SpectraSense

SpectraSense™
Acton Research
Ver. 4.0

User's Guide

Version 4.0

Roper Scientific Acton Research

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Chapter 1: Introduction

SpectraSense is a comprehensive spectral acquisition and data treatment package. It is designed to work exclusively with Roper Scientific Acton Research instrumentation and accessories. It runs under Windows 98 and Windows NT operating systems. SpectraSense software will control and acquire data from both single channel detection systems, which require scanning of a monochromator, and CCD based detection systems that may or may not require repositioning of a spectrograph. Depending upon the hardware purchased, either one or both of the modes of acquisition will appear during normal operation.

SpectraSense is presented as a series of tabbed screens. Depending on the desired operation, you may jump between any tabs. The tabs are presented in a logical order for acquiring and interpreting quality spectra. All tabs except the Hardware Configuration tab will be accessible as long as there is hardware to support their operation. The Hardware Configuration tab can only be accessed from the Select Tab menu level. A brief discussion of the purpose and operational capabilities of each tab follow.

Hardware Configuration

The hardware configuration screen is used to configure the software to recognize and operate with the various automated components of your system. It is in this screen that you tell the software what you have and where you have put. A diagrammatic representation of your system is created by placing icons that represent components and accessories on a monochromator diagram. Once the elements are put in place, it is no longer necessary to use this screen unless you have physically moved or changed one of your computer controlled components. The only exception is that you define your working spectral units; i.e. nm, A, microns, Ev, or wavenumbers in this screen. If you switch between working units on a regular basis you will have to return to this screen from the menu level.

Hardware Status

The hardware status screen is used to quickly verify the states of all of the current operational parameters. At a glance you can verify or change gratings, adjust automated slits, change from one mode of detection to another, verify or change the position of your spectrometer(s), and change the states of your triggers, filters, high voltage, and shutters.

Survey Mode

The survey screen is used to quickly set up and optimize the parameters that affect the quality of your spectra. In real –time you can adjust factors such as integration time, slit width, high voltage, areas on a CCD detector, and spectrometer positioning. When working with a CCD you can evaluate the signal as either an image or a spectrum. With a single channel detection system you can sit on a peak and watch how the signal level varies as you change operating parameters.

You can do real-time manipulation of data that is coming in and see the effects in varying parameters associated with one detector relative to another. And finally you can store the spectra that you have taken here. All of the optimization and tweaking that you that you have done in this screen is automatically transferred to Acquisition screen so that you can be sure that the spectra being collected are as good as you can get.

Acquisition

In the acquisition screen you define how your experiment is to be performed. It is here that you create routines that can be recalled at any time to exactly reproduce the experimental conditions used in a previous session. It is also here that you can add anecdotal information to be stored with the data. It is from this screen that you acquire you spectral data.

Live Data

The live data screen shows the data as it is being acquired. In certain high speed acquisitions using CCD Detectors however, it may not be possible to see the data until it has been collected.

Post Processing

After you have collected the data, you can view it, compare it to other data, and perform mathematicaly manipulate it. It is also from this screen that you can create hard copies of the spectra.

Expanding Spectra and Images

All screens, windows, and dialog boxes that contain spectra can be expanded. To expand around a section of a spectrum draw a box around the section by clicking the left mouse button and dragging the cursor from the top left corner of the section to the bottom right. To return to full scale expansion, click and drag the cursor anywhere on the display from bottom right to top left. You can move an expanded display left, right, up, or down by clicking and holding the right mouse button. Images taken with the CCD can be expanded only if they are in the primary display

File Formats

Spectral data files can be stored in one of three formats: Spectrum**.arc_data**, Spectrum**.txt** or Spectrum**.SPC**. The arc_data format contains all of the acquisition, instrumentation, and data manipulations information in a text header as well as the data. This is an ASCII format. The .txt format contains only the data in as X and Y coordinates in a tab delimited ASCII file. The SPC format is a proprietary file format used by Galactic Industries' Grams software. This format is only available as an option. Data stored in this format can be directly imported into Grams. You select the storage format in the Save dialog box in the Save as choice field. Use the drop arrow to select the format you wish to use.

Images can be stored as a Windows bitmap (*.**BMP**). They can also be saved as in a Galactic (*.**SPC**) format which will import the image into Grams as a series of spectra, one for each row of the image. Two **Tiff** formats are also available, 8.bit RGB and 16 bit gray scale. Select format you wish to save in by clicking on the drop arrow in the Save as field in the Save dialog box.

Software Installation

In order to install SpectraSense you must have a computer with at least a Pentium processor or equivalent, 32mb of RAM or more, a hard disk drive with 200mb of available space, a SVGA or better graphics card, a monitor, a CD ROM reader, a Windows compatible mouse and a Windows compatible printer. The operating system must be Windows 95 or higher or Windows NT.

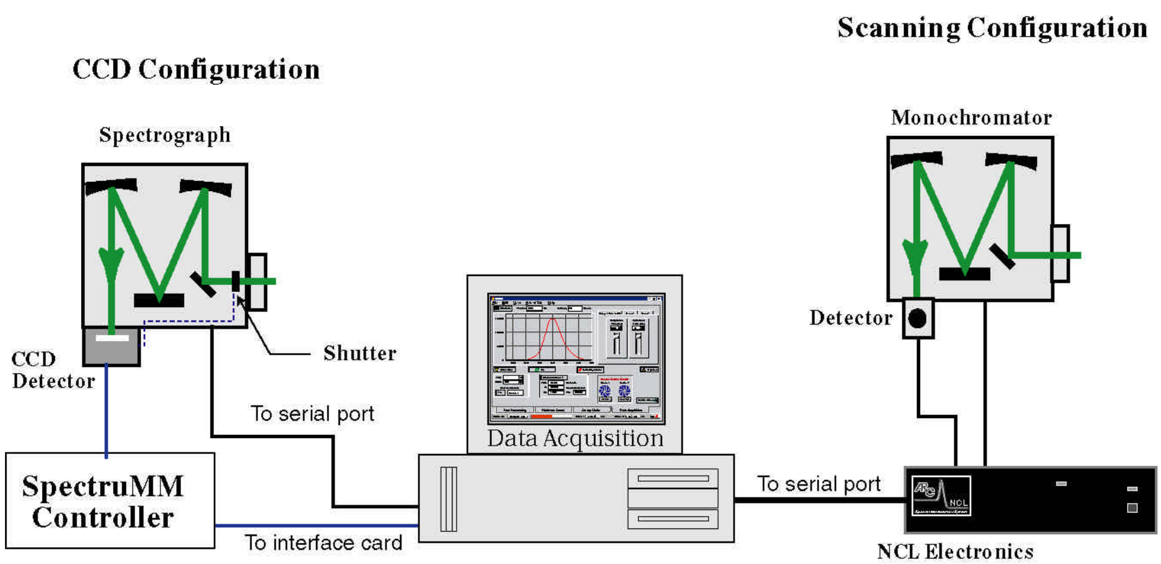
Place the SpectraSense CD-ROM in the drive. Click on the Start button, go up to Run. Click on the Browse button and find the drive and directory that contains Autorun.exe. Click on Autorun.exe and then Open. Click on OK.

An installation panel will appear. Click on the install button that is appropriate for your operating system. Follow the directions on the screen to complete the installation. Your computer must be rebooted before you can use the software.

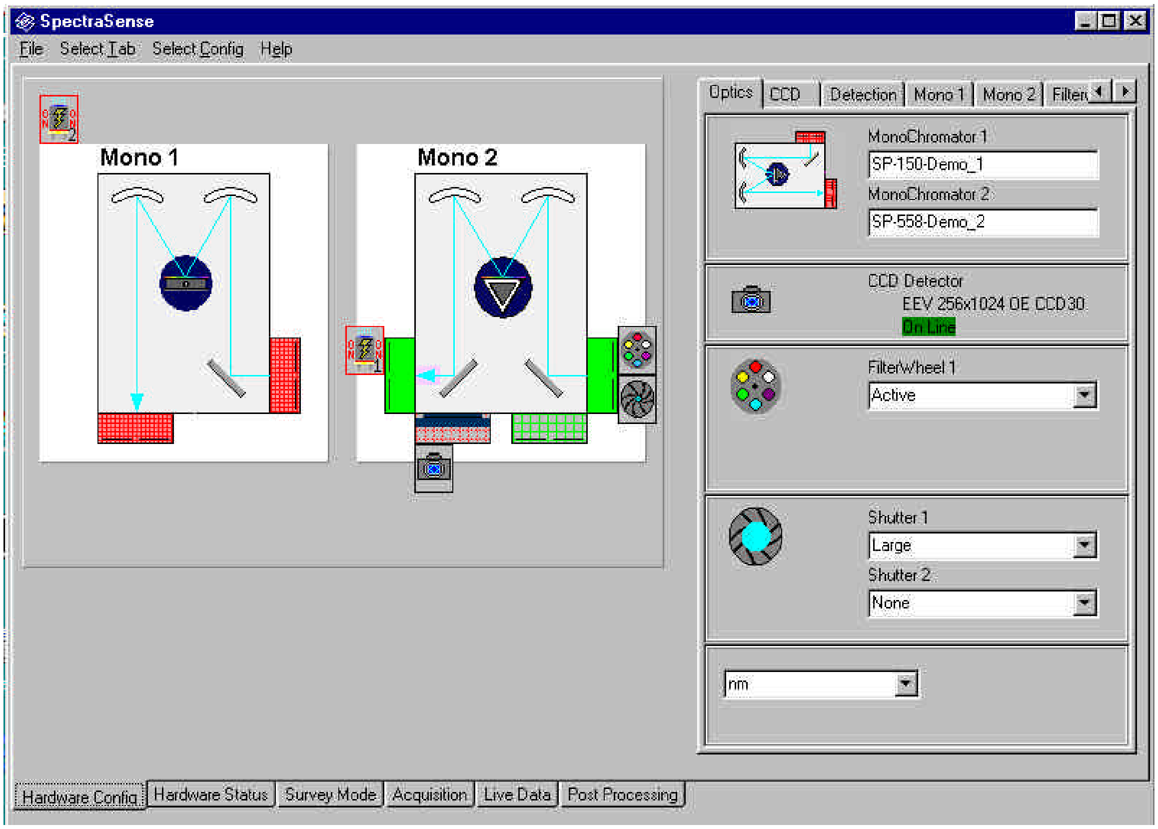
The complete manual in PDF format is also included on the installation CD-ROM. All topics in the table of contents and index are hot linked to the appropriate pages in the manual. In order to read the manual, you must have an Adobe Acrobat Reader on your computer. If you do not have one, click on the install Adobe Acrobat Reader button. A complete catalog of Acton Research products and technical notes are included on the CD-ROM.

Hardware Installation

Your hardware must be set up and all of the appropriate cables attached before the software can work. Refer to each component's installation manual for specifics. The diagram below shows typical cabling configurations. If your system includes both single channel and CCD detectors, the monochromator(s) should be connected to the NCL rather than directly into the computer's serial port



Chapter 2: Hardware Configure Screen



The Hardware Configuration screen is used turn on or off software control features related to the specific hardware in your experimental set up. In principle, the diagram represents the physical placement of all of the software controllable components in your system. Once the system is configured, there should be no need to return to this tab unless there is a physical modification to the system. For that reason the hardware configuration screen is only accessible from the Select Tab menu level.

The system diagram to the left is updated with icons for the specific hardware included in your system as you activate components from the panel to the right. Monochromators, the NCL data acquisition system, and CCD detector systems are automatically detected when the system is turned on. Shutters and filter wheels must be specified as being active on the OPTICS tab. The following tabs may show up on the panel depending upon the hardware specified in your system:

OPTICS Shows monochromators present, CCD if present, allows activation of filter wheels and shutters.

CCD This tab appears only if a CCD detector system is detected.

DETECTION This tab appears if a NCL is present and is used to configure the system for single channel detectors.

MONO 1 This tab appears if a monochromator is detected

MONO 2 This tab appears if a second monochromator is detected

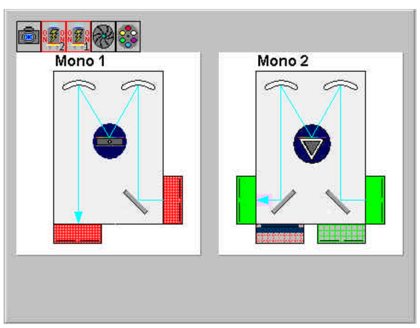
FILTER WHEEL This tab appears if on the OPTICS tab a filter wheel has been specified as being active.

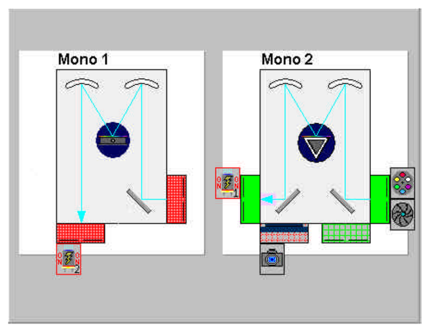
SHUTTERS This tab appears if on the OPTICS tab a shutter is specified.

NCL TRIGGERS This tab appears if a NCL is present. It is used to configure the triggering conditions and actions that start an acquisition or terminate it .

CCD TRIGGERS This tab is used to configure the CCD triggers.

PRINTER This tab is used to configure printing parameters.

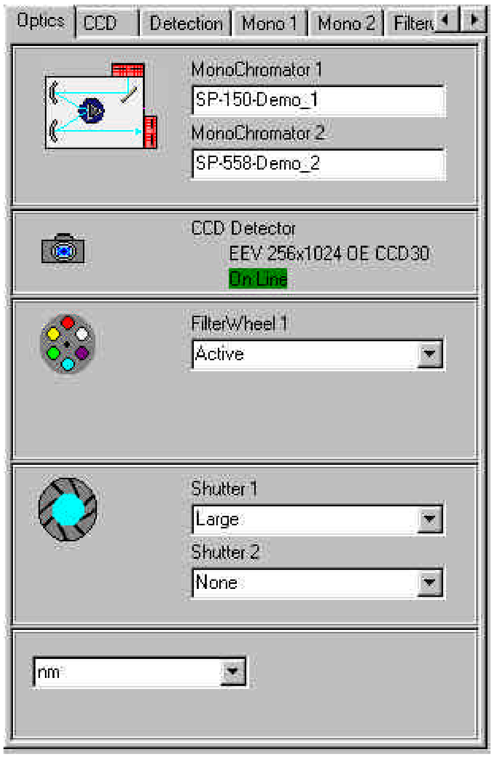




As components are activated through the tabs on the panel, icons are created and placed on the top of the system diagram. You then place the icons in the appropriate position in the experimental set up. (Click on an icon, drag the cursor to the appropriate port and release.) In this way the software associates the specific components to specific ports on the monochromator(s).

The Optics Tab

The optics tab shows the found monochromator(s) and CCD detection systems. It is here that you specify if there are filter wheels and shutters in your system. You also specify your working spectral units from this tab:



Display of spectrometers detected by the software

Display of CCD camera detected by the software

Filter Wheel

NONE	You do not have a filter wheel
ACTIVE	You have one and want software control.
INACTIVE	You have one but do not want software control

Shutters

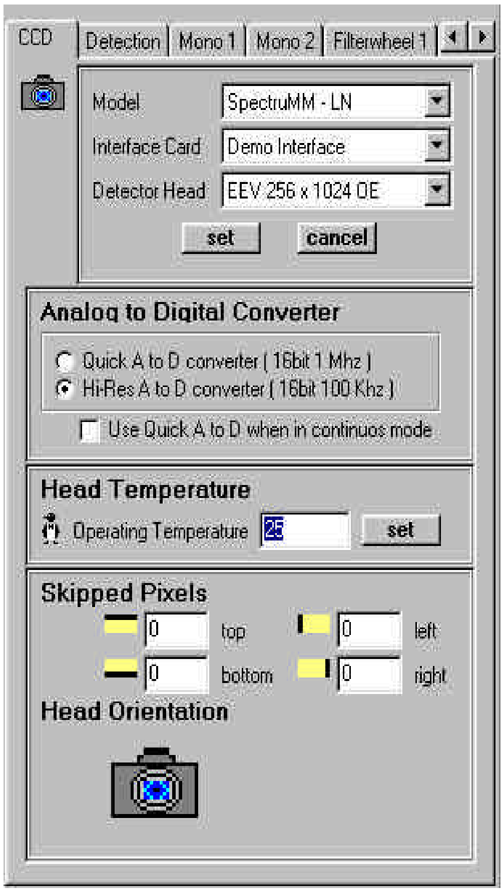
NONE	You do not have a shutter
SMALL	To be used with CCD shutters
LARGE , ELECTRIC, REMOTE	for future use

Working spectral units.
Select from nm, microns, EV, Angstroms, absolute wavenumbers or relative wavenumbers with a laser wavelength specified in nm.

All displacements of the monochromators will be in the specified units. If motorized slits are present, slit width adjustments can be specified in band passes of the selected working unit.

The CCD Tab

This tab appears if a CCD camera is detected by the software.



Use the model drop button to select the model of CCD you have.

Select the PCI interface card

Select the type of chip supplied in your camera head. This will be specified in the documentation that came with the detector.

Press the set button when all fields have the correct information.

Select either the high speed A to D converter or the slower high resolution converter for pixel read out. If the use quick A to D box is checked then the camera will use the high speed A to D in continuos update mode. This mode is recommended only for image updating and not for spectral acquisition.

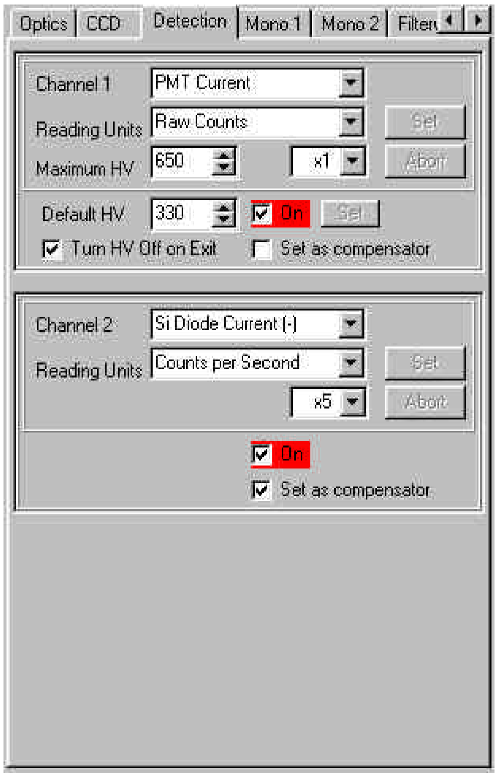
Set the head temperature to the lowest value specified for that model. Refer to the camera documentation for the appropriate value.

Some chips may have defects in their edge columns or rows. Specify how many rows or columns to skip for all read outs. Start out with zero in these fields and change only if you find non-uniform rows or columns. Click on the camera icon to change the head orientation. If your spectra come out backwards, either invert the head or click on this button to invert the icon.

The Detection Tab

The detection tab appears if an NCL is part of your system. In this tab you define the type of detectors that are supplied with the system, the output units, high voltage settings, if appropriate, and the gain. The standard NCL comes with two detector channels, a third panel will appear in systems supplied with three detector inputs. Be sure to verify which detector is attached to each labeled input on the NCL back panel.

Channel 1 select your detector type from the drop box. The choices are:



None
PMT current
Silicon diode (Si diode) current –
Silicon diode (Si diode) current +/-
Preamp voltage + for certain IR detectors
Preamp voltage - for certain IR detectors
Photon Counting

Reading Units select:
Raw counts
Counts per second
PicoAmps
Microvolts

Gain : select X1, X2, X5, X50, X200

These fields will have a pink background until the **SET** button is pressed. Use the Abort button to change the values.

Maximum HV Enter the highest safe voltage setting for your specific PMT. No values larger than this will be accepted for input from any other screen. Refer to the PMT manufacturer's documentation for the maximum safe operational voltage.

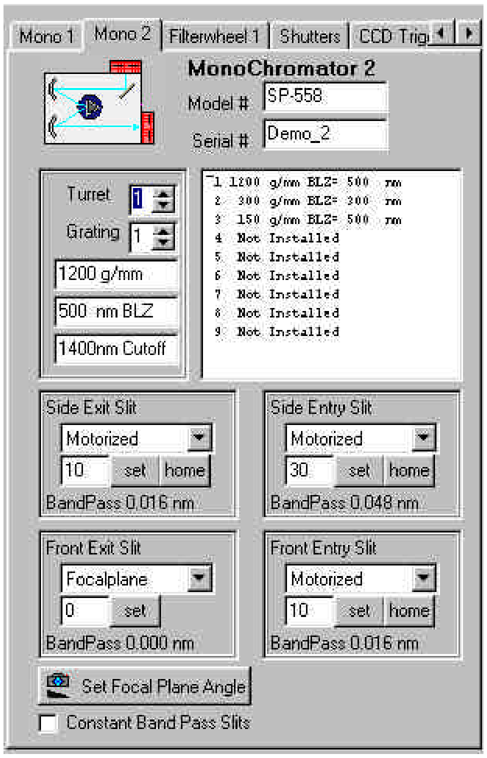
Default HV Enter the normal working voltage for your PMT. The value entered into this field will have a pink background until it is confirmed with the **SET** button.

The **On** check box is used to have the HV come on when the NCL is turned on.
The **Turn HV Off on Exit** check box is used to turn off the HV when SpectraSense is exited. If it is not checked the HV will remain on until the NCL is turned off. In general it is better to leave the HV on for better PMT stability.

The **Set as compensator** check box is used when you want to divide the primary input channel by this one. Check this box if your system is supplied with the source compensation accessory and the output from it is connected to this channel.

The Monochromator Tab

The monochromator tab is for the most part informational. All of the monochromator characteristics including grating types and port configurations are read directly from a flash ram in the monochromator. Although it is possible to change the specification of a port, for field upgrade, it is recommended that these fields not be modified by the user.



The model number and serial number of the monochromator are automatically entered into the specified fields.

Your monochromator may be supplied with interchangeable turrets. If that is the case gratings 1 through 3 are installed on turret number 1, gratings 4 through 6 on turret number 2 etc. Turrets must be manually changed and the corresponding turret number selected in the turret field. The grating field will toggle through the available gratings on the specified turret showing their groove density, blaze wavelength, and wavelength at maximum rotation.

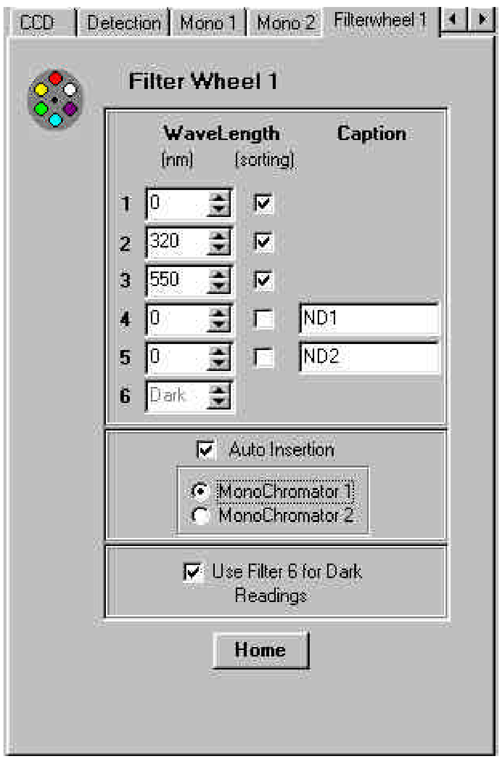
Slits

If your monochromator is supplied with motorized slits you can set a specific width in microns by entering a value in the field and clicking on the **SET** button. You can recalibrate the slit setting by clicking on the **home** button. The band pass for that specific slit width with the specified grating at the current central wavelength is shown below. If the **Constant Band Pass Slits** box is checked, then the values entered into the fields should be the band pass in the selected units. The width in microns will be shown below. Selecting constant band pass slits is only appropriate with motorized slits as the software must adjust the widths during operation.

The **Set Focal Plane Angle** button is used when an angled CCD adapter flange is supplied with the spectrograph. The default values are the specified focal length of the instrument and 0 degrees for the angle. If an angled adapter is supplied with the spectrograph the value should be changed to 11 degrees.

The Filter Wheel Tab

If you have specified in the Optics tab that you have an automated filter wheel in your system, the filter wheel tab will appear. The filter wheel holds up to six filters. The wheel can be set up to automatically insert cut off filters at specified wavelengths and to allow insertion of a specific filter to remain in place for the entire acquisition.



If a sorting filter is installed in a specific position, enter the wavelength in nm that it is to be inserted and check the sorting box. In a scanning acquisition the monochromator will momentarily stop while the appropriate filter is inserted if the **Auto Insertion** box is checked. Other types of filters such as neutral density filters can be installed in the wheel. For these types of filters the sorting box is left unchecked and a caption box is opened for naming the filter.

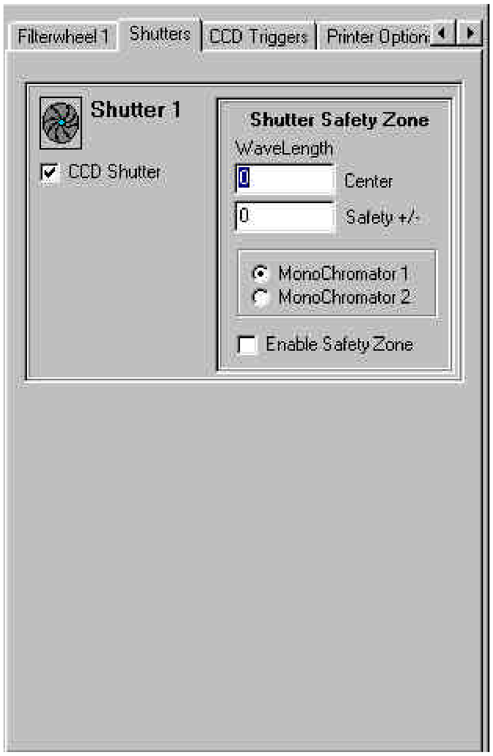
An opaque filter can be inserted in the sixth position to be used as a shutter for dark subtraction. If this is the case, check the **Use Filter 6 for Dark readings** check box**.**

In the case where two monochromators are supplied with the system, a panel with both monochromators will appear. Click on the monochromator on which the filter wheel is attached.

The **HOME** button will reset the wheel in the case where the knob was used to move the wheel.

The Shutters Tab

The shutters tab will appear if shutters were specified in the Optics tab. There are two classes of shutters: CCD and blocking. The CCD shutter is intimately integrated with the readout of the CCD. Non CCD shutters are used for dark subtraction and PMT protection in scanning operation.



Click on the CCD shutter box if the specified shutter is to be associated with a CCD. It may also be associated with an entrance slit for scanning operation.

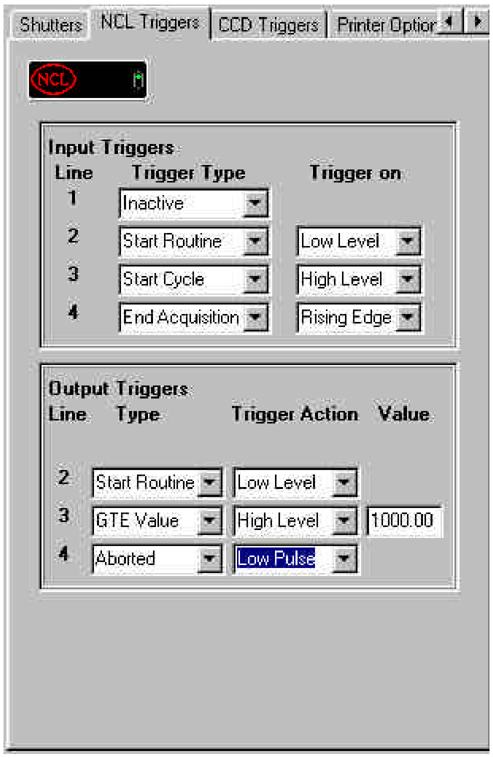
Shutter Safety Zone

The shutter safety zone is used to protect sensitive detectors from overexposure to sources such as lasers. Enter the wavelength to be protected from in the center field. Enter the number of working units, nm, cm-1 as specified in the Optics tab, on either side of the center wavelength over which the shutter will remain closed. For example, for a Raman experiment 0 relative wavenumbers would be specified as the center with a safety zone of +/- 20 wavenumbers. The shutter would remain closed between –20 and 20 cm-1.

If two monochromators are supplied in the system specify which monochromator the shutter is to be associated with. **The Enable Safety Zone** check box activates this feature.

The NCL Triggers Tab

The NCL triggers tab is used to specify the triggering conditions for the input and output trigger lines included in the NCL. It is the user's responsibility to determine the type of trigger output is needed to communicate with ancillary devices. Refer to the NCL manual for pin assignments for each trigger.



There are four input triggers in the NCL they can be used to initiate the following actions:
Inactive
Start an acquisition routine
Start a cycle within an acquisition routine
Acquire the next data point
End the acquisition (Abort)

These triggers may be of the following type as provided by the triggering device:
Low level
High level
Rising Edge
Falling Edge

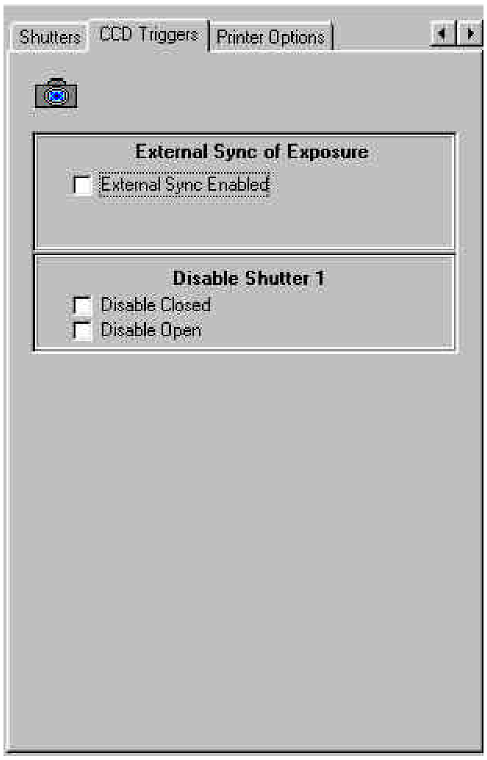
The NCL is also capable of outputting TTL triggers to ancillary equipment. Triggers may be initiated by the following conditions:
Inactive
Start of acquisition routine
Start of acquisition cycle
End of acquisition cycle
End of acquisition routine
Computed value Greater than or equal to a specified value
Computed value Less than or equal to a specified value

The type of output signal provided can be:
Low level
High level
Low pulse
High pulse

When using the GTE or LTE conditional triggers, the values monitored are the computed values based upon any ratioing of channel inputs and or division or subtraction of reference files for channel 1.

The CCD Triggers Tab

The CCD triggers tab will appear only if there is a CCD camera detected by the software.



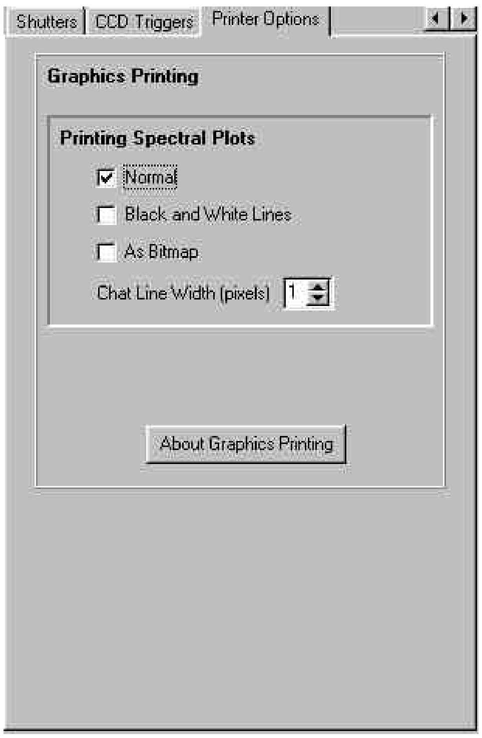
Check the External Sync box to synchronize the read out of the CCD to an external signal provided by another device. Refer to the SpectruMM manual for specifications of the type of triggers accepted.

The shutter is normally closed when there is no acquisition in progress. By checking the Disable Closed box you can prevent the shutter from opening even during acquisition. Checking the Disable Open box will open the shutter and leave it open until manually closed.

The Printer Options Tab

The printer options tab is used to correct for known problems with several printers and to switch between back and white and color printing. The Normal check box should be used as your default option if your printer is 100% compatible with Windows 98/NT. The Black and White Lines check box should be used if your laser printer has problems converting the color lines into gray scale. The As Bitmap check box is used as a last resort if your printer is not responding correctly.

The Chart Line Width choice field is used to make the axis and plots thicker. Some printers have a problem printing one pixel width.



Menu

File
- exit

Select Tab
- Hardware Config
- Hardware Status
- Survey Mode
- Acquisition
- Live Data
- Post Processing
- Terminal

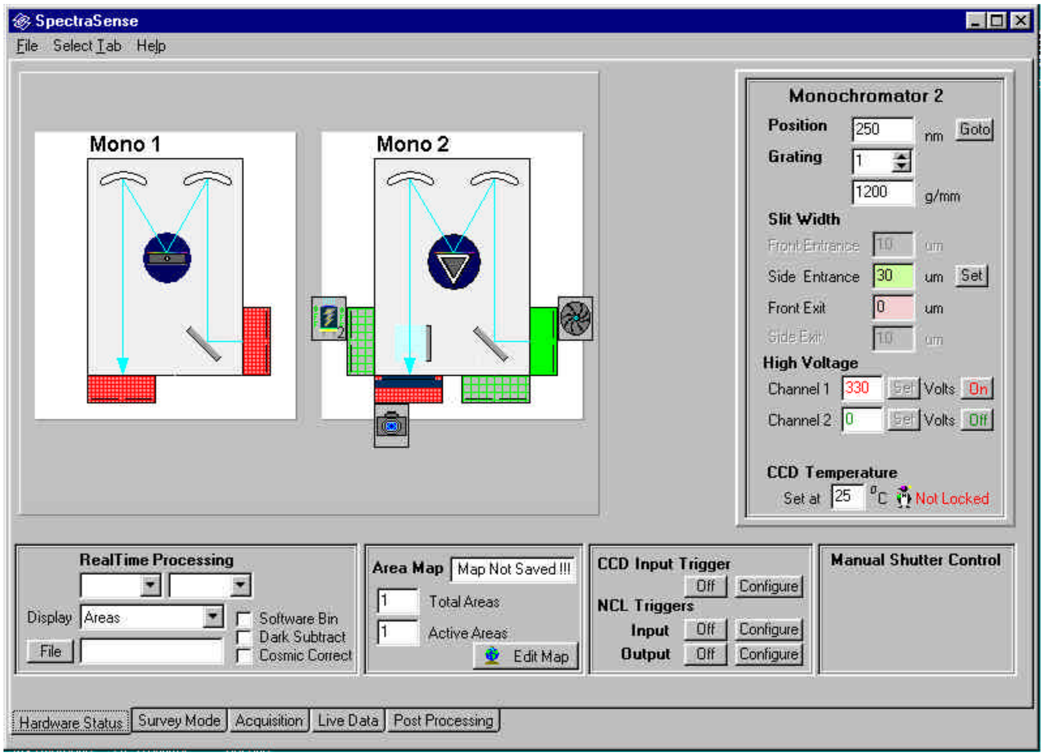
Select Config

Set up Optics	Jumps to Optics tab on panel
Set up CCD	Jumps to CCD tab on panel if a CCD is detected
Set up Detectors	Jumps to Detectors tab if an NCL is detected
Set up Mono 1	Jumps to Mono 1 tab
Set up Mono 2	Jumps to Mono 2 tab if a second monochromator is detected
Set up Filter Wheel	Jumps to Filter wheel tab if one is specified in the Optics tab
Set up Shutter(s)	Jumps to Shutters tab if shutters are specified in the Optics tab
Set up NCL triggers	Jumps to NCL triggers tab if NCL is detected
Set up CCD triggers	Jumps to CCD triggers tab if a CCD is detected
Set up Printer	Jumps to Printer tab

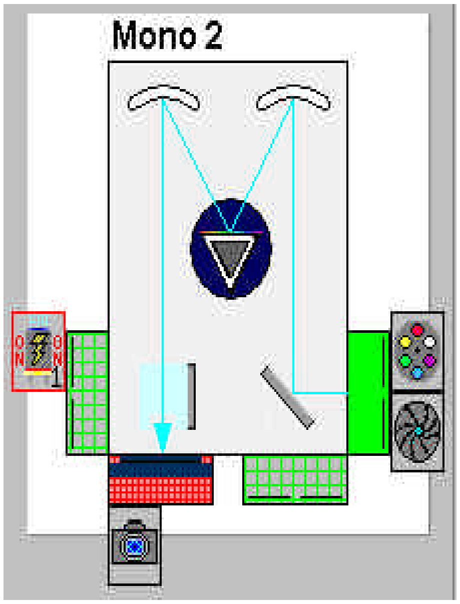
Help

Chapter 3: Hardware Status Screen

The hardware status screen is the one place where the current system settings such as grating choice, active detector(s), slit settings, and real time data processing methods can be viewed all at once. The real time processing options will change depending on the selected optical path and type of detector employed.

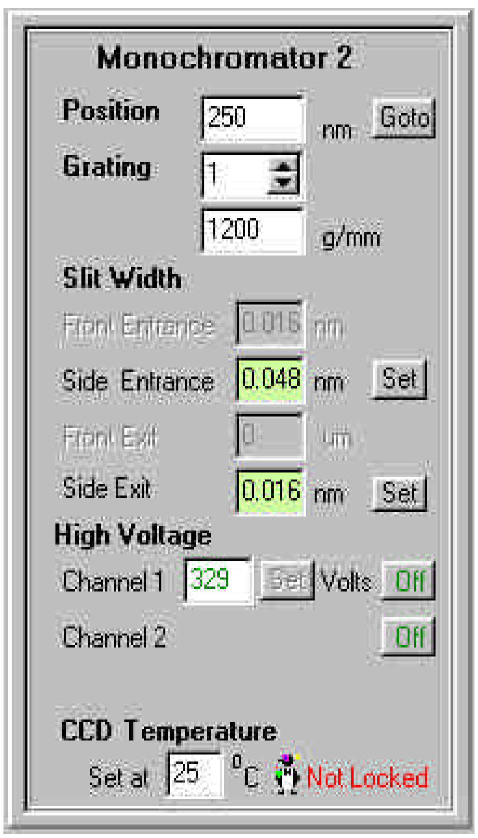


You select from this screen which entrance and exit ports to use for you next series of experiments. It is also only from this screen that you can select which grating will be employed.



The optical layout with the current optical path is shown on the system diagram. If there are two spectrometers, both will be shown and you select the one you want to work on by simply clicking on it. The layout to the left shows the light entering from the side entrance slit and going to the CCD camera. The optical path can be changed in either of two ways; by clicking on the turning mirrors or by clicking on the desired entrance and exit ports. The blue optical path will change to reflect the selected entrance and exit ports. If your spectrometer has multiple exit ports but only one has a detector associated with it, when the empty port is selected, the survey and acquisition screen tabs will disappear.

The current grating can be verified or changed by clicking on the grating turret. A drop down menu with all of the available gratings will appear. Solid green slits are motorized and software controllable. Solid red slits are manual and any information about the slit width must be manually entered for storage in the data file. Checkered slits are out of the optical path.

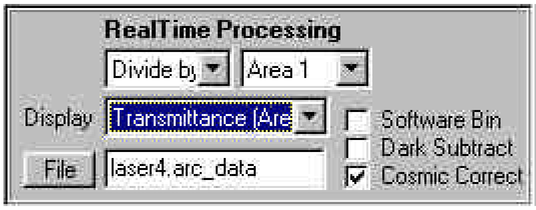


The information panel shows the state of the currently selected monochromator and associated detectors. The position field shows the current central wavelength of the monochromator or spectrograph. It can be changed by entering a new value and clicking on the Go to button.

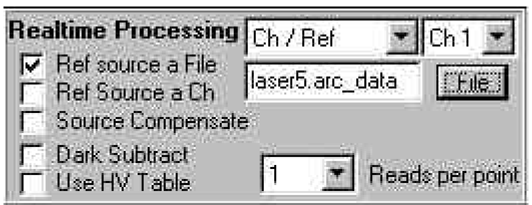
You can see the current grating and change it in the grating field. The grooves per millimeter field will up date with the grating number selection.

The active slit positions are shown in the slit width fields. Fields with green backgrounds indicate software controlled operation and the slits will open the values entered and set. Fields with a red background represent manually adjustable slits and the current values should be entered here for accurate inclusion in data files.

If there is a PMT(s) in the system, the High Voltage fields will appear. You can turn the HV on or off by clicking on the On/Off button(s). You can change the HV by entering a new value in the field and clicking on the Set button. If there is a CCD in the system, the specified cooling temperature will appear in the temperature field. The penguin icon indicates if the temperature has been attained.



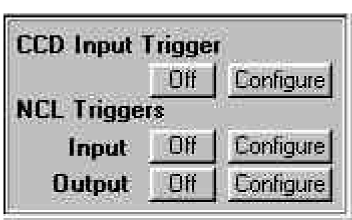
The CCD real time processing panel shows how the incoming data is being treated before presentation on the screen. The top left dialog box has three options; no op, subtract, and divide by one of the areas that are being readout on each acquisition. The area number to be subtracted or to be the divisor is selected from the right drop down field. The data can be displayed in raw areas, areas/file, absorption, %transmission, and %reflectance where a reference file must be specified in the file field. The data may be software binned, have a dark spectrum subtracted, and use the cosmic correction algorithm. Detailed discussions on these operations are covered in the glossary.



The single channel or scanning real time processing panel appears if there is a single channel detector in the light path. The real time processing of the incoming data can be selected from the drop down field. The choices include: CH1, CH/Ref(erence), CH1-Ref, Absorption, Transmission, Reflectance, and All Channels displayed.

The Ref source a File check box indicates that a stored file will be the reference data used in any real time calculations. The Ref Source a Ch(annel) indicates that one of the detectors, which has been defined as a reference channel in the Hardware Configuration screen, will be used as the reference. If there is a source compensation accessory installed in the system, checking the Source Compensate box will automatically divide all other inputs by the source compensation signal. The Dark Subtract check box is used to take a dark reading and subtract that value from all subsequent readings. The Use HV Table will vary the high voltage as the monochromator is scanned to compensate for the variation of the quantum efficiency of the photomultiplier tube as per a table of HV values created in the survey screen. The Reads per point drop box specifies that 1, 3, or 10 readings of the detector will be averaged at each data point.

If a CCD is in the light path, the area map information panel will appear. It shows the name of a stored map if loaded, in the top field, the total number of areas created on the chip and how many of these areas are going to be actively read out. Clicking on the Edit Map button brings you to the map creation panel in the survey screen.



The triggers panel indicates if the triggers functions are on (active) or off. Clicking on the Configure button, will open the triggers configuration dialog box from the Hardware Configuration screen to modify or verify the triggers that have been created.

If a CCD is in the current light path, the CCD manual shutter control panel will appear. The shutter is normally closed, opening only for the specified integration time. By clicking on either of the options boxes here, you can keep the shutter permanently open or permanently closed.

If a shutter is in the system and the light path includes a single channel detector, the manual shutter control panel will appear. Click on the shutter icon to open or close the shutter. The current status of the shutter is shown by the icon (closed in this illustration).

Menu Level

File

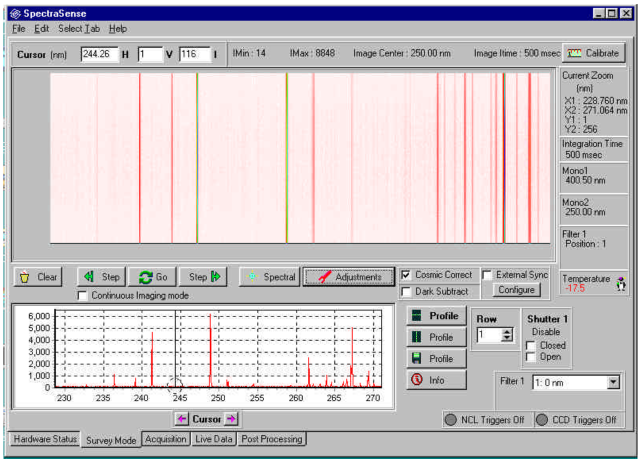
Exit

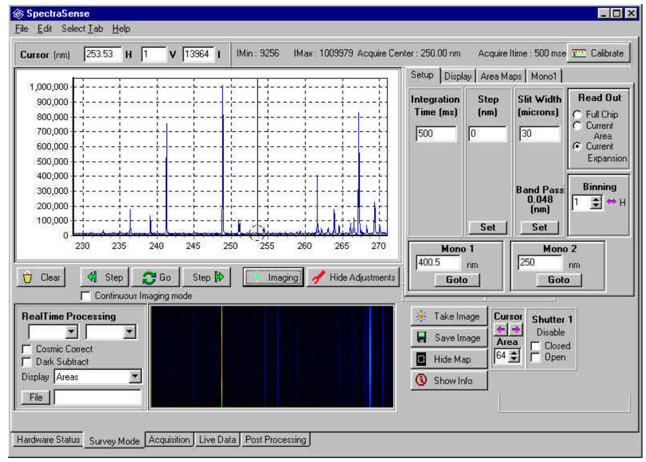
Select Tab

Hardware Config	Calls up the Hardware Configuration screen
Hardware Status	Calls up the Hardware Status screen
Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen
Live Data	Calls up the live data screen
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

Help

Chapter 4: CCD Survey Screen





The CCD survey mode screen appears when the CCD is in the optical path and the Survey screen tab is selected either from the menu level or from the tab at the bottom of the page.

The purpose of the survey screen is to optimize the acquisition parameters for taking spectra. From within this screen you can adjust the spectrograph position, the integration time, area(s) of the chip from where the spectra will be acquired and slit widths. These parameters control the signal to ratio of the spectra and the spectral range that will be covered.

You can adjust these parameters in both a spectral mode and an imaging mode. The combination of both modes provides an accurate and precise method for optimizing spectral acquisition. The top window of this screen shows the active mode. The bottom window is used to help evaluate the active mode. Spectra and images can be directly stored from within this screen, however the main purpose is to transfer the operating parameters to the acquisition screen which provides more flexible data acquisition and storage of routines that can be called upon repeatably. The spectral and image displays in both windows can be expanded or returned to full scale using the mouse dragging procedure discussed earlier in this document.

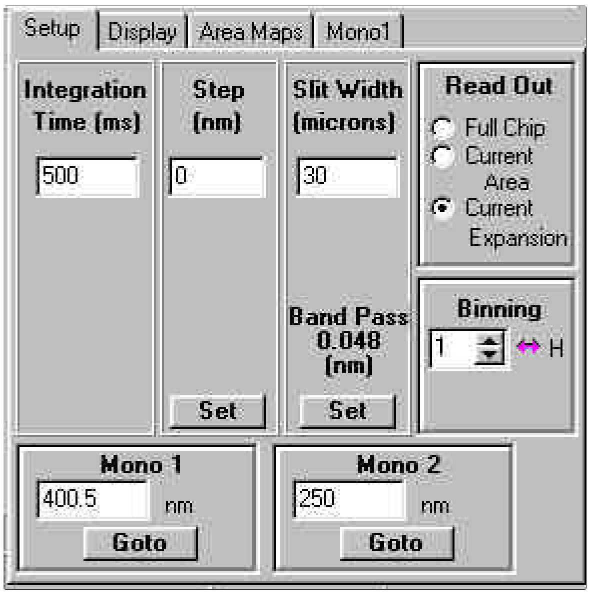
You select your acquisition mode by clicking on the two state Imaging/Spectral button.

The present state of the button indicates what mode will be active if the button is clicked on.

The two state Adjustments button is used to toggle between a larger primary display and access to the panels which control the acquisition and viewing parameters. In the illustrations above the adjustment panels are hidden on the left and visible on the right.

The Go/Stop two state button is used to acquire data. If the continuos box is checked, data will be continually acquired and the display updated until the Stop button is pressed. The Step buttons are used to move the spectrograph a specified number of wavelength units to either higher or lower wavelength before each read acquisition. If the continuos box is checked the spectrograph will continuously move to either high or lower wavelength and update the display. The increment for the motion is specified in the Setup tab.

The clear button will erase the image or spectrum displayed in both windows.



The **Setup tab** controls most of the parameters that affect the spectral quality and wavelength coverage. The integration time is how long the CCD will be exposed before the data is read out. Doubling the integration time will double the signal intensity.

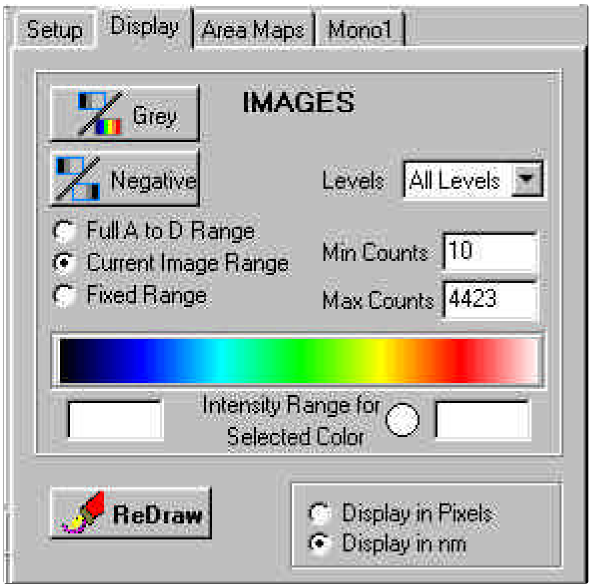
The Step panel is used to define the incremental position change for each click of the left or right step arrows. After entering a step increment in your selected spectral units, click on the Set button to validate the change.

The Slit width panel is used to set the width of the slit (if motorized) or for entering the final slit width that has been manually set. The spectral band pass for the width is shown on the panel. (If you have selected band pass units for the adjustments in Hardware Configuration the field will show the band pass and the information below will show how wide the slit is in microns. You must validate your entry for automated slits before the change will occur by clicking on the Set button.

The Read Out panel defines what portion of the chip will be displayed in image mode only. If Full Chip is selected the entire chip will be displayed. If Current Area is selected, only the defined areas of the chip will displayed. If Current Expansion is displayed only and you have expanded the image, only that portion visible will be updated and displayed. The smaller the portion of the chip you select, the faster the image will update. For focusing fiber optics for example it would wise to expand the image to show only a few of the fibers. In this way you can iteratively adjust the focus more quickly.

The binning panel will have both H(orizontal) and V(ertical) adjustments in imaging mode and only horizontal in spectral mode. By binning pixels together you can increase the signal to noise at the expense of spectral or image resolution. In many cases binning by two pixels or more will not degrade the spectral resolution and will increase the signal to noise ratio.

The Mono panels show the current central wavelength of the spectrogaph(s). You can move the spectrograph by changing the value in the position field and clicking on the Goto button. The background of the field will be red as the spectrograph is repositioning and will return to white when it has reached the desired position.



The **Display tab** is primarily used to enhance the images displayed in the top window. It also here that the x axis of the spectrum and image can be shown in wavelength units or horizontal pixel position.

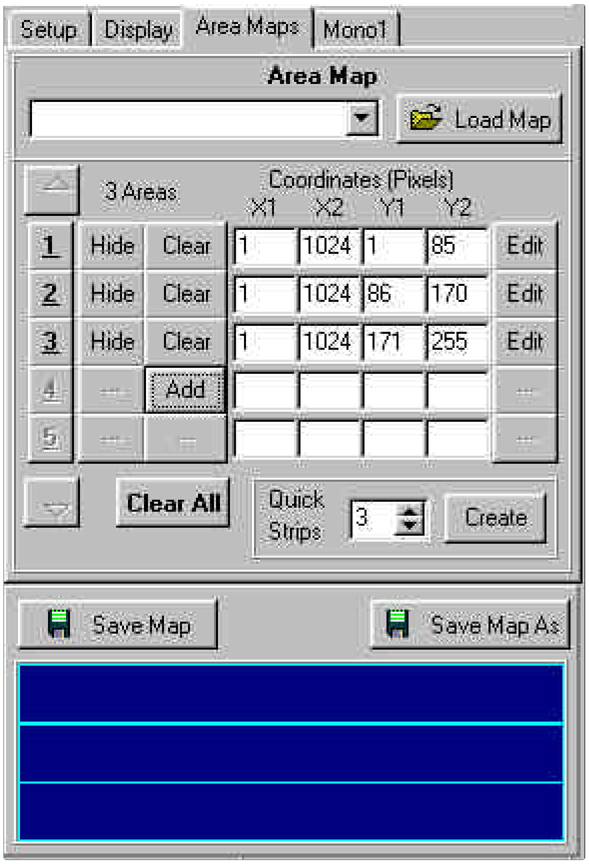
The Grey/Color button changes the image between false color or gray scale. The Positive/Negative button reverses the color scale. Sometimes weak features are best visualized in negative grey scale.

The Levels field is used to define how many shades of grey or number of colors will be used in the image display. The choices are 2, 3, 4, 8,16,32, and All levels which is a function of your graphics board.

The Full A to D Range radio button will display the full level of colors between 0 and 65,535 counts irrespective of the actual count range for the image. The Current Image Range will set the color levels from the minimum intensity value to the maximum intensity value in the current image. The Fixed Range button allows you to set arbitrary minimum and maximum intensities over which the color levels will be displayed.

To find the count range for any color in the image, click on the same color on the color band in the panel. The minimum and maximum counts for that color will appear in the intensity range fields.

If you have changed any of the parameters discussed above, you can redraw the image with the new settings by clicking on the ReDraw button. You must re-acquire the image or spectrum after changing the display between pixels and spectral units.



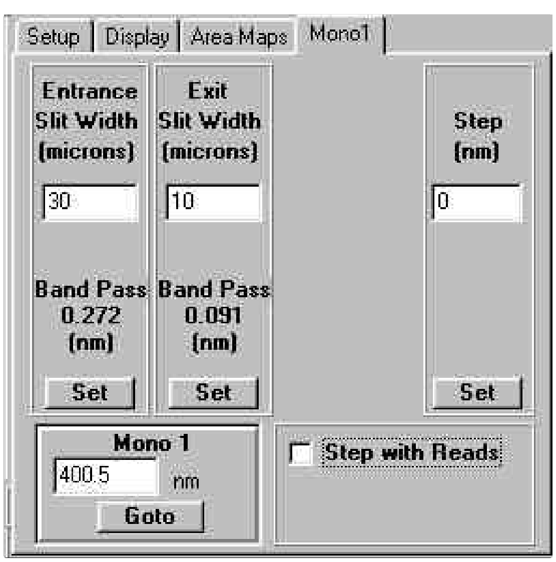
The **Area Maps tab** is used to define the areas on the CCD chip from which spectral or image data will be acquired. Multiple areas can be defined as long as there is no overlap between areas. Areas are important in that the size of an area can have a significant effect on the signal to noise ratio of a spectrum and in reducing saturation in cases where there is a strong signal. In working with fiber optics, you would normally define areas that just cover the height of each fiber and the width of the chip.

There are three ways in which areas can be defined. However before any new area maps can be defined you should first click on the Clear All button and then on the Add button.

You can draw areas on an image that is displayed in the top window by clicking and dragging the mouse to draw a box around the area. You can enter x and y limits, in pixel positions into the coordinates fields or you can user the Quick Strips to create up to 64 equal height areas across the chip. You can clear or add areas by clicking on the clear/add button. You can edit the values in the coordinates fields by clicking on the Edit/Set button. You can choose to display or hide any of the areas by clicking on the Hide/Show button.

As you define the areas they will be displayed in the diagram at the bottom of the panel. After you have created a map of the desired areas you can save it for future use by clicking on the Save Map button. You can reload the map at any time by clicking on the Load Map button. If you modify a saved map and wish to keep both the original and modified versions use the Save Map As button to save the modified version.

When using the Quick Strips method of creating areas, sometimes there will be a group of pixels left over that is smaller than the others. These will show up as another area. You may chose to clear this area or hide it from display.

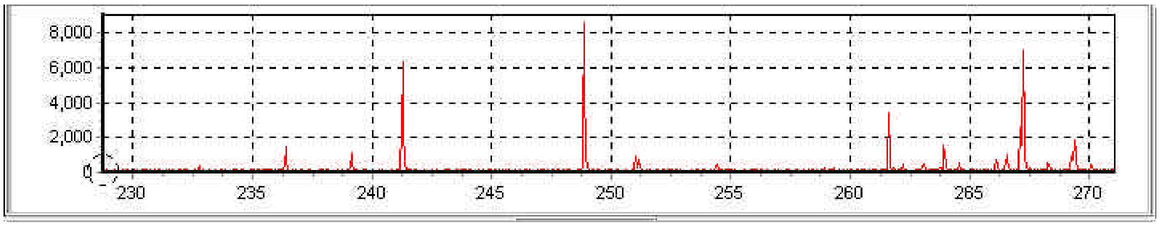


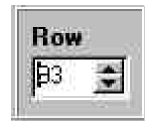
If there is a second monochromator in your system a **Mono tab** will appear. In this tab you can adjust the slit widths by entering the desired values in the fields and clicking on the Set button, if the slits are motorized. Otherwise you should enter the values for the width that you have set manually so that they can accurately be stored with the data file.

The second monochromator can be set to step the number of spectral units entered into the Step panel. If the Step with Reads box is checked each time the CCD is read out the monochromator will move to the next position. This is useful for acquiring fluorescence excitation emission matrices.

The position of the monochromator is visible in the Mono panel and can be changed by entering a new position and clicking on the Goto button.

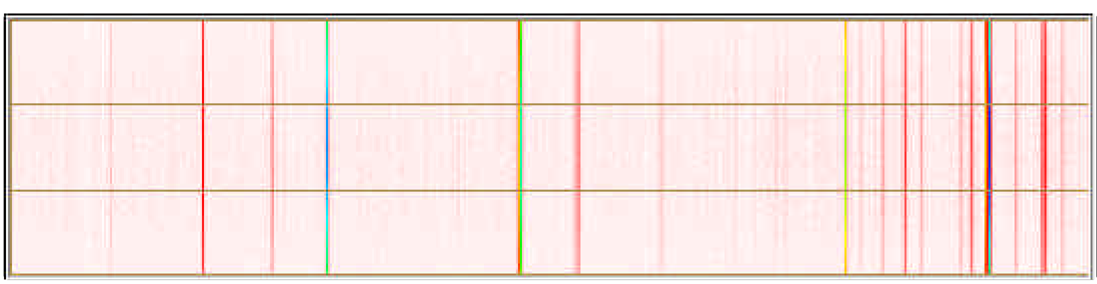
The Lower Display Window

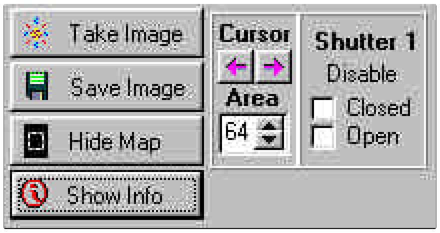




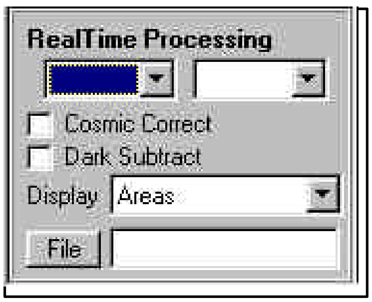
If your are in image mode the smaller window can be used to analyze the image by providing either horizontal or vertical profiles of the image. These show up in graphical form. The horizontal Profile button will display the intensities across a single row of pixels. The row can be specified by either moving the cursor to the desired position on the image or by entering a value in the row panel. A vertical profile will give a graph of intensity versus height along the entrance slit. You can select the column to be displayed by either moving the cursor to the desired position or entering a value in the column panel. You may save the profile data in a file by clicking on the Save Profile button. Clicking on the Info button will clear the display and show a panel containing all of the acquisition parameters.

If you are in spectral mode the primary window will display the current spectrum and the lower display window will show the last image taken, with or without outlines of the areas defined on the chip.





The options available for the lower window when in spectral mode include: Take Image where in a new image is taken and displayed in this window. Save Image will save the current image in the window to a BMP, Tiff or SPC file. Hide/Show Map will trace the current map on the image in the window. The Show/Hide Info button will toggle between the information screen shown above and the last image taken. The Area and cursor arrows will show the intensity and wavelength values for the specified area in the spectrum display window. The Shutter panel is used to open or close the shutter during periods when the CCD is not active.



The Real Time Processing panel is used to do spectral manipulations on the data as it is being acquired and displayed. The top left hand choice box is used when doing mathematics between specified areas on the chip. The choices are NoOp, Divide, and Subtract. The right hand choice box lists all of the current areas. The area specified in this box will be the area that will either subtracted from or divided into all of the current areas on the chip. If there are 4 areas and Divided is specified in the left box and 2 is specified in the right box , then the spectral display will show A1/A2, A3/A2, and A4/A2.

The Cosmic Correct check box is used mainly with long exposures to eliminate any spurious peaks that may appear due to cosmic rays. When this is selected, two spectra with the specified integration time will be taken. If there are any peaks in one that are not in the other then these peaks will be removed from the displayed spectrum.

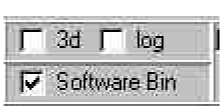
The Dark Subtract check box is used to subtract the contribution of temperature dependent signal from a spectrum. Since the dark component is constant for any temperature and integration time, a spectrum of only the dark component can be subtracted from each spectrum. This is accomplished by taking a spectrum with the shutter closed and subtracting it from each subsequent read out. This has the effect in survey mode of doubling the time for each acquisition.

The Display choice box will display the spectral data of the areas with any of the manipulations discussed above, the area(s) divided by a file specified below, Absorbance, %T, and %R using a reference file specified in the field below.

The filter panel appears if there is a filter wheel in your current experimental setup. The field shows the current filter position, or cut off wavelength, if specified, or name specified in the filter wheel set up tab in the hardware configuration screen. Click on the arrow to display all possible choices and highlight the desired filter.

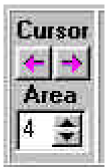
The triggers indicator panel shows whether user defined trigger are active or inactive. To change the state of the triggers return to the Hardware Status screen. To redefine the trigger ports or triggering criteria return to the Hardware Configuration screen.

The Cosmic Correction and Dark Subtraction panels appear in imaging mode. These functions appear in the real time processing panel in spectral mode. Refer to the descriptions above.

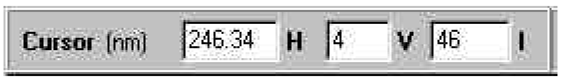


The 3d check box will cause successive spectral readouts to be displayed in a 3 dimensional plot in the primary window. The log check box will cause the intensity range to be displayed on a logarithmic scale.

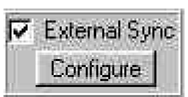
The Software Bin check box causes each row in the specified area to be individually read out and coadded in memory. This is fundamentally different from the normal read out where all the rows in the area are shifted into the chip's read out register and read out at once. The advantage of using software binning is that it allows for higher dynamic range in that individual rows may not oversaturate the read out register, while the simultaneous readout of all of the rows might. The disadvantage to using this option is that the read out process takes significantly more time than in the normal hardware binning.



The cursor area selection panel only appears in spectral mode. It is used to select from which area the cursor will display the intensity value in the cursor coordinates panel at the top of the screen. Do not enter a value larger than the number of areas collected on the current acquisition.



The cursor coordinates panel displays the horizontal position of the cursor in the selected working units. In imaging mode the second field, V, displays the column number of the cursor. In spectral mode it displays from which area the intensity value is being displayed in the intensity field. In imaging mode the intensity field shows the intensity at the specific pixel with the displayed H and V coordinates.



The external sync check box is used to synchronize the start of a read out with an external device. There must be the correct connection between the device and the ST133 controller for the CCD.

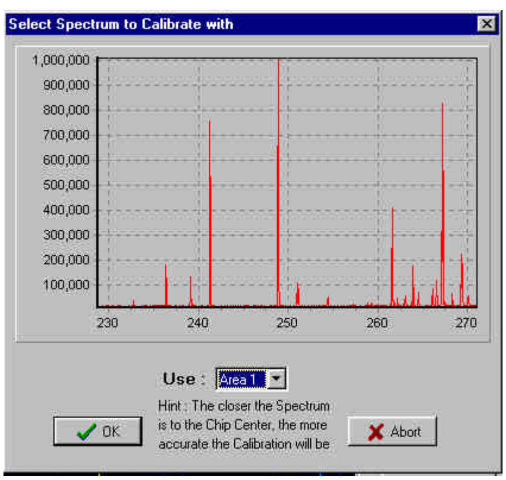
The Shutter control panel allows you to disable the mechanical shutter opened or closed for subsequent read outs. For experiments where spatial information in the vertical direction is not important, and read out speed is, it may be advantageous to disable the shutter in the open position.

Calibration

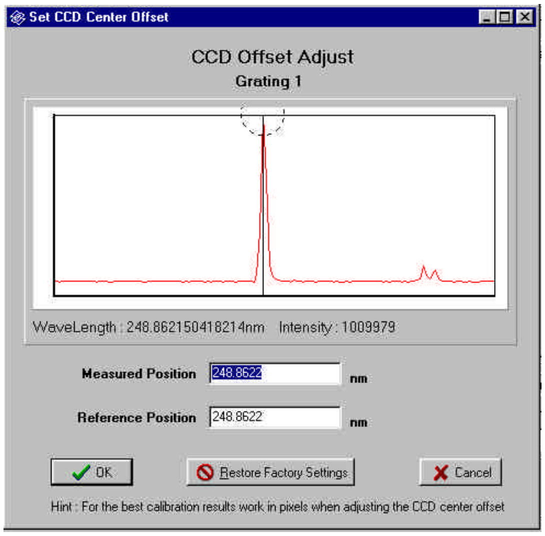
Wavelength (or wavenumber) calibration of a spectrograph takes many parameters into consideration; the focal length of the instrument, the angle of the focal plane relative to the plane of the CCD chip, the difference in the spectrograph's dispersion at different center wavelengths, and the grating groove density. With SpectraSense once the calibration is computed for any central wavelength, it will remain valid for all central wavelengths. However, a separate calibration function must be created for each grating in the spectrograph. Once the gratings are calibrated, the software knows which function to apply for each grating when they are interchanged. To begin the process, a known wavelength standard must be available to measure. Typically mercury pen lamps or fluorescent lights are used for calibration as they have very sharp, well know peaks. Usually the 435.8nm peak or the 546.1nm peak is used in the calibration procedure.

You begin by selecting the grating that you wish to calibrate in the Hardware Status screen. Once it is selected, return to the survey mode screen and click the image/spectrum button so that you will be collecting spectra. Illuminate the entrance slit of the spectrograph with light from your calibration source. Take a spectrum with good signal to noise with the spectrograph centered at your reference peak. Click on the Calibrate button.

The introductory screen for the calibration procedure will be displayed. Note that you will repeat the procedure three times to accurately calibrate your system. Start out by selecting Step 1 and then click on the OK button. If at any time you feel that you made an error you can always click on the Restore Factory Defaults button.



You will come to a screen that shows the spectrum or spectra from multiple areas that you have just acquired. Select one area to work with by clicking on the arrow on the area Use panel. Click on the OK button to continue.



You will come to the third screen in the calibration procedure. Expand the spectrum around your reference peak so that you can easily place the cursor exactly on the center of the peak. If the reference peak is the highest peak in the spectrum, the software will automatically move the cursor on it. If the reference peak is not the highest peak, move the cursor to it and enter the wavelength value displayed below it into the Measured Position field. In general there is no need to enter the value to more than two decimal places. Next enter the know wavelength of the peak into the reference field. Click on OK.

You will be returned to the survey mode screen. Move the spectrograph so that the reference peak is located very near the left-hand edge of the spectrum. Click again on the Calibrate button. Select Step 2 and repeat the procedure described above. Next move the spectrograph such that the peak is now located near the right edge of the spectrum and repeat the above procedures. After you have completed this three-step process your spectrograph is calibrated for the selected grating. Change the grating and repeat the process again. If you have a third grating in your system perform the calibration procedure for it also.

Once your system is calibrated it should remain so unless you move the CCD detector head or if there is a noticeable change in ambient temperature. It would be good laboratory practice to verify the calibration from time to time by running a spectrum of you calibration source and noting the displayed value for the reference peak.

Menu Options

File

Open		Open saved chip area map
Save		Saves the current spectrum to a file.
Print	Frame	Sends a bit map image of the entire screen to the printer
	Spectrum	Prints a plot of the spectrum, or spectra displayed
	Data	Prints out the entire data file including parameters and data coordinates
Print Setup		Calls Windows printer control screen
Exit		Closes SpectraSense

Edit

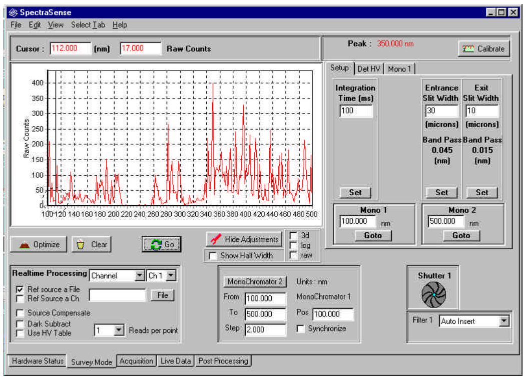
Export to Grams	Puts the data in the active working window in Grams software
Export to Grams 3D	Exports multi-file data into Grams 3D program. Program must be running concurrently with SpectraSense
Overlay Spectra	Recalls a stored spectrum to be displayed concurrently with incoming spectra.

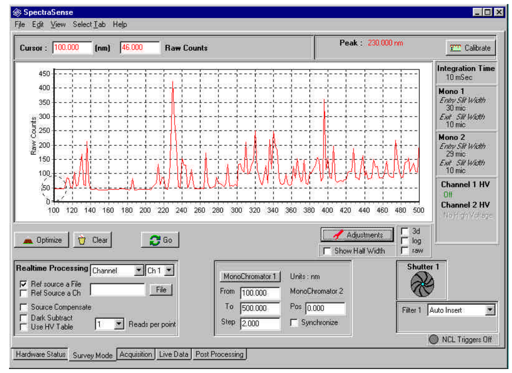
Select Tab

Hardware Config	Calls up the Hardware Configuration screen
Hardware Status	Calls up the Hardware Status screen
Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen
Live Data	Calls up the live data screen
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

Help

Chapter 5: Scanning Survey Screen

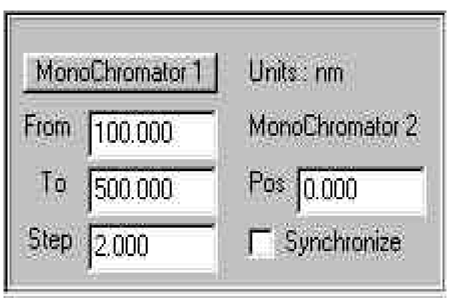




The Scanning Survey Screen is used to optimize the acquisition parameters when acquiring data using a single channel detector such as a silicon cell, PMT, or IR detector. This screen will appear when the Survey Mode tab is selected if there is a single channel detector in the light path specified in the Hardware Status Screen.

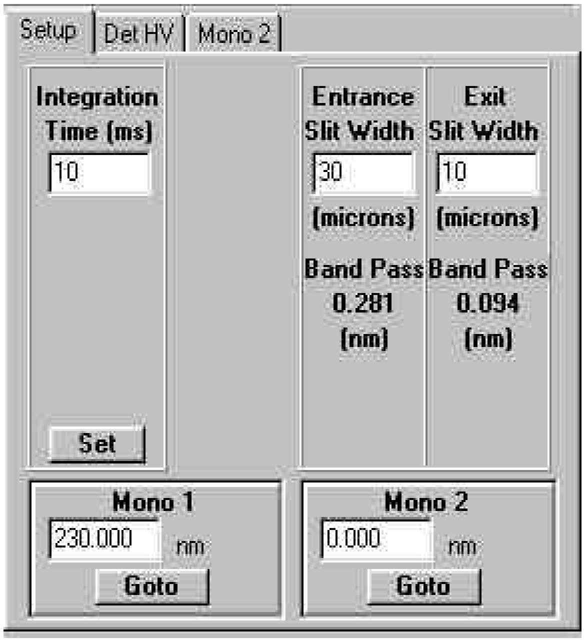
The spectral display screen shows the incoming data as it is being acquired. As previously described, the display can be expanded or contracted by dragging the mouse over the desired section of the spectrum.

Certain parameters must be defined before an acquisition can occur. There must be starting point and ending point of the acquisition, there must be step increment to tell the spectrometer how far to move between data points, there must be an integration time to define how long the signal will be collected at each data point, and there must be a definition of which detector or detectors are going to used for acquiring the spectrum and what real time manipulations of the data are required. It is in this screen that these parameters are adjusted and optimized to produce spectra with the desired signal to noise ratio and acquisition time.



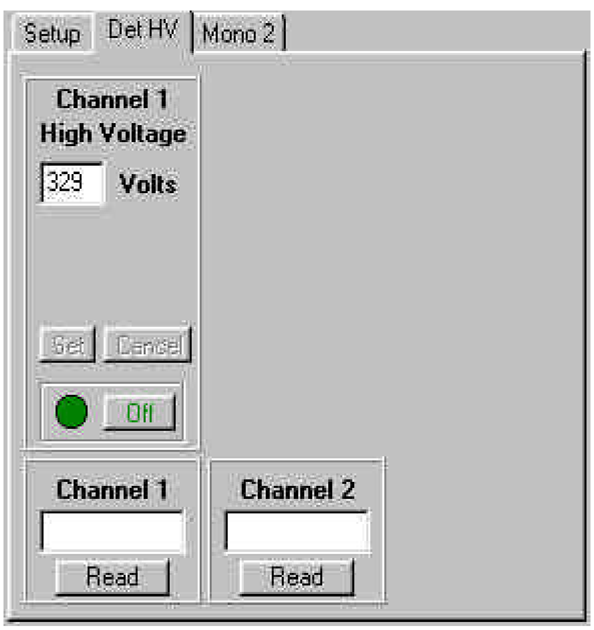
The scan range selection panel is used to input the start and end limits for the scan. The step is how many spectral units (nm in this case) the grating will turn before data is again taken. If there are two monochromators in your system, you can select which one will be scanned by clicking on the Monochromator button which will toggle between monochromator 1 and 2. You can specify a specific position for the other monochromator if desired, and can have it scan an equal number of steps as the primary monochromator starting at the wavelength entered in the position box by checking the synchronize button.

The two state adjustments button opens access to the parameters that will affect the signal to noise quality of your spectra. Click on this button to access or hide these parameters.

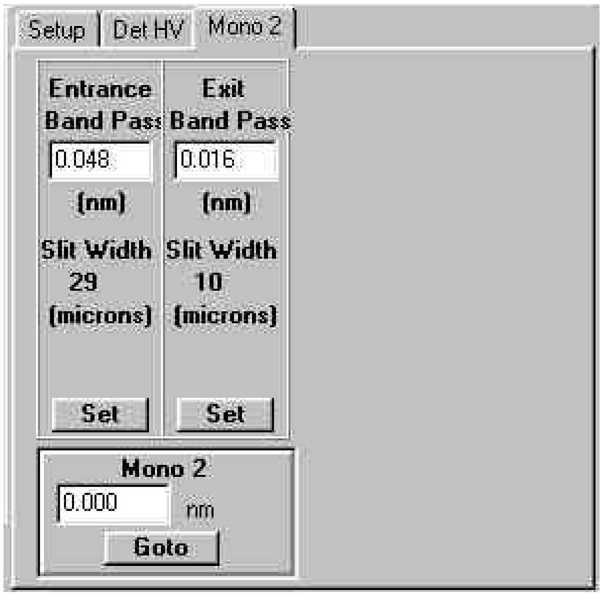


The **Setup tab** is where the integration time for each data point is specified. After entering a value (in milliseconds) click on the set button to validate your entry. The longer the integration time, the better the signal to noise ratio, and the longer the time to collect a spectrum. If your monochromator has motorized entrance and exit slits, you can adjust the widths by entering values in the slit width fields and pressing on the Set buttons to validate. The values entered into these fields are stored with the spectrum, therefore even if your system has manually adjusted slits the correct values should be entered into the fields so that you can accurately reproduce the acquisition parameters at a later date.

You can quickly set the monochromators to a specific wavelength by entering the desired value and clicking on the Goto button. The position field will change color while the monochromator is moving.

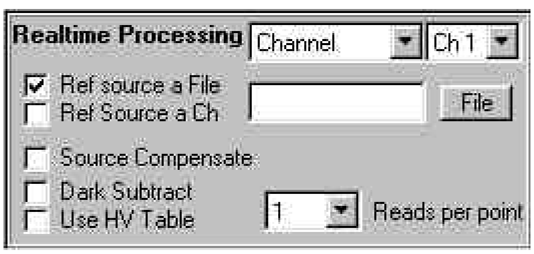


If your system includes a photomultiplier tube, you can adjust the high voltage setting. Within a certain high voltage range, specified by the manufacturer of the specific tube, increasing the high voltage will increase the signal. You change the high voltage by entering a new value in the Volts field and verifying it by clicking on the Set button. If you wish to change the value you have entered, click on the cancel button and the previous value will return. You can manually turn the high voltage on or off by clicking on the On/Off button on this panel. Clicking on the Channel read buttons will display the intensity at the current wavelength using the current integration time. You will note that Channel 2 does not have a high voltage associated with it. It may be a silicon cell or other solid state detector. None-the-less clicking on the Read button will display the intensity at the current position and integration time.



If there is a second monochromator in your experimental setup the Mono2 (or Mono 1 if Mono2 is your primary monochromator) tab will appear. It is from this tab that you can change the slit widths, if automated slits are included in the spectrometer, or you can enter new values to be stored in the data file when using manually adjustable slits. You will note that in this diagram the default setting units are in spectral band pass, i.e. you specify the desired spectral band pass and the slits will open to the appropriate widths. As spectral band pass varies with wavelength the slits will automatically adjust to maintain the specified values. You specify if you wish to work in microns or band pass in the Hardware Configuration screen. It is not recommended that use select the band pass option if your slits are manually adjustable. If there is no set button on the panel, the slits are manual.

You can also reposition the monochromator to a new central wavelength by entering the value in the Mono 2 panel and clicking on the Goto button. The field will have a red background will the monochromator is moving to the new position. A white background indicates that the monochromator is at the wavelength shown in the field.



The Real Time Processing panel is used to define which detectors are to be read out for display and how the incoming data is to be processed before it is displayed. The top left choice field contains all of the display options available, which will vary depending on your system configuration. The typical choices are: Channel #, Chan #/reference, Channel #/ Channel #, Channel #/file, Absorbance, %Transmission, %Reflectance, and All Channels. The channel number is chosen from the choice field to the right. There must be a reference for the absorbance, transmission, and reflectance measurements. This reference can be either a stored file, or the output from another detector.

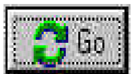
The **Ref source a File** check box is used if a stored data file will be used as the reference for the absorbance, transmission, and reflectance measurement. The **ref Source a Ch** check box is used if a detector is used as the reference. If this box is checked, a field will appear in which you specify which channel will be used as the reference.

The Source Compensate check box is used if a source compensation accessory is included in the system and you wish to divide each data point by the signal from this accessory.

The Dark Subtract check box is used if you wish to subtract the dark signal of the detector from each reading. All detectors produce a signal output that is temperature dependent. This signal can be subtracted from all readings when the detector is making a measurement. The software will close any automated shutter and take an initial reading or, if the 6^{th} position on the filter wheel has been specified for dark subtraction, the wheel will move to this position and take a reading and then return to the appropriate position for the scan. If your system has neither a shutter of filter wheel, you will be requested to block the light from entering the monochromator by any means of your choice, the dark reading will be taken and you will asked to unblock the light before the actual scan is taken.

The use HV Table check box is used to automatically adjust the high voltage on the photomultiplier tube as the monochromator is scanned. In order to use this option a HV table must be created. This automatic procedure is discussed later in this document.

You can specify 1, 3, or 10 reads per data point. If the signal is extremely weak, at times it is reasonable to average several read outs at each data point. If 3 is selected, the monochromator will sit at each position and take three readings at the specified integration time and then output the average value from the three readings. If ten is selected this procedure will take 10 read outs at each point. For most cases one read out per point is sufficient.

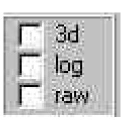


After all of the parameters that are necessary to perform an acquisition are specified, it is only a matter of clicking on the GO button. The button changes to a Stop button once the scan is started.

After you have acquired your initial spectrum, it is possible to optimize the peak signal by using the Optimize button. In optimize mode the monochromator will move to the highest peak and start taking intensity read outs at the specified integration time. The display will look like a strip chart recorder where you can seen in real time how the signal intensity changes as you modify acquisition parameters such as integration time, slit width, and high voltage. Once you have made the adjustments to your liking, click on the Stop button to go back to scanning mode. You can also set the monochromator to a specific wavelength by entering the value in the Mono panel of the Set up tab.

The Clear button will clear the spectral display window. If the window is not cleared at the end of a scan, the subsequent scan will overlay on the previous one.

The cursor information panel displays the current position and intensity information for all active detectors.



The display format options include 3D display of multiple spectra, the intensity displayed on a log scale, and the raw data input rather than any preprocessed data. The raw option is useful helping to determine the cause for spectra that do not appear as expected. It will show the raw data from all detectors on the same intensity scale.

When the Show Half Width box is checked. The wavelength position and spectral resolution of the highest peak on the spectral display window will be shown in the information panel at the top of the screen. To determine the spectral resolution of a smaller peak, expand the display such that that peak is the highest displayed.

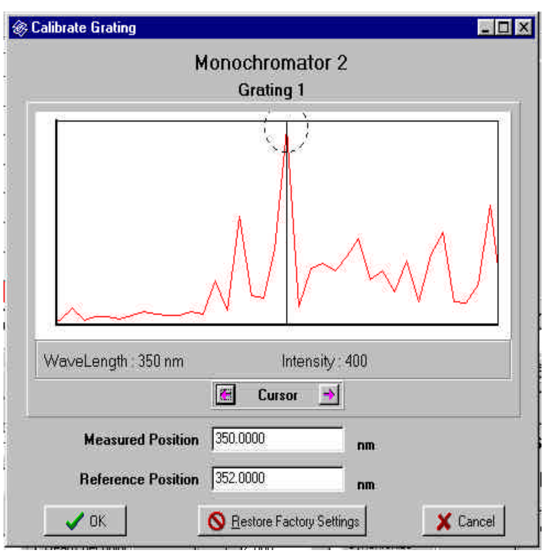
If your system has an automated shutter its current status, i.e. open or closed is shown in the shutter panel. Click on the shutter icon to change the state of the shutter. If an automated filter wheel is present, the Filter panel will appear. The choice field shows the current filter in place or Auto Insert if this option has been defined in the Hardware Configuration. You can insert any filter by clicking on the choice arrow and highlighting the appropriate filter.

The trigger status information panel will indicate if triggers you defined in the Hardware Status screen are active (red) or inactive (gray). To change the status of the triggers, return to the Hardware Status screen.

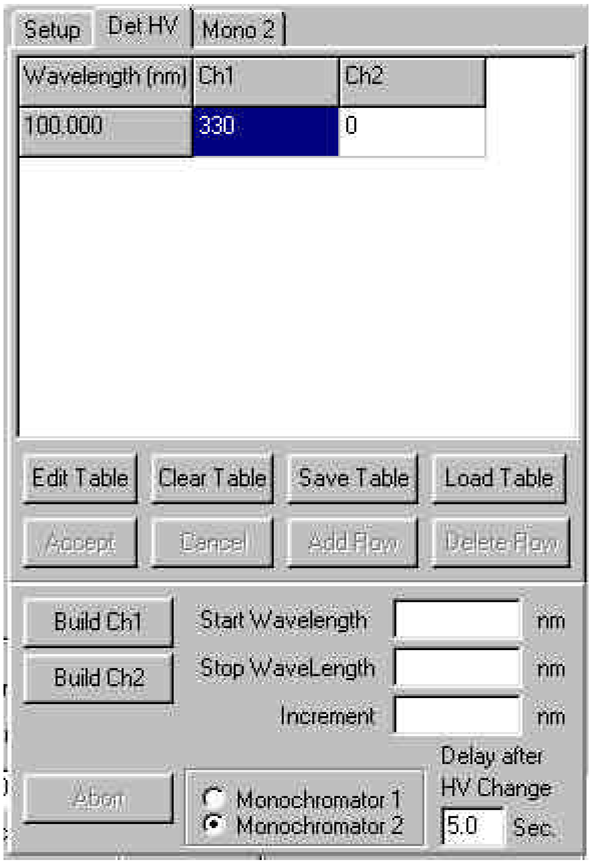
Calibration

The Calibrate button is used to verify or adjust the wavelength calibration of the currently active monochromator. A precisely known spectral line must be scanned over in order to use this function. Usually a Hg pen lamp or the mercury lines in a typical fluorescent light can be used. Known lines that can be used from these sources include the 435.8nm line and the 546.1nm line. Scan the monochromator over one of these lines such that the peak is very well above the noise level. Press on the Calibrate button to continue.

The calibration adjustment screen will appear. The cursor will automatically line up on the highest peak on the display. If the peak you are using for calibration is smaller, you can expand around it or move the cursor to its position. If you have expanded the display, you must click on the peak again to update the measured position. The Measured Position field will show the spectrometer position of the peak at the present calibration. The Reference position represents the real wavelength of the peak. Using the 546.1nm line as an example, the measured position and reference position may both say 545.5nm. By changing the reference position to 546.1nm, you have recalibrated the wavelength of the monochromator. Click on OK to accept the new values.



While the monochromator is a very stable instrument, calibration shifts can occur with temperature changes and misalignment of input optics. It is a good idea to verify the calibration of your monochromator on a regular basis. The calibration procedure must be repeated for each grating in the system, as the calibration offset for each one may be different.



When the **HV table** box is checked, the high voltage on the photomultiplier tube will change as the monochromator scans in order to ensure that spectral response of the system remains within a reasonable working range. In order to do this a high voltage table must either be created or recalled. The first time that you click on the HV tab, you will enter the high voltage table creation panel. In order to create the table, a broad band light source in the region of interest must be placed at the entrance of the monochromator. You specify the range over which you want the correction to be made by entering a start and stop wavelength. You specify how finely you want to make the adjustments by entering an increment. Enter a delay after HV change in the several seconds range to allow the photomultiplier tube to stabilize to the new voltage. Specify which monochromator the specific detector is attached to in order for the program to display the appropriate input channels. Click on the Build Ch1 or Build Ch2 (if present) to start the procedure. The table will automatically be generated by the software with the wavelength and HV values shown in the chart above. You have the option to edit the HV values in the table, clear the table, save the table to a file, or recall a previously stored table.

Menu Options

File

Save	Saves the current spectrum to a file.	
Print	Frame	Sends a bit map image of the entire screen to the printer
	Spectrum	Prints a plot of the spectrum, or spectra displayed
	Data	Prints out the entire data file including parameters and data coordinates
	Exit	Closes SpectraSense

Edit

Export to Grams	Puts the data in the active working window in Grams software

View

Autoscale	Automatically scales the axes of the plot so that the full spectrum is shown.
Full Width coverage.	Show the spectrum with the current vertical expansion but full wavelenght
Full Height	Shows the spectrum with full vertical expansion but with current horizontal expansion
Zoom In	Expands the spectrum to show half the current values as full scale on the display.
Zoom Out	Shrinks the current expansion to twice the current level
Overlay Spectra	This allows you to recall stored spectra and display them on the same axis as the most recently acquired spectrum in the display window

Select Tab

Hardware Config	Calls up the Hardware Configuration screen
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Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen
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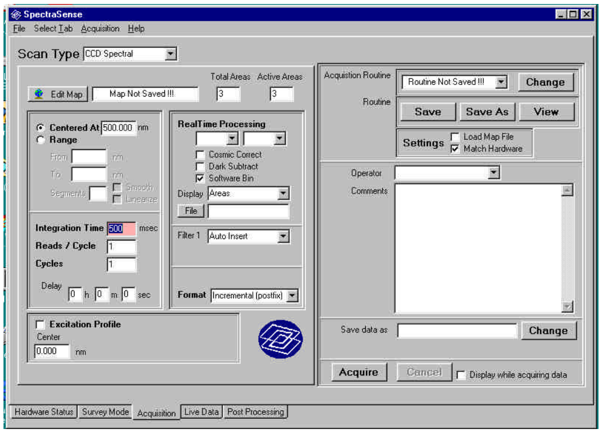
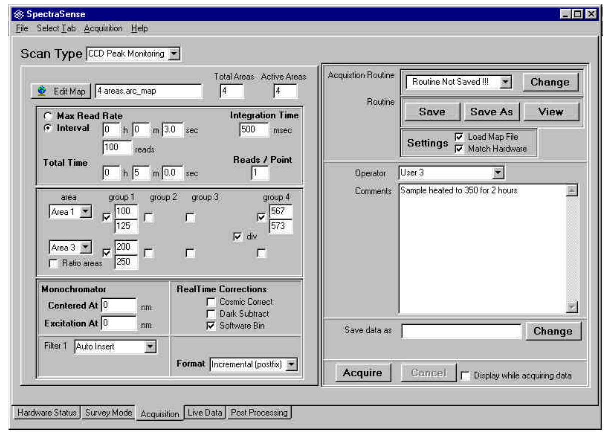
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

Help

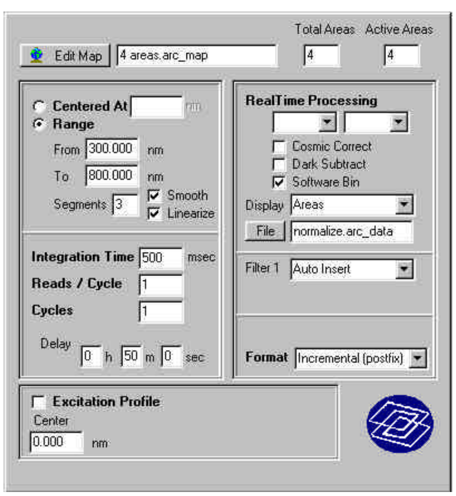
Chapter 6: CCD Based Acquisition



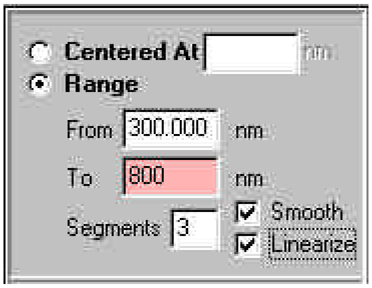


The Acquisition screen is used to collect spectra or time based intensity at a specific wavelength measurement. The acquisition parameters that were optimized in the Survey Screen are carried over to the Acquisition screen to ensure that the spectra are collected with the desired signal to noise ratio and resolution. It is from these screens that routines can be created that will reproduce acquisition conditions that can be recalled at a later date. There are two acquisition modes associated with CCDs; spectral acquisition and peak monitoring. Either can be accessed form the Scan Type field at the top of the screen. If your system also includes single channel detectors, the acquisition types associated with them will also be accessible from the Scan Type choice box. If you inadvertently choose an acquisition mode not associated with the detector in the current light path, the parameter input fields will not appear. If the acquisition mode you wish to use will not come up, go to the Hardware Status screen and change the light path such that the desired detector will be activated.

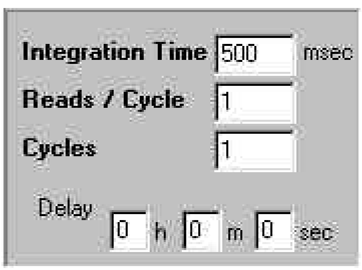
CCD Spectral Acquisition



In the spectral acquisition mode individual spectra may be acquired, multiple spectra collected with a specified delay between read outs can be acquired, multiple spectra "glued" together to produce a data file which covers and extended spectral range can be acquired, and excitation/emission profiles can be acquired. The left side of the acquisition screen is used to define how the spectrum or spectra will be acquired.

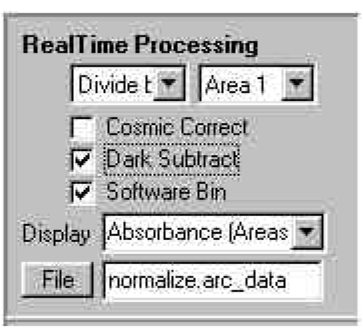


In all cases the spectrometer must be positioned to capture the spectral region(s) of interest. This information is entered into the position panel. If the entire spectral region of interest can be dispersed on the CCD chip, the Centered At option is selected and you enter the wavelength that will be in the center of the range in the field. If the spectral range to be covered is wider than can be captured by the CCD all at once, the Range choice should be checked. When the range choice is checked you must enter a starting and ending wavelength to be covered. You then select the number of segments needed to cover that range. This can be estimated by noting the wavelength coverage on a single read out and determining how many of these segments will be needed to cover the full range. It is advisable to allow an extra segment if the coverage is close. For example; if in the Survey screen you noticed that the spectrum covered the range from 200 to 400nm, you can make the rough assumption that 200nm will be covered in every segment. To cover the range from 300nm to 800nm would require 3 segments and would have sufficient overlap between segments to ensure continuity. The Smooth check box will automatically average the intensity differences in the overlap regions and produce a smooth continuous spectrum. The Linearize check box is used to extrapolate the data so that the spacing between data points is in equal wavelength units as opposed to pixel spacing.



The Read out panel is used to define the integration time for the spectral acquisition and how many spectra are to be collected. The value shown in the Integration Time field is initially the value used in the Survey screen, as under normal operation the integration time is optimized in the Survey screen. This can be changed by enter a new value into this field.

The Reads/Cycle determines how many read outs will be averaged together for each spectrum. In general one read out is sufficient. In cases where the integration time is long, it may be useful to coadd reads to reduce the chances of cosmic induced peaks. The Cycles field determines how many spectra are to be acquired in the experiment. The Delay, in hours, minutes, and seconds, determines the time between each acquisition. Note that the delay includes the integration time; if the integration time is 500ms and the delay is one second, the camera will integrate the signal for 500ms and wait an additional 500ms before starting the next acquisition.



The incoming data from the CCD can be pretreated before being displayed and saved by selecting options in the Real Time Processing panel. If more than one area of the chip is being read out, it is possible to either divide the intensities of all other areas by one, or to subtract the spectrum from one area from all of the others. These options are initiated by selecting No op, Divide by, or Subtract from the top left choice box and selecting one of the areas from the top right choice box. If there is only one area being used, these options will not be accepted and an error message will appear.

The incoming data can also be manipulated using data previously stored. The incoming data from all channels can be divided by the stored spectrum. Real time calculations of absorbance, %transmission, and % reflection can be calculated and displayed where a stored file is used for the reference.

The incoming data can be corrected for cosmic interference by checking the Cosmic Correct box. This will cause two acquisitions with the defined integration time to be taken. The two spectra will be compared and any peak not found in both spectra will be removed. This option should only be used for long integration times, usually above 60 seconds.

The dark subtraction box will cause a spectrum to be taken with the shutter closed which will then be subtracted from all subsequent read outs.

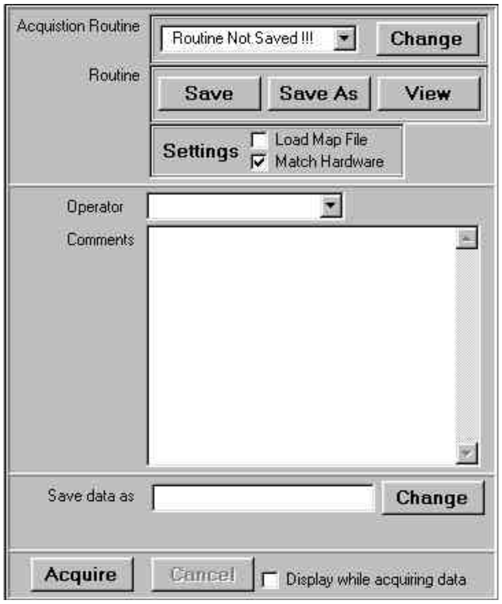
The software binning option will cause each row of pixels in the active area(s) to be read out individually and have the intensities from all of the rows coadded in memory. This will result in a noticeable delay in the acquisition but may eliminate saturation of strong peaks.

If a filter wheel is present in the system optical path, the filter panel will appear. The current state of the filter wheel is displayed in the choice field. Clicking on the arrow will present all of the installed filters and allow you to select which one to use in this acquisition.

The Format panel allows you to specify whether files from the same acquisition program are specified with a numerical prefix or suffix. Example: 02myfile.dat or myfile02.dat.

The Excitation Profile panel will appear if your system includes two spectrometers and you are using one in conjunction with a light source for fluorescence excitation. If the check box is not checked only the wavelength position of the excitation monochromator will appear in a field named center. Entering a value in this field will cause the monochromator to go to that wavelength before all acquisitions are made. If the box is checked, three fields will appear. An excitation profile takes a spectrum or series of spectra as defined above, for each excitation wavelength defined in this panel. The results can be viewed as a 3D surface plot using programs such as Grams 3D. The excitation range is defined by the From and To limits entered into these fields. The Steps field defines how many wavelength units (nm in this example) the excitation monochromator will move before the next spectrum or series of spectra will be taken. In this example 12 spectra will be taken in the profile.

The area map information panel shows at a glance the total number of areas currently defined on the chip. It is possible to change the size and number of areas by clicking on the Edit Map button. The area map creation panel will appear allowing you to either load previously stored area maps, modify the current area map, or change which areas in the current map are read out or ignored. Refer to the CCD Survey Screen chapter for more information on this subject.



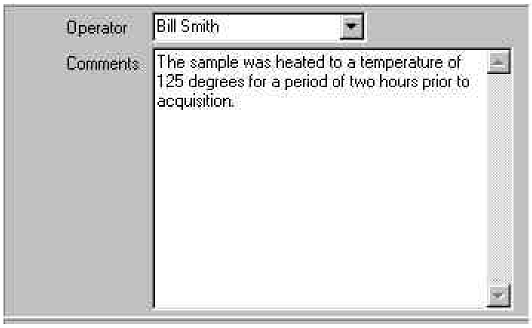
The Acquire panel is used to save all of the parameters entered in the Acquisition panel into a file that can be recalled at any time to collect spectra under identical instrumental conditions. Routines can also be recalled in this panel which will override the current hardware and operating parameters to those defined in the stored routine file. Although they are not present in this screen, the grating choice and slit width settings used in the original acquisition can also be recalled and set.

The Routine panel is used to recall or create new acquisition routines. The choice box will display "Routine Note Saved!!!" if the current conditions have not been recalled from a stored routine file. The most recently used stored routines are shown as choices in the panel. If the desired routine is not displayed here, clicking on the Change button will allow you to browse through your directories and recall the desired routine.

The Save button is used to store the currently displayed acquisition parameters and hardware status such as grating used and slit widths in a new routine file. The Save As button is used if you have recalled a routine, modified it and wish to save the original routine and the modified routine. The View button will open a window that shows all of the instrumental parameter settings used when the routine was stored.

You may wish to reproduce the acquisition parameters defined in a routine but not necessarily all of the instrumental parameters. If you do not care if the area map is identical to the one stored with the routine you can uncheck Load Map File. If the area map settings are critical, check the box to ensure that the same area map is loaded before the acquisition starts.

Hardware parameters that can be matched or ignored include the grating choice and slit width settings. If the Match Hardware box is checked, any differences between the current setting and stored settings will be noted in a pop up dialog box.



The User field is used to store the name of the person who acquired the spectra in the file information header. The comments field is used to store comments or other experimental conditions in the data file.

Enter the file name you wish to use to store your spectra in this field. Click on the Change button to bring up the store dialog box.

Check on the Display while acquiring data button to see the acquisition in real time on the Live Data screen. If the acquisition time is very short and the delay between reads is also very short, the data may not be displayed in real time so as to not affect the timing of the experiment.

Click on the Acquire button to start the acquisition. If you have not specified a file name, a dialog box will appear asking if you wish to continue or enter a name. You may stop an acquisition at any time by clicking on the Cancel button.

Menu

File

Exit

Select Tab

Hardware Config	Calls up the Hardware Configuration screen
Hardware Status	Calls up the Hardware Status screen
Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen
Live Data	Calls up the live data screen
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

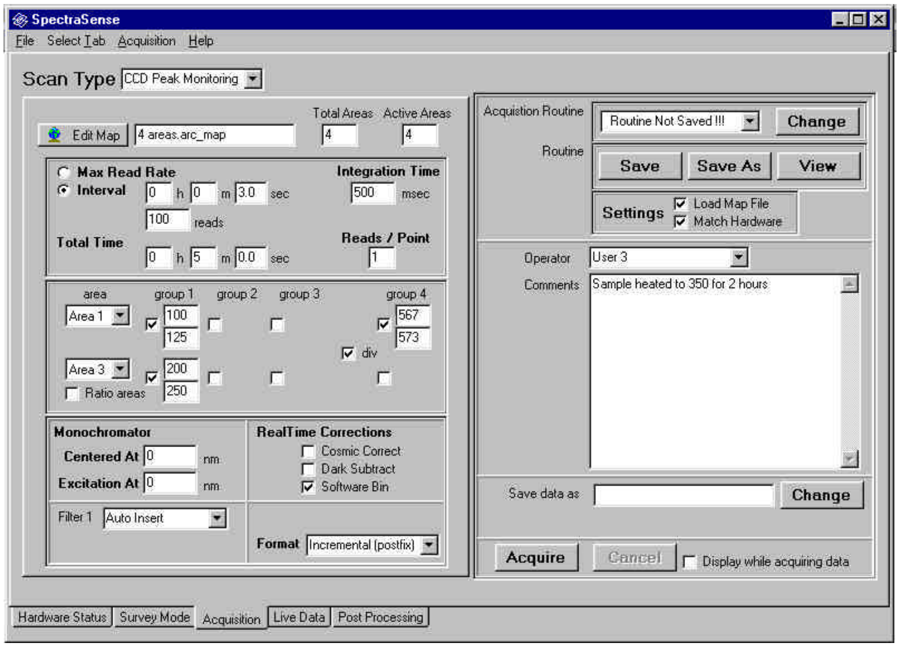
Acquisition Parameters

Default path	This is the directory path that the software will use to find and store routines and data

Default routine	You can specify a default routine which will be loaded each time the SpectraSense is run
Default user	The operator's name that will be stored with the data unless specifically changed

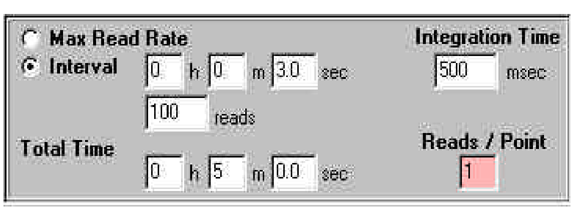
Help

CCD Peak Monitoring Acquisition



The CCD Peak Monitoring Acquisition is used to monitor and compare peaks within a spectrum or spectra as a function of time. Typical applications include monitoring the relative intensity of one peak in a spectrum compared to another where the peaks are signatures of a chemical or physical change in the analyte. The program also allows the comparison of peaks within one sample and a reference, if the spectra from each can be separated by collecting data from different areas on the CCD chip. The data displayed is either the integrated intensity under a peak versus time, or the ratio of two integrated peak areas versus time.

This mode of operation requires that the x-axis of the spectra being analyzed or compared be in pixel units. It is therefore necessary to first acquire the spectra in pixel units in the Survey screen. This is accomplished by selecting the display in pixels option in the display tab. The starting pixel number and ending pixel number for each peak must be selected and noted.

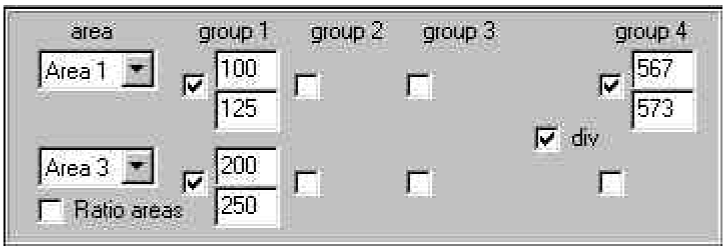


The Integration and timing panel is used to define the integration time for each data point and the time between measurements. The integration time initially displayed in the field is the current value in the Survey screen. This value can be changed by entering a new value manually or by recalling a routine that has a different integration time.

You have the option of collecting data points as fast as possible by clicking on the Max Read Rate button. In this case there will be no delay between the termination of one acquisition and the start of the next. There is however, a mechanical lower limit to this if the shutter is employed. That limit is approximately 100ms. Shorter times may result in variable integration times. Enter the total measurement time in hours, minutes, and seconds fields. The exact number of reads per second depends on factors such as the height and number of areas defined on the chip.

If you wish to take data points at specific time intervals you must click on the Interval button. In a slow decay experiment, the integration time needed for good signal to noise may be 500ms but the time between data points can be much longer, such as the 3 seconds in the illustration above. The 3 second interval includes the 500ms integration time. In this case the shutter will open for 500ms and there will be a delay of 2.5 seconds before it is opened again for the next data point. Enter the total measurement time in the hours, minutes, and seconds, fields. The reads field will update according to the total time.

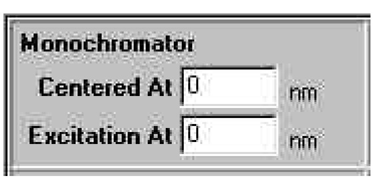
The number of reads per data point field is used to coadd multiple reads within an interval. Generally speaking, one read per data point is preferred. Only in cases where there may be short term variability in the signal or when the integration time is so long that the probability of cosmic ray induced peaks is high, should values greater than 1 be used.



The program allows simultaneous monitoring of up to four peaks in any one spectrum and up to two areas. If up to 8 peaks are to be monitored it may be possible to create two areas that receive the same signal and define four peaks on one to be monitored and four different ones on the second area. The integrated area under a peak is defined as a **group** of pixels, to avoid confusion with areas on the CCD chip. Using the pixel spaced spectrum collected in the Survey screen, note the starting pixel and ending pixel for each group (peak) you wish to monitor. If spectra are to be taken on more than one area, click on the area choice box arrow to select which area you wish to monitor. The positions of the groups on a spectrum do not have to be in ascending pixel order, i.e. group (peak) 2 may be between pixels 200 and 220 while group 4 may be between pixels 150 and 170. Click on the check box to access the starting and ending input fields for each peak to be monitored.

By definition if peaks are to be ratioed within one spectrum (area) the divisor must be group 4. Clicking on the div check box will cause all of the defined peaks in that area to be divided by the peak defined as group 4.

In the case where spectra are being acquired in multiple areas it is possible to get the peak intensity ratio between peaks in two areas. Define the groups (peaks) in each area such that the peaks to be ratioed have the same group number. Click on the Ratio areas box to have the ratio of the integrated peak intensity between the top specified area and the same defined group number in the bottom specified area. In the example above a peak defined by group 1 in area 1 on the chip is divided by the area of another peak in the same area (spectrum) defined as group 4. Additionally another peak in area 3 of the chip is also being monitored.



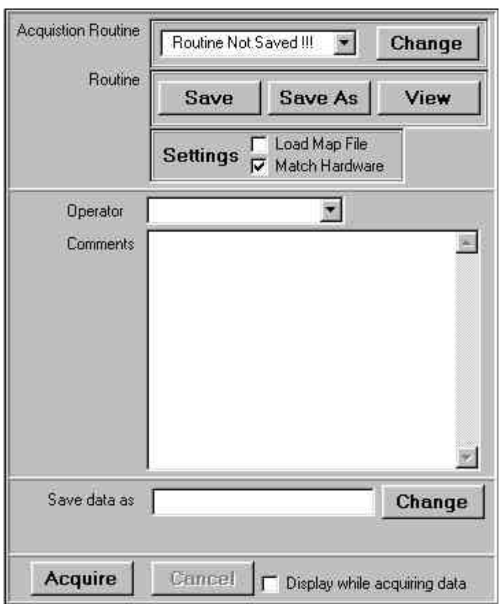
The monochromator position panel will show the current positions of the monochromators in the system. The positions used in the Survey screen to acquire a spectrum there are automatically transferred here. You may change the positions by manually entering new values. If a routine is recalled, the positions will change to those stored in the routine.

The options selected in the Survey screen are automatically updated in the Acquisition screen. These can be changed by clicking on the check box to activate or deactivate the option. Recalled routines will also reset these parameters to those stored.

If a filter wheel is present in the system optical path, the filter panel will appear. The current state of the filter wheel is displayed in the choice field. Clicking on the arrow will present all of the installed filters and allow you to select which one to use in this acquisition.

The Format panel allows you to specify whether files from the same acquisition program are specified with a numerical prefix or suffix. Example: 02myfile.dat or myfile02.dat.

The area map information panel shows at a glance the total number of areas currently defined on the chip. It is possible to change the size and number of areas by clicking on the Edit Map button. The area map creation panel will appear allowing you to either load previously stored area maps, modify the current area map, or change which areas in the current map are read out or ignored. Refer to the CCD Survey Screen chapter for more information on this subject.



The Acquisition panel is used to save all of the parameters entered in the Acquisition panel into a file that can be recalled at any time to collect spectra under identical instrumental conditions. Routines can also be recalled in this panel which will over ride the current hardware and operating parameters to those defined in the stored routine file. Although they are not present in this screen, the grating choice and slit width settings used in the original acquisition can also be recalled and set.

The Routine panel is used to recall or create new acquisition routines. The choice box will display "Routine Note Saved!!!" if the current conditions have not been recalled from a stored routine file. The most recently used stored routines are shown as choices in the panel. If the desired routine is not displayed here, clicking on the Change button will allow you to browse through your directories and recall the desired routine.

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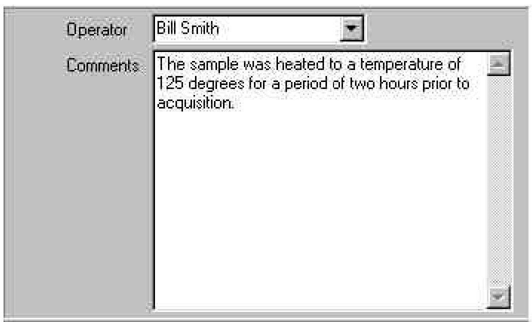

The User field is used to store the name of the person who acquired the spectra in the spectrum's information header. The comments field is used to store comments or other experimental conditions in the data file.

Enter the file name you wish to use to store your spectra in this field. Click on the Change button to bring up the store dialog box.

Check on the Display while acquiring data button to see the acquisition in real time on the Live Data screen. If the acquisition time is very short and the delay between reads is also very short, the data may not be displayed in real time so as to not affect the timing of the experiment.

Click on the Acquire button to start the acquisition. If you have not specified a file name, a dialog box will appear asking if you wish to continue or enter a name. You may stop an acquisition at any time by clicking on the Cancel button.

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Help

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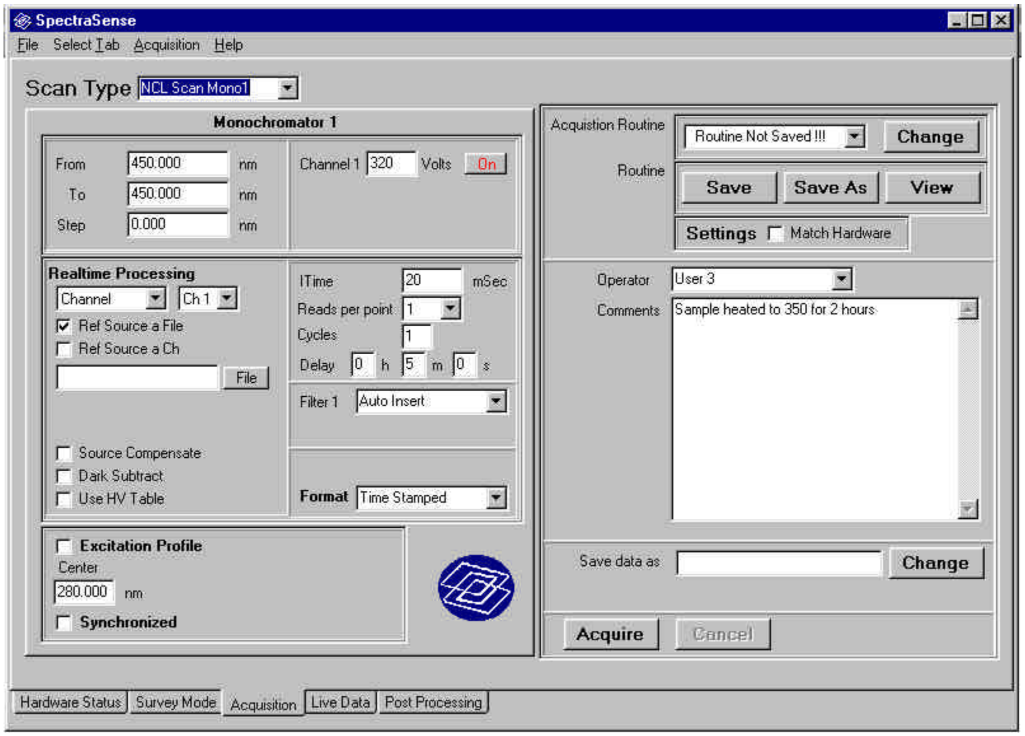
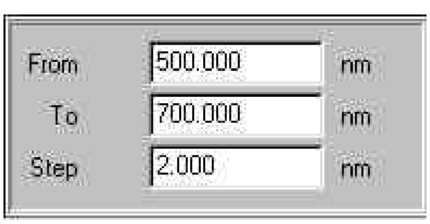
Chapter 7: Scanning Spectral Acquisition



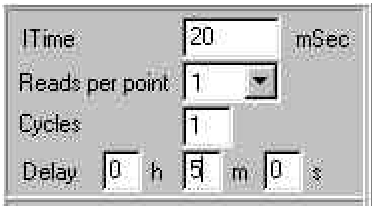
The Scanning Acquisition screen is used for collecting spectra from single channel detectors such as photomultiplier tubes, silicon cells, and most solid state infrared detectors. In the normal progression in setting up and acquiring good spectra, the Scanning Acquisition screen is usually employed after the parameters that affect spectral quality are optimized in the Survey Mode screen. For the most part, all of the previously adjusted parameters are automatically transferred over to this screen. It is from this screen that single spectral experiments as well as those requiring multiple spectral acquisitions can be defined and run.

If there are two monochromators in your system there will be two NCL scan choices, one for Mono 1 and one for Mono2. This allows you to set up two discretely different experiments.

The Scanning Acquisition screen is also used to create and recall experimental routines. A routine contains all of the acquisition parameters and hardware settings to exactly reproduce spectral acquisition conditions. Creating routines for often repeated experimental procedures ensures that all spectrometric conditions will be identical and that all of the information on the system parameters is safely stored within the data file.



The scanning parameters specify the spectral range to be covered and the increment between data points. When you open this screen the last values used in the Survey mode are loaded into the fields. You have the option of changing any or all of the parameters by highlighting and a field and entering new values. If you recall a routine, these values will be changed to those stored in the routine. As a rule of thumb, if you know the spectral resolution of the narrowest peak you will be measuring, set the Step to approximately 1/5 that value. For example, if the narrowest peak you expect to see in your spectrum is 10nm wide at half maximum intensity, set the step to 2nm. Fewer steps may cause loss of resolution and data while very much smaller steps will, for the most part, only make the acquisition time longer and the data file larger.

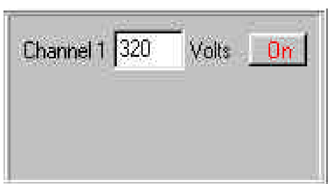


The integration time used to optimize your signal to noise ratio in the Survey screen is automatically transferred to the I Time field. You can if you wish change the integration time by highlighting the field and entering a new value.

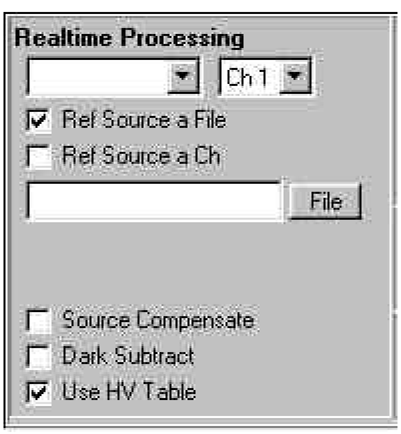
The Reads per point field indicates how many times the detector will be read out at each new position. The choices are 1, 3, and 10 where the multiple readings are averaged. For most applications it is advisable to set the integration time and slit widths wide enough so that there is good signal to noise on a single read out of the detector. Multiple read outs may be necessary under conditions where the signal is so weak that it is just distinguishable from the noise.

The Cycles field is used to indicate how many times spectral are to be collected during the experiment. Each spectrum can be saved individually or all of the cycles signal averaged together to create one file.

Enter the delay in hour, minutes, and seconds between cycles (spectra). The delay must be longer than the time to acquire one spectrum and slew back to the starting wavelength. The time to acquire a spectrum and return to the starting wavelength depends not only upon the integration time and number of increments, but also the time to move between data points and the time to slew back. These parameters change under different acquisition conditions and can not be defacto calculated. It is advisable to take a single scan and measure the time it takes to acquire. The time to slew back is normally 10 seconds or less. The combination of these represents the minimum allowable delay between cycles.



The High Voltage panel will appear if there are photomultiplier tubes in your system. The current value is that last used in the Survey mode. You may change the high voltage by highlighting the field and entering a new value. A set button will appear to validate the change. If a stored routine is loaded, the high voltage will be changed to the value stored in the routine. You can turn the high voltage on or off by clicking on the On/Off button.



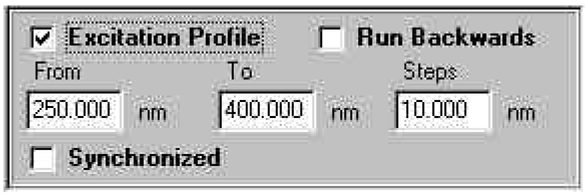
The Real Time Processing panel will normally have values in all of the fields and appropriate check boxes checked. These values are carried over from the Survey Screen or reloaded from a stored routine. You can however change any of the values or check box options.

The Real time Processing panel is used to define which detectors are to be read out for display and how the incoming data is to be processed before it is displayed. The top left choice field contains all of the display options available, which will vary depending on your system configuration. The typical choices are: Channel #, Chan #/reference, Channel #/ Channel #, Channel #/file, Absorbance, %Transmission, %Reflectance and all channels. The channel number is chosen from the choice field to the right. There must be a reference for the absorbance, transmission, and reflectance measurements. This reference can be either a stored file, or the output from another detector channel. The Ref source a File check box is used if a stored data file will be used as the reference for the absorbance, transmission, and reflectance output. The ref Source a Ch check box is used if a detector is used as the reference.

The Source Compensate check box is used if a source compensation accessory is included in the system and you wish to divide each data point by the signal from this accessory.

The Dark Subtract check box is used if you wish to take a reading of the detector when there is no light hitting it. All detectors produce a signal output that is temperature dependent. This signal can be subtracted from all readings when the detector is making a measurement. The software will close any automated shutter and take an initial reading or, if the 6th position on the filter wheel has been specified for dark subtraction, the wheel will move to this position and take a reading and then return to the appropriate position for the scan. If your system has neither a shutter of filter wheel, you will be requested to block the light from entering the monochromator by any means of your choice, the dark reading will be taken and you will asked to unblock the light before the actual scan is taken.

The use HV Table check box is used to automatically adjust the high voltage on the photomultiplier tube as the monochromator is scanned. In order to use this option a HV table must be created.



The Excitation Profile panel will appear if there are two monochromators in the system. The purpose of this panel is to allow a series of fluorescence emission spectra to be taken at different excitation wavelengths. For each excitation wavelength there will be an emission spectrum taken with the parameters defined in the panels above. The data is usually displayed as a 3D surface plot. Specify the shortest excitation wavelength desired in the From field. Specify the longest excitation wavelength in the To field. Specify excitation wavelength step increment in the Steps field. Check the Run Backwards box, if your sample is subject to photodegradation at short wavelengths.

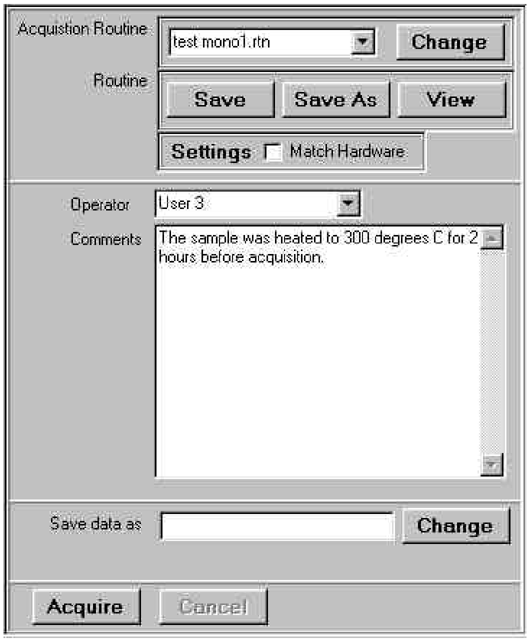
If the Synchronized option is checked the excitation monochromator will move one step increment in lockstep with the emission monochromator. You specify the starting wavelength in the From field and the step increment in the Steps field. The number of steps taken will be the same number of steps taken by the emission monochromator.

If neither the Excitation Profile nor Synchronized boxes are checked, the monochromator will move to the specified wavelength and stay there through all of the spectral acquisitions specified in the panels above.

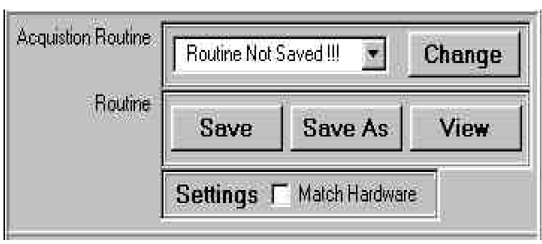
The filter wheel panel appears if there is a filter in your system. The filter number or auto insertion option will appear in the choice field. You may change the filter by clicking on the arrow and highlighting the desired filter.

The format panel is used to define the nomenclature for the storage of the spectra. The choices are: Incremental prefix, Incremental postfix, Averaged cycles, and Time stamped. If in your experiment you are collecting multiple spectra you have the option of storing each spectrum individually or signal averaging them into one data file. Assuming a filename of "my spectrum" the prefix option will save the spectra as **01my spectrum.arc_data** to **##my spectrum.arc_data**. The post fix option will store the spectra as **my spectrum01.arc_data** to **my**

spectrum##.arc_data. The average data option will produce one data file named **my spectrum._arc.data**. The time stamp option will name each spectrum as **my spectrum_date_time.arc_data.**



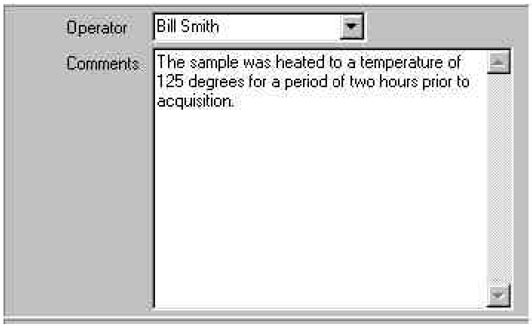
The Acquisition panel is used to save all of the parameters entered in the Acquisition panel into a file that can be recalled at any time to collect spectra under identical instrumental conditions. Routines can also be recalled in this panel. The parameters in the stored routine will overwrite the current hardware and operating parameters to those defined in the stored routine file. Although they are not present in this screen, the grating choice and slit width settings used in the original acquisition can also be recalled and set.



The Routine panel is used to recall or create new acquisition routines. The choice box will display “Routine Note Saved!!!” if the current conditions have not been recalled from a stored routine file. The most recently used stored routines are shown as choices in the choice field. If the desired routine is not displayed here, clicking on the Change button will allow you to browse through your directories and recall the desired routine.

The Save button is used to store the currently displayed acquisition parameters and hardware status such as grating used and slit widths in a new routine file. The Save As button is used if you have recalled a routine, modified it and wish to save the original routine and the modified routine. The View button will open a window that shows all of the instrumental parameter settings used when the routine was stored.

You may wish to reproduce the acquisition parameters defined in a routine but not necessarily all of the instrumental parameters. Hardware parameters that can be matched or ignored include the grating choice and slit width settings. If the Match Hardware box is checked, any differences between the current setting and stored settings will be noted in a pop up dialog box.



The User field is used to store the name of the person who acquired the spectra in the spectrum's information header. The comments field is used to store comments or other experimental conditions in the data file.

Enter the file name you wish to use to store your spectra in this field. Click on the Change button to bring up the store dialog box.

Click on the Acquire button to start the acquisition. If you have not specified a file name, a dialog box will appear asking if you wish to continue or enter a name. You may stop an acquisition at any time by clicking on the Cancel button.

Menu

File

Exit

Select Tab

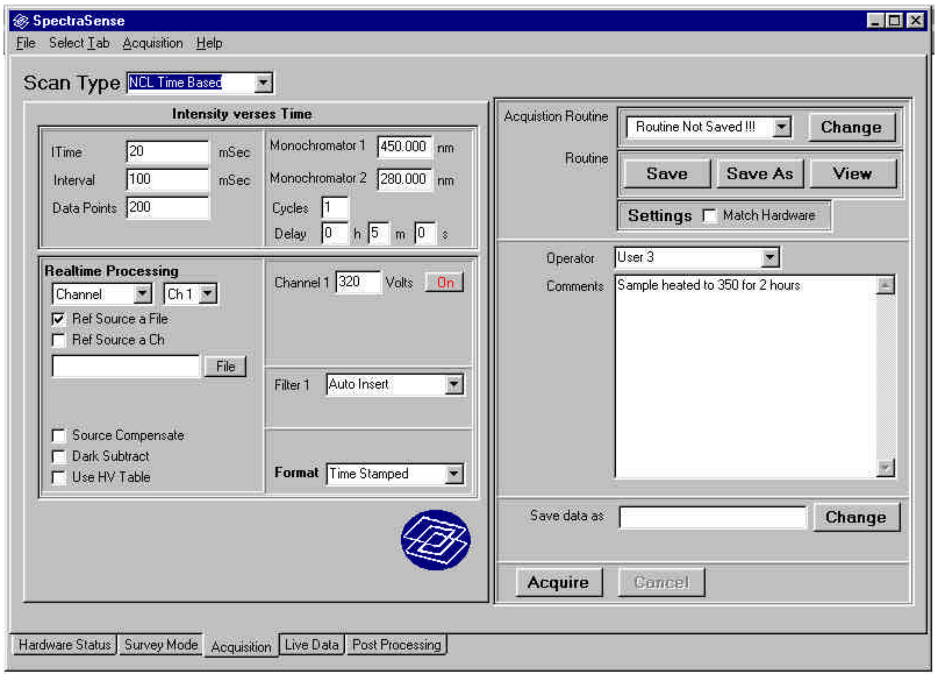
Hardware Config	Calls up the Hardware Configuration screen
Hardware Status	Calls up the Hardware Status screen
Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen
Live Data	Calls up the live data screen
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

Acquisition Parameters

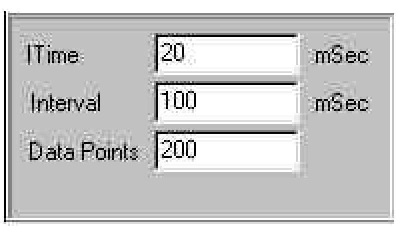
Default path	This is the directory path that the software will use to find and store routines and data
Default routine	You can specify a default routine which will be loaded each time the SpectraSense is run
Default user	The operator's name that will be stored with the data unless specifically changed

Help

Chapter 8: Scanning Time Based Acquisition



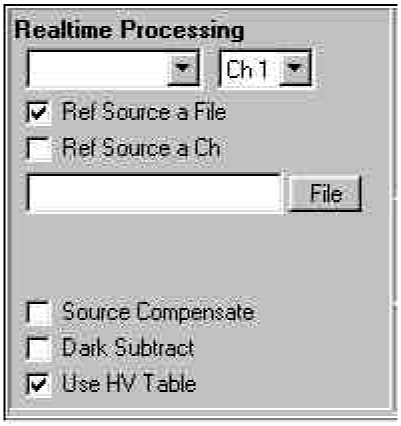
The Scanning Time Based acquisition mode is used to monitor the intensity at a specific wavelength as it changes over time. The spectra created are in intensity versus time units. This mode is valid for measuring intensity changes in intervals as short as 5 milliseconds up to hours.



The time panel is where the signal integration time, interval between measurements, and number of data points are specified. The only parameter passed from the Survey screen is the integration time. You may change this by highlighting the value in the field and enter a new one. The interval is the time between measurements. The interval must be equal to or larger than the integration time and includes the integration time. The Data Points field is used for specifying how many data point are to be taken in the spectrum. If you know how long you wish to make the measurements, divide that time by the interval and enter the value in the Data Points field.

In the wavelength panel you specify the wavelength at which the measurement will be made. If your system includes two monochromators two position fields will appear.

If you wish to make the measurement more than one time, you can specify a number of cycles, where each cycle produces another time base spectrum. You can specify a delay between cycles by entering values in the hours, minutes, and seconds fields.



The Real Time Processing panel will normally have values in all of the fields and appropriate check boxes checked. These values are carried over from the Survey Screen or reloaded from a stored routine. You can however change any of the values or check box options.

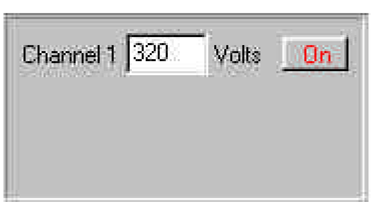
The Real time Processing panel is used to define which detectors are to be read out for display and how the incoming data is to be processed before it is displayed. The top left choice field contains all of the display options available, which will vary depending on your system configuration. The typical choices are: Channel #, Chan #/reference, Channel #/ Channel #, Channel #/file, Absorbance, %Transmission, %Reflectance and all channels. The channel number is chosen from the choice field to the right. There must be a reference specified for the absorbance, transmission, and reflectance measurements. This reference can be either a stored file, or the output from another detector. The reference file must be an intensity versus wavelength spectrum. The intensity at the wavelength specified above will be used as the reference value.

The Ref source a File check box is used if a stored data file will be used as the reference for the absorbance, transmission, and reflectance output. The ref Source a Ch check box is used if a detector is used as the reference.

The Source Compensate check box is used if a source compensation accessory is included in the system and you wish to divide each data point by the signal from this accessory.

The Dark Subtract check box is used if you wish to take a reading of the detector when there is no light hitting it. All detectors produce a signal output that is temperature dependent. This signal can be subtracted from all readings when the detector is making a measurement. The software will close any automated shutter and take an initial reading or, if the 6th position on the filter wheel has been specified for dark subtraction, the wheel will move to this position and take a reading and then return to the appropriate position for the measurement. If your system has neither a shutter of filter wheel, you will be requested to block the light from entering the monochromator by any means of your choice, the dark reading will be taken and you will asked to unblock the light before the actual scan is taken.

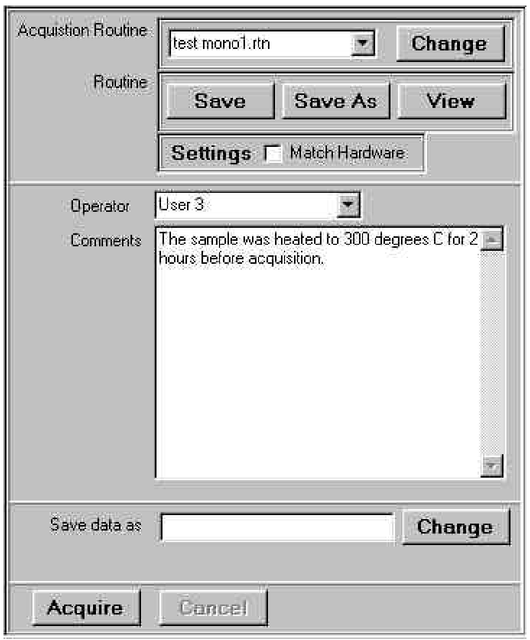
The use HV Table check box is used to automatically adjust the high voltage on the photomultiplier tube as the monochromator is scanned. In order to use this option a HV table must be created.



The High Voltage panel will appear if there are photomultiplier tubes in your system. The current value is what was last used in the Survey mode. You may change the high voltage by highlighting the field and entering a new value. A set button will appear to validate the change. If a stored routine is loaded the high voltage will be changed to the value stored in the routine. You can turn the high voltage on or off by clicking on the On/Off button.

The filter wheel panel appears if there is a filter in your system. The filter number or auto insertion option will appear in the choice field. You may change the filter by clicking on the arrow and highlighting the desired filter.

The format panel is used to define the nomenclature structure for the storage of the spectra. The choices are: Incremental prefix, Incremental postfix, Average cycles, and Time stamped. If in your experiment you are collecting multiple spectra you have the option of storing each spectrum individually or signal averaging them into one data file. Assuming a filename of "my spectrum" the prefix option will save the spectra as **01my spectrum.arc_data** to **##my spectrum.arc_data**. The post fix option will store the spectra as **my spectrum01.arc_data** to **my spectrum##.arc_data**. The average data option will produce one data file named **my spectrum._arc.data**. The time stamp option will name each spectrum as **my spectrum_date_time.arc_data.**

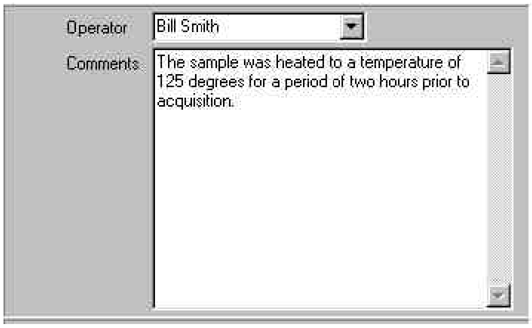


The Acquisition panel is used to save all of the parameters entered in the Acquisition panel into a file that can be recalled at any time to collect spectra under identical instrumental conditions. Routines can also be recalled in this panel. The parameters in the stored routine will overwrite the current hardware and operating parameters to those defined in the stored routine file. Although they are not present in this screen, the grating choice and slit width settings used in the original acquisition can also be recalled and set.

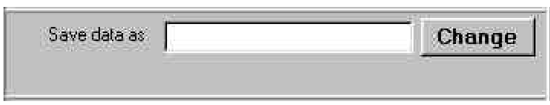
The Routine panel is used to recall or create new acquisition routines. The choice box will display "Routine Note Saved!!!" if the current conditions have not been recalled from a stored routine file. The most recently used stored routines are shown as choices in the choice field. If the desired routine is not displayed here, clicking on the Change button will allow you to browse through your directories and find the desired routine.

The Save button is used to store the currently displayed acquisition parameters and hardware status such as grating used and slit widths in a new routine file. The Save As button is used if you have recalled a routine, modified it and wish to save the original routine and the modified routine. The View button will open a window that shows all of the instrumental parameter settings used when the routine was stored.

You may wish to reproduce the acquisition parameters defined in a routine but not necessarily all of the instrumental parameters. Hardware parameters that can be matched or ignored include the grating choice and slit width settings. If the Match Hardware box is checked, any differences between the current setting and stored settings will be noted in a pop up dialog box.



The User field is used to store the name of the person who acquired the spectra in the spectrum's information header. The comments field is used to store comments or other experimental conditions in the data file.



Enter the file name you wish to use to store your spectra in this field. Click on the Change button to bring up the store dialog box.

Click on the Acquire button to start the acquisition. If you have not specified a file name, a dialog box will appear asking if you wish to continue or enter a name. You may stop an acquisition at any time by clicking on the Cancel button.

Menu

File

Exit

Select Tab

Hardware Config	Calls up the Hardware Configuration screen
Hardware Status	Calls up the Hardware Status screen
Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen
Live Data	Calls up the live data screen

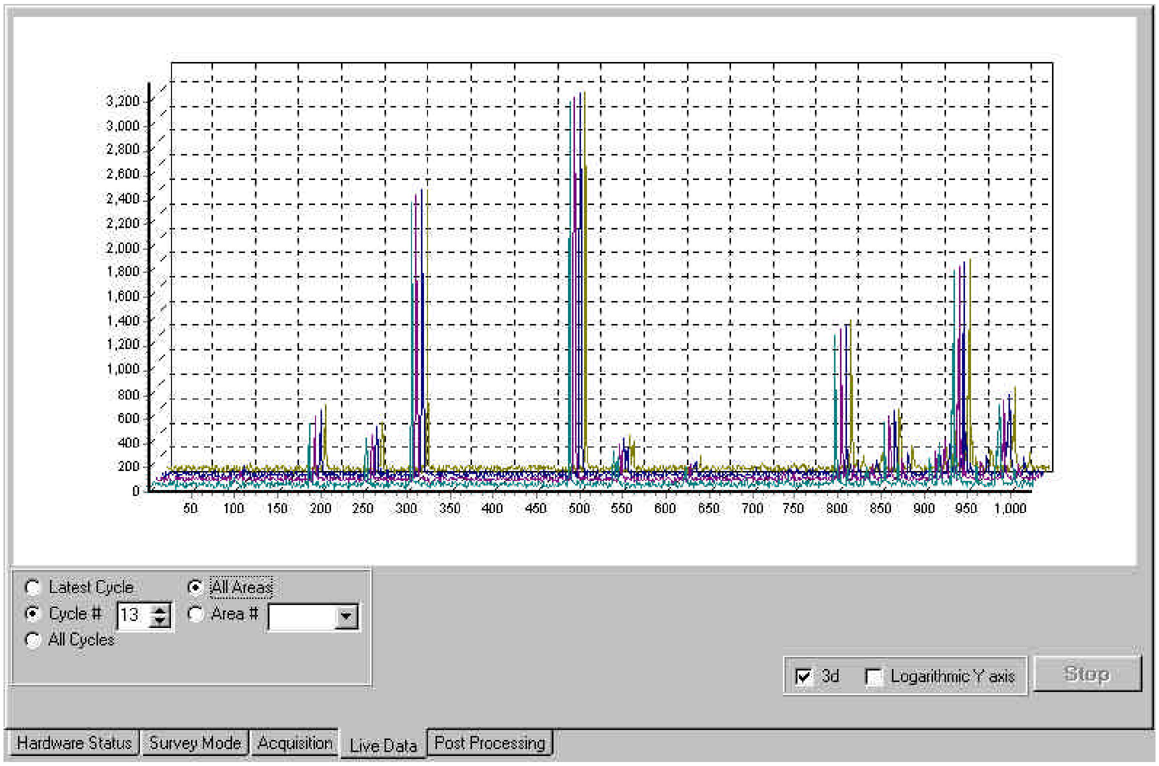
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

Acquisition Parameters

Default path	This is the directory path that the software will use to find and store routines and data
Default routine	You can specify a default routine which will be loaded each time the SpectraSense is run
Default user	The operator's name that will be stored with the data unless specifically changed

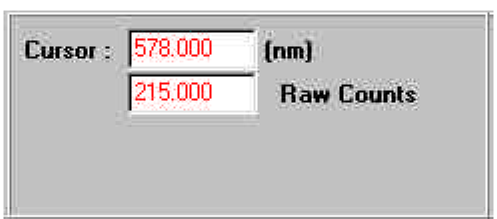
Help

Chapter 9: Live Data Screen

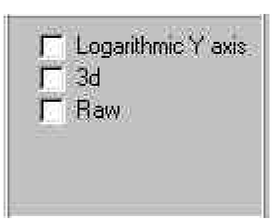


The live data screen is used to view spectral data as it is being acquired. The screen will update in near real time in all cases except for high speed CCD spectral acquisition.

Scanning Mode Display Options



The cursor panel will display the current position and intensity values for all active detectors.



The display options include:

Logarithmic Y axis scaling

3D display of multiple cycles in a multicycle acquisition

Raw. The specified real time display may be the resultant of channel1/channel2 or a channel divided by a stored data file. When this box is checked, the raw intensity values for all detectors in use will be displayed. This option is generally used for debugging unexpected results by verifying that all the detectors are functioning and are in the light path.

CCD Mode Display Options

When acquiring spectra it is possible to display the data in different ways. If there were multiple cycles specified in the acquisition it is possible to view at any time, the latest cycle (spectrum) acquired, or the Nth previous cycle (spectrum) individually or all of the currently acquired cycles.

It is also possible, if multiple areas of the chip were read out, to view the spectra from a specific area by selecting it from the Area # choice box or to view all of the areas' spectra simultaneously.

The data can be presented on a logarithmic scale for data with a very wide dynamic range or on a linear scale. If the 3D box is checked multiple spectra will be displaced that the latest collect spectrum appears in front of the previous ones. If the 3D box is not checked, the spectra will be overlaid.

In the CCD peak monitoring mode it is possible to look at the data for an individual peak (pixel group) or all of the groups simultaneously.

It is possible to acquire data from two areas in the CCD peak monitoring mode. You may see the data from only one area at a time or both areas simultaneously.

The stop button will stop an acquisition in progress. All valid data collected up until the button was clicked on will be saved in the data file.

Menu

File

Exit

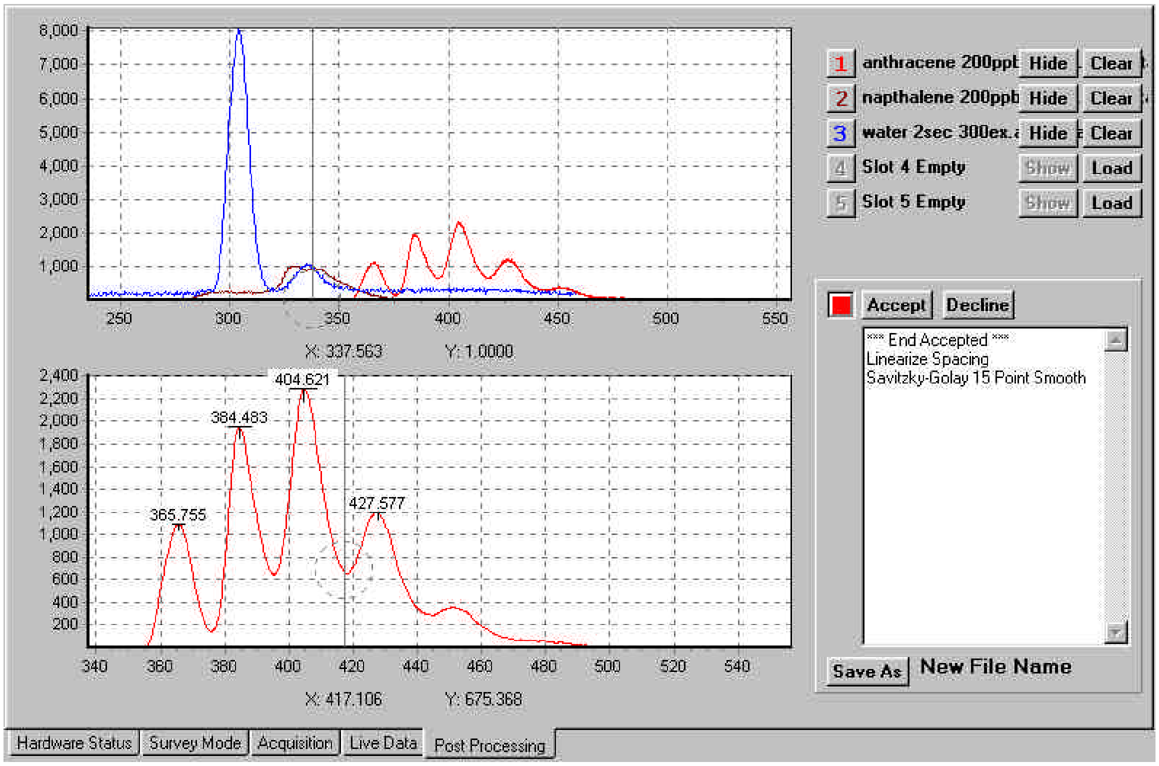
Select Tab

Hardware Config	Calls up the Hardware Configuration screen
Hardware Status	Calls up the Hardware Status screen
Survey	Calls up the Survey screen
Acquisition	Calls up the Acquisition screen

Live Data	Calls up the live data screen
Post Processing	Calls up the Post Processing screen
Terminal	Used for diagnostics in communications between the hardware and computer

Help

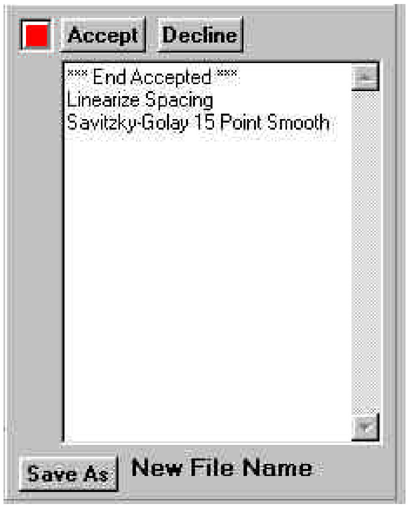
Chapter 10: Post Processing Screen



The Post Processing screen is used for evaluation and treatment of your spectral files. Up to five files may be viewed simultaneously. The Post Processing screen has a full compliment of classically used mathematical manipulations employed in spectral analysis.

The Post Processing screen has two display windows. The top window shows the unaltered spectra. The bottom shows the resultant spectrum after it has been operated on. The spectra in each window can be independently expanded or contracted. A cursor in each window displays the position and intensity information at its location.

Up to five spectra can be loaded for display in the top window. Once loaded, a spectrum can be shown or hidden from view by clicking on the Show/Hide button. A spectrum can be cleared or loaded by clicking on the Load/Clear button. The numbered buttons to the left of the spectrum's name are used to select which spectrum the cursor will track and the spectrum to be manipulated. The chosen spectrum is also displayed in the bottom window.



The manipulations log panel keeps track of every operation performed on the spectrum. Each operation or series of operations can be accepted or declined by clicking on the appropriate button. If you wish to save the treated spectrum, click on the Save As button. The save file as dialog box will appear. All of the operations performed on the spectrum and the date they were performed are saved in the new data file's header.

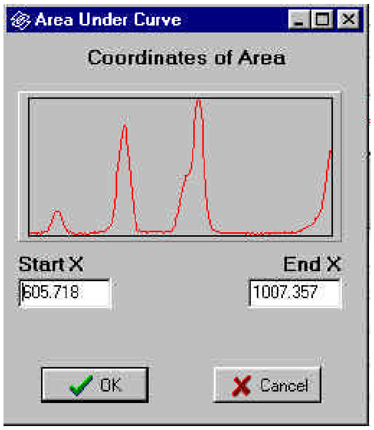
Mathematical Operations

Scalar Operations

Scalar	Data + - * / k , k-data, k/Data
Log	
Ln	
Antilog	Antilog e, Antilog 10

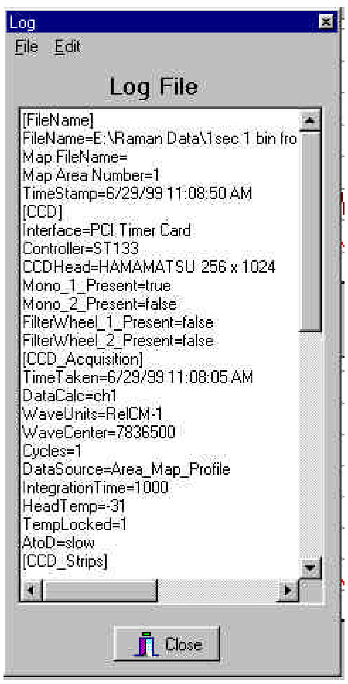
File Operations

Math	addition, subtraction, division, multiplication with another file
Smooth	Savitzky-Golay 5, 9, 15, points
Derivative	First, Second
Area	Finds the area under a peak
Peak Find	Finds the highest peak in the spectrum gives coordinates and half width.
Truncate	Discards data points from ends of spectra.
Join	Attaches another spectrum to the end of the selected spectrum
X shift	Changes the wavelength calibration of the spectrum by shifting the x-axis coordinates by the shift value.
Linearize	Specific to CCD spectra. Extrapolates the data such that the data point spacing is in equal wavelength units.
Change Units	Converts calibration between all supported working units in the software; nm, A, microns, eV, absolute and relative wavenumbers.



A dialog box similar to the Coordinates of Area to the left, appears when, area, and truncate are selected from to File Operations Menu. In each case you can expand the spectrum so that the desired limits fill the display. The Start X and End X fields will update and the operation will take place over the range specified in the fields. You may also enter specific values into the fields if you know exactly the limits you wish to include in the operation.

History



Show Pair List — Opens a dialog box with the X Y coordinates of the data. The data may be printed out or copies to the clipboard.

Show Peak List — Show all found peaks at the specified discrimination level. The data may be printed out

Discrimination — Used to define peaks to be labeled. Enter a value between 1 and 100 percent of full scale. All peaks with heights above that level will be marked.

Show/Hide Peaks — Labels or clears peak position labels on the lower display screen.

Show Log File — Opens a dialog box with all of the stored hardware, acquisition, and data treatment parameters.

Recalculate Components — If a spectrum is acquired where there are two detectors used in the acquisition such as CH1/CH2, the raw data from each of the detectors is also stored in the file. Although only the resultant spectrum is normally displayed, the raw data is always available for diagnostic and reconstructive purposes. The Recalculate Components option allows to perform mathematical procedures on the individual components and to reconstitute the derived spectrum from the raw data.

Show/Hide Components — Allows you to switch between seeing the spectrum as defined in the real time processing or to see the raw input from each of the detectors.

The Log File contains all of the information on how and when the data file was acquired. This information can be printed out from the File menu. The log file can be saved as an individual file without the data by selecting Save from the File menu. Data can be cut and pasted from the Edit menu level. There is no way to modify the information directly within SpectraSense. If you wish to do so, you may open the data file in a text editing or word processing software package.

Menu

File

- Load — Loads a data file into a slot
- Save As — Saves a data file under a new name
- Wave Calculator — Spectral units converter
- Wavenumber Calculator — Calculates spectral positions for relative wavenumber units
- Clear — Clears a data slot
- Delete — Deletes a data file
- Print
    - Spectrum
    - Screen
    - History
    - Data list
    - Peak list

View

- Autoscale
- Full Height
- Full Width
- Fixed Expansion
- Zoom In
- Zoom Out

Select Tab

- Hardware Config — Calls up Hardware Configuration screen
- Hardware Status — Calls up Hardware Status screen
- Survey Mode — Calls up Survey mode
- Acquisition — Calls up Acquisition screen
- Live Data — Calls up Live Data screen
- Post Processing — Calls up Post Processing screen
- Terminal — Calls up terminal mode for communications debugging

Scalar Operations

- Scalar
    - Scalar
        - D-k
        - D+k
        - D/k
        - D*k
        - k-D
        - k/D
    - Log
    - Ln
    - Antilog
        - Base 10
        - Base e

File Operations

Math	addition, subtraction, division, multiplication with another file
Smooth	Savitzky-Golay 5, 9, 15, points
Derivative	First, Second
Area	Finds the area under a peak
Peak Find	Finds the highest peak in the spectrum gives coordinates and half width.
Truncate	Discards data points from ends of spectra.
Join	Attaches another spectrum to the end of the selected spectrum
X shift	Changes the wavelength calibration of the spectrum by shifting the x-axis coordinates by the shift value.
Linearize	Specific to CCD spectra. Extrapolates the data such that the data point spacing is in equal wavelength units.
Change Units	Converts calibration between all supported working units in the software; nm, A, microns, eV, absolute and relative wavenumbers.

History

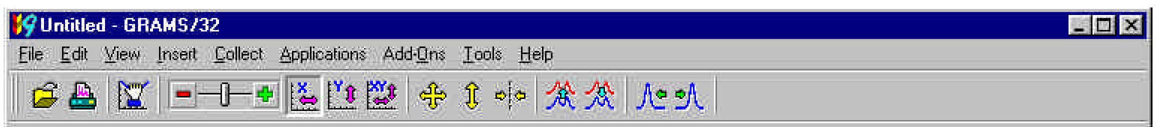
Show Pair List	Shows the X and Y values for each data point in the file
Show Peak List	Show the wavelength and intensity values for each peak found.
Discriminate	Enter the value for percentage of full scale to be used mark peaks
Show/Hide Peaks	Shows or hides the peak labels from on the lower plot.
Show Log File	Show all of the information stored with the data.
Recalculate Components	If a data file was collected as one channel divided by another, the raw data from each channel may be recalled separately and used in subsequent calculations.
Show/Hide Components	Shows the raw data from each channel from a data file created by performing real-time calculations between two channels.

Help

CHAPTER 11: Importing Data into Grams

SpectraSense software can automatically transfer data into Galactic Industries' Grams/5 and all of the related programs such as Grams/3D and PLSplus/IQ. There are two methods of working with Grams. The first method is to run the two programs concurrently and let SpectraSense send the data to Grams via DDE, direct data exchange. This accomplished in the Survey Mode by clicking on the Edit menu level. You will have the option to export the data to Grams or Grams 3D when using a CCD or only Grams when working with a single channel detector.

In the Acquisition screen, if you specify a filename using the SPC format in the Save dialog box, two check boxes will appear. They are Export to Grams and Export to Grams 3D. If one of these boxes is checked, the data will be passed to the program and will appear in the working window. This method has the advantage, when taking long acquisitions, of allowing you to continue to work with previously collected in the Grams window.



The second method of transferring data directly into Grams is to use the Collect option on the menu bar in Grams. When you select Survey Mode or Scan, a window will open with the selected SpectraSense operation. You can then input the parameters necessary for the acquisition and initiate it. When the acquisition is complete you will be returned to the main Grams screen. If you use this method you can not change to another Grams window or work on another data file until the acquisition is completed.

Glossary

Acquisition A spectral acquisition is the displayed or stored results of a single or group of read outs. A spectral acquisition may generate several spectral data files or a multifile with several spectra in it depending on the parameters selected.

Area An area is a user defined portion of the chip from which an image or spectrum will be acquired. Multiple areas can be created on the chip and information from each area can stored as separate data sets as either spectra or images as desired. Areas may not overlap. In spectral mode, the data from each are may be stored as an individual data file or a subfile in a multifile.

Cleaning Cleaning is the continuous read out of the CCD without digitization between acquisitions. This eliminates the accumulation of dark charge in each read out of interest

Cosmic Correction Cosmic rays are always traveling through the atmosphere. When high energy cosmic rays strike the CCD chip they release electrons in a manner similar to photons. The result is spurious peaks. To differentiate between photon induced peaks and comic ray peaks two spectra are taken under the identical conditions. They are compared. If there is a peak in one spectrum and not the other it is assumed to be produced by a cosmic ray and the resultant spectrum which is saved does not show this peak.

Dark subtraction Electrons generated from thermal processes rather than interactions with photons are always present on each read out. The rate at which they are generated is constant for any given temperature. By taking a read out with the shutter closed, and subtracting the data from a read out of the same integration time with the shutter open, you can subtract out the thermionic contributions to the data. In most acquisitions, when dark subtraction is selected, a single readout of the array is made first with the shutter closed

Group A group is a user selected set of contiguous columns in an area in which all the data will be added into one intensity value. A group is only applicable in Peak Monitoring mode and is used in comparing the integrated intensity under one peak with another.

Horizontal binning Horizontal binning is the combining of adjacent columns into one wider column. Horizontal binning is valid in both spectral and image modes. In image mode it reduces horizontal spatial resolution but increases the intensity of each superpixel. In spectral mode horizontal binning will increase the signal to noise ratio by the square root of the binning factor but will reduce the measurable spectral resolution inversely to the binning factor. In low light applications where the spectral features are broad compared to the pixel size, it would be advantageous to employ horizontal binning.

Image An image is a three dimensional data set where each data pint has an intensity value, a horizontal pixel position, and a vertical pixel position. Images are used mainly for diagnostic and set up purposes in SpectraSense CCD software.

Multifile When data is stored in Grams® compatible format, multiple spectral read outs can be stored in a single data file. These read outs may be either the spectra from multiple areas on the chip or spectra taken sequentially with a time delay.

Read out A read out is the result of digitizing the data from the chip. A read out can result in a spectrum, a subset of a spectrum, if a final spectrum is to be made from the addition of several readouts, or an image. It can also produce an image.

Segment A segment is part of a spectral acquisition taken with the range option. Multiple segments are "glued" together to construct a large spectral coverage spectrum.

Software binning Software binning is the coaddition of the intensity values from each row in the selected area of the chip. In this case each row is individually sent through the chip's read out register and digitized rather than filling the readout register with all of the charge from every row in the area before digitizing. It is only applicable in spectral mode. Software binning can prevent saturation of intense spectral features while improving the signal to noise ratio on weaker features. The penalty for using this option is that the time to read out a spectrum is significantly increased. To read out a full 1024 x 256 array using software binning can take about 3 seconds. Without spectral binning it takes milliseconds.

Spectrum A spectrum is a two dimensional data set where each point contains an intensity value and a position value or a time value. The positional value can be stored in terms of dispersed wavelength or horizontal pixel number on the chip.

Vertical binning Vertical binning is the co-addition of adjacent rows into a single value. In image mode it will reduce the vertical spatial resolution of the image with a linear increase in intensity. In spectral mode all of the rows are combined automatically by the hardware in the read out process, therefore vertical binning is valid parameter.

Appendix A

Focussing Your CCD Detector

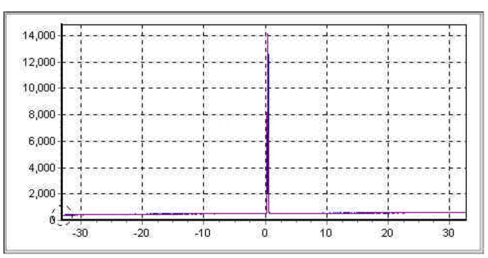
Attach the CCD detector mounting flange to the face of your CCD detector hear. Slide the adapter into the axial exit port of the spectrograph and align the head so that the long axis of the chip is parallel to the table-top. Make all of the connections between the CCD, shutter and computer. Turn on the CCD and the computer. Run SpectraSense and go to the Survey screen. Wait for the CCD to reach operating temperature.

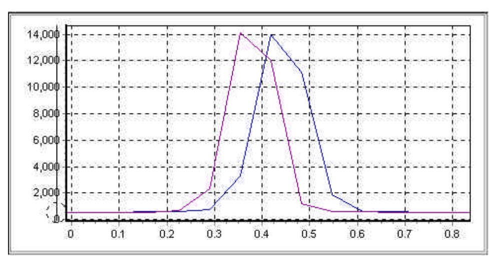
Illuminate the entrance slit of the spectrograph with a Hg pen lamp or light from an overhead fluorescent lamp. Open the entrance slit to approximately 50µ. If your spectrograph has more than one entrance slit, be sure that you are illuminating the slit with the CCD shutter and that the turning mirror is in the correct position. (verify this by looking at the optical path in the Hardware Status screen).

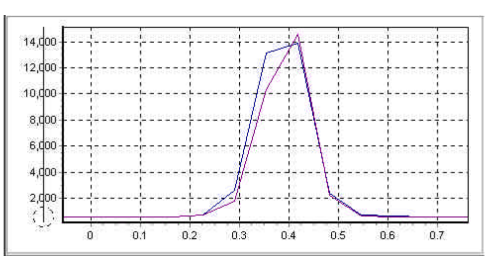
Set the monochromator position to 546nm. Set the integration time to approximately 250 ms. Click on the Spectral/Imaging button so that the display is in spectral mode. Press the GO button. You should see a peak in the center of the display. You may have to adjust the integration time so that it is clearly visible and not over saturated. Click on Stop.

Click on the Area Maps tab. On the Quick Strips panel enter 4 in the field and click on the Create button. This will create 4 equal areas on the chip. Click on the Hide buttons for areas 1 and 4. This will leave you with two areas in the center of the chip.

Click on the Setup tab and then click on GO. Adjust the integration time so that the two 546nm peaks are clearly visible. Expand the display around the peak so that you can easily see how their shapes change. Slide the adapter in and out slowly until the peaks are at their maximum height and minimum width. Next slowly rotate the detector so that the two peaks are superimposed. Once you are satisfied with the adjustment lock the adapter in place using the two locking screws located on the top and side of the spectrograph.







Appendix B

Improving the signal to noise ratio of your CCD spectra

The name of the game in acquiring spectra is to get a good signal to noise ratio (s/n), that is to be able to say with certainty that a feature is a true spectral peak and not just a randomly higher noise spike. There is no fixed value that must be attained in order to say that the spectrum is good or noisy. For strong phenomena it is not uncommon to have a s/n of over 1000. In certain very weak Raman and fluorescence experiments, attaining a s/n of 3 or 5 may be considered to be sufficient.

There are several factors that contribute to the noise component of a spectrum. They include the random component of the dark signal generated in the detector, the random component of the signal being measured, and the random signal added by the electronic circuitry. The random components of the dark signal and analytical signals being measured are the square root of the signals. For a signal of 400 counts the noise would be 20 counts thereby giving a s/n of 20. If a detector has an intrinsic dark signal of 2500 counts/sec and the signal being measured is 30 counts/sec, it would not be possible to detect the analytical signal because, even if we could subtract out the dark signal, its random component would be 50 counts /sec, which is greater than the signal we are trying to measure.

The advantage of using CCD detectors is that the random components due to the dark signal and the readout are so low that for most applications the s/n of the spectrum is only limited by its own random component. When this condition is met the measurement is said to be shot noise limited.

Most scientific CCD detectors are cooled. The colder the CCD chip is the lower the dark signal will be. A general rule of thumb is that for every 7 degrees C that the CCD is cooled, the dark signal halves. With a liquid nitrogen cooled CCD the dark signal can be less than 1 electron/pixel/hour. Typically as there are between 5 to 8 electrons per "count", it would therefore take about 8 hours to produce 1 count with such as detector. Light levels which are much less than 1 photon/sec can be detected with a LN cooled CCD. A typical thermoelectrically cooled CCD produces approximately 5 to 8 electrons/pixel/second, which can be roughly translated to 1count/sec/pixel. The most commonly used CCD chips in spectroscopy are 256 pixels high. If all of the pixels are binned for a data point, there will be 256 dark counts/sec producing a 16 count/sec none subtractable noise component to any measurement.

It should be clear that to improve the s/n the measured signal level must be increased. All other external parameters aside, there are only a few things that you can do to improve the s/n. They are:

1. Increase the integration time. As all of the electrons being released by the experimental signal are being held before read out, the more collected the more counts will be produced. Doubling the integration time will double the number of counts measured for a steady state experiment. By doubling the integration time you are increasing the s/n by the square root of 2 or 1.4. It is noticeable but not dramatic. A s/n gain of 2 is noticeable.

2. Open the entrance slit of the spectrograph to let more light in. Double the width, you double the signal as long as the illumination spot is wider than the slit width. Increasing the slit width has the adverse effect or reducing the spectral resolution. However unless you are looking at very narrow spectral features, you probably can afford to double the slit width without degrading in resolution.

3. You can increase the effective size of your detector. You increase the size of your detector by binning pixels together horizontally. This procedure is very effective for broad band phenomena such as fluorescence and absorption. You can increase the horizontal binning factor to the number of pixels it takes to equal your entrance slit width, without degrading spectral resolution. If your entrance slit is 100 microns and your pixels are 25 microns wide, you can bin four pixels horizontally without changing the spectral resolution and increase your s/n by a factor of 2!

4. You can decrease your effective detector size by reading out as few rows as possible assuming the light from your experiment is focussed down to a spot with a diameter less than the height of the CCD. This is especially important when measuring weak signals through a fiber. If a fiber is 200 microns in diameter and the chip is 256, 25micron pixels high, the dark signal and its inherent noise component from the 248 pixels not being illuminated can visibly degrade the s/n of the spectrum. In this case you would take an image and create an area encompassing only the spectrum from the fiber.

5. In cases where the measurement includes very strong peaks as well as very weak peaks, software binning can be used to increase the dynamic range allowing you to integrate long enough to get a good s/n on the weak peaks without clipping the strong peaks. This is possible because when a spectrum is normally taken, all of the charge from all of the rows in a column is dumped into the read out register of the CCD at one time. It is possible, that perhaps, 50 rows worth of charge might not saturate the read out register but 250 would. By reading each row out individually and coadding the values in software, it is possible to collect the maximum signal for the weak peaks as well for the strong peaks without saturation. The penalty that is paid for this is that the readout noise associated with electronics is added 256 times instead of one. However since the read out noise is very low, it probably will not degrade the s/n too much from the theoretical gain. A second penalty is that it takes much longer to read out a spectrum because all of the pixels must be individually digitized.

6. If you are not resolution limited, you can select a grating with a coarser groove density. This will reduce the dispersion and increase the “number of wavelengths” on each pixel. Changing from a 1200g/mm grating to a 600g/mm grating with the same blaze characteristics will increase the s/n by 1.41 and double the spectral coverage.

The trick is to use any combination of these techniques to get the highest quality spectra in the shortest amount of time possible. You can see the effect each has in real time by using the adjustments in the Survey Mode screen.

APPENDIX C

Trigger order of operation.

Trigger operations for each of the 6 phases of a cycle occur in four phases

Input triggers that need to be reset are reset

1. Output lines for a complementary phase are reset
2. Output lines that need to be set are set
3. Wait for external I/O for the phase

The order in which events occur during a scan

1. Before a routine starts
    1. Clear and setup all input triggers
    2. Set all Output line initial states
        1. High output trigger lines are set low
        2. Low output trigger lines are set high
        3. Rising edge trigger lines are set low
        4. Falling Edge trigger lines are set high
    3. Set all start routine output line trigger states (1 first, 4 last)
    4. Wait for all start routine input line trigger states or abort trigger states (in order 1 first, 4 last)
        1. Check for the start routine trigger (in order 1first, 4 last)
        2. Check for any abort scan triggers (in order 1first, 4 last)
    5. Check for any abort scan input triggers (in order 1first, 4 last)
    6. If Scan Aborted set any Scan abort output lines (in order 1first, 4 last)
2. Before a cycle starts
    1. Set all start cycle output line trigger states (1 first, 4 last)
    2. Clear and set all End Cycle output lines to initial states
        1. High output trigger lines are set low
        2. Low output trigger lines are set high
        3. Rising edge trigger lines are set low
        4. Falling Edge trigger lines are set high

3. Wait for all start cycle input line trigger states or abort trigger states (1 first, 4 last)
    1. Check for the start routine trigger (in order 1 to 4)
    2. Check for any abort scan triggers (in order 1 to 4)
4. Check for any abort scan input triggers (in order 1first, 4 last)
5. If Scan Aborted set any Scan abort output lines (in order 1first, 4 last)

3. Before a point is taken (if GTE, LTE, Input Abort, or wait for trigger are set, otherwise skipped)
    1. Wait for all each point input line trigger states or abort trigger states (1 first, 4 last)
        1. Check for the start routine trigger (in order 1 first, 4 last)
        2. Check for any abort scan triggers (in order 1 first, 4 last)
    2. Check for any abort scan input triggers (in order 1first, 4 last)
    3. If Scan Aborted set any Scan abort output lines (in order 1first, 4 last)
4. After a point is taken (if GTE, LTE, Input Abort, or wait for trigger are set, otherwise skipped)
    1. Clear and setup all each point input trigger lines (1 first, 4 last)
    2. Set all GTE output line trigger states (1 first, 4 last) (set when GTE, cleared when not GTE)
    3. Set all LTE output line trigger states (1 first, 4 last) (set when LTE, cleared when not LTE)
    4. Check for any abort scan input triggers (in order 1first, 4 last)
    5. If Scan Aborted set any Scan abort output lines (in order 1first, 4 last)
5. After a cycle completes
    1. Clear and setup all start cycle input trigger lines (1 first, 4 last)
    2. Reset all start cycle output line trigger states (1 first, 4 last)
    3. Set all cycle complete output line trigger states (1 first, 4 last)
    4. Check for any abort scan input triggers (in order 1first, 4 last)
    5. If Scan Aborted set any Scan abort output lines (in order 1first, 4 last)
6. After a routine completes
    1. Reset all start routine output line trigger states (1 first, 4 last)
    2. Set all routine complete output line trigger states (1 first, 4 last)
    3. Check for any abort scan input triggers (in order 1first, 4 last)
    4. If Scan Aborted set any Scan abort output lines (in order 1first, 4 last)

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