addIXS

A MatLab based user interface for converting and adding together inelastic x-ray scattering (IXS) spectra at ID28

Andrew Walters October 2010

Introduction to addIXS

addIXS is a MatLab based program which takes the raw inelastic x-ray scattering (IXS) data from a SPEC file and converts it into an xye file, where:

x is the energy transferred to the sample
y is the normalized intensity (normalized to monitor ‘ione’)
e is the square-root error on the intensity

Step 1: Starting addIXS

1. Open a terminal on Leonov at ID28 (this can be done remotely)
2. Type “matlab” in the terminal window
3. Once MatLab has loaded, choose your working directory (the path given at the top of the screen). This is the folder in which your IXS spectra will be saved
4. Type “addIXS” at the MatLab prompt
5. The addIXS user interface will appear

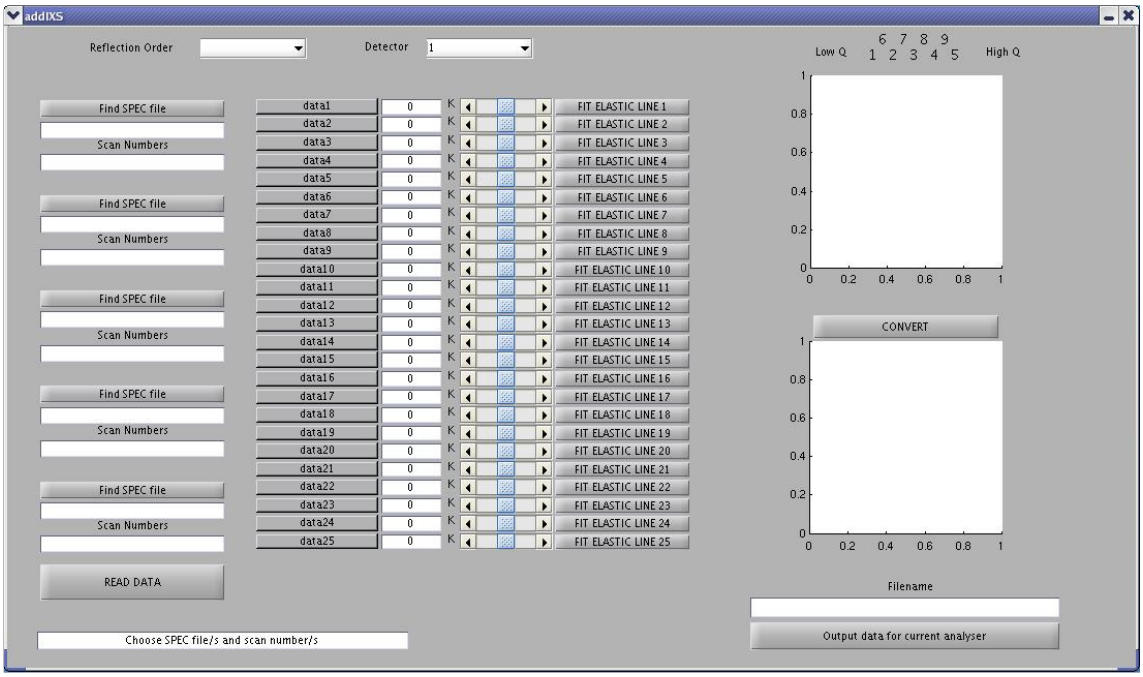


Figure 1: addIXS at startup

Step 2: Loading SPEC data into addIXS

1. Choose the Si reflection order of the monochromator which was used for the IXS scans. This is done via the drop-down menu labeled "Reflection Order". The Si reflection order is used in the calculation which converts the temperature of the monochromator into the energy of the monochromated beam
2. To select the SPEC file/s which contain/s the data to be converted or summed together, click on the top button which says "Find SPEC file". The data can be found in /data/id28/archive/galilee/. Ask your local contact which subdirectory your data are in. When you have selected the SPEC file, the name of the SPEC file will appear below the "Find SPEC file" button. The other "Find SPEC file" buttons can be used to read from other SPEC files.

Please note that a maximum of
5 SPEC files can be read simultaneously

3. Below the name of the SPEC file there is a window labeled "Scan numbers". Enter the scan numbers which you wish to convert and/or sum. Note that normal MatLab array conventions can be used (e.g. 212:214 will load scans 212, 213 and 214).

Note that a maximum of 25 scans
can be read simultaneously

4. Press the "READ DATA" button. This can take a few seconds.
5. When the scans are loaded, the intensities measured by Detector 1 will appear at the top right, and a set of buttons corresponding to each scan will appear in the centre of the user interface panel.

By default when the scans are first loaded, all of the scans are selected (the toggle buttons on the left are all down). To deselect any scan, simply press on the corresponding toggle button. The button will appear to be up, and no data measured in that detector will be plotted. Data measured in different detectors can be

accessed using the drop-down menu labeled “Detector”. addIXS should now look something like Figure 2.

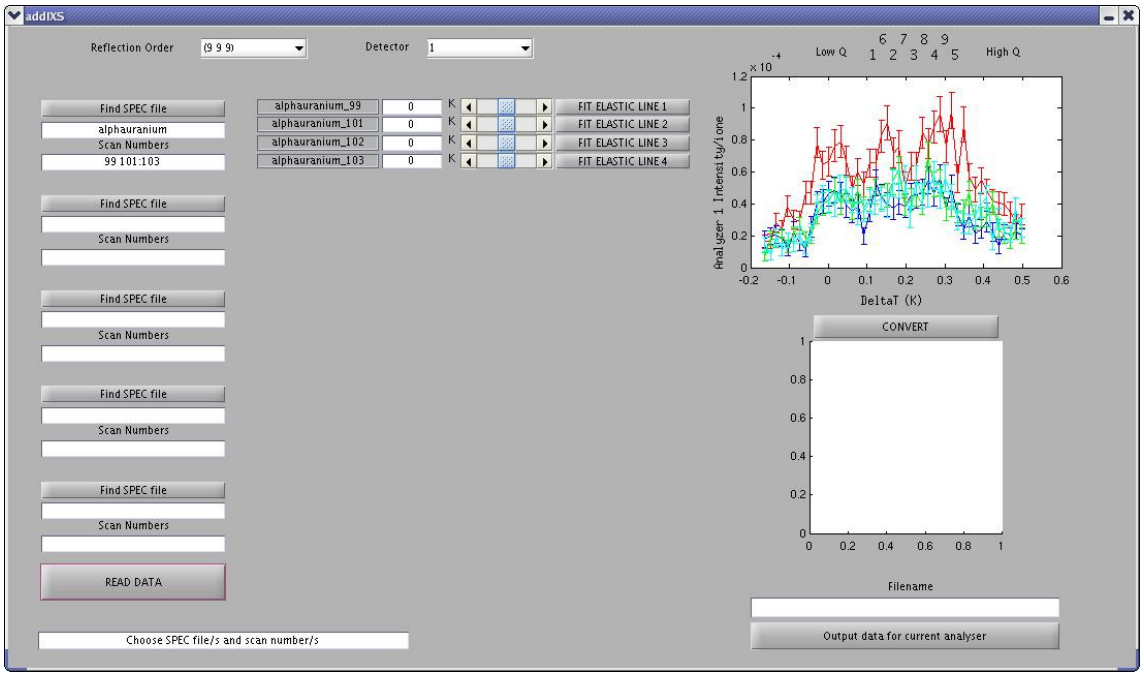


Figure 2: addIXS screen after clicking “LOAD DATA”

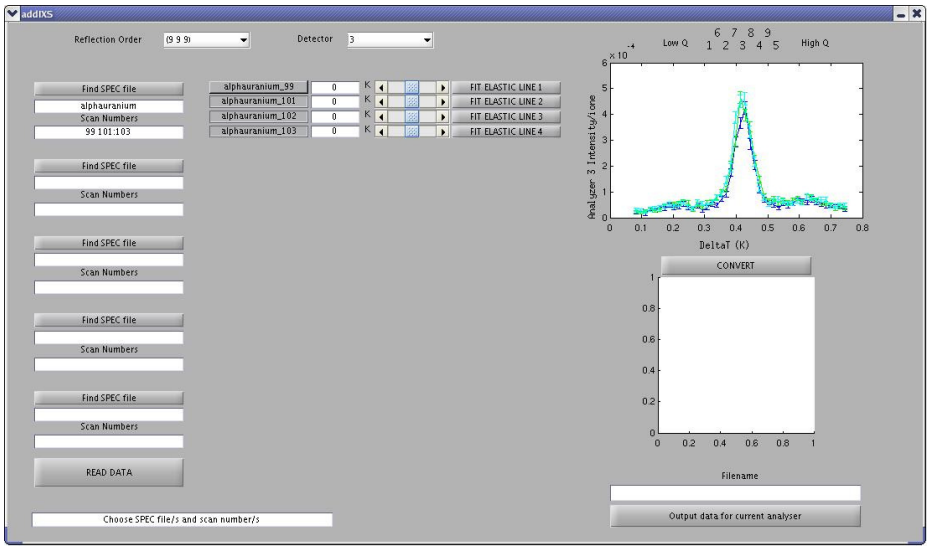
Step 3: Finding the temperature offsets for each analyzer crystal

The next step is to find the appropriate temperature offset for each analyser crystal. Although the temperatures of the analysers are kept as stable as possible, there can be some drift over a week-long experiment. In addition the measured temperatures of the analysers are very different to each other, due to the different contact resistances on the thermistors. Depending on the type of IXS data being measured, the temperature offset can be found in different ways.

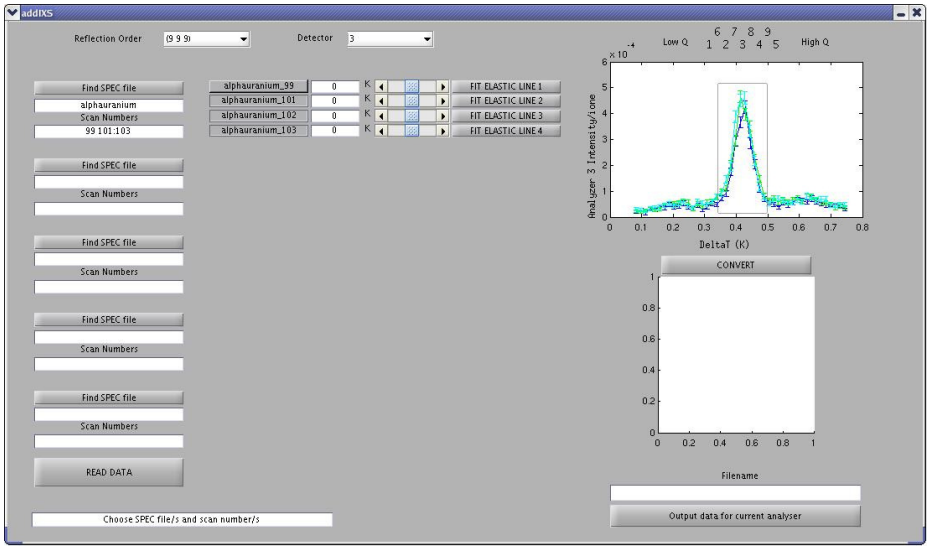
Perhaps the most common way is to include an elastic line in the IXS scan and then fit the elastic line in the immediate vicinity of the elastic line (so that any low energy phonons do not affect the fit). The elastic line can be fitted easily in addIXS, as can be seen in the following example.

Finding the temperature offsets for an analyzer: an example

1. We would like to sum the data measured in detector 3 in scans alphauranium_101, alphauranium_102 and alphauranium_103, as shown above. Note that alphauranium_99 has been deselected.

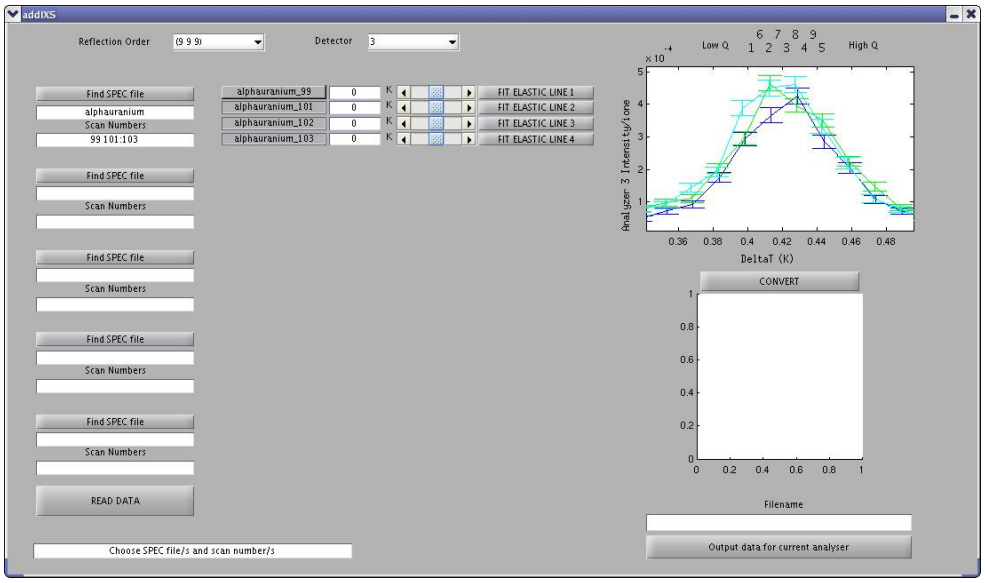


2. Select the range of temperatures over which the elastic line will be fitted for alphauranium_101. This is done by simply dragging a box around the region of interest. The scale can be put back to the default values by clicking the right mouse button and selecting “Reset to Original View”

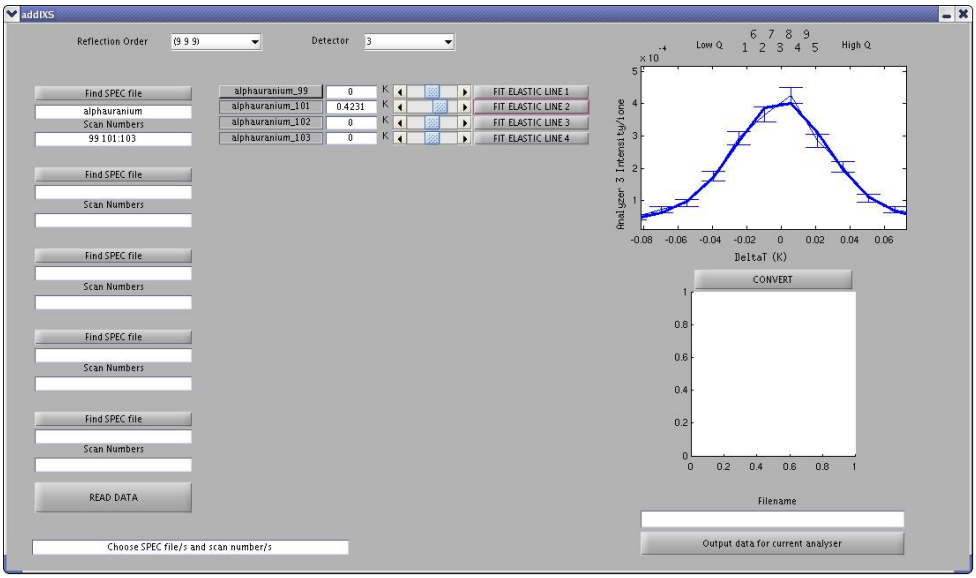


Note that it may be easier in terms of visibility if you select only the scan of interest, although this is not necessary

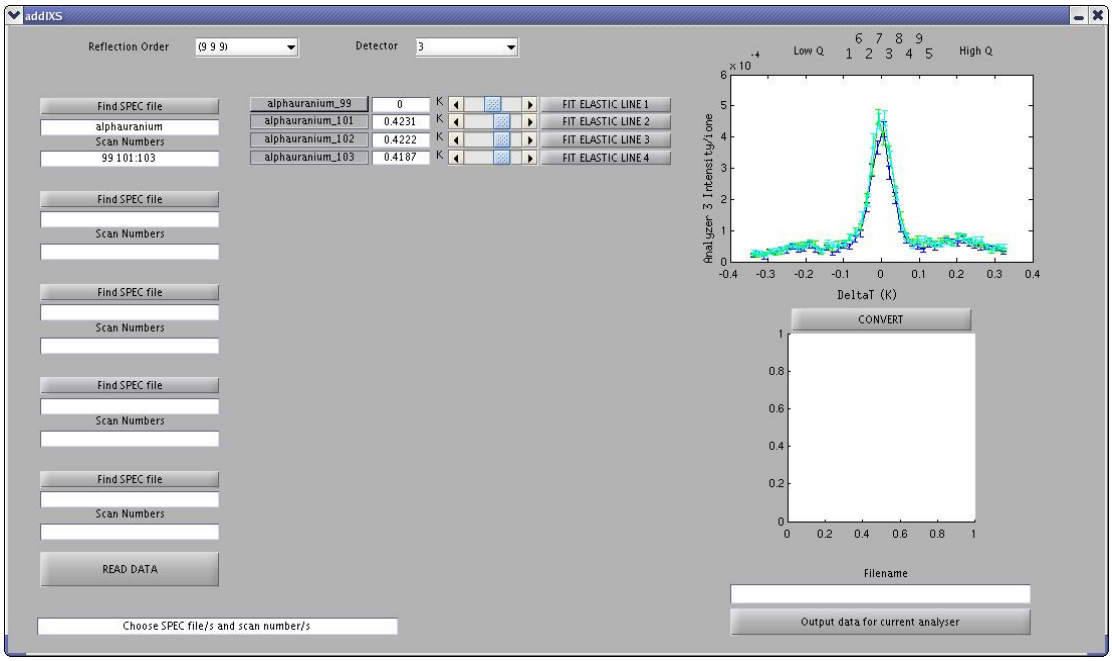
3. Click "FIT ELASTIC LINE X", taking care to press the button which corresponds to the scan you are interested in.



4. The fitted value of the centre of the elastic line will appear in the box next to the scan of interest. The fit to the elastic line will also appear in the plot window. addIXS automatically subtracts this temperature offset from the plotted data. So if you have found the offset correctly, the elastic line should be at precisely 0.



5. This process is then repeated for the other two scans (alphauranium_102 and alphauranium_103).



In addition to the fitting option described above, the zero temperature offset can be typed in by hand (press the Enter key to update the value) or tweaked with the aid of a slider button.

Step 4: Converting the data onto an energy transfer scale

Once you are satisfied with the temperature offset/s, press the "CONVERT" button to convert the selected datasets onto an energy transfer scale. When the convert button is pressed, all of the selected datasets for the chosen detector are converted onto an energy transfer scale and summed. The result is plotted in the panel at the bottom right of the addIXS user interface.

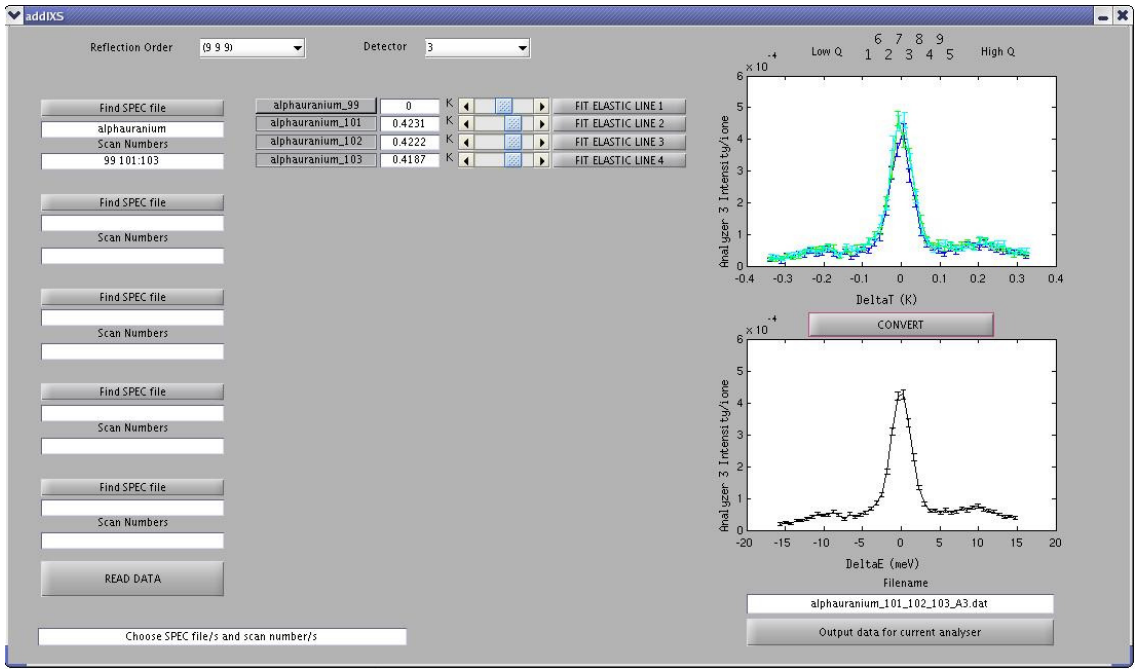


Figure 4: addIXS screen after clicking "CONVERT"

The name for the output datafile is automatically chosen in the format

<SPEC filename> _ <scan number> _A <detector number> .dat

This name for the output file can be changed if preferred by simply clicking on the filename and retyping. The output file will be saved into the MatLab working directory. This process should then be repeated for each detector, as the temperature of the corresponding analyser will be different in each case.

If you have any further questions, please email me at andrew.walters@esrf.fr or call on +33 (0)4 76 88 26 78. **Good luck!**