

# SPEC\_SOFT Manual

Gratingworks LLC

# Catalogue

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## 1. Spectrometer Overview

The spectrometer is powered through USB. Current consumption is under 150mA at 5Vdc. USB is either 2.0 Full Speed or 2.0 High Speed depending on the model.

### Terminal block interface

- Pin 0** 5Vdc from USB. Can be used as power supply for external units (<100mA) or as a input for 5Vdc power supply. (Closest to the USB connector.)
- Pin 1** External Acquisition Trigger, Falling Edge.
- Pin 2-7** GPIO 0-5. Output is 3.3Vdc, Input is 3.3-5Vdc compatible. Current is limited by the microcontroller.
- Pin 8** Lamp PWM Strobe, can be used to control Xenon/LED lamps.
- Pin 9** RS232 RX, Not implemented, OEM only.
- Pin 10** RS232 TX, Not implemented, OEM only.
- Pin 11** GND.

## 2. Software Usage Overview

Spec\_soft GUI on windows provides a basic interface to the CONCAVUS and PSP family of spectrometers. It has the following functions.

- Graphical display of the spectrum in pixel or wavelength.
- Averaging, dark noise subtraction, CCD dark pixel subtraction.
- Wavelength Calibration.
- Find peaks and measure FWHM.
- Absorbance, Transmittance, Reflectance or oscilloscope measurement.
- 3D display of the spectrum.
- DFT of the spectrum.
- Pixel linearity correction.
- Filter out the Nyquist noise from CCD.
- Supports multiple CONCAVUS/PSP spectrometers.

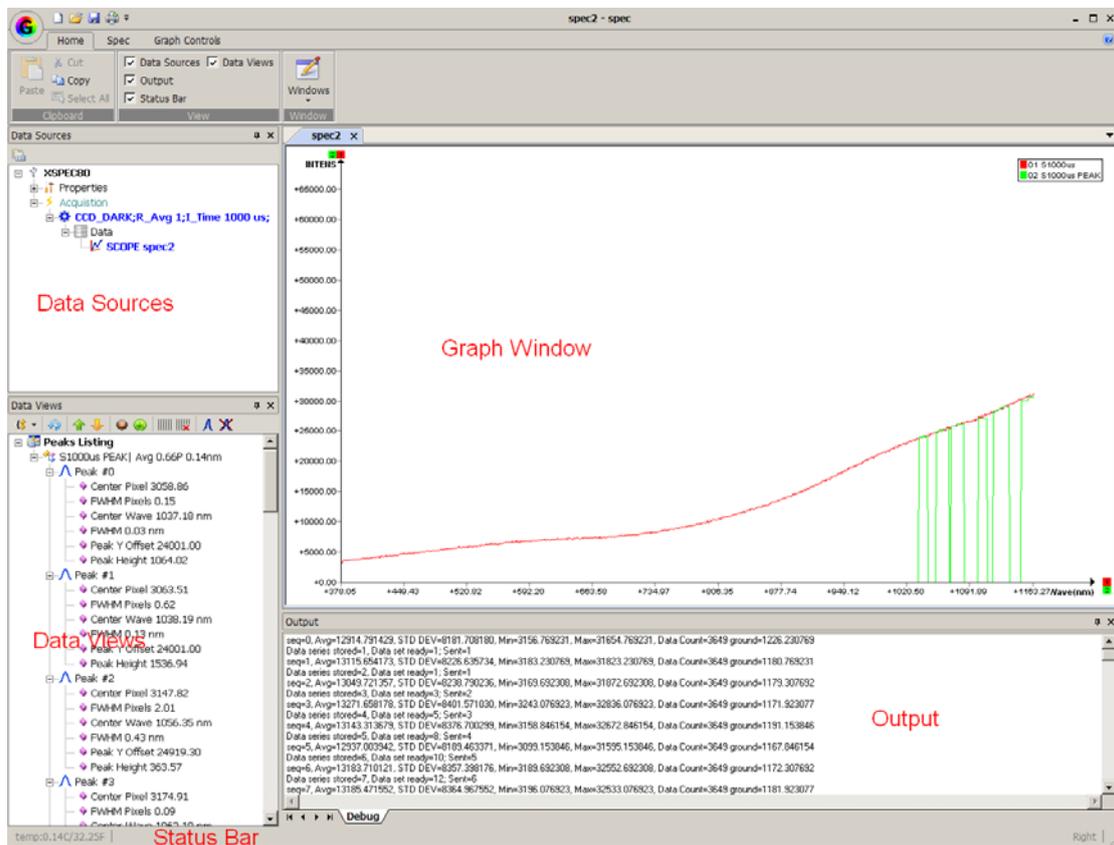


Figure 2.1 Main Screens

## 2.1 Home

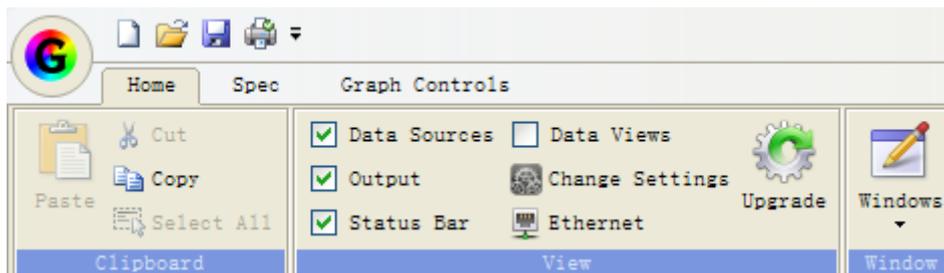


Figure 2.2 Home Panel controls

### 2.1.1 Data Sources

List all the spectrometers connected.



Figure 2.3 Data Sources

**Name of the spectrometer** The name “XSPEC801” is user configurable. Right mouse click on “XSPEC801” to rename. The name is saved in the firmware.

#### Properties

List the properties of the spectrometer.

#### Acquisition

- Add Profile, F8. Add an acquisition profile with different parameters.
- Terminate Acquisition, F5, stop acquisition.

#### Profile

Profile name contains the description of the acquisition. Subtracting CCD Dark, Running Average, Integration Time, FIR filtering.

- Use it as Dark Spectrum.
- Use it as Reference Spectrum.
- Delete this Profile.
- STOP F5.
- Run Once F6.

- Run continuously F7.

**Data** Export the data to a text file for Excel import.

### SCOPE spec6

- Overlay Saved File.
- Overlay Exported File.
- Remove Overlay File.

## 2.1.2 Data Views

List the data related to the spectrometer selected in the Data Sources.



Figure 2.4 Data Views

### First Button

- Peak Zoom. Default is on. Zoom in on each peak when click on 3<sup>rd</sup> & 4<sup>th</sup> buttons.
- Only show peak information in a single line.
- Continuously find peak. Used during assembly.
- Insert Hg/Ar lines. Insert the reference Hg/Ar line to check the calibration.
- Export Peak. Export the peak data in a text file.

### 2<sup>nd</sup> Button

Refresh Peak.

### 3<sup>rd</sup> Button

Select the above peak.

### 4<sup>th</sup> Button

Select the next peak.

### 5<sup>th</sup> Button

Open the calibration dialog.

### 6<sup>th</sup> Button

Add the selected peak for calibration.

### 7<sup>th</sup> Button

Add a marker for each peak.

### 8<sup>th</sup> Button

Remove all markers.

### 9<sup>th</sup> Button

Do a peak calculate and add the peak curve to the graph.

### 10<sup>th</sup> Button

Remove the peak curve.

In the peak below, you can right mouse click on a peak and select:

- Use the peak for calibration.
- Insert all the peaks for calibration.

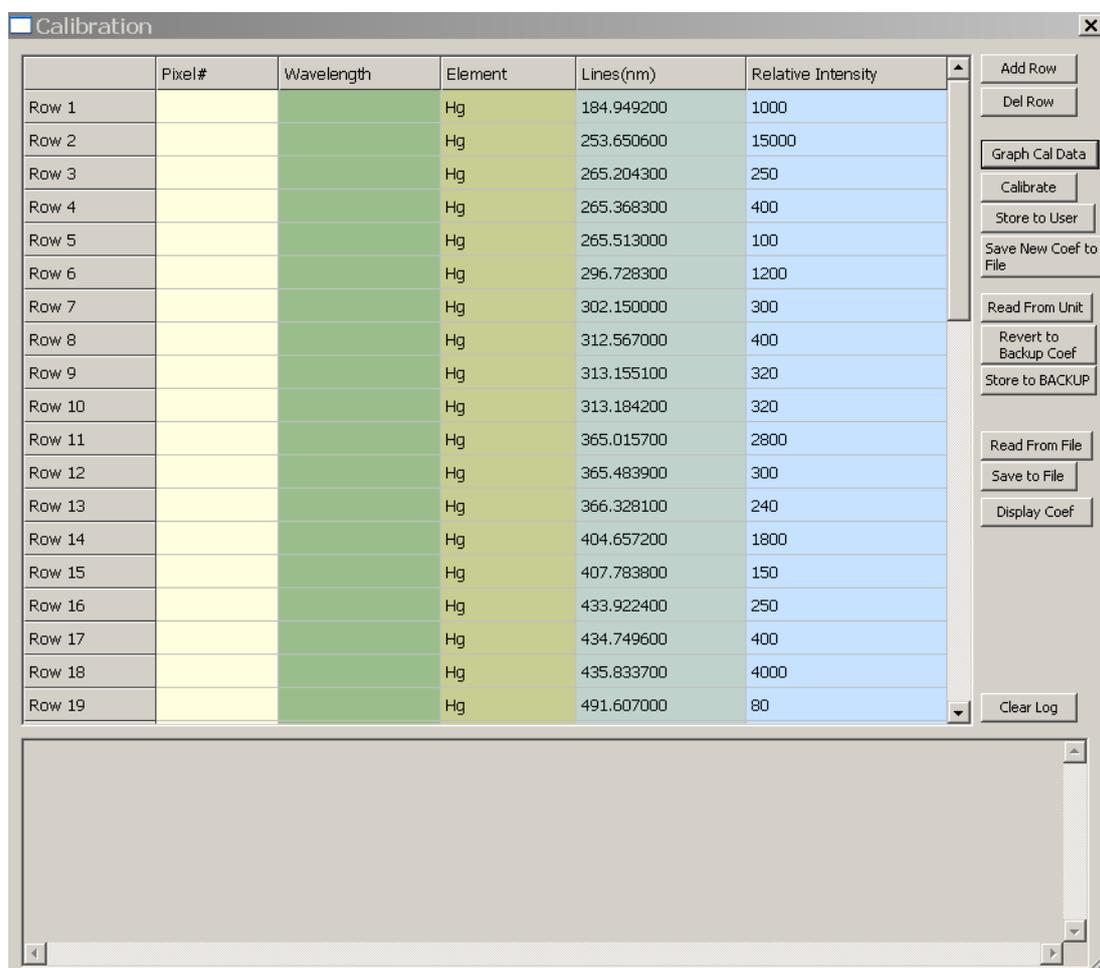
## 2.1.3 Calibration

The calibration method use the data points given, let the user select a polynomial from 1<sup>st</sup> order to 5<sup>th</sup> order. It can graph the original data points with fitted data points so user can select the best fit.

First row has the pixel number. Second row has corresponding wavelength.

To achieve a good calibration:

- More points the better.
- Have points cover the beginning and end of the wavelength range.
- Use graph to check the data points. If a point has a high deviation from the calibrated line, then the validity of the point is put into question and maybe it should be removed.
- From the graph, select an order that give a good STD DEV and also does not deviate at the wavelength range ends. You might not have data points at the two ends of the wavelength range and the polynomial fitting has no constraint at the ends.



The screenshot shows a software window titled "Calibration" with a table of data points and a control panel on the right. The table has six columns: Pixel#, Wavelength, Element, Lines(nm), and Relative Intensity. The data points are as follows:

Row	Pixel#	Wavelength	Element	Lines(nm)	Relative Intensity
Row 1			Hg	184.949200	1000
Row 2			Hg	253.650600	15000
Row 3			Hg	265.204300	250
Row 4			Hg	265.368300	400
Row 5			Hg	265.513000	100
Row 6			Hg	296.728300	1200
Row 7			Hg	302.150000	300
Row 8			Hg	312.567000	400
Row 9			Hg	313.155100	320
Row 10			Hg	313.184200	320
Row 11			Hg	365.015700	2800
Row 12			Hg	365.483900	300
Row 13			Hg	366.328100	240
Row 14			Hg	404.657200	1800
Row 15			Hg	407.783800	150
Row 16			Hg	433.922400	250
Row 17			Hg	434.749600	400
Row 18			Hg	435.833700	4000
Row 19			Hg	491.607000	80

The control panel on the right includes buttons for "Add Row", "Del Row", "Graph Cal Data", "Calibrate", "Store to User", "Save New Coef to File", "Read From Unit", "Revert to Backup Coef", "Store to BACKUP", "Read From File", "Save to File", "Display Coef", and "Clear Log".

Figure 2.5 Calibration Dialog

After calibration is done, click on both "Store to User" and "Store to BACKUP" to save the data into the firmware. Or only "Store to User" if you don't want to erase the backup.

To enable the Output, select the Output Spectrum Info checkbox in the Graph Controls Panel.

## 2.1.4 Graph Window

Show the spectrum graph.

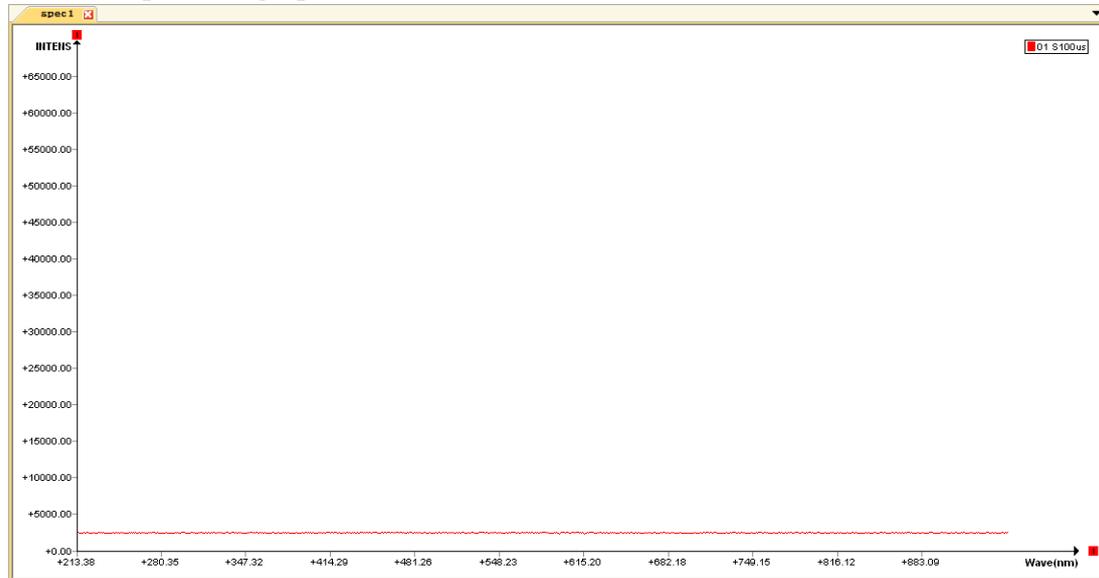


Figure 2.6 Graph Window

## 2.1.5 Status Bar

Control the On/Off of the status bar on the bottom. There is a temperature sensor inside the Analog to Digital Converter. And it shows the temperature reading on the left side.

## 2.1.6 Output

Show some statistic information about the spectrum.



Figure 2.7 Output Window

## 2.2 Spec Pane



Figure 2.8 Spec Panel

## Trigger

- Software Trigger: Acquisition initiated by software by sending over a command.
- External Hardware Trigger: Pin #2 (2<sup>nd</sup> PIN from left, closest to the USB connector) Negative edge trigger the

start of Single/Continuous acquisition. Single/Continuous mode is still controlled by the software command.

<b>Skip</b>	To slow down the reading rate, #numbers of readings are thrown away inside the firmware and are not sent to the USB.
<b>INT Time</b>	In micro second 10 us to 65,000,000 us. Change the integration time here. To take effect, change the number and press enter. To save to the firmware, press “Save Int Time” button.
<b>Number of Readings</b>	Take # of reading and then stop.
<b>GPIO &amp; LAMP</b>	Open the GPIO&LAMP control dialog.
<b>Load Int Time</b>	Load the Integration Time stored in the firmware and display/use them on the GUI.
<b>Save Int Time</b>	Save the current Integration Time to the firmware.
<b>ACQUIRE</b>	Continuously acquire data.
<b>STOP</b>	Stop the acquisition.
<b>ACQUIRE ONCE</b>	Acquire once.
<b>Scope</b>	Display in Scope mode. Default Mode.
<b>Absorbance</b>	Absorbance mode. Make sure there is a Reference data set saved.
<b>Transmission</b>	Transmission Mode. Make sure there is a Reference data set saved.
<b>Reflectance</b>	Reflectance Mode. Make sure there is a Reference data set saved.
<b>Running Avg #</b>	Display the graph in running average mode. The weight of the latest reading has 1/# weight in the averaging.
<b>DFT</b>	Display the graph in Directe Fourier Transform.
<b>Use as Dark</b>	Save the current displayed spectrum as the dark spectrum.

<b>Use Dark</b>	Check box to enable subtracting the dark spectrum.
<b>Use as REF</b>	Save the current displayed spectrum as the reference spectrum.
<b>3D</b>	Check box to enable the 3D display.
<b>3D Controls</b>	Open the 3D control dialog.
<b>-CCD Dark</b>	Subtract the dark pixel reading from each data pixel.

### 2.3 Graph Controls



Figure 2.9 Graph Controls

<b>Select Mode</b>	Cursor in select mode.
<b>Cursor Mode</b>	XY cursor mode. Display cursor x,y, Integration time, Data point x,y.
<b>Pan</b>	Pan graph.
<b>Reset Pan</b>	Reset Pan.
<b>Measure</b>	Measure distance.
<b>Edit</b>	Edit the data point. Change the value of a data point.
<b>Print Graph</b>	Send the graph to a printer.
<b>Properties</b>	Open the properties dialog. Change properties for the chart, axis, curve, and peak.
<b>Reset All</b>	Reset all the default.
<b>Remove Markers</b>	Remove all makers. Markers can be added by click on the X or Y axis first.
<b>Zoom Controls</b>	Various zoom controls.
<b>Output Spectrum Info</b>	Check box to enable/disable the output of the statistical data of the spectrum. Disable for performance.

<b>Wavelength or Pixel</b>	Set the X axis as Wavelength or Pixel.
<b>Update Graph</b>	Enable/Disable update of the graph. Can be disable to achieve the fastest data throughput.

### **3. Graph Control**

### 3.1 Peak

In turn, click Graph Controls, Properties, and then Peak.

依次点击“Graph Controls”，“Properties”，选择“Peak”标签页。

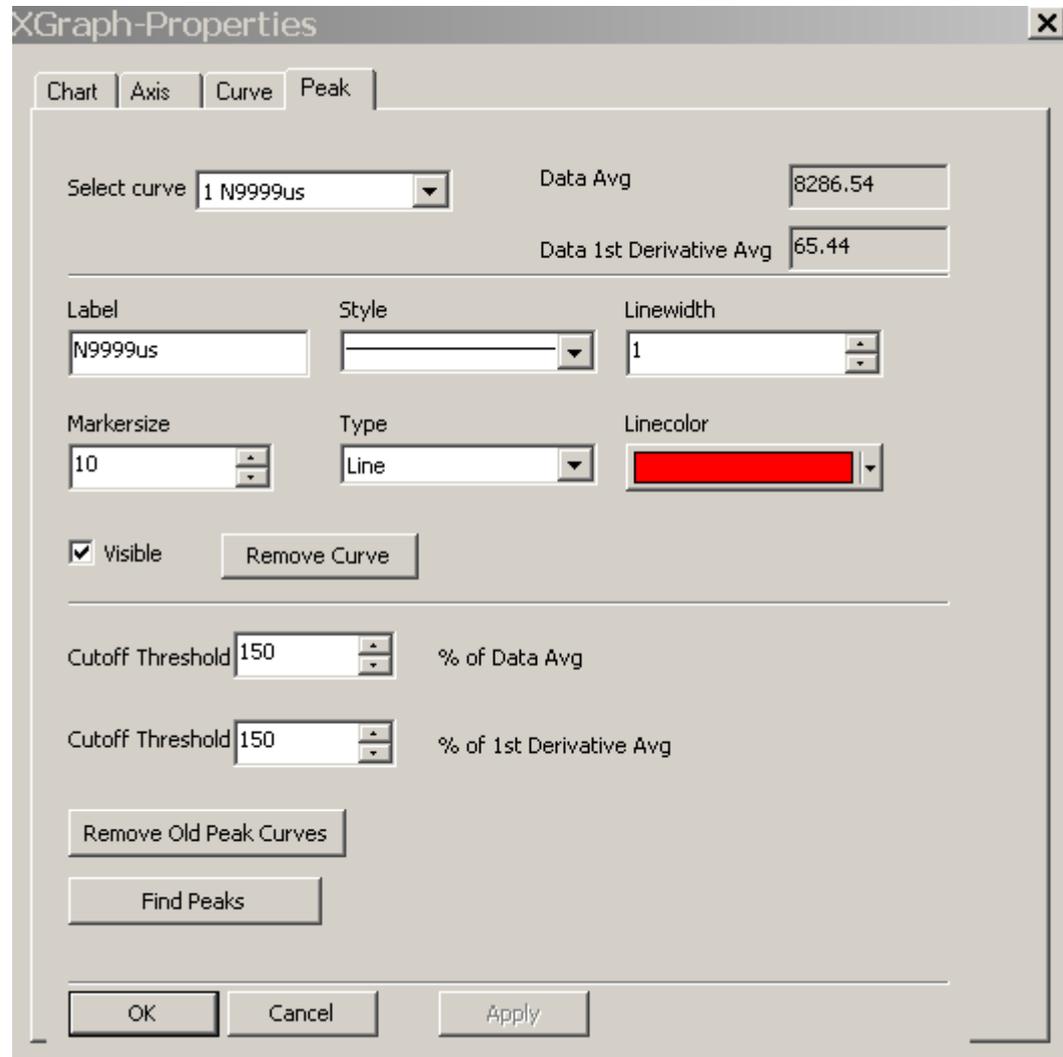


Figure 3.1 Peak Controls

There are 2 threshold settings that control the peak selection. Peaks below the threshold are ignored. They are used to filter out the noise. First one is the data average, 2<sup>nd</sup> one is the average of the 1<sup>st</sup> derivative. Default settings are 150 for both.

### 3.2 GPIO & Lamp Control

In turn, click Spec, and than GPIO&LAMP.

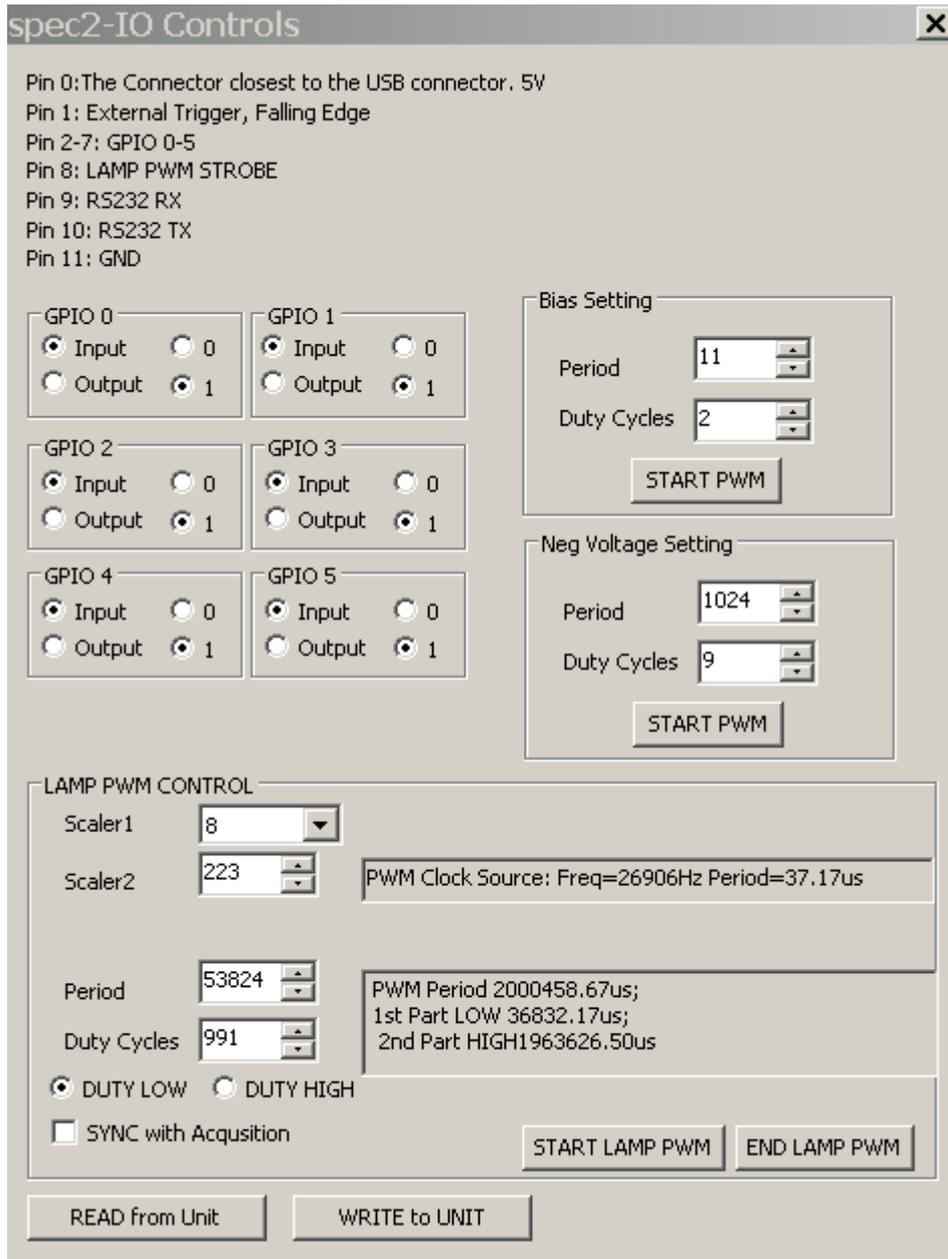


Figure 3.2 GPIO&amp;LAMP Controls

GPIO control the input and output of the signal. When set to output, click on the “Write to Unit” to output the setting. When set to input, click “Write to Unit” to change to input and then “Read from Unit” to read the GPIO value.

### Bias Setting

Every TCD1304 CCD detector has small variation on the output bias voltage. The bias voltage also changes with temperature. Adjust the PWM setting so the output has the lowest dark reading (Closest to zero) at 10us integration. During the adjustment, make sure uncheck the –CCD Dark at the right corner of the Spec panel.

**Negative Voltage Setting** This is a factory setting. Adjust the negative voltage for the OPAMP so it can work in the 0vdc region.

## 4. Firmware Settings

In turn, click Home, Change Settings.

**SETTINGS** [X]

3720 Integration Time DACNov 17 2013:::12:31:55;Flash Size 0X10000; Flash Page Size 128; Flash Setting Start 0XF000

0 (S)Int Mode 0=regular 1=shutter XSPEC80 User String

0 Trig mode 0=normal 1=external XSPEC80 Description

0 (N)External Trigger Delay 2.00 Detector Linearity Coef

0 Skip Count 20131108-165019 Firmware Version 0 0 4 0

0 (N)Dark Offset TCD1304 Serial 1 0 5 0

65000000 Lamp PWM Setting 0 Auto Adj CCD DC 5100 Detector 2 0 6 0

64946176 Lamp PWM Setting 1 0 360nm Grating 3 0 7 0

0 Multiple Count 25um Entrance Filter

0 Lamp Mode DOUBLE Slit Size

0 GPIO Port IO

63 GPIO 0 Wave Start 0 Wave End

0 (S)Temp System Coef 0 0 0 0 0 0 0

58100 BIAS PWM User Coef 0 0 0 0 0 0 0

328704 NEG PWM MAC HEX 18 52 86 120 154 188 12.34.56.78.9a.bc

3694 # of Pixels IP DEC 100 0 0 100

19 Dark Start Pixel Gateway DEC 100 0 0 1

31 Dark End Pixel Net Mask 255 255 255 0

35 Data Start Pixel

3682 Data End Pixel TCP PORT 8888  
If USE\_THIS NOT 123, then default ist: (MAC:12.34.56.78.9a.bc, IP:100.0.0.100, GATEWAY:100.0.0.1, MASK:255.255.255.0, TCP:8888, HTTP:80)

HTTP PORT 80

USE\_THIS (123) 123

[READ] [REFRESH] [Set Default] [WRITE]

Figure 4.1 SETTINGS

**Read/Refresh** Read and refresh the values.

**Set Default** Change the values to system defaults values before initial calibration.

**Write** Write to firmware.

**Note** User can change all the values on this dialog, including the calibration values.

## 5. Setup the CCD DC Bias.

In turn, click Spec, GPIO&LAMP.

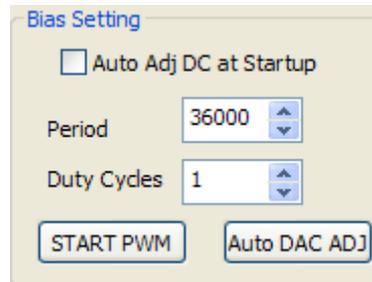


Figure 5.1 Bias Setting

To set the DC bias, Set INT time to 10us, and block all light input into the SMA fiber connector. You can either manually change the period value or click on “START PWM” button to change the DC bias. Then observe the spectrum taken with 10us INT time, the spectrum should be flat, and set the average DC value to 100-200 range. Or you can click on “Auto DAC ADJ” and the firmware will adjust the DC bias automatically to 100-200 range.

If you enable the “Auto Adj DC at startup”, every time the unit is powered up by plug in the USB cable; it will perform an auto DC bias adjustment.

## 6. GPIO Controls

In turn, click Spec, GPIO&LAMP.

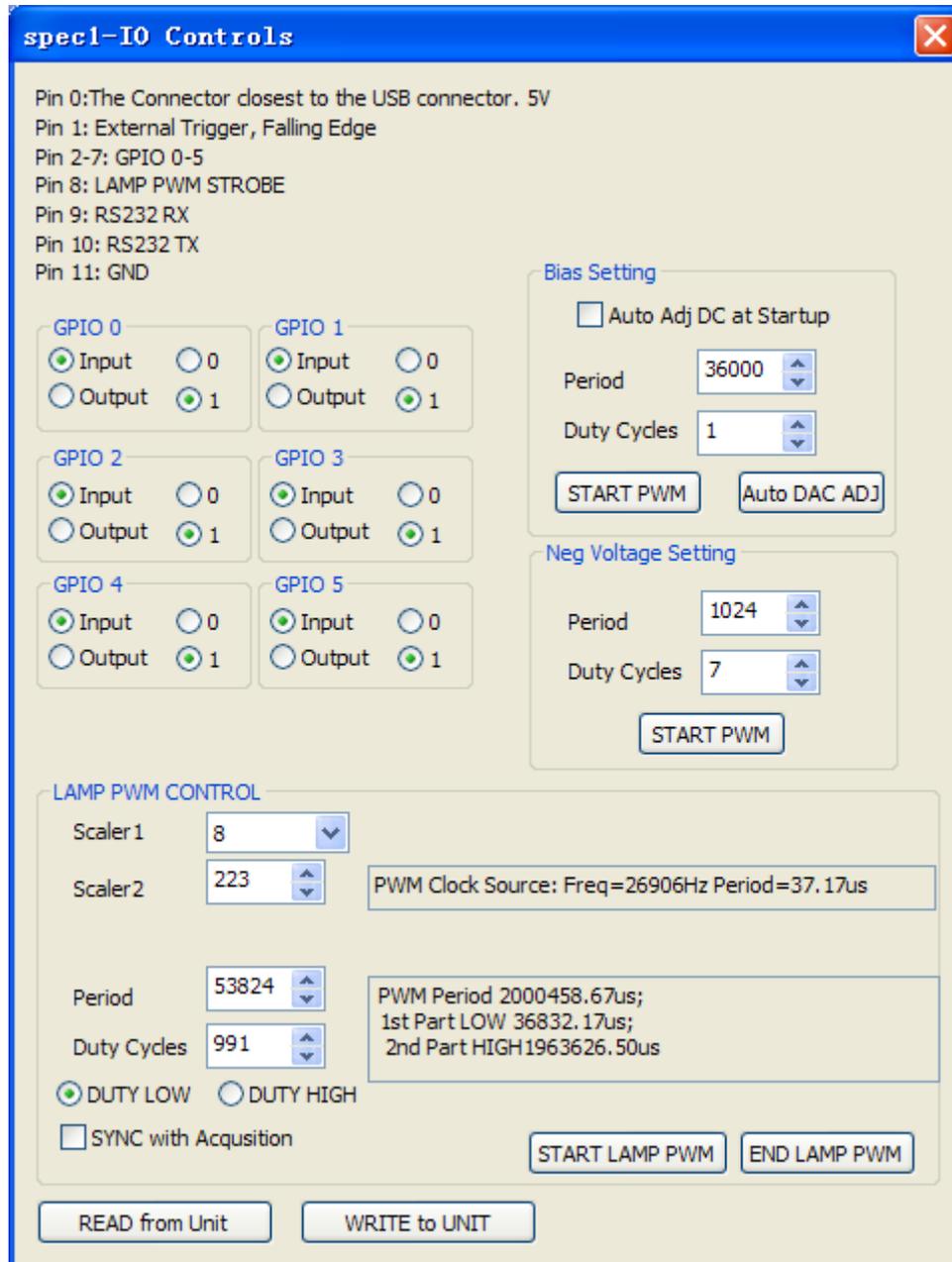


Figure 6.1 GPIO Controls

Change the input/output status for GPIO 0-5. If set to input, “Write to UNIT” first to change the state to INPUT, then do “READ from UNIT” to read the GPIO values. If set to output, set the value as well and then click “WRITE to UNIT”.

**Read from Unit** Load the setting from the firmware.

**Write to Unit** Save the setting to the firmware.

## 7. PWM Control

In turn, click Spec, GPIO&LAMP.

**LAMP PWM CONTROL**

Scaler1: 8

Scaler2: 223

Period: 53824

Duty Cycles: 991

DUTY LOW  DUTY HIGH

SYNC with Acquisition

PWM Clock Source: Freq=26906Hz Period=37.17us

PWM Period 2000458.67us;  
1st Part LOW 36832.17us;  
2nd Part HIGH1963626.50us

START LAMP PWM END LAMP PWM

Figure 7.1 PWM Controls

- Scaler1, 2** Change the scaler divider for the input clock for the PWM. See the right text for the resulted frequency and period.
- Period, Duty Cycle** Change the period and duty cycle for the PWM signal.
- Duty Low/High** Set to low/high during the Duty cycle.
- SYNC with Acquisition** When checked, a pulse rising edge occurs at the start of integration, and falling edge occurs at the end of the data acquisition, which is 3.7ms. In another word, the on time of the pulse for every integration is 3.7ms. If uncheck, PWM pulse turns on after user update the setting.
- Start/End LAMP PWM** Send command to firmware to start/end the PWM.
- Read/Write from/to Unit** Load/Save the setting from/to the firmware.

## 8. Measurements

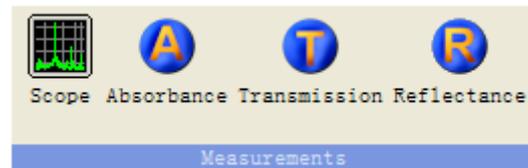
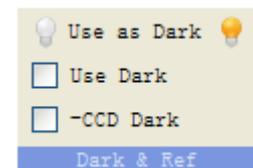


Figure 8.1 Measurements

### 8.1 CCD Dark

CCD TCD1304DG has some pixels that are light blocked and are used as dark reference. Dark current is temperature sensitive and values changes with temperature. To keep reading constant over a temperature range, enable –CCD Dark during measurement.



- Dark Noise  
If you intend to use a spectrum as Dark noise, click on “Use as Dark”, then enable “Use Dark”.
- Reference  
If you intend to use a spectrum as reference, click on “Use as REF”.

### 8.2 Scope measurement

Default setting is Scope mode. Click on ACQUIRE or ACQUIRE Once to acquire data and STOP to stop acquiring.

- A. Make sure you see a spectrum when there is no light signal into the SMA connector, when –CCD Dark, and Use Dark are not enabled. If all pixel readings are zero, adjust the DC Bias according to section 3.
- B. Enable –CCD Dark.
- C. Set the INT time, and click on ACQUIRE, make sure there is no light signal into the SMA connector. And click on “Use as Dark”, and “Use Dark”. The signal should fluctuate around zero.
- D. Turn on the light input and start Acquire.
- E. If you change the INT time, make sure you repeat III & IV again.

### 8.3 Absorbance

- A. Use Scope measurement to get a reference curve with maximum value around 60,000.
- B. Click on “Use as Ref”.
- C. Click on Absorbance button. You should now get a curve around zero. If the reference signal is very weak, you will get noisy readings.
- D. Insert a filter or a solution in the light path that needs to be measured.

- E. Click on ACQUIRE.

#### **8.4 Transmission**

- A. Use Scope measurement to get a reference curve with maximum value around 60,000.
- B. Click on “Use as Ref”.
- C. Click on Transmission button. You should now a get a curve around 100%. If the reference signal is very weak, you will get noisy readings.
- D. Insert a filter or a solution in the light path that needs to be measured.
- E. Click on ACQUIRE.

#### **8.5 Reflectance**

- A. Use Scope measurement to get a reference curve with maximum value around 60,000.
- B. Click on “Use as Ref”.
- C. Click on Reflectance button. You should now a get a curve around 100%. If the reference signal is very weak, you will get noisy readings.
- D. Insert a filter or a solution in the light path that needs to be measured.
- E. Click on ACQUIRE.

### **9. Calibration**

Calibration is done in the factory. The following description is a guide only. Make sure you save the coefficients before any modifications.

In turn, click Date Views, and then the 5<sup>th</sup> Button , open the Calibration dialog.

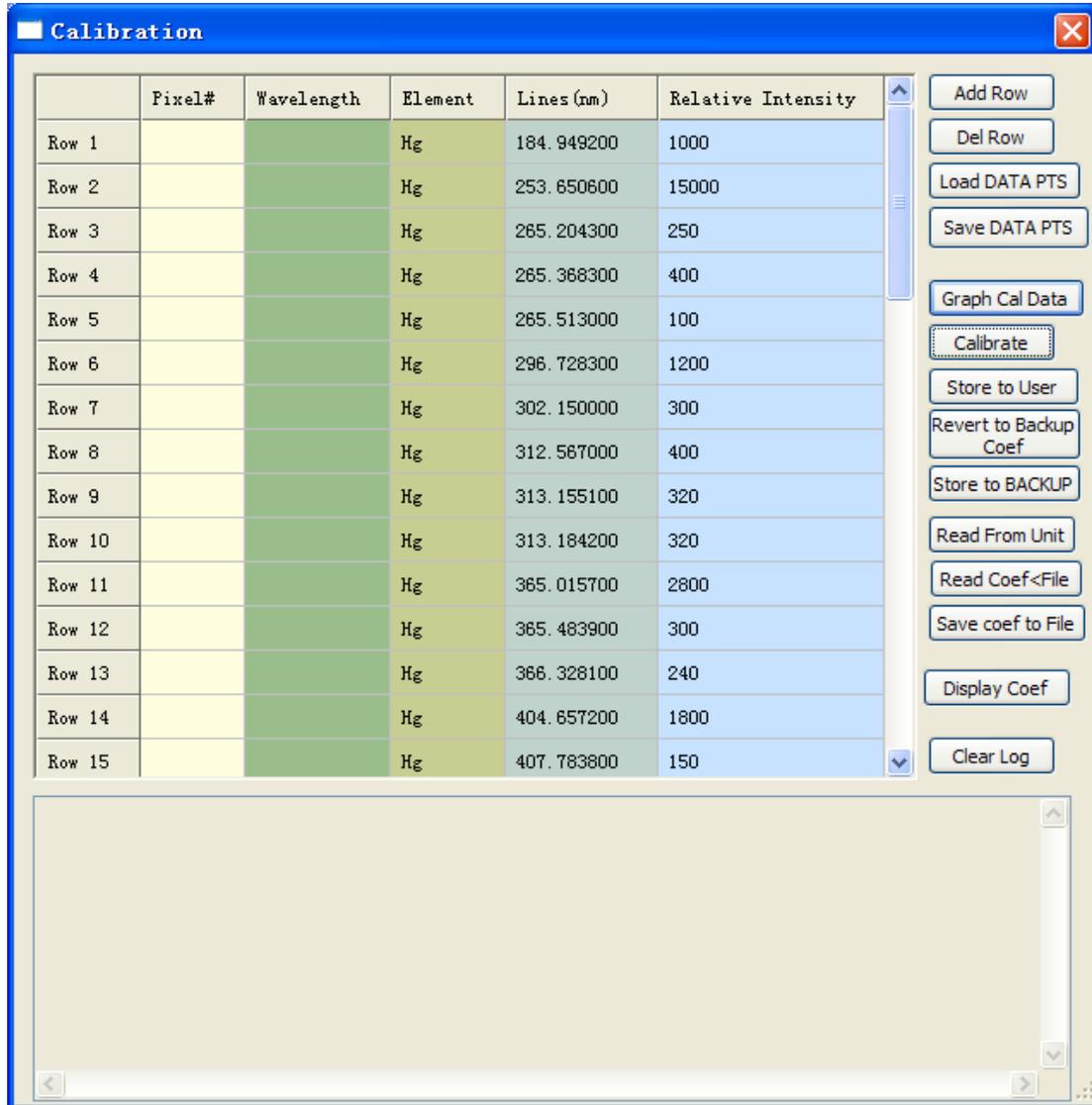


Figure 9.1 Calibration Dialog

- A. Click on “Read From Unit”;
- B. Click on “Display Coef”;
- C. Click on “Save Coef to File”; then input pixel/wavelength pairs into the Excel-like spreadsheet in the Calibration dialog.
- D. Click on “Calibrate”;
- E. Click on “Store to user”;
- F. Click on “Store to BACKUP” if you wish to replace the BACKUP.

## 10. Linearity

In turn, click Spec, and then Lin Cal, open the Detector Linearity dialog.

Figure 10.1 Detector Linearity

For fixed pixels, diagnose the linearity of readings of each pixel with respect to integration time. We found the linearity of TCD1304 is excellent that requires no linearity correction.

## 11.FIR filtering

In turn, click Spec, and then FIR Filter, open the Filter Setting dialog.

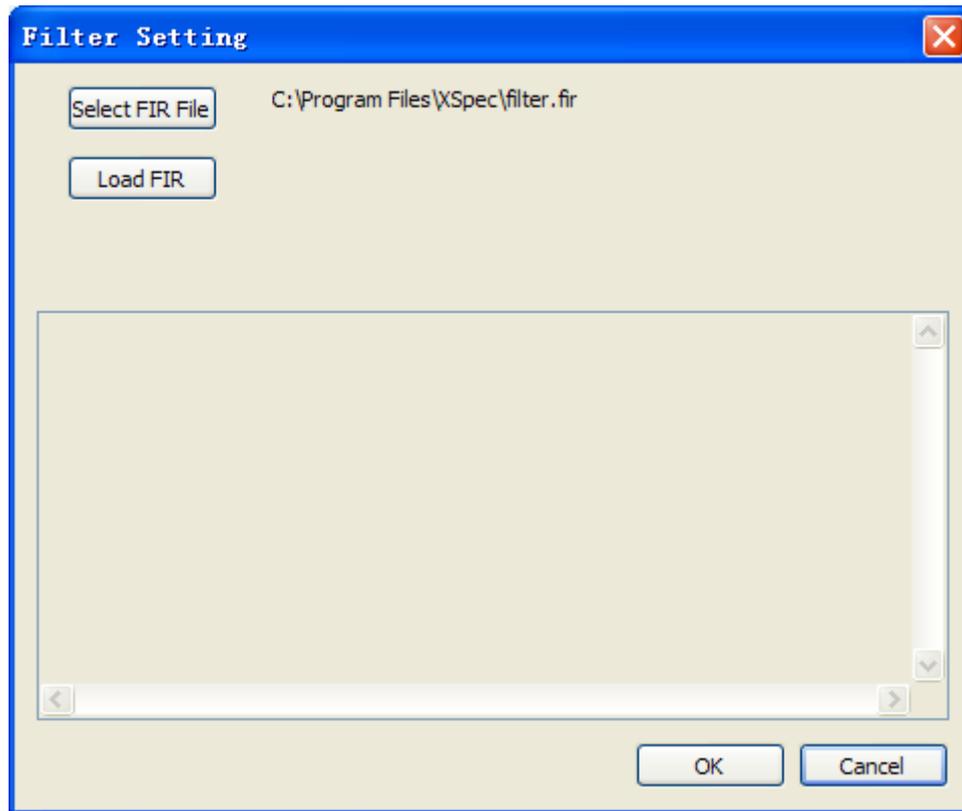


Figure 11.1 Filter Setting

Select a file with FIR coefficients, Format of the file:

-----  
 #comments 450000 is the cutoff frequency, ADC is 1MHz. 32 is number of taps.

“Description” 450000 32

Coef 0

Coef 1

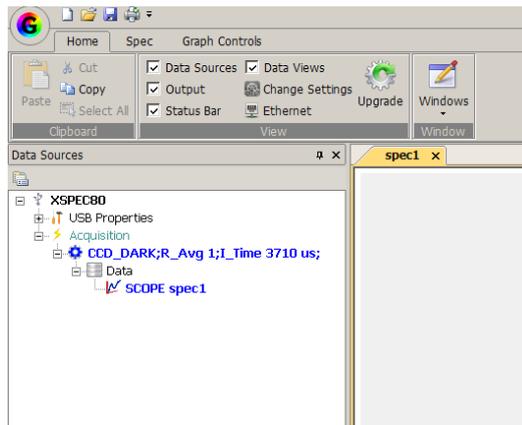
...

Coef 32

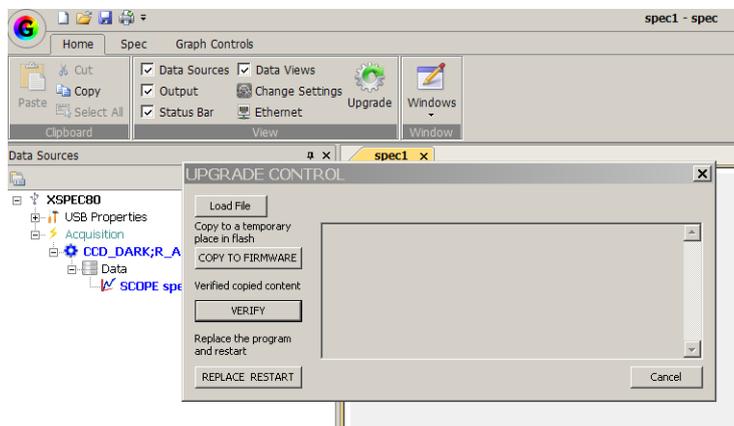
-----  
 Enable “Use FIR” to apply the FIR. The defaults FIR file is used to remove the CCD Nyquist noise at 500 KHz.

## 12.Firmware Upgrade

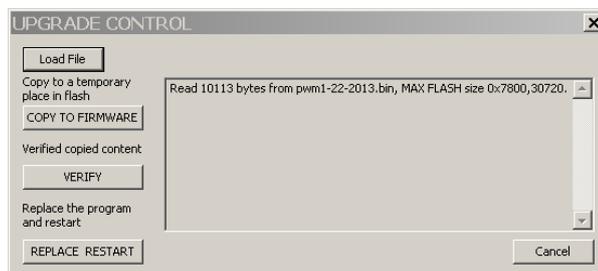
A. Connect device, make sure you see the device.



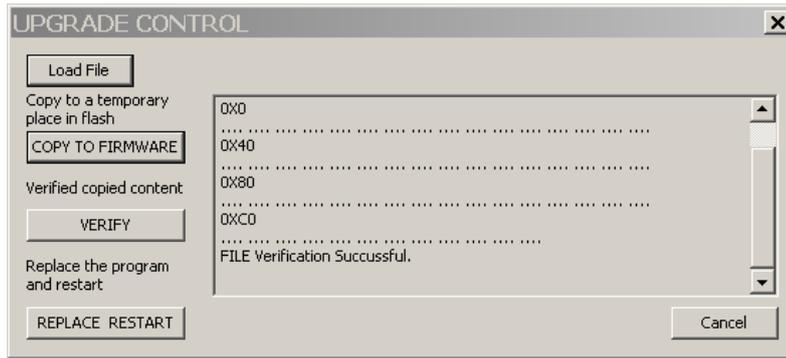
B. On Home TAB, click on Upgrade



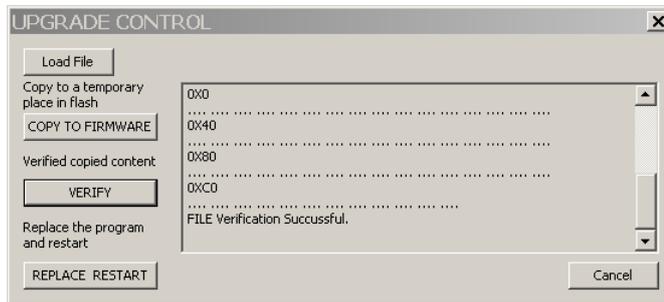
C. Load File, Download Firmware file from <http://www.gratingworks.com/products/tech.htm>, Unrar and load the bin file.



D. Click on copy to firmware, it will copy the new file to a temporary place in flash. It does not replace the running program yet. If you see X or error, pull out the USB cable and restart the operation.



E. Verify, make sure download is correct.



F. Click on REPLACE&RESTART to replace the running program and restart the unit. You will hear the USB power off/on sound.

G. UPGRADE DONE.