

SPEC 64

Spectrometer for Raman-Mapping



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GENERAL INFORMATION

SPECIFICATION OF THE SPEC64

GENERAL CHARACTERISTICS

Single Grating Czerny-Turner Spectrometer	
Focal Length	200 mm
Numerical Aperture	Max. 0.12
Grating Size	50 mm x 50 mm
Grating	1800 l/mm (optional gratings available)
Remote Control	USB 2.0
Min. Acquisition Time	10 ms

SPECTRAL RESOLUTION

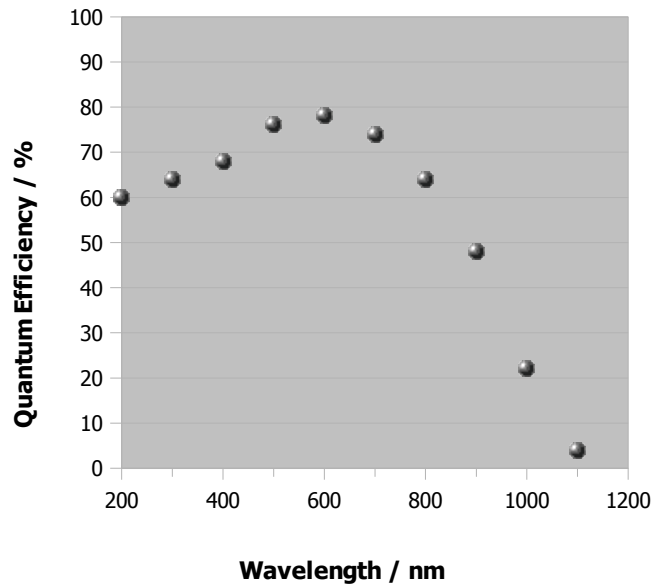
Center Wavelength	532 nm	633 nm	785 nm
Spectral dispersion [nm/mm]	2	1.8	1.4
Technical resolution [cm^{-1} /pixel]	1	0.64	0.3
Spectrometer resolution (100 μm fiber) [cm^{-1}]	9	6.5	4
Spectrometer resolution (100 μm fiber) [nm]	0.27	0.26	0.24
Spectral coverage for full CCD [cm^{-1}]	2100	1300	650
Spectral coverage for full CCD [nm]	60	52	40

POSITIONING RESOLUTION

Grating Positioning Resolution [°]	0.00006
Wavelength Accuracy [nm]	± 0.2
Wavelength Repeatability [nm]	± 0.01
Wavelength Range [nm]	400 – 1100 (with appropriate gratings)

CHARACTERISTICS OF THE CCD

Sensor Image Size [mm]	$\sim 27 \times \sim 0.5$ (100 % fill factor)
Active Pixels	2048 (horizontal) x ~ 60 (vertical)
Hermetic Sealing	Quartz glass window
Time per Spectrum [ms]	Min. 10
CCD Node Sensitivity [$\mu\text{V}/\text{e}^-$]	< 8
CCD Dark Current at 25 °C [$\text{e}^-/\text{pixel}/\text{s}$]	Typ. < 80 (max. 500)
Operation Temperature [°C]	11 ± 0.5
Dynamic Range	1:50000
Spectral Response [nm]	200 – 1100



• Figure 1: Typical spectral response of the CCD detector (without window)

CHARACTERISTICS OF THE FIBER

Type	Multimode fiber patch cable
Connector	FC/PC
Core diameter [μm]	105
Numerical Aperture	0.22
Wavelength Range	400 nm – 2400 nm
Tubing	Metal tubing as ambient light protection

GENERAL

Interface	Plug & Play USB 2.0 interface
Drivers	Windows NT/2000, Windows XP, Win7
	32 bit
Power consumption	12 Vdc, 1.3 A
Warranty	2 years

STANDARD PART LIST

Spec64 Spectrometer	1
Power Supply 12 V dc	1
USB cable M-M , 2 m long	1
Manual	1
Software on USB-stick	1
Optical Fiber FC/PC 105 μm core	1
Noble Gas Calibration Lamp (Ne, Ar)	1

LICENCE FOR THE SOFTWARE

The Source code for the remote control software and the DLL source code are provided with the General Public Licence (GPL). All examples for LabView can be freely implemented and changed by the user.

INSTALLATION

SYSTEM REQUIREMENTS

- compatible PC
- 1 MB hard disk space
- Windows NT 4.0 / Windows 2000 or Windows XP (32 bit) / Windows 7 (32 bit)

SOFTWARE INSTALLATION

On the delivered USB Stick, you find

Driver	in	.\Driver	run "setup.bat"
Software	in	.\	Start "CCD.exe" to control the device

NOTE: In Windows7, the ini-file "user.ini" might be copied automatically in another directory. If you want to avoid this, make the directory that contains the ini-file writeable by any user.

The easiest way is to copy the whole content into a suitable directory (%YourPath), e.g. "C:/Users/CCD". If working under Windows 7, one needs to set the user rights as follows:

- right click on the top most folder and select properties
- select the tab "Security"
- select "Users" and click on "Edit"
- allow "Full control" and use "Apply" and "OK" to verify

DRIVER INSTALLATION

Connect the 12 V power supply to the Spec64 and then connect the USB cable between Spec64 and your PC. If the system asks for a driver, select the "...sys" in the directory "..\Driver". If the system does not ask automatically, one has two possibilities:

A) install through device manager

- open the device manager
- select the "Unknown Device" and right click to "Update Driver Software"
- "Browse for driver software on your computer"
- provide the path "%YourPath/Driver/"
- select the driver "CCD"
- Say OK when Windows recommends not to install from an unknown driver vendor

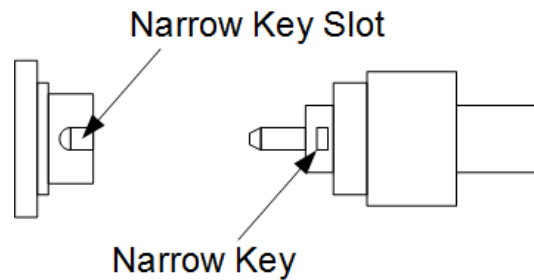
B) install with setup program in "C:.\Driver"

In Windows7, Windows XP and Windows 2000 start "setup.bat".

Allow the setup.bat program to do changes on your PC. During installation, a command window is opened and closed when finished. For the 1st installation, this procedure might take about 20 seconds.

GETTING STARTED

- ☑ Connect the delivered optical **FC/PC multimode fiber** (50 μm or 105 μm core diameter) to the spectrometer and couple a light source (e.g. calibration lamp) into the other end of the fiber
- ☑ Make sure that the narrow key of the FC/PC fiber fits into the narrow key port of the FC/PC spectrometer fiber port during fixing
- ☑ Connect the power supply
- ☑ Connect the USB interface to your PC
- ☑ When the PC asks for a driver, install the driver provided on the USB-Stick under "Driver" with "setup.bat" (see Software Installation on page 7)
- ☑ Make sure the provided user.ini is in the same folder as CCD.exe
- ☑ Start the software CCD.exe as Administrator¹
- ☑ Move on with the Initialization Procedure of the Spectrometer on page 15



CONNECTIONS TO THE SPEC64

Power – requires 12 V dc, 1.3 A. The inner pin is positive.

USB – interface for remote control via USB2.0



• Figure 2: Power Supply for 12 V dc (left) and USB-Connector (right)

DRIVER UPDATE

One has two possibilities:

A) install through device manager

- ☑ open the device manager
- ☑ select the "Unknown Device" and right click to "Update Driver Software"
- ☑ "Browse for driver software on your computer"
- ☑ provide the path "%YourPath/Driver/"
- ☑ select the driver "ccd"
- ☑ Say OK when Windows recommends not to install from an unknown driver vendor

B) install with setup.bat

- ☑ In Windows 7, XP and 2000, run the delivered "setup.bat"

¹ This ensures that the same calibration parameters are used in CCD.exe and VistaScan.

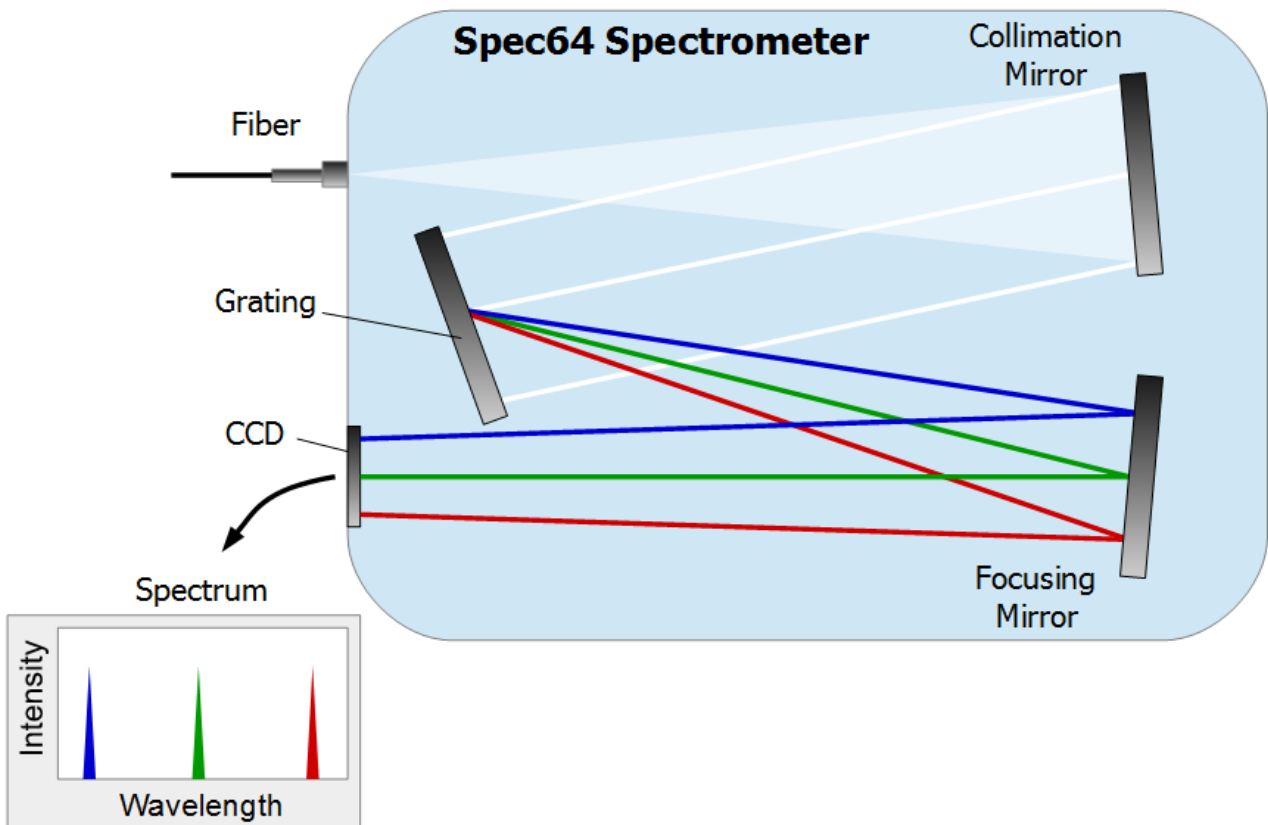
SPECTROMETER BASICS

PRINCIPLE

A spectrometer splits light into its wavelength components and projects them onto an array detector called Charge Coupled Device (CCD). The spectrometer software assigns the position of the light on the CCD detector to the corresponding wavelength.

A spectrometer consists of the following main parts (see Figure 3):

- Optical fiber
- Collimating mirror
- Diffraction grating
- Focusing mirror
- CCD detector



- *Figure 3: Schematics of the working principle of a Czerny-Turner Spectrometer. White light is dispersed by the grating and refocused to the CCD. The CCD signal is transformed to a spectrum.*

OPTICAL FIBER

The fiber is a very important part of the spectrometer hardware for the user. The light from the experiment (or light source) is focussed into the fiber core. The polarization and the beam shape are not maintained inside the fiber. The full diameter of the core will be illuminated at the spectrometer entrance. Therefore, using a fiber with double the core diameter will decrease the resolution and the signal to noise ratio by a factor of 2.

It is important that the numerical aperture of the incoupled light is preserved as long as it is smaller than the NA of the fiber. The maximum numerical aperture of the Spec64 spectrometer is 0.12. Therefore, the **collimating optics for the fiber should have a numerical aperture of max. 0.12.**

COLLIMATING MIRROR

The divergent light from the fiber illuminates the first spectrometer mirror and the collimated light is reflected to the grating.

OPTICAL DIFFRACTION GRATING

The grating consist of a periodic structure which diffracts the light in different directions depending on its wavelength. For higher the wavelength, the diffraction angle increases. Therefore, the resolution of the spectrometer is higher for larger wavelengths at the expense of wavelength range covered by the CCD width (horizontal direction).

FOCUSING MIRROR

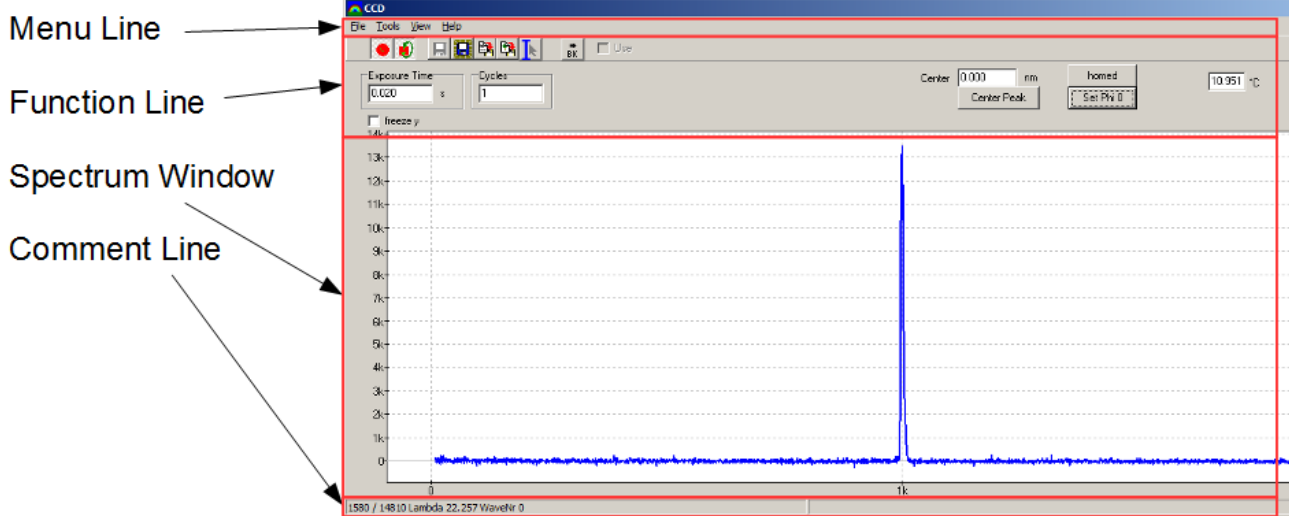
The light coming from the grating is still collimated but it has a different inclination angle on the mirror in dependence of its wavelength. The second mirror focusses the light to a wavelength dispersed image of the optical fiber on the CCD.

CCD DETECTOR

The detector consists of an array of small detectors called pixels. A photon impinging on a pixel is transformed into a charge. This charge is detected by an analogue digital converter to a count value displayed by the spectrometer software. The spatial distribution of the light is preserved during the read-out process. The Software CCD.exe transforms the signal obtained by the CCD into a spectrum.

SOFTWARE DESCRIPTION

OVERVIEW



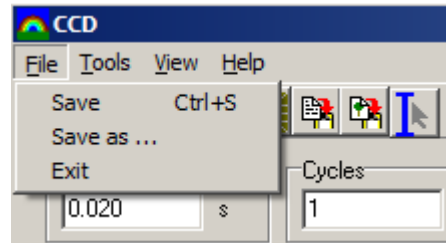
• Figure 4: Main window of the spectrometer software CCD.exe.

Figure 4 shows the main window of the spectrometer software, which appears when the program is opened. Starting from the top, you will find the menu line, the function line, the spectrum window and the comment line

FUNCTIONS IN THE MENU LINE

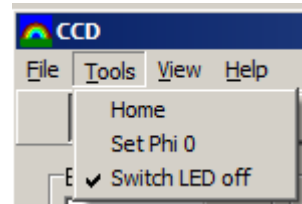
FILE

- Save* – Save the spectrum in the current folder
- Save as* – Save the spectrum in a selectable directory
- Exit* – Exit the program



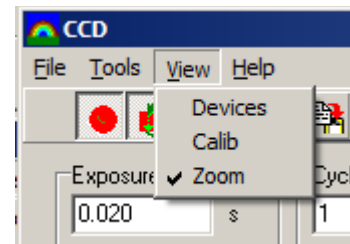
OPTION

- Home* – Move the grating to its home position. This procedure is recommended after every restart of the spectrometer
- Set Phi 0* – Set the actual grating position to the 0th order position. This needs to be done after the homing procedure (see section Initialization Procedure of the Spectrometer)
- Switch LED off* – During movement of the grating, an internal LED is switched on. This LED can be switched off during measurements to decrease the background signal



VIEW

- Devices* – show an additional window below the spectrum window with device details
- Calib* – open the calibration data window. There you can set the laser wavelength used for Raman measurements. Additionally you can set the groove density of the grating and the order of the grating you want to use. The other values strongly influence the



spectrometer calibration and should be changed during service only.

Zoom – only the center of the CCD will be displayed in the spectrum (Pixel 900 to 1100)

Calib Data	
	0
Gear	311.421068
	0
Grid Groove Density [1/mm]	300
LASER WaveLength [nm]	532
EncPhi0 [mm]	12.306017
Dv [rad]	0.4485
Focal Length [mm]	196.75
Order	1
Diameter GridTower[mm]	75.161
Kippangle[deg]	-3

HELP

About – shows the current program version and the version of the used hardware driver

FUNCTIONS IN THE FUNCTION LINE

START MEASUREMENT BUTTON



Start a measurement with the selected settings.

CONTINUOUS MEASUREMENT MODE



A measurement is continuously repeated until the start button or the continuous measurement mode button is pressed

SAVE



Press the save button to save the current spectrum. Hold shift pressed and click on the save button to activate the autosave function. The save button will remain pressed and every spectrum will be saved automatically. An incrementally increasing number will be appended to the file name.

SAVE AS



Press the save as button to save the current spectrum in the desired directory with a specific file name.

COPY DATA TO CLIPBOARD



Copy the wavelength and the intensity data values of the current spectrum to the clipboard. You can past the data to data evaluation software.

COPY IMAGE TO CLIPBOARD

Copy the image of the spectrum to the  clipboard.

MARKERS



Activate red markers. Move both markers by left click and movement of the mouse. The distance between the markers can be changed by hold the shift key pressed while left click and mouse movement. The markers have two functions. First, within the markers the mean value and the rms noise of the spectrum intensity are calculated. Second, if a peak is within the markers, press *Center Peak* to move the grating that the peak is in the center of the CCD. It might be necessary to repeat the centering procedure to bring the peak in the very center.

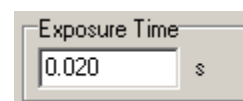
BACKGROUND



The software can subtract a predefined background from the measured spectrum. This is helpful in applications with strong but stable background light or for Raman mappings. Measure a spectrum of the background signal with a sufficiently high number of cycles and the same exposure time of the later measurement. Press the background button and this spectrum will be internally saved as background. In order to subtract the background signal from the displayed spectrum, check the check box next to the background button. If the background subtraction is activated, the saved spectrum files will contain the background corrected and the background spectrum as well.

EXPOSURE TIME

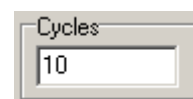
The exposure time defines how long the signal will be integrated before the data is read out from the CCD. The shortest value possible is 10 ms.



Exposure Time
0.020 s

CYCLES

Cycles gives the number of single measurements that will be averaged for the final displayed spectrum.



Cycles
10

CENTER



Center 0.000 nm

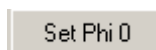
The current grating position refracts a specific wavelength to the center of the CCD. The value of the current center wavelength is displayed in the *Center* field. In order to change the grating position, insert the desired wavelength (in nm) in the *Center* field and press ENTER. In spite of the very high positioning resolution of the grating, the displayed value might differ slightly to the set value.

HOME INDICATOR



Press *Home* to move the grating to its home position. This procedure is recommended after every restart of the spectrometer. After homing the window is labelled with *homed*.

SET PHI 0



Set the actual grating position to the 0th order position. This needs to be done after the homing procedure (see section Initialization Procedure of the Spectrometer).

TEMPERATURE DISPLAY

The temperature of the CCD is displayed.

10.936 °C

FREEZE Y

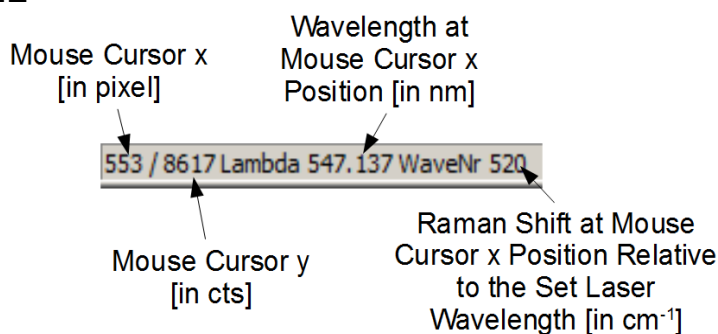
freeze y

After checking the *freeze y* check box, the intensity of the spectrum is not automatically scaled and will remain at that value.

SPECTRUM WINDOW

The spectrum window shows the current spectrum. The x axis is in the units of pixels with a grey dashed line at 1000 pixel (labelled as *1k*). The spectrometer is calibrated for pixel 1k being the center. The grating position value displayed in the *Center* field is the wavelength at pixel 1k. The y axis is in counts. The CCD saturates at approximately 100 k counts. A slight over-saturation will not harm the CCD but the most intense peak will be cut at the top. Therefore it is recommended to adjust the exposure time in a way that a measured peak has a maximum intensity of 5 to 10 % below the saturation counts.

COMMENT LINE



The comment line is a very useful tool for the spectrum evaluation. It shows the data values of the mouse cursor position on the spectrum window. By moving the mouse to a measured peak, one can read the peak position in CCD pixel, the wavelength of the selected peak in nm and the Raman Shift of the peak relative to the set laser wavelength. Additionally the peak height in cts can be estimated.

TUTORIALS

INITIALIZATION PROCEDURE OF THE SPECTROMETER

The initialization procedure has to be performed after every restart of the spectrometer (reconnection to power supply).

After connecting the Spectrometer to the power supply and the PC, start CCD.exe **as administrator**. The spectrometer will warm up during operation. For high wavelength accuracy, it is recommended to wait 30 minutes after switching on the spectrometer for thermal stabilization. Make sure that the most recent user.ini file is in the same folder as CCD.exe.

- Press the *Home* button (or Menu: *Tools > Home*). The grating moves to its home position.
- Insert a "0" in the *Center* field of the function line and press ENTER.
- Connect the first end of the delivered optical fiber to the spectrometer and the second end to a weak light source or use the room light. A single peak close to the center of the CCD is visible. Adjust the light source intensity to not saturate the CCD (e.g. less than 70k counts).
- Press the button *Center Peak* several times until the peak is in the center of the spectrum. The *Zoom* functionality (*View => Zoom*) might be helpful.

Note: The markers (see Markers on page 13) have to be switched off or the peak has to be within the red markers. Otherwise the procedure will not work correctly.

- Press the button *Set Phi 0*

The spectrometer is calibrated and you can start a measurement.

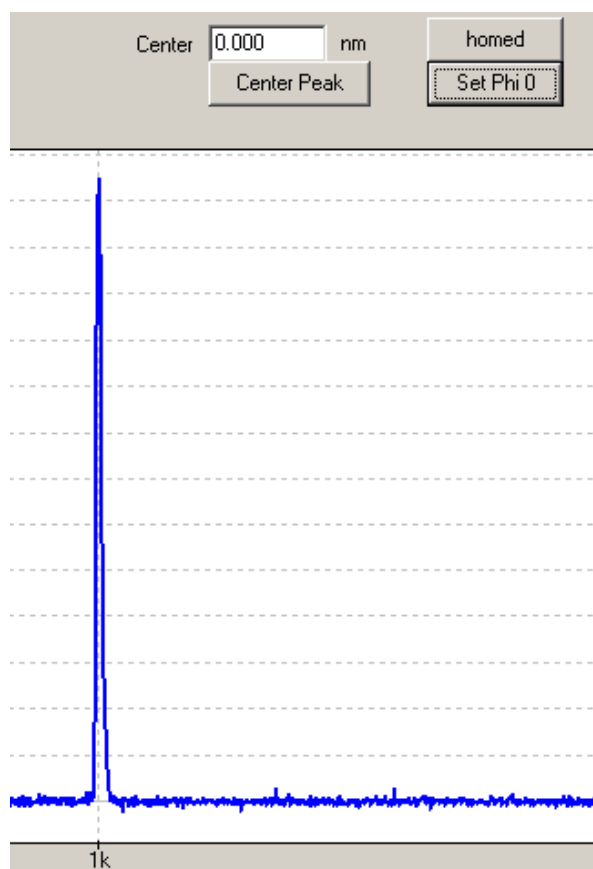
SET A LASER WAVELENGTH

For displaying the right Raman Shift in the Comment line, it is necessary to set the wavelength of the laser used for excitation.

Click on *View* in the *Menu Line* and press *Calib*. Enter the desired wavelength value in the field *LASER WaveLength* in nm units.

PERFORMING MEASUREMENTS

Insert the desired center wavelength in the *Center* field of the function line. Set the *Exposure Time* and the number of *Cycles* and press the green start button.



PERFORMING RAMAN MAPPINGS WITH SXM

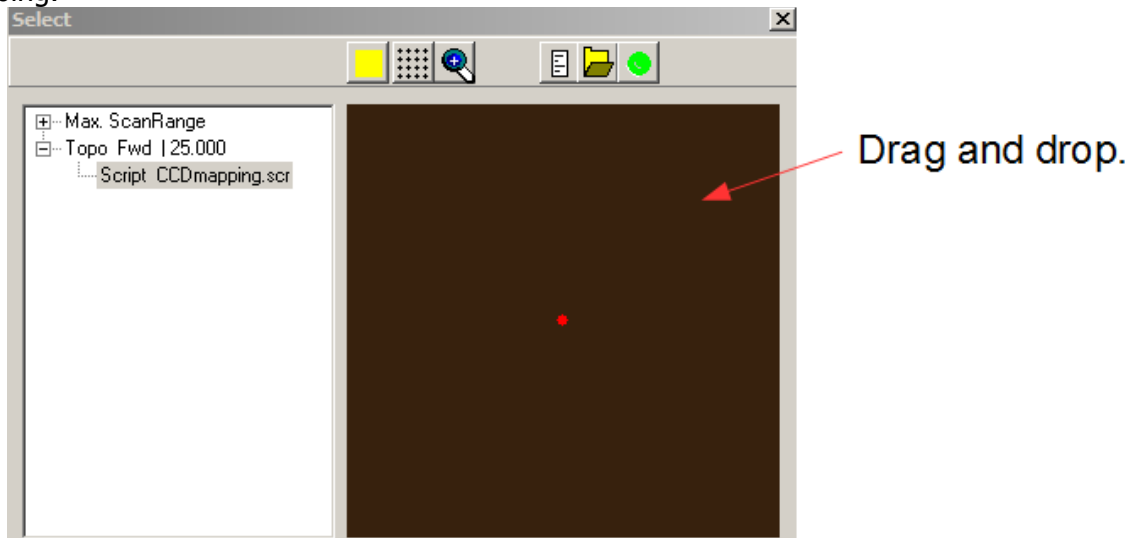
Set the center wavelength for the Spec64 with CCD.exe. Choose a proper exposure time. The signal to noise should be sufficient but do not use too long exposure times. A 128 pixel times 128 pixel image with 100 ms will take a total time of approximately 27 minutes.

Close CCD.exe. If necessary, open SXM.

In SXM, open the *Select* window (Menu: *Window* => *Select*).

Set the desired scan range in the SXM parameter window (F1 => *Range*).

Drag and drop a scan image (could be blank) into the *Select* window like shown in Figure 5: The Select Window of SXM. This will set the scan range and the scanning speed of the scanner for the mapping.



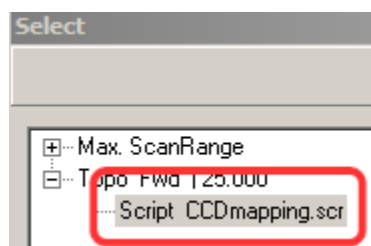
• Figure 5: The Select Window of SXM.

Activate scripting in the Select Window and open the script: "CCDmapping.scr".

Open the CCD software in SXM with the following icon:



In order to change the pixel resolution, double click on "Script CCDmapping.scr" in the Select Window and edit the variable n (e.g. n = 128) in the notepad editor. Save the script.



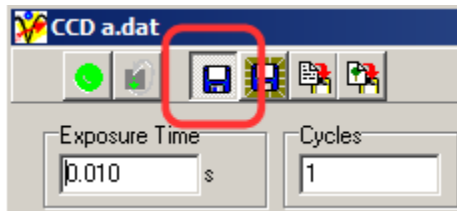
Set the *Exposure Time* and the *Cycles*.

Uncheck the continuous measurement mode.

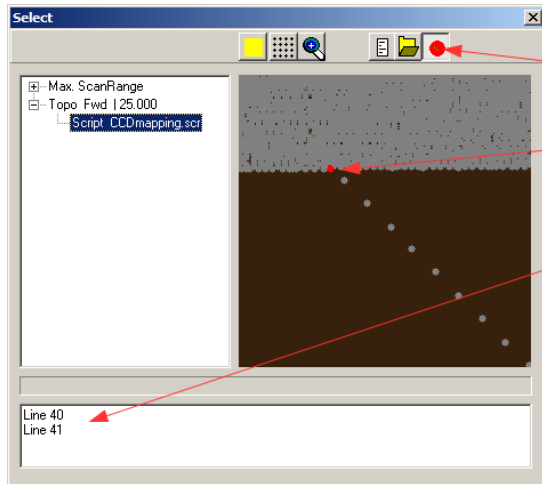
Save the initial file of the mapping with the *save as ..* function into a separate folder (e.g. a.dat).

Activate the auto-save function. Hold the shift key pressed and left click on the *save* button.





Run the script by pressing the green button in the SXM *Select* Window.



Run the script.

The red dot indicates the scanner position.

The note window gives information about the progress

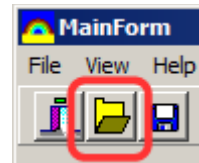
The file names in the SXM CCD software header should start count upwards.

EVALUATION OF RAMAN MAPPING DATA

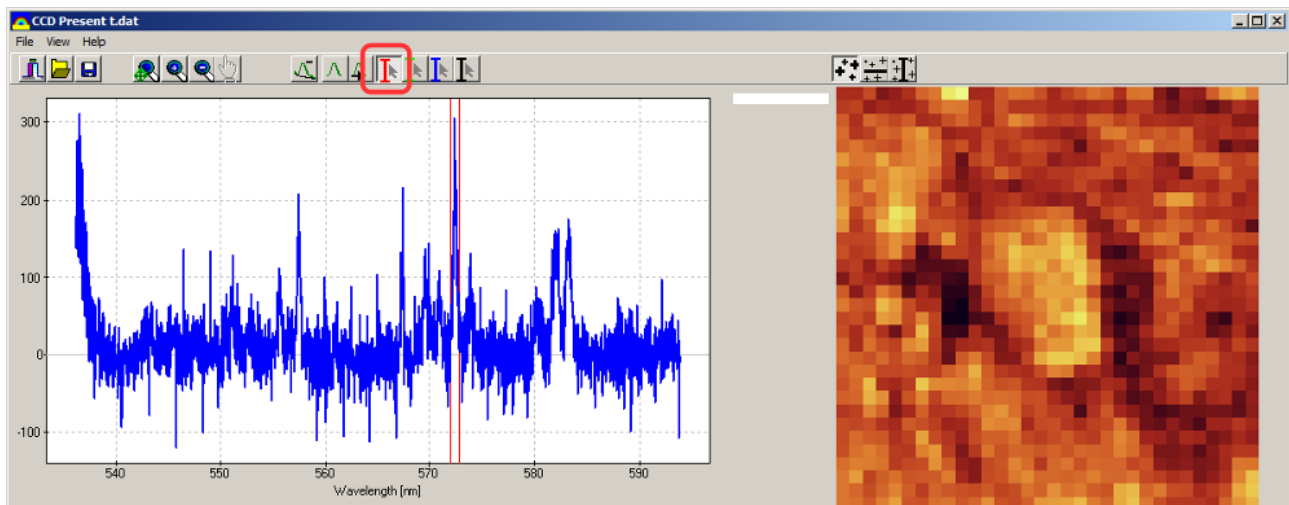
Open CCDPresent.exe.

Open the first file of the mapping (e.g. e.dat).

The progress indicator starts to count upwards in the left bottom corner of the CDDPresent window.



After the data has been loaded successfully, a spectrum will be displayed at the left side and an intensity map on the right side. In order to show an intensity map of a desired (spectral) peak position, activate the red markers.



Change the distance of the markers by holding the shift key and the left mouse key pressed and

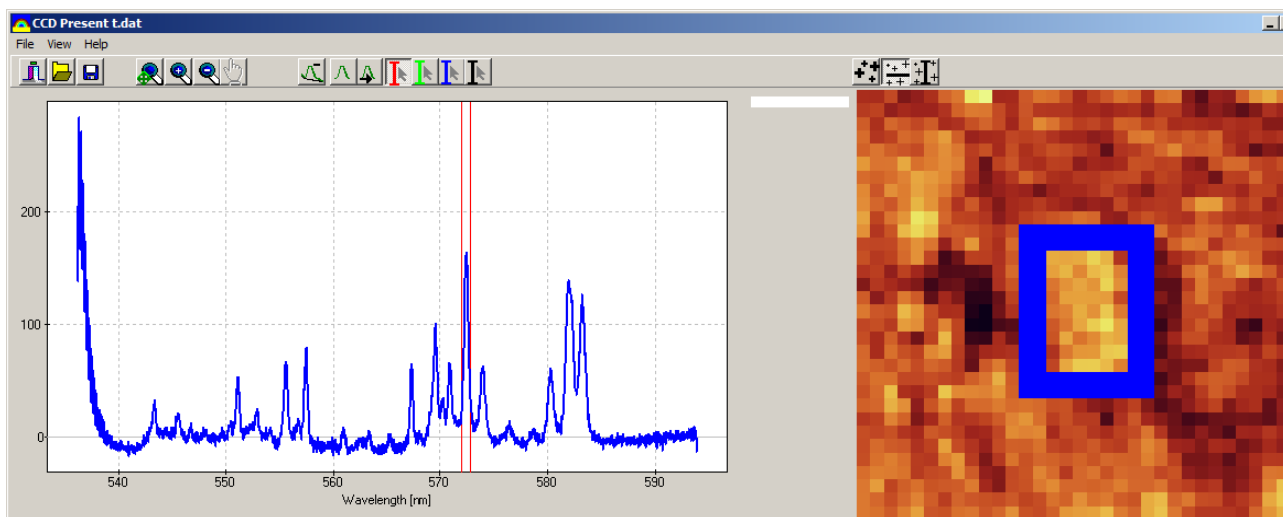
move the mouse. Move the markers to the peak of interest with left click and mouse move.

With the three buttons on the right, one can display a spectrum of a desired (spatial) position of the map.

Point Spectrum: Click in the map image and the corresponding spectrum will be displayed on the left.



Average Spectrum of Area: Shows an average spectrum (left) of all the selected spectra in the map (right).



Max of area: Shows an overlap of all spectra in the left window of the selected area on the right side.



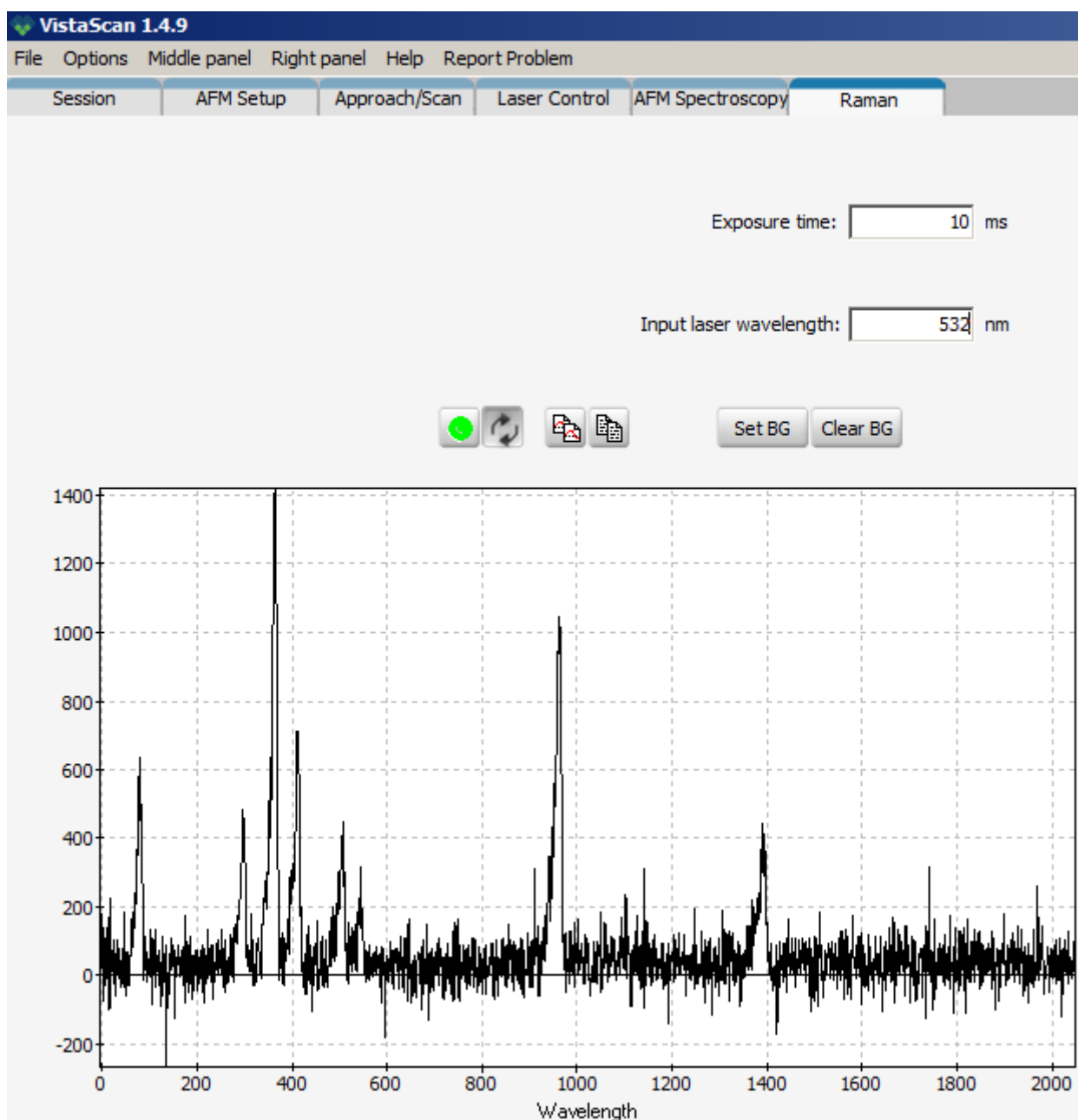
The spectra of specific points in the map or specific areas can be displayed as reference. After selecting a point spectrum or an area average, right-click into the spectrum window. Select *Ref* and the spectrum and the corresponding point (or area) will be displayed in a different color. In order to remove references, right-click on the legend and select *Clear Ref* or *Hide Ref*.

PERFORMING RAMAN MAPPINGS WITH VISTA SCAN

In order to perform a map of Raman spectra with the VistaScan software, follow the routine below.

Make sure that the spectrometer is connected to the PC via USB and that the Spec64 power supply is plugged in.

Prepare the hardware of the spectrometer in CCD.exe by setting the desired center wavelength. Close CCD.exe and open VistaScan.raman3.exe.



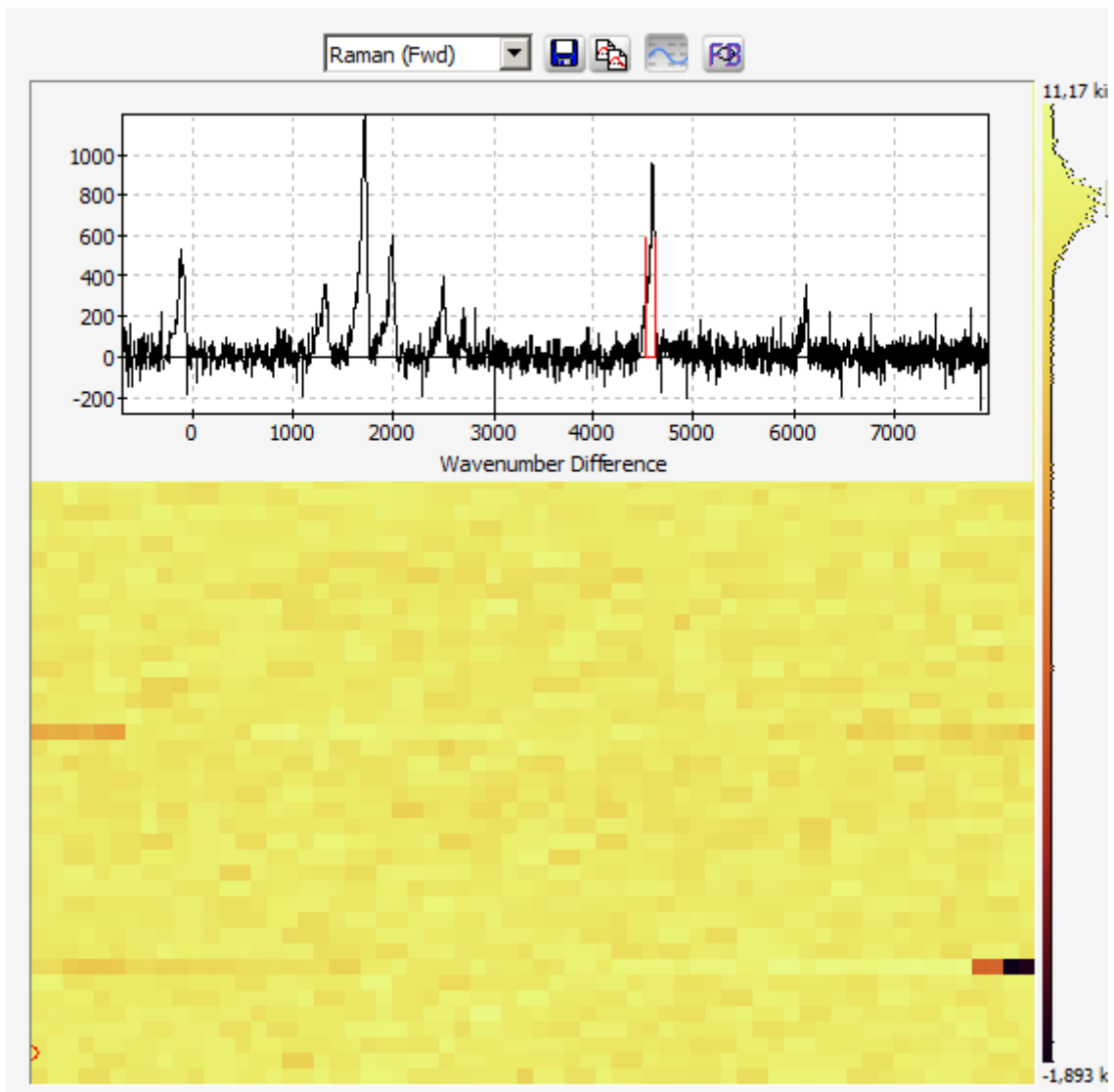
• Figure 6: Raman Mapping user interface of VistaScan

Set the desired *Exposure Time* and the laser wavelength in the field *Input laser wavelength*. The green button starts a measurement and the button with the circled arrows sets the continuous measurement mode. This helps to find a suitable exposure time. With *Set BG* you can define a background spectrum. If a background spectrum is set, it will be subtracted from the following spectra. With *Clear BG* the background spectrum is deleted.

Calibrate the x axis by right-click on a known peak (e.g. laser wavelength) in the spectrum window and select *add calibration point*. Insert the known wavelength. Repeat this for a second known wavelength (e.g. peak of the calibration lamp).

Make sure that the Raman channel is acquired (*Session Tab* → *Channels to acquire*).

Go to the *Approach/Scan* tab, select *Raman (Fwd)* as channel to be displayed and start a scan.



After the scan is done, click into the image and a spectrum of that point will be displayed. Move the red markers from the sides (left and right side of the spectrum window) with the mouse to a desired peak and the intensity distribution will be displayed in the image.

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