

XC Spectro

Users Guide

XC Spectro is an IDL application used to analyze the spectral data obtained from an x-ray crystal diagnostic. XC Spectro is configurable for different crystals and for different experimental conditions and as such has several configuration files that change the behavior of the application.

### Configuration Data Files

XC Spectro uses several data files to allow for the most general program execution. Each file is tab delimited with “!” (exclamation points) marking the divisions between one parameter and the next. IDL uses these marks to distinguish between one parameter and the next when it reads these files, therefore the formatting of these files should not be changed and care is necessary when modifying the parameters inside these files. Also the “;” (semicolon) is a comment symbol which can be used to comment out an entire line in any of the configuration files. This can be useful if you want to change a setting but retain the value of a previous setting for future reference, you can just comment out the line and make a new line for that parameter. The parameters in each of these files are detailed in the appendix, however here is a brief description of the contents of each file. Also see the section entitled Setting up analysis for a new Data Set for the most common setting changes and examples.

analysis.dat	Example ascii file containing the name of the theory file (see vainshtein.dat) and the name of the idl function that will do the analysis
default_settings.dat	Default setup parameters for program execution such as name of file containing crystal information to use and number of dimensions in data set
crystal.dat	Contains possibly several but at least one set of crystal parameters
datafile.dat	Describes input data files to be read
mds.dat	Describes MDSplus name of tree and nodes where input data is contained if running in mdsplus mode (set in default_settings.dat) Used as an alternative to datafile.dat
lines.dat	Contains list of lines to fit and their corresponding characteristics
vainshtein.dat	Theoretical configuration file containing excitation rate coefficients and theoretical wavelengths etc.
vainshtein_restore.dat	An idl restore file that contains the structure of the theory file for idl function read_ascii
vars.dat	Contains a list of variables with initial guess values, max/min

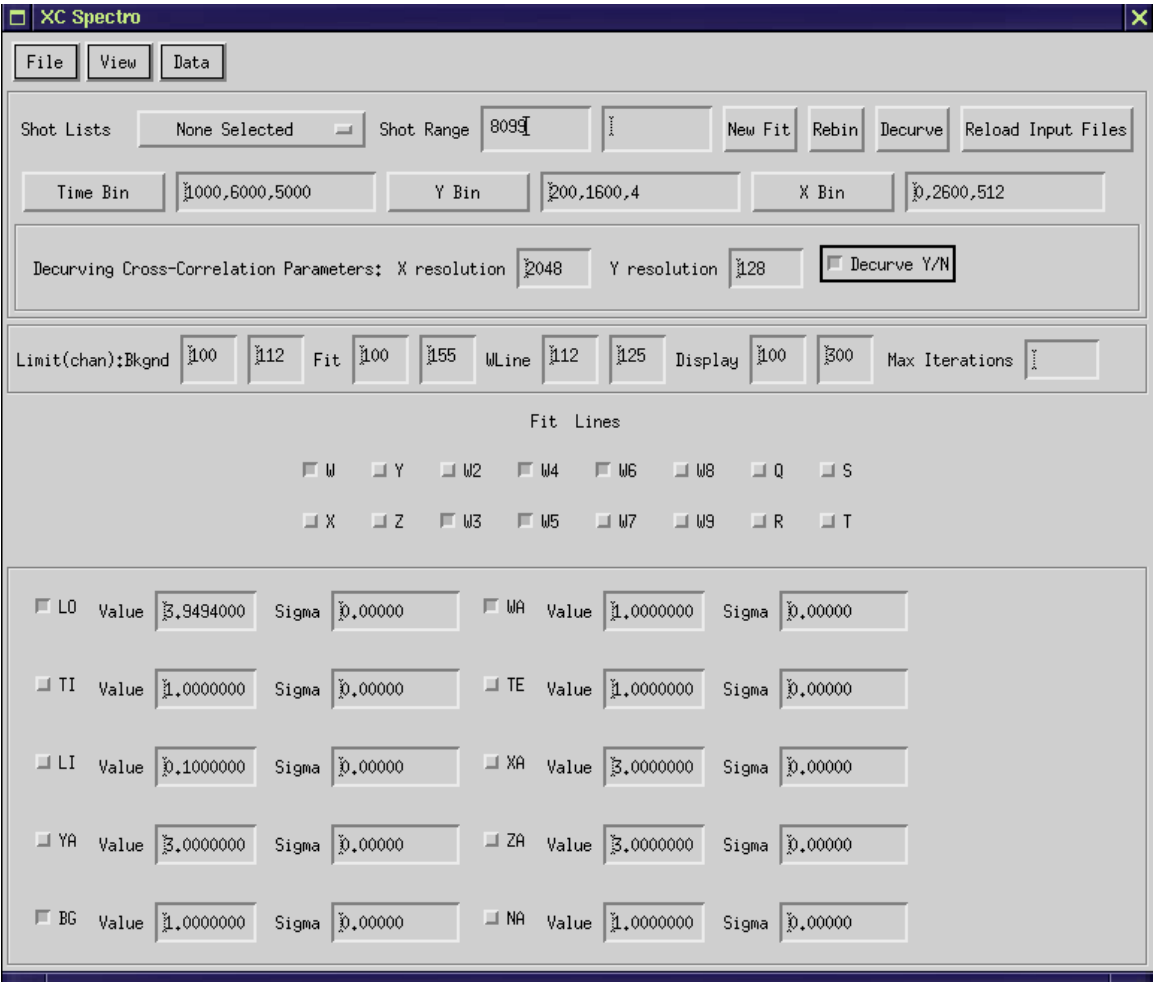
	and correction values for each as well as initial conditions for varying each variable in the fit.
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### Starting XCSpectro

To start the application first start the idl program. Once inside IDL type at the prompt:

```
IDL> a=xc()
```

This will begin the XC Spectro application and create the following widget which functions as the main window/interface of the XC Spectro application.



Doing the above assumes that you have a license for the IDL application which can be obtained/purchased from <http://www.itvis.com/>. However, if an IDL license cannot be obtained the XC Spectro application can also be run using a previously compiled version of the application with the freely available IDL Virtual Machine.

In this section I will review all the options, features and functions available from the XCSpectro main application window.

## The File Menu

At the top left of the main application window you will see the “File” menu. From the “File” menu there is only one menu option “Exit”. Use “Exit” to exit the program cleanly, memory will be cleaned up when the application is exited this way.

## The View Menu

The “View” menu contains several menu items each of which is used to view the settings as they are listed in the various input files listed in the first section of this document. entitled “Configuration Data Files“. The “View” menu contains the following options:

- “Default Settings” -- displays default\_settings.dat
- “Parameter Settings” – displays vars.dat
- “Line Settings” – displays lines.dat
- “Crystal Settings” – displays crystal.dat
- “Data Settings” – displays datafile.dat or alternatively mds.dat depending on the settings in default\_settings.dat
- “Analysis Settings” – displays analysis.dat

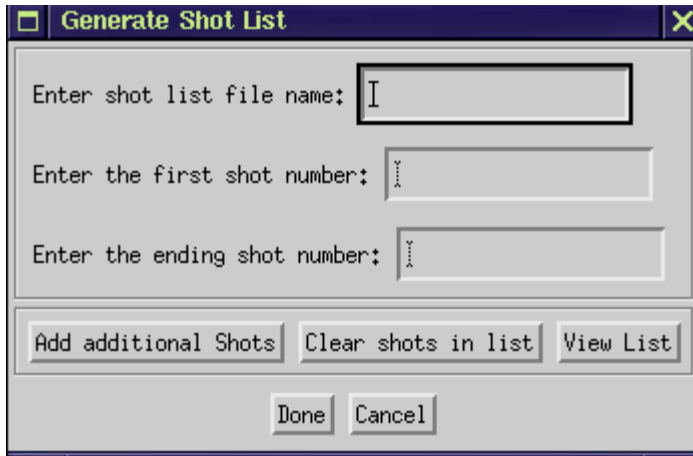
When any of these are selected a new window will appear displaying the contents of the file selected. The left most column displays the name of the parameter while the columns to the right indicate the value associated with that parameter. Parameters can be changed from these windows and changes can be saved by clicking the “Save” button on the bottom left corner of the window. The save button on these windows will save changes to the actual files. Therefore, once you have changed the settings those changes will be in effect even if you re-open the application. Once changes have been made and saved you must click the “Reload Input Files” button on the main window for the changes to be used in your analysis. The one exception to this is the crystal settings file. If you chose “Crystal Settings” from the view menu you will see a window containing a drop-down list of the previously defined crystal settings from which you can choose by name. Changes can be made to the settings for use during your analysis but these changes are not written to the file. Permanent changes to the crystal settings can only be made by manually editing the crystal.dat file. Clicking the “Reload Input Files” button on the main menu after making changes to the crystal settings using the “View”->“Crystal Settings” function will cause your changes to be overwritten by those contained in the crystal.dat file.

## The Data Menu

The “Data” menu contains the majority of the applications functionality. Most of the steps needed to complete data analysis are called from within this menu.

### Generating Shot Lists

If you choose “Generate Shot List” from the “Data” menu, you will see the following window:



The screenshot shows a dialog box titled "Generate Shot List". It has a standard Windows-style title bar with a green icon on the left and a close button (X) on the right. The main area of the dialog contains three text input fields. The first field is labeled "Enter shot list file name:" and has a cursor in it. The second field is labeled "Enter the first shot number:" and the third is labeled "Enter the ending shot number:". Below these fields are three buttons: "Add additional Shots", "Clear shots in list", and "View List". At the bottom of the dialog are two buttons: "Done" and "Cancel".

First give your list of shots a filename. The shot list you generate will be stored in this file and can be recalled for future use by this name. The default\_settings.dat file contains a parameter called Shot\_File\_Dir which controls the location of the output of this feature. Next, enter a first shot number and an ending shot number in the remaining fields. At this point your shot list will include all the numbers from the ‘first shot number’ up to and including the ‘ending shot number. So for example, if your first shot number is 123456 and your ending shot number is 123458 your shot file would look like this:

```
123456
123457
123458
```

Lets say that in addition to these three shots you would also like to include shots 123460 and 123461. You would then click the button “Add additional Shots” and put 123460 as the first shot number at 123461. At this point if you were to click the button “View List” you would see that your shot file contains the following shots:

```
123456
123457
123458
123460
123461
```

If you also want to include shots 123470 and shots 123480-123485 you would then click “Add additional Shots” and this time enter only a starting shot number, 123470. Then click the “Add additional Shots” button one final time and enter 123480 and 123485. At any time you can click the “Clear shots in the list” button to remove all shots from the list and start again. Once you are satisfied with your list, you would click the “Done” button which would result in your setting shots 123456-1234458, 123460-123461, 123470, 123480-123485 as the current shots to work with. The file you just created will appear as the chosen shot file in the “Shot Lists” drop down on the main XCspectro window. When you begin your analysis your dataset will contain all the data accumulated over all the chosen shots.

### Viewing your Data

To view your data choose “View Raw” from the “Data” menu. At this point the application will go looking for your input files or for your data as you specified and it is at this point that your data files will be read for the first time. This is a necessary first step to completing your analysis. Choosing “View Raw” from the “Data” menu will bring up a new window with plots in 3 tabbed sections. The exact appearance of this window and the number of plots displayed depends on the binning parameters that are set on the main window. For this reason I will address the binning parameters here.

### Binning your Dataset

On the main window there are three fields labeled “Time Bin”, “Y Bin”, and “X Bin”. These are the binning parameters. The Time Bin field expects values of starting time, ending time, and # of points in each bin with all values entered in milliseconds. If you forget how to enter the values, you can click on the “Time Bin” button and a messagebox will appear that will remind you. For example, you could enter the following:

1000, 6000, 5000

This entry would indicate that binning should start at 1 second and go through 6 seconds with 5 seconds in each bin, or just one bin. Another possibility would be:

0, 8000, 2000

This entry would indicate that binning should start at time zero, go through 8 seconds with 2 seconds in each bin for a total of 4 bins. This would result in 4 plots on the Time tab of your “View Raw” window.

The “Y Bin” and “X Bin” fields expect entries in the form of starting channel #, ending channel #, and number of final bins. If you forget how to enter the values, you can click on the “Y Bin” or the “X Bin” button and a messagebox will appear that will remind you. For example, if you entered the following in the “Y Bin” field:

200, 1600, 4

This entry would indicate that binning should begin at channel 200, go through channel 1600 and bin those channels 200-1600 into 4 groups. Likewise for the “X Bin” field. If you entered the following:

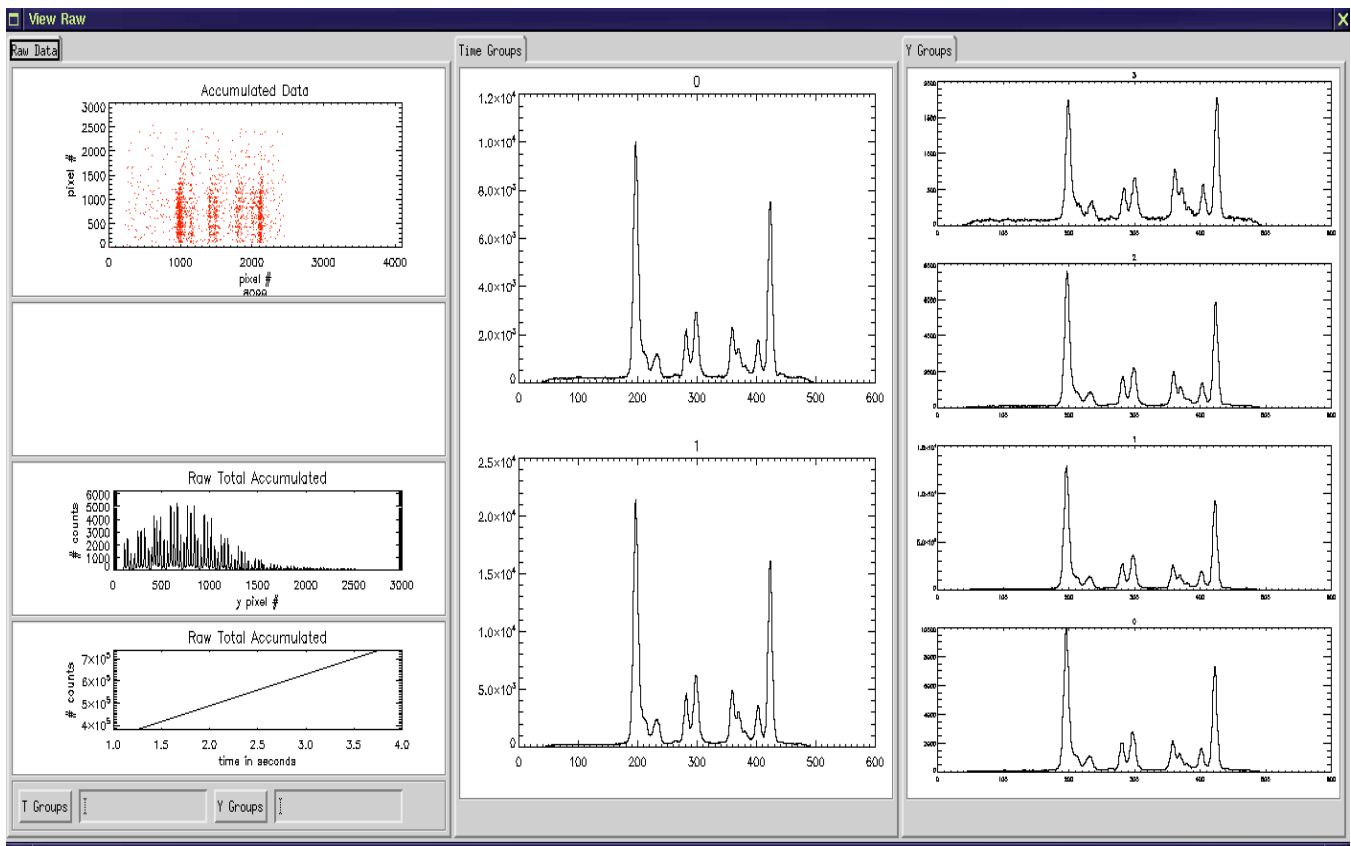
0, 2600, 512

This entry would indicate that binning should occur between channels 0 and 2600 and the final resolution should be 512, or 512 final groups/values.

So if we had the following binning parameters:

“Time Bin”	1000, 6000, 2500	(2 bins)
“Y Bin”	200, 1600, 4	(4 bins)
“X Bin”	0, 4096, 512	(512 bins)

We might see returned the following “View Raw” window:



The first tab/column of plots shows various representations of the raw data. The first plot is a histogram by channel number of all the raw counts. By default the 2<sup>nd</sup> plot remains

empty. The 3<sup>rd</sup> plot shows the data collapsed over the x-channels and bins counts in the y direction. The 4<sup>th</sup> shows the number of counts in each time bin. The second tab is the “Time Groups” tab and shows two time bins/groups, labeled 0 and 1, with time increasing from top to bottom (1 being later in time). The last tab is the “Y Groups” tab and shows four time bins/groups, labeled 0-3, with channel number increasing from the bottom to the top as it appears in the “Accumulated Data” raw plot (group 3 displaying the highest channel numbers). Each of the plots displayed in this window have a ‘context sensitive menu’ that can be brought up by right clicking on the plot. If you right click (click on a plot using the right-most mouse key) you will see a small menu appear with the following options:

Save – Saves a postscript version of the plot to your Output directory as defined in the default\_settings.dat file

Zoom – Brings up a larger version of the plot/tab.

Save text – Saves to a text file in your output directory the numerical values used to create the plot

Any files saved due to the save, zoom, or save text functions will be named according to the shots used for the fit and the name of the plot saved. So for example, If you were using shot number 7011 and you saved the top left plot a file would appear in your output directory named raw\_7011.ps The text version of the file would be named raw\_8099.txt. Postscript files can be read by any postscript viewing program such as ghostview and can also be converted to pdf.

Bin values can be changed. After modifying the bin parameters on the main window as described above, click the “Rebin” button. This will cause the data to be re-binned according to the new parameters and will cause a new “View Raw” window to open displaying your newly binned data.

**IMPORTANT NOTE:** The mm/channel parameter listed in the crystal.dat file is dependent on the number of x-channels chosen by your binning parameters. If you do not get a good fit a likely culprit is the mm/ch parameter which may need to be reset after having binned your data.

## Viewing your Data – Part II

As stated above, the default behavior is that the 2<sup>nd</sup> plot on the “View Raw” window is left empty. This plot has two optional functions.

The first possible use of the second plot is for an addition view of raw data. It is achieved by choosing “View Raw Calib” from the “Data” menu instead of “View Raw”. Doing so results in a 2<sup>nd</sup> plot that shows “Raw Total Accumulated” data with the y-dimension collapsed, counts per x channel. The 2<sup>nd</sup> use of this plot is for displaying de-curving information as described below.



## De-Curving

Since the detector makes use of a spherical crystal data is typically curved in the y direction. For this reason, the W line in 1 Y bin/group may not fall into the same x channel as that of another bin as you traverse the Y dimension of the detector. A “Decurve” feature has been added for this reason. Once you have displayed your raw data, you can de-curve by first selecting the “Decurve Y/N” button and then clicking the “Decurve” button on the main window. The de-curve feature uses cross-correlation to find the W and Z lines in each of the bins specified and then shifts them to make them line up with each other. The bins used for the cross-correlation are not the same as those used to display/analyze the data. The cross-correlation parameters can be set on the main window in the section labeled “Decurving Cross-Correlation Parameters:” “X resolution” and “Y resolution”. By default these values are set to 2048 and 64 but they can be changed. Once you have clicked the “Decurve” button the “View Raw” window will update with a straightened raw data set and the 2<sup>nd</sup> plot will then be filled with the curve used to straighten the data-set.

**IMPORTANT NOTE:** The “Decurve Y/N” selection determines whether the application straightens your data-set by default. If it is selected before choosing “View Raw” from the “Data” menu, data will automatically be de-curved at the time of initial binning.

## Selecting Bins/Groups for Analysis

Once you are satisfied with the binning selections you have made for your data, you can choose specific groups/bins to use in your analysis. At the bottom of the “View Raw” window you will notice two fields labeled “T Groups” and “Groups”. Here you can enter the number/s of the groups you wish to use in your analysis. The group numbers can be entered like:

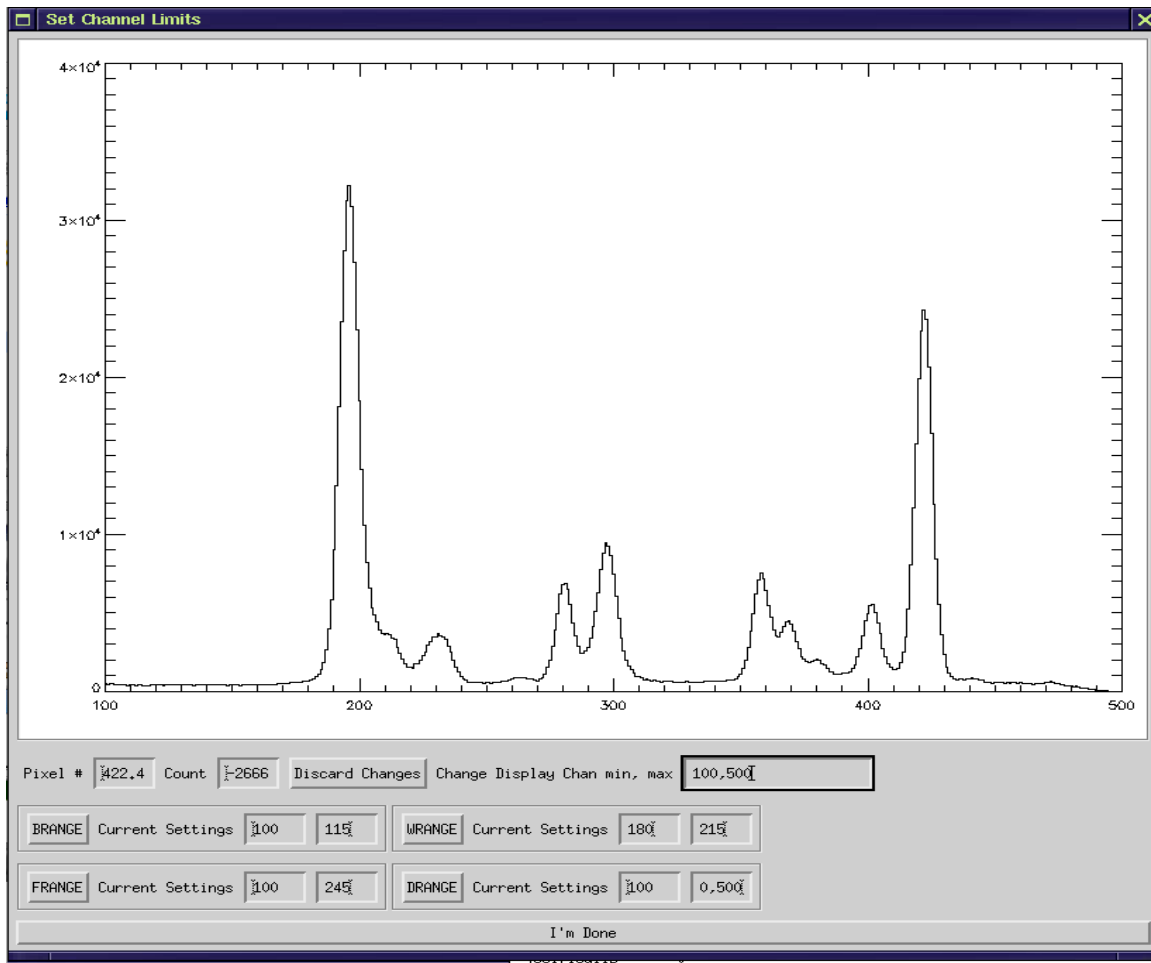
0,1  
1-3,5  
2

If you forget the format accepted by these fields you can click on the buttons labeled “T Groups” and “Y Groups” for a reminder. If you do not enter anything in these fields all groups binned will be used in your analysis.

## Setting Fit Limits

Typically the x-ray crystal analysis is completed by a series of fits varying different parameters and over different regions. A typical starting point is to fit first over the W-line region. For this reason it is often necessary to set the channel limits over which to do a fit. It is possible to select the time and Y groups desired for this selection. This is useful mainly for the case of data that has not been de-curved or if there is a particular bin/group that has very poor statistics that may throw off your channel selections. You

can select the groups you wish to include by following the instructions above in the section entitled “Selecting Bins/Groups for Analysis”. Once you have selected the groups you wish to use, there are two ways you can set your fit limits. The first method, if you know what channels you wish to use, you can set them on the main program window in the fields labeled “Limit(chan):Bkgnd,”Fit”,”WLine”,”Display”. The Bkgnd channel limits are those over which you want to fit the background. The “Fit” channel limits are the channels over which you want to complete the fit, which initially is often smaller than the total number of x channels after binning. The “W Line” channel limits are those channels where the W line lies. Alternatively, these channels can be selected graphically by choosing “Set Limits” from the “Data” menu. Doing so will result in data from the chosen time and Y groups to be collapsed and the displayed in the following window:



The “Set Channel Limits” window allows you to select graphically your channel limits. As you move your mouse over the plot, you will notice that the “Pixel #” and “Count” fields update with the current value over which the mouse moves on the plot. For a better view, you can change the channel limits on the plot by entering channel numbers in the “Change Display Chan min, max” field. For example, above you can see the channel limits have been set to 100,500. This is only used to help select your fit channel limits.

The “BRANGE” is the background channel limits. You can set the background limits by entering the channel numbers in the fields after the “BRANGE” heading. Alternatively, you can click on the “BRANGE” button and then click on the plot to select first a starting and then again to select an ending channel. Likewise for the “WRANGE” or W line limit, “FRANGE” or fit limits, and “DRANGE” or display limits. For example, above the limits for each are set to reasonable values for the first fit. Once you are satisfied with your limits, click the “I’m Done” button to close the “Set Channel Limits” window. You will notice that channel limit fields on the main window will update with the values you have chosen.

**IMPORTANT NOTE:** The “Set Channel Limits” window is a blocking window. The rest of the application will not respond until this window has been closed by clicking the “I’m Done” button.

### Selecting Lines to Include in your Fit

The lines included in the fit are set on the section of the main window labeled “Fit Lines”. Typically, a first fit would include the lines:

W  
W3 satellites  
W4 satellites  
W5 satellites  
W6 satellites

Lines that are selected on the main window are the ones that will be included in the fit. Each button is a toggle button so you can add or remove lines from your fit by clicking on the line you wish to add or remove.

### Selecting Parameters to Vary in your Fit

The fit parameters are listed at the bottom of main application window, along with their current value and the sigma from the last fit, 0 if no fit has been yet executed. The values assigned to each parameter before a fit is executed come from the vars.dat file.

The default or starting values for the fit can be modified in this file, as well as the maximum allowed and minimum values allowed. Fits whose results return values outside of these min-max values will not be used. Also in the vars.dat file there are optional correction factor that can be applied to any of the variables. Variables that are selected on the main program window are those that will be varied on the next fit. Those that are not selected will be held constant during the fit. Again these buttons are toggle buttons, so variables can be changed to be varied or held constant by clicking on them. A typical first fit would vary the parameters:

LO  
WA

BG  
TI  
TE

And keep all the rest fixed.

### Executing a Fit

Once you have binned your data, set the limits of your fit, chosen the lines to include in the fit and the parameters to vary in your fit, you are now ready to execute a fit. A fit can be executed by selecting “Analyze” from the “Data” menu. . The application will complete a least squares fit for each Time and Y group selected on the “View Raw” window, comparing each spectra to a synthetic spectra constructed by the theoretical predictions of Vainshtein and Safranov, Dubau and Gu. The values of the parameters that were varied in the fit will update on the main application window as well as the sigma values from the fit. The results of each fit are then displayed in a separate window

If you are unsatisfied with the results of the last fit and want to change a parameter and repeat it, you can do so by choosing “Undo Last Fit” from the last.

### Starting a New Fit

On the main window you will see a button labeled “New Fit”. Clicking this button will cause all the fit parameters to return to default values and clear the raw data to allow a new dataset to be read in. After clicking the “New Fit” button you will need to re-enter a shot number in any of the ways described above in order to continue.

### Example Steps for completing Data Analysis

In this section will attempt to cover the basic steps required to complete analysis on a set of Xray Crystal Data. All of these functions are discussed in detail in the sections above, but here I have tried to outline the basic steps involved in completing analysis on a data set. As you will see later, in the section entitled “Scripting”, it can be very useful to keep track of the steps you are taking to complete your analysis if you will want to do the same

steps for other data sets. For this reason, it is a good idea to keep note of the binning, values, groups, channel limits etc. that you use for your analysis as you are doing it.

1) Edit the setup files.

Default\_settings.dat

Verify that the Crystal Name parameter reflects the crystal used to create your data. (If it does not you can find or add the correct crystal parameters in the crystal.dat file and change the Crystal Name parameter in this file to match)

**IMPORTANT NOTE:** The millimeters/channel (mm/ch) parameter in the crystal.dat file is dependent on the x dimension binning that you choose. The mm/ch are calculated by comparing the distance on the detector between the W and Z lines with the number of channels measured between the W and Z lines. The number of channels between the W and Z lines is dependent on the number of bins/resolution of your data, which is set by the X Bin value on the main XC Spectro window. Therefore, if you change your x binning, you will need to modify the mm/ch parameter in the crystal.dat file for the crystal you are using to reflect your change.

If your data is located in files:

Modify the Data\_Dir parameter to reflect the location of your data files.

Paths for input and output can be absolute or relative, but be sure that they exist!

Verify the settings in the datafile.dat file. As an example if your data file is named:

XCS0008099.SIK

Then datafile.dat should contain:

shotfile_prefix	XCS000
shotfile_suffix	.SIK

If your data file is one of a split data set where the full data set is split horizontally, having a top and a bottom then you will want to use the read\_sik\_split\_xyt as your read\_program and you will need to specify which file contains the top and which contains the bottom. So if your dataset was made up of

XCS0008099\_1.SIK (containing the top)

XCS0008099\_2.SIK (containing the bottom)

Then you would have the prefix and suffix as above and you would have the parameters

```
top          _1
bottom       _2
read_program read_sik_split_xyt
```

Parameters such as top and bottom are for data sets that are made up of two files each representing one half of the total data set. In this case you would use the read\_sik\_split\_xyt (or your own idl function) to read your data.

If your data is located in mds:

Change the Data File parameter to mds.dat

Modify the mds.dat file to reflect the tag/node names where your data resides.

Modify the Output\_Dir parameter to reflect the location where you would like to put the results of your analysis files, i.e. output plots etc. (don't forget to create this directory if it does not already exist – on unix this is done by typing mkdir <dirname> at the command line)

Analysis.dat

Verify that the timebase is set correctly for your data set. The timebase should reflect the conversion of your data timestamps into seconds.

Verify that the tmin and tmax values are set correctly (values are entered in seconds).

## 2) Using the interface

### Selecting Shots to use

The application allows several methods for selecting shots. The simplest is that you can select a single shot and enter its number into the first box on the interface following the heading “Shot Range” on the GUI and then pressing ENTER.

Alternatively if you wish to gain better statistics by combining data from more than one shot you can either enter a 2<sup>nd</sup> shot number in the 2<sup>nd</sup> box following the heading “Shot Range” on the GUI and press ENTER. As a final option, you can use the “Generate Shot List” feature. If you chose the former, the application will assume you want to use every shot from the first entered through the 2<sup>nd</sup> entered. So for example, and continuing with the example of the naming convention prefix and suffix described above, if you put the number 8099 in the first box and the number 8102 in the 2<sup>nd</sup> box XCSpectro will attempt to find files XCS0008099.SIK, XCS0008100.SIK, XCS0008101.SIK and XCS0008102.SIK in the directory you specified in the default\_settings file. If any one of these files

is missing or unreadable this will result in an error. XCspectro will then combine the data of all 4 shot files for analysis.

If for example you do not have data for shot 8101 but you want to combine data from more than one shot then you will most likely use the “Generate Shot List” feature. This feature can be invoked by choosing “Generate Shot List” from the “Data” menu on the GUI. See the section “Generating Shot Lists” for more information on this feature.

### 3) Viewing your data

The next step would be to view your raw data. This would be done by choosing “View Raw” from the “Data” menu on the main window.

### 4) Binning

At this point you would be able to determine how you want your data to be binned and which time and y slices of your data you want to analyze. The Binning parameters are set on the main XCspectro window under the headings “Time Bin”, “Y Bin”, and “X Bin”. Once you are satisfied with your bins, you can select specific Time and/or Y groups to analyze or use them all. To select a specific time region/s put the Time group number/s that you wish to use in the “T Group” field at the bottom of the “View Raw” window. You can enter groups like 0-1,3. This is also true for the Y groups.

### 5) Setting Fit Limits

Next you must set the channel limits for your fit by choosing “Set Limits” from the “Data” menu. Set the channel ranges limits for the W line, the background fit, the whole area to fit and the area to display. Typically more than one fit is used to fit your data and initial fits use a smaller subset of the total spectra. After completing a fit you can repeat this process to expand the channels over which the fit will be done. You can also do this by editing the fields for the limits on the main XCspectro window.

### 6) Analysis

You must select the Fit Lines you wish to be included in your fit and the variables you wish to fit on the main XCspectro window by clicking the things you wish to include/vary and deselecting those you wish to exclude or keep constant. Then choose “Analyze” from the “Data” menu. This will return the values of the parameters varied in the fit and a plot of the fit over the ranges selected in step 5. This step can be repeated as many times as necessary. Fits can also be “undone” by choosing “Undo Last Fit” from the “Data” menu.

## Scripting

XC Spectro allows the user to set the program up for unattended execution or for quicker execution of repetitive steps. For this reason it's a good idea to keep track of the settings and values for each of the parameters you set up so that once you have the fit exactly as you desire you can repeat the exact steps. XC Spectro has built in functionality that allows you to save a series of commands in a file and execute them as a batch. Each of the steps described above can be executed from a script. There is a command that can be put into a file that corresponds to setting values for the Time binning and another that will allow choosing bins to use for your analysis. An example script is contained in the file `xc_script.pro` which can be run by choosing "Execute Script" from the "Data" menu and then navigating to your script with the file dialog box that will open. Scripts can also be run from the IDL command line if interactive IDL is available/licensed as follows:.

```
IDL>@xc_script
```

If your file is named `xc_script.pro`

The following is a list of command with a comment on their use:

<code>a-&gt;SetCrystal, "EAST"</code>	<code>; Set the active crystal to the one named ;EAST in the crystal.dat file</code>
<code>a-&gt;SetShots,file='east_shots.shot'</code>	<code>;set a shot file for use in your analysis</code>
<code>a-&gt;SetShots, shot0=7311</code>	<code>;set a single shot for use number 7011</code>
<code>a-&gt;SetShots, shot0=7311, shot1=7315</code>	<code>;Set shots in range 7311-7315 for use</code>
<code>a-&gt;set_xyt,[1000,6000,2500],'t'</code>	<code>; sets time bin 1 second to 6 seconds in 2 ;groups of 2.5 seconds</code>
<code>a-&gt;set_xyt,[1000,6000,5000],'t'</code>	<code>; sets time bin 1 second to 6 seconds in 1 ;group of 5 seconds</code>
<code>a-&gt;set_xyt, [200,1600,4],'y'</code>	<code>;sets y bin channels 200-1600 into 4 groups</code>
<code>a-&gt;set_xyt,[0,2600,512],'x'</code>	<code>; sets x bin channels 0 - 2600 binned into ;512 points</code>
<code>a-&gt;viewraw</code>	<code>;Read input data and open the "View Raw" ;window</code>
<code>a-&gt;set_ygrps, [0,1,2,3,4]</code>	<code>;Set y groups 0-4 for analysis</code>
<code>a-&gt;set_tgrps, 1</code>	<code>;Set T group 1 for analysis (all groups are ;zero based)</code>
<code>a-&gt;setBLimits,88,126</code>	<code>;Set background fitting limits from channel ;88 to 126</code>
<code>a-&gt;setFLimits,81,197</code>	<code>;Set fitting limits from channel 81-197</code>
<code>a-&gt;setWLimits,137,157</code>	<code>;Set W line limits from channel 137-157</code>
<code>a-&gt;setDLimits,36,473</code>	<code>;Set display limits from channel 36-473</code>
<code>a-&gt;decurve,1,2048,64</code>	<code>;Execute Decurve function with X res 2048 ;and Y res 128</code>



a->SetVars,'TI',1	;Vary Ti
a->SetVars,'TE',1	;Vary Ti
 a->Analyze	 ;Execute a fit
 a->SetFLimits,58,269	
a->SetDLimits, 39,349	
 a->SetLines,'X',1	;Include the line X in the fit
a->SetLines,'Y',1	;Include the line y in the fit
a->SetLines,'Z',1	; Include the line z in the fit
a->SetLines,'W2',1	; Include the line W2 in the fit
a->SetLines,'Q',1	;Include the line Q in the fit
a->SetLines,'R',1	;Include the line R in the fit
a->SetLines,'S',1	;Include the line S in the fit
a->SetLines,'T',1	;Include the line T in the fit
a->SetVars,'LO',0	;Fix the parameter Lo in the fit
a->SetVars,'WA',0	;Fix the parameter Wa in the fit
a->SetVars,'TI',0	;Fix the parameter Ti in the fit
a->SetVars,'TE',0	;Fix the parameter Te in the fit
a->SetVars,'XA',1	;Vary the parameter Xa in the fit
a->SetVars,'YA',1	;Vary the parameter Ya in the fit
a->SetVars,'LI',1	;Vary the parameter Li in the fit
a->SetVars,'ZA',1	;Vary the parameter Za in the fit
a->Analyze	;Execute another fit

In this way all the functionality of the application can be utilized from a script.

As a final note, the XC Spectro program is also possibly extensible to other kinds of spectral analysis. The binning, input reading, and fitting routines used are all named in input files and can be replaced by other routines if so desired. Additionally the user interface itself reads the names and values of the parameters to fit from input files. Replacing those files with others would allow the interface to display and fit a completely different kind of data.

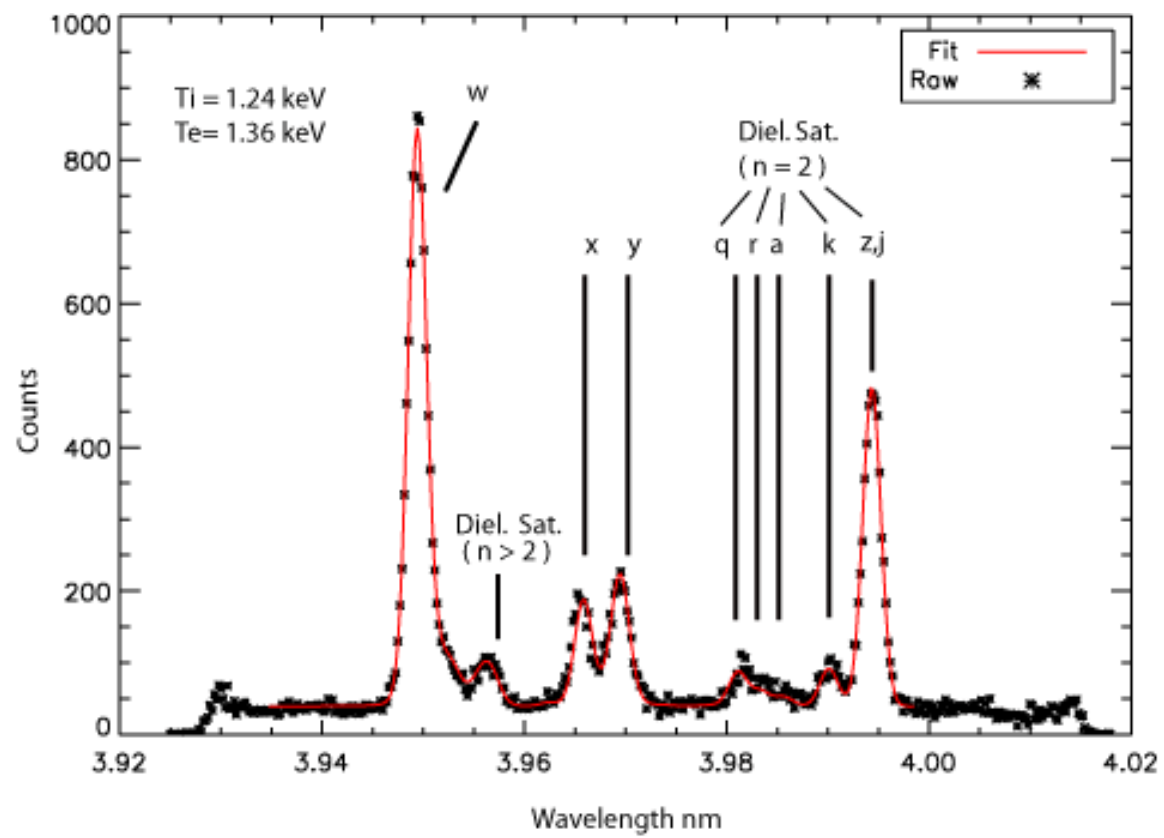


Fig 4.