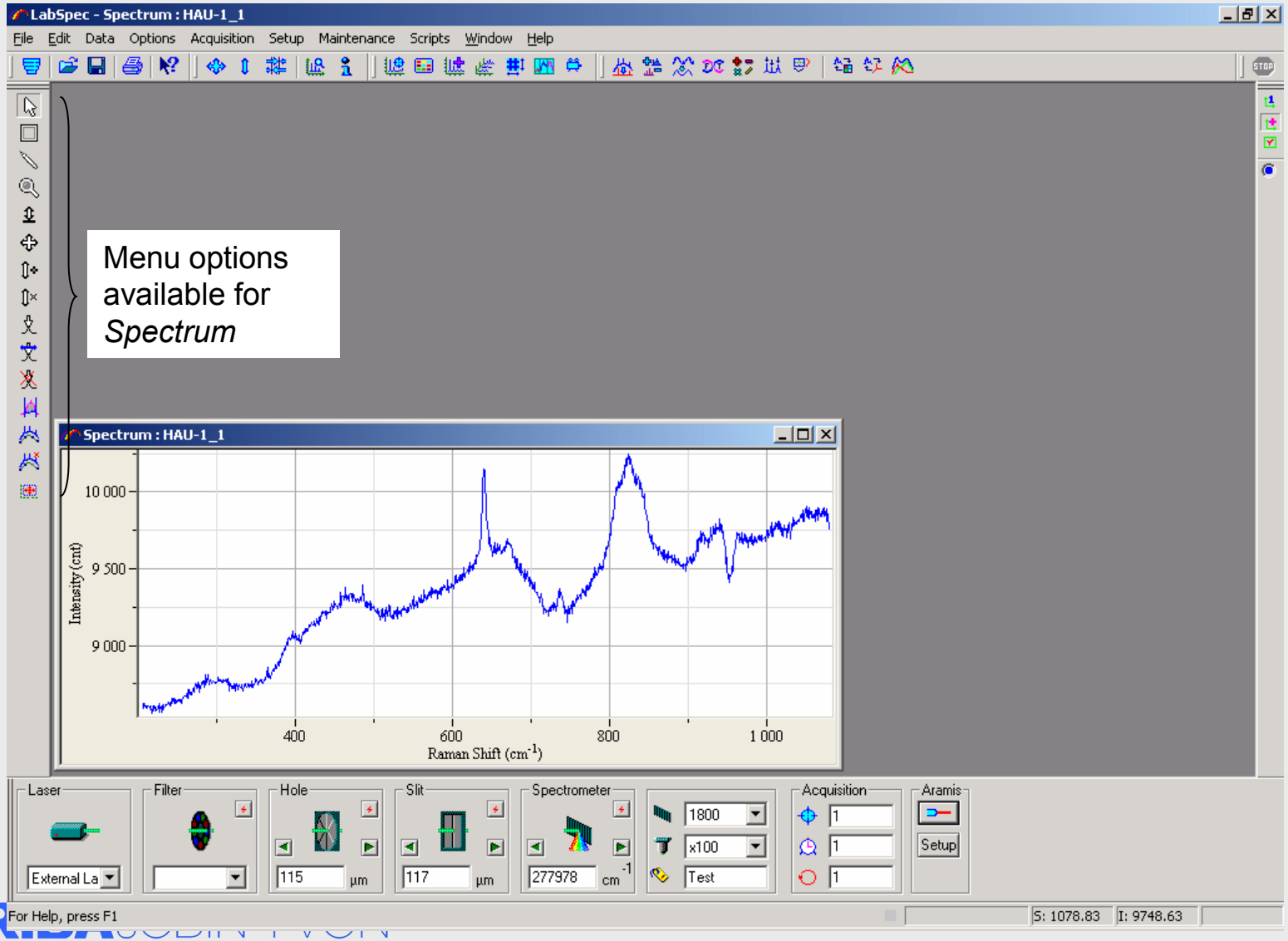


Spectrum RTD
Continuously capture and display the spectrum at the current spectrometer position

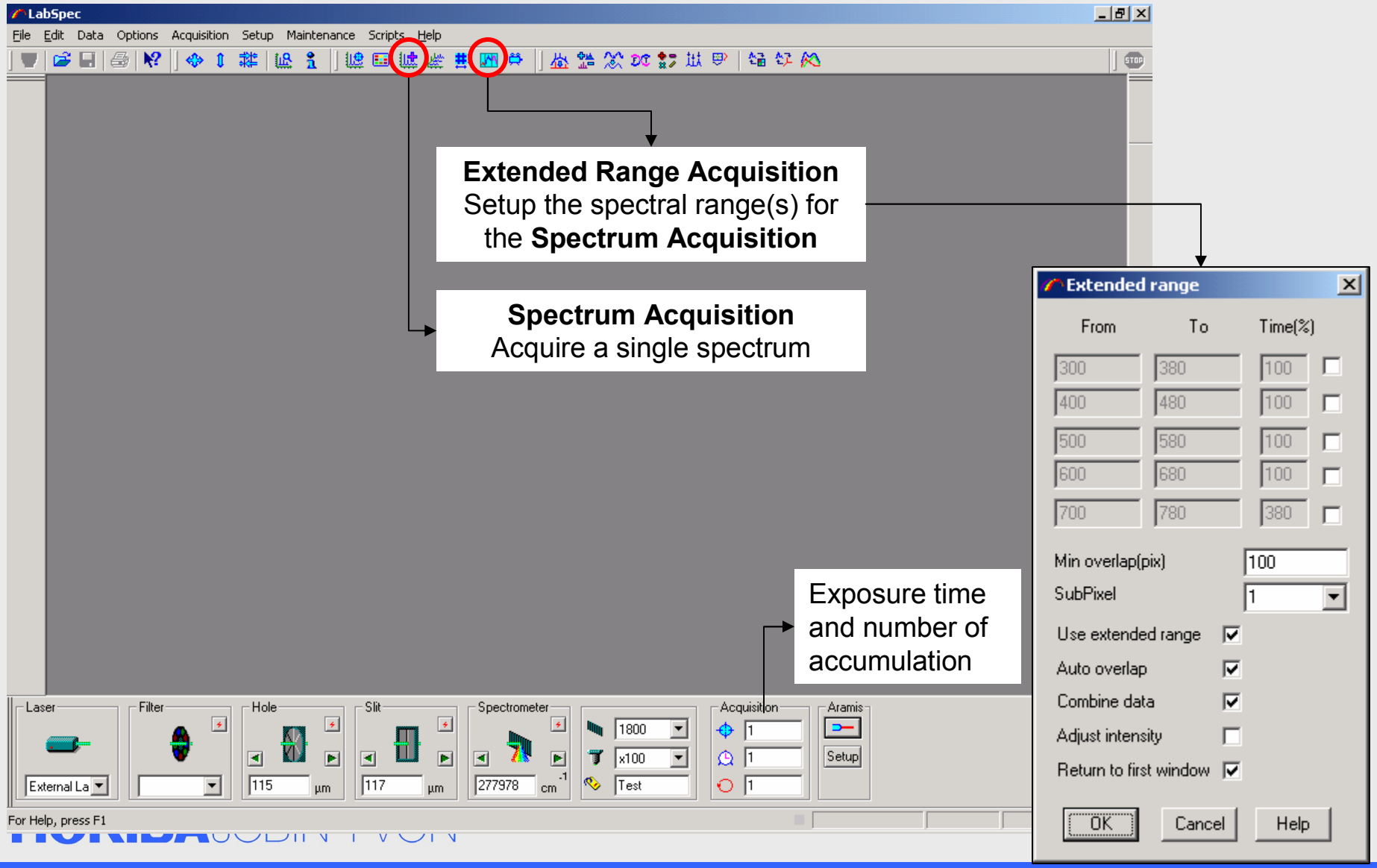
Spectrometer position
The spectral range is defined by the size of the CCD, laser wavelength and grating

RTD exposure time is set separately from the Data Acquisition exposure time

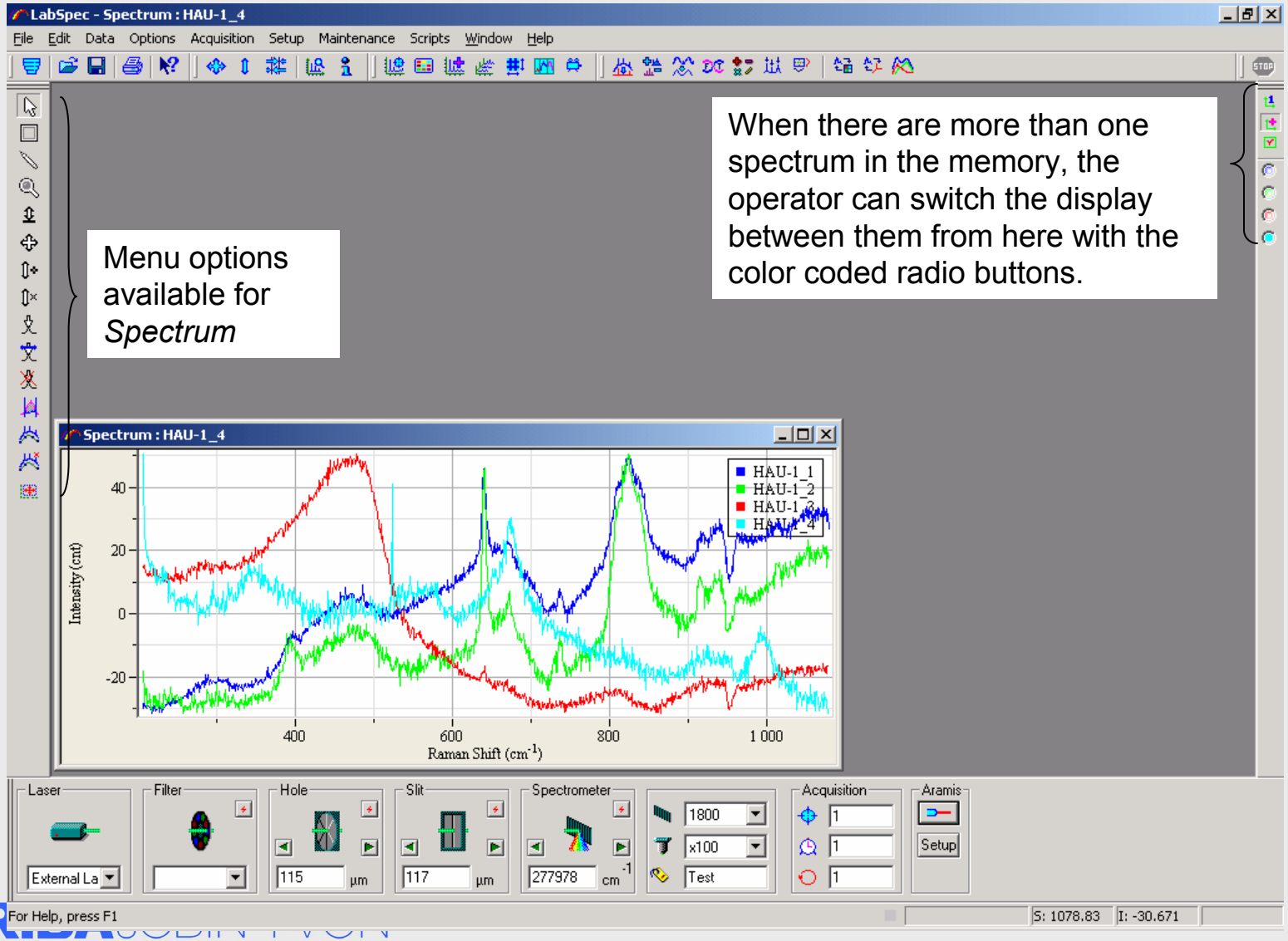
Spectrum


LabSpec - Spectrum : HAU-1_1
File Edit Data Options Acquisition Setup Maintenance Scripts Window Help
Menu options available for *Spectrum*
Spectrum : HAU-1_1
10 000
9 500
9 000
Intensity (cnt)
400
600
800
1 000
Raman Shift (cm-1)
Laser
Filter
Hole
Slit
Spectrometer
Acquisition
Aramis
External La
115 µm
117 µm
277978 cm-1
1800
x100
Test
Setup
For Help, press F1
S: 1078.83
I: 9748.63

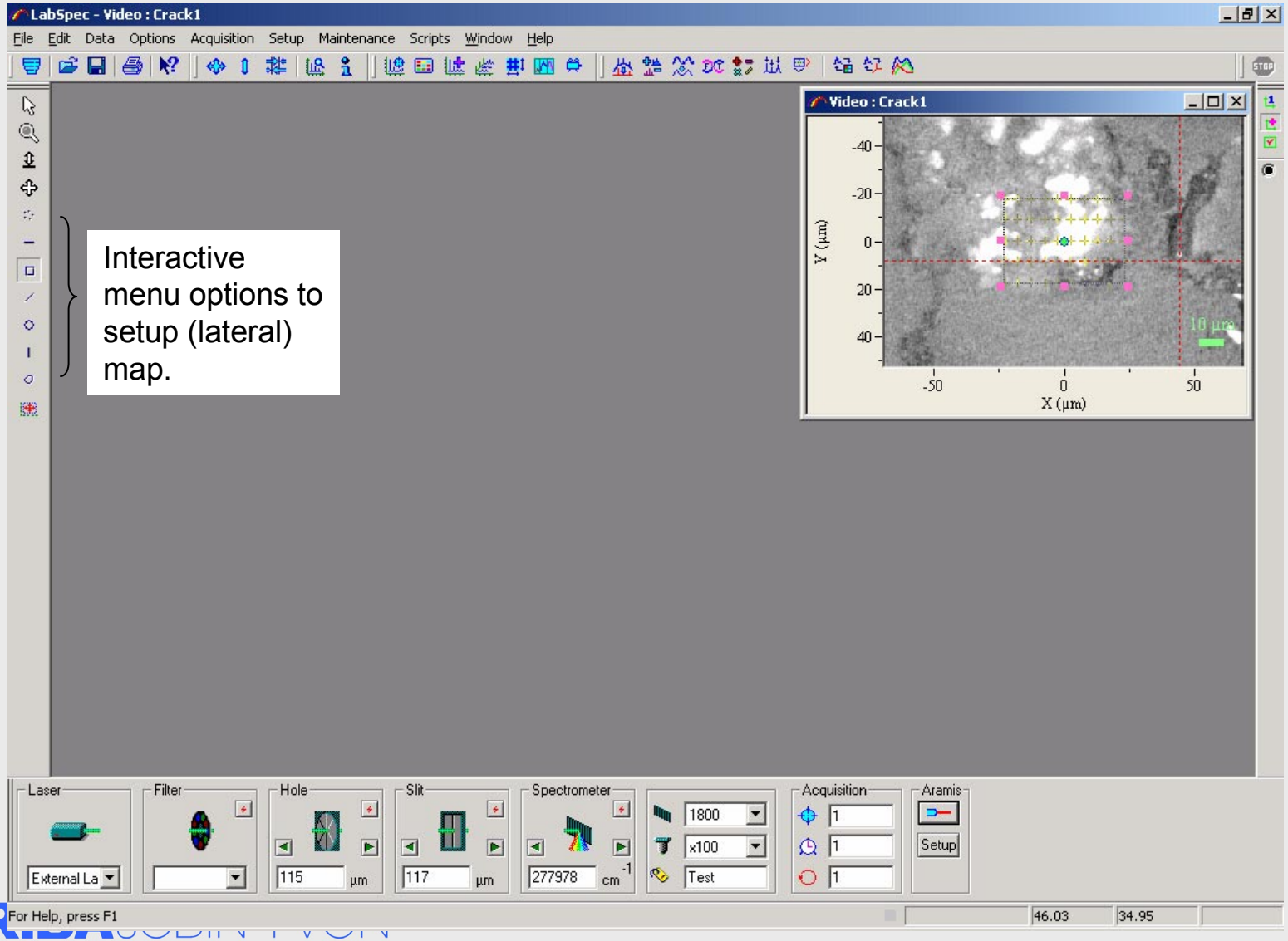
Spectrum Acquisition



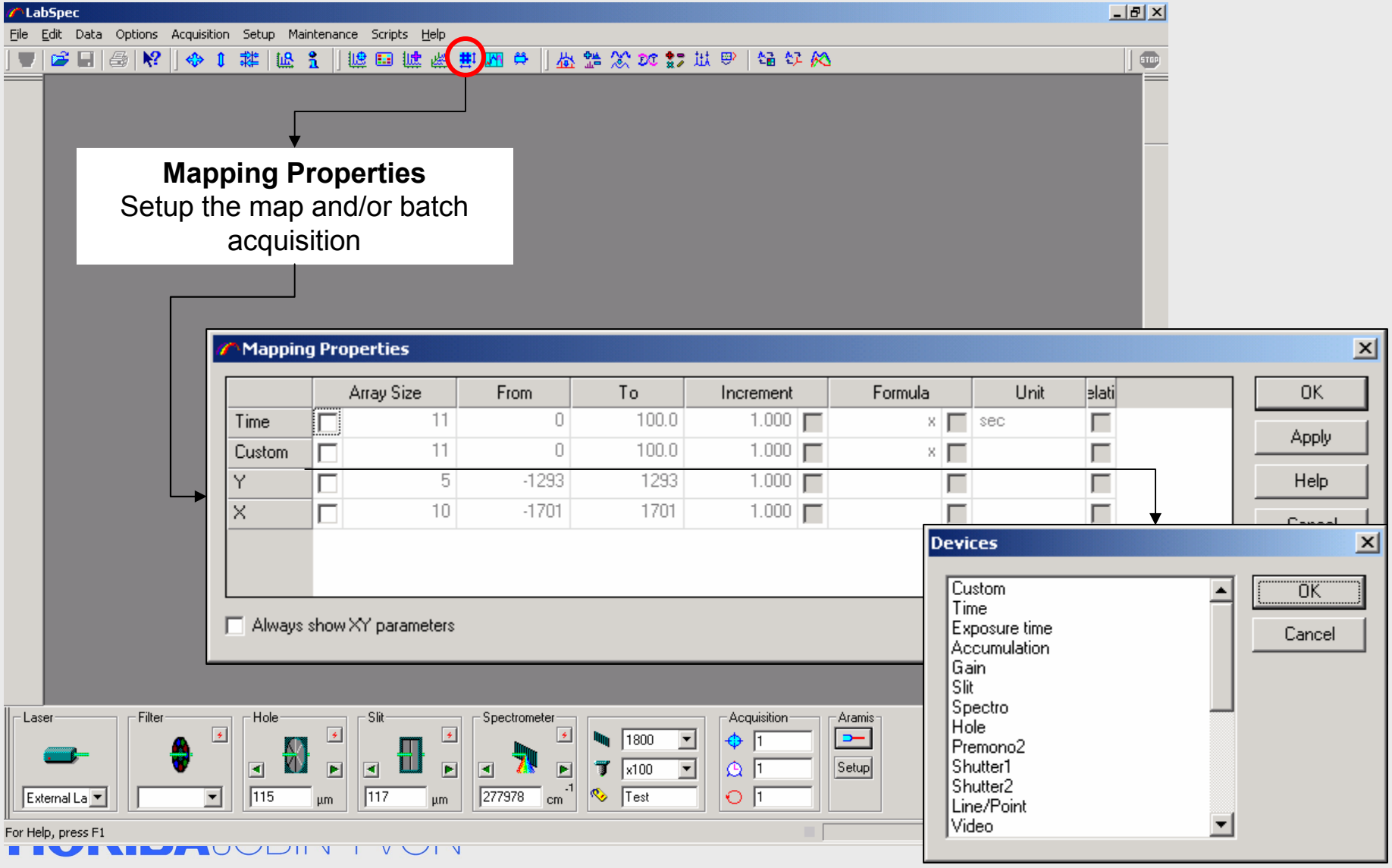
Spectrum


LabSpec - Spectrum : HAU-1_4
File Edit Data Options Acquisition Setup Maintenance Scripts Window Help
When there are more than one spectrum in the memory, the operator can switch the display between them from here with the color coded radio buttons.
Menu options available for *Spectrum*
Spectrum : HAU-1_4
HAU-1_1
HAU-1_2
HAU-1_3
HAU-1_4
Intensity (cnt)
Raman Shift (cm-1)
Laser
Filter
Hole
Slit
Spectrometer
Acquisition
Aramis
External La
115 µm
117 µm
277978 cm-1
1800
x100
Test
Setup
For Help, press F1
S: 1078.83
I: -30.671

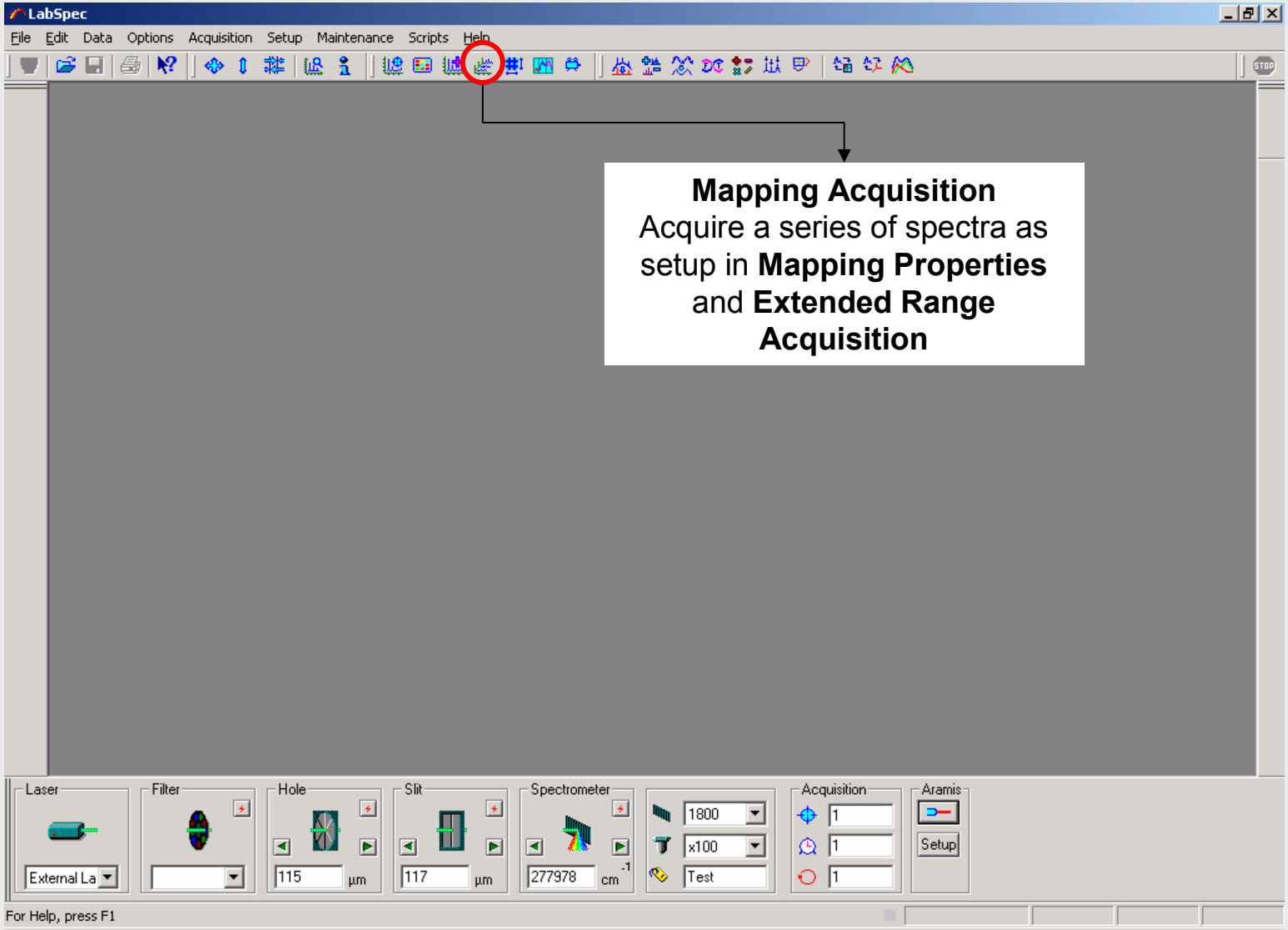
Map Acquisition



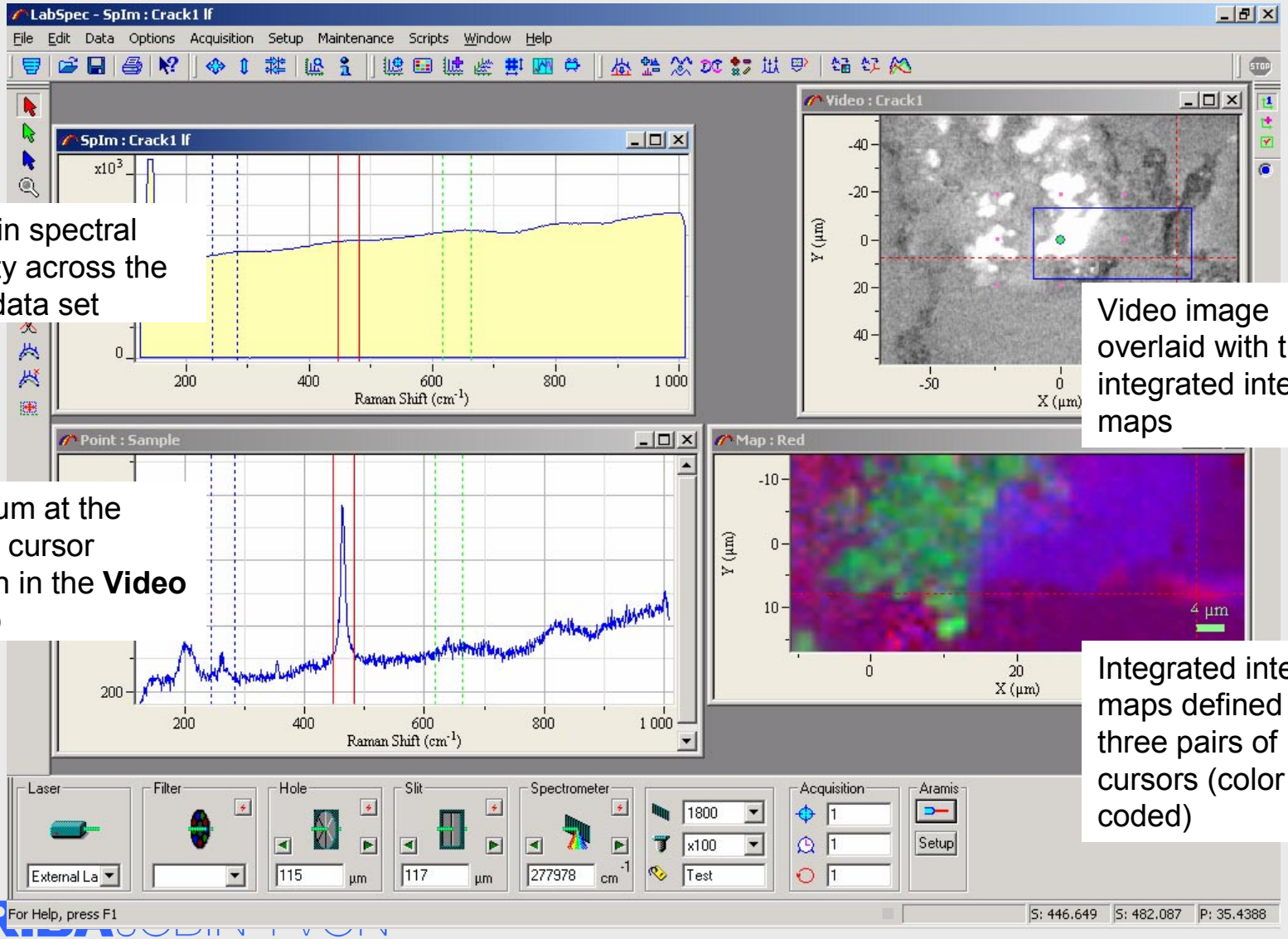
Map Acquisition



Map Acquisition



Map



Max/min spectral intensity across the entire data set

Video image overlaid with the integrated intensity maps

Spectrum at the current cursor position in the **Video** or **Map**

Integrated intensity maps defined by three pairs of cursors (color coded)

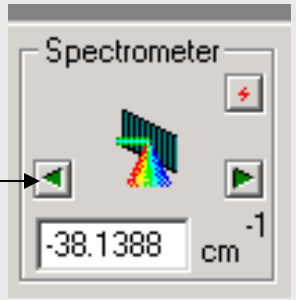
Maintenance

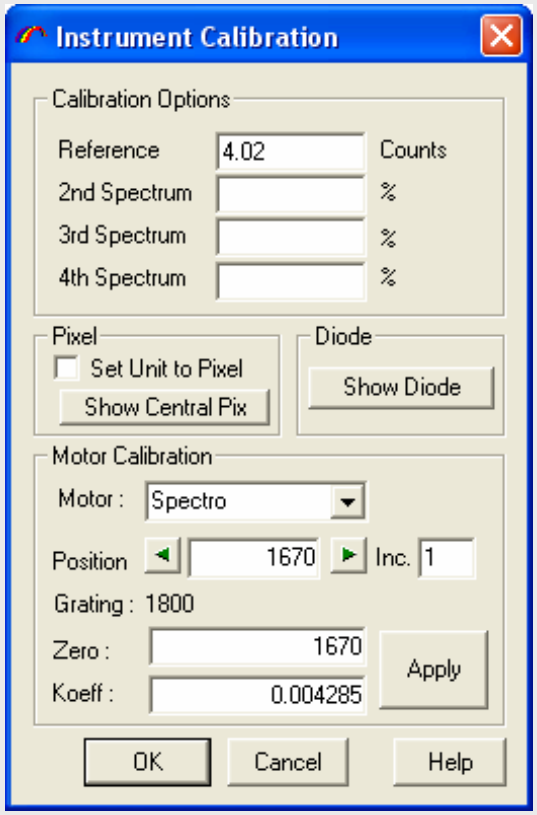
Spectral Axis Calibration

- X-axis (spectral axis) of a Raman microscope is calculated using the full trigonometric relationship involving the included spectrometer angle.
- When the instrument is well aligned, there is a linear relationship between the spectrometer parameters and the spectral axis coordinates.
- The slope (KOEFF) and intercept (ZERO) of this linear relationship can be ‘tweaked’ to adapt to the daily fluctuation of the environment (e.g. temperature).
- The best practice is to keep record of changes made to these parameters.
- Please contact HORIBA Jobin Yvon if a significant drift in spectral axis is suspected or observed.

Spectral Axis Calibration

1. Place Si reference target on the sample stage
2. Change the X-axis unit to nm by selecting **Options** / **Unit** / **nm**
3. Set Spectrometer to **Zero Order**





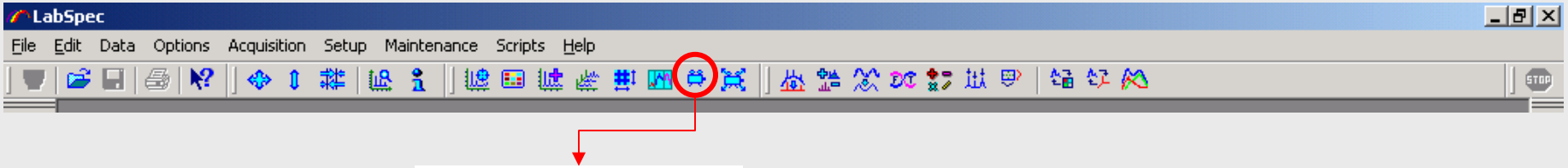
4. Check zero position (laser line) using **Spectral Real Time Display**
5. If the laser line position is off zero, select **Setup** / **Instrument Calibration** and adjust the value for ZERO. Make sure to check zero position after every adjustments by repeating steps 3 and 4.
6. Change the X-axis unit back to 1/cm by selecting **Options** / **Unit** / **1/cm**
7. Set Spectrometer to 520 cm^{-1}, where Si line should appear.
8. Check Si line position using **Spectral Real Time Display**
9. If the laser line position is off 520, select **Setup** / **Instrument Calibration** and adjust the value for KOEFF. Make sure to check line position after every adjustments by repeating steps 7 and 8.

Spectral Axis Calibration

- To ensure the linearity over the full spectral range, the procedure in the previous page can be repeated with different spectrometer position.
- From the step 7, set the spectrometer to 600, 700, etc., and repeat the rest of the steps.
- Sharp and strong peaks from other samples of well known spectra can be used as well. (e.g. Aspirin, Chloroform)

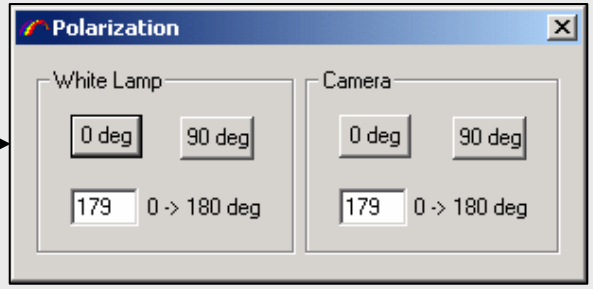
Data Acquisition

Video Acquisition – Real Time



Video
Continuously capture and display the video image

Both light source (white lamp) and detector (camera) can be polarized



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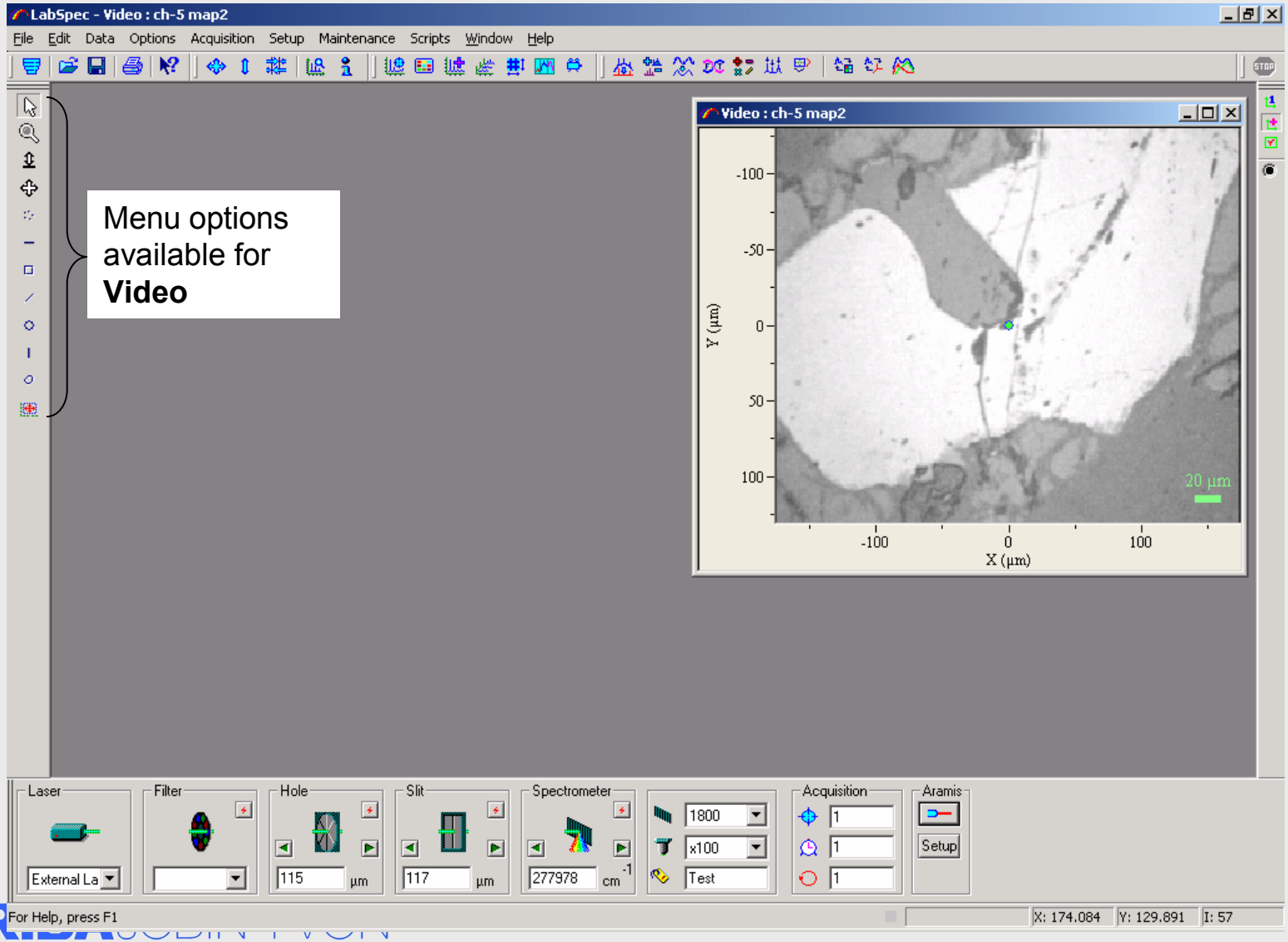
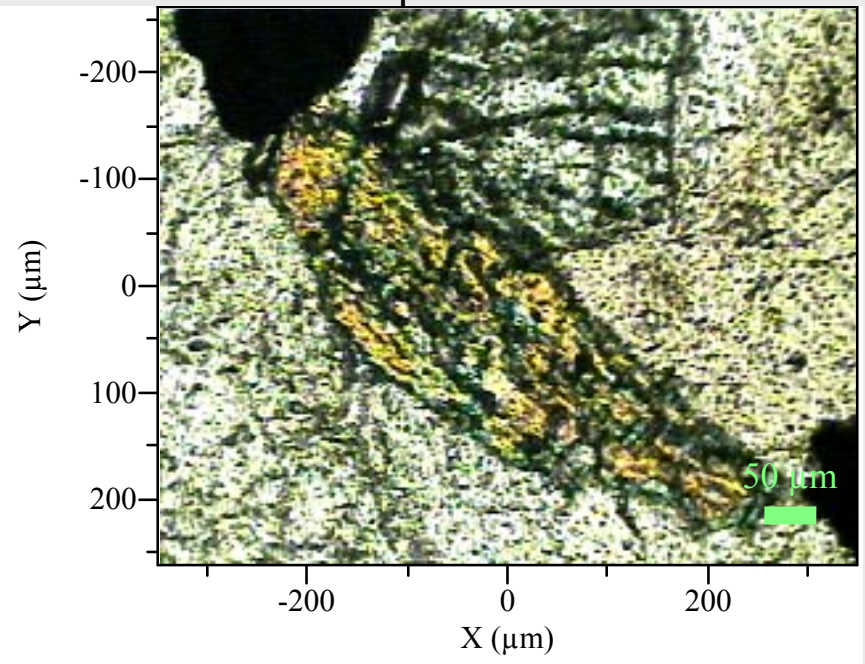
Video


LabSpec - Video : ch-5 map2
File Edit Data Options Acquisition Setup Maintenance Scripts Window Help
Menu options available for **Video**
Video : ch-5 map2
-100
-50
0
50
100
Y (µm)
-100
0
100
X (µm)
20 µm
Laser
External La
Filter
Hole
115 µm
Slit
117 µm
Spectrometer
277978 cm-1
1800
x100
Test
Acquisition
1
1
1
Aramis
Setup
For Help, press F1
X: 174.084
Y: 129.891
I: 57

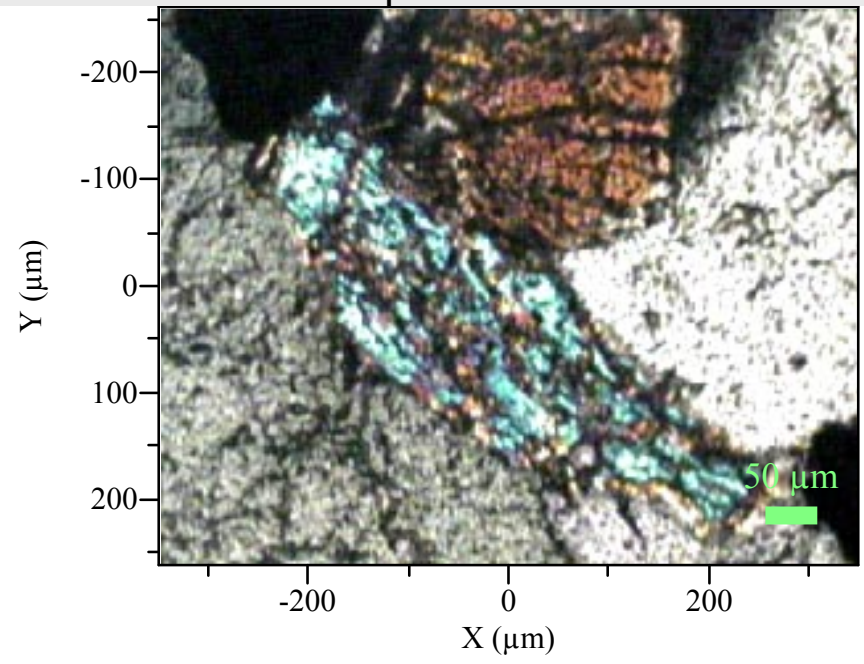
Transmission Light

Pyroxine

Parallel polarization

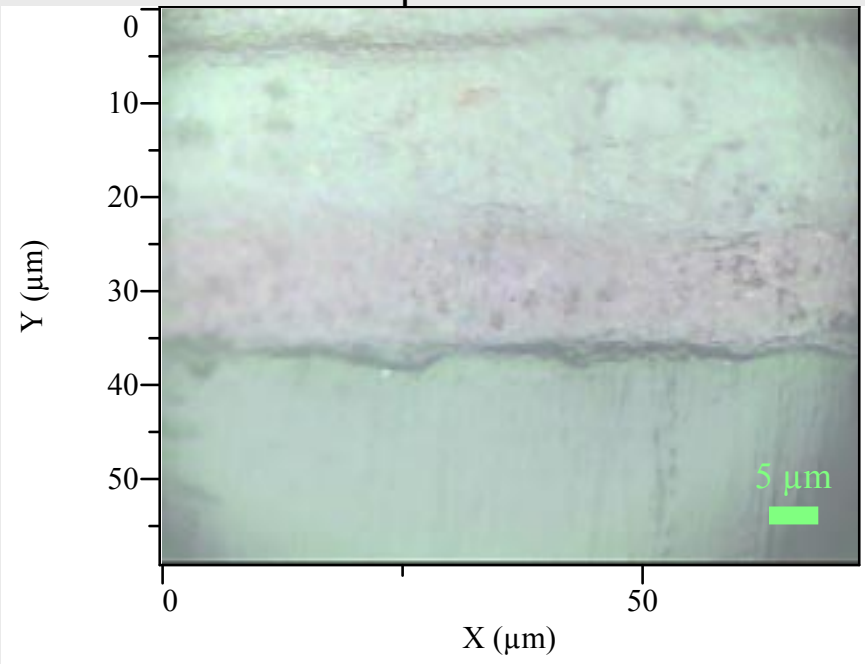


Cross polarization

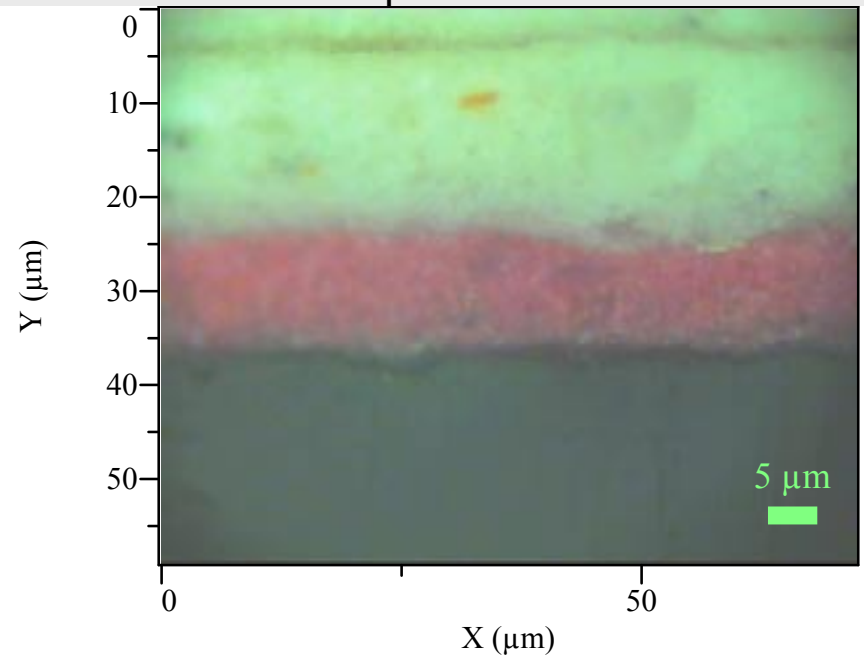


Reflection Light

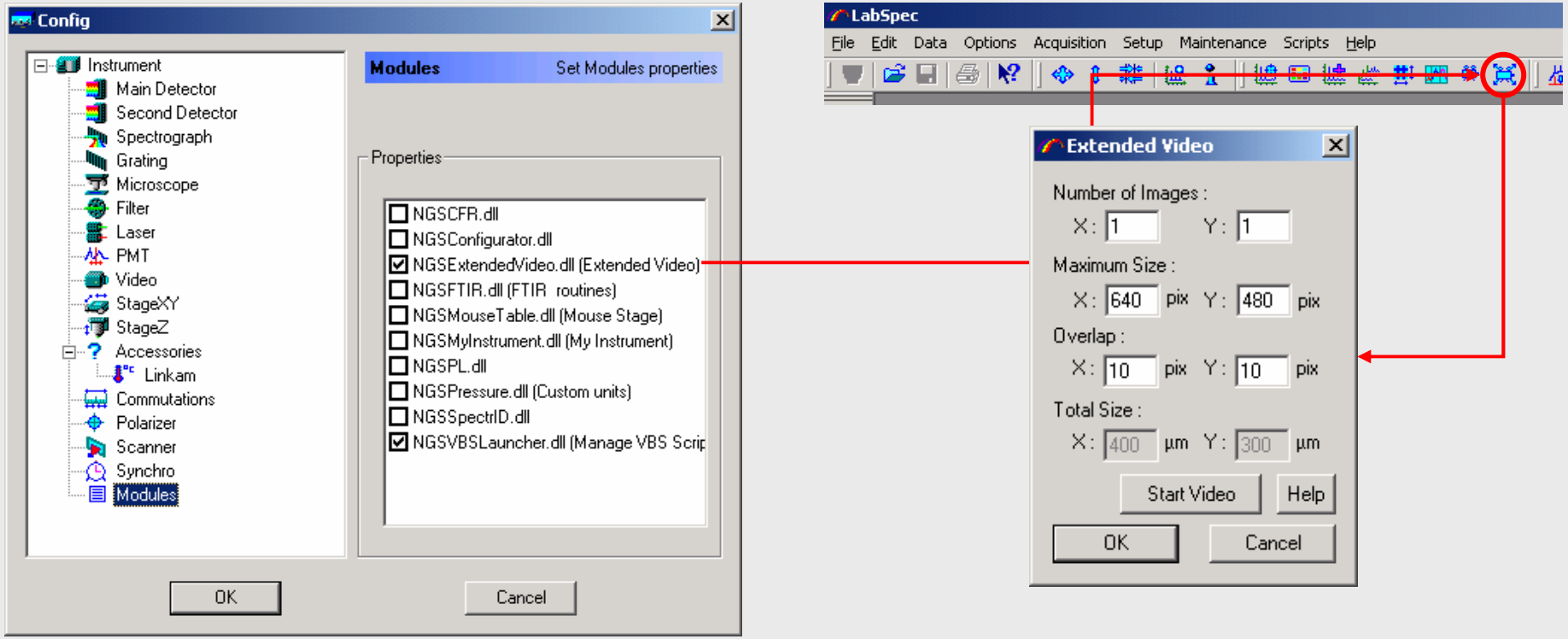
Parallel polarization



Cross polarization

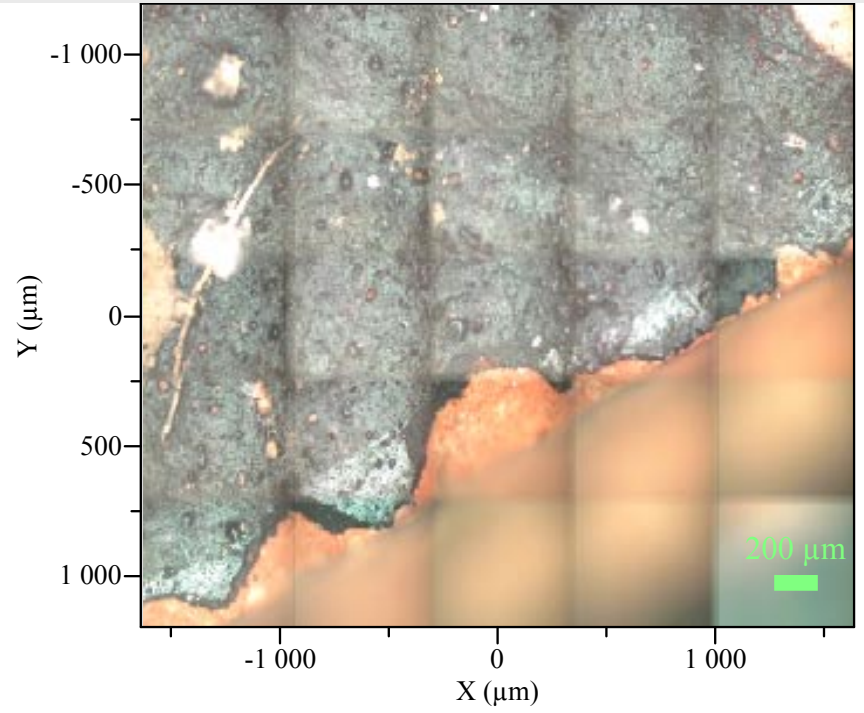


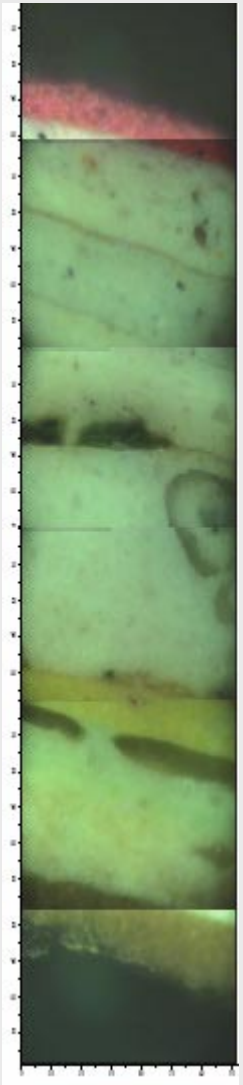
Extended Video Acquisition



- Requires a motorized xy-stage.
- Select NGSExtendedVideo.dll in *Config* to activate, which adds an additional icon to the LS 5 tool bar
- Selecting the icon opens the *Extended Video* window for setting up the extended video acquisition.

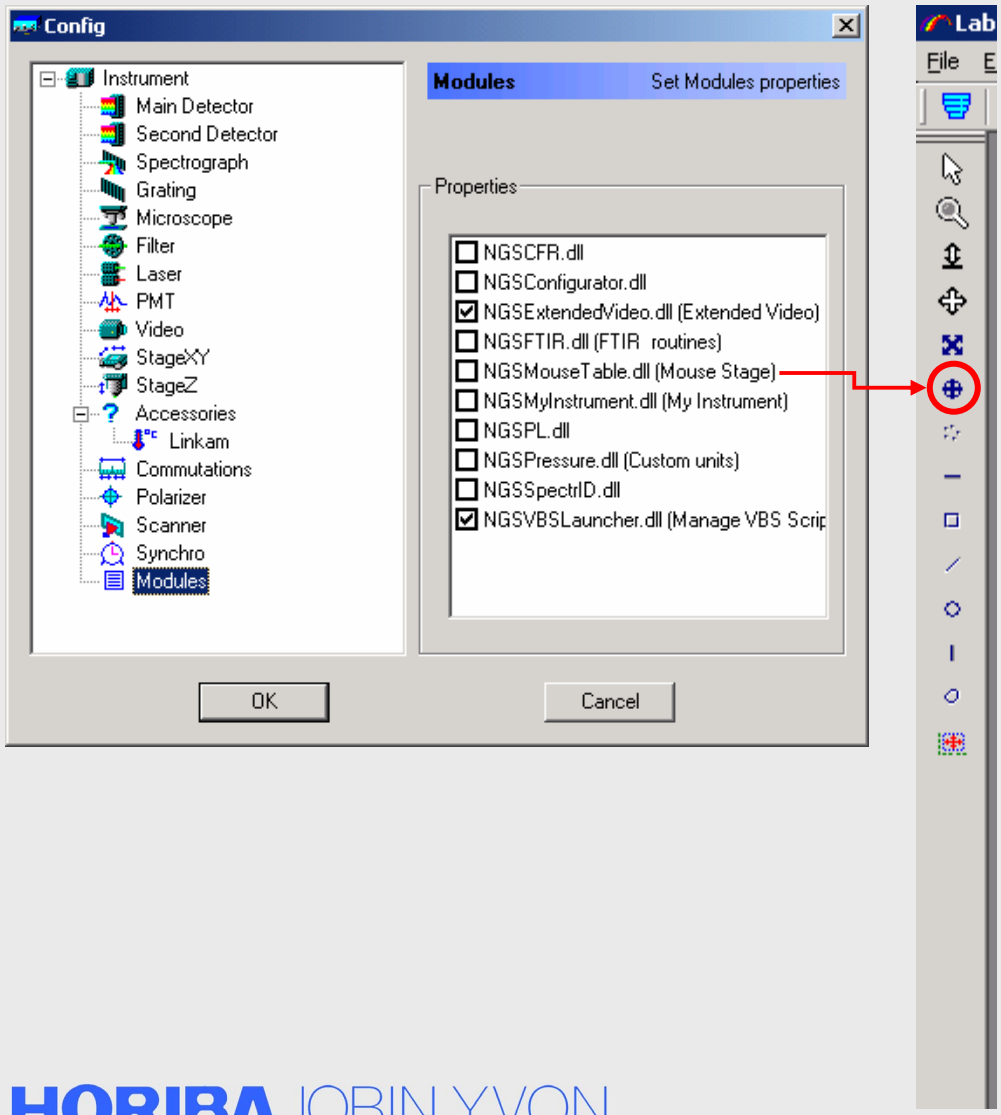
Extended Images





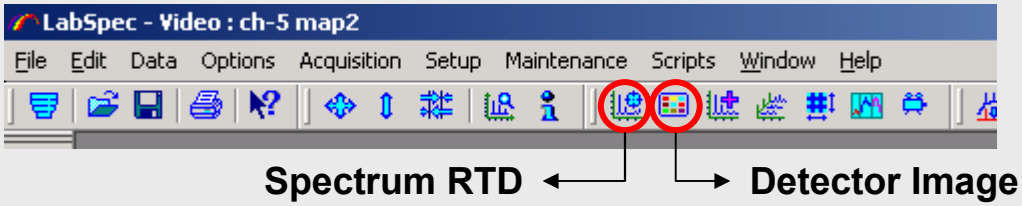
- Extending the field of view by patching multiple images together.
- This is **NOT** a real time image.

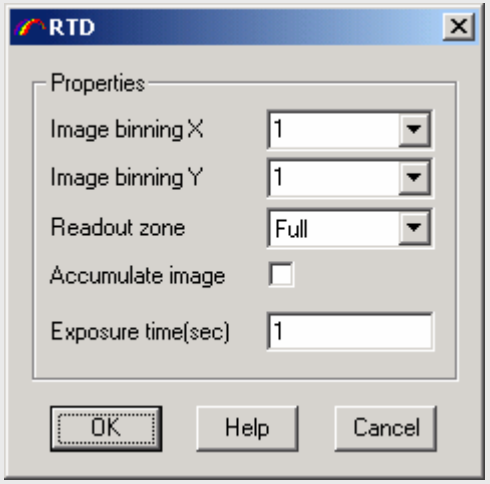
Move to the Cursor Position



- Requires a motorized xy-stage.
- Select NGSMouseTable.dll in *Config* to activate, which adds additional icons to the left tool bar of **Video**
- When the **Target** is selected, a bulls-eye appears on the video image, which defines the current center.
- Clicking on a new location in the image moves the bulls-eye and the stage moves automatically to center at the new position.

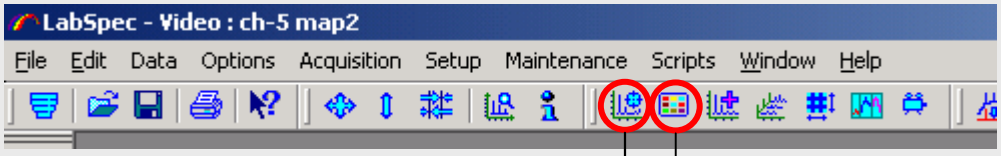
Spectrum Acquisition – Real Time

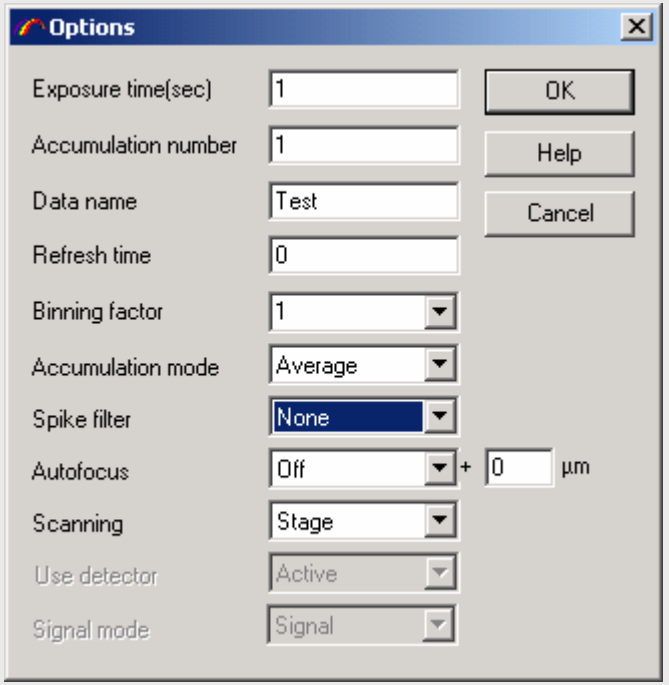




- **Acquisition / RTD**
  - There are two Real Time Display (RTD) modes
  - Selecting **Acquisition** / **RTD** menu opens RTD window
  - Image binning X and Image binning Y apply to **Detector Image RTD**.
    - Number of pixels specified here are added and read out as one pixel.
    - Increasing number of binning speeds up the read-out process.
  - Readout zone applies to both **Detector Image RTD** and **Spectrum RTD**.
    - There are three Readout zone modes: **Spectrum**, **Image** and **Full**
    - **Spectrum** and **Image** are defined in **Acquisition** / **Detector** and window the detector read-out regions
    - Usually, Readout zone is set to **Spectrum**
  - When selected, Accumulate image takes the number of accumulations (set in the bottom tool bar) into account.
  - (RTD) Exposure time can be modified here as well as in the bottom tool bar.
- RTD is triggered on by clicking Icons on the LS 5 tool bar.

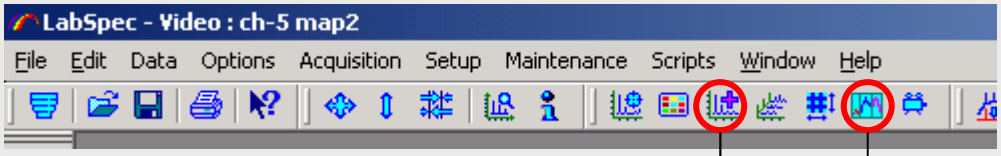
Spectrum Acquisition - Options



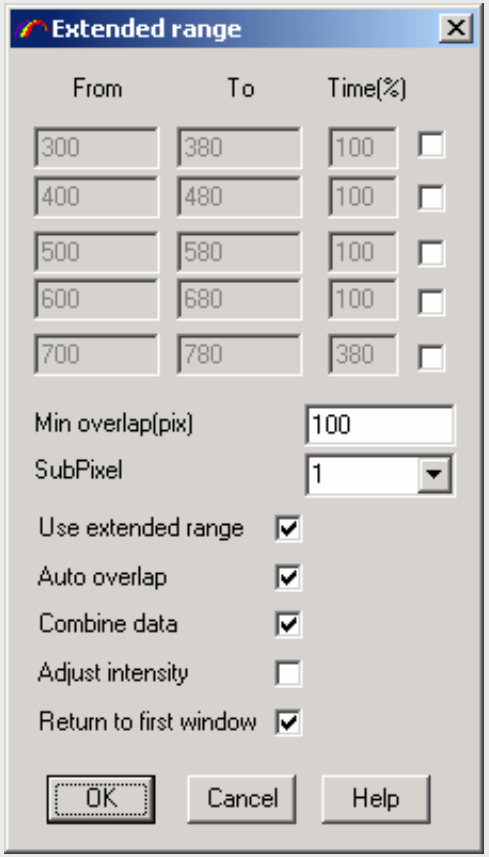


- **Acquisition / Options**
  - Exposure time and Accumulation number can be set here as well as in the bottom tool bar
  - The name of the spectrum (or the data set) is set to Data name and a increasing integer suffix by default
  - Refresh time: Refresh the data measurement in progress at the set interval
  - Binning factor: Read out the set number of pixels as one. Increasing binning factor lowers the spectral resolution while increasing the signal.
  - Accumulation mode: Average, Sum, Detector
  - Spike filter: None, Multi (auto add), Multi, Single
  - Autofocus: Off, Before acquisition, Before each point
  - Scanning: Stage (point mapping mode), Scanner (line scanning mode).
  - Use detector : Active detector, Both
  - Signal mode : Signal, Signal-Dark

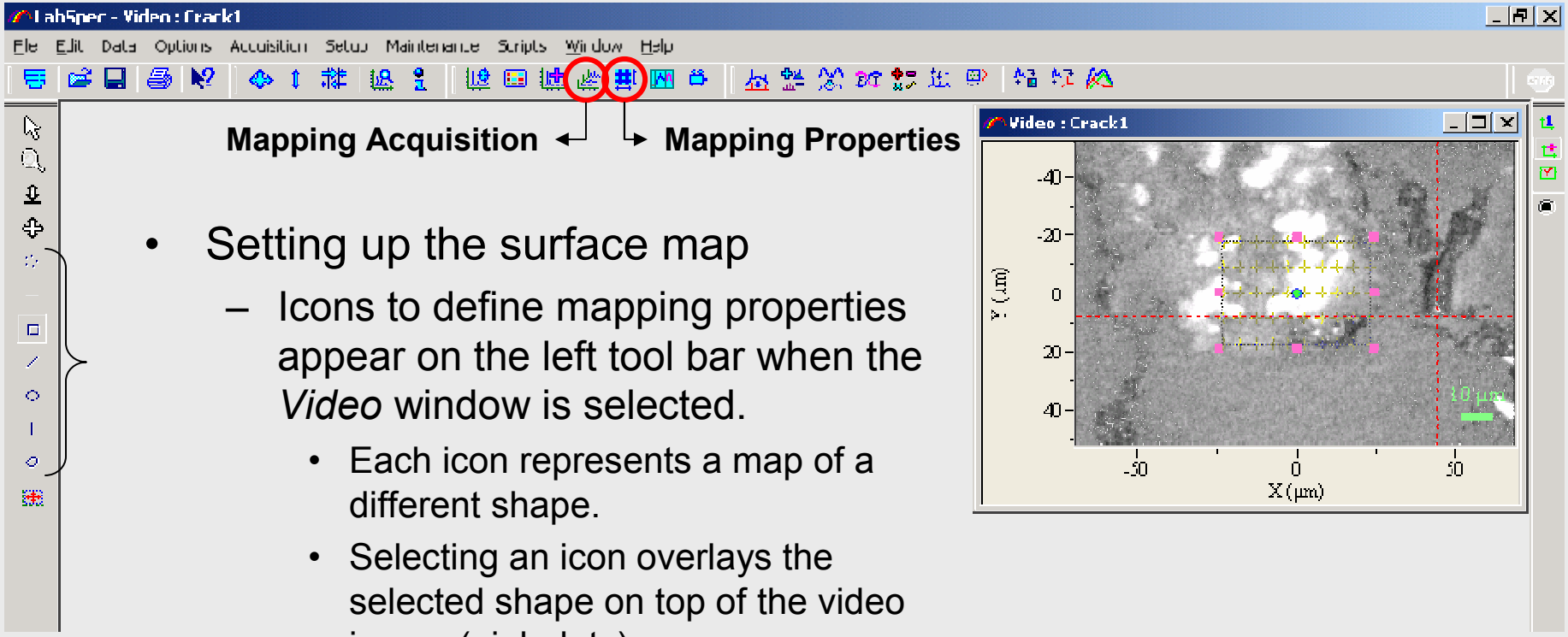
Extended Range Acquisition



- Selecting **Acquisition** / **Extended Range** menu or **Extended Range** icon opens *Extended Range* window
- Select Auto-overlap and Combine Data options to use CREST (Continuous Rapid Extended Scanning Technology) to measure the spectrum.
- Spectrum acquisition is started by clicking **Spectrum Acquisition**.



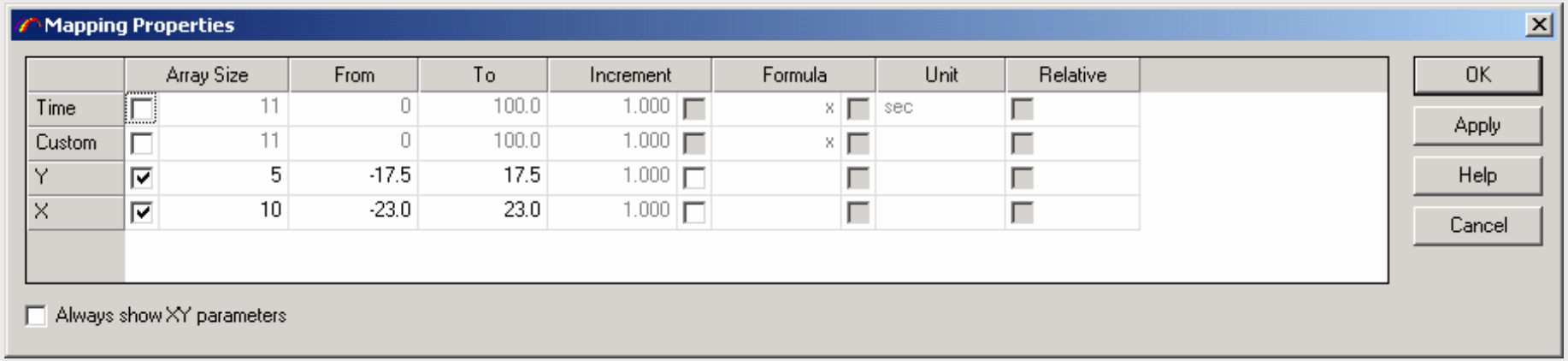
Map Acquisition



- Setting up the surface map
  - Icons to define mapping properties appear on the left tool bar when the *Video* window is selected.
    - Each icon represents a map of a different shape.
    - Selecting an icon overlays the selected shape on top of the video image (pink dots).
    - The size of the map is adjusted by clicking and dragging with the mouse.

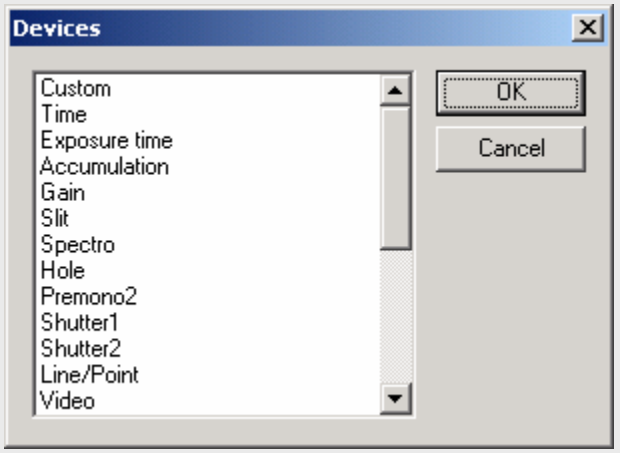
Map Acquisition

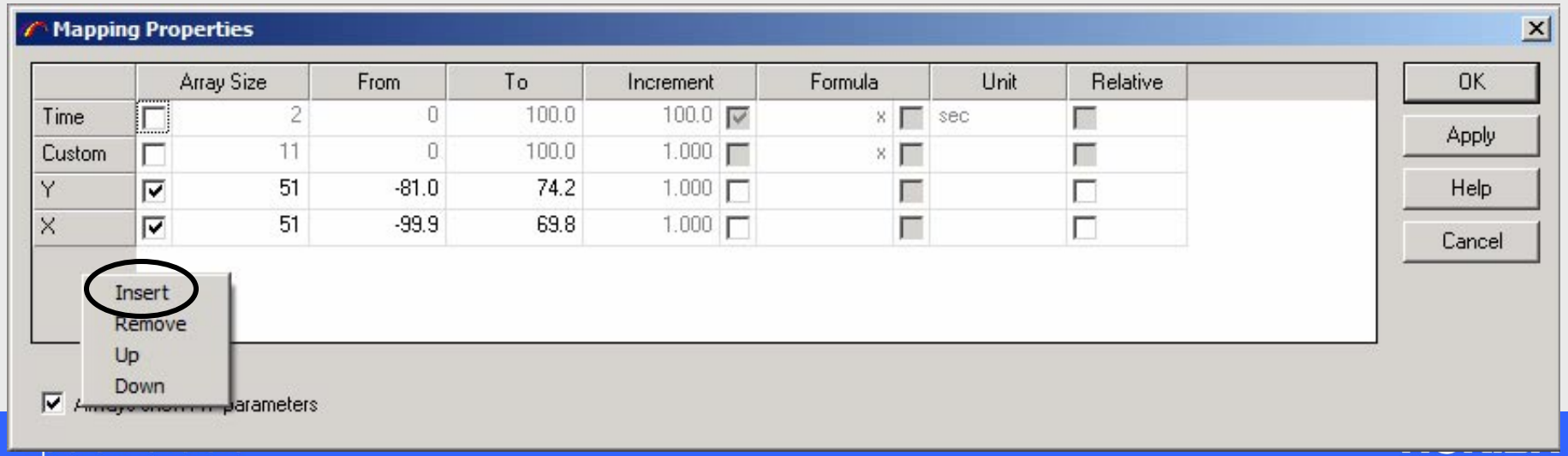
- Setting up the surface map
  - **Mapping properties** icon opens *Mapping properties* window
    - Array Size and Increment must be defined here.



Map Acquisition – Other Parameters

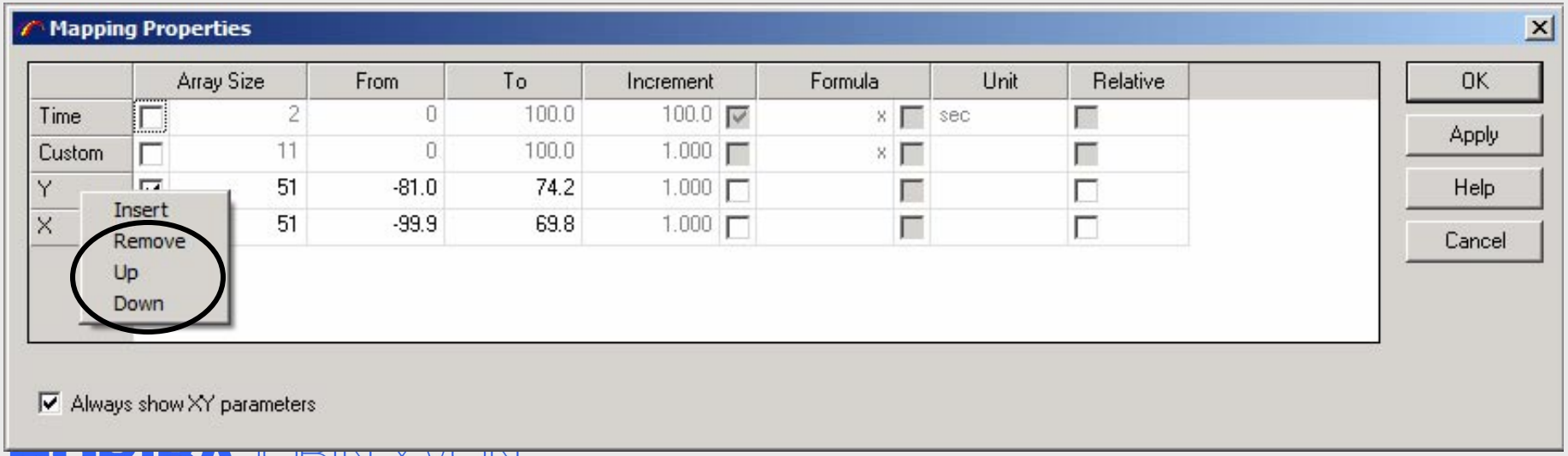
- *Mapping properties* window provide the place to set up parameters other than x and/or y scanning.
  - Depth profile is performed by employing the parameter Z
  - Other variables such as slit width and confocal hole diameters can be set to scan over a range at an increment.
  - Right clicking on the parameter list activates context menu. Select **Insert** to open *Device* window. Select variables to scan. (e.g. SLIT, HOLE)





Map Acquisition – Other Parameters

- Priorities of the variables
  - The order of the variables sets their priority during the mapping. The bottom parameter has higher priority, the top parameter has lower priority.
  - When set as below, the measurements will be made along x-axis at a constant y position before moving to a new y position to repeat the process.
  - To change the order of variables, right click on the variable name to activate the context menu Use **Remove**, **Up**, **Down** menus to change the list and order of variables.

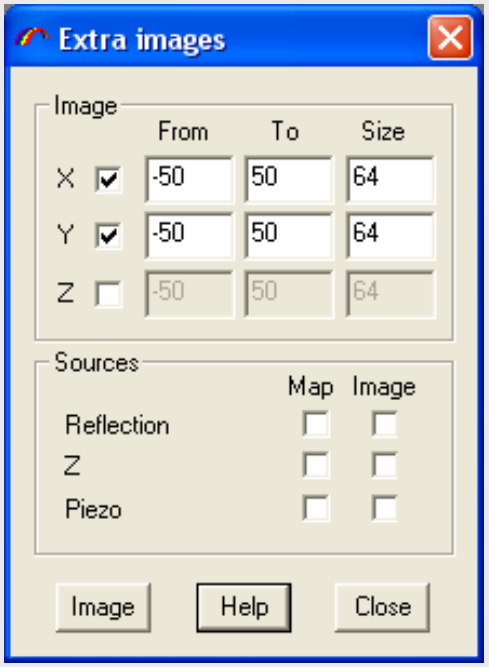


Map Acquisition – Options

- Increment
  - When the INCREMENT box is checked, the measurements are performed at the set increment.
  - When the INCREMENT box is not checked, measurements are performed at the increment calculated from FROM, TO and ARRAY SIZE.
- Relative
  - When the RELATIVE box is checked, then the current position of the image is the (0,0,0) position of the map table.
  - When the RELATIVE box is not checked, then the (0,0,0) position of the image is the (0,0,0) position of the map table.

Map Acquisition – Options

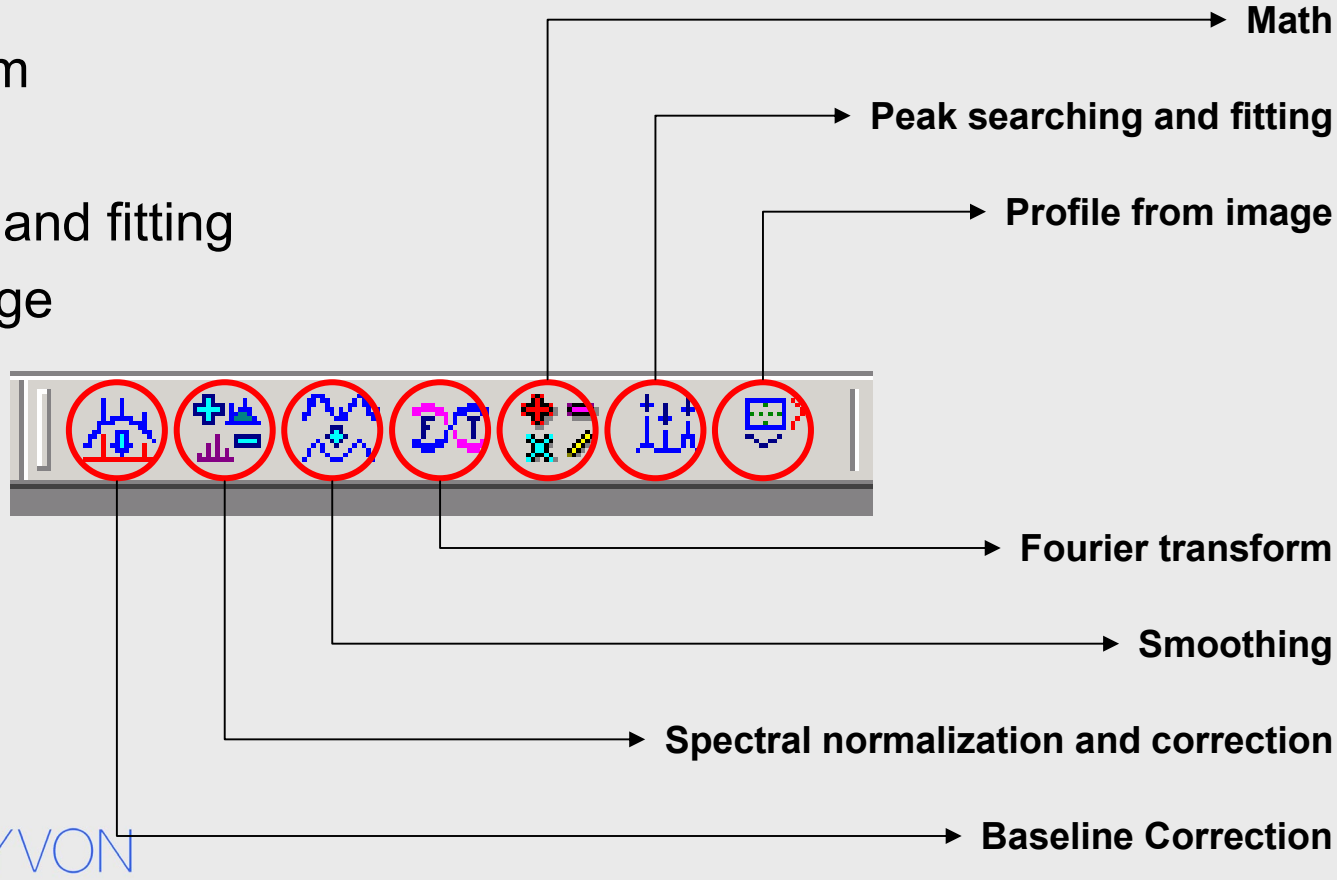
- Extra Images
  - **Acquisition / Extra images**
  - When the autofocus is activated, extra images like the Reflection (on the autofocus detector) and the Z position (after each autofocusing) are available.
  - These are recorded
    - At the same time as the Raman mapping if you select MAP
    - Without recording any spectrum if you select IMAGE and click on IMAGE.
    - If you use IMAGE then you only obtain a topographic picture of the sample and the variation of reflectivity over the surface of the sample.



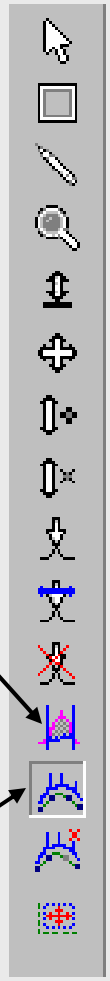
Data Treatment

Basic Data Treatment

- Baseline correction
- Spectral normalization and correction
- Smoothing
- Fourier transform
- Math
- Peak searching and fitting
- Profile from image

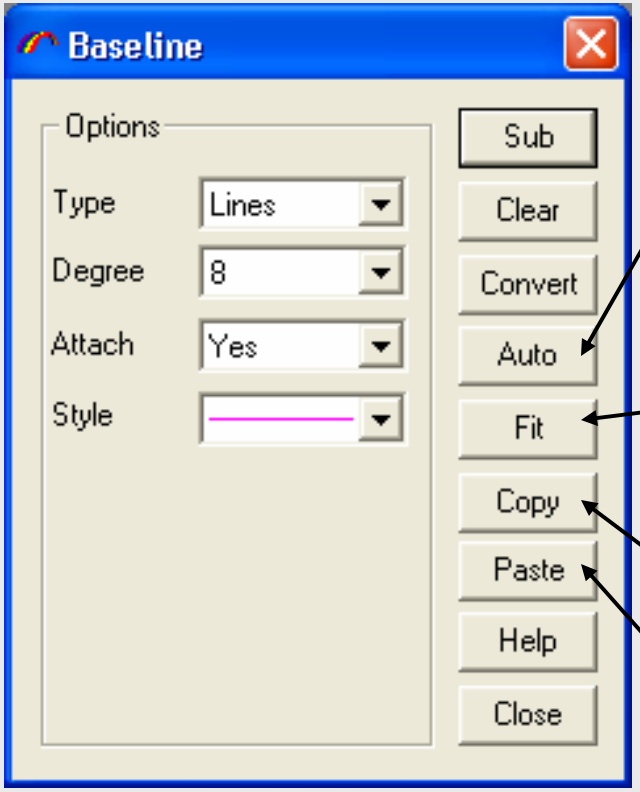


Baseline Correction



Build the baseline by adding points at the cursor position

Remove the points defining the baseline



Build the baseline automatically and subtract from the current spectrum

Build the baseline automatically but NO subtraction

Copy the baseline

Paste the baseline to an other spectrum

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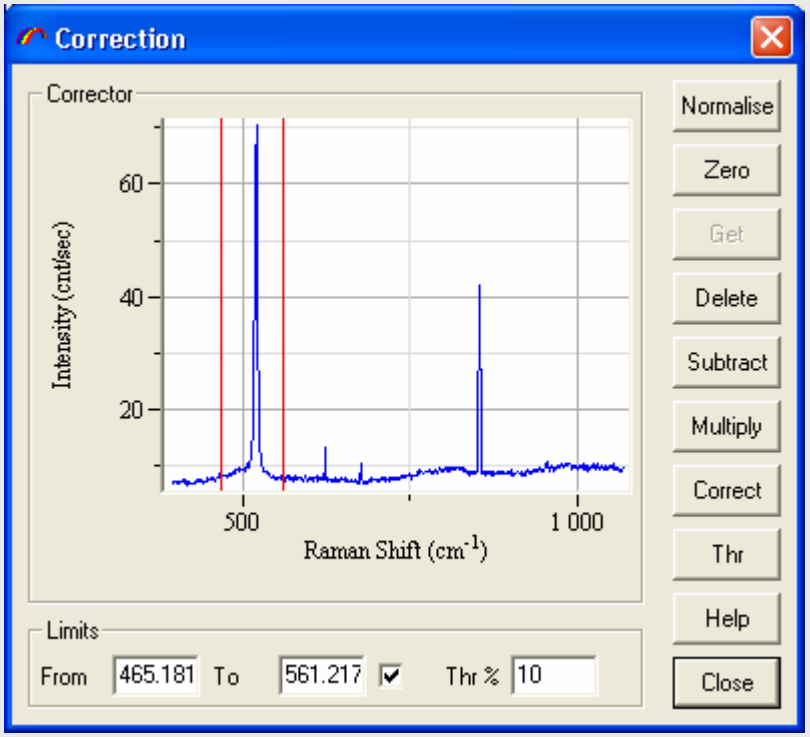
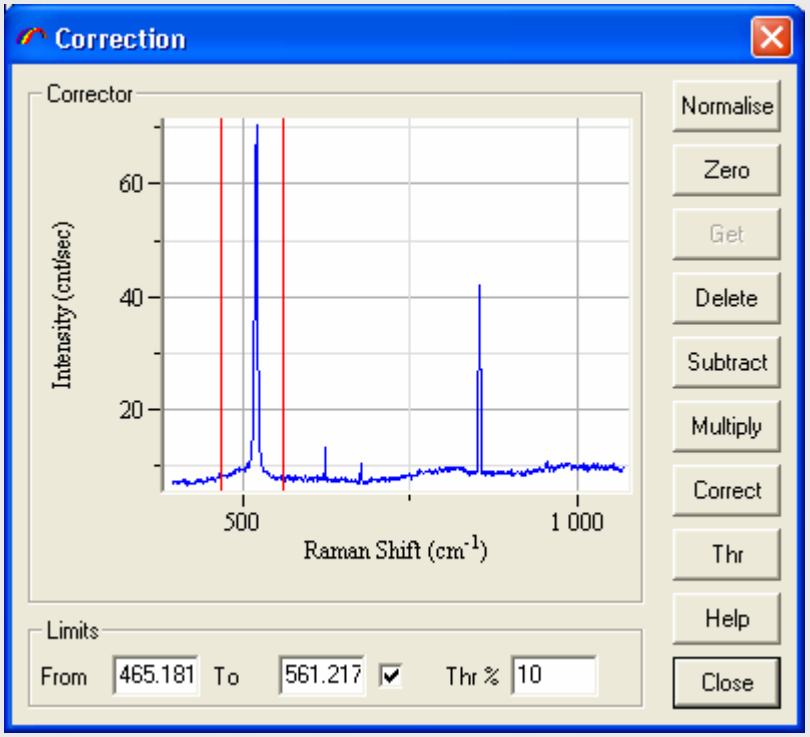
Spectral Normalization and Correction

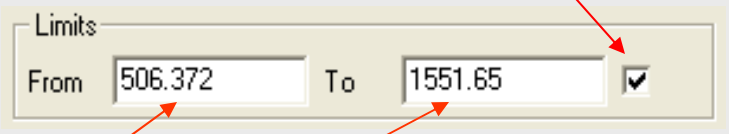


- **Normalize**: Normalizes all traces to same area value (100).
- **Zero**: Moves all traces to the minimum intensity level.
- **Get**: Takes the activated spectrum and put it in Corrector frame. This data object will be used as parameter.
- **Delete**: Removes the Corrector spectrum.
- **Subtract**: Subtracts the Corrector spectrum from all traces.
- **Multiply**: Multiplies the trace on the Corrector spectrum.
- **Correct**: Subtracts the Corrector spectrum from all traces. The intensity of the Corrector is multiplied to fit the intensity of the trace
- **Thr**: Remove all trace with maximum intensity less then threshold value (in % to maximum data intensity)

Spectral Normalization and Correction

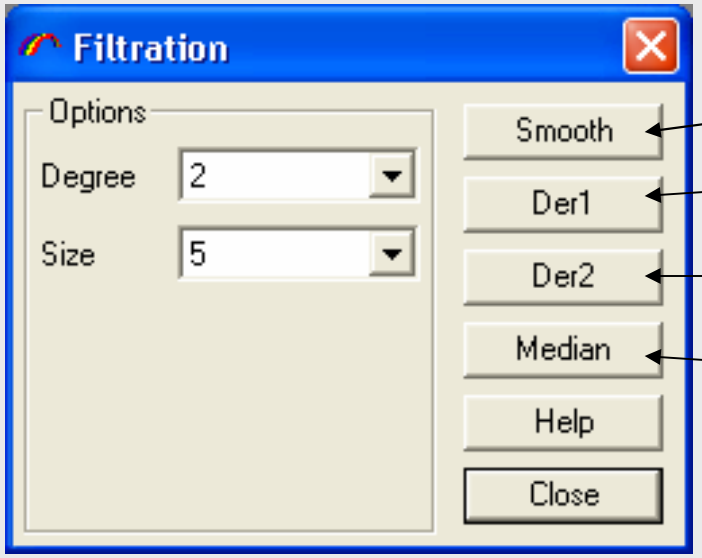


LIMITS: Check the box if you want that only a part of the trace is used for operation. This parameter is used for **Normalize** and **Correct** operation.



FROM and TO: Edit these fields to modify the limits of the selected region (linked to the red vertical cursors)

Smoothing



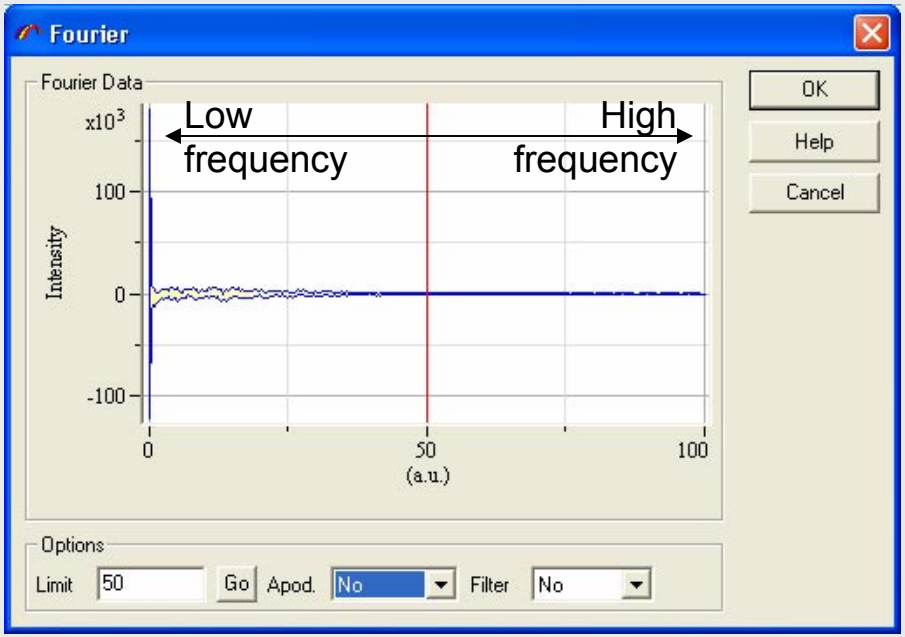
Savitsky-Golay smoothing.

First derivative

Second derivative

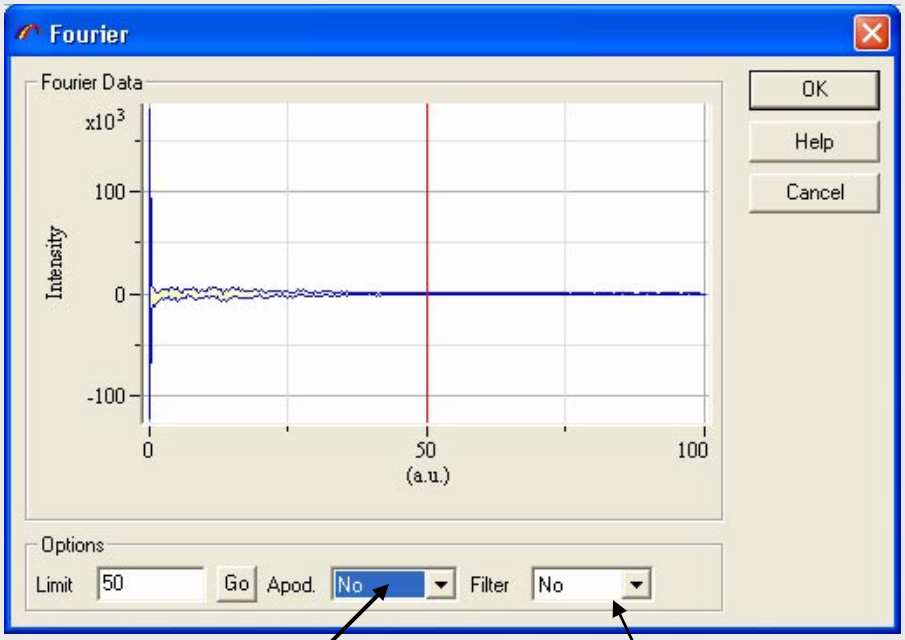
Median filter smoothing

Fourier Transform



- This is another smoothing tool
- When a spectrum is Fourier transformed, the low frequency data (spectral features) and high frequency data (noise) are separated.
- Therefore, eliminating high frequency region in the Fourier transform domain removes high frequency noise.
  - Fourier transform the spectrum
  - Cut off high frequency region
  - Reverse Fourier transform to spectrum

Fourier Transform

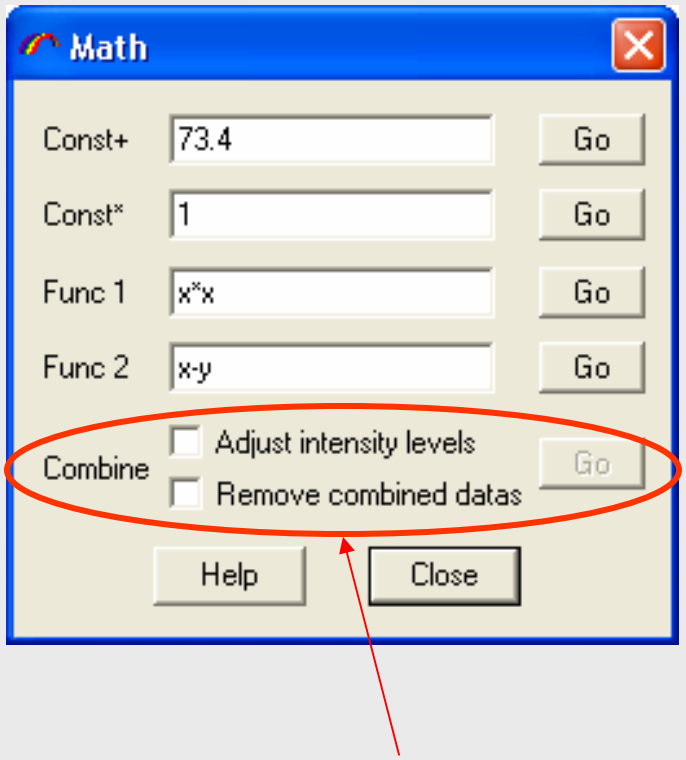


- LIMIT: Position of the cut off point in %. This parameter defines the smoothing factor.
  - 0: Fully smoothed,
  - 100: No smoothing.
- Click on the **Go** button to apply the value or drag the pointer to select the LIMIT visually.
- APOD: Type of the apodization function with apodization value reaching zero at a Limit point.
- FILTER: Select here the type of the filter function

None	No apodization function
Line	Linear function
Sqr	Parabolic function
Cos	Cosine function

None:	No filter function
Traffic:	Traffic function

Math



Combine data objects into a single object

- FUNC 1 and FUNC 2: Basic math functions (+, -, *, /, ^), negating, power, log, exp, sin, cos, asin, acos, atan, abs, sqrt, step.
- **Go**: Perform the operation
- x : denotes the active object
- y : denotes other objects of the active window
- a, b, c, d……. : values of the axes for each data points (next slide)

Examples

If we apply the formula '**x+2*a**' to a spectrum, **x** is the intensity and **a** the Raman at each point.

Before operation

Raman shift	100	200	300	…	**a**
Intensity	200	250	500	…	**x**

After operation

Intensity values	20000	50000	150000	…

If we apply the formula '**x+b-a'** to an image, **x** is the intensity, **a** is the x distance and **b** is the y distance

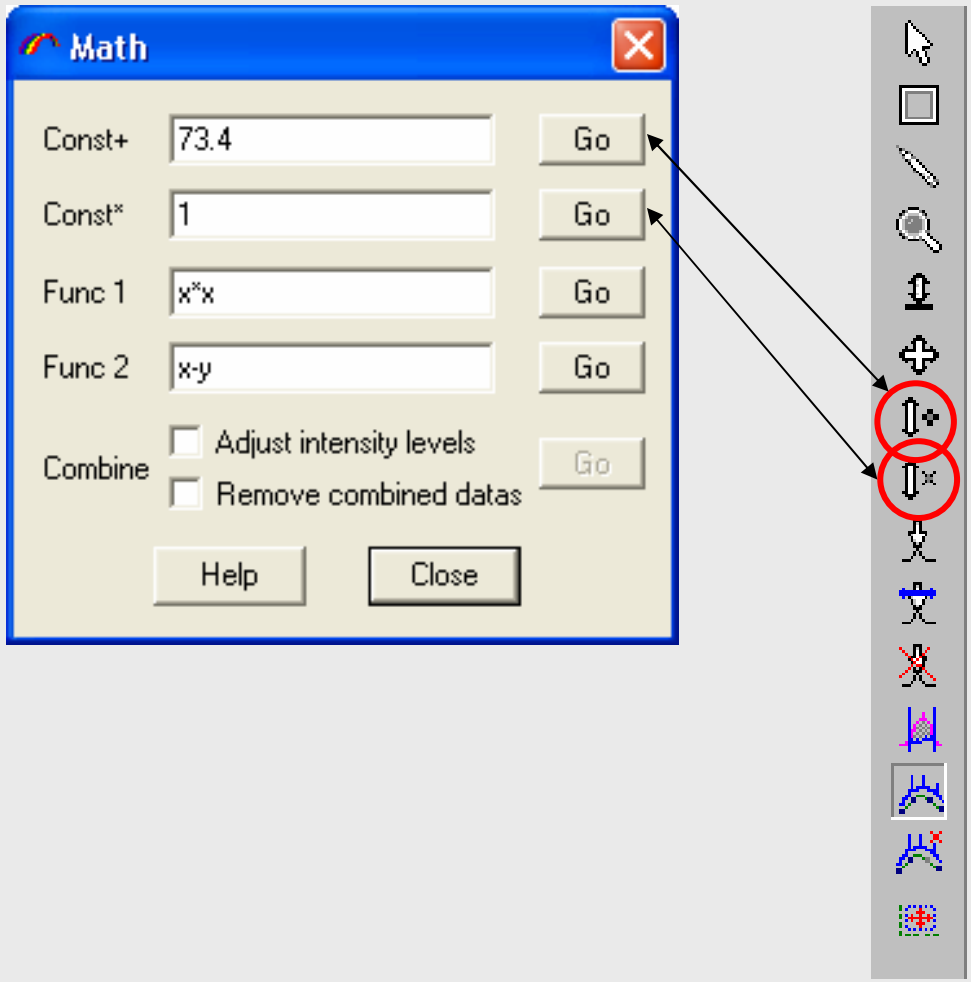
Before operation

	10	20	30	…	**a**
40	500	250	500		
50	50	120	400		
60	30	0	500		
…					
b					

After operation

530	270	510
90	150	420
80	40	530

Math



Operations using constants can be performed interactively using icons as well.

Add/subtract a constant

Multiply/divide by a constant

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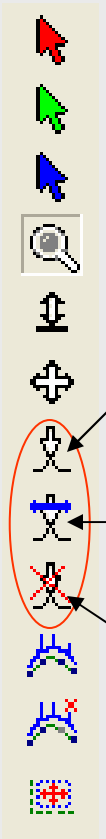
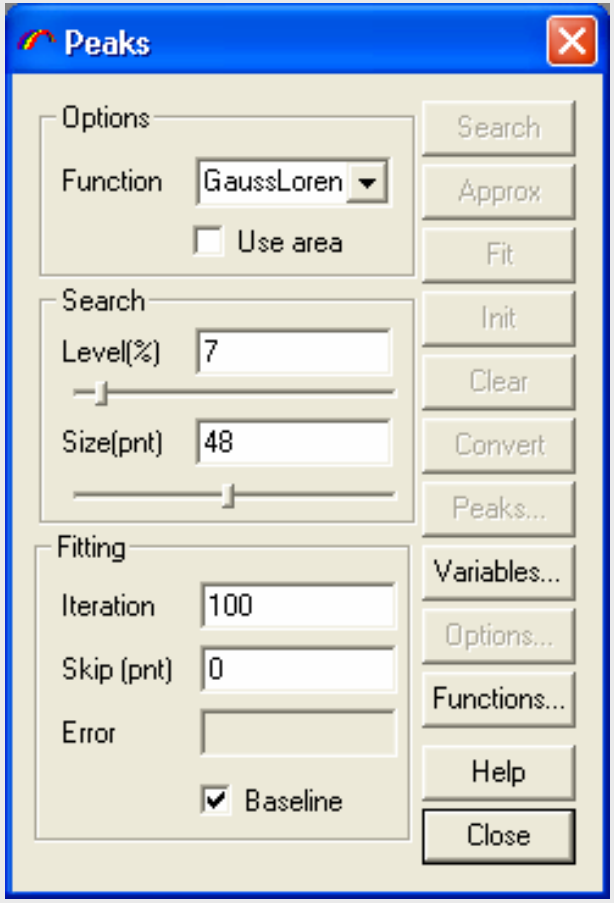
Peak Searching and Fitting



Insert a peak

Adjust position, height and width

Remove the selected peak



Search: search peaks automatically

Approx: approximate the peak position, height and width without fitting

Fit: start iteration

Init: initialize

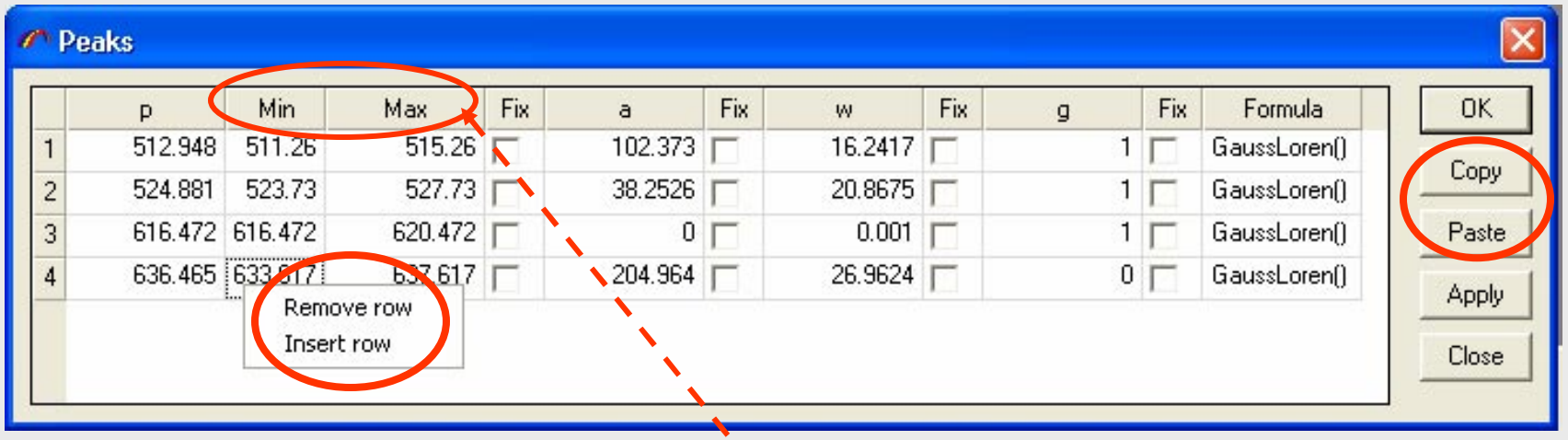
Clear: clear all peaks and calculation results if there is any

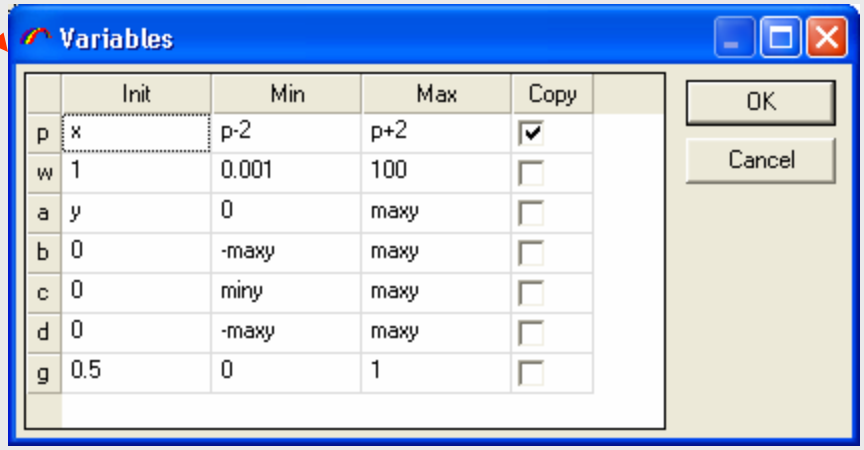
Convert: convert the fitted spectrum with the calculation result

Peaks: open *Peak* window

Variables: open *Variables* window

Peak Searching and Fitting





Right clicking in the table activate the context menu, which allows add or remove peaks to fit.

Parameters of fitting functions can be adjusted for each peak from *Variables* window

The entire peak fitting table can be copied and pasted using the **Copy** and **Paste** button.

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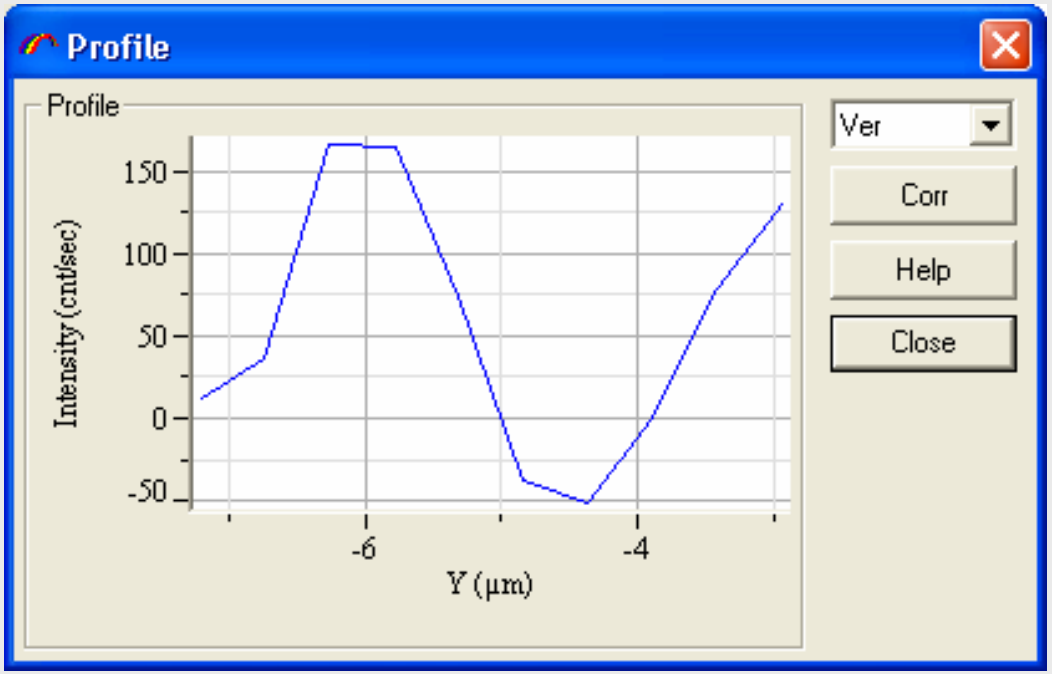
Profile from Image



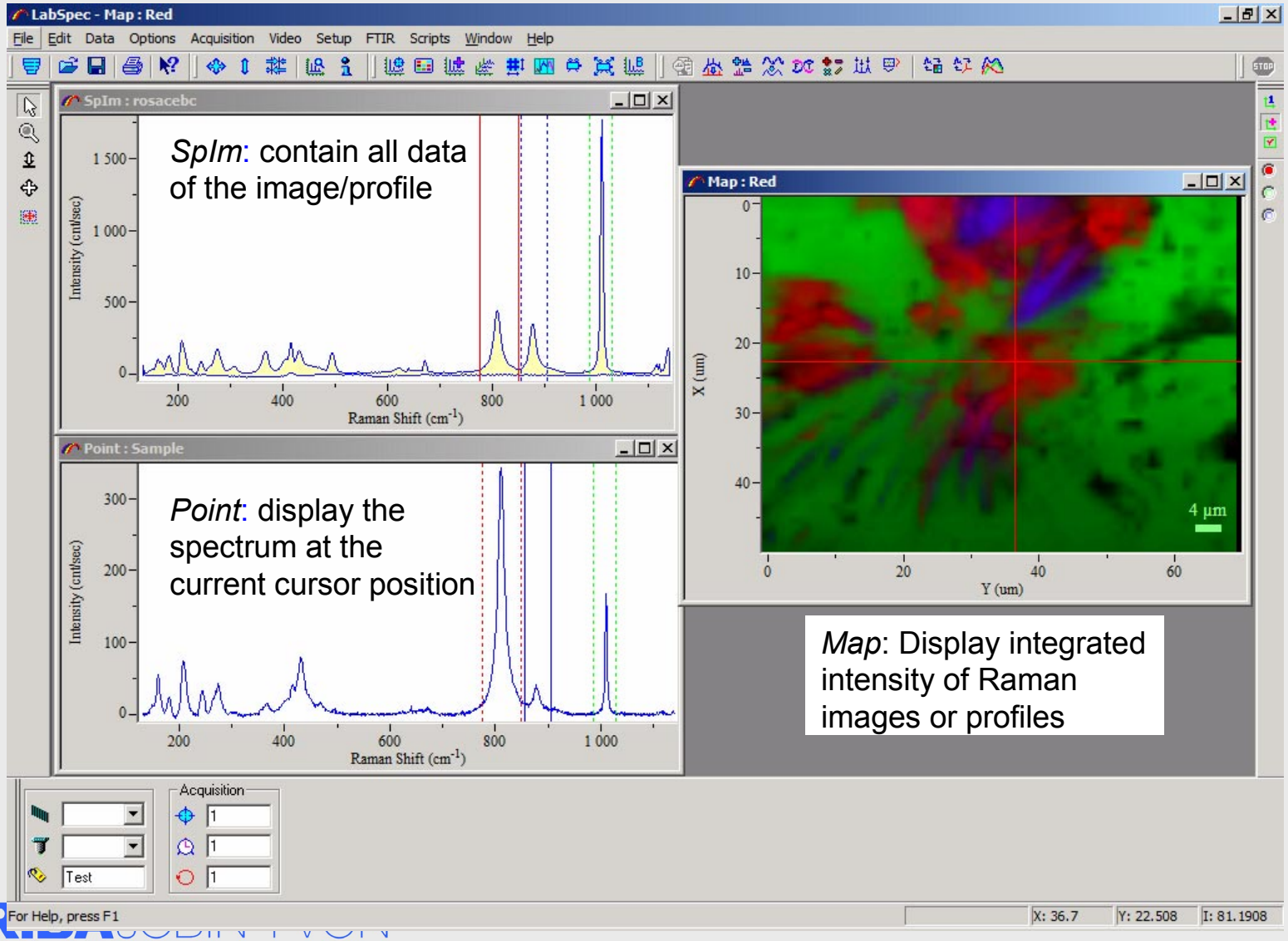
Vertical or horizontal profile over an image can be obtained from Profile window.

You can apply to a profile the same operations as for a spectrum, then using the **Corr** button to put the corrected data back to the image where the profile was extracted

Advanced Data Treatment

- Analyzing map image and profiles
- New spectral profile

Analyzing Images and Profiles

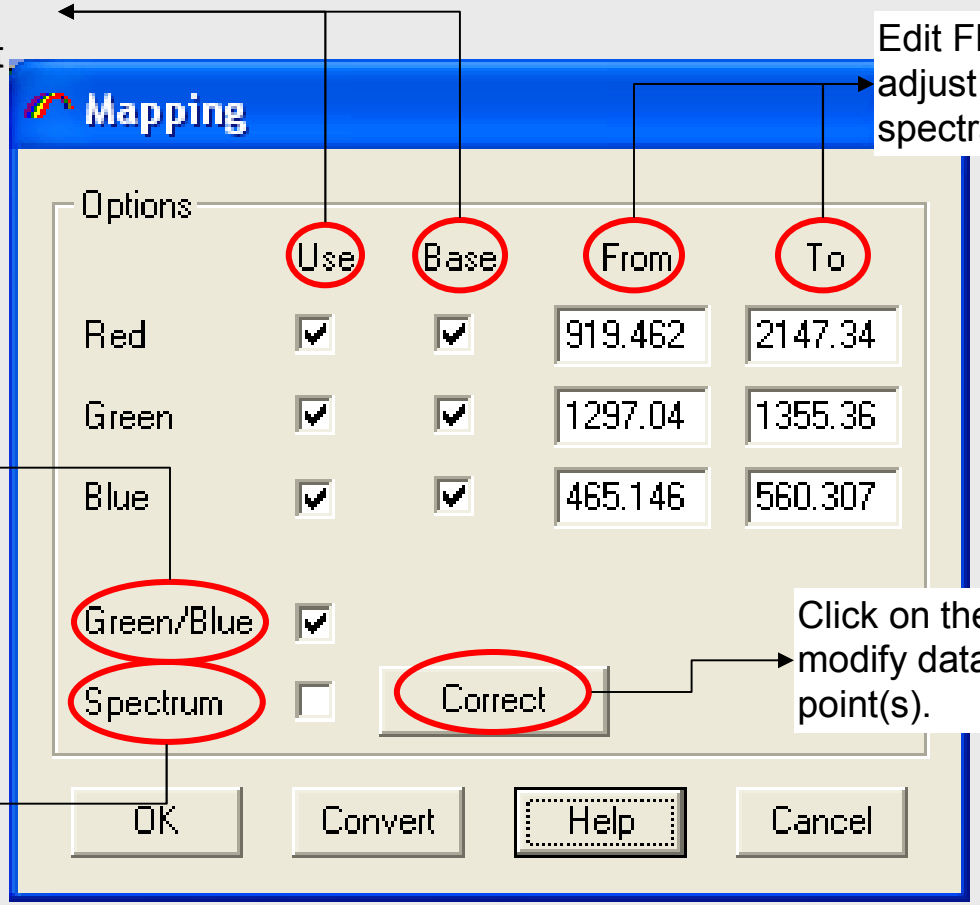


Analyzing with Cursors

Check USE box to generate the corresponding map.

Check BASE box to subtract baseline.

Edit FROM and TO fields to adjust the limits of the spectral regions.



Check GREEN/BLUE box to generate the map of the corresponding ratio.

Click on the **Correct** button to modify data on the selected data point(s).

Check SPECTRUM box to see the spectrum of the selected data point(s)

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Analyzing with Cursors

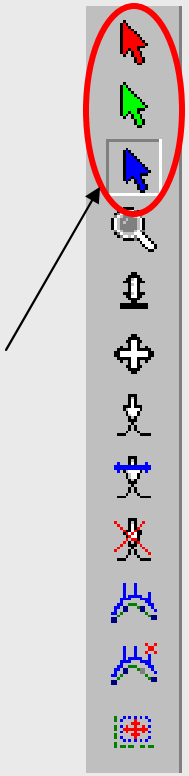
The initial method for analysing a mapped image or profile is to use three cursors (**R**, **G** and **B**) to define regions.

The image is generated by displaying the spectral intensity between these cursors.

The three cursors are simply selected from the three coloured cursor.

These three cursors appear when the window SpIm is activated.

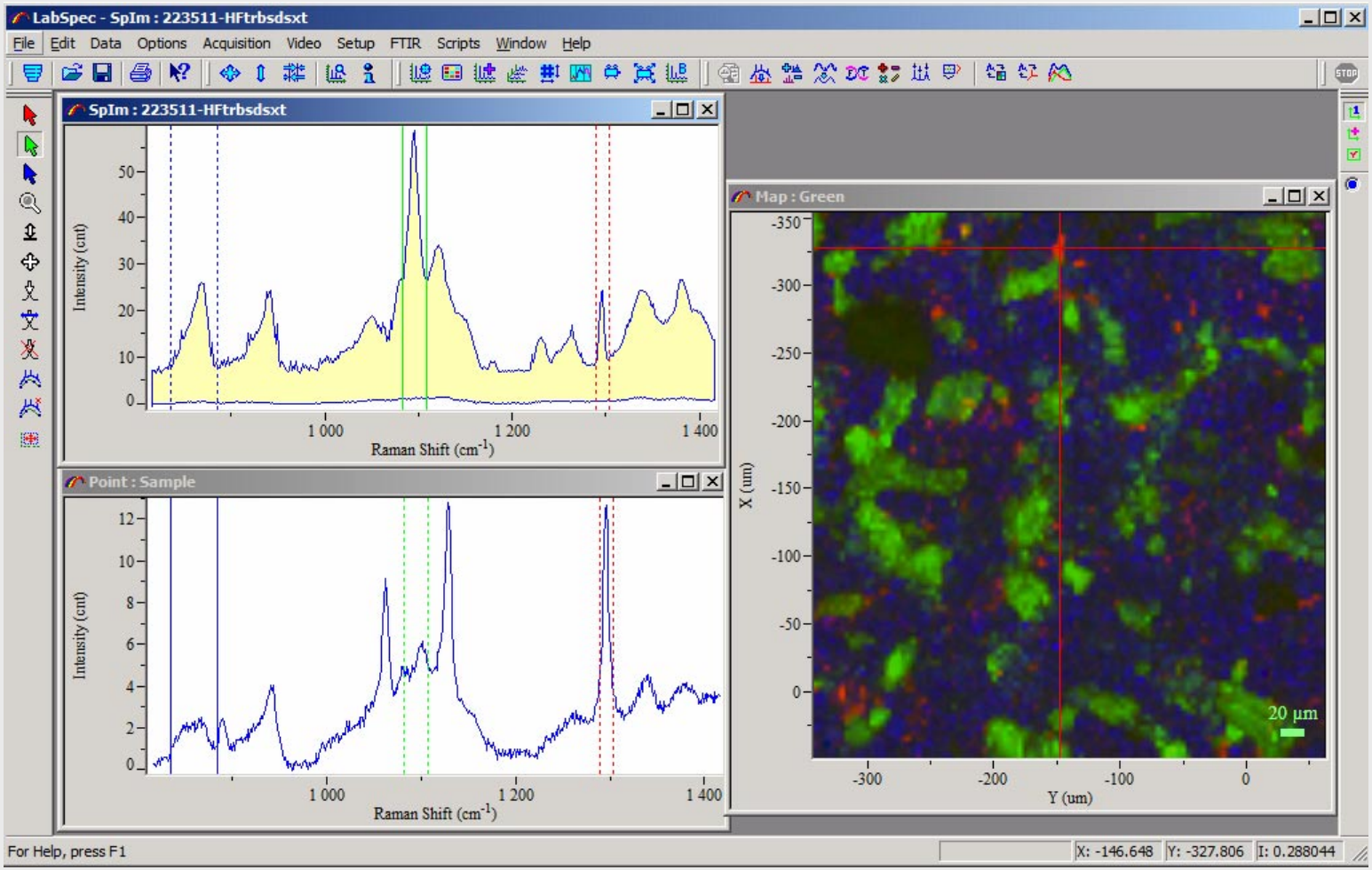
If one or more of the cursors aren't currently displayed on screen, they can be returned by clicking on the **Cursor normalization** icon on the toolbar.



Example

- Sample description
  - A raw pharmaceutical pellet. The map shows the distribution of 3 widespread fillers in pharmaceutical pellets: Cellulose, Starch and Magnesium stearate.
- Measurement
  - A large map is recorded onto the surface of the pellet.
- Acquisition conditions
  - Instrument: LabRam HR
  - Laser wavelength : 633 nm
  - Grating : 600 gr/mm
  - Confocal hole : 600 µm
  - Objective: ×50
  - Map size: 400 × 400 µm and 36 × 36 data points
  - Acquisition time: 10 s/point

The map displays the distribution of 3 components: Starch, Cellulose, and MgStearate



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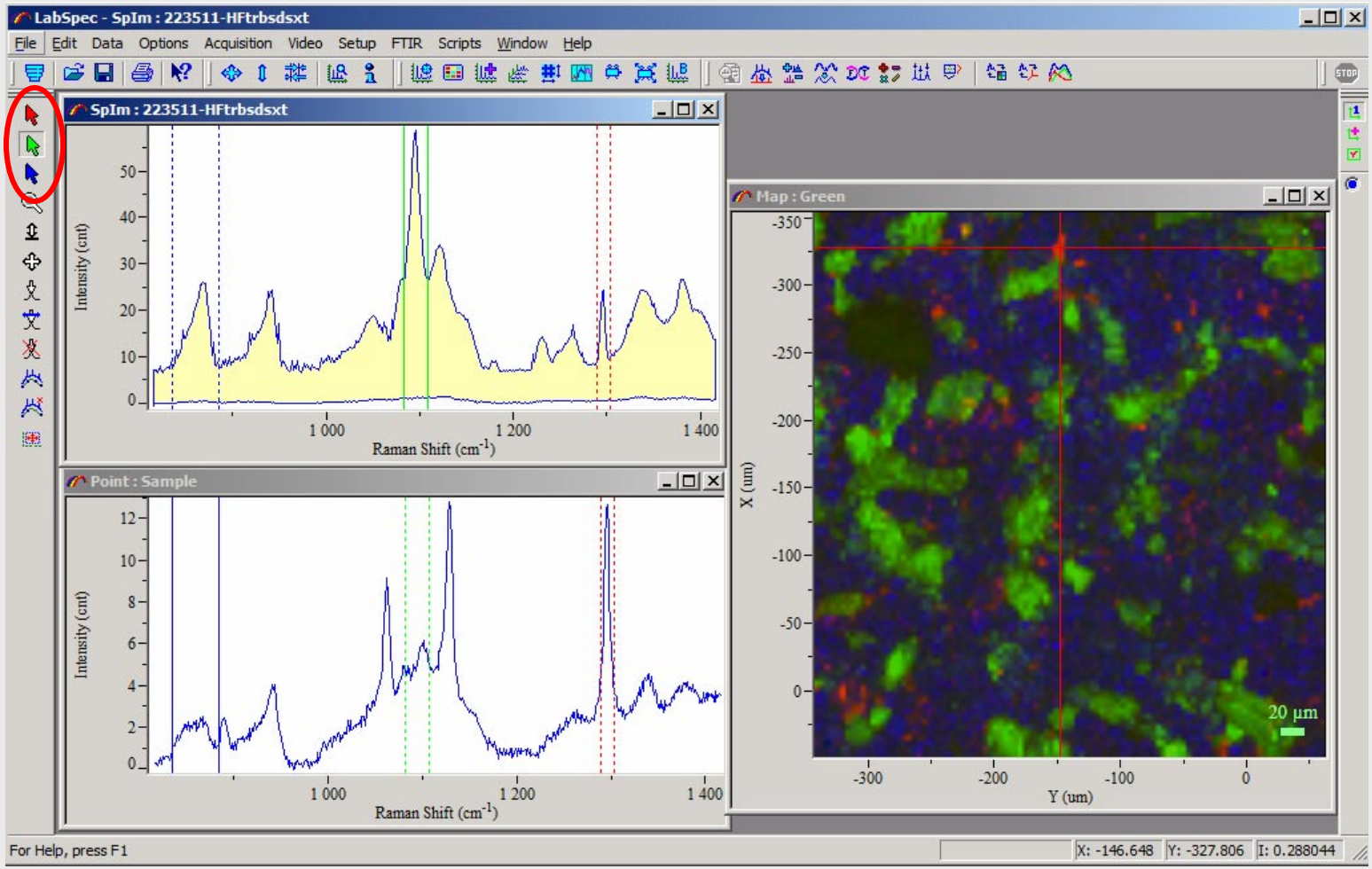
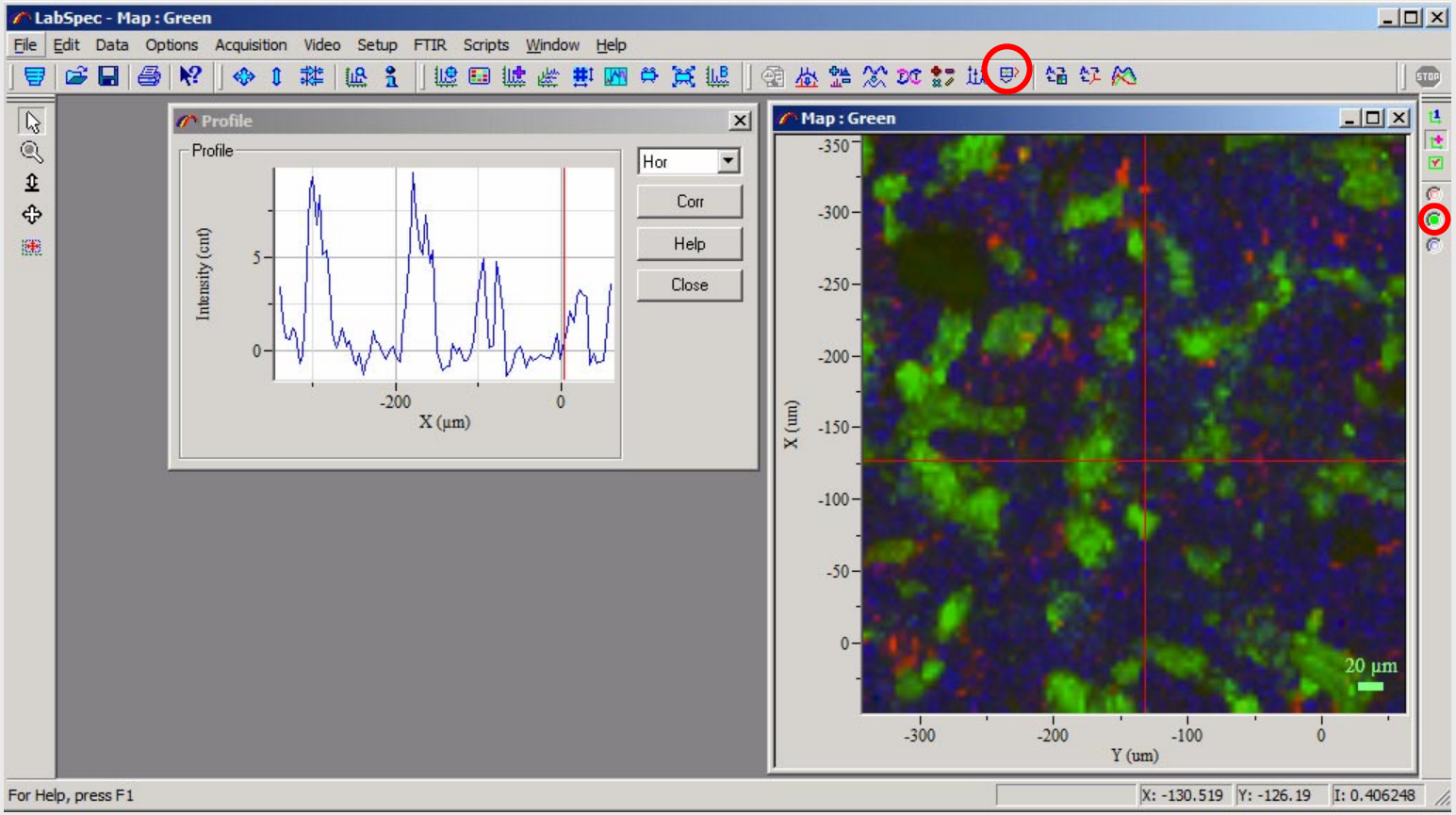
To display the integrated intensity map, position pairs of Red, Green, and Blue cursors around selected Raman bands in *Point* or *SpIm* by selecting the corresponding color arrow on the left toolbar.

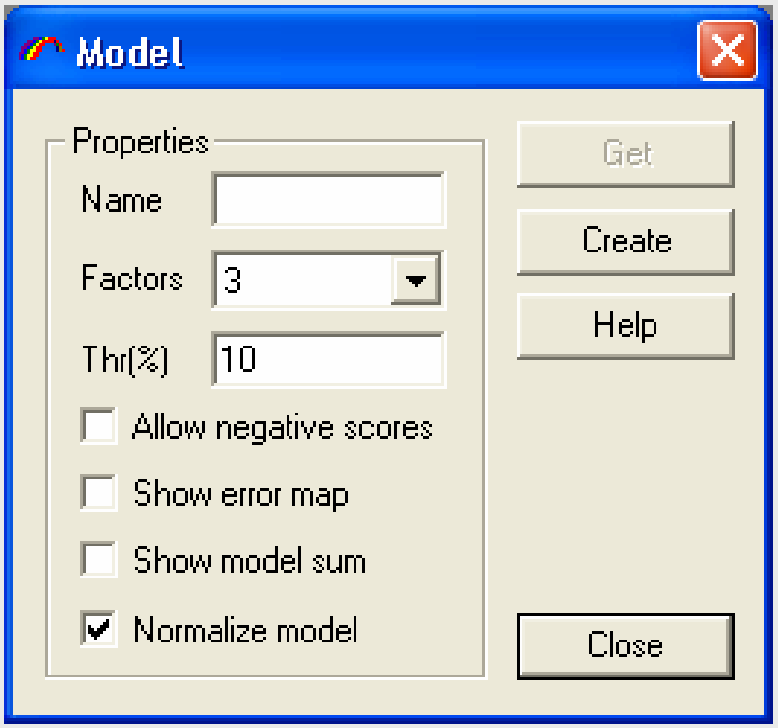


Sometimes, an intensity profile along a line can provide useful information such as diameter of agglomerations. Select a map (right tool bar) and click **Profile** icon (top tool bar). The intensity profile of the selected intensity map is displayed along the vertical or horizontal cursor line (red cross in *Map* window).



Select intensity map

Modeling



Supervised or unsupervised factors

Normalize model

If the spectra of the pure components are available, they can be taken into the modeling program.

If not, LabSpec 5 allows you to create a model automatically by using a factor analysis algorithm.

In terms of normalization of the reference spectra:

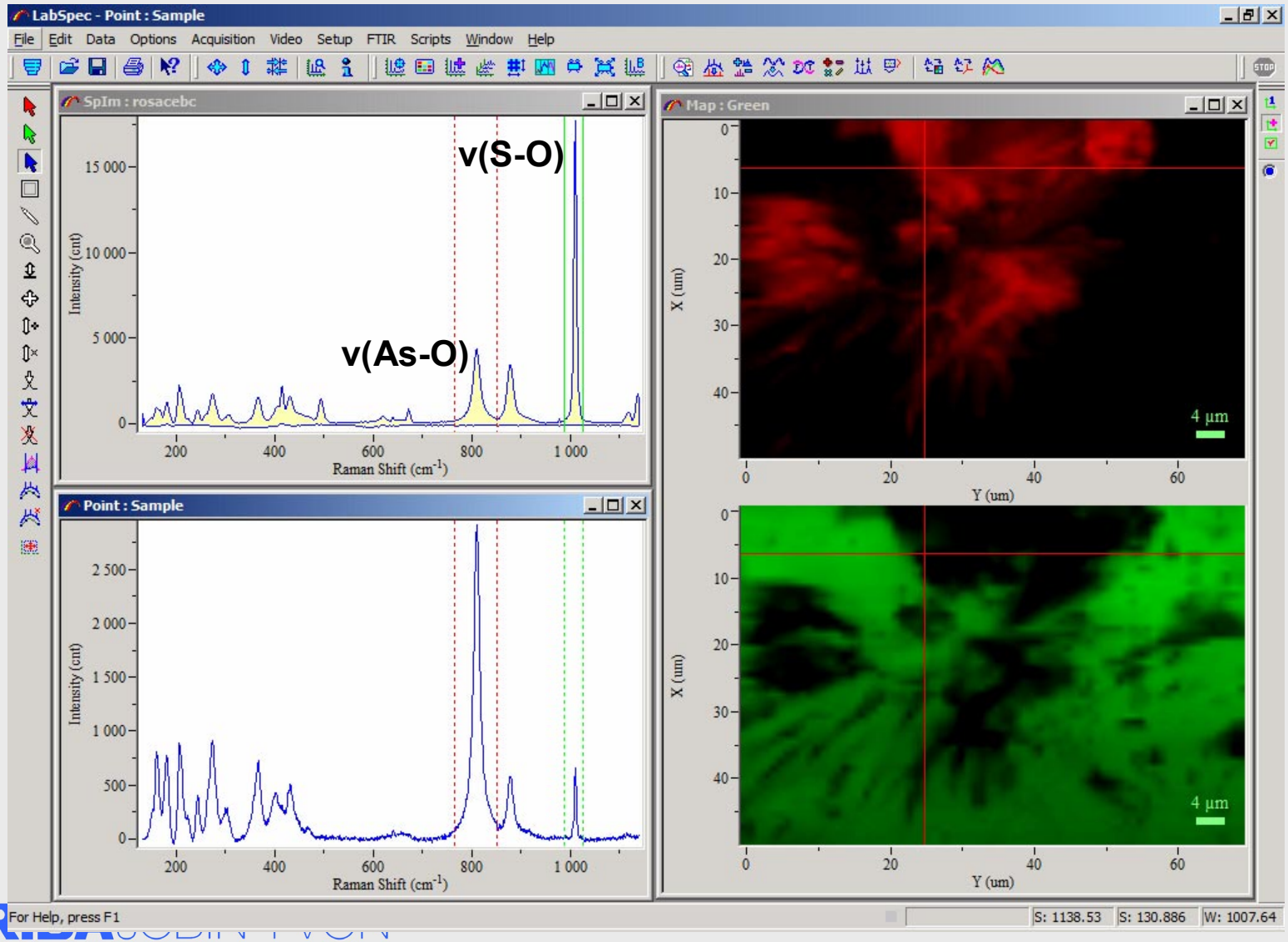
If the original spectra had not been recorded in the same conditions you wouldn't loose any information by normalizing because the relative intensities were already unreliable.

But, if the spectra have been recorded in the same conditions, the relative intensities are representative of the relative Raman scattering power of each components. In this latter case, you loose information by normalizing.

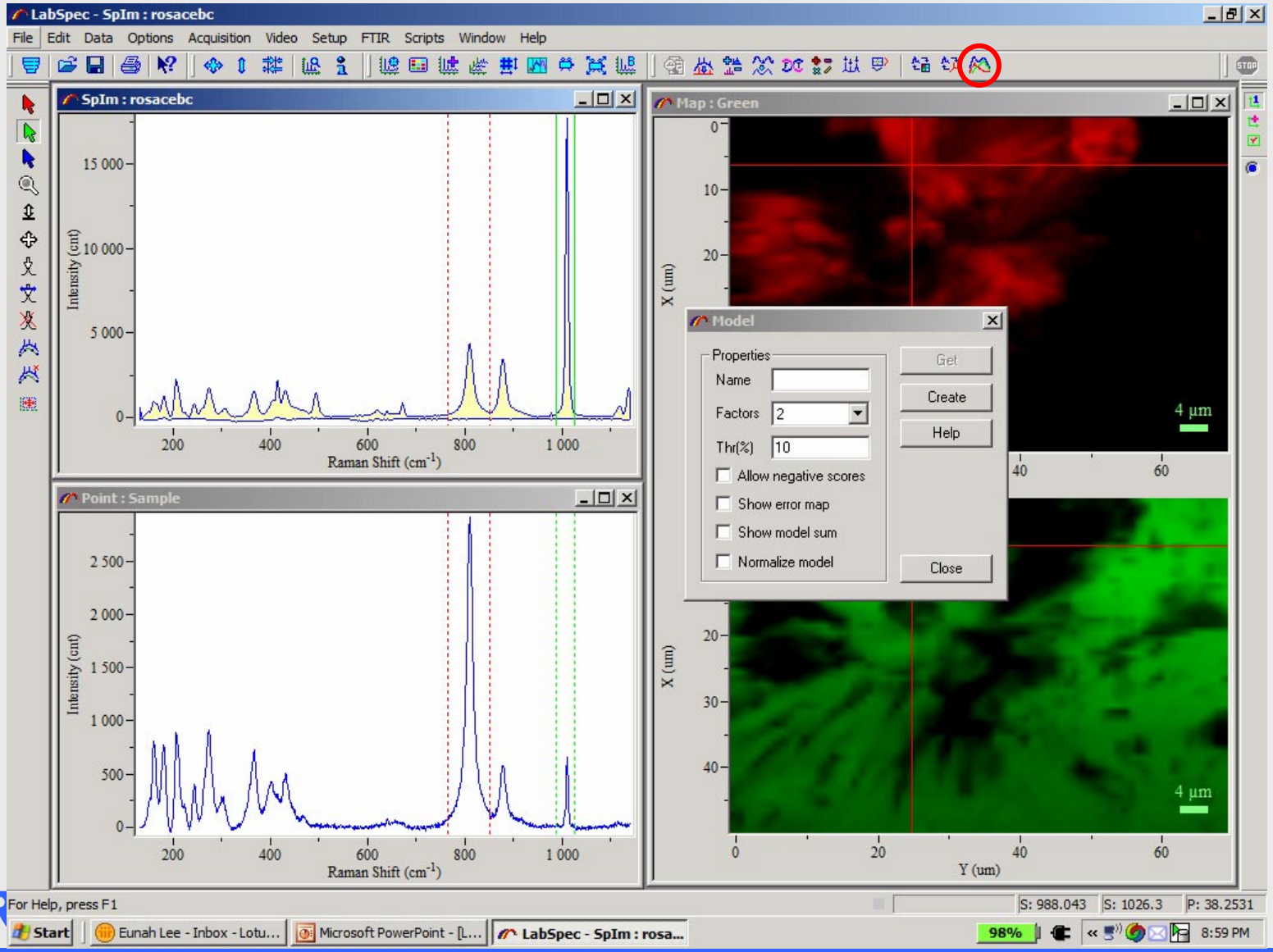
Example

- Sample description
  - AsO_4^{3-} can substitute for SO_4^{2-} in sulfate minerals. Raman spectrometry proved very useful for investigating the formation of SO_4^{2-} - AsO_4^{3-} intermediate phases.
  - The sample comes from a former industrial site in France comprising mainly sulfate minerals similar to gypsum ($CaSO_4.2H2O$) and thenardite (Na_2SO_4) and with a high As content (8 to 18% w/w).
- Acquisition conditions
  - Instrument: LabRam HR
  - Laser wavelength : 633 nm
  - Map size: 51 × 70 µm
  - Step size: 1µm
  - Acquisition time: 10 s/point

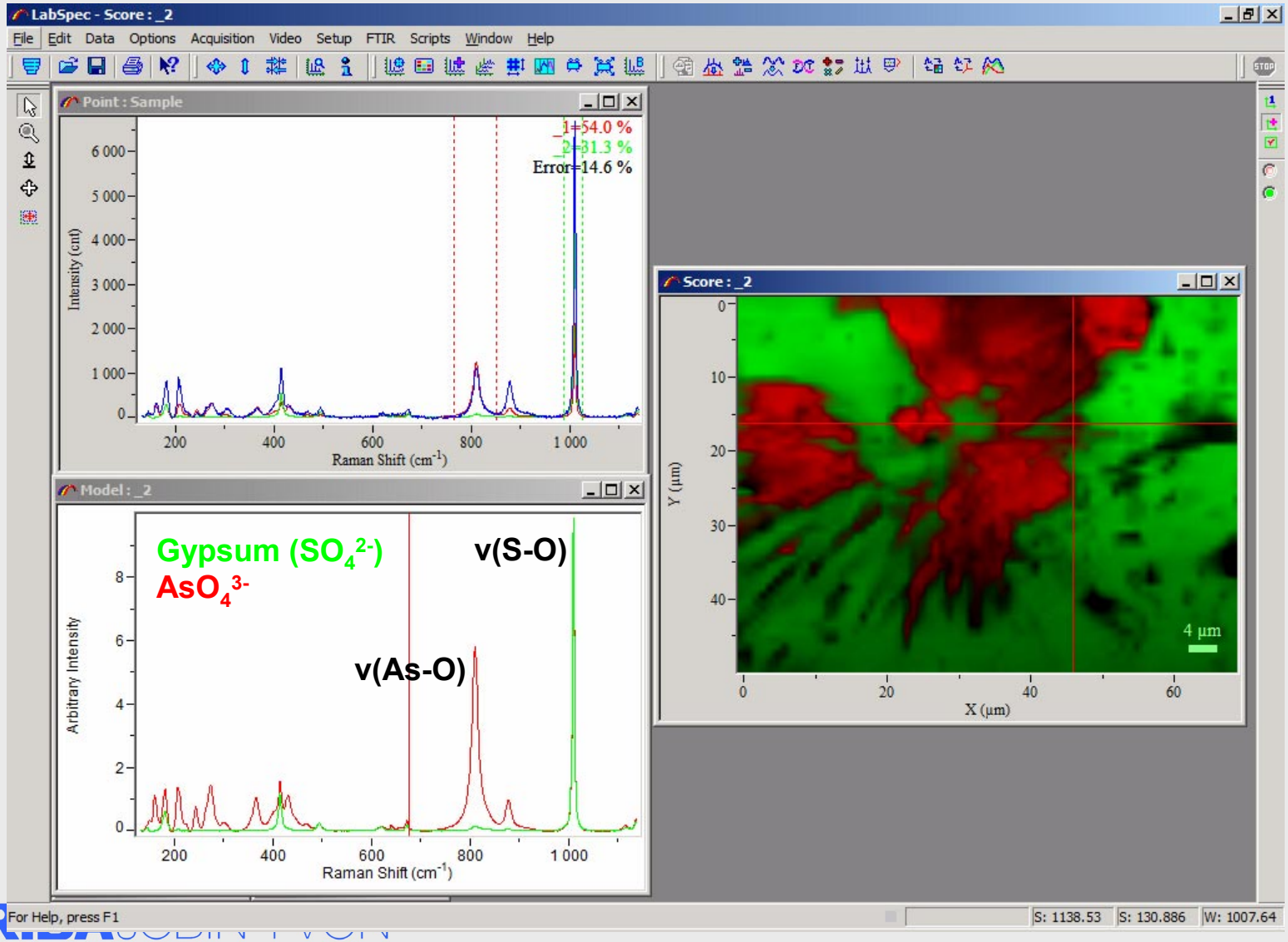
Two phases are observed. The characteristic peak of each phase is displayed between Red and Green cursors:



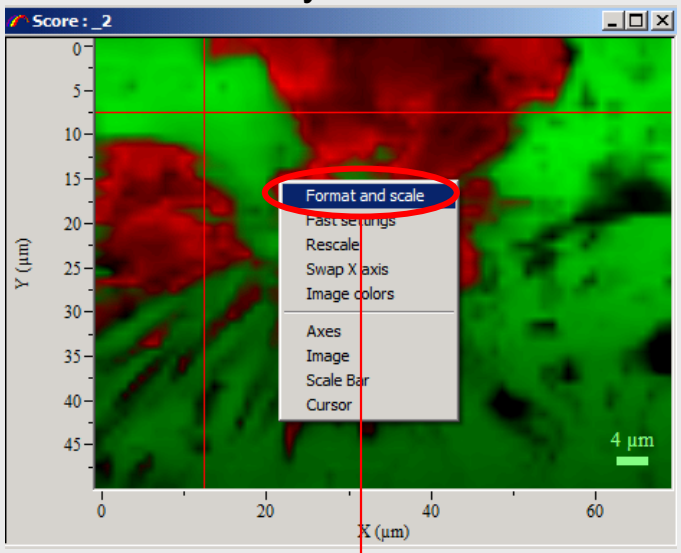
To extract two pure spectra constituting the sample, click **Modeling** icon to open *Model* window. Set FACTORS to 2 and click **Create**.



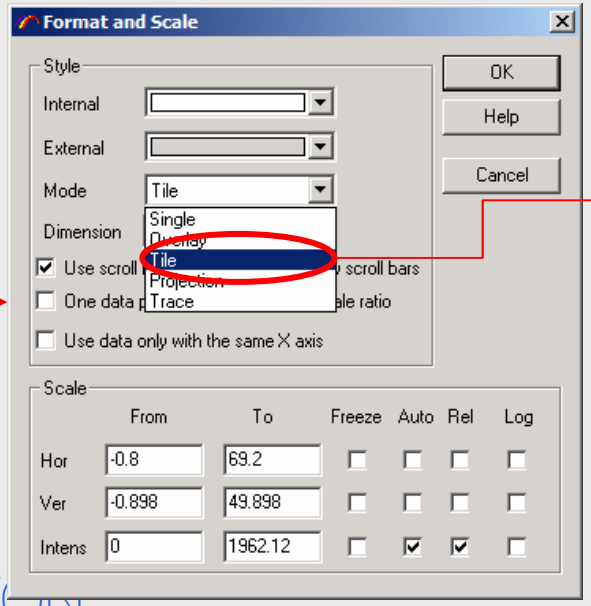
Two phases are extracted by the Modeling procedure. The characteristic peak of each pure phase is displayed in Red and Green.



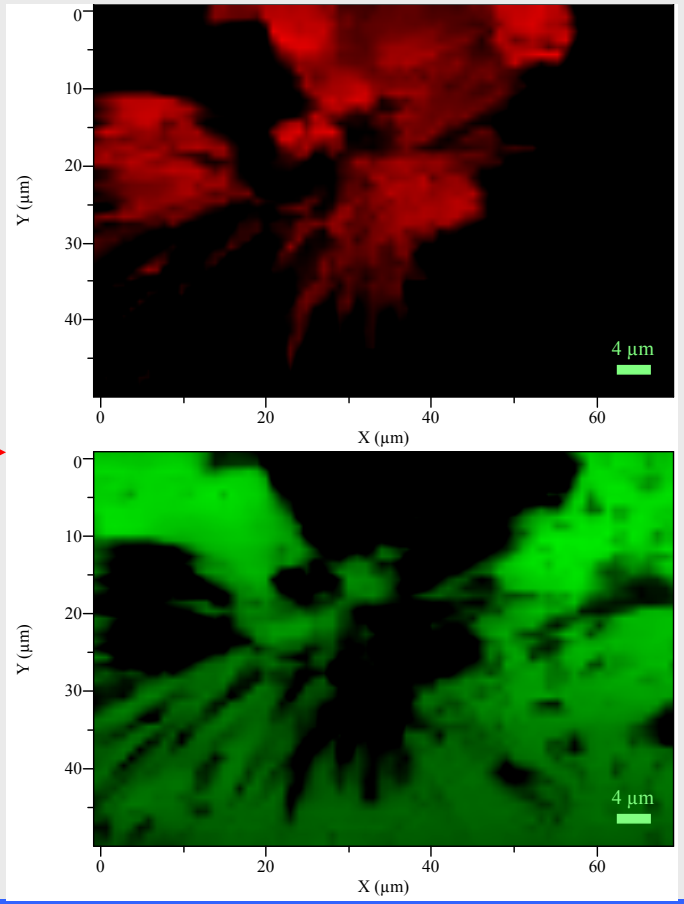
MODE: Overlay



To change the display mode of score images, right click in the image to activate window context menu and select **Format and scale**. Select TILE from MODE.



MODE: Tile



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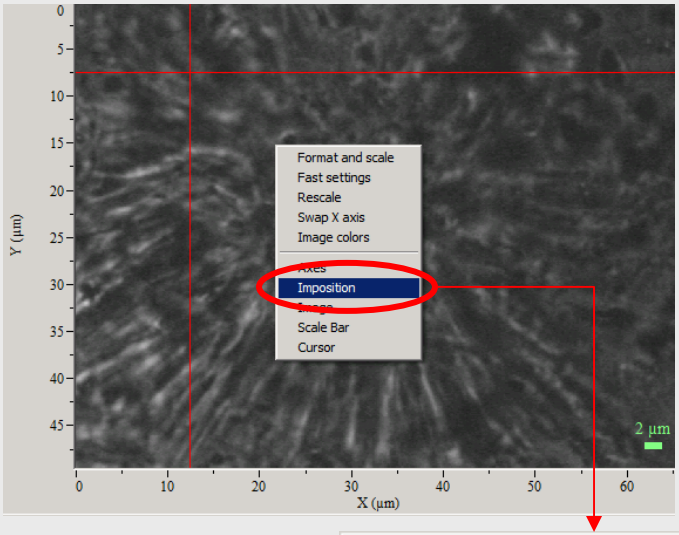
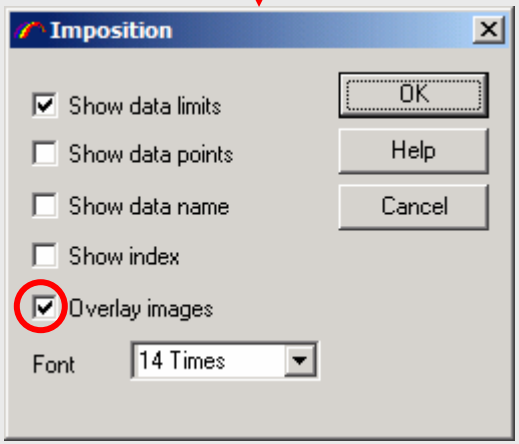
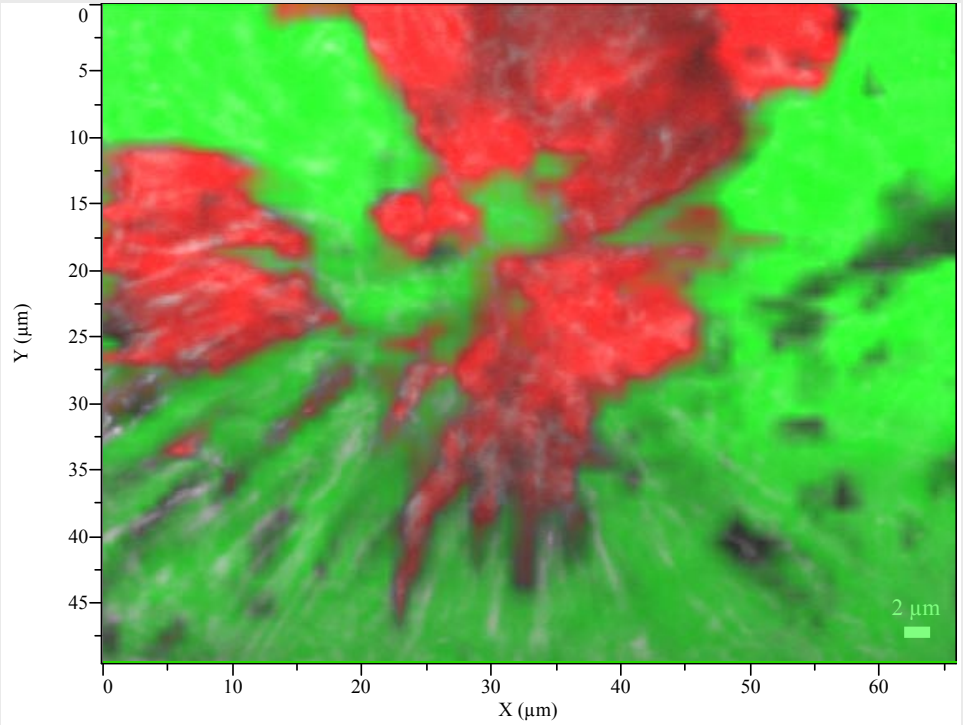
Open the corresponding video image, right click in the image to activate the window context menu, and select **Imposition**. Check OVERLAY IMAGES box. Select an intensity map or a score map to overlay.







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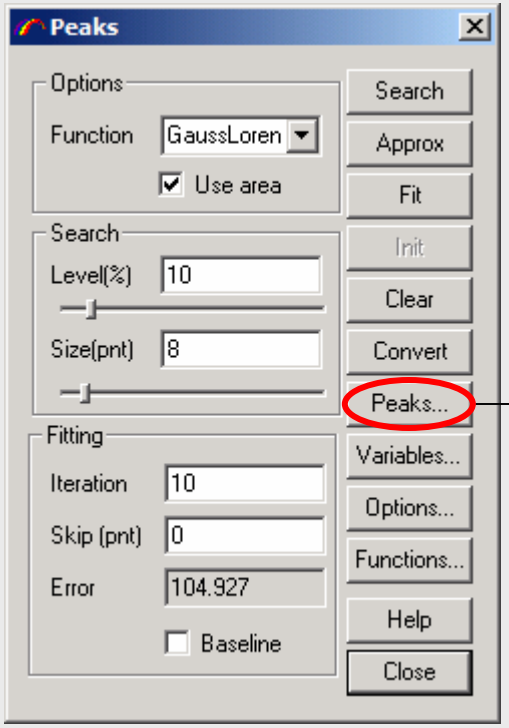
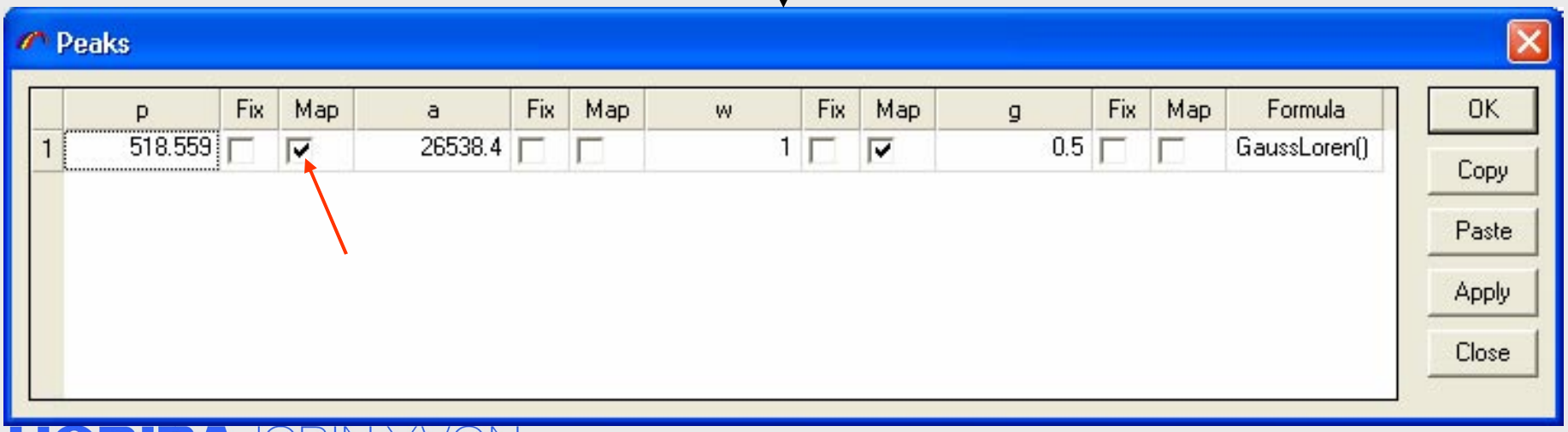


It is also possible to use the band fitting results to create a map of peak position (p), amplitude (a), band width (w) and the area (a) of the peak.

Check MAP box of the parameter to map and click **Apply**.

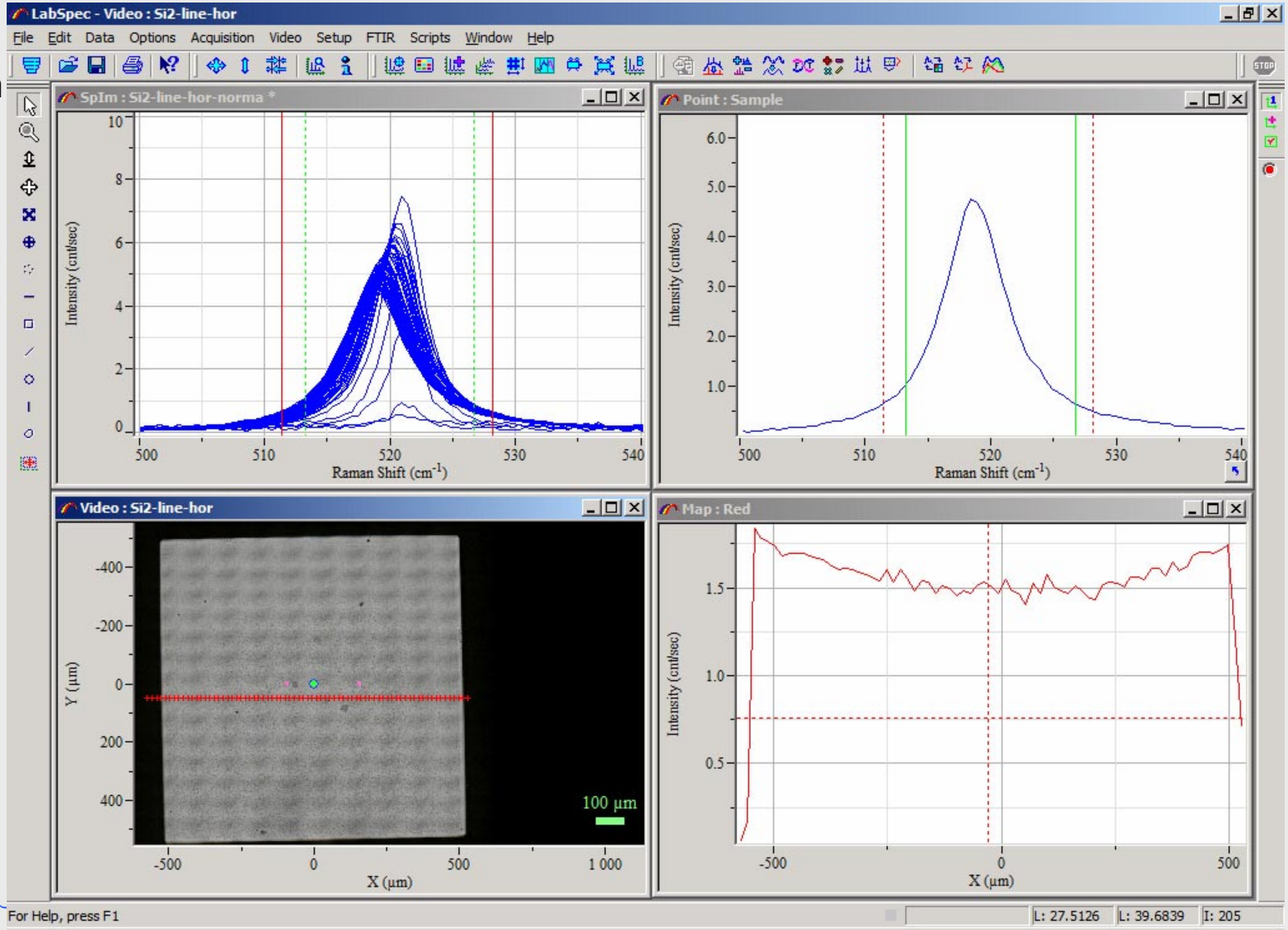


Example

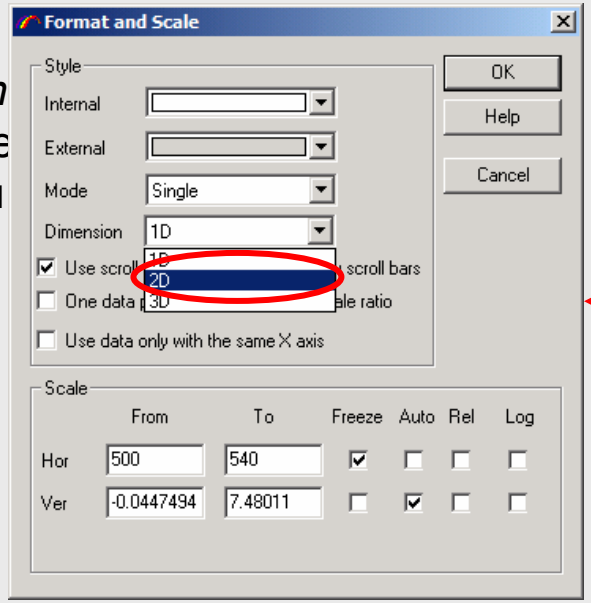
- Sample description
  - 1 mm square silicon structure.
- Measurements
  - A line measurement is recorded at mid-height of the square from one edge to the other.
  - A spectrum is recorded at every 15 µm.
  - The Silicon peak position in a non-stressed Si crystal is 520.7cm^{-1}.
  - If a tensile or a compressive stress is occurring in the structure (due to a defect, a coating, a boundary, etc.), then the position of the peak shifts to lower (tensile) or higher (compressive) wavenumbers.
- Acquisition conditions
  - Instrument: LabRam HR
  - Laser wavelength : 532 nm
  - Grating: 1800 gr/mm
  - Confocal hole diameter: 200 µm
  - Step size (x-axis only): 15 µm
  - Extended video image: the picture is recorded over a very large surface area.

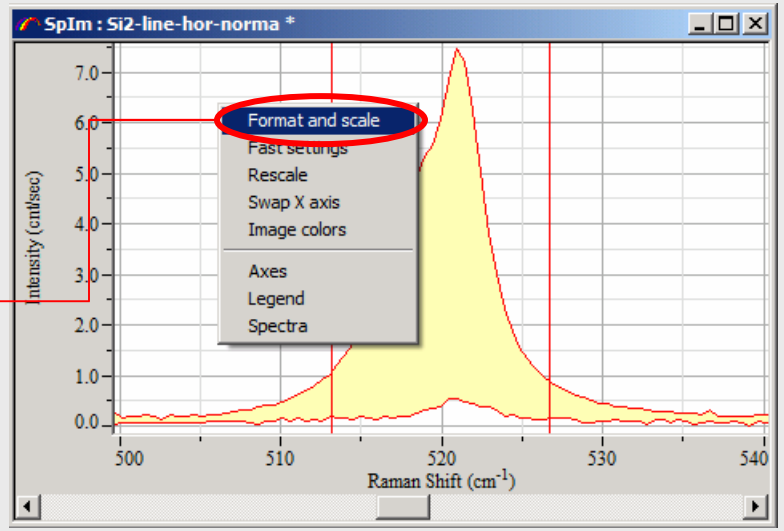
SpIm displays all the spectra recorded along the line. *Point* shows the spectrum at the cursor position selected either in *Video* or *Map*. The line of analysis is superimposed on the video image. *Map* displays up to three parameters that are selected in *SpIm*.

Red cursors are position in *SpIm* to map the intensity of the silicon peak along the line. The intensity drops at the edge of the silicon square.

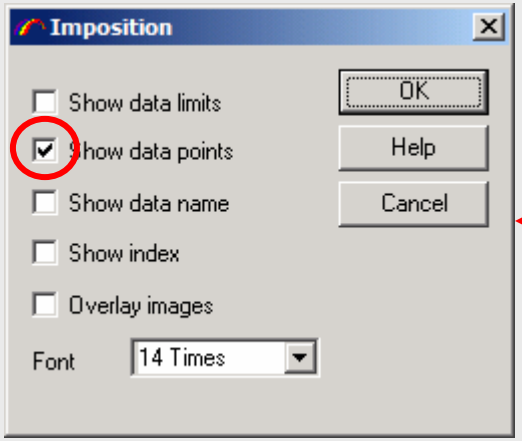


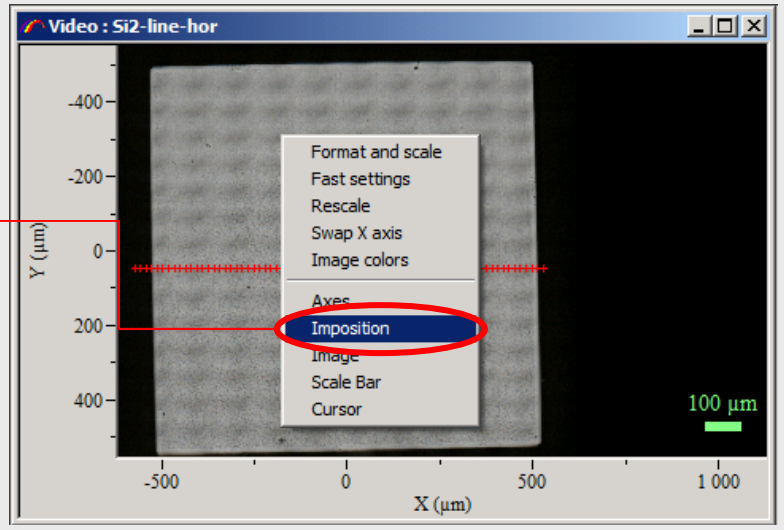
To display *SpIm* in 2D, right click in *SpIm* window to activate the window context menu and select **Format and** scale. Select 2D from DIMENSION





To display the line of measurement on the sample image, select *Video* and right click in the image to activate the window context menu. Select **Imposition**. Check SHOW DATA PPOINTS box.





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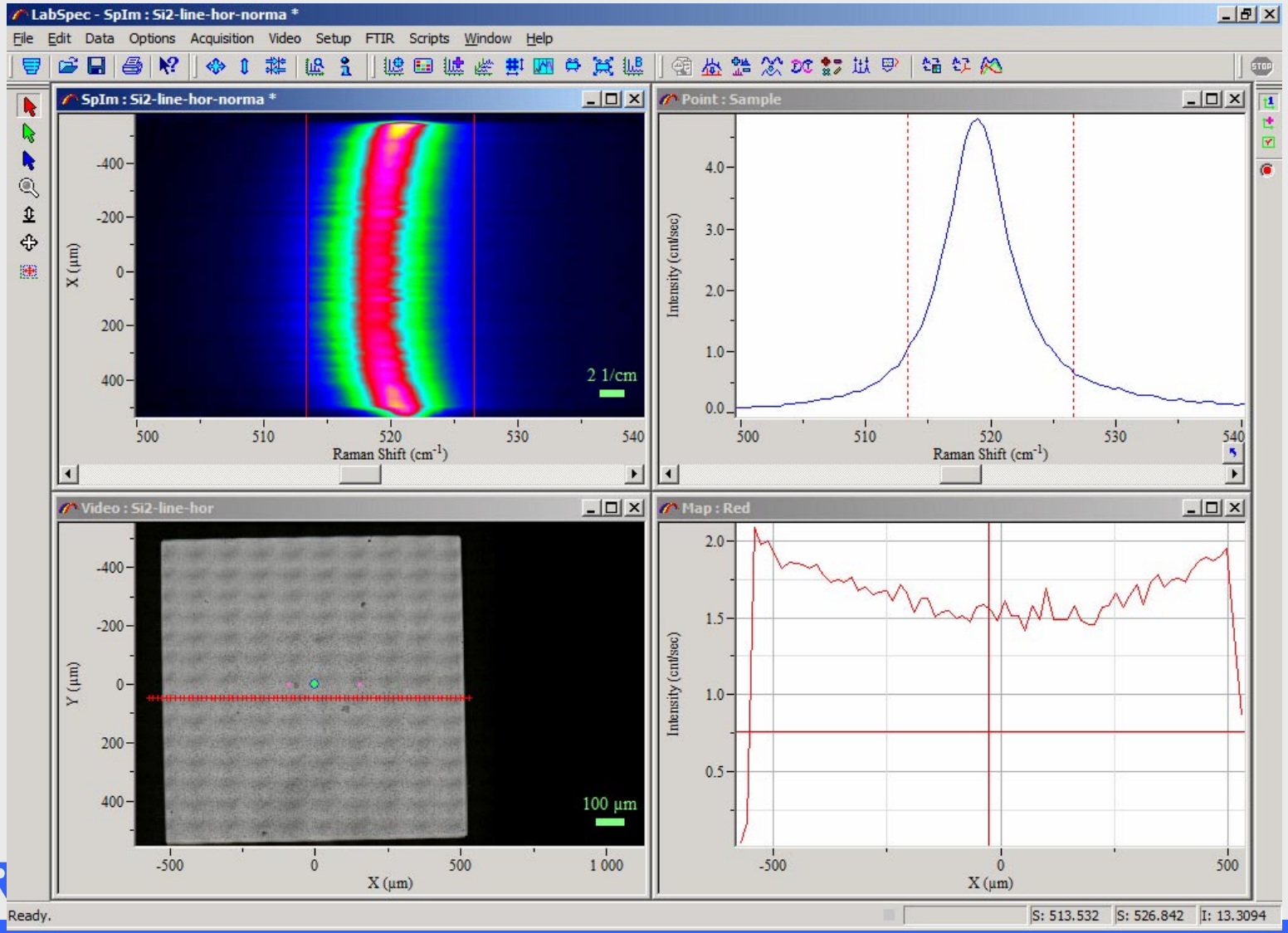
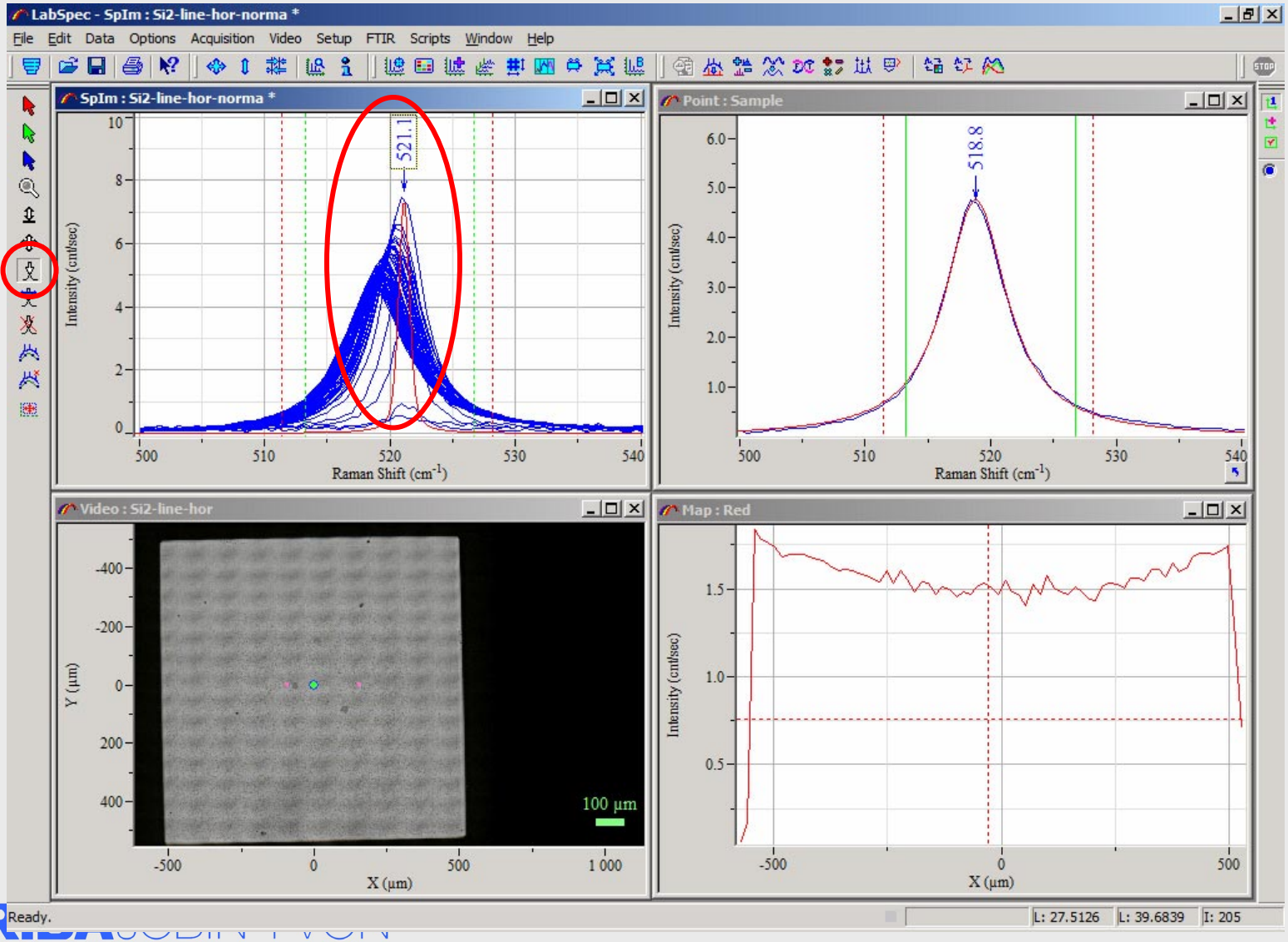
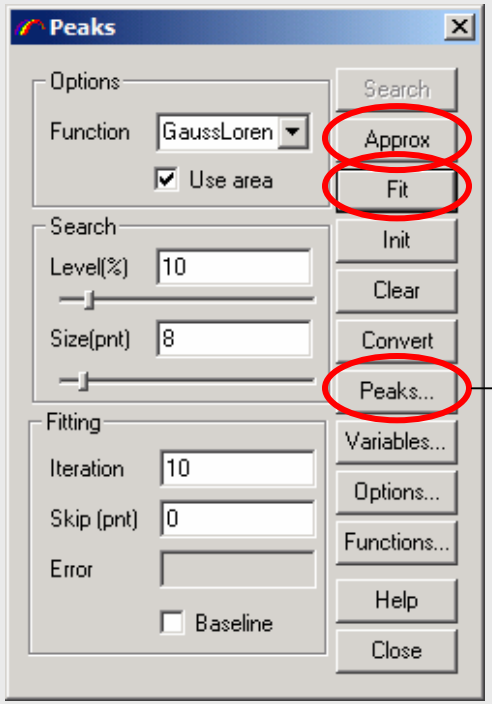
The profile is displayed in 2D in *SpIm* such that the color scale corresponds to the Raman intensity. The curve shape of the 2D map illustrates the shift of the Silicon position along the line of analysis that is displayed on the video image.

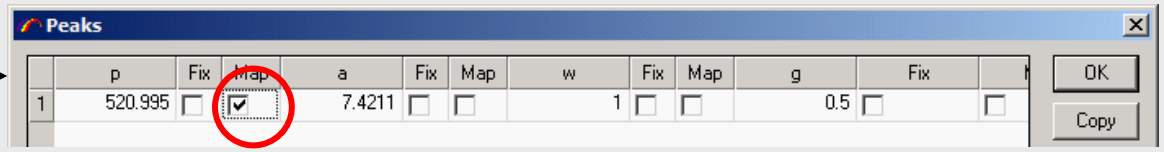


When the profile is displayed in 1D, peak fitting can be applied to the image in order to map the peak positions. Select **Add peak**. Click at the peak position. This adds a peak to be fitted.

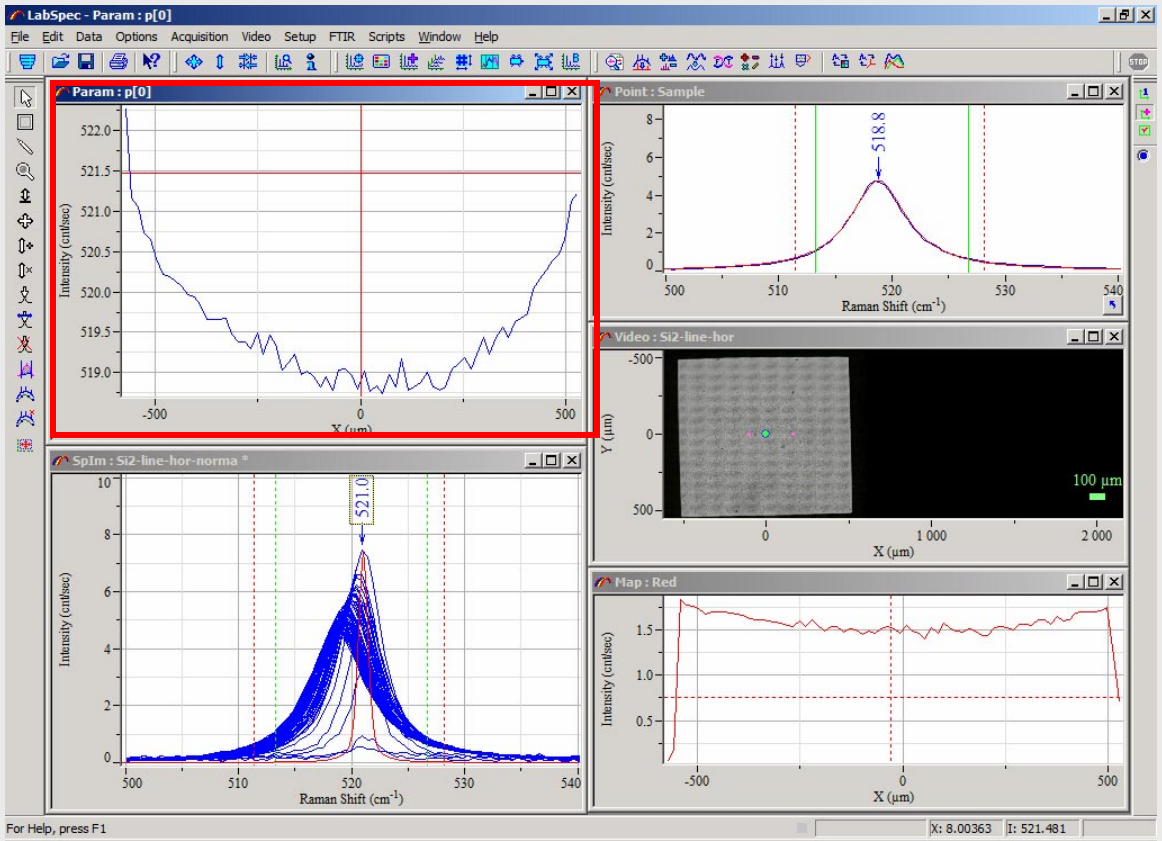




Click **Approx** and then **Fit**.
When finished, click **Peak**. From *Peak* window, check MAP box for P, and click **OK**.



A new window appears with the plot of the peak positions along the line. It gives an accurate idea of the strain in the silicon structure:



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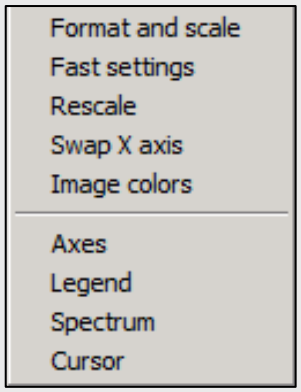
Spectral Profile

- Create a Raman map out of spectra that were recorded separately.
  - Open the files that are to be made into a map
  - Select the first spectrum of the new spectral profile.
  - Input a name and click New. New SpIm window with the given name is created automatically showing the selected spectrum. Corresponding Map window is also created.
  - Add other spectra one by one by selecting and clicking **Add** or **Insert** button.
  - **Add** – adds the selected spectrum to the end of the spectral file.
  - **Insert** – inserts the selected spectrum to the position selected in the Map window

Graphic Tool Panel

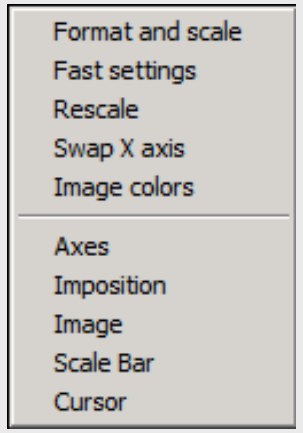
- Window Context Menu
- Activated by clicking right mouse button with the mouse positioned in a window.
- Graphic Tool Panel is sensitive to the characteristics of the window it is linked to. Therefore, the specific elements listed change depending on the window the menu has been called for.
- Each Graphic Tool Panel is composed of two sections, separated by a line. Elements in the top section are common to all windows. Elements in the bottom section are window specific.

Graphic Tool Panels

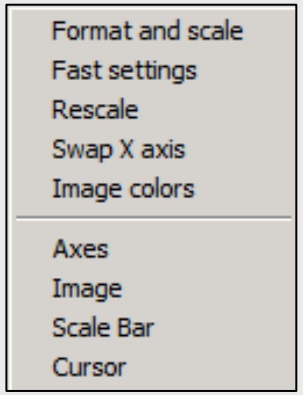


Window displaying individual spectra.
Spectrum
Model

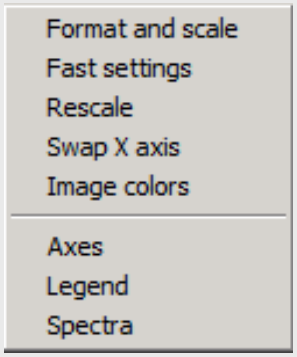
Window displaying individual video images.
Video



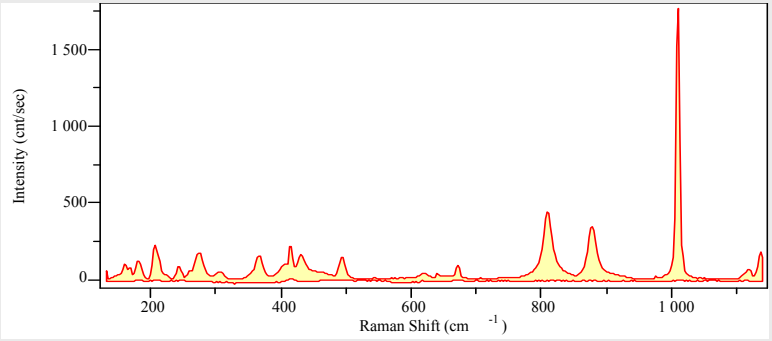
Window displaying maps.
Map
Score

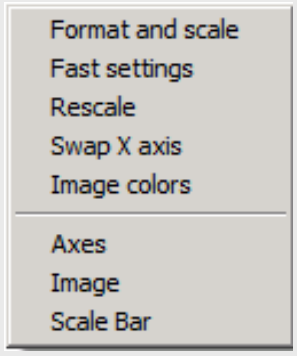


Graphic Tool Panels

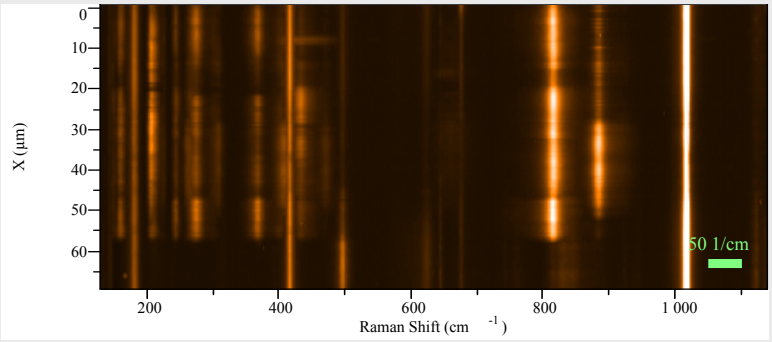


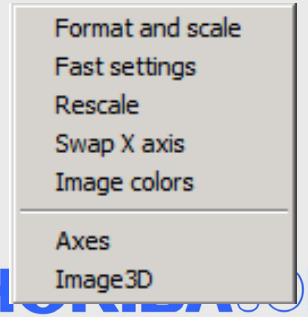
Window displaying a collection of spectra in 1D.
SpIm



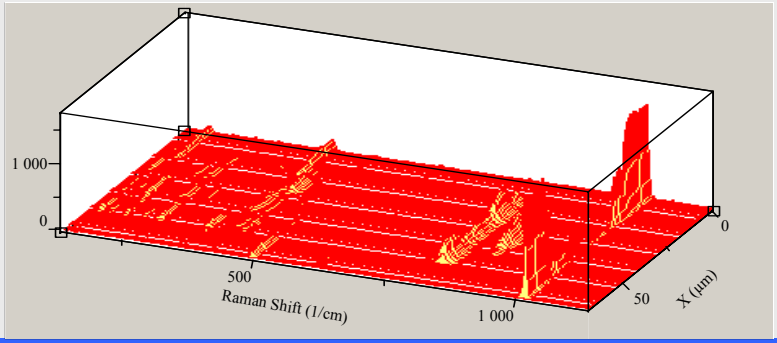


Window displaying a collection of spectra in 2D.
SpIm

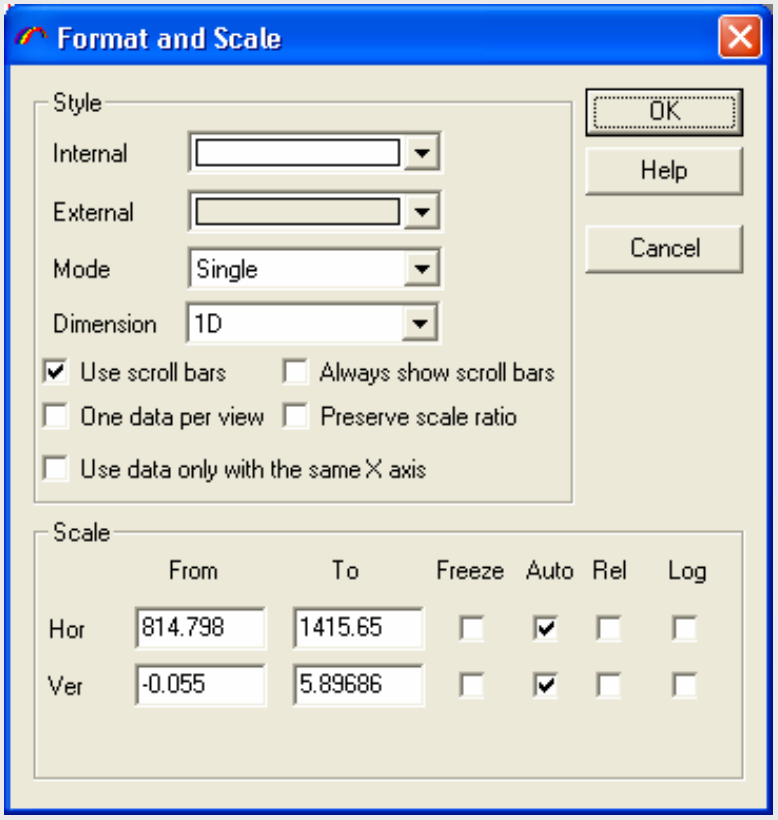




Window displaying a collection of spectra in 3D.
SpIm



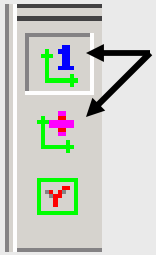
Common Elements



Format and scale

Format the window setting. Often used options are

- Mode: Select display modes out of Single or various Multi modes.
- Rel: Allow multiple spectra/images be displayed with independent scale for easy comparison.



Shortcut icons on the right tool bar
Toggle between single and selected multi display modes

Common Elements

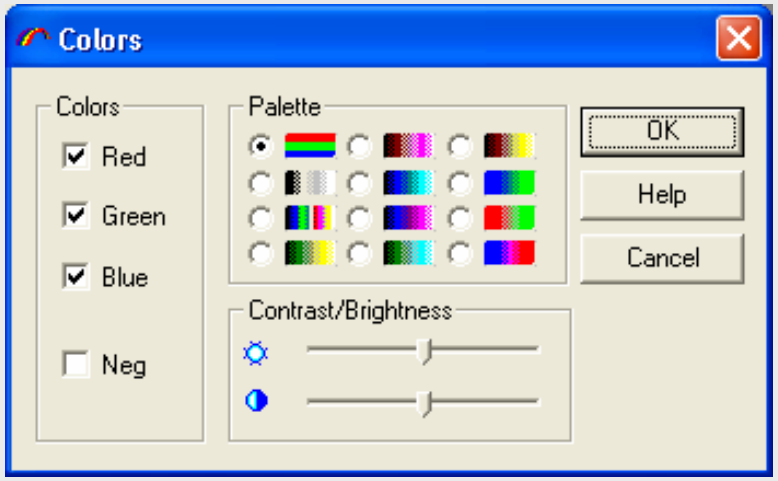
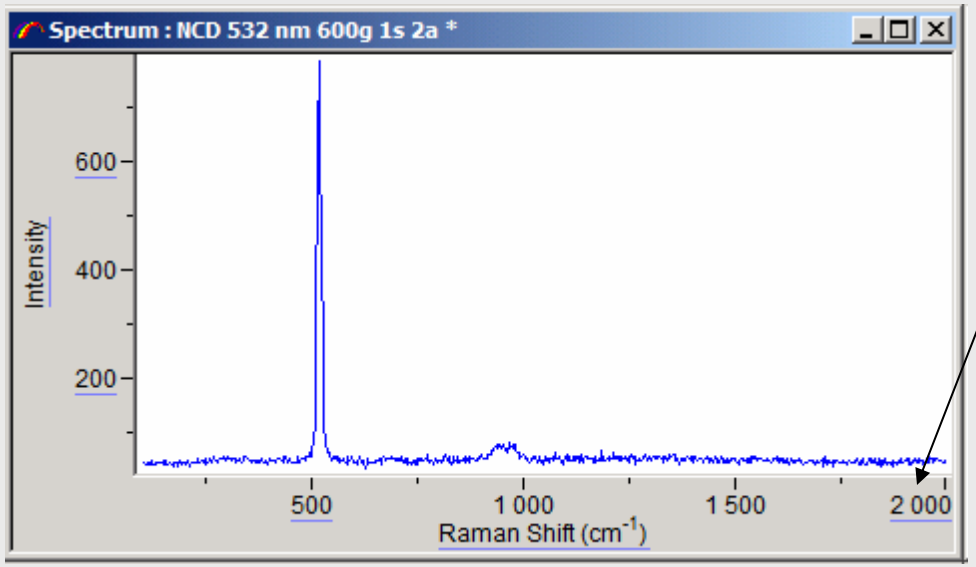
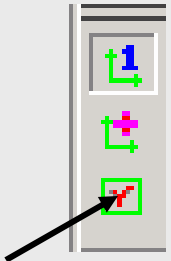


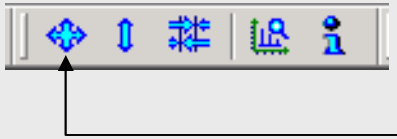
Image colors
Select and format color palette for the window

Common Elements



Fast settings
Activate the interactive formatting from the data window itself.
Elements that can be changed are underlined.
Shortcut icon on the right tool bar

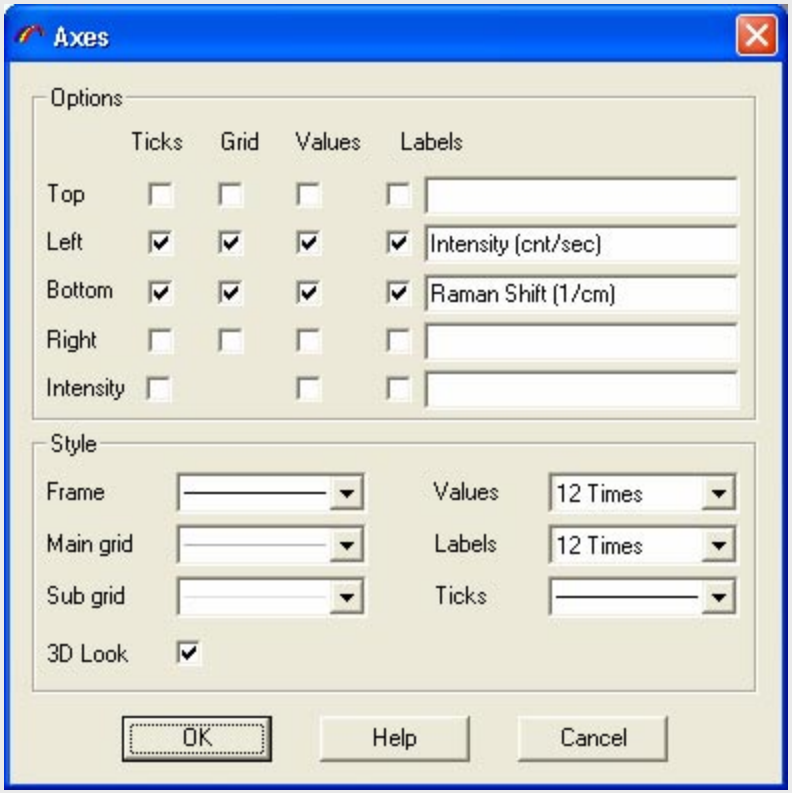




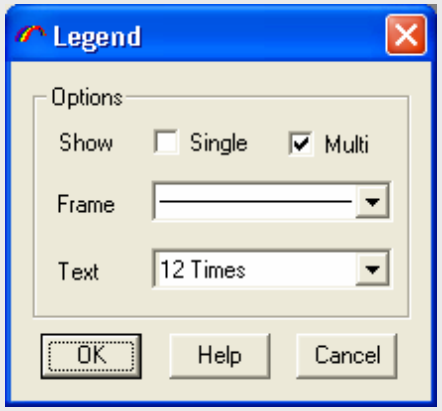
Rescale
Rescale both X and Y axes to show the full data range.
Shortcut icon on the top tool bar

Swap x axis
Reverse x-axis direction

Window Specific Elements



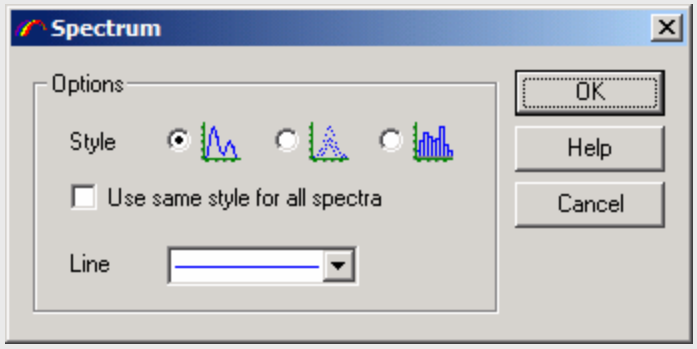
Axes
Format axes and grids.



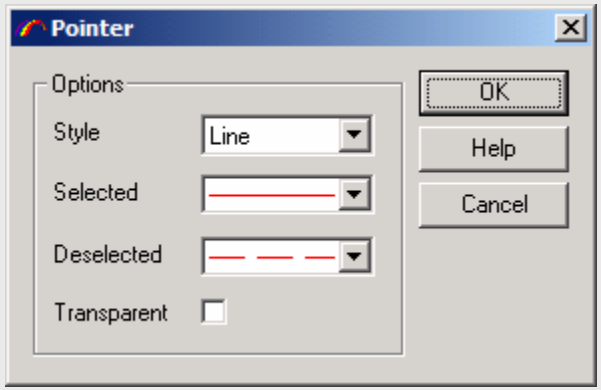
Legend

- SINGLE: Legend is displayed when Single display mode in **Formatting and scale** is selected.
- MULTI: Legend is displayed when one of Multi display mode in **Formatting and scale** is selected.

Window Specific Elements

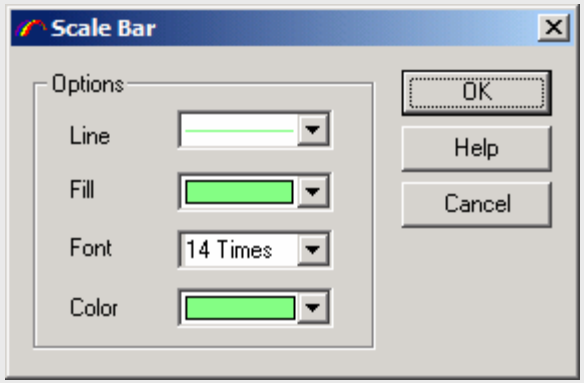


Spectrum
Select to display spectrum as a set of Lines, Points or Bars.
Format line style, color and thickness.



Cursor
Select pointer types:
- Line: single vertical line
- Cross: vertical and horizontal lines
- Level: vertical and horizontal lines with the horizontal line position locked to the intensity
- Double: two vertical lines
- Peak: three vertical lines with positions of two outer lines locked to the approximated FWHM.

Window Specific Elements



Scale bar
Format color and font of scale bar.

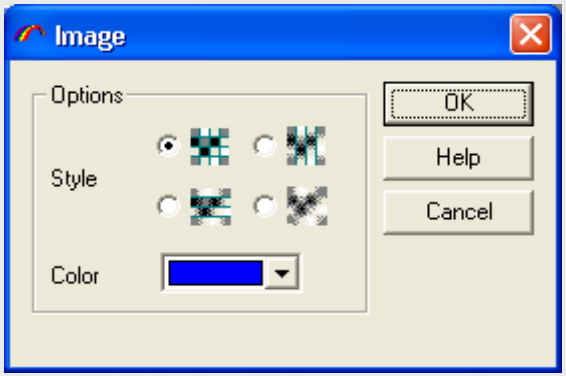
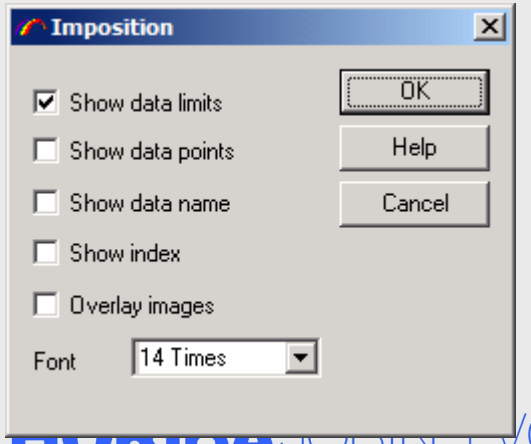
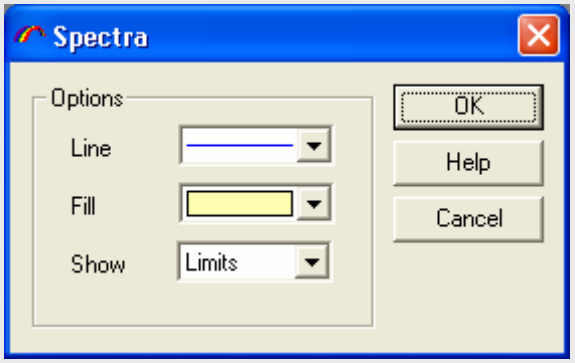


Image
Select to display image with or without interpolated rendering, and change the default image color.



Imposition
Overlay elements of *Maps* or *Score* windows on top of *Video* image. Check boxes of desired elements and then select the *Map* or *Score* window to overlay.

Window Specific Elements



Spectra
Format 1D rendering of SpIm window

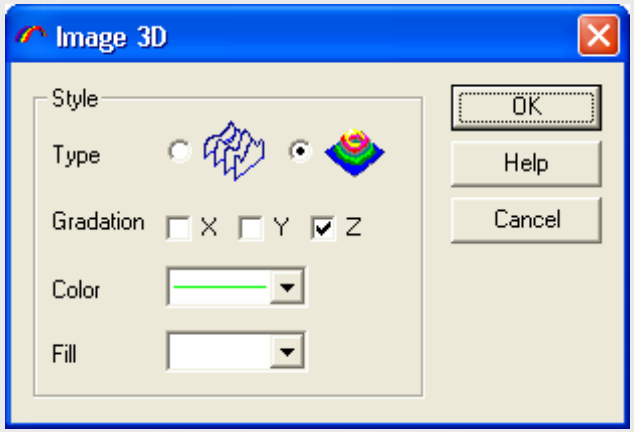


Image 3D
Format 3D rendering of SpIm window

Visual Basic Script (VBS)
A scripting language to automate LabSpec

What is VBS ?

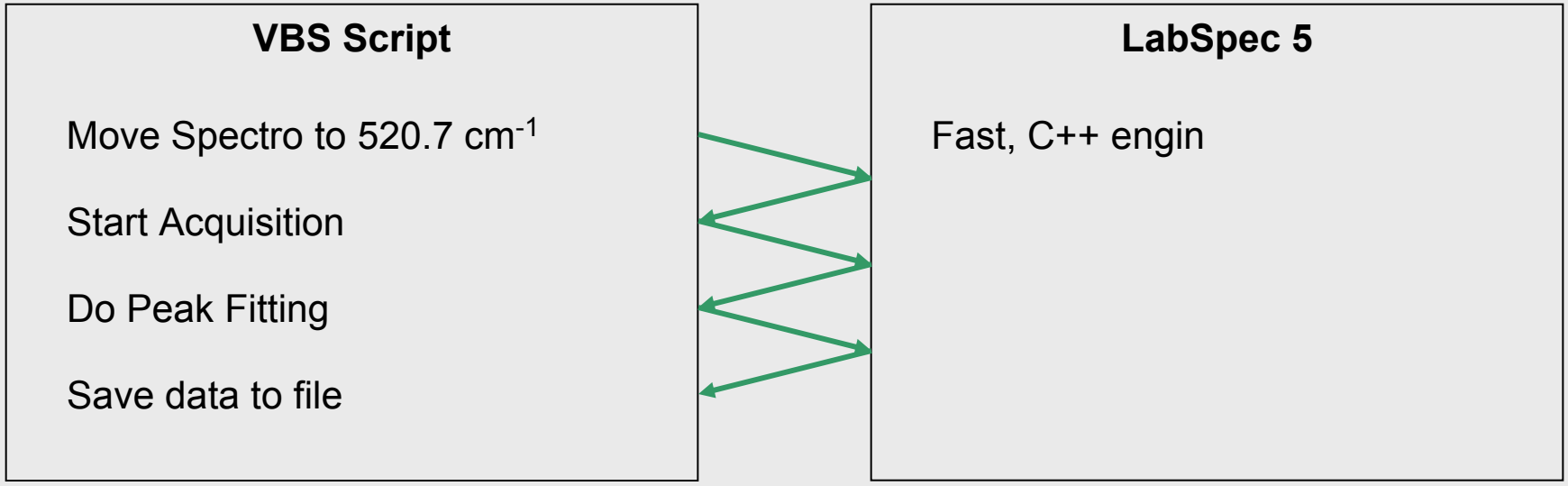
- What is VBS?
  - In order to simplify complex or repetitive tasks, LabSpec 5 can be automated, using VBS, a well known Scripting Language.
  - Visual Basic Script is an interpreted, scripting language.
  - It allows very fast implementation, high level programming.
  - It does not requires an external development environment.
- What can be automated ?
  - Motor movements
  - Data Acquisition
  - Data Treatment
  - 2D Map or 1D Profile Generation
  - Instrument calibration
  - File import/Export
  - Video

What is Different about VBS ?

- There are basically two kinds of programming languages :
  - Compiled languages (C, C++, Pascal, Delphi, etc..)
    - They are low level programming languages that require a program called compiler to convert source code to the machine language.
    - Advantages: Very powerful, flexible and fast to execute.
    - Disadvantages: Hard to code, require a compiler, not intuitive.
  - - Interpreted languages (VBS, JavaScript, Python, PHP, ASP, etc..)
    - They are high level programming languages that do NOT require a compiler.
    - A program called interpreter converts at execution time the commands to the machine language.
    - Advantages: Very fast to implement, easy to code, very intuitive
    - Disadvantages: Much more limited and slower than compiled languages, no visual interface.

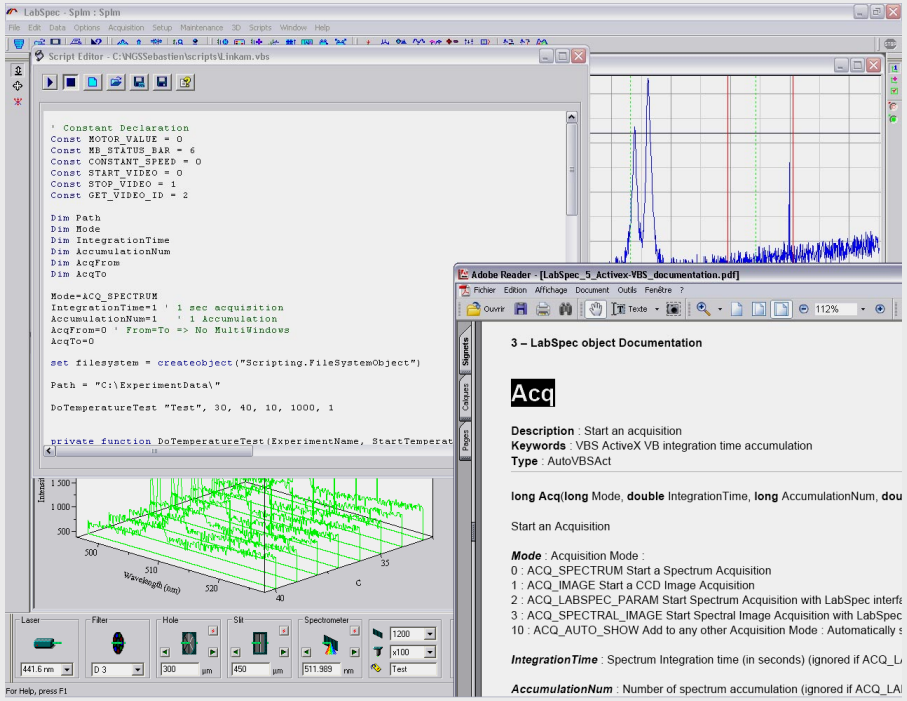
How Does it Work ?

- You said VBS is slow, but I want fast measurements !
  - LabSpec automation allows VBS (easy to code, but slow) to call LabSpec C++ (hard to code, but very fast) functions !
  - This way, you can have both an easy to code scripting language and very fast functions for acquisition and treatment.



What do I Need ?

- LabSpec 5 has an integrated script editor, with auto-completion and syntax colouring.
- It includes Full pdf documentation.
- A ‘Getting Started’ tutorial to get familiar with VBS and LabSpec programming is also available.



Where Can I Use ?

- Examples in Data Acquisition
  - Spectra with different lasers
  - Spectra with different gratings
  - From low power to high power (D2, D1, D0.6,….)
  - Depth profiles with different confocal hole diameters
- Examples in Data Processing
  - Sequences
    - filter + baseline + peak fitting
    - peak fitting + plasma position correction
  - Create new functions
    - create special data smoothing functions

Where Can I Use (cont'd) ?

- Examples in Data Display
  - Create a profile from single spectra
    - 1 D profile with access to axis definition + possibility to have non-equidistant data
    - 2 D profiles (re-create maps from single spectra)
- Examples in Data Export
  - Export in specific format for other software

Visual Basic Script (VBS)
One Practical Example in Detail

Step 1

- Objective: Automate a Linkam heating/cooling stage
  - This example will show you how easy and how fast VBS prototyping can be, even with a relatively complex project.
- Requirements:
  - Manage a temperature ramp (From T_1, to T_2, Step, Speed, Holding time and Experiment name)
  - Take a video snapshot before each spectrum (save image to file)
  - Do a Raman Acquisition (save spectrum to file)
  - Create a profile Intensity vs. Temperature (save profile to file)

Step 2

1. Create a function to manage the temperature ramp
   - Temperature ramps are defined by 6 parameters. Let's write a function that can handle these parameters.

   Function DoTemperatureTest (ExperimentName, StartTemperature, StopTemperature, Speed, HoldingTime, TemperatureStep)

   End Function
2. Setup the Linkam stage with the correct speed and holding time
   - LabSpec specific functions are identified by "LabSpec." prefix. These functions are fully documented, specific parameters are explained and a short example is provided.

```
'Set Heating/Cooling Speed
LabSpec.ManageTemperature CONSTANT_SPEED, Speed, 0, Speed, 0, HoldingTime
```

ManageTemperature

- Overview
  - Description: Manage Linkam stage parameters
  - Keywords: Cooling, heating, speed
  - Type: AutoVBSAct
- Syntax
  - **long** ManageTemperature (**long** *Mode*, **double** *HeatingSpeed*, **double** *HeetingTime*, **double** *CoolingSpeed*, **double** *CoolingTime*, **double** *HoldingTime*)
- Parameters
  - *Mode*: Heating and Cooling mode
    - CONSTANT_SPEED: Use constant speed (ºC/min) during heating/cooling
    - CONSTANT_TIME: Use contstnat time (sec) for heating/cooling
    - FREE_TEMPERATUREL Free the cooling stage (other parameters are ignored)

Step 3

3. For each point, heat or cool the Linkam stage
   - The Linkam stage can be used as any other motor (spectro, hole, slit, etc.)
   - The unique command to drive all motors is “LabSpec.MoveMotor”
   - MotorName is “Temperature” and MotorPosition (ºC) for point i can be calculated by: Temp (i) = StartTemperature + i × TemperatureStep

```
‘Calculate the number of spectra
NbSpectra = (StopTeperature – StartTemperature) / TemperatureStep + 1

‘Heat/Cool to the first/next step
For i = 0 To NbSpectra – 1
      LabSpec.MoveMotor “Temperature”, StartTemperature + I * TemperatureStep,
      “”, MOTOR_VALUE
Next
```

MoveMotor

- Overview
  - Description: Moving a specific motor
  - Keywords: Script, step value, string index
  - TypeL AutoVBSAct
- Syntax
  - **long** MoveMotor (**LPCTSTR** *MotorName*, **double** *PositionValue*, **LPCTSTR** *PositionName*, **long** *Mode*)
- Parameters
  - *MotorName*: Motor name (see Motor Name List)
  - *PositionValue*: Value to reach
  - *PositionName*: Position name (only for named position motors such as microscope)

Step 4

4. Capture a video snapshot
   - Waiting for the video to be ready may take some time, for example to move the beam splitters in ARAMIS.
   - The video image is being saved to a native “*.ngv” file here, but it can also be saved as a TIFF or JPEG image

```
'Take Video Image
LabSpec.Video START_VIDEO        'Start the live video

Do                               'Wait till video is ready
    VideoID = LabSpec.Video (GET_VIDEO_ID)
Loop Until VideoID > 0

'Save the live video image
LabSepc.Save VideoID, Path & ExpermentName & "\Video_" & i+1 & "_" &
CurrentTemperature & "deg.ngv", "ngv"

LabSpec.Video STOP_VIDEO         'Stop the live video image
```

Video

- Overview
  - Description: Display video image
  - Keywords: Camera
  - Type: AutoVBSAct
- Syntax
  - **long** Video (**long** *Mode*)
- Parameters
  - *Mode*: Start/Stop video
    - START_VIDEO: 0, Start video
    - STOP_VIDEO: 1, Stop video

Step 5

5. Spectrum Acquisition
   – Raman Acquisition is totally similar to the video acquisition

```
'Take Spectrum

'Start acquisition
LabSpec.Acq Mode, IntegrationTime, AccumulationNum, AcqFrom, AcqTo

'Wait till spectrum is ready
Do
      SpectrumID = LabSpec.GetAcqID()
Loop Until SpectrumID > 0

'Save the spectrum
LabSpec.Save SpctrumID, Path & ExperimentName & "\Spectrum_" &
CurrentTemperature & "deg.ngs", "ngs"
```

Acq

- Overview
  - Description: Start an acuqisition
  - Keywords: VBS ActiveX, VB, integration time, Accumulation
  - Type: AutoVBSAct
- Syntax
  - **long** Acq (**long** *Mode*, **double** *IntegrationTime*, **long** *AccumulationNum*, **double** *From*, **double** *To*)
- Parameters
  - *Mode*: Acquisition modes
    - ACQ_SPECTRUM: 0, Start a spectrum acquisition
    - ACQ_IMAGE: 1, Start a CCD image acquisition
    - ACQ_LABSPEC_PARAM: 2, Start spectrum acquisition with LabSpec interface parameters
    - ACQ_SPECTRAL_IMAGE: 3, Start spectral image acquisition with LabSpec interface parameters
    - ACQ_AUTO_SHOW: 10, Add to any other acquisition mode to automatically show acquired data
  - *IntegrationTime*: Spectrum integration time (sec). Ignored if ACQ_LABSPEC_PARAM mode is selected.

Step 6

6. Add each spectrum to a profile

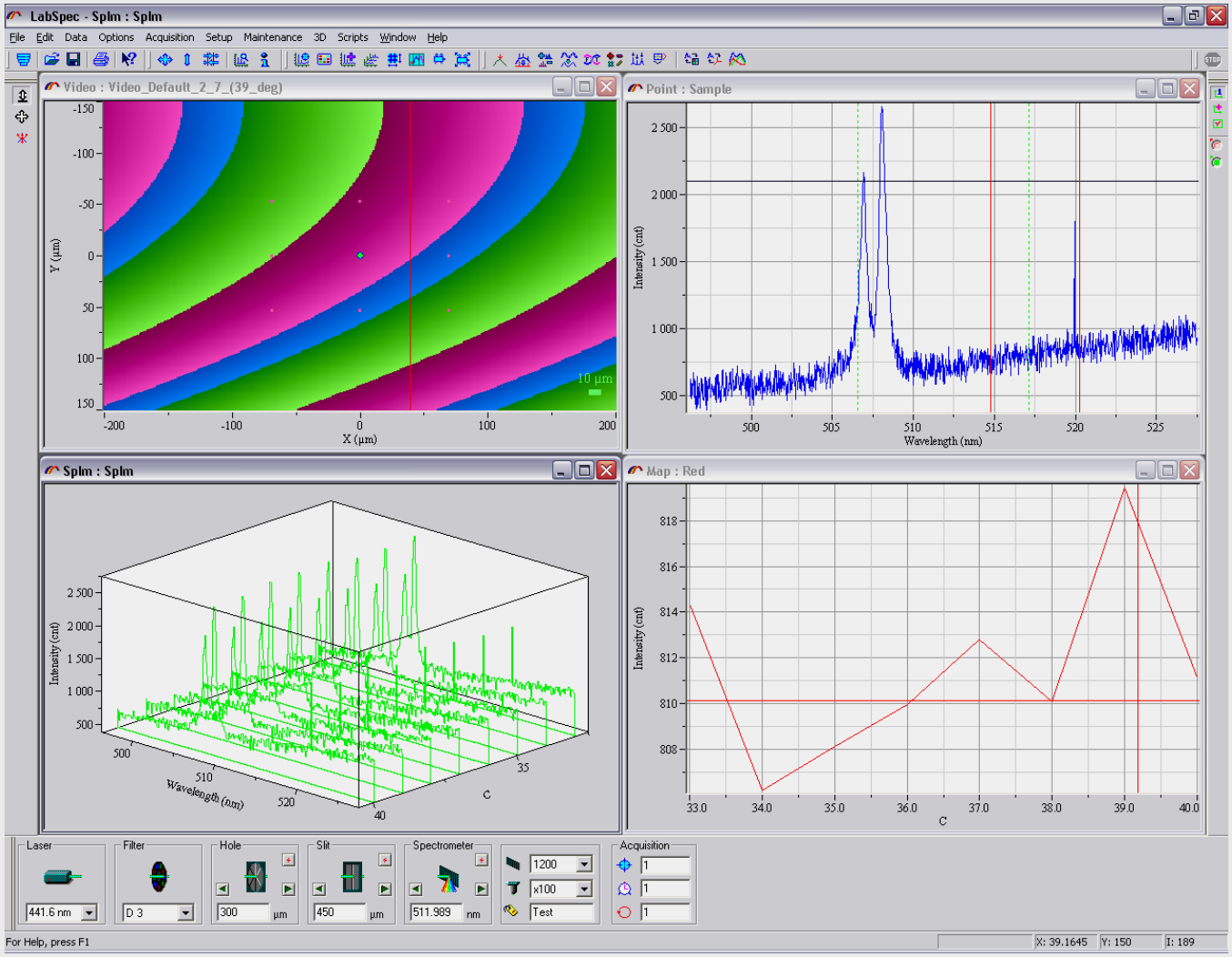
```
'If the profile does not exist and the current spectrum is the first spectrum of the profile, the profile is created.
If i = 0 then ProfileID = LabSpec.Profile (0, 0, SpectrumID, CurrentTemperature, "Degree", "Temperature")

'If the profile exists, the current spectrum is added the profile, and the profile is updated.
If i > 0 then ProfileID = LabSpec.Profile (1, ProfileID, SpectrumID, CurrentTemperature, "", "")
```

Profile

- Overview
  - Description: Create spectral image from spectra
  - Keywords
  - Type: AutoVBSAct
- Syntax
  - **long** Profile (**long** *Mode*, **long** *profileID*, **long** *SpectrumID*, **double** *Value*, **LPCTSTR** *Unit*, **LPCTSTR** *Label*)
- Parameters
  - *Mode*: Profile modes
    - CREATE_PROFILE: 0, Create a profile with one spectrum (ProfileID is ignored)
    - ADD_TO_PROFILE: 1, Add a spectrum to the profile
    - ProfileID: ID of a previously created profile. Relavent only for ADD_TO_PROFILE mode
  - *SpectrumID*: ID of a spectrum to add to the profile
  - *Value*: Extra dimension value for the current spectrum

Results



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