

# Guide to the XAFS Data Acquisition Software at PNC-XOR BM20/ID20

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Prepared by ASI staff, edits and updates RGC and PAC (2006, 2009, 2010).

This is a work in progress - All new info and adjustments to be reported to RGC

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## 1. Introduction and Starting Up

This document is an informal guide, written from the viewpoint of a beamline (BL) user, to the XAFS software and BL control suite on the PNC-CAT BM20/ID20 BL, which are located at the Advanced Photon Source (APS).

After you arrive at APS, the BL staff will set up the BL equipment for your experimental needs so that it is ready for your measurements. They will show you how to mount and change samples inside the BL hutch, and how to operate the XAFS data acquisition software. Subsequently you will be left to carry out XAFS measurements by yourself as far as possible. The BL staff will be available for consultation if problems arise, or if you do not know (or forget) how to do something.

Initially it is appropriate to setup a data collection area for YOUR data on the sector computers.

- Define a workspace (in iduser or bmuser (psw access provided by BL staff)
- Named Folder (Your names or Project leader name with date is appropriate)
- Setup sub folders to separate your data sets if desired)

You can define files in the various setup programs when you setup scans but you must have these folders in place and these are best defined in the op system (XP looking like W2000 as of Feb 2006).

In the "scan setup" (see later) you will have opportunity/ability to switch folders.

Select desired directory (with mouse) then activate/press "Select Current Directory" (see p 9)

The main operations which have to be completed by a user after mounting a new sample may be summarized by the following list:

- a) Set widths of  $I_0$  slits
- b) Set sample ( $x, y$ ) position
- c) Set scan configuration
- d) Set amplifier sensitivities
- e) Set data storage information (folder, file group name, comments)
- f) Set number of scans
- g) Initiate a simple scan or a program of scans

The following sections of this document contain task-oriented descriptions of these operations ('how do I do this?'). In contrast, the Appendix contains a module-oriented description ('what does this do?') of the parts of the software suite which might be of interest to users (some of the software controls elements of the BL hardware which users do not need to know about, and should avoid disturbing). The guide assumes that the software modules which you need for each task are already open on the desktop, or that you know how to access them. But they may not be, or you may have accidentally closed (and lost) them. If so, refer to the Appendix to locate them.

Note that much of the software is similar or identical on both the bend magnet (BM20) and insertion device (ID20) stations. Many of the same tricks are or can be done at either station. The principal difference is in what experiments are more likely to be done at the different

stations. As a focused beam (KB-mirrors) is available on both lines mapping can in principle, be done on either beamline. Mapping is not usually done on BM20 because the flux is much lower (by about  $10^{*-3}$ ) than on ID20. The following sections labeled ID or BM are those experiments most likely done at those stations. If an experiment is not in that section it may be in the other section. The Appendix contains many menus that are common to both stations. Also note that in most cases the only difference between the software at the stations is a label of either BM or ID.

### 1.1. Detectors and Sensitivity Settings

The simplest detectors used on the both beamlines are ion chambers in the beam. These are typically used for measuring  $I_0$  and  $I_1$ . There are displays of these detectors which tell you the current signal. These are useful to watch when making any adjustments to the setup.

- Set sensitivity for the usual "scalar" channels (ion chambers and the like) so that reading is  $\sim 3v$
- A value of 5-7 on these meters indicates saturation, it may be much bigger than this so absolute signal has been greatly attenuated - reduce gain.
- $I_1$  may be simple transmission. It maybe called  $I_2$  and  $I_2$  sometimes called I-trans!!! Make sure you know which is which (the BL staff should make this clear)
- $I_0$  is generally always labeled as such.
- FY refers to a fluorescent detector (a Lytle box or a Vortex or a multi detector array sometimes called a "multi element detector" (This latter does not mean the number of Chemical elements which can be detected, rather it is the number of individual detectors assembled in the head. A 13 element has 13 separate detectors and so collects 13 times the count of one. Often some of the channels do not work properly and should be deleted from the recording.)

Caution: make sure you have correctly linked/labeled detectors so that it is clear which signal is coming in and what it is called. Labels may not always match. This is particularly true in the software where channel names may not match the input device. It is up to the user to name/label inputs in a consistent/logical manner. (Do ask the BL scientist to be clear on this.)

In general make sure you know where in the stream the signal is measured and how (ion chamber, pin diode, etc) it is measured and what control you have over it. You will need to know this to analyze your data.

Detectors that are listed as 'scalar' detectors include simple Ion Chambers ( $I_0$ ,  $I_1$ ,  $I_2$  etc), Lytle Type boxes, a TOTAL fluorescence (non selective as to chemical element) detector (both FY), TEY (Total electron yield) current detectors or a PIN diode fluorescence (FY) detector.

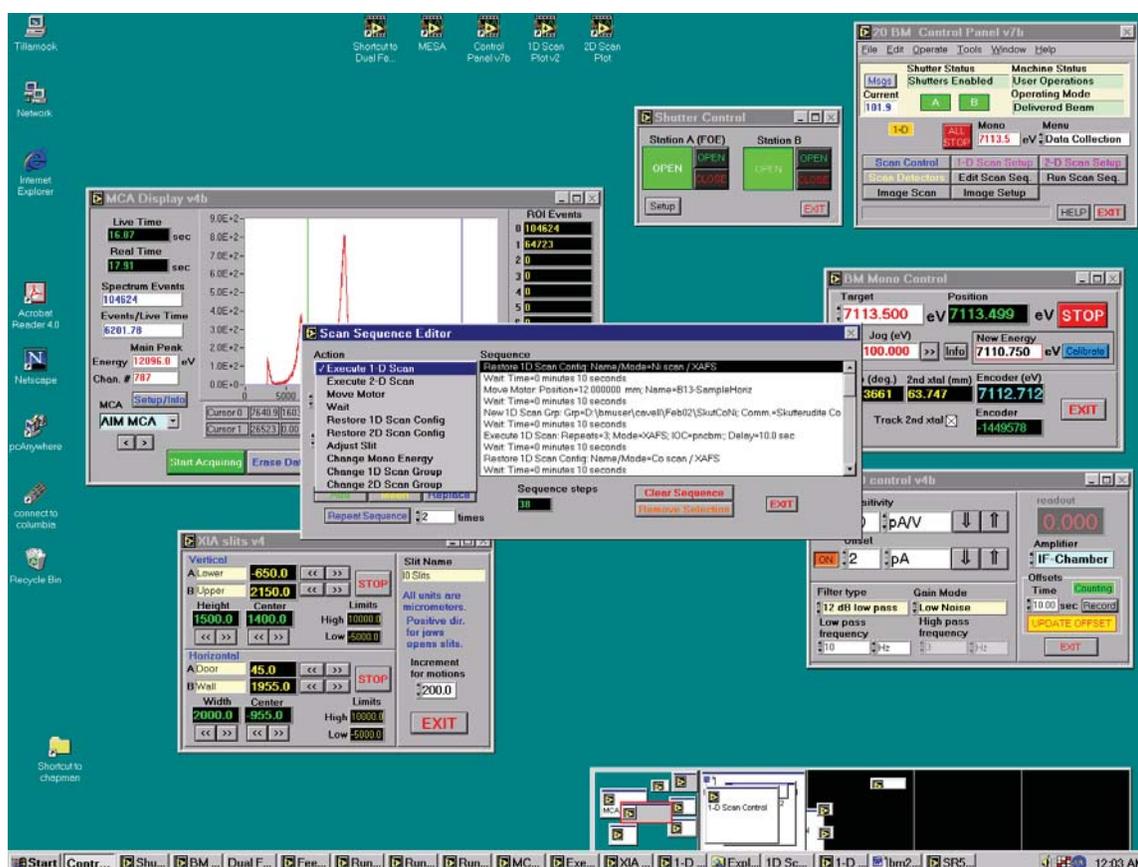
Fluorescence is also recorded by single component (element) solid state detector or multicomponent (ex. 7 element and 13 element units are available at PNC) solid state detector. These detectors discriminate on X-ray emission energy and so collect signals specific to a particular Chemical Element. You will need to select Regions of Interest (ROI) to direct your info to appropriate "bins". See MCA directions for further information.

ALL UNITS controlled by software (detectors - measured signals , motors - mono position (energy) etc) are called "Process Variables" and each has a specific numerical label in the system. Typically at PNC you will not be aware of that number BUT you must know what the "Labelled signal" properly corresponds to.

## 2. The BM20/ID20 data acquisition system desktop

Fig. 1 shows the desktop on the computer which is used to acquire XAFS data. It runs a familiar Win32 operating system. Typically the desktop presents a cluttered view, with many open programs (not all of which may be relevant for your purposes).

The computer runs a desktop management program called WinSpace which creates a number of so-called 'virtual screens' on to which running programs may be dragged. You can display a virtual screen on the main screen by clicking (with the mouse) the relevant rectangle of the WinSpace display. This will hide all programs from the current display. By distributing different programs among the five WinSpace screens you can reduce desktop clutter on the main screen.



**Fig. 1.** View of the BM20/ID20 data acquisition system desktop. The rectangular areas at bottom right are the WinSpace virtual screens.

### 3. Common User tasks

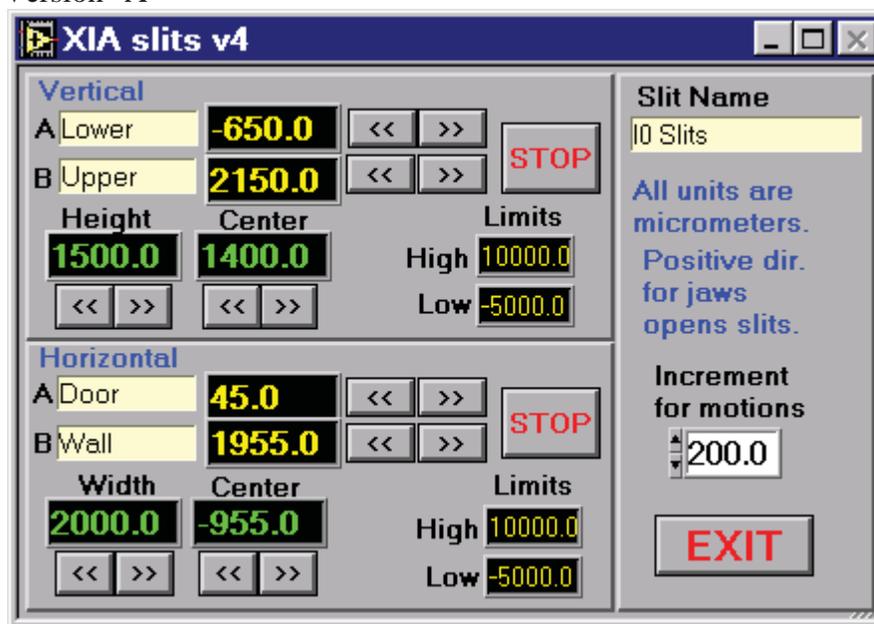
#### 3.1. Set widths of $I_0$ slits

Fig. 2 shows the **XIA Slits** dialog box which is used to change slit widths. This is more important for BM operation than ID operation (in the latter the beam is inherently narrow). This is not a frequent operation, but some samples may require it. The caption of the figure explains how to make the adjustment. (Note that there are possibly two different panels - see below). The slits define the shape of the beam which is allowed to enter the ionization chamber just in front of the sample ( $I_0$  refers to the current measured by this chamber, which is used as a photon flux normalization reference for XAFS spectra).

Typical maximum values for the BM (unfocussed) slit widths are 3000 (horizontal) and 1500 (vertical), both measured in microns ( $\mu\text{m}$ ). There is no point in opening up further than this. However, under some circumstances you may wish to narrow the slits, e.g. to study a small region of the sample.

The effect of reducing the slits is to reduce the photon flux impinging on your sample. You can see the effect of this by looking at the 'Io Monitor' output which is displayed on the rack near the computer.

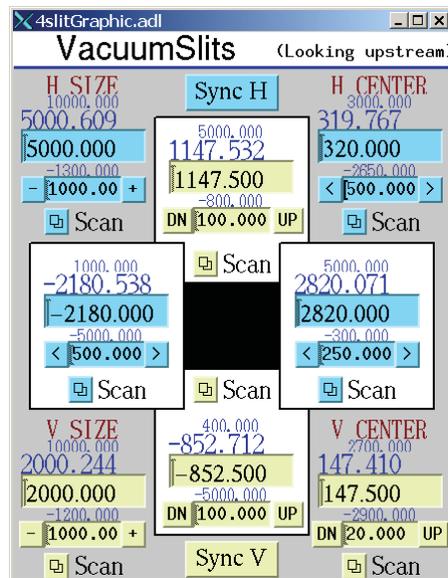
Slit Control Version "A"



**Fig. 2A.** Set widths of  $I_0$  slits. All units are microns ( $1000 \mu\text{m} = 1 \text{ mm}$ ). Note **Slit Name** at top right – there are other slits in the system which you should not change. Note that at the bottom of this panel you can set the increment for each motion step. Under normal circumstances, users should only modify the Height and Width settings. This is achieved by clicking the **Increase** [ >> ] and **Decrease** [ << ] width buttons on the vertical and/or horizontal slits. **EXIT** will close the dialog box, while **STOP** will halt the operation.

### Slit Control Version "B"

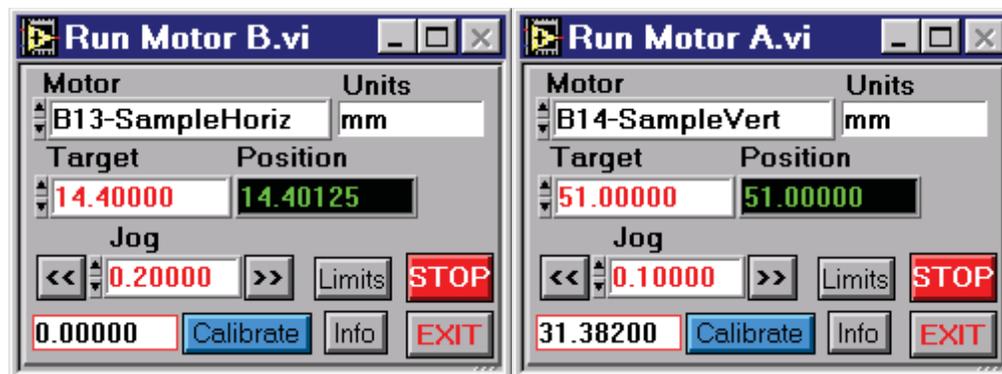
The installation of vacuum slits led to the revision of the slit control panel. The 2009 onward version is illustrated in Figure 2B



**Fig. 2B.** Control panel for Vacuum Slits. These define the width and height of the beam just before the Io chamber. Note **Slit Name** at top – there are other slits in the system which you should not change. Horizontal (width) and Vertical (height) pairs of blades are controlled simultaneously and each half moves relative to the center of the beam. The centering of the beam on the slits is something that the Beamline Scientist will have done prior to your arrival and you should NOT need to adjust the two "Center" items. All units are microns ( $1000 \mu\text{m} = 1 \text{mm}$ ). The actual size (e.g. H size 5000.609, a 5mm beam width) is given above the blue highlight box. The upper highlight value (5000 even) is the target width. Below is a second blue highlight box with +/- buttons - these are the "jog" increments for opening or closing the slits. Similarly the Vertical size controls are coded with yellow highlight boxes. Also indicated under each name is a number which gives the limit settings - you cannot exceed these (and generally you want a reasonable size Since the BM beam is already limited by the characteristics of the bending magnet there is usually nothing to gain by opening the vertical. You can set the increment for each motion step. Under normal circumstances, users should only modify the height and width settings. This is achieved by clicking the + or - buttons on the vertical and/or horizontal slits.

### 3.2. Set sample (x, y) position

The sample (x, y) position is modified by defining new coordinates which are set up by the mechanical drives (translators). Fig. 3 shows the dialog box for the horizontal (x) and vertical (y) translations. These will normally be open somewhere on the desktop. Note the description of the motors (e.g. B13-SampleHoriz) which identifies which is which. Different terms are used on BM and ID so be sure you know which motor controller controls the device you are using.



**Fig. 3.** Set sample (x, y) position (left: horizontal position; right: vertical position). You can either set a **Target** value (followed by the enter key), or **Jog** the position by the stated amount (which you can modify) using the arrow buttons [ >> ] and [ << ]. This illustration refers to the positioning of the multiple sample holder on the BM.

[Note careful- In focused (KB mapping) the x,y positions (of the beam on the sample) are labeled KB-Horiz, KB-Vert. These are the beam positions on the sample. Units are in microns because you will be working with micron-sized beams. In unfocussed operation (typically on the BM) the x,y positions are "Sample-Horiz, Sample-Vert and an array of samples can be placed on a multi sample holder and scanned automatically. The units of motion here are mm and this is appropriate because the beam size in the mm range and the new sample is to be moved into beam position. The size of the beam is controlled by the upstream slits (Sec 3.1).]

### 3.3. Set 1D Scan Configuration

The scan configuration defines the scan intervals, scan rate, and scan ranges of your XAFS measurement (intensity versus photon energy), which in BM20/ID20 terminology is known as a 1-D scan. The 1-D scan set-up is shown in Fig. 4, the caption of the figure explains how to do the set-up. (To map, a 2-D scan is setup - see later)

**Fig. 4.** Set scan configuration (XAFS scans are known as 1-D scans at BM20/ID20). The user must provide values for the step edge (**E<sub>0</sub>**), the **Boundaries** of the ranges, the sizes of **Steps**, and the **Integration Times**. The values shown here are for Ga. The **Integration Times** are often 1 or 2 s, rather than 4 s as shown here. Otherwise, the values are the standard ones which you will probably use yourself. (Often only **E<sub>0</sub>** is changed from scan to scan.). Note that the upper limit of the EXAFS range is expressed in terms of the wave-vector, **k**, ranging here up to 16 Å<sup>-1</sup> (**k** = 0 is assumed to coincide with **E<sub>0</sub>**). The corresponding energy width for the **k** extension in eV is listed below the input box (973 eV) and it is useful to note this. "Time Kwgt in EXAFS Region" is typically set to 0.0 as shown. Other parameters should be left at their default values - they refer to detector characteristics established by the BL scientists. Changes made to this dialog box are not transferred to the system until you click the button which has the word **Apply** in its caption. A red text message will come up when you edit any parameters to advise you that the changes have not been applied.

A scan set-up must be explicitly **applied** before it is ‘known’ to the system (This is UNIX at work). If you modify a setting and press exit, the next scan will continue to use the old scan settings. Scan set-ups can be saved to, or read from, the computer disk. A maximum of 10 set-ups is allowed, and usually all 10 have will already been defined by previous BL users. You will have to select an existing set-up, and replace it, if you wish to save your own settings (**Apply & Save** command). This command brings up the alarming orange-coloured warning box (telling you that 10 set-ups are already defined), which you can ignore.

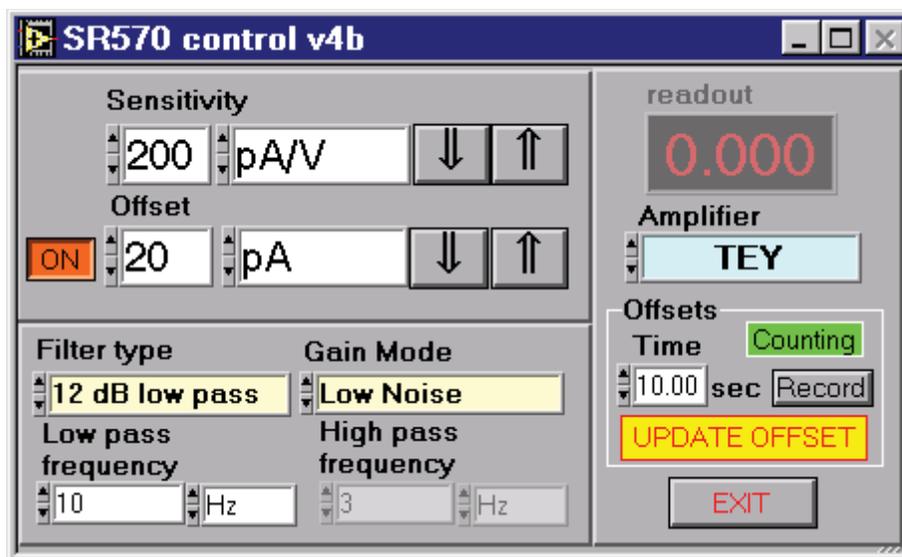
In summary, use the button commands at the bottom of the dialog box to:

- Read and apply a setup (**Restore & Apply**)
- Apply the set-up and then save it (**Apply & Save**)
- **Apply** the set-up (but don’t save it)
- Apply the set-up, and then start the scan (**Apply & Start Scan**)
- **Exit** (but don’t apply)

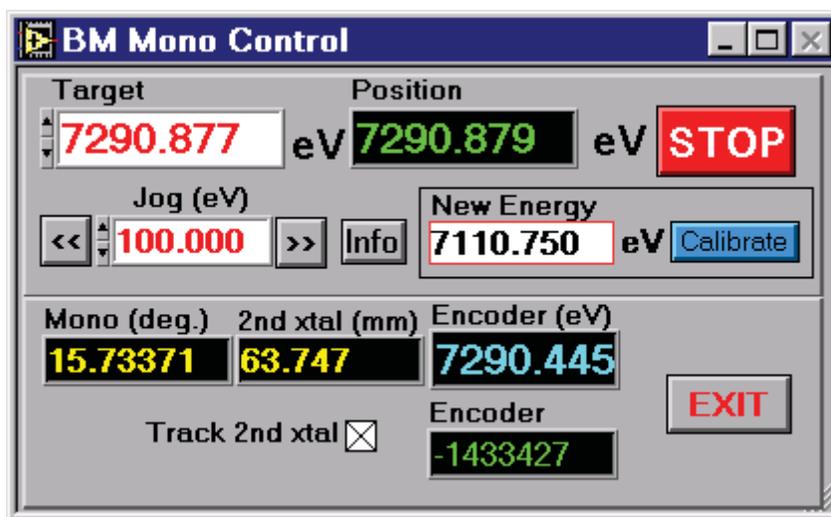
XAFS scans are divided into 3 regions (pre-edge, XANES, EXAFS), which are scanned differently. You can disable any of the region scales by depressing the **YES** buttons shown in Fig. 4. The standard scan mode scans EXAFS spectra on a linear range in  $k$ -space. The scan shown in Fig. 4 uses energy intervals of about 2-8 eV; the intervals increase as the scan moves further from the edge. Make sure the time intervals are the same in each portion of the spectrum to be collected otherwise you might

### 3.4. Set amplifier sensitivities

The need for this operation arises because the amplifiers are not linear over their full range. It is necessary to set their sensitivities so that the signal received from your sample falls in the middle of the amplifier working range. Fig. 5 shows the SR570 control dialog box which is used for this task, and explains what is involved. It will be necessary to check or set the sensitivity for every amplifier which you are using (including the  $I_0$  amplifier). Typically, that means setting 3-4 amplifiers:  $I_0$ ,  $I_2$ , (transmission), fluorescence, TEY. In practice the  $I_0$  sensitivity does not need adjusting very often. To prevent the output falling to near zero **or below**, an offset of 10% is added once the sensitivity range has been determined.



**Fig. 5.** Set amplifier sensitivities. First you must select an amplifier from the set which you are using: the **TEY** amplifier (used for total electron yield measurements) is indicated here. Then move the mono (monochromator) to the energy region(s) where you want to test the response (see Fig. 6), and adjust the sensitivity so that the readout never exceeds about 3.0 V (lower readouts, 1.0-2.0 V, are adequate). These energy regions are those in which you expect to get the highest amplifier response. Except for transmission data ( $I_2$ ) this corresponds to the region above the absorption edge. The  $I_2$  amplifier sensitivity should be set up in a region *below* the edge. Set the offset to 10% of the sensitivity range value (as shown in the figure). Other parameters should be left at the default values. After changing sensitivity or offset the 'UPDATE OFFSET' warning comes on. Press **Record** to update. This will automatically close the shutter and count for the time indicated. This will update all of the amplifiers.

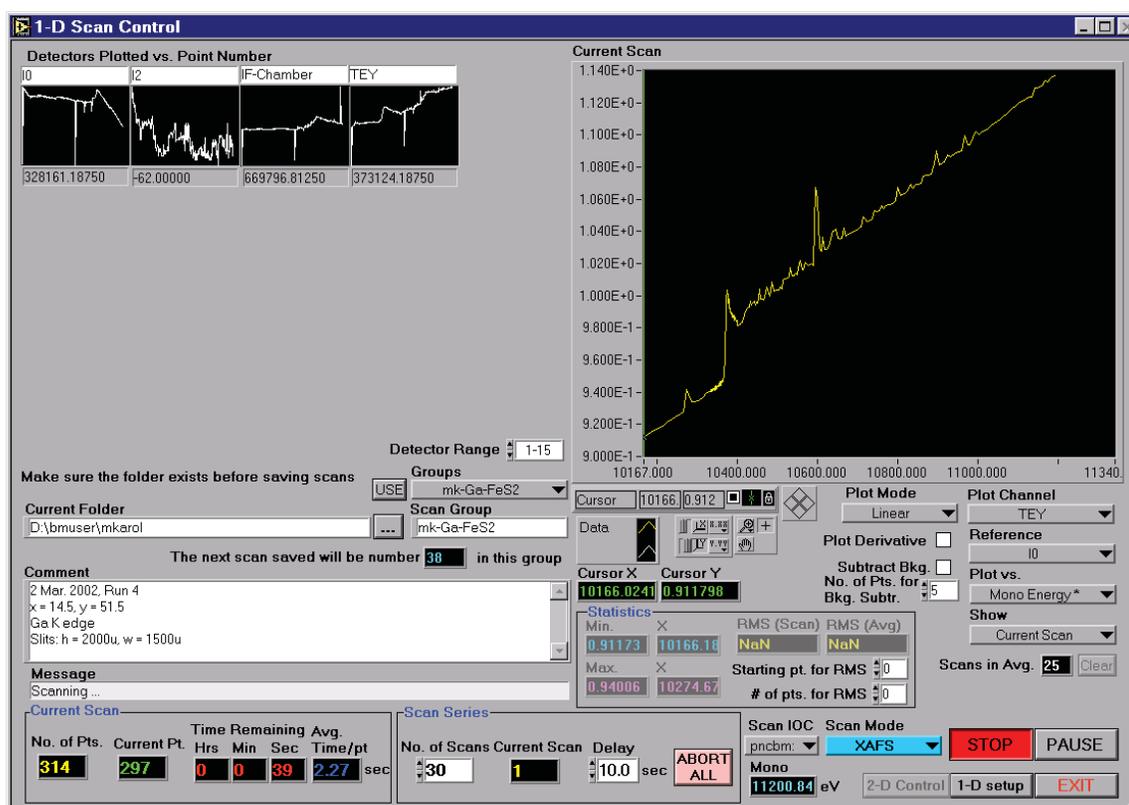


**Fig. 6.** Monochromator control. This control is used to manually adjust the current photon energy by changing the double crystal monochromator settings. You can select a **Target** energy, or you can **Jog** the monochromator by the amount specified. For example, you could move to an energy of ~8000.0 eV by entering '8000', or by hitting the **Jog** [ >> ] button 7 times in succession. If you choose to make a large move (1000 eV), you will be prompted for confirmation ('Whoa, Nelly!'). A move operation can be aborted by clicking **STOP**. The option to **Track 2<sup>nd</sup> xtal** (crystal) should be set as shown [X]. If you switch it **off**, the beam may move to a different position on the second monochromator crystal or even worse move completely off the second crystal completely making a disastrous reduction in flux (so no signal!!). Sometimes a small move is beneficial (e.g. if that spot happens to be bad), but usually this **is to be avoided**. Tracking the second crystal is kept "off" if working below 6000 volts of energy. Other buttons/parameters should not be clicked/adjusted by users.

Calibration is usually done by BL staff (especially at the beginning of your shift) but more seasoned users might want to do this.

### 3.5. Set data storage information

At this stage you should locate the 1-D scan control dialog box (Fig. 7). Recall info about setting folders in Introduction.



**Fig. 7.** 1-D Scan Control dialog box. This is the main window which you will use for monitoring the progress of XAFS scans. Most of the controls below the large chart on the right are concerned with how the data are displayed. The **STOP** button stops the current scan and moves to the next scan. It becomes a green **START** button when scanning is complete. To stop all scans, click **ABORT ALL**, or set the **No. of Scans** to the same value as the **Current Scan** index. **Pause/Resume** allows you to pause the scan and then resume.

Before starting the scan, you must specify the folder (which must exist before the scan starts), and enter a file group name, as well as any comments which you wish to attach to the data files. These tasks are straightforward, so long as you understand the file naming convention used by the software:

- **Current Folder:** folder in which data are stored (select via [...] button).
- **Scan group:** stem of data file names. For example, if the scan group is specified as **test** then scan 1 will be saved as **test.0001**, scan 2 as **test.0002** etc. You can either define a new name (simply by typing it into the Scan Group box (enter via "return" will immediately assign that name to the scan) , or use an existing group name (see next item)
- **Groups:** brings down a list of the scan groups found in the folder specified. If you choose one and press 'USE', the name will be transferred to the scan groups edit box. The next scan will be assigned the first free index number e.g. if **test.0009** is the last existing file in the group, the next spectrum you scan will be named **test.0010**.

### 3.6. Set number of scans

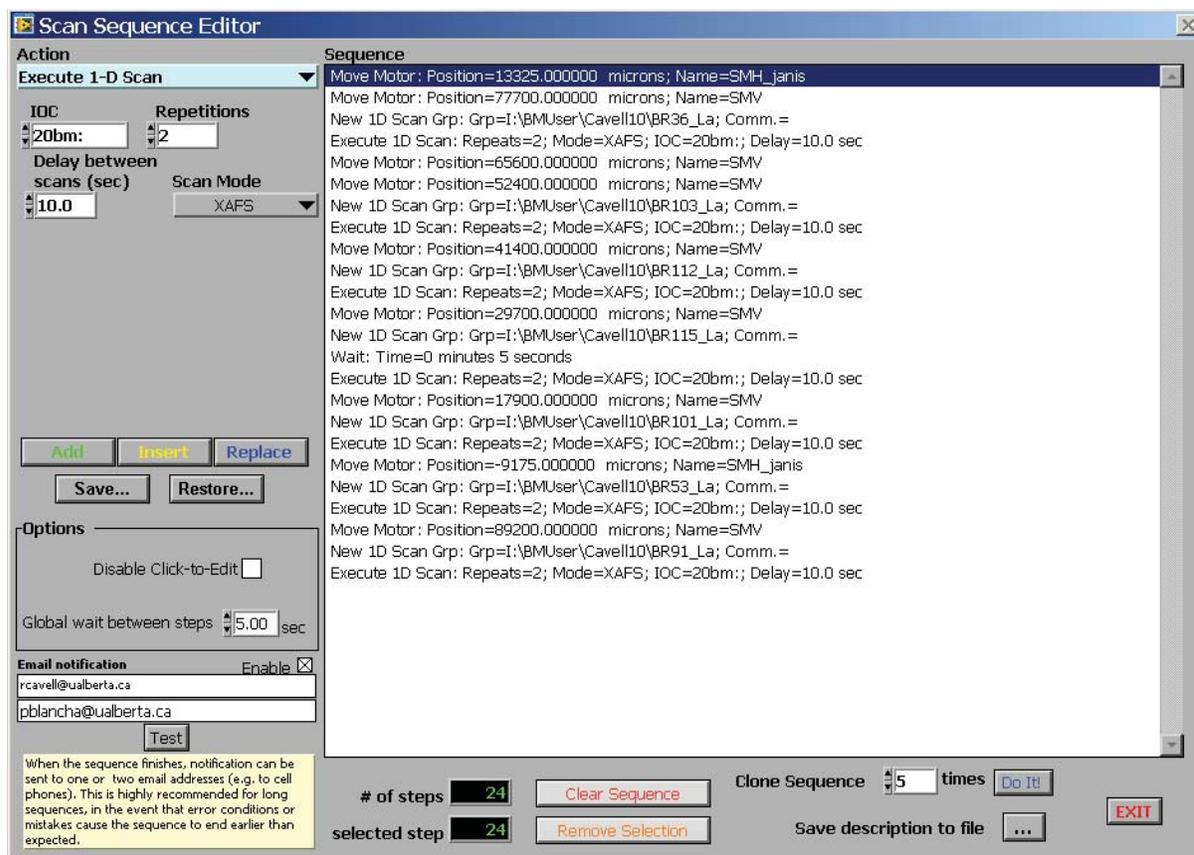
The **No. of Scans** parameter determines how many scans will be accumulated. It can be increased or decreased while the spectrometer is running. The **Current Scan** index indicates the progress of the scanning procedure during data measurement. The message **The next scan saved will be number XX in this group** indicates the number that will be attached as an extension to the data file (e.g. **test.0024**); if this is the first time you are using this group it will be identical to the current scan index.

### 3.7. Initiate a simple scan

Simple scans which involve a fixed set of parameters are initiated by clicking the **START** button in the 1-D Scan Control dialog box (see Fig. 7). The scan will follow the specifications defined in the 'set scan configuration' stage (section 3.3). You can stop, pause, restart or abort the scan. Each time a new scan starts, it will produce a data file with a unique name (e.g. **test.XXXX**, where the digits XXXX number the file). There are many other (optional) data display features of the 1-D Scan Control box. One useful feature which should be mentioned here is the **Show** option which allows you to display averaged spectra and/or the current scan. To use this feature, you must click the **Clear** button before the scan starts. This sets the accumulator to zero (clears previously collected data). The button is disabled during scanning.

### 3.8. Initiate a program of scans

Scans may be programmed to operate automatically. The program is specified via the Scan Sequence Editor (Fig. 8). The (blue) drop-down list provided under the **Action** field allows the user to select a series of operational steps (actions) and their accompanying parameters. It is recommended that after each action you insert a wait statement of about 10s which will allow the system to settle down.



**Fig. 8.** Scan sequence (i.e. scan program) editor. The actions are selected and defined by the controls on the left side of the window. An action can be **Added** at the end of the existing sequence, **Inserted** above the current position of the selection bar (black), or used to **Replace** an existing action. **Clear Sequence**: deletes all actions from the editor; **Remove Selection**: deletes the action under the selection bar; **Repeat Sequence**: duplicates the current sequence of actions  $N$  times, and appends them to the editor (this is very useful for writing long programs).

Note: Above, Line "New 1D Scan Group...SkudCoNi..." This is the specification to put the data in a new data file. Very IMPORTANT if you want to segregate results. All scans will be numbered sequentially .0002, 0003 etc as described above.

Note also that you can email to up to two addresses a notification of completion of sequence.

Most of the set-up operations described in preceding sections can be programmed. This is useful if you have to execute a sequence of highly repetitive tasks (e.g. scan three points on the same sample, or scan 4 elements on the same sample or measure one particular edge on many samples. The multiple sample holder will allow the order of 16 samples to be mounted, and moved into position with the sample motor controls (Sec 3.2).). However, the sensitivity settings of the amplifiers cannot be programmed. This restricts the use of programmed scans to jobs which have mutually compatible sensitivity settings.

Once you understand how to set up a simple scan, the individual programmed scan operations are quite easy to understand. However, as with all programming tasks, it is easy to do things in the wrong order. To reduce complexity, the following approach is suggested:

- Write the scan sequence for a single scan job, without using wait statements.
- After reviewing the program for correctness, insert wait statements after each action.
- Use the **Repeat Sequence** command to generate the number of scan jobs which you require.
- Make changes as necessary to actions in the program using the **Replace** function.

The program may be executed by clicking the Start Sequence button which is found on the Execute Scan Sequence window (Fig. 9). The button controls are self-explanatory (**Abort Sequence** will halt the execution of the sequence). The Pause, Stop, Start control buttons on the 1-D Scan control window (Sec 3.5) are operative - for example you can "pause" when an injection is being done.

The ID or 2D scan sequence must be defined.

Mode = "Co Scan" means the 1D XAFS scan parameters generated in "1D Scan Setup" AND Saved under that name in the list allowed. (If you are not changing ranges etc. then "Mode=XAFS" (etc) will pick up the currently available file instructions and execute those instructions - this is used when you are scanning the same edge in multiple samples.)



**Fig. 9.** Execute scan sequence window. The **Start Sequence** button will initiate the execution of the sequence (program) in a step-by-step fashion.

### 3.9. Display a scan

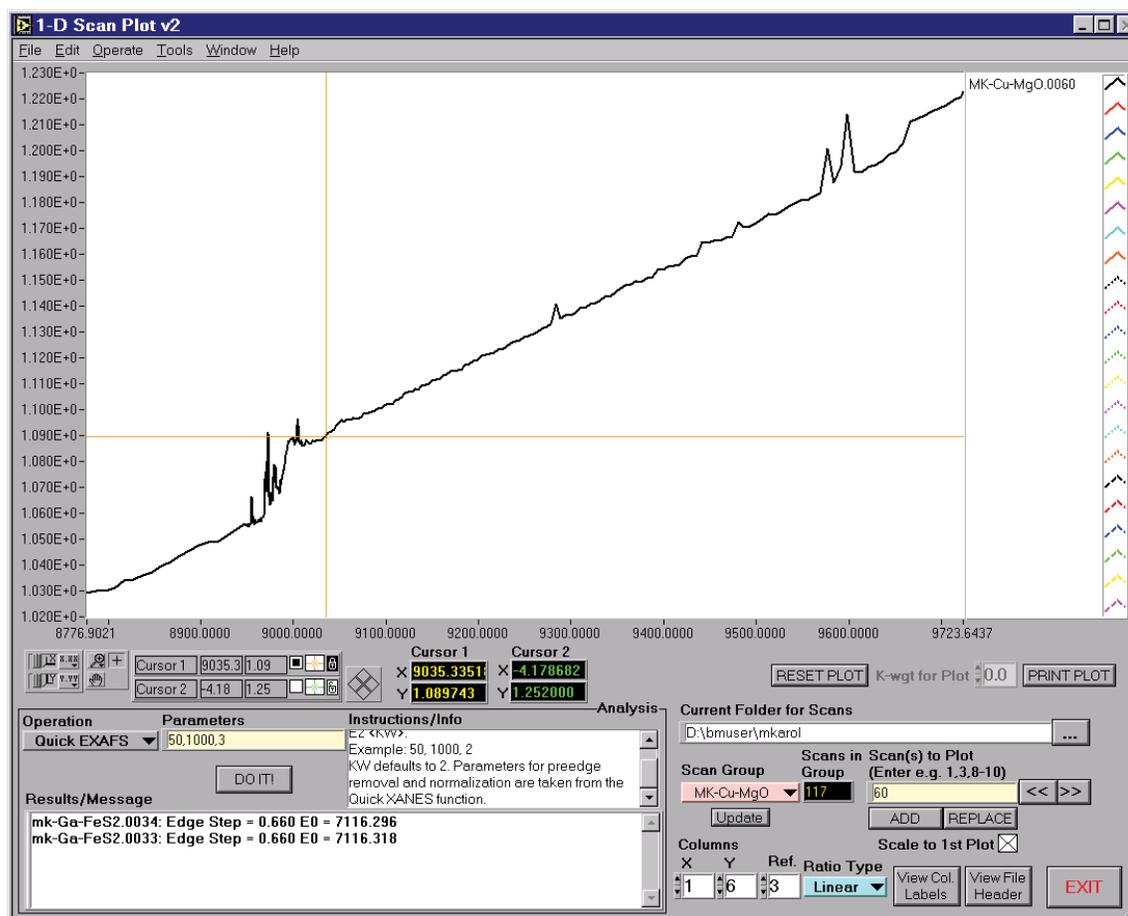
Fig. 10 shows the 1D scan plot window which can be used to display and print XAFS scan data files.

- Select **Current Folder for Scans**, (button marked [...]), and **Scan Group** of interest (via the drop down window). NB. the Scan Group information is only updated when you hit the update button.
- Set the number of the scan (i.e. scan 1 of scan group **test** refers to the file **test.0001**).
- Set the **Columns** to plot (**View Column Labels** will list the file format if you are uncertain).

- d) Don't forget to set the **Ratio Type** (**linear** for fluorescence or TEY spectra, or **log** for transmission spectra) and **Reference** ( $I_0$ ) column.
- e) To plot the spectrum alongside the existing plot click **ADD**, or click **REPLACE** to plot the spectrum by itself. If using the **ADD** option, note the **Scale to 1<sup>st</sup> Plot** option, which you will probably use.
- f) **View File Header** provides information about the data file, including user comments.

In the analysis box, there are various quick data processing options (intended to help the user assess the quality of the data). These operations (if you wish to use them) are accessed via the drop down box, e.g. Quick EXAFS in Fig. 10. You can use this option to extract some EXAFS oscillations, e.g. to assess the signal/noise ratio, or to compare data from two sources.

The buttons and labels just below the plot (**RESET PLOT**, **Cursor 1** and **Cursor 2** etc) are used for data display purposes. It probably better to explore these by yourself. These controls provide data display and exploration capabilities, e.g. area zooming, coordinate mapping.



**Fig. 10.** 1D scan plot window which is used to display and print XAFS spectra.

## 4. ID 20: Producing 2-D scan (Map)

### Abbreviations

<b>2-D</b>	two dimensions
<b>ID</b>	insertion devices
<b>ROI</b>	regions of interest
<b>MCA</b>	multiple channel analyzer
<b>Proc. Vars.</b>	process variables

### 4.1. Description

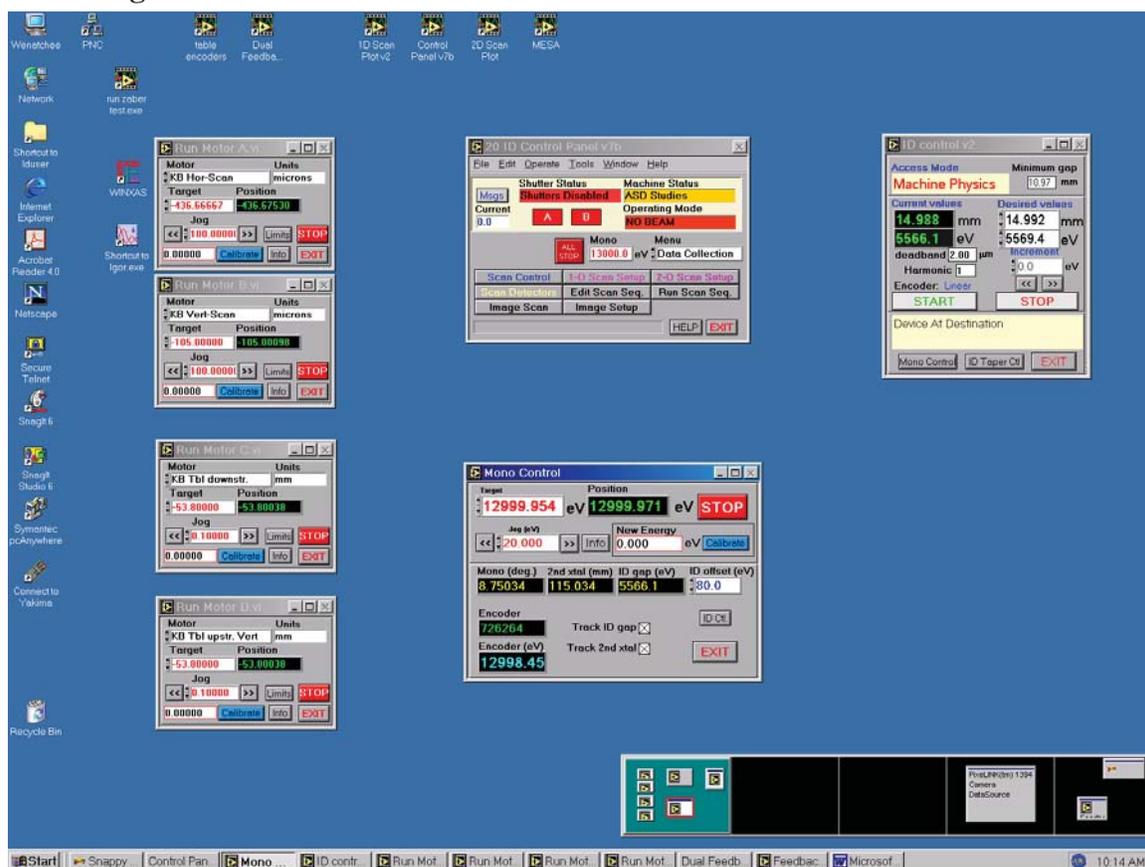
A 2-D scan is a map of elemental abundances within a selected rectangular area of the analytical sample. Maps are usually collected at one X-ray energy - high enough to excite all chemical elements of interest. The X-rays are analyzed in the Energy Dispersive detector and binned into separate files according to energy (and therefore identity). These files are displayed during the collection. The user can collect data on several elemental peaks during one 2-D scan by specifying the (energy) regions of interest (ROI) from a spectrum generated prior to map production. A 2D scan is most productive when the sample has been analyzed with other types of spectroscopy or examined by optical microscopy. 2D scans are a useful tool to identify interesting points for further EXAFS study. Caution should be exercised however as 2D mapping can consume much of the available beamtime. Many of the set-up procedures are identical to those undertaken on the BM beamline, and it is suggested that the user read BM sections of this manual..

This guide is intended as a work in progress, basic step-by-step guide to the manipulation of the computer software in the production of a 2-D scan and assumes that the analytical sample has been prepared, mounted within the beamline assembly, and properly lit. The identification of any errors in this text, or suggestions for its improvement would be gratefully received.

### 4.2. Active desktop configuration.

The production of a 2-D scan requires the user to specify various parameters before the scan can commence e.g. specifying the co-ordinates of the area to be mapped, setting the amplifier sensitivities etc. Therefore, at any one time during the procedure, the user will often find it easier to have several windows open, see **Fig 4.1**. In the bottom right of the screen five Winspace panels are visible. Four are black (inactive) and one is blue (active). The user can activate any panel by clicking on the black portion. The user can bring all the windows required at any stage in the procedure into a single panel by clicking and dragging the windows. Visible on the desktop are some of the windows for the program. Some of the following is identical to that described in the BM section above and some is described in the Appendix section of this manual.

**Figure 4.1: ACTIVE DESKTOP CONFIGURATION**



### 4.3. Check beamline orientation

#### Reason

To ensure accurate positioning of the beam and determination of the area to be mapped.

#### Action

Tape fluorescent or photographic ('burn') paper to the mount, ensuring that the paper is attached securely, and that it lies flat on the sample surface.

Open the beamline and record the beam dimensions on the screen in the console area by drawing around the beam rectangle using **non**-permanent marker.

(If this paper were also gridded you could confirm the actual dimensions of the beam as recorded on the screen).

Alternatively, phosphor can be placed around the sample to check the beam position by moving the beam over the phosphor. This assumes that the phosphor is at the same plane as the sample. As the sample is moved the apparent position of the beam will move outside of the marked box due to parallax. However, you can check the horizontal and vertical positions separately.

Ideally the cross-hairs on the screen should tally with the beam position. If the screen cross-hairs and the beam are in widely different positions, the user **MAY** consider **CAREFULLY** altering the camera position.

The beam takes several minutes to affect the burn paper but the result is more accurate than a determination using fluorescent paper.

*Carefully remove the burn paper without disturbing the position of the mount or sample or the cameras.*

#### 4.4. Defining the area to be mapped

##### Reason

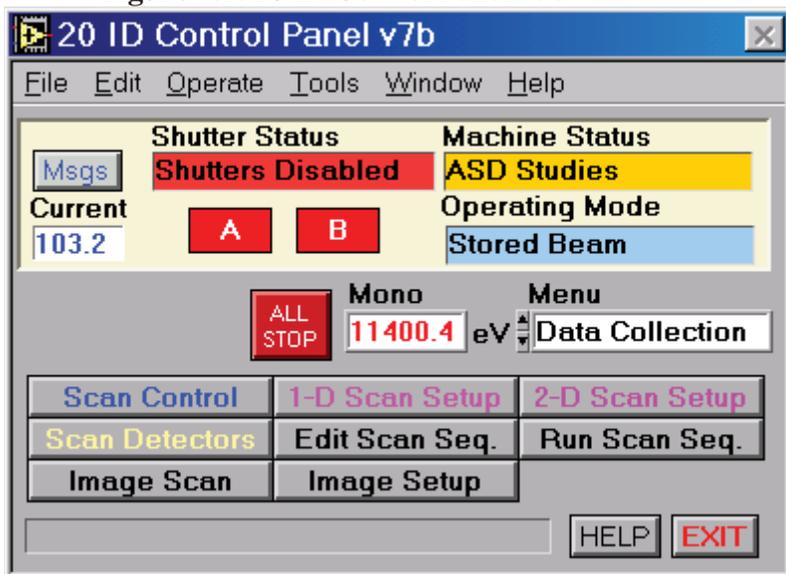
To provide the co-ordinates of the rectangular area to be mapped.

##### Action

Using ‘Run Motor A.vi’ and ‘Run Motor B.vi’ windows (Section 3.2) position the beam on the base-line left, base-line right, top left and top right corners in turn, of the rectangle to be mapped, and record in notebook the four co-ordinates on an annotated sketch.

Note that different motor selections within the ‘Run Motor ...vi’ window are associated with different units of measurement e.g. the ‘B13-SampleHoriz’ motor is measured in mm, whereas the ‘KB Hor-Scan’ (or the appropriate motor) which performs the same function is measured in microns.

**Figure 4.2.** 20 ID Control Panel v7b



Click on the up/down arrows on the ‘Menu’ box and select ‘Data Collection’.  
Click on ‘2-D Scan Setup’.

This takes the user to '2-D Scan Setup' window. The X-ray energy has been set with Mono Control by this time. Now the area to be mapped is defined by these motor controls.

**Figure 4.3. 2-D Scan Setup**

The screenshot shows the '2-D Scan Setup' window with the following configuration:

Lead Dimension				2nd Dimension			
Positioner	Start	End	Step Size	Positioner	Start	End	Step Size
#1 KB Hor-Scan	0.5000000	2500.0000	15.000000	#1 KB Vert-Scan	4000.0000	6000.0000	15.037594
#2 None	0.000000	1.000000	0.005000	#2 None	0.000000	1.000000	0.007519
#3 None	0.000000	1.000000	0.005000	#3 None	0.000000	1.000000	0.007519
#4 None	0.000000	1.000000	0.005000	#4 None	0.000000	1.000000	0.007519

Integration Time: 0.500 sec, Detector Settling Time: 0.200 sec, Scaler IOC: pncid: [dropdown], Estimated Scan Time: 5 Hrs 59 Min 21 Sec.

In the 'Lead Dimension' box, set the 'Positioner Settling Time' at around 0.1 sec. Under 'Positioner', click on the '#1' drop-down box and select e.g. 'KB Hor-Scan'. Enter the x (horizontal) co-ordinates, with the left-hand vertical co-ordinate in the 'Start' column and the right-hand vertical co-ordinate in the 'End' column.

In the '2<sup>nd</sup> Dimension' box, set the 'Positioner Settling Time' at around 0.1 sec. Under 'Positioner', click on the '#1' drop-down box and select e.g. 'KB Vert-Scan'. Enter the y (vertical) co-ordinates, with the base-line horizontal co-ordinate in the 'Start' column and the top horizontal co-ordinate in the 'End' column.

Note that you can use whatever motor or other control that is desired in the place of the KB controls mentioned above. In this way it is possible to make numerous kinds of 2D scans in addition to the physical scan of the sample described here.

The scan will then start in the base-line left corner and proceed through to the top right corner.

At the bottom of the '2-D Scan Setup' window, check the 'Integration Time' is around 0.1 sec (select time as appropriate for the sample), and the 'Detector Time' is around 0.3 sec.

Note that the 'Estimated Scan Time' is shown. The estimated time tends to be shorter than the actual time needed.

The scan time can be increased or decreased by

- changing the 'Step Size' in the 'Lead Dimension' and '2<sup>nd</sup> Dimension' boxes (this alters the 'Number of Pts' recorded in that dimension),
- changing the 'Number of Pts' (this alters the 'Step Size' in that dimension)
- changing the total area of the scan by entering different co-ordinates.

Make the step sizes the same in the 'Lead' and '2<sup>nd</sup> Dimension' boxes.

Depending on the purpose of the scan, a larger, coarser grained map or a smaller, more finely grained map can be produced.

Click 'Apply' and then 'Exit'.

The scan will not yet proceed.

#### 4.5. Produce MCA scan

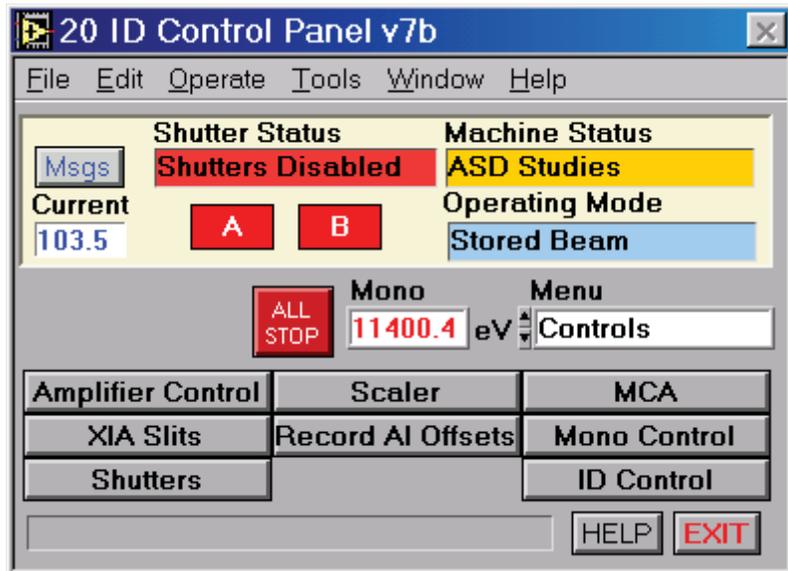
##### Reason

A MCA scan needs to be produced from a point on the sample to enable selection of the regions of interest (ROI), i.e. the range/s of the spectrum that encompasses the elemental peak/s the user has chosen to record and reproduce on the map.

##### Action

Position the beam on a spot (user choice) within the area to be mapped using 'Run Motor A.vi' and 'Run Motor B.vi' windows (Section 3.2) to adjust vertical and horizontal position.

Figure 4.5 20 ID Control Panel v7b



Click on the up/down arrows on the 'Menu' box and select 'Controls'.  
Click on 'MCA' which takes the user to 'MCA Display v4b'

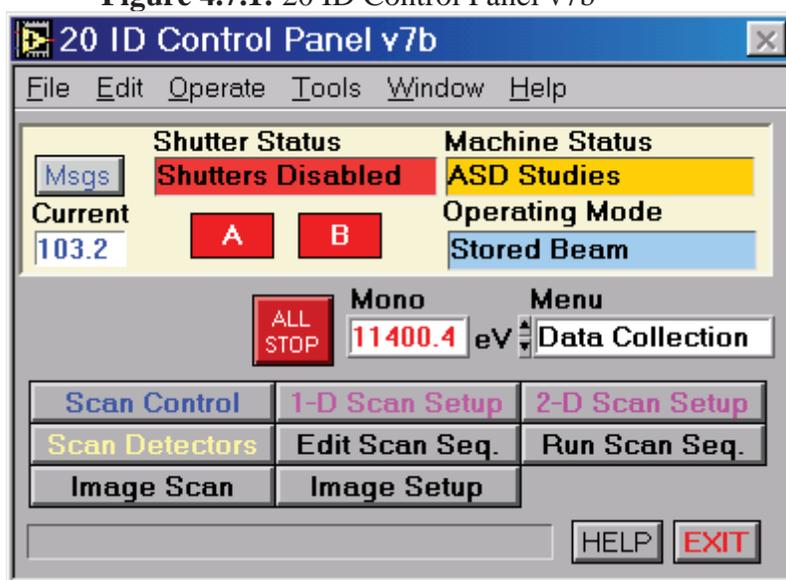
#### 4.6. Select ROI

A MCA scan is collected and the ROI's are selected. The details of collecting a MCA scan and setting ROI's is in Appendix B2.3: MCA controls.

## 4.7. Produce Map

Use scan control to produce the map. Go back to 20 ID control panel and select 'Scan Control'

**Figure 4.7.1:** 20 ID Control Panel v7b



You will then be asked to choose between 1D and 2D controls: select 2D (Appendix B1.1). This will bring up the 2D control panel.

### Insertion Device and Harmonic Control

The insertion device (ID) produces a peaked Energy distribution and to maintain signal it is necessary to (a) scan the ID Energy and (b) switch Harmonic Values.

In the case of (a) the Energy, this setting is offset by several eV from the output of the monochromator (the output off peak is smoother). It is possible to scan approx 5 eV range before resetting the ID energy. This increases the speed of data collection by reducing the number of "waits" between ID resets.

Harmonic	Energy Max or Range	Offset
1	11500	
3	12500 - 25000	

The feedback numbers are oft times a more precise value of the actual energy than the set points. The former is an encoder value which gives the Precise position of the monochromator

setting. It is of course only as good as the calibration. Consult with beamline staff before doing any recalibration - it may not be necessary!

### Tracking Second Crystal

As with BM operation, it is necessary to have "Track Second Crystal" ON to ensure that the geometrical relationship between the beam diffracted off the primary crystal is maintained so that the second crystal is able to again diffract the beam and send the X-ray beam out to the exit slit.

should be ON when making large energy region changes.

"Track Second Crystal" is usually turned OFF during EXAFS scans because this motion is a source of noise in the signal. Since an EXAFS scan is generally smaller than 1500eV, the beam remains focused on the second crystal for the duration of the scan.

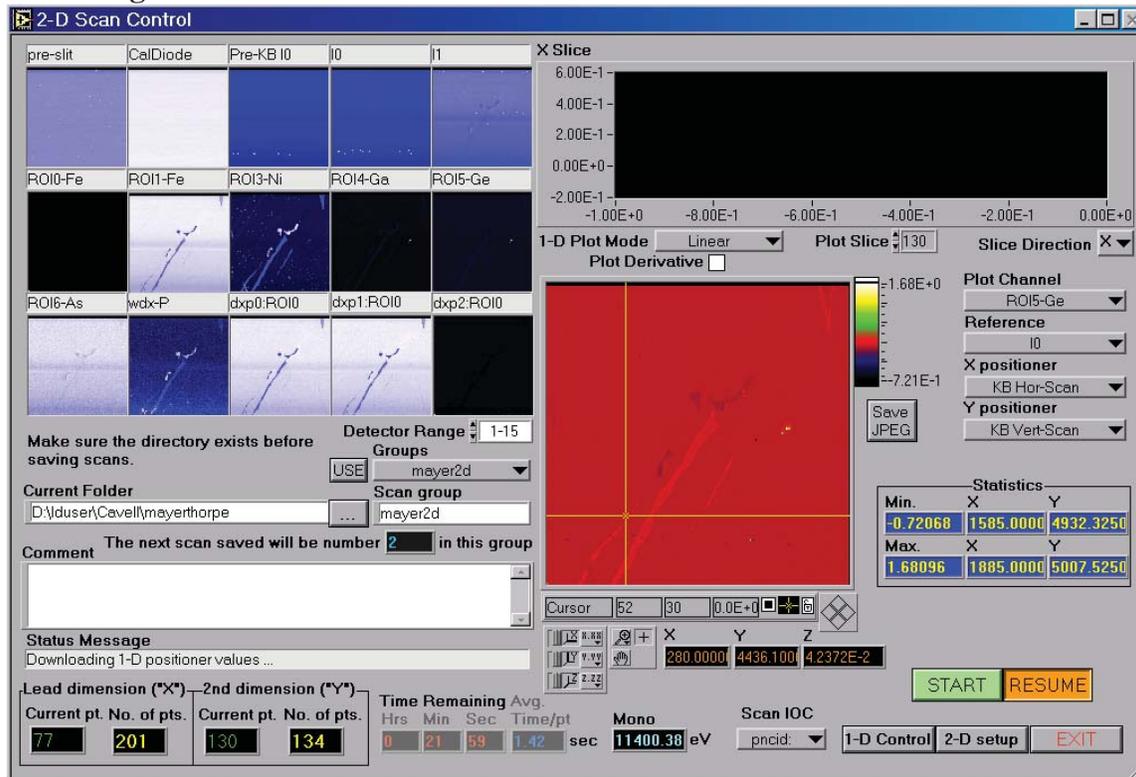
The strategy is to move the monochromator with "Track Second Crystal" ON to the mid point of the EXAFS scan and then turn it OFF. The second crystal will generally maintain a correct relationship through the EXAFS scan.

Caution: Consult Beamline Staff before doing any recalibration. It may not be necessary.

### Calibration Procedure:

[Note: The encoder may return an erroneous value for E; the encoder will have the exact angular position of the monochromator crystal (which rotated to do the Bragg Energy selection) BUT its conversion factor may be incorrect. Thus (encoder x conversion factor) gives a value on screen as "Mono Energy" which may be grossly incorrect.] See Caution above.

Figure 4.7.2 2D Scan Control



Choose the folder to put the spectrum in using the Current folder control. The Groups menu gives groups that are present in the folder or a new group can be entered under Scan group. Pressing 'enter' after typing a name in the scan group box will update the groups menu as well as select that group for the current scan group. The comment field can be used to add any comments to the saved file. It is a good idea to put information in the comments file such as the identity of the sample and the coordinates used for the map.

The boxes on the upper left will show the maps for each of the selected detectors. Note recent changes to the detectors may not be in the list but will be updated when the scan is started.

The field in the center shows the map as it is scanned. The map that is displayed is controlled by the pull down menus on the right hand side of the control panel.

The scan is started using the 'START' button. The scan can be paused and resumed using the 'PAUSE/RESUME' button. The 1-D control panel and the 2-D setup panel are accessed using the buttons in the lower right hand corner.

NB: If you pause (Beam Dump etc) note that the map is NOT saved at this point. To save the map (and the data that you have collected to this point which may well be very useful) you must activate "STOP". You will get the violent orange message "ABORT" screen with 2 options - "Stop immediately" or "Stop at end of scan" Choose most appropriate for your

situation and "Select". The data collection will cease AND THE SCAN FILE WILL BE SAVED.

### Observing the Map

On working with the displayed maps it is useful to remember that if one moves the cursor to a point on the map and clicking "move to cursor" the (x,y) stage will move to put the beam on that point on the map.

## Appendix

### A. CONTROL PANEL

The BM20/ID20 Control Panel windows (see Fig. A1) provides access to all functions of the BL (NB. don't confuse this with the Windows Control Panel). The functions are organized into several categories, which are selected from the **Menu** list, as shown in Fig. A1 for BM20.

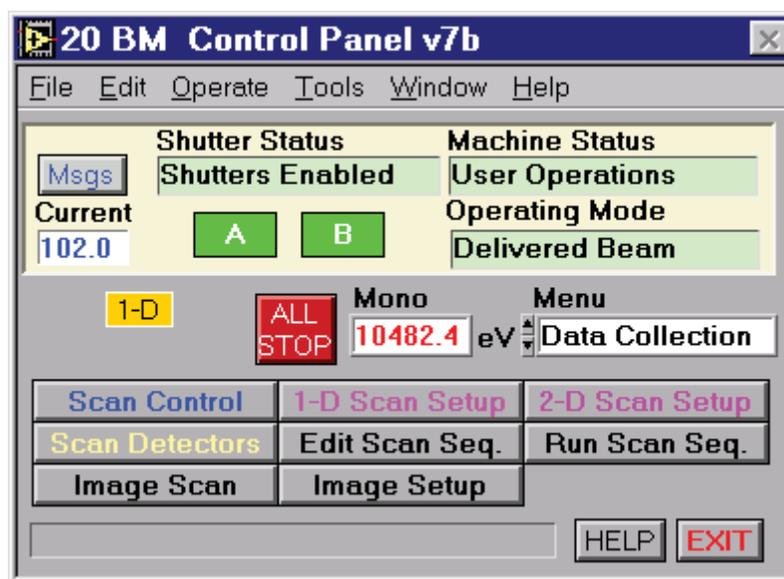
#### Beamline Setup

**Motors** (rarely needed)

**Displays** (rarely needed)

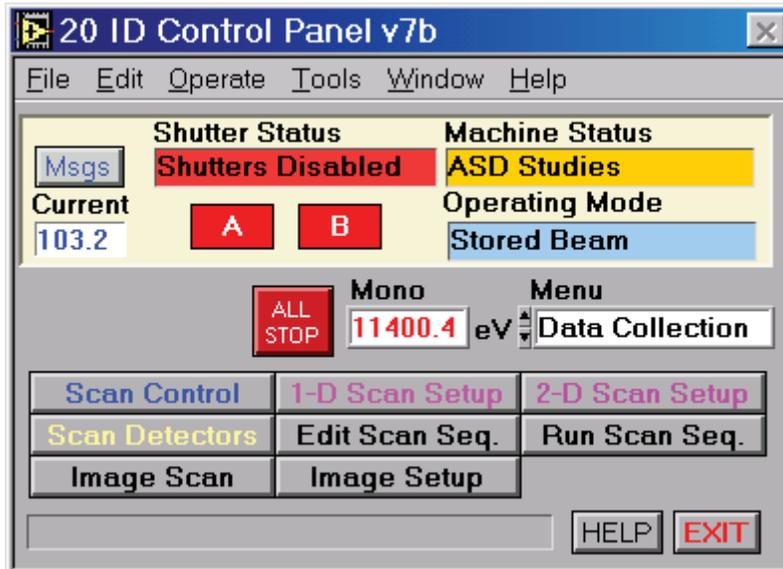
**Tables** (rarely needed)

For each menu category, a new set of buttons comes up, which changes the appearance of the window drastically. Each of the buttons has an associated window or dialog box which comes up when you click the button. These are the same dialog boxes that are normally found scattered around the computer desktop. Therefore, if you close a dialog box by mistake, and want to reopen it, you can probably find it by looking carefully through the menu items on the Control Panel dialog box.



**Fig. A1.** BM20 Beamline Control Panel showing the Data Collection menu items as buttons (Scan Control etc.). The Control Panel buttons in themselves don't initiate any commands, so you can explore them without risk. In 2 or 3 cases, a warning box will come up telling you that something has not been set up. If in doubt, just exit. If the dialog box is already open somewhere it will be brought to the fore of the screen. The default virtual screen will also be displayed.

The ID20 Control panel is similar. And is used in the same manner as the BM20 control panel.



**Figure A2.** ID20 Control Panel showing Data Collection menu. The current beam status is shown here.

## B. MENU ITEMS

The menu items in this section are found in the software on both beamlines. In some cases a panel may be labeled as BM or ID.

### B1. DATA COLLECTION MENU

Fig. A1. Shows the appearance of the Beamline Control Panel when the **Data Collection** menu item is selected. The functions of the various buttons associated with this menu item are now summarized.

#### B1.1. Scan Control

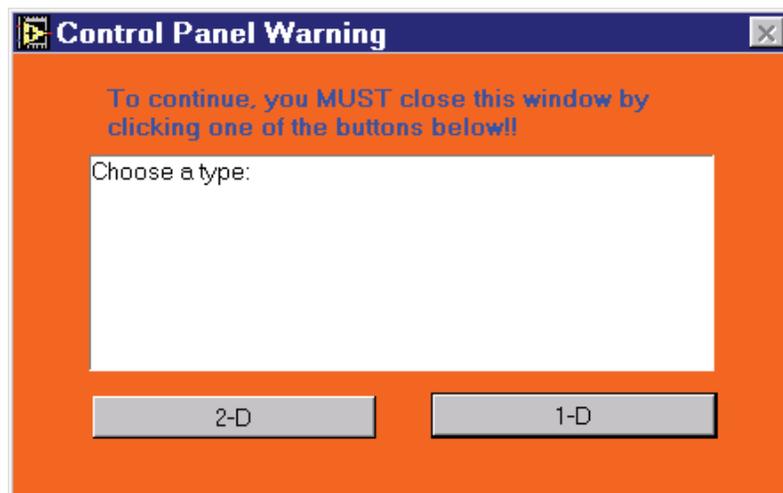


Fig. B1.1.

The 'Scan Control' brings up a cryptic warning box, Fig. B1.1, which asks the user to select a 1D or 2D scan). On the BM station the 1D scan is typical while 2D is often used on the ID station.

## B1.2. 1D Scan Setup

This button has the same function as the button with the same title which is found on the 1-D scan.control dialog, i.e. it brings up dialog box used to set up EXAFS/XANES scans (Fig. B1.2). See section 3.3 (above) for a description.

**1-D Scan Setup**

File Edit Operate Tools Window Help

**Scan Mode**

XAFS Multiple-region scan of monochromator energy.

E0: 10367.000 eV No. of Pts.: 314 Positioner Settling Time: 0.100 After Scan: Stay at scan end point

Include Region?	Boundaries	Steps	Integration Times
Pre-edge YES	-200.000 eV	10.000 eV	4.000 sec
XANES YES	-30.000 eV	0.500 eV	4.000 sec
EXAFS YES	30.000 eV	0.075 (k)	4.000 sec

16.000 (k) Time Kwgt in EXAFS Region: 0.0

Estimated Scan Time: 0 Hrs 21 Min 43 Sec (Not including time to move positioners)

Integration Time: 0.500 sec Scaler IOC: pncbm: Detector Settling Time: 0.050 sec Dummy positioner dwell time: 0.050 sec

Scan IOC: pncbm:

"Apply" saves changes for *displayed* scan mode

Select Detectors Define a Positioner Restore & Apply Apply & Save Apply Apply & Start Scan EXIT

Fig. B1.2

### B1.3. 2D Scan Setup

This is irrelevant for XAFS scans. The button brings up the window shown in Fig. B1.3 (which is used for imaging applications, Section 4.4).

**2-D Scan Setup**

File Edit Operate Tools Window Help

**Lead Dimension**

Positioner Settling Time Number of Pts  
 #1 None 0.10 sec 10  
 #2 None 0.10 sec 10  
 #3 None 0.10 sec 10  
 #4 None 0.10 sec 10

Positioner	Start	End	Step Size
#1	0.000000	1.000000	0.111111
#2	0.000000	1.000000	0.111111
#3	0.000000	1.000000	0.111111
#4	0.000000	1.000000	0.111111

\* denotes a generalized EPICS positioner. \*\*denotes a non-EPICS positioner.

Dwell time for dummy positioner: 0.050

**2nd Dimension**

Positioner Settling Time Number of Pts  
 #1 None 0.10 sec 10  
 #2 None 0.10 sec 10  
 #3 None 0.10 sec 10  
 #4 None 0.10 sec 10

Positioner	Start	End	Step Size
#1	0.000000	1.000000	0.111111
#2	0.000000	1.000000	0.111111
#3	0.000000	1.000000	0.111111
#4	0.000000	1.000000	0.111111

\* denotes a generalized EPICS positioner. \*\*denotes a non-EPICS positioner.

Dwell time for dummy positioner: 0.100

Integration Time: 0.100 sec  
 Detector Settling Time: 0.050 sec  
 Scaler IOC: pncbm  
 Estimated Scan Time: 0 Hrs 0 Min 26 Sec  
 (Doesn't include time to move positioners)

Scan IOC: pncbm

Changes have not been applied!

Buttons: Clear Positioners, Select Detectors, Define a Positioner, Restore & Apply, Apply & Save, Apply, Apply & Start Scan, EXIT

Fig. B1.3

## B1.4. Scan Detectors

This button brings up a dialog box (**Scan Detector Selection**), Fig. B1.4, with a list of detector-derived quantities ('process variables') whose output can be selected for use in an XAFS scan. Various list-editing functions are provided by buttons on the dialog box. This window is used after a new detector has been installed.

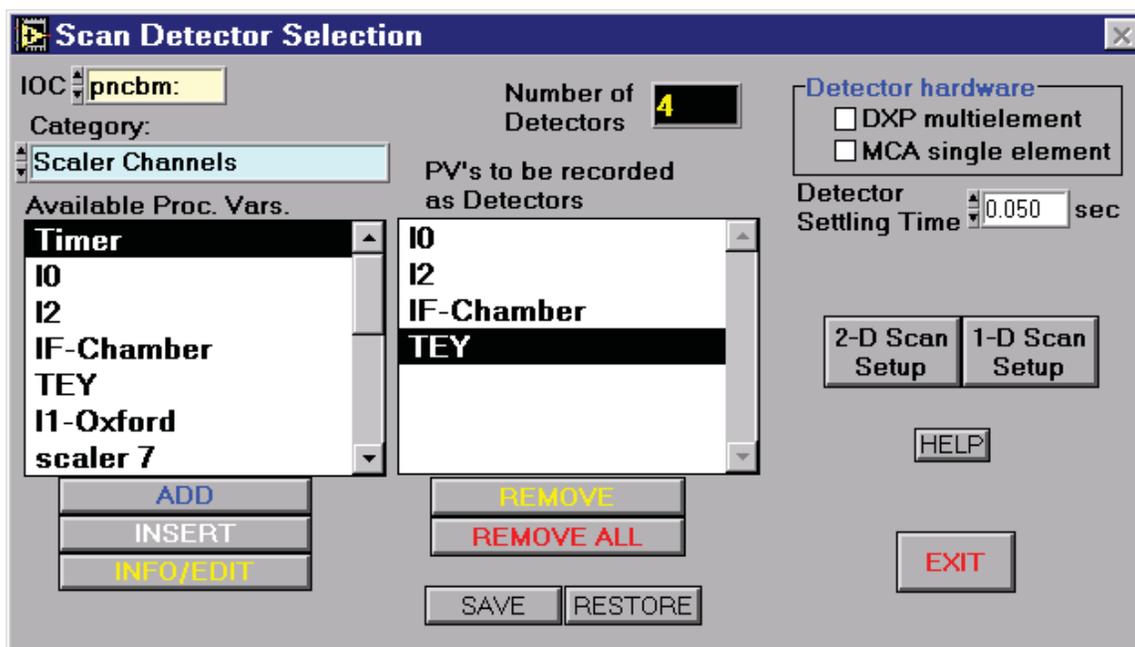


Fig. B1.4

The '**Scan Detectors**' is used to select which detectors are being used and direct the output of the detectors to the display and output file. The detectors are divided into categories and it may be necessary to search to find the desired detector. The desired detector is highlighted under '**Available Proc. Vars.**' and the '**ADD**' button is pressed. This adds the detector to the '**PV**' list next to it. Note that the name put in the PV list is not necessarily the same as the detector name. The name in the PV list is edited by selecting the detector and pressing '**INFO/EDIT**'. The name chosen for the PV list will be the one used for display purposes and for labeling in the data file. It is best if the name chosen is somewhat meaningful to avoid confusion later on.

The UserCalcs (Appendix E) are selected here. A typical application is to define a UserCalc to take the output from each element of (say) the 13 element detector and sum the signals for one particular ROI. In this case, it is useful to number the UserCalc and the ROI with the same number. It is also useful to name the PV with the element that was chosen.

NB Cannot do 1 scan here - i.e a line scan changing only H or V alone. This must be done with the generic 1D scan control.

### B1.5. Edit Scan Sequence, Run Scan Sequence

These buttons bring up the dialog boxes used to program (Fig. B1.5.1) and execute scan sequences (Fig. B1.5.2). See section 3.8 (above) for description.

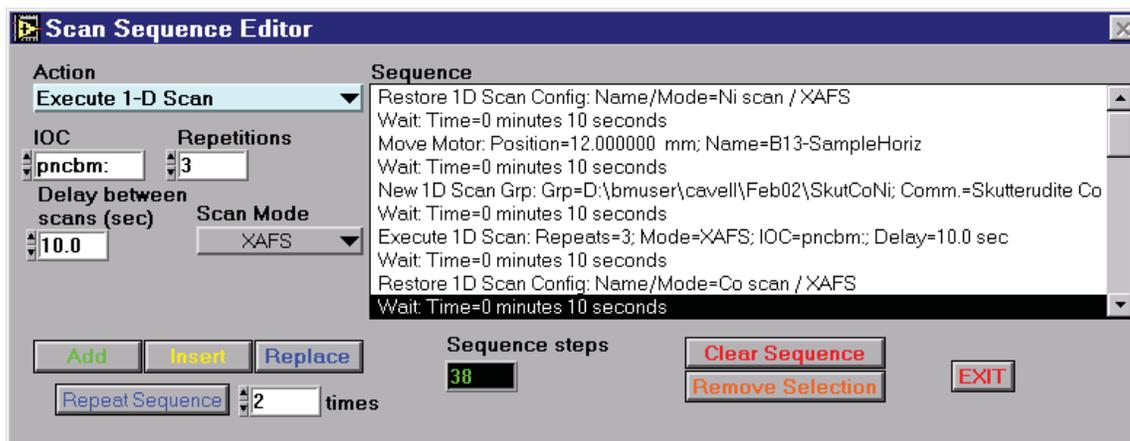


Fig. B1.5.1



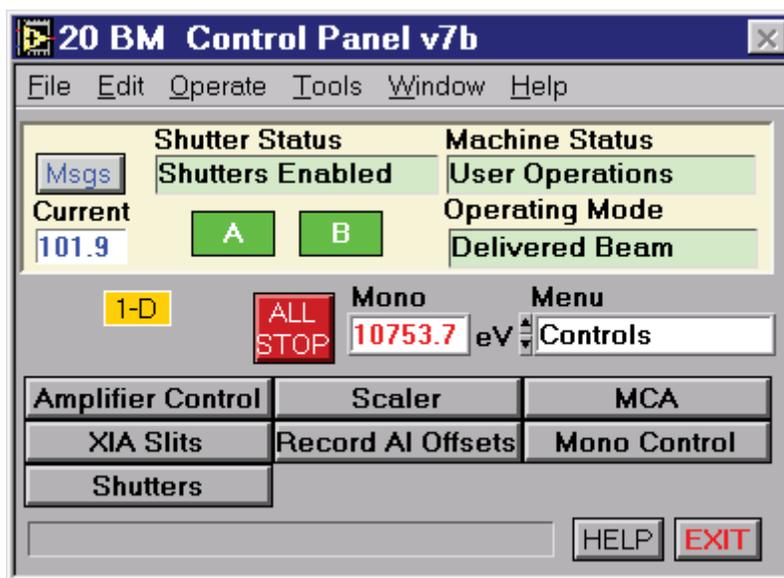
Fig. B1.5.2

### B1.6. Image Scan and Image Setup

These functions refer to imaging applications. They are not used for XAFS scans.

### B2 Controls Menu

Fig B2 shows the Beamline Control panel with the Controls menu item selected.



**Fig. B2.** Beamline Control panel with Controls menu item selected.

## B2.1. Amplifier control

The associated dialog box is shown in Fig. B2.2. The controls are discussed in section 3.4 (above). You will probably get a warning if you have reason to open this dialog box for the first time (just ignore it).

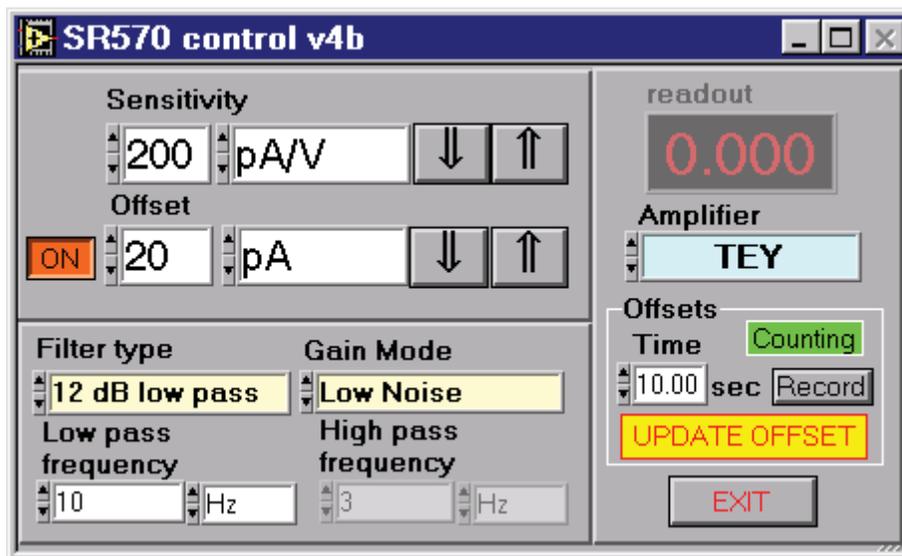


Fig. B2.1.

## B2.2. Scaler control

This window (Fig. B2.2) is used by BL staff to define the quantities which constitute the measurable process variables. Once set, the general XAFS user should have no need to modify the parameters.

**Scaler Control**

NOTE: Display shows offset-corrected scaler counts

Channel	Name	Counts
1 (A)	Timer	0
2 (B)	I0	472612
3 (C)	I2	-51
4 (D)	IF-Chamber	361975
5 (E)	TEY	618423
6 (F)	I1-Oxford	0
7 (G)	scaler 7	0
8 (H)	IF-AmpTek	0
9 (I)	scaler 9	0
10 (J)	scaler 10	0
11 (K)	scaler 11	0
12 (L)	scaler 12	0
13 (M)	scaler 13	0
14 (N)	scaler 14	0
15 (O)	scaler 15	0
16 (P)	scaler 16	0

STOP

Preset Time: 2.00 sec  
Elapsed Time: 0.10 sec

**Scaler Calcs**

Name	Expression	Result
I1-IonChamber	C/B	-0.0001
I1/I0	F/B	0.0000
I2/I0	C/B	-0.0001
PIN-Down/I0	E/B	1.3085
(Up-Down)/I0	(D-E)/B	-0.5426

Enter calculations using the variable assignments shown at left (1->A, 2->B, etc). Enter a descriptive name in the fields next to the scaler channels and scaler calcs.

Integration time: 10.00 sec

Offset

Record Offset

UPDATE OFFSET

EXIT

Fig. B2.2.

### B2.3. MCA controls

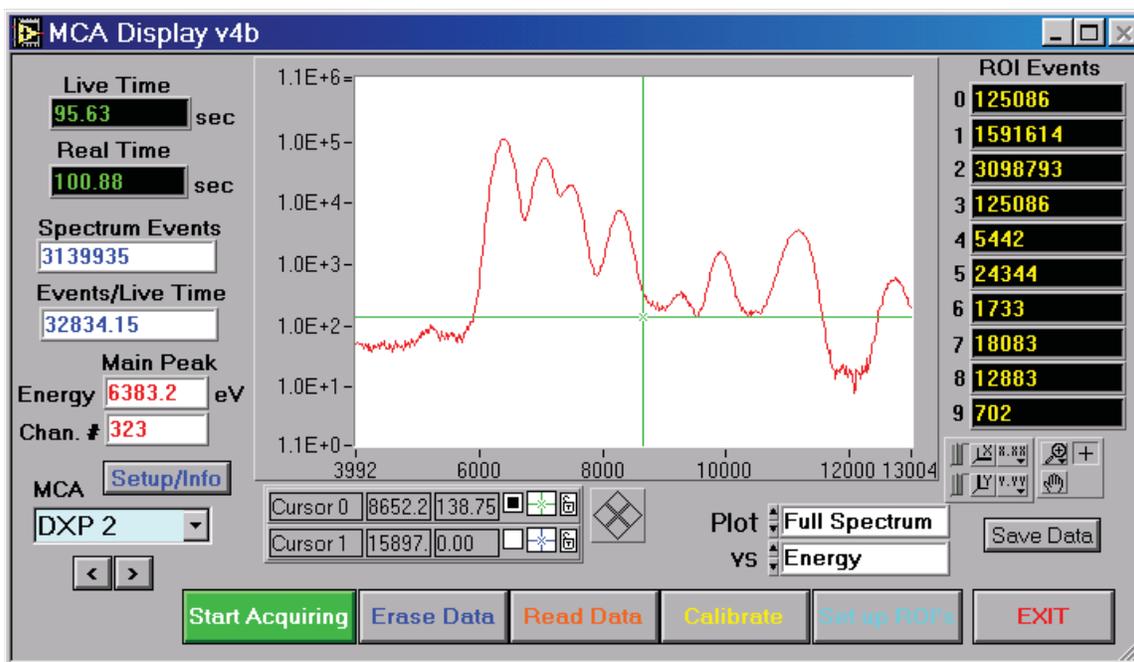


Fig. B2.3.1

The MCA controls shown in Fig B2.3.1 are used to run a MCA scan to set the ROI's for the solid-state detectors. Running a spectrum with the MCA is straightforward: select detector under **MCA**, click **Erase Data** followed by **Start Acquiring**. DXP 2 is the usual selection for the 13-element detector. Plot 'Full Spectrum vs Energy'. It takes ~60-300s to get a good spectrum. Keep the MCA screen open so you can check back: this screen is calibrated and shows energy as the scale.

The '**Live time**' and the '**Real time**' should be fairly close to each other. The '**Events/Live Time**' shows you how much signal you are getting. For a map, a signal in the range of 50,000 to 75,000 is best. For an EXAFS scan a signal of less than 50000 works better to avoid saturation of the detector.

To set up ROIs hit the **Set up ROIs** button. The regions are defined by manipulating the positions of the vertical lines with the mouse.

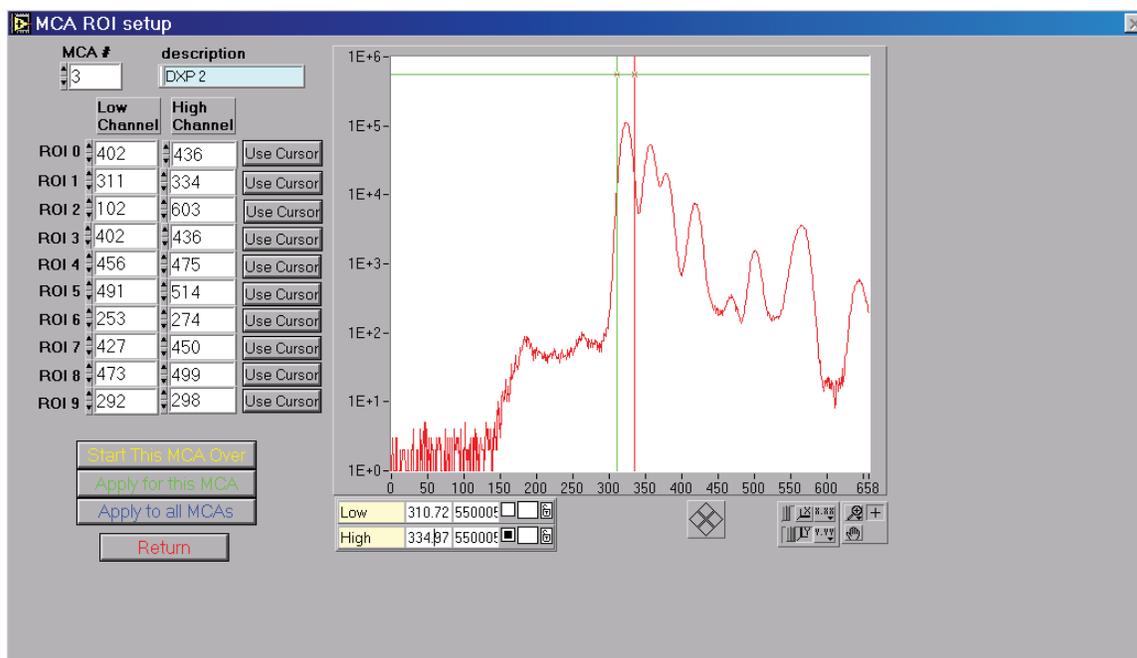


Fig B2.3.2

The green line defines the left edge and the red line defines the right edge. Note that you cannot move the left line past the red or vice-versa. When the area is selected a ROI is defined by pressing the 'Use Cursor' button next to the desired ROI. The area can also be entered manually in to the 'Low Channel' and 'High Channel' columns. Each region of interest is set up in this manner. Note that the x-axis scale is not in energy but in channels. Refer to the previous panel for energy of each peak. Once all the regions are selected press the 'Apply to all MCAs' button to apply the regions of interest. A small window will appear and ask which detectors to apply to. In general you want to apply to all detectors 'of this type'. You will then return to the main MCA display.

**CAUTION:** The detector type is displayed under 'description'. Be sure that the correct detector is selected as the panel may start with a different detector than the one selected in the previous panel.

Note: Matching ROI numbers and UserCalc numbers is a good way to ensure that it is clear which UserCalc is being used for a particular ROI. Record the ROI's and the elements in your notebook.

It is possible to calibrate the energy scale in the main MCA panel. To do so press 'Calibrate' in the main window. The calibrate window appears. For example to calibrate to a known peak, use the blue cursor to select a peak for which you know the energy value. The new energy is entered into the control box and press 'Calibrate'.

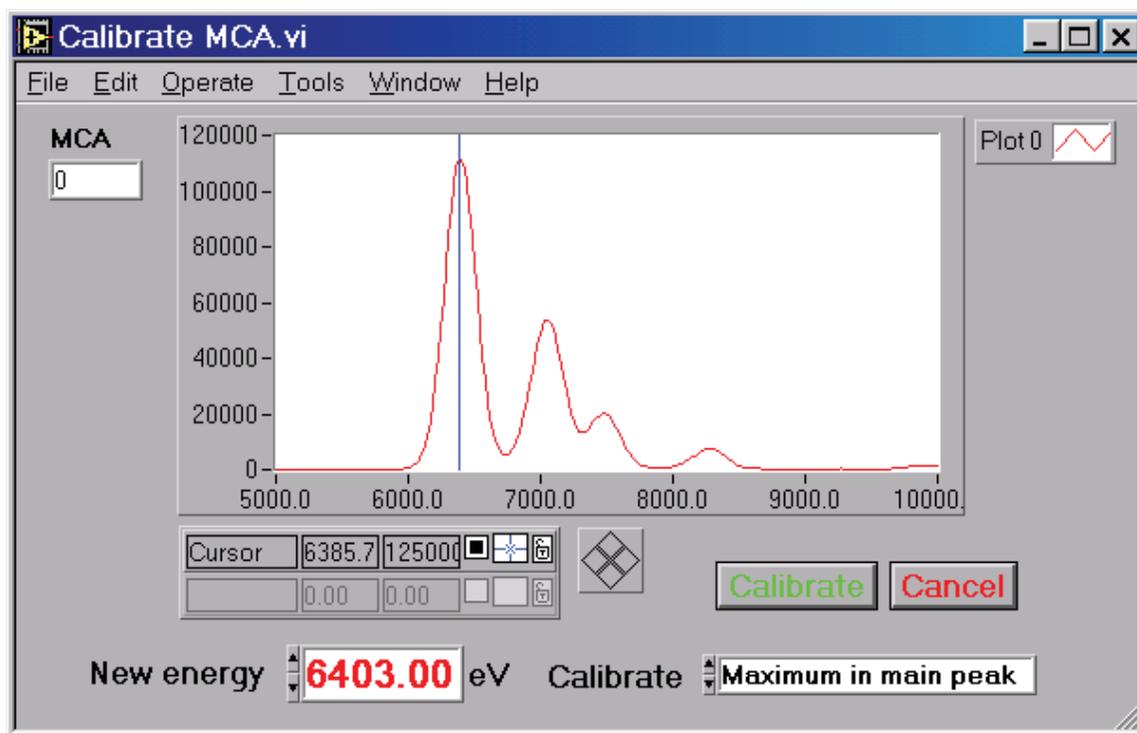


Fig B2.3.3

#### B2.4. XIA slits

Fig. A12 shows the XIA slit selection dialog box. The  $I_0$  slits dialog box is what is normally needed, so click **OPEN** (or click exit to do nothing). This will bring up the slits dialog box shown in Fig. A13 which is discussed in section 3.1.



Fig. B2.4.1

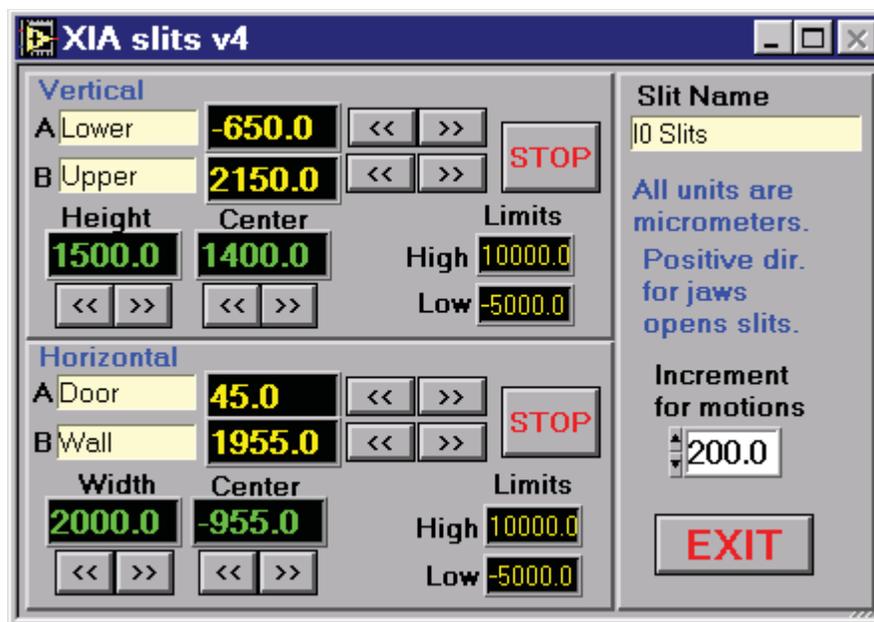


Fig. B2.4.2.

## B2.5. Record AI offsets

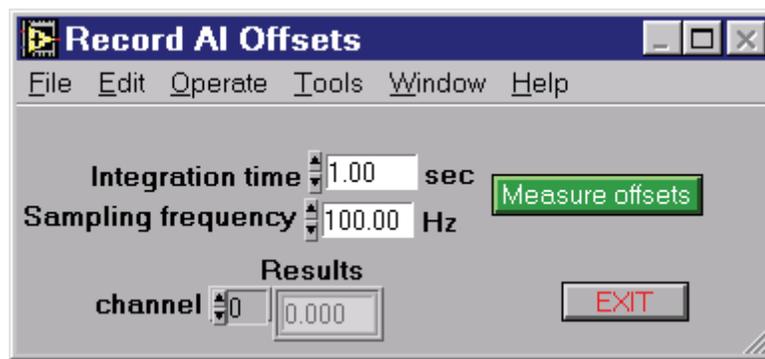


Fig. B2.5

The associated dialog box is shown in Fig. B2.5. It doesn't seem to be important.

## B2.6. Mono Control

The Mono Control window is shown in Fig. A15. A description is given in section 3.4 (above).

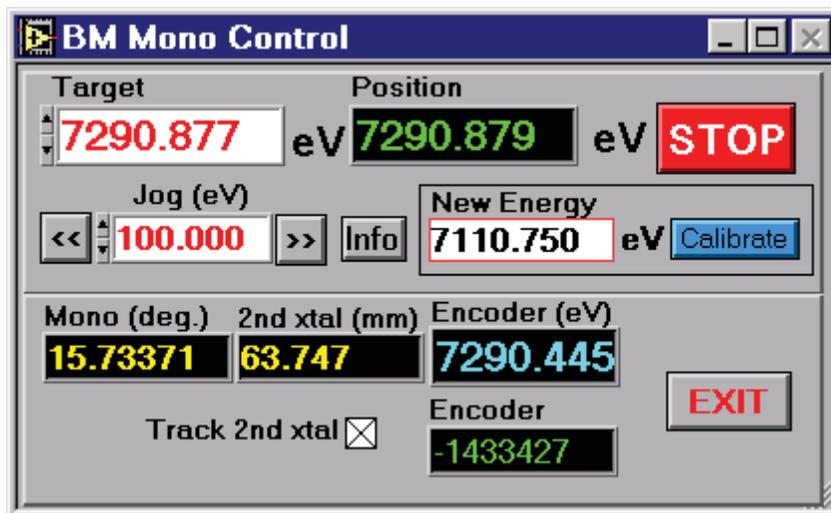


Fig. B2.6

The target 7290.877 here is set to the value shown by the encoder in the lower half of the panel.

New Energy is the literature value of the edge being used for calibration.\*

(\*You can make little adjustments here to get encoder spot on).

TBA ID version procedure.

## B2.7. Shutters

Fig. B2.7 shows an old version of the Shutters control window. This window simply duplicates the function of the *real* shutters control buttons on the BL hutch wall. In general, there is no need for users to interact with this control window.

From 2007 on, the shutter control is offered on a secondary computer which monitors feedback.

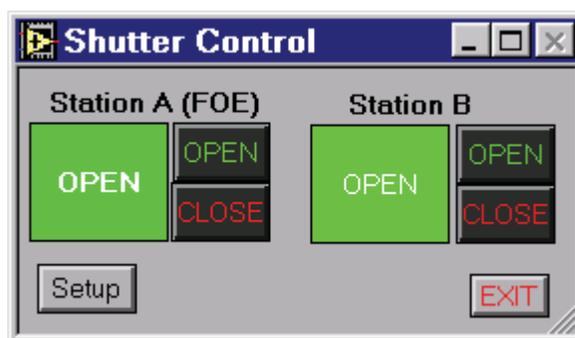


Fig. B2.7

### B3. BEAMLINe SET-UP MENU

Fig. B3 shows the appearance of the Beamline Control Panel window when the Beamline Set-Up menu is selected. The **Analog Inputs** and **Pager** buttons can be ignored by the user, and are not discussed here.

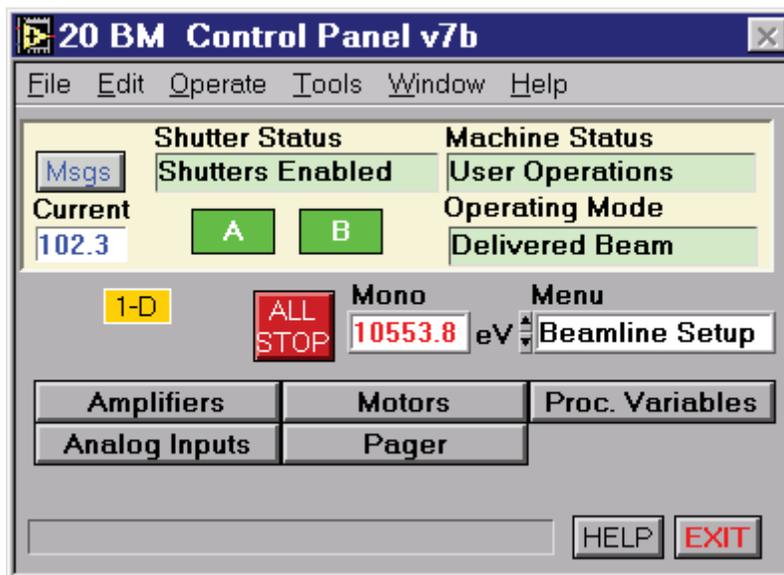


Fig. B3.

### B3.1. Amplifiers

This window (Fig. B3.1) cannot be accessed while the **Amplifier Control** panel (sensitivity control, on Controls menu, Fig. B2). A warning message will advise you of this if you attempt to do so. You should not attempt to modify any parameters in the window without consulting the BL staff.

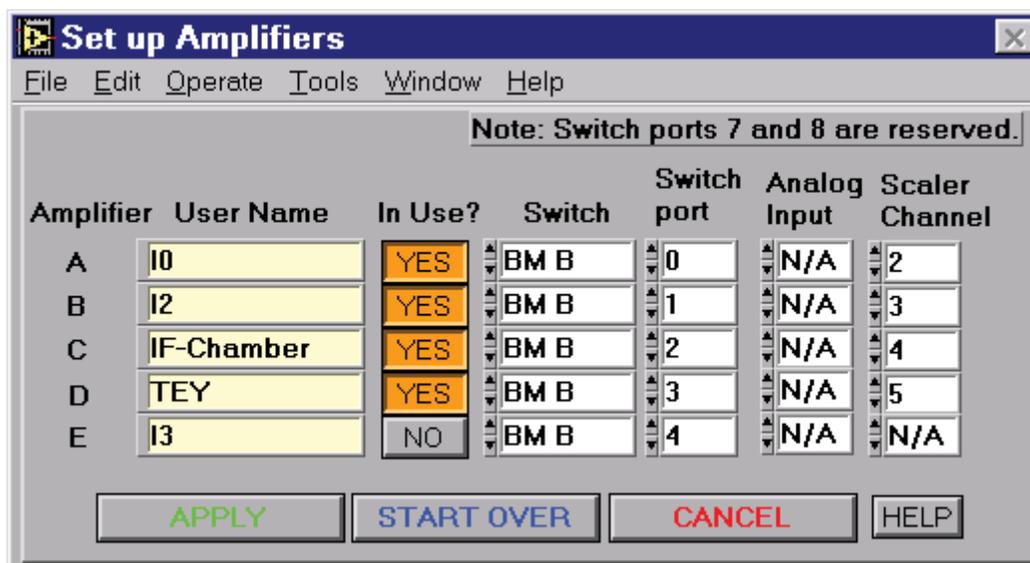


Fig. B3.1.

### B3.2. Motors

The window which controls the sample position motors is shown in Fig. 3 and is discussed in section 3.2. There are several other types of motors in the system which are controlled by similar windows. Make sure you are moving the right one (often **B13 Sample Horiz** or **B14 Sample Vert**). The correct motor will depend on which beamline you are using as well as what it is you wish to move. You may need to consult with the BL staff to determine which motors you are using.

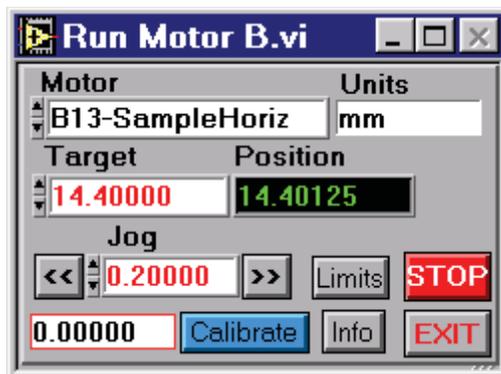


Fig. B3.2

## B3.3. Process Variables

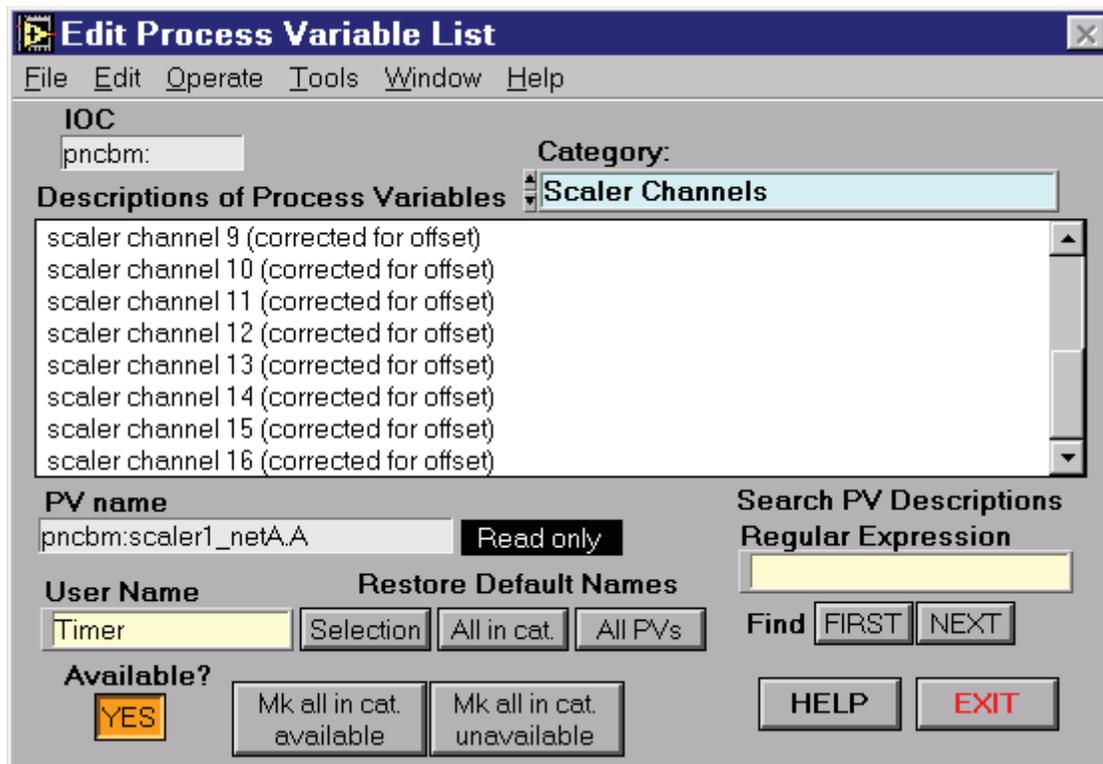


Fig. B3.3.

Fig. B3.3 shows the Process Variables window. This is yet another window used for interfacing output data to the computer control system. Users should not modify its settings without assistance from BL staff.

### C. ID20 CONTROL PANEL

The ID20 Control Panel window (see Fig. C1) provides access to all functions of the BL. The functions are organized into several categories, which are selected from the **Menu** list, as shown in Fig. A1:

**Data Collection**

**Controls**

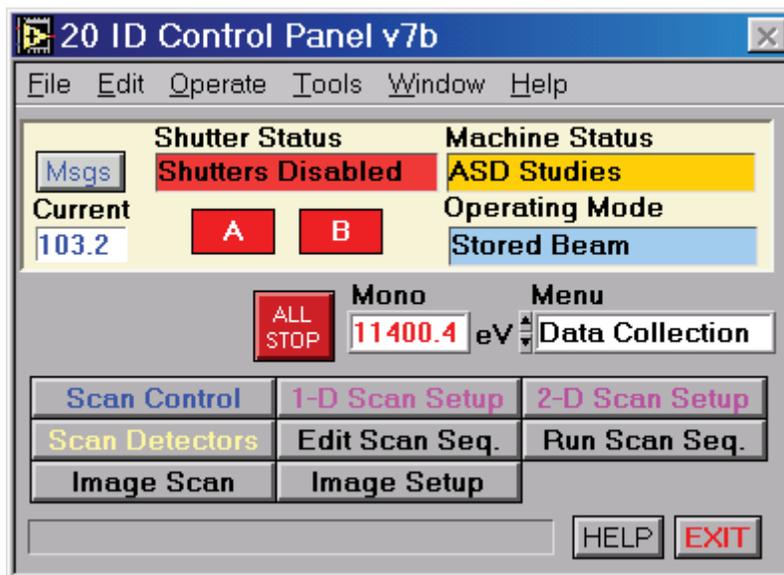
**Beamline Setup**

**Motors** (rarely needed)

**Displays** (rarely needed)

**Tables** (rarely needed)

For each menu category, a new set of buttons comes up, which changes the appearance of the window drastically. Each of the buttons has an associated window or dialog box which comes up when you click the button. These are the same dialog boxes that are normally found scattered around the computer desktop. Therefore, if you close a dialog box by mistake, and want to reopen it, you can probably find it by looking carefully through the menu items on the Control Panel dialog box.



**Fig. C1.** ID20 Beamline Control Panel showing the Data Collection menu items as buttons (Scan Control etc.). The Control Panel buttons in themselves don't initiate any commands, so you can explore them without risk. In 2 or 3 cases, a warning box will come up telling you that something has not been set up. If in doubt, just exit. If the dialog box is already open somewhere it will be brought to the fore of the screen. The default virtual screen will also be displayed.

## D. Detuning

Detuning is the process of reducing contributions from higher order reflections of the monochromator crystals. The process of selecting an energy using the mono involves Bragg diffraction. If, for example, you are using a set of Silicon (111) crystals in the monochromator, you are using the Si(111) reflection. The reflections have finite width in energy, and the width is energy-dependent, becoming narrower with increasing energy. The next-higher reflection from Si(111) that can contribute is Si(333) which occurs at 3 times the energy and is approximately 3 times narrower in width. By detuning to 75 – 85% of maximum for the Si(111), one reduces the Si(333) contribution to a few % or less. (The use of harmonic rejection or KB focusing mirrors, set to an appropriate angle, can further reduce harmonic contamination.)

Detuning on ID and BM is done on both beamlines in reference to the detector labeled “Preslit”. On BM, this is a small He-filled ion chamber located before the HR mirror. On ID, this is done using the summed signal (i.e. total current) from the horizontal BPM near the front of ID-B. Detuning is also linked to feedback settings. Feedback is used on ID and on BM when using the focusing mirror.

The feedback on either line uses a pair of split-plate transmission ion chambers (BPMs): one for vertical and one for horizontal. Output from the two plates is measured and one can examine the sum and difference signals. The difference signal is used to provide feedback to piezo-electric motors called dtheta (vertical) and dchi (horizontal) which control the position of the beam and attempt to keep the beam steady on the slits. As mentioned above, on ID, the sum signal from the horizontal is used for detuning and is recorded in the datafile as “Preslit”. On BM, Preslit is a separate chamber upstream of the HR mirror tank.

Detuning is done in the following steps:

1. Pause the feedback (if being used).
2. Move the mono energy to the detuning energy, remembering to track the 2<sup>nd</sup> crystal (and undulator on ID). This detuning energy is usually 200 – 300 eV above the absorption edge being targeted – near the middle of the XAFS range.
3. Adjust dtheta to maximize the signal in the Preslit detector. Note, if the range of dtheta is insufficient, adjust dtheta to near-mid-range, and use the 2<sup>nd</sup> crystal theta motor to get close to maximum flux in Preslit.
4. Detune to your preferred level (75% if no HR mirror is typical, 85% if using an HR mirror or KB mirrors set to reject harmonics). This can be done by adjusting dtheta knob clockwise or counterclockwise. Usually on ID, counterclockwise motion is used. On BM, clockwise is used with the focused beam (gives a better range of control for feedback). Just be consistent.
5. Adjust the table height to maximize the signal in the detector after the slits

6. Adjust dchi to maximize the signal in the detector after the slits. Note, if the range of dchi is insufficient, adjust dchi to near-mid-range and use the 2<sup>nd</sup> crystal chi motor to get close to maximum flux in Preslit. When operating in unfocused mode on BM, this step is not needed.

ID:

The detector after the slits for the KB-mirrors will be called “PreKB”. After step 4, the vertical feedback can be restarted by taking the difference readout and putting that value in to the set-point of the feedback control, and un-pausing the feedback. One adjusts the vertical position of the KB table in step 5 to maximize the signal in PreKB. In step 6, one adjusts dchi to further optimize the flux in PreKB. Once this is done, the difference signal from the horizontal feedback is input to the feedback control, and control un-paused.

For LERIX, the detector after the slits is I0 (LERIX-I0). Since LERIX typically uses the toroidal mirror, staff will modify the vertical feedback (switch upstream and downstream amplifiers) to allow for the mirror.

At very high energy (e.g. Sb K-edge near 30,491 eV), the gain on the vertical feedback control needs to be changed from 0.5 to -0.5 and the control limits lowered to near 1.00V for the feedback to be stable and recover from shutter closure or return-to-scan-start.

BM, no focusing:

The current set-up on BM has the feedback split-plate chambers mounted on the experimental table before the slits, and I0 after the slits. In step 5, one adjusts the table height to maximize the signal in I0. With no focusing, step 6 is unnecessary. Note the readout of the dtheta piezo control and check the value over time in case the piezo motor “twitches” and causes the value (and hence detuning level) to change.

BM, focused, with feedback:

The current set-up on BM has the feedback split-plate chambers mounted on the experimental table before the slits and I0 after the slits. In step 5, one adjusts the table height to maximize the signal in I0. The slits are aligned to the centre of the BPM chambers. Optimizing the vertical and horizontal beam positions result in set-point values near zero. The user (generally) does not need to adjust settings, only optimize the table after setting the tuning. Once in position, the feedback can be un-paused. Small adjustments of the slit position may be needed to get the difference values of the feedback chambers right to zero. Note also, sometimes it is better to run with the horizontal feedback off, even in focused mode.

NOTE: Large temperature changes in the monos (start-up after machine studies, lengthy beam dump, large change in undulator gap) will result in thermal drift. The user should monitor the output voltage and feedback output levels. If they are drifting out of range, the motors will need to be adjusted to bring the feedback back into control.

## E. User Calcs

UserCalcs are defined to determine how the signals from the solid-state detectors are processed. Typically, a ROI for an element is summed up for each element of the detector to give a total signal. This may be divided by I0 automatically at this time if desired. The channels can also be averaged.

The UserCalcs are accessed using the Sun computer rather than the Labview program used for other tasks.

-each detector component is specified in a labeled line\*

```

A pncaux:dxp_mca0.R1
(region of interest #1 for mca detector component "0")
-
-
-
-
-
L pncaux:dxp_mca9.R1

```

-components say 0-12 except 11 (not working) and 9 (selected for ref later appears at end)

so: User Calc #1 = A+B+C+D+.....+L

(note: in this case no normalization. Ratioing/subtraction/etc is applied. They may be if desired)

For another ROI say #2, starts all over  
User Calc #2

```

A pncaux:dxp?mca0.R2
-
-
-
L 9.R2

```

A+B+C+D+.....+L

Since .R1, .R2 is part of the PV name, there is no confusion

\*order is not necessary but desirable for accuracy

User Calc limit: 10

Each user calc can have 12 items (if all 13 components were working one would have to be left out)

Making User Calcs:

Use Sun computer (sign on)

Bring up user calcs (on bmmain.adl)

Select on user calc with LH button – User Calc full

Screen comes up, edit as decided (see before)

Typ: 1/I0 TRIGGER – one must be triggered

Typ dxp 12 – yes

To transfer (activate) to list, which can be picked up by Labview controller press PROC for proceed. This then becomes defined.

Now to receive this data stream in Labview, go to detector list in appropriate Labview screen (where these user calcs just prepared have been added) and then add them into the active list.

Note: Sun Editing (UNIX IN OPERATION)

The keys copy, cut and paste on keyboard work

BUT To select item, pointer must be on the item

Pointer must not move out of box to copy, cut etc as desired

Move to new box, put pointer within box, keep pointer in place, paste, ENTER

If not “ENTERED”, item is not kept in new box

## F. Other Useful Aids

Supporting information of use to operations is available on the ancillary computer on the desk. These capabilities are provided by the IFEFFIT suite of Data Analysis programs. To use pull up the Hephaestus program by clicking on the shortcut of the same name. Follow the menu to access the items listed below.

### F 1. Calculation of Gas Proportions.

As the X-ray energy is changed it is necessary to change the gas mix/proportions in the ion chambers to obtain an appropriate absorption profile. Enough absorber to give a signal but not so much as to attenuate the beam. Selecting the Ion Chamber menu item will give the following screen:

The screenshot shows the 'Hephaestus' software window with the title 'Compute Absorption of Ion Chambers'. The interface includes a menu bar (File, Units, Resource, Xsection, Help) and a sidebar with icons for Absorption, Formulas, Data, Ion Chamber, Transitions, Edge Finder, Line Finder, f & f'', and Document.

The main panel contains the following controls and data:

- Using Elam database**
  - Photon energy: 9000
  - Chamber Length:
    - 3.3 cm Lytle Detector
    - 6.6 cm Lytle Detector
    - 10 cm
    - 15 cm
    - 30 cm
    - 45 cm
    - 60 cm
    - Choose your own
  - Input field: 20 cm
- Gas and Pressure Settings:**
  - Primary Gas: N2
  - Secondary Gas: He
  - Pressure (Torr): 760
- Absorption Sliders:** Three vertical sliders for Primary Gas, Secondary Gas, and Pressure. The Primary Gas slider is set to approximately 60, Secondary Gas to 40, and Pressure to 760.
- Percentage absorbed:** 15.16 % (with a Reset button)
- Photon flux:** Amplifier gain 8 with 0 volts gives 0 photons/second
- Rules of thumb:** 10% absorption in 10; 70% absorption in 1t or 1f (1 Atm = 760 Torr)

Select appropriate chamber length, select primary and secondary gases from the pull down list and manipulate the slider to get the appropriate percentage of absorption. Note guiding rules at bottom.

## F 2 Absorption Edges

Pull up the Absorption menu item to see the following screen. Click on an element to get the full set of absorption edges Energies, identification and transition profile.

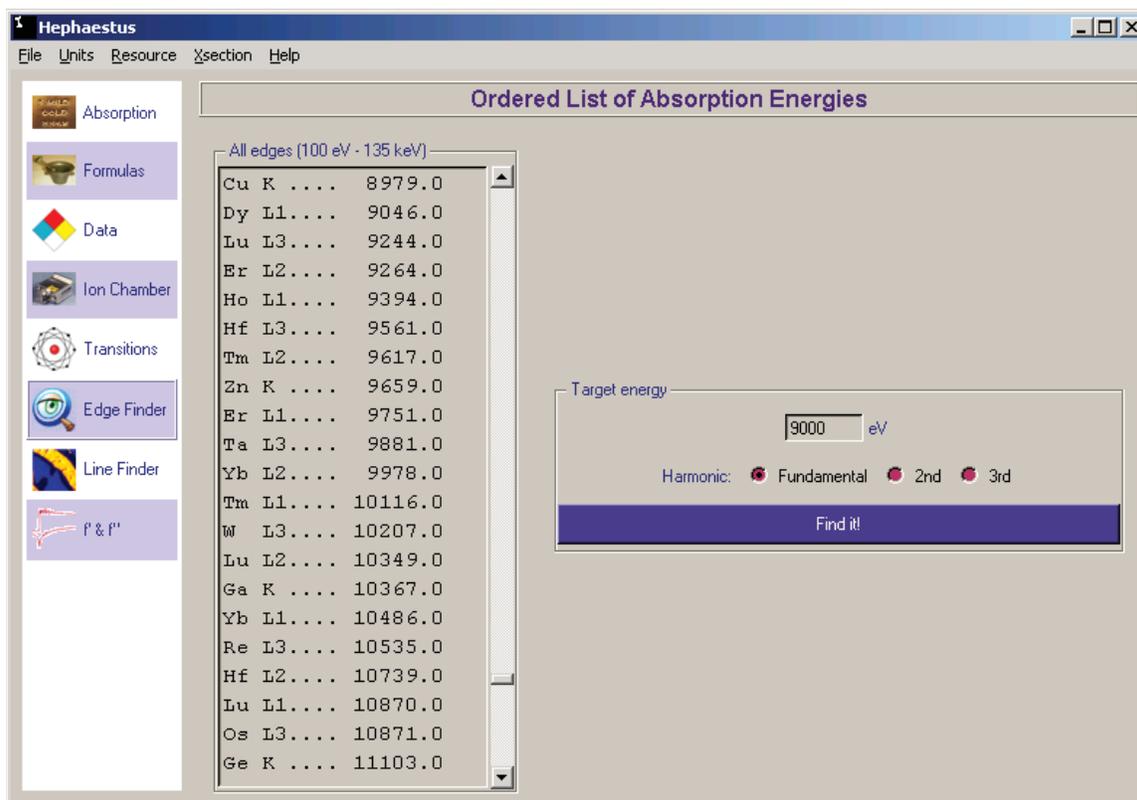
The screenshot shows the Hephaestus software interface. The main window is titled "Hephaestus" and contains a menu bar (File, Units, Resource, Section, Help) and a sidebar with icons for Absorption, Formulas, Data, Ion Chamber, Transitions, Edge Finder, Line Finder, and f & f'. The central area displays the "Periodic Table of Absorption Data" with the text "Using Elam database Computing total cross-section". The periodic table is color-coded by groups. Below the table, the element Neodymium (Nd) is selected, and its properties are listed: Name (Neodymium), Number (60), Weight (144.27 amu), Density (6.96 g/cm<sup>3</sup>), Energy (input field), Thickness (input field), Absorption Length, and Transmitted Fraction. Two tables are displayed: one for absorption edges and one for transition lines.

Edge	Energy
K	43569
L1	7126
L2	6722
L3	6208
M1	1575

Line	Trans.	Energy	Prob.
Kalpha1	K-L3	37361	0.5210
Kalpha2	K-L2	36847	0.2861
Kalpha3	K-L1	36443	0.0001
Kbeta1	K-M3	42272	0.0973
Kbeta2	K-N2,3	43325.7	0.0432

### F 3 List of Absorption Energies

The menu item "Edge Finder" gives an ordered list of Absorption Energies. Search by Energy value.



The screenshot shows the Hephaestus software interface. The main window is titled "Ordered List of Absorption Energies". On the left, there is a sidebar with several menu items: "Absorption", "Formulas", "Data", "Ion Chamber", "Transitions", "Edge Finder", "Line Finder", and "f' & f''". The "Edge Finder" menu item is highlighted. The main area displays a list of absorption edges for various elements and shells, sorted by energy. The list is titled "All edges (100 eV - 135 keV)". The elements and their corresponding absorption energies are as follows:

Element	Shell	Energy (eV)
Cu	K	8979.0
Dy	L1	9046.0
Lu	L3	9244.0
Er	L2	9264.0
Ho	L1	9394.0
Hf	L3	9561.0
Tm	L2	9617.0
Zn	K	9659.0
Er	L1	9751.0
Ta	L3	9881.0
Yb	L2	9978.0
Tm	L1	10116.0
W	L3	10207.0
Lu	L2	10349.0
Ga	K	10367.0
Yb	L1	10486.0
Re	L3	10535.0
Hf	L2	10739.0
Lu	L1	10870.0
Os	L3	10871.0
Ge	K	11103.0

Below the list, there is a search box labeled "Target energy" with the value "9000 eV" entered. To the right of the search box, there are radio buttons for "Fundamental", "2nd", and "3rd" harmonics. The "Fundamental" radio button is selected. A "Find it!" button is located below the search box.

## F 4 List of Emission Energies

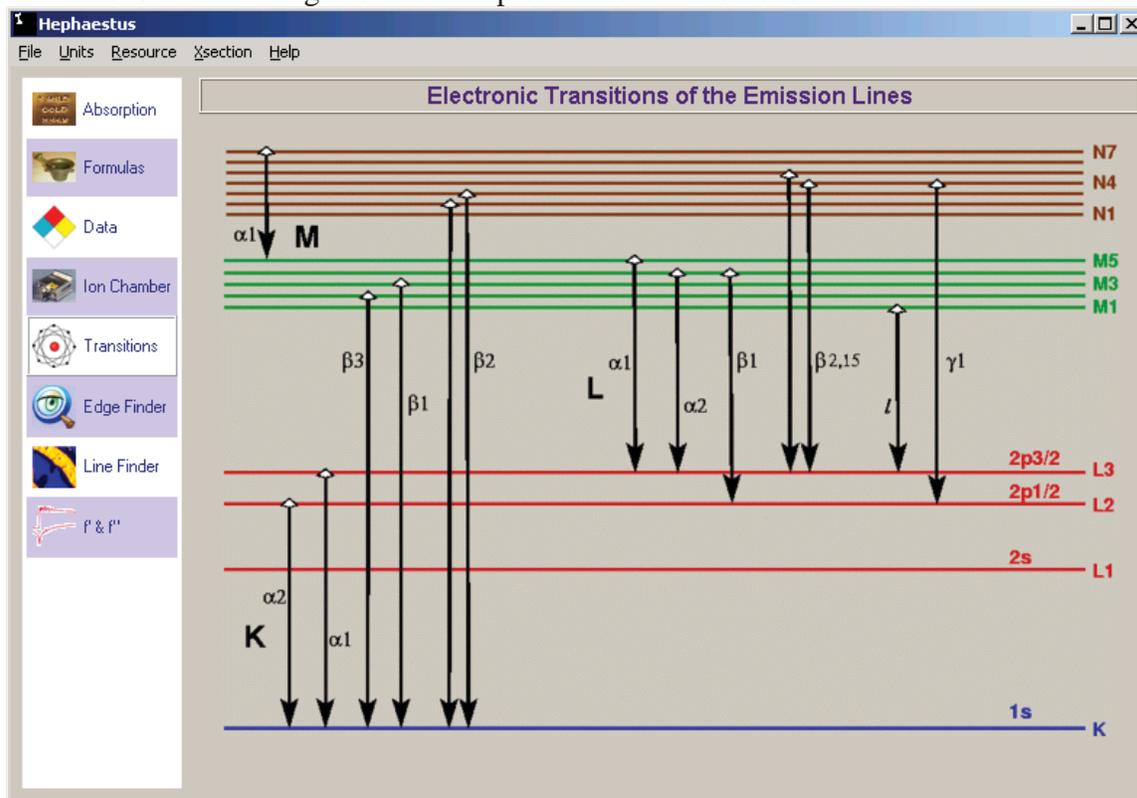
The Line Finder menu item gives an ordered list of Emission Energies

The screenshot shows the 'Hephaestus' software interface. The main window is titled 'Ordered List of Fluorescence Line Energies'. On the left, there is a sidebar with menu items: Absorption, Formulas, Data, Ion Chamber, Transitions, Edge Finder, Line Finder, and  $f' & f''$ . The main area displays a table of fluorescence lines. The table has columns for Element, Line, Transition, Relative Intensity, and Energy (eV). The 'Cu Kalpha1' line is highlighted in blue. To the right of the table, there is a 'Target energy' input field with the value '8047' and a 'Find it!' button.

Element	Line	Transition	Relative Intensity	Energy (eV)
Hf	Lalpha2	L3-M4	(0.0831) ....	7845.0
Lu	Lnu	L2-M1	(0.0182) ....	7858.0
Cu	Kalpha3	K-L1	(0.0003) ....	7882.3
Hf	Lalpha1	L3-M5	(0.7455) ....	7899.0
Er	Lbeta6	L3-N1	(0.0084) ....	7908.2
Ho	Lbeta2	L3-N4, 5	(0.1529) ....	7911.0
Er	Lbeta3	L1-M3	(0.4713) ....	7939.0
Tm	Lbeta4	L1-M2	(0.3012) ....	8026.0
Cu	Kalpha2	K-L2	(0.2943) ....	8026.7
Ir	L1	L3-M1	(0.0037) ....	8041.0
Cu	Kalpha1	K-L3	(0.5771) ....	8046.3
Ta	Lalpha2	L3-M4	(0.0827) ....	8088.0
Gd	Lgamma2	L1-N2	(0.0932) ....	8090.0
Tb	Lgamma1	L2-N4	(0.1432) ....	8101.5
Tm	Lbeta1	L2-M4	(0.8323) ....	8102.0
Gd	Lgamma3	L1-N3	(0.1306) ....	8105.0
Hf	Lnu	L2-M1	(0.0181) ....	8138.0
Ta	Lalpha1	L3-M5	(0.7414) ....	8146.0
Tm	Lbeta6	L3-N1	(0.0086) ....	8177.1
Er	Lbeta2	L3-N4, 5	(0.1510) ....	8190.4
Tm	Lbeta3	L1-M3	(0.4678) ....	8231.0

## F 5 Transitions

Transitions Menu item gives a roadmap of K and L transitions:



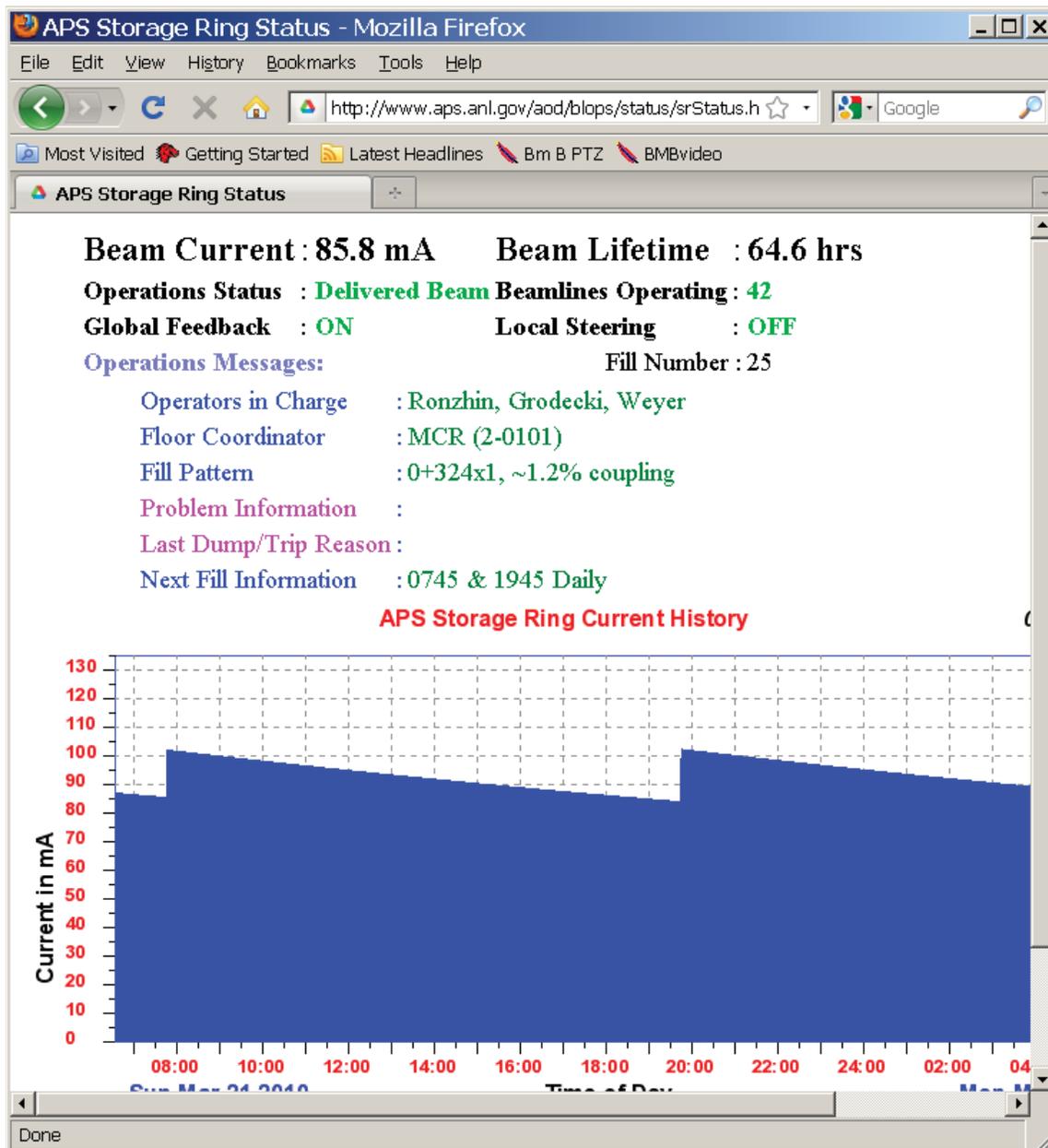
## F 6 Complex Scattering Factors

Provided by the  $f'$   $f''$  Menu item. Can calculate the scattering factors over the range selected in the windows.

The screenshot shows the Hephaestus software interface. The main window is titled "Periodic Table of Complex Scattering Factors". The periodic table is displayed with elements color-coded by group. Below the table, there are input fields for "Starting energy" (3000), "Ending energy" (7000), and "Energy grid" (5). There is a checkbox for "Convolute by the natural core-level width" which is checked. Below this are five radio button options for plotting: "New plot", "Overplot", "Plot just  $f'$ ", "Plot just  $f''$ ", and "Plot both  $f'$  and  $f''$ ". A "Save data for Pt" button is located at the bottom.

## F 7 Ring Condition

Access via APS home page; You can display this which is easier to read than the station monitors or other monitors in the building. On the right hand side of the box (not shown here) is more detailed information - expand window to see.



Additional items TBA

Log spiral detectors