

VM92

Software Manual

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Installation

The operating software is compatible with Windows XP 32-bit systems. Windows Vista and 7 support exist only if the photodiode detector is to be used. Hardware drivers for the currently used CCD do not exist for Windows Vista & 7. 64-bit support can requested for XP, Vista, or 7 for photodiode only, although the 32-bit version is recommended on all 3 operating versions since the software does not utilize any optimizations that 64-bit operating systems can provide. The following procedure will guide the user through the steps necessary to fully install the VM92 Spectrometer application & hardware drivers.

*Note: all support folders & files can be found in the "Support Files" directory on the included installation CD. The main application installer is found in the "VM92 Installer" folder.

- 1. Make sure all hardware (LabJack, CCD, & Stepper electronics box) is disconnected from the computer before attempting to install anything.
- 2. Locate and run the "setup.exe" file in the "VM92 Installer" directory. This will launch the LabVIEW installer which installers the main application and shortcuts to the Start Menu and Desktop. The installer is simple and the user merely needs to choose an install location (default recommended) and follow the on-screen instructions to continue. A reboot of the system is not necessary after this step despite the recommendation to do so.
- 3. If the CCD is to be installed proceed with the next steps, otherwise reboot the computer to finalize the installation. The application may be initialized after the computer boots.
- 4. Locate and run the "setup.exe" file in the "Support Files\Spectronic Drivers and Demo" folder. After CameraServer is installed, the installer copies the serial interface drivers to the program install folder. The default location is:

C:\Program Files\Spectronic Devices\CameraServer\drivers\usb

- 5. The CCD may now be plugged in. When Windows asks to search for the driver, select "No, not this time" and then "Install from a list or specific location" (same as above, for stepper electronics). Browse to the directory listed in step 7. The installation should proceed and the user should ignore any warnings about the driver being unverified. The CCD camera should now be installed.
- 6. Reboot the computer to finalize the installation. The application may be initialized after the computer boots.



Overview

The software written for the VM92 VUV Spectrometer is a complete control application designed to offer the user a complex set of functions without the complex graphical user interface. The various functions are organized into their own respective tabs, grouped with their supporting options and controls. In this way, the various functions can be cycled through simply by selecting the desired tab.

CCD Mode

The CCD detector is a 1 x 2048 pixel array which allows an entire spectrum to be acquired and displayed without moving the diffraction grating. The span is approximately 150 nm, but if repeatable results are an absolute must there is no better alternative than a fixed hardware setup such as this. The grating can of course be moved to different wavelengths so the CCD can display different regions of the full capable spectrum of the spectrometer. These different regions can even be stitched together as one continuous spectrum using the software's multiple graphing abilities, where up to 4 plots can be

Settings File (settings.ini)

The software uses a single settings file to store important parameters. The file is found in the program's root directory (which changes depending on your operating system but for Windows XP by default is C:\Program Files\VM92\) and is named "Settings.ini". It can be edited in notepad (simply by double-clicking) and the various parameters directly changed. In the program's graphical user interface (GUI), the tab called "Settings" allows the user to edit and save all the program's parameters without manually opening the INI file.

Whenever the settings file is written to from within the "Settings" tab of the GUI, a backup copy is placed in the program's \data directory and given a date and time stamp. The \data directory is a folder named "data" contained in the path to the program executable (by default C:\Program Files\VM92\data\). If for any reason the existing (or missing!) settings file needs to be corrected, replaced, or if the user needs to revert to older settings one of the files found in the \data folder can be opened in notepad and its values copied to the active "Settings.ini" file. Alternatively, one of the backup files can simply be renamed to "Settings.ini" and copied to the program's root directory, overwriting the existing file.



Error Log

The program's error log can be found in the "Settings" tab. When errors occur during the operation of the software, they are reported and appear with a timestamp in the error log. The log is also written to a text file, stored in the program's data directory (the same folder the executable resides, as explained above), in a folder called "data". When errors occur they are automatically appended to the error log text file. There can only be 1 error log file per day, and each file is given a file name with a time stamp. This is to prevent the log from reaching an unmanageable length if they fill with too many errors over time. Typical errors have to do with serial handshaking and transmission. Do not be alarmed if errors appear in this section. The software is designed to respond to errors and keep any operations active. Unless the program becomes unresponsive or behaves erratically the error log can usually be ignored, otherwise it becomes an invaluable debugging tool.



Global Functions



Figure 1: The global controls available at all times (highlighted).

Independent of the currently selected GUI tab, the following indicators and controls are available to the user at all times:

Indicators

WL (nm)

Displays the current wavelength the grating drive is currently positioned for. This is a user entered value and is obtained from the manual dial on the spectrometer itself.

Status:

Displays useful information while the software performs various operations. For example if the CCD is running or if an "exit" command has been given etc.



Global Functions (continued)

CCD Timer

Displays the amount of time remaining before the next CCD acquisition (and screen refresh) is due, based upon the selected integration time and number of averages. This control will be grayed if the photodiode is in use.

Connection LE

An indicator LED has been placed on the front panel of the software to give the user a convenient and quick way of determining if connection has been made with the CCD and it is functioning properly. The "Connection" LED is lit when valid pixel data has been processed.



Figure 2: The CCD Connection indicator LED.

Exit

The "Exit" button found in the GUI's top-right corner attempts to properly stop all running processes and close the executable, leaving the hardware devices in a state ready for proper initialization when the software is started again for another session. Note that in order to close properly the current CCD integration must complete – and since integrations can be 10's of minutes, the user may have to wait that long for it to complete.



Figure 3: The exit program button



CCD Tab



Figure 4: The "CCD" tab.

Store Dark

Stores the latest spectrum in memory. This spectrum can be subtracted from any future or stored spectra by toggling the "Subtract Dark" button.

Subtract Dark

Subtracts the saved "dark" spectrum from a stored or real-time (current) spectrum. The button affects all graphed spectra simultaneously.

X Axis

Selects which units to apply to the x-axis. Pixel number or wavelength is available. Wavelength is displayed in nanometers.

Store Spectrum

Stores the latest spectrum in memory for the purposes of graphing and data manipulation. Stored spectra can be graphed simultaneously over current spectra or operated on to produce a result spectrum (see the "Data Manipulation" section).



Integration Time (ms)

Specifies the length, in milliseconds, the CCD waits until reading out the intensities of its pixels to produce a spectrum.

Averages

Specifies how many spectra to acquire and average to produce a final resulting spectrum.

Save

The save function writes a .csv file renamed to an .xls file extension so it opens natively in Microsoft Excel. A pop-up window will appear prompting the user to enter the file name and path. A header is written which contains all the pertinent program settings that affect the scan, followed by the data. A comment box is supplied for the user to enter in any pertinent information about the data to be saved, and will appear in the file header. The column format is displayed below:

WL	Intensity	Intensity	Intensity (Dark	Avg Intensity (Dark	Pixel	Dark
(nm)	(Counts)	Averaged	Subtracted)	Subtracted)	Number	(Counts)

Figure 5: Save file header format

Calculate Result

Launches another window in which mathematical operations can be applied to various plots to generate a result spectrum. The new spectrum will be graphed automatically when the window is closed. See the section "Data Manipulation" for more information.

Revert

Restores the plots that were visible before "Calculate Result" was pressed.



Cursors

Cursors can be added or removed and told to snap to a plot or to be freely movable. The X and Y columns indicate the position of the cursor and can also be edited to place the cursor at an exact location. A context menu allowing the user to change cursor attributes such as point style, colour, and X/Y scales can be accessed by right-clicking in the cursor window (Figure 16 below).



Figure 6: The "CCD" tab cursor controls.

Graphing Controls

The software is tailored for repeating scans and therefore allows the user to plot up to 4 scans on the same graph, as well as a "Result" plot, which is explained later in the section "Data Manipulation".

Avg?	}		Spec.	# Vis?		Spectrum Par	ameters
	Plot 1	$\wedge \vee$	1		۲		Date
	Plot 2	$\wedge \wedge$	2	i ii 🔾	0		Time
	Plot 3	$\wedge \wedge$	÷)3	ealt 🔾	0		Centre WL
	Plot 4	$\wedge \wedge$	()4	° 🔾	0		Int. Time
	Result	$\wedge \wedge \vee$		۲			Averages
Avgs 3 Total: 4							





Graphing Controls (continued)

The area is structured around 4 static plots, each assigned a colour. Note that the colour and other parameters such as line width and point style can be changed by directly clicking on the black box with the plot colour icon; to produce a menu. Each plot displays a scan, as denoted in the scan box directly to its right, in the "Spec. #" column. Whenever the user initiates a scan, even if it is stopped, the application holds it in memory and assigns it an index, from 1 to infinity. Therefore, if 100 scans were performed, Plot 1 can display a scan from 1 to 100. The "Vis?" column directly to the right selects whether the plot is visible or not. By clicking the round green button the user can choose which plots to display (and therefore which scans). The "Spectrum Parameters" to the right of the "Vis?" column displays the parameters associated with a given scan, selectable by the vertical "radio selection" box. These parameters for the 3rd plot will be shown, and remember, the 3rd plot is not necessarily the 3rd scan, it is whatever scan is selected in the respective "Spec. #" column.

The "Real-time" check box toggles whether plot 1 should display the latest acquired spectrum or a stored spectrum of specified index.

The "Avg?" column selects whether to apply a running average to the respective plot. The sample length, or "Avgs" as denoted in the software, is how many samples are to be averaged together to produce a point. This parameter can only be an odd integer, and the software will filter even entries. A side effect of a typical running average is a shift in data by ½ the sample length rounded down. That is, if a peak was displayed on a graph and a running average of 11 was applied, the peak would shift to the right by 5 samples. The software compensates for this by deleting the first 5 points on the graph. This is the reason only odd numbers are permitted. The user should be aware that during a scan, if the plot is being averaged, no data will appear until there are more data points than half the average value, since they are being chopped off the beginning of the data array. It could appear as though nothing is happening until enough points are acquired to have something to graph.

The bottom right of the "CCD" tab allows the user to set the autoscale or manually applied limits for the wavelength and signal axes. When in manual mode, the limits can be changed using the increment arrows on the controls themselves or a new value can be typed in. When focus is lost from the control (preferably by pressing "enter") the new values are instantly applied to their respective axis. Note that for usability purposes, the values are not checked to see if they make sense. Therefore, for example, the user could enter in a maximum value that is actually lower than the current minimum value, which will cause the graph to incorrectly display data. Changing the lower value to something lower will naturally solve this problem.

The graph palette (at the bottom right corner of the graph) can also be used to zoom in on a section data quickly and easily. All apply/autoscale buttons must be un-clicked in order for this function to work. Simply click on the middle button on the palette and choose a selection type. A region may now be drawn on the graph to define the zoom area. Refer to Figure 18 below for an illustration.





Figure 8: The "CCD" zoom area control

Data Manipulation

One feature of the software is the ability to apply mathematical operations to 1 or more plots to produce a "result" spectrum. This function allows the user to perform mathematical operations on any of the 4 displayed plots. All 4 plots can be involved in the operation, or just 1 or more plots with or without constants. The calculation follows the mathematical order of operations, respecting the parentheses around the values.



Figure 9: The Data manipulation pop-up window invoked by pressing "Calculate Result" on the "Photodiode" or "CCD" tabs



To access this function, "Calculate Result" needs to be pressed on the "Photodiode" or "CCD" tabs. A separate window will pop up asking the user for the parameters of the operation.

There are two list boxes that hold savable constants in case the user needs to add, subtract, multiply, or divide by the same number from session to session. The list boxes can be edited by triple-clicking the values and typing a new number. Pressing the "Save" buttons beneath them will write the constants to files in the application root directory called "constant1.txt" and "constant2.txt". These are simple text files which can be manually edited if needed. The sliding switch to the right of each box allows the user to use a value from the list box or a manually entered temporary constant above.

The operators themselves are selectable via drop-down boxes, and 4 choices are given: add, subtract, multiply, and divide. When the "Calculate Result" button is pressed, the operations are carried out on the 4 plots and a "Result" plot is created and graphed on the tab which called the function. When a data operation is in progress the status indicator will display "Calculating result" to let the user know the operation is in progress.

Figure 19 above shows the data manipulation window and the selected function: Plot 1 is to be added to Plot 2. The First two plots in the equation are meaningless since they are being multiplied by a constant of 0. Figure 20 below shows the resulting spectrum in yellow graphed with Plot 1 and 2 to show that the operation was successful.

The result spectrum is also padded according to the source scans used in the operations. That is, if the start and end wavelengths of the scans do not match the result spectrum will range from the lowest of the scan wavelengths to the highest of the scan wavelengths, and will pad the scans so they all match this range before operating on them. The CCD is exempt from this additional feature since there are always the same number of pixels, and the beginning and end wavelengths are simply a function of the calibration polynomials. It wouldn't make sense to manipulate spectra of different regions for the CCD mode of operation.



Settings Tab

This section of the application allows the user to modify some very important parameters essential to the proper operation of the instrument. Each setting will be explained below.



Figure 8: The "Settings" tab.

Save Settings

Saves all entered parameters in this tab to an ".INI" file in the application's root directory. See the "Overview" section at the beginning of this manual for more information.

Error Log

As can be seen from Figure 21 above, the error log contains information about an error that occurred during operation of the instrument. In this case, the error was caused by a physical interruption of the USB cable from the instrument's stepper control electronics to the laptop computer running the software. The error window allows the user to scroll through past messages which are all time stamped. Refer to the "Error Log" section under the "Overview" heading for more information about where the logs are automatically saved.



CCD Wavelength Calibration

CCD WL Calibration							
(r) -1.9	CCD Centre Offset	CCD "ax Coeff" WL correction					
5.98613	ax Coeff 🔫	5.9147 Offset					
0.003	ax^2 Coeff	0.0003 ax Coeff					
0.014	Pixel Width (mm)	JO ax^2 Coeff					

Figure 9:	The	"CCD	Wavelength	Calibration"	settings.
	-				

There is a 3rd-order polynomial which converts the pixel number to wavelength, based on the currently set wavelength. Because the dispersion will change with the angle of the diffraction grating (and therefore wavelength) the 1st coefficient of this polynomial (ax Coeff) needs to be modified by the current (center) wavelength. It is called the center wavelength because the set wavelength will be incident upon the center of the CCD. To modify this 1st coefficient, yet another 3rd order polynomial (on the right) is used to calibrate it against center wavelength. The result is a CCD-spectrometer system which can remain accurate over a large range of wavelengths, and which can set any particular wavelength to the center of the CCD instead of being confined to certain regions of calibration.

Calibrating the CCD is a complex task and involves a lot of trial-and-error tweaking. The coefficients shipped with the instrument should not be tampered with unless Resonance Ltd. is consulted.

CCD Centre Offset

Due to potential variations in the CCD positioning during the manufacturing process and the combined effect of the shifting dispersion with respect to wavelength of the grating and the non-linear spectral response of the CCD, it is possible that the set wavelength may not fall on the center pixel of the CCD as expected. If this occurs, a shift in the wavelength calibration may be observed when scanning to various spectral regions with the CCD. To compensate for this a CCD center offset option has been included in the software to allow the user to compensate for this effect. The entered offset is in nanometers.



Contact

Resonance Ltd. stands behind every product we sell. We welcome feedback and encourage any of our customers to contact us with questions, or concerns. You may contact us through e-mail, our website, telephone, or fax!

Resonance Ltd.

143 Ferndale Drive North

Barrie, ON

L4N 9V9

Tel: 705-733-3633

Fax: 705-733-1388

Email: res@resonance.on.ca

Web: www.resonance.on.ca