



# GeoPIXE®

## Quantitative PIXE / SXRF Trace Element Imaging and Analysis

A GUI analysis environment for GeoPIXE ® including quantitative PIXE and SXRF analysis and image projection using the *Dynamic Analysis* method

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Building on the established methods of the GeoPIXE software for PIXE analysis, a graphical user interface front-end has been designed for PIXE and SXRF imaging and analysis using IDL to provide greater portability between computer platforms. The heavily vectorized code in GeoPIXE works efficiently with the vector and matrix features of IDL to yield fast and efficient operation.

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# GeoPIXE

*Quantitative PIXE and SXRF Trace Element Imaging and Analysis*

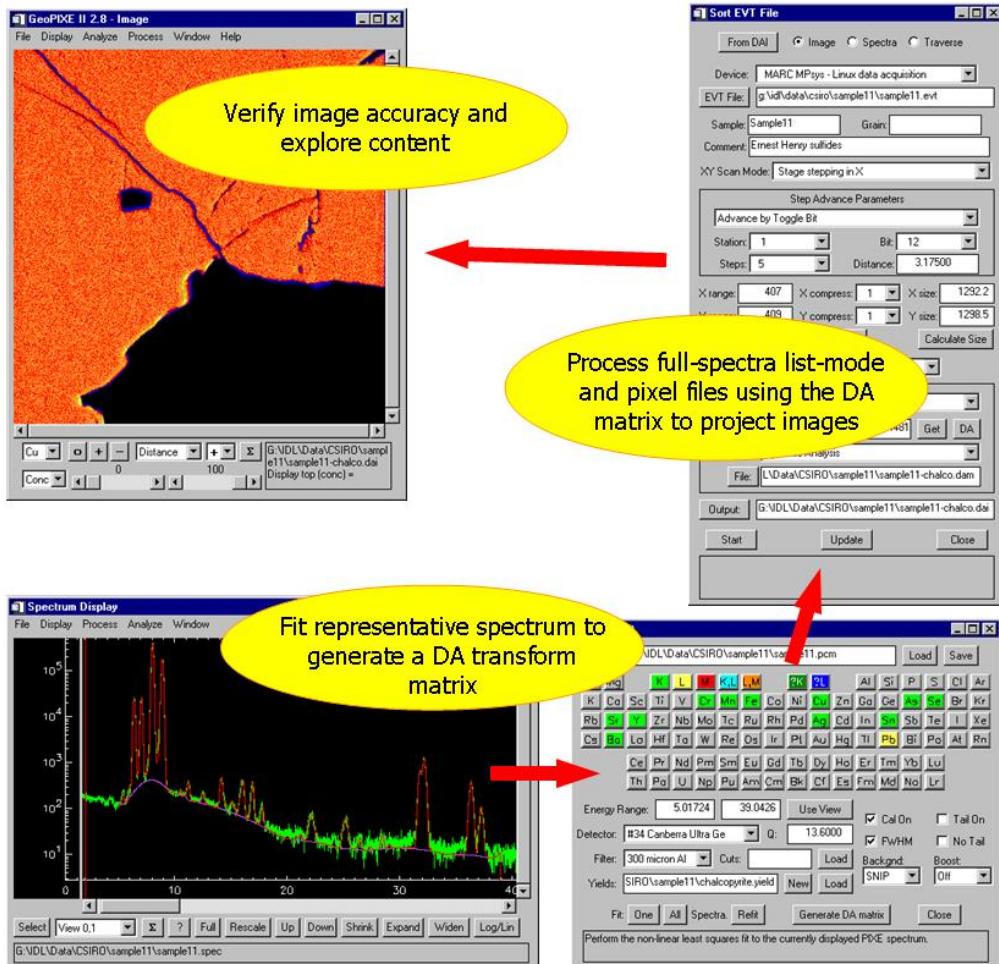
## Overview

The main first section of the manual “**GeoPIXE User's Guide**” provides a description of the various windows of GeoPIXE in the order in which they are typically used for building quantitative PIXE (proton induced X-ray emission), monochromatic SXRF (synchrotron X-ray fluorescence) and laboratory XRF images and exploring their content.

The last main section “**GeoPIXE Analysis Scenarios, Data Flow and Worked Examples**” provides a number of worked examples using sample PIXE and SXRF full-spectral image data-sets.

*A more extensive source of worked examples can be found in the Workshop notes and GeoPIXE Worked Examples PDF (see the “Help” directory). These provide step-by-step tutorials on various data analysis scenarios using the Demo data available from the DAP site.*

Both provide examples of the main tasks of fitting spectra to generate the **Dynamic Analysis** (DA) image projection matrix; using this DA matrix to process full-spectral data to deconvolute elemental components and project separated elemental images; and exploration and processing of the images to first verify their accuracy and make corrections and then to explore their content.



For a quick tour of main features and data-flow, using worked examples with sample data, see the Scenarios examples “**Notes on PNC-CAT full-spectral SXRF data and imaging**” to illustrate SXRF imaging, and “**Raw PIXE Data to Elemental Images**”, which illustrates PIXE imaging. With these as starting points, read the “**GeoPIXE Users Guide**” sections and pursue other worked examples.

*A very good starting point is to work through the worked examples (with sample data) found in the GeoPIXE Workshop notes, located in the Help directory.*

A description of the DA method of image projection can be found in the paper “C.G. Ryan, **Quantitative Trace Element Imaging using PIXE and the Nuclear Microprobe**, International Journal of Imaging Systems and Technology (Special issue on Quantitative Imaging) 11, (2000) 219-230”. Recent refinements to the DA method for SXRF imaging can be found in the papers “C.G. Ryan et al., 2010, ‘**Elemental X-ray imaging using the Maia detector array: The benefits and challenges of large solid-angle**’, Nucl. Instr. Meth A 619, 37-43 (DOI: 10.1016/j.nima.2009.11.035)” and “C.G. Ryan et al., 2010, ‘**The New Maia Detector System: Methods for High Definition Trace Element Imaging of Natural Material**’, X-Ray Optics and Microanalysis, AIP Conference Proc. 1221, 9-17; doi:10.1063/1.3399266”.

The basic philosophy is to use a representative spectrum (one that contains all elemental lines likely to be encountered in a particular series of samples and image areas) to generate a DA transform matrix. This enables the projection of EVT data (list-mode, event-by-event data or pixel spectra) directly onto quantitative elemental images. This process resolves element overlaps, strongly rejecting artefacts from overlapping elements and detector response effects (escape peaks, tails) and subtracts background. Pileups are well treated in many cases which involve a single dominant element or majors in fixed ratios. (A more general approach that corrects for the spatial variation of pile-up components has also been developed and can be found in this manual.) The results are quantitative images in ppm.flux units.

Concentration variance images are also accumulated (at half resolution to minimize memory usage), so that error estimates (which include contributions from overlap and background subtraction) and detection limits can be provided for all extracted concentration values and line profile projections, etc. The DA method is treated elsewhere (C.G. Ryan, D.N. Jamieson, C.L. Churms and J.V. Pilcher, "*A New Method for On-Line True Elemental Imaging using PIXE and the Proton Microprobe*", *Nucl. Instr. Meth.* B104 (1995b), 157-165; C.G. Ryan, "*Quantitative Trace Element Imaging using PIXE and the Nuclear Microprobe*", *International Journal of Imaging Systems and Technology (Special issue on Quantitative Imaging)* 11, (2000) 219-230; C.G. Ryan, "*Developments in Dynamic Analysis for Quantitative PIXE True Elemental Imaging*", *Nucl. Instr. Meth.* B181 (2001) 170-179.; C.G. Ryan and D.N. Jamieson, *Nucl. Instr. Meth.* B77 (1993) 203-214). Extension of the DA method to SXRF is outlined in C.G. Ryan, B.E. Etschmann, S. Vogt, J. Maser, C.L. Harland, E. van Achterbergh and D. Legnini, 2005, "*Nuclear Microprobe – Synchrotron Synergy: Towards Integrated Quantitative Real-time Elemental Imaging using PIXE and SXRF*", *Nucl. Instr. Meth.* B231, 183-188 and "C.G. Ryan et al., 2010, '*The New Maia Detector System: Methods for High Definition Trace Element Imaging of Natural Material*', *X-Ray Optics and Microanalysis, AIP Conference Proc.* 1221, 9-17; doi:10.1063/1.3399266".

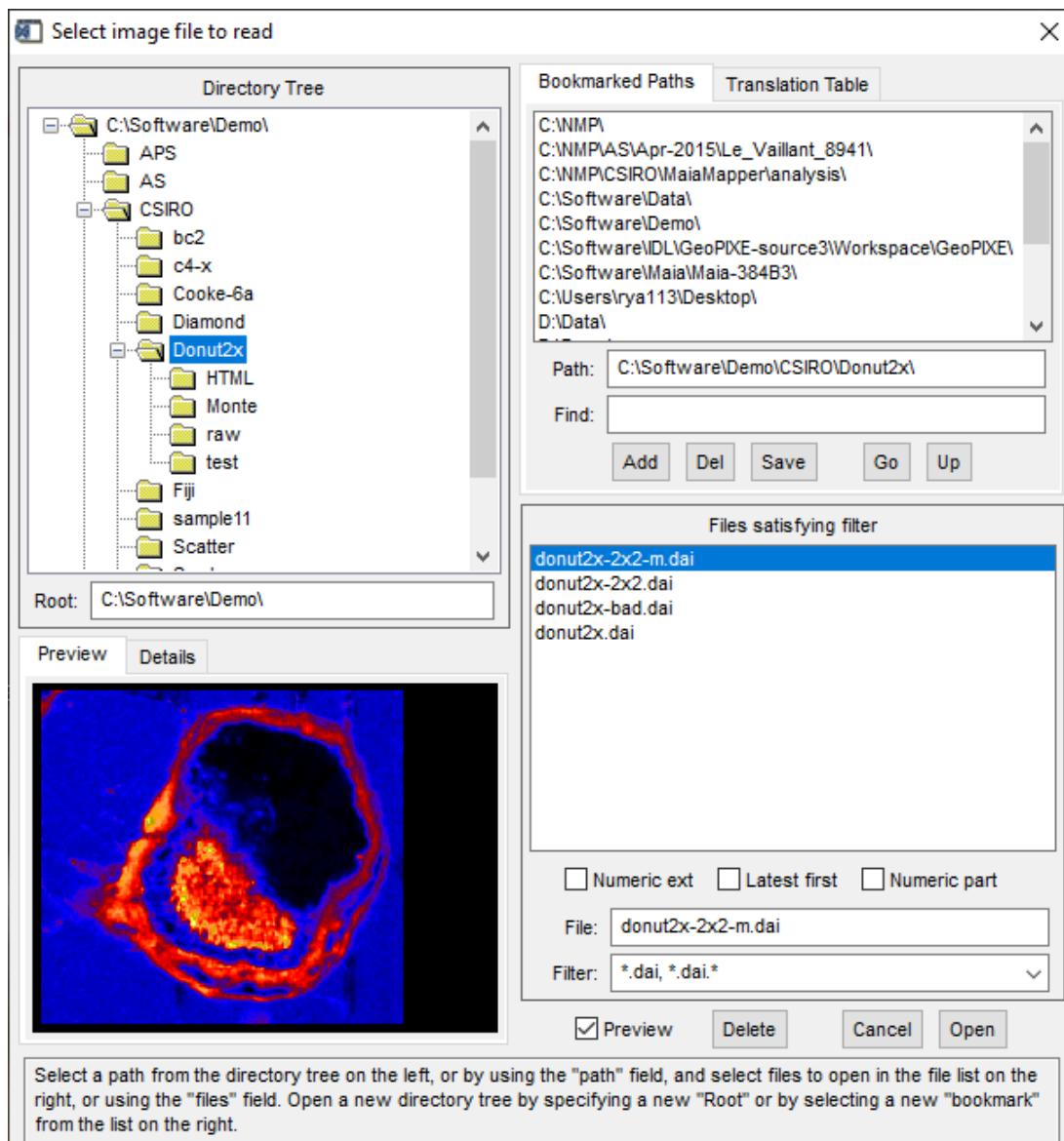
## GeoPIXE User's Guide

The following sections provide a guided tour of GeoPIXE, in an order commonly encountered in data analysis. Following the user's guide is a chapter entitled “**GeoPIXE Analysis Scenarios, Data Flow and Worked Examples**”, which aims, through the use of data analysis scenarios, to provide a working picture of how data flows between window elements, how data is shared, and how windows are interdependent; the actions taken in one window flow onto to affect changes or update the contents of other windows.

### **File Requester in GeoPIXE**

The GeoPIXE *File Requester* is used for I/O of various GeoPIXE files. It includes a tree directory display, bookmarked paths (that can be saved), a path translation table, a preview of certain data-types, a file list in the selected directory path, sometimes with multiple file selection, and file filters. A check box enables the display and sorting of only files with numeric file extensions, useful for many raw data formats.

The *File Requester* is often called behind the scenes in GeoPIXE to search for files needed for analysis. If files get moved on a file system, or between computers, the paths saved in various data-files (e.g. image DAI files) will become unresolved on the new file-system. The *File Requester* is used to search for missing files in the local directory tree, or in another “Config” dir tree. If the file is found, it is quietly used. If not, the *File Requester* will open to enable you to locate it on its new path.

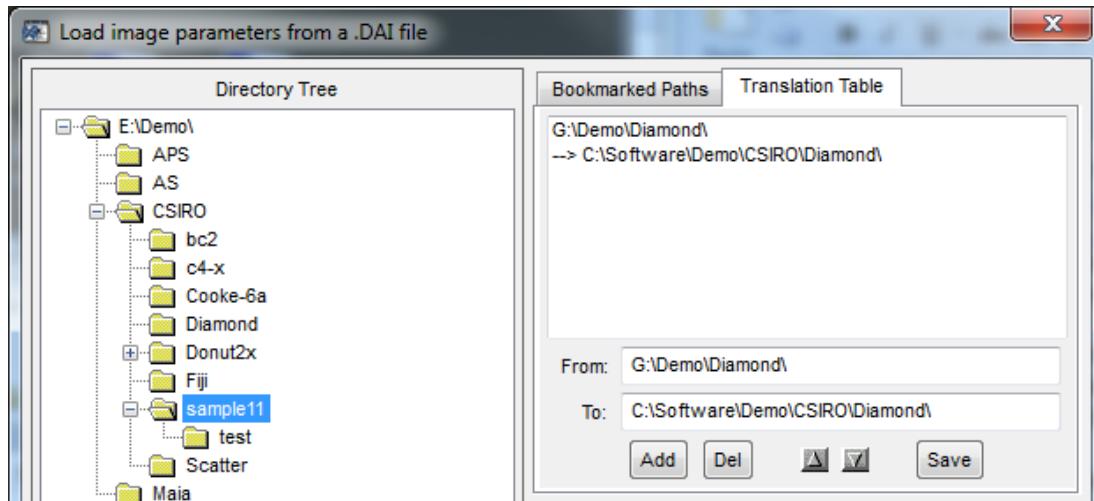


Select a directory tree root from the Bookmarked list (double-click to select) or type in a new root path in the “Root” text field (and hit <return>). Navigate in the directory tree by opening directory nodes (you may need to click on a node to display the “+” symbol to open a directory and display its sub-directories). Single click a directory name to open it in the tree and view its files in the Files list below.

*Note: Initial paths for raw data, analysis and results and config files can be established using the GeoPIXE config file “geopixe.conf”.*

The selected path is shown in the “Path” text field. This can be bookmarked for later use by clicking “Add”. Use “Save” to save these to disk for a later session. Select a file from the file list. The list is sorted in alphabetical order. Use the “Numeric extensions” check-box to display only files with numeric extensions and sort these numerically in ascending order. Some uses of the File Requester in GeoPIXE allow multiple file selection (e.g. raw data sorting for certain data types), in which case use “shift” and “ctrl” modifier keys and drag-selection to select files. Click “OK” to open the selected file(s) or simply double click on a selected file.

Entries can be added to a “Translation Table” to enable the translation of the path roots (perhaps from another computer system) to local paths. A hint is to set-up translations for the path root towards the top of the directory tree.



Selected files are previewed in the “Preview” area for many file types, and various details are shown under “Details”. File selection can be modified using one or more Filters. Separate multiple filters by commas (e.g. \*-m.dai,\*-x.dai” or select multiple files using control-click and drag). Select a file and click “OK”. Cancel file selection using “Cancel” or return a blank file name.

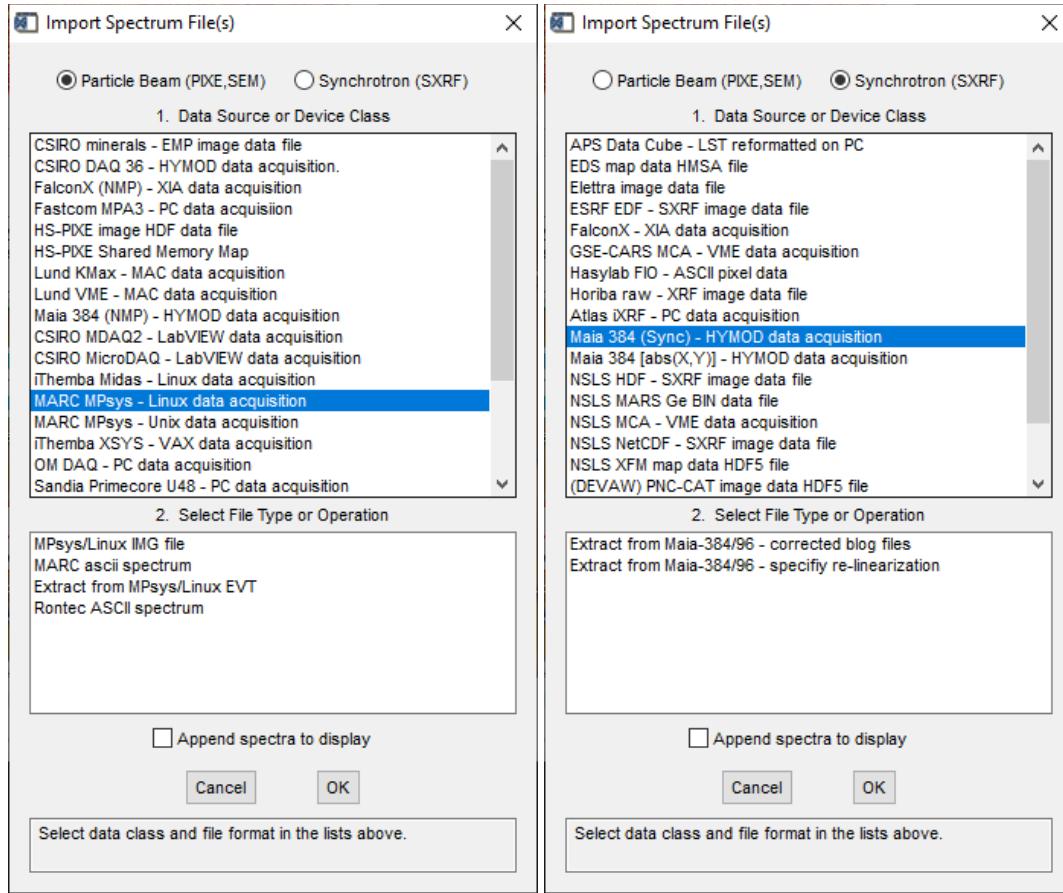
The *File-Requester* endeavours to find files provided by searching in the local directory tree, if they are not found where expected from their complete filename with path. Hence, if dir structure has been changed, or files moved to a new system, the *File-Requester* (called behind the scenes from various window, such as *Sort EVT* and *Image Regions*) will work to find them locally on the new system. You may see a progress bar appear when a search is underway. If it is taking too long, or clearly wandering into unwanted parts of a dir tree, you can “Cancel” it and navigate to the lost file.

## **Import and Calibrate Raw Spectrum Data**

Start GeoPIXE by double clicking on GeoPIXE.sav (or a shortcut to it; see the Installation Notes below). Select “Spectrum Display” from the Windows menu to open the *Spectrum Display* window (a *Spectrum Display* window may be open already, if selected for start-up in config file “geopixe.conf”). To import a raw spectrum, use the “Import” menu under the File menu of *Spectrum Display*.

Select data groups between “particle beam” and “synchrotron”, and select a category of data file, usually by source laboratory or data device. The bottom panel will list various data format options for that group. Select one and click “OK”. This will overwrite the spectra in *Spectrum Display*. To append to the existing spectra, check the option “append spectra to display”.

The “extract” options will scan list-mode data files and extract total energy spectra for each detector (E), the total projection of each onto the X axis (X), the Y axis (Y), and for Maia format data the total time-over-threshold spectra for each detector (T). Use the “select” button in *Spectrum Display* to display the list of detectors and E, X, Y and T spectra found for each.



Import file types are provided by Object Oriented device driver plugins. Plugins for the following devices have been written, and new ones can be created using these as templates:

- 1) Histogram files (.HIST) generated by the Lund Sparrow Kmax data acquisition system, and written on a MAC.
- 2) XSYS spectrum files (.DAT) generated by the XSYS data acquisition system at NAC, and written under VAX/VMS.
- 3) MPsys raw spectrum files (.IMG) generated by the MARC MPsys data acquisition software, and written under PC/Linux.
- 4) MPsys raw spectrum files (.IMG) generated by the MARC MPsys data acquisition software, and written under Unix.
- 5) PIXE, PIGE and RBS RPT spectrum files generated at ANSTO.
- 6) Rontec ASCII format spectrum files.
- 7) 3MCA spectra files generated at the APS.
- 8) MCA spectra files generated at the NSLS.
- 9) Simple ASCII formats.
- 10) Total spectra extracted from Lund Kmax list-mode files, and written on a MAC.
- 11) Total spectra extracted from XSYS list-mode files (.EVT) generated by the XSYS data acquisition system at NAC, and written under VAX/VMS.
- 12) Total spectra extracted from MPsys list-mode files (.EVT) generated by the MARC MPsys data acquisition software, and written under PC/Linux.
- 13) Total spectra extracted from MPsys list-mode files (.EVT) generated by the MARC MPsys data acquisition software, and written under Unix.
- 14) Total spectra files extracted from OM DAQ list-mode files (.LMF) generated by Oxford Microbeams OM DAQ

- data acquisition software, and written under PC Windows.
- 15) Total spectra files extracted from Sandia data-cube files (.EVT) generated at Sandia, and written under PC Windows.
  - 16) Total spectra files extracted from MPAWIN and MPA3 list-mode files (.LST) generated by Fastcom Tec data acquisition software, and written under PC Windows.
  - 17) Total spectra files extracted from BDA12 list-mode files (.BD12) generated by Rontec data acquisition software, and written under PC Windows.
  - 18) Total spectra files extracted from Primecore list-mode files (.pixieU48) generated by the Primecore data acquisition software for the Rontec BD12 detector, and written under PC Windows.
  - 19) Total spectra (E,X,Y) extracted from APS Data Cube files reformatted to LST format.
  - 20) Total spectra (E,X,Y) extracted from NSLS MED/MCA pixel spectra files.
  - 21) Total spectra files extracted from Labo list-mode files (.LST) generated by Laboratory Equipment Co. multiparameter data acquisition software, and written under PC Windows.
  - 22) APS and NSLS MCA spectrum files.
  - 23) Total ‘traverse like’ spectra extracted from 1D PNC-CAT full-spectral scan files.
  - 24) Total spectra files extracted from LIBI Zagreb list-mode files (.LST).
  - 25) Total spectra extracted from the Maia 96 data acquisition system files, with and without pileup extracted and/or gain linearization. Select the pileup limits file for pileup rejection and/or the linearization function parameters and lookup table for gain linearization.
  - 26) Total spectra extracted from the HDF format NSLS image scan files (.HDF).
  - 27) Ortec Maestro SPE spectra from Wakasa Wan Energy Research Centre, Japan (.SPE).
  - 28) Total spectra extracted from Wakasa Wan ACC UniDAQ list-mode data.
  - 29) Total spectra extracted from MCA image files from the SLS (preliminary support).
  - 30) Hasylab FIO spectra files (basic support).
  - 31) Total spectra extracted from Hasylab FIO image spectra files (basic support).
  - 32) Total spectra (E,X,Y,T) extracted from CSIRO Maia detector event mode data streams.
  - 33) New formats are added regularly ...

In the case of general ASCII spectra, various formats are handled. One reads spectra, one from each column, into consecutive spectra (“File→Import” – “Generic ASCII” – “ASCII Spectrum (data only)”). Another reads ASCII spectra files that contain channel energy as the first column (e.g. as produced by the “File→Export→CSV Table” menu) and one or more spectra channel counts as the subsequent columns (“File→Import” – “Generic ASCII” – “ASCII Spectrum (Energy, data)”). These files can be white space, comma or tab delimited, or a combination of these. For files that contain an energy column, it is assumed that all spectra have the same linear energy calibration, which is deduced from this energy column. The first row of the file is assumed to contain column labels. In energy mode, the first label gives the energy units.

### **Example**

```
keV, CAL_T2.02
-0.02425769, 0.0000000
0.008927912, 0.0000000
0.04211353, 0.0000000
0.07529914, 0.0000000
0.1084847, 0.0000000
0.1748559, 0.0000000
.
.
.
```

3.792087,	386.0000
3.825273,	597.0000
3.858459,	1552.000
3.891644,	4614.000
3.924830,	11969.00
3.958015,	24700.00
3.991201,	39311.00
4.024386,	47487.00
.	.
.	.
.	.

## Loading Multiple Spectra Files

Multiple files can be selected from the file requester to load multiple files into consecutive spectra regions in memory. The behaviour depends on whether spectra are extracted from a list-mode file and whether the list-mode data is in a file sequence as opposed to a single list-mode file.

### *Spectra files*

Use multiple file selection using the control or shift keys to select multiple files in the file requester.

A sub-set of files in a directory can be viewed in the file requester by typing a file-name with a wild-card character (or many) and hitting “return” or “enter”. The file requester then only shows these files. To select all of them, click on the first one, and then hold down “shift” and click on the last one.

If a spectrum file contains multiple spectra, then all spectra will be loaded. Spectra files created using the “EVT” button in the Image Regions window, for example, will contain multiple spectra in general.

To append the loaded files to the ones currently in memory, use the “File→Import” pop-up and check the “Append spectra to display” check-box.

### *Extraction from List-mode files*

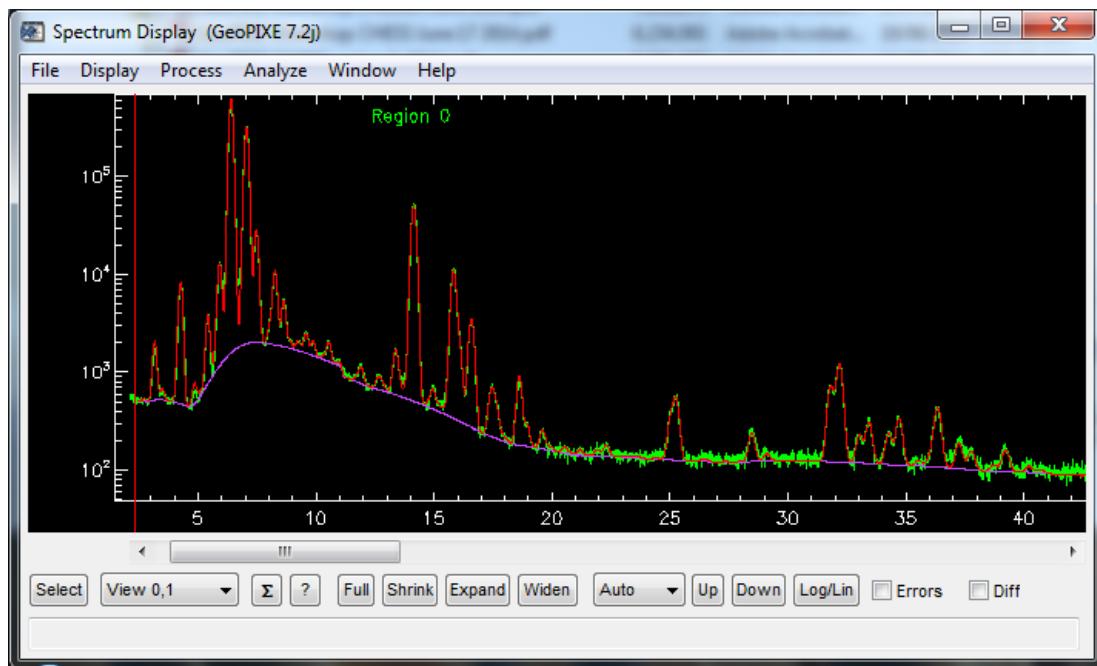
For list-mode data stored in a single file, multiple file selection will cause a number of list-mode files to be scanned for E,X,Y [,T] data. These will be accumulated into a single set of E,X,Y [,T] spectra one for each ADC or detector channel in an array.

Some list-mode formats use a sequence of files to hold the list-mode data (or a series of pixel spectra). In this case, it is normal to select the First file and be prompted to select the Last file; all files in the sequence (files with the same file-name root) will be processed between the First and Last file, in numerical order.

You can use multiple file selection to select files in a sequence for a single list-mode set or select files that include other list-mode sequences. The E,X,Y [,T] spectra data from the specific files selected will be accumulated into a single set of E,X,Y [,T] spectra, one for each ADC.

## Spectrum Display Window

On import, all spectra contained in the file will be displayed by *Spectrum Display*, using an energy horizontal scale for the first spectrum (if calibrated, else channels). You may need to scroll to see the spectrum or click on “Full”. The *Spectrum Display* window can be resized or made full-screen.



Alternatively, you can sort through the list-mode data file and extract the full energy spectra for all ADCs/ detector array channels, and their corresponding X,Y [,T] spectra, using the *Import " Extract from ... "* formats items. This will also automatically create a SPEC file with the same name as the list-mode file, but with “.spec” appended.

*Note that for some formats, this may be missing an energy calibration read from other files (e.g. mp files in MARC format data). Once the spectra are read and calibrated, save the spectra to a new SPEC file using the “File→Save” menu.*

## Spectrum Display Menus

### File Menu:

- Load SPEC Load spectra from GeoPIXE format binary files. Spectra in memory are lost.
- Append SPEC Load spectra and append these to existing spectra in memory.
- Import→Spectra Import spectra in various formats from various platforms, with options to clear memory first, or to append loaded spectra to those already in memory.
- Import→Energies Scan raw data files for beam energies (for XANES).
- Load DA Matrix Load a Dynamic Analysis matrix to examine rows as spectra.
- Load TRAV Load traverse data for multiple elements as spectra.
- Save SPEC Save spectra to a .SPEC file.
- Save TRAV Save traverse data to a .TRAV file.
- Export→CSV Table Export spectra as columns in a comma separated CSV text file
- Export→CSV Table w/ overlays Export spectra as columns including the spectra overlays
- Export→CGM Plots Plot selected spectra in Computer Graphics Metafile format.
- Export→WMF Plots Plot selected spectra in Windows Metafile format.
- Convert→ ... File format conversion programs.
- Print Plot Plot selected spectra to the default printer.

### Display Menu:

- Spectrum Select Open the Spectrum Select window (or use button on bottom left of window).
- Calibrate Energy Open the energy calibration window, and select the Cal 0,1 markers.
- Get ALL Energy Cals from SPEC Get energy Cals for all stations or detectors in an array from a selected spectrum file.
- Get ALL Energy Cals from DAI Get energy Cals for all stations or detectors in an array from a selected image file.
- Clear ALL Energy Cals Set all energy Cals to display “channels” only.
- Identify X-rays Open the X-ray identification window, and select the Identify marker.

- **Mark→...** Select various marker groups, as an alternative to the drop-list at the bottom-left of the window.
- **Clear All Markers** Clears all markers, even those that are not displayed at present.
- **Pileup→from Single Spec** Calculate a pileup spectrum using the first displayed spectrum.
- **Pileup→using Image products** Calculate a pileup spectrum using the full image products.
- **Ge Escapes** Calculate and overlay the Ge escape spectrum.
- **Si Escapes** Calculate the Si escapes spectrum.
- **Show Negative** Display negative channel values. Use this to examine DA matrix rows.

**Process Menu:**

- Smooth Perform a simple 2 channel boxcar smooth operation on all selected spectra.
- Median Filter Perform a 3 channel Median digital filter on spectrum.
- Compress Combine channels in pairs.
- Add Add all selected spectra and store results in the first.
- Add (re-map cal) Add all spectra, but re-map energy calibrations to match first.
- Fold (bit #12) Merge two halves of a spectrum when a most-significant toggle bit has been used (bit #12), i.e. ‘fold’ it over on itself to half length, adding channel counts.
- Fold (bits #11,12) Merge two halves of a spectrum when two toggle bits has been used (bit #11,12), i.e. ‘fold’ it over on itself to half length, adding channel counts.
- Correct Throttle Remove “Throttle” statistics reduction.
- User Plugins→... Execute one of the available spectrum processing user plug-ins.
- Reload user plugins Force a reload of all plugins, if a new one is added or recompiled.

**Analyze Menu:**

- Analyze Cut Integrate peak counts using the currently selected Cut. View results in the Cuts Setup window. Can also use Cut markers and the “” button.
- X-ray Spectrum... Opens the X-ray Spectrum Fit window for fitting PIXE or SXRF spectra. You can also use the menu “Window→X-ray Spectrum Fit”.
- Fit Curve Select a curve fitting function or perform the fit using X markers to define channel ranges to constrain parameters (e.g. X0-X1 for left background, X2-X3 for central peak or slope, X4-X5 for right background).
- Throttle Using the current spectrum as a model, develop a Throttling factor spectrum to be used to selectively reduce Maia data acquisition system data-rates.

“Throttle” uses a pop-up panel of parameters to derive a ‘factor’ by which the count-rate must be reduced, while minimising loss of image quality and trace element statistics. Once this ‘factor’ is derived interactively, the routine uses the current spectrum as a model to calculate a spectrum of factors to reduce each channel count-rate by. This is saved to a TXT file for use with the Maia data acquisition system and also for replay and correction of Throttled event file collected in this way. (See also the *Image Display* “Analyze→Throttle” menu for a better method, and *Sort EVT* for the use of Throttle files on play-back.)

**Window Menu**

- Spectrum Select Another way of opening the *Spectrum Select* window, equivalent to the “Select” button.
- Spectrum Properties Displays details from the spectrum header.
- Calibrate Energy Open the *Energy Calibration* window and select the Cal 0,1 markers.
- Identify X-rays Open the *X-ray identification* window and select the Identify marker. Can also use the “?” button below the spectrum.
- Cuts Setup Open the *Cuts setup* window to view/manipulate energy cuts.
- X-ray Spectrum Fit Open the *X-ray Spectrum Fit* window.
- Fit Results Open the *Fit Results* window, which shows results from X-ray Spectrum Fit.
- Yield Calculation Open window to perform *PIXE/SXRF yield modelling*.
- Depth profile Plot ratio of inner/outer detectors in a Maia array (better to use Depth Wizard)
- Time Amplitude Display Display *Time-Amplitude* for Maia detector records.
- PIGE Fit Open *PIGE fit* window.
- Edit Filters Open the *Filter Setup* window to edit and create X-ray absorber filter files. X-ray Spectrum Fit will need to be closed and reopened to use new filters.
- Edit Detector Open the *Detector Setup* window to edit and create detector files. X-ray Spectrum Fit will need to be closed and reopened to use new detectors.

- Blog Browser Open the Maia event stream raw data browser *Blog Browser*.

***Help Menu***

- GeoPIXE Users Guide Advice on accessing the GeoPIXE Users guide and other PDF guides.
- Query IDL Environment Probe the IDL installation.

**Spectrum Display Widgets**

This list summarises the functions of all widgets on the *Spectrum Display* window, including buttons, sliders, drop-lists and text entry widgets. These are listed from left to right, top to bottom.

***First row below spectrum:***

- X Scroll Bar Control to scroll spectrum in X to show areas off screen.

***Second row:***

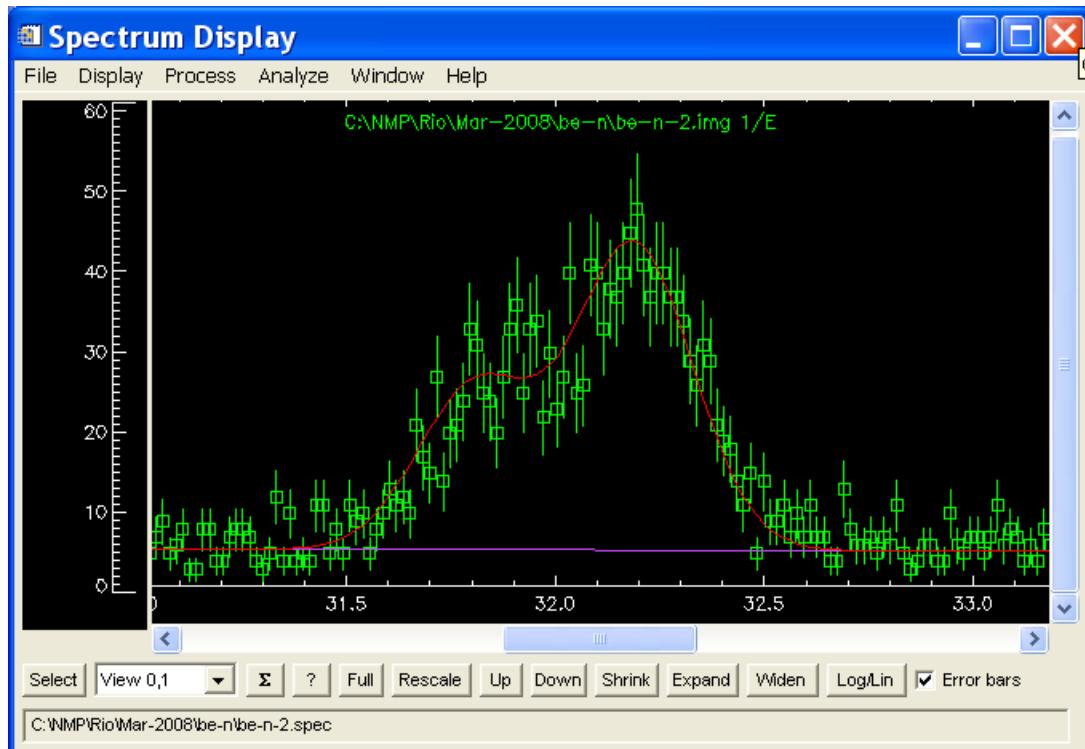
- “Select” Button Open the *Spectrum Select* window to select spectra to display.
- Marker Drop-list Select which marker set is active on the display.
- “ $\Sigma$ ” Button Analyze between the current markers. When used with Cut and X markers, results appear in the *Cuts Setup* window.
- “?” Button Opens the *X-ray Identification* window and sets the marker to “Identify”.
- “Full” Button Display the full spectrum range.
- “Shrink” Button Shrink the spectrum in energy; increase the energy range visible.
- “Expand” Button Expand the spectrum in energy; decrease the energy range visible.
- “Widen” Button Expand to display the range between the View 0,1 markers.
- Scale Drop-list Set the Y scale display mode.
- “Up” Button Expand the spectrum up; reduce the Y maximum value displayed.
- “Down” Button Compress the spectrum down; increase the Y maximum value displayed.
- “Log/Lin” Button Toggle between log and linear display on the Y axis.
- “Show errors” option A check-box to display spectra as points with error bars.
- “Errors” select Display curve with error bars given by error array.
- “Diff” select Overlay the difference between data and fit.

***Bottom row:***

- Help Text Context-sensitive help area, shows help prompts for widgets as the mouse pointer moves over them.

Markers are set by first selecting the marker-set type using the “Marker” drop-list and then clicking on the spectrum to position these, starting with the right-most marker for a group. For example, to set View markers select the “View” markers in the drop-list. If no View markers are set, click to the right of the spectrum to position the V1 marker. Click to the left to position the V0 marker. Either can be moved by clicking on them and dragging. If markers are already positioned, then click and drag them to re-position. Markers may be out of view. In this case scroll the spectrum to find them or click on “Full” to show the entire spectrum.

The Scale mode drop-list selects between: (i) Fixed – Fixed vertical scale, adjusted with Up, Down buttons, (ii) Auto – Vertical scale set to make all spectra visible, (iii) Norm – Scale is set for first spectrum, as for “Auto”, and then all other spectra are scaled to this Y range, (iv) and, Cut – like “Norm”, but uses the sum integrated over the Cut range, between the C0 and C1 markers. Re-apply this drop-list to recalculate the normalizations for re-display, if needed.



Spectrum Display showing data displayed with points and error bars, using “Error bars” option.

### Spectrum Select Window

To select (or hide) spectra open the *Spectrum Select* window using the "Select" button beneath the spectrum (or "Spectrum Select" in the Windows menu). This shows a list of spectra loaded along with parameters for each in a table. All spectra that are visible (all to start with) are marked with "\*" in the row labels on the left of the table. To hide a range of spectra, select them by clicking and dragging a range within the table. Then click "Display" to toggle their visibility. Similarly, the visibility of overlays can be toggled using the “Overlay” button (they are labelled with “F” when on).

Alternatively, while all spectra are visible (all with "\*" initially, or after using “All” button) use “Prev” as a shortcut to display just the first one. Then “Next” to move to the next one, etc. Alternatively, select a row by clicking in it, and then click on “One” to select and display just that row. This window can be resized and scrolled in X and Y. Click on “All” to display all spectra.

Normally *Spectrum Display* colours each spectrum and overlay differently. The colour legend is shown in the “Sample” column of the table. Alternatively, you can select “Highlight” mode, using the left drop-list at the bottom of the *Spectrum Select* window. This highlights or draws in green, the spectrum selected in *Spectrum Select*. To select a spectrum, simply click on that row label. All other spectra are displayed in grey.

	Label	Sample	Grain	Comment	ADC	Mult	Charge	IC Count	Conversion	DT Corr	Size	Cal A
0 *F	3199Q23199.0 4/E				0	1	0.00928585	5.49459e+006	1.69000e-009	0.981104	4096	0.00911867
1 *F	3199Q23199.0 2/E				2	1	0.00928585	5.49459e+006	1.69000e-009	0.979171	4096	0.00930213
2 *F	3199Q23199.0 4/E				4	1	0.00928585	5.49459e+006	1.69000e-009	0.978165	4096	0.00936783
3 *F	3199Q23199.0 5/E				5	1	0.00928585	5.49459e+006	1.69000e-009	0.978834	4096	0.00911867
4 *F	3199Q23199.0 6/E				6	1	0.00928585	5.49459e+006	1.69000e-009	0.977750	4096	0.00911867
5 *F	3199Q23199.0 8/E				8	1	0.00928585	5.49459e+006	1.69000e-009	0.981564	4096	0.00918620
6 *F	3199Q23199.0 9/E				9	1	0.00928585	5.49459e+006	1.69000e-009	0.981052	4096	0.00935129

Buttons at the bottom include Colour, Display, All, One, Overlay, Prev, Next, Array..., Delete:, and a dropdown for 'all Odd detectors'.

Spectra can be deleted using the “Delete:” buttons, which deletes spectra based on the selection of the Drop-list to the

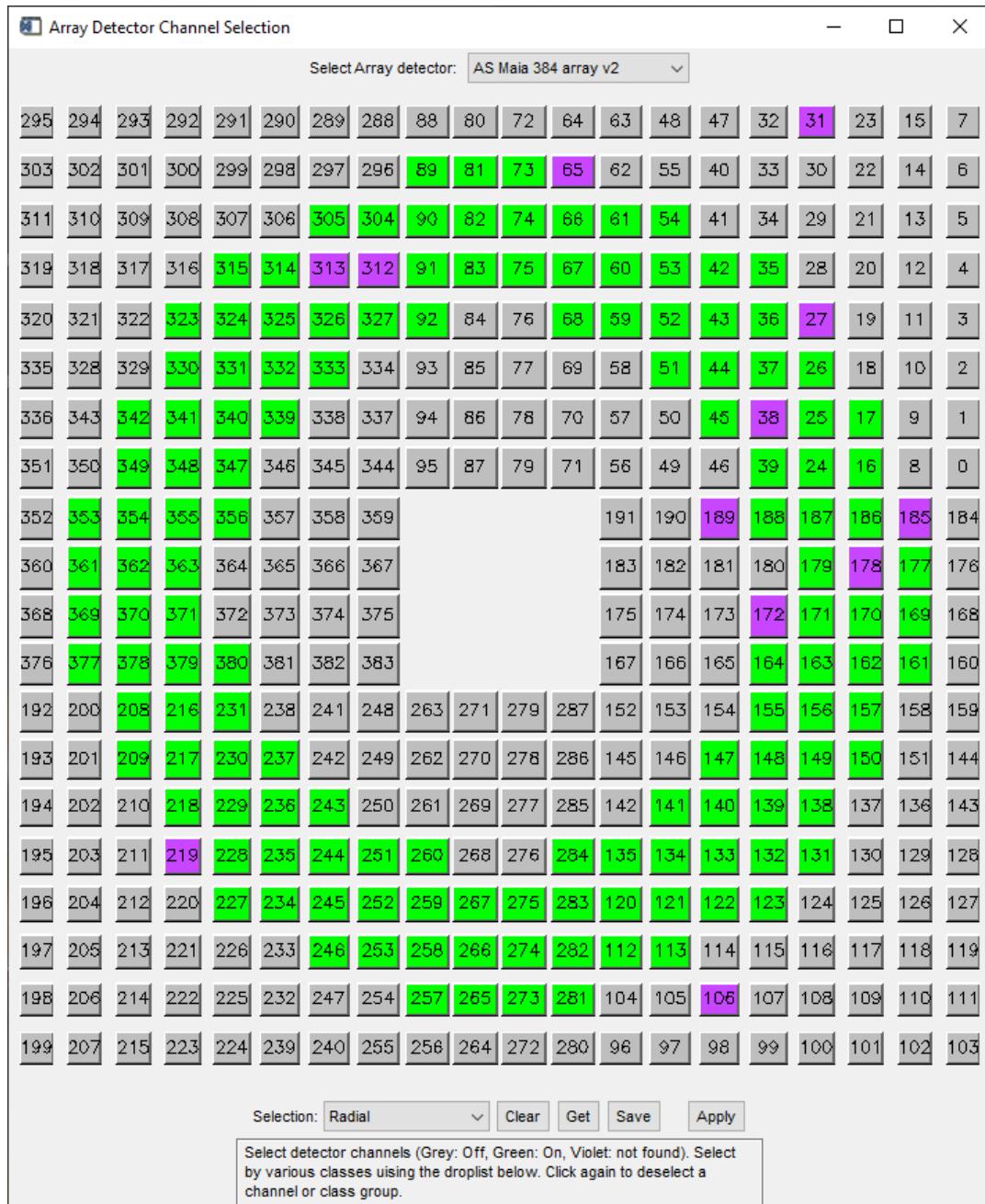
right. To delete spectra, first select a row (or a range of rows by clicking and dragging) and select “Selected range” and then the “Delete” button. To delete all XY spectra, select “all XY spectra” on the drop-list and delete use the “Delete:” button. Similarly, E and T spectra can be deleted as well as all Odd or Even detector channel spectra using the appropriate drop-list selection. These options ignore the current row selection. The “Displayed spectra” drop-list option selects all spectra currently displayed (and showing a “\*” in the row title on the left of the table). The “Fit overlays” option deletes successive overlays (e.g. fit, background, escape peaks, pileup overlays, etc.) of selected rows, starting with the last one added. A special case is the “Charge values” option, which zeroes all charge for all spectra in the table. There are also drop-list items to delete all Not selected or Not Displayed spectra or spectra with No Valid Energy Calibration.

Values in the *Spectrum Select* window can be edited. “Cal A” and “Cal B” change the energy calibration and “Charge” affects the selected charge. “DT Corr” is the relative dead-time (and pileup) correction factor between detector channels, as the Charge is generally already dead-time corrected. It reflects any differences in dead-time/pileup correction applied between detector spectra in a detector array. “Y Low” and “Y High” affect the displayed Y scale and “Y Log” selects between Log (1) and Linear (0) scales.

The “Array...” button brings up a new *Array Detector Channel Selection* window designed for spectra selection based on detector channels in an array.

### **Array Detector Channel Selection Window**

First select the appropriate detector array using the drop-list at the top of the window. Only detector setups are listed that specify a detector array (see the *Detector Setup* window description later in the manual).



Click on a detector pad to toggle its selection state (green=On, grey=Off, violet=not found in *Spectrum Select* table), as well as other members of the selected class. Class is selected using the “Selection Class” drop-list. This allows groups of detectors to be selected or deselected based on column, row radial position, odd and even detector channels. Relevant to the Maia detector, it also allows selection based on the custom chips (12 for Maia 384) and detector quadrant (4 for Maia 384). Use the buttons “Save” and “Get” to save or load detector channel selections to/from a file.

Once the desired detectors are selected, use “Apply” to apply them to the *Spectrum Select* table and *Spectrum Display*.

### Adjusting the View in Spectrum Display

To adjust the viewed energy range in the *Spectrum Display* window, use the horizontal scroll bar to slide the spectrum, or the "Expand" and "Shrink" buttons. The vertical scale can be controlled using "Up", "Down" or "Log/Linear". Leave this on “Auto” normally. You can also use the View markers. These can be selected by using the Marker drop-list below the spectrum and to the left. Select "View 0,1", then click first to set the HIGH end of the desired view range, and then click again to set the LOW end of the view range (or click and drag these, if they are present already). Then

click on the "Widen" button to expand this view. The vertical scale can be optimized using the vertical scale drop-list. Set this to "Auto" to automatically rescale the vertical scale and suppress zero on log scales. The full spectrum can be displayed using "Full".

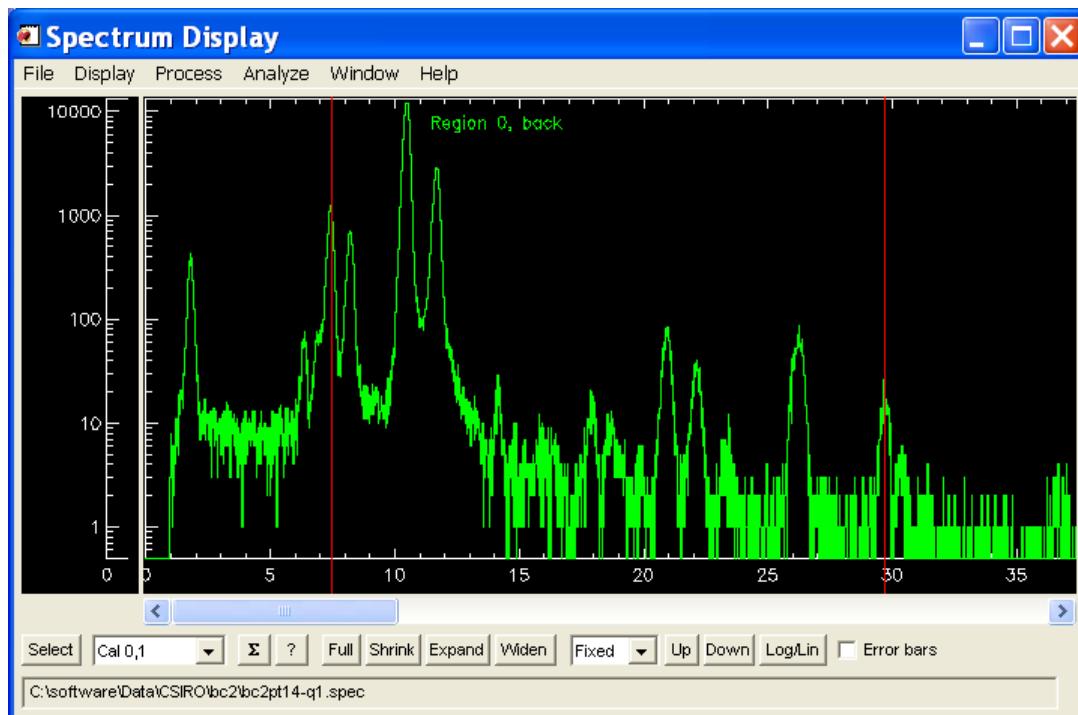
All markers in *Spectrum Display* are set from HIGH to LOW energy (i.e. for View markers, set the high V1 markers first and then click away from it to the left to set the V0 low View marker). If they are on the spectrum already, move them using the mouse and the left mouse button to click and drag them. If they are out of sight, try scrolling the spectrum view or using "Full" to display the entire spectrum. If you lose track of the markers, you can clear them using the "Display→Clear All Markers" menu.

### Context Sensitive Help

*Note that you can get help on buttons and drop-lists, etc. in many GeoPIXE windows by moving the mouse over the widget. Context-sensitive help then appears in the text area at the bottom of the window (if present).*

### Energy Calibration Window

The imported spectrum data are often without energy calibrations or integrated charge (except for some formats, e.g. Maia, MPsys, Lund, NAC and OM DAQ formats). To calibrate the spectrum, open the *Energy Calibration* window using "Calibrate Energy" under the Display or Windows menus. This automatically selects the two Cal markers used to select two peaks to determine a linear calibration. Click in the spectrum to first set the HIGH energy marker, then click again to set the LOW energy marker. These can be dragged by selecting them with the left mouse button. To select the Cal markers again at any time, use the drop-list on the left below the spectrum and select "Cal 0,1".



*The bottom field in the Cal window provides context-sensitive help on any widget the cursor is over. Simply move the cursor around to get help/reminders on the functions of each widget.*

There are two ways to specify the energy of each marker using the groups of three widgets in the *Cal* window on the top-left. Firstly, you could simply type the energy of a line in the lower of these three widgets (use the context-sensitive help to verify what each does). Secondly, for PIXE or SXRF you can enter the element mnemonic and select an X-ray line using the widgets on the top row. Repeat this for the high marker and enter units for the energy (e.g. keV) in the units field (or use the "keV" button to set the units to "keV"). If you select a line mnemonic, then "keV" will be set for you. For PIXE and SXRF, always use "keV" for energy units in GeoPIXE.



The A and B calibration coefficients are dynamically updated on the right. Hit <return> after each typed in entry to update A and B. Now select "Apply One" (click on the "One" button) to have this cal transferred to the displayed spectrum to calibrate the currently viewed spectrum (only). Click on "All" to set the energy calibration for all spectra.

"RA" or 'Re-Assign' is similar, setting the calibration of the first spectrum, but then sets the calibration of all others maintaining the current relative calibration between spectra. Use this for a detector array if you find that you want to globally adjust existing calibrations for spectra for the array.

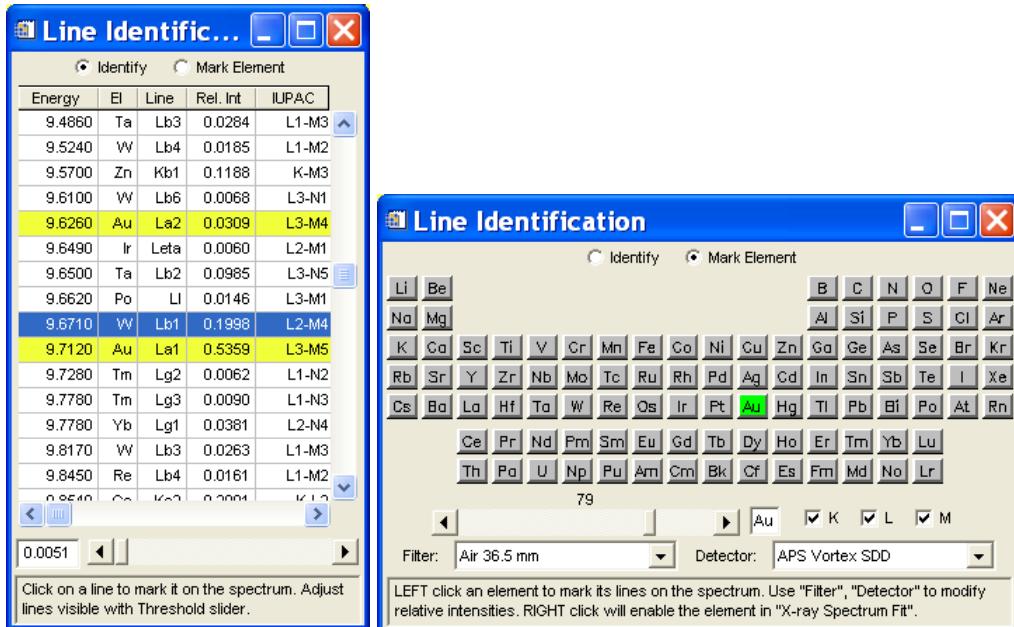
You can also type in A and B coefficients directly. In this case, also remember to click on "keV" and enter A and B in "keV" units, or type in other units in the text widget (e.g. "MeV").

You can also retrieve an existing energy calibration from a SPEC file using the "Get" button. This will retrieve the Cal A,B coefficients from the file for the ADC # specified in the drop-list to the right of "Get". If the drop-list is set to "Any", "Get" will just return the first Cal in the SPEC file.

*Note: It is a good idea to save the spectrum to disk after calibration. Use the Spectrum Display menu "File → Save SPEC" for this.*

### X-ray Identification Window

X-ray lines can be identified using the *Identify* popup window. Click on the "?" button in the *Spectrum Display* window to bring up *Identify* (or select "Identify X-rays" in the Display or Windows menus). This switches to the "Identify" marker. Now you can click and drag within the spectrum to identify the closest match in energy for any feature or peak. The scrolling list in *Identify* shows the closest match and those nearby. You can tailor the relative intensity threshold of lines that are displayed using the scroll bar at the bottom. View the context-sensitive help to get information about each widget in *Identify*. You can also click on a line to set the marker to that energy. In this case, all lines for the corresponding element will be highlighted in yellow in the line list table.



All lines for selected elements can be marked by switching *Identify* into “Mark Element” mode, using the radio buttons at the top. This brings up a periodic table. Click on any element to show the lines for that element, or use the scroll bar at the bottom, which controls atomic number. X-ray lines are marked in orange and the sub-shell edges are marked in dashed light blue. The relative intensities of the marked lines can be modified by the choice of filters and detector. These can be selected from the drop-lists at the bottom of the window.

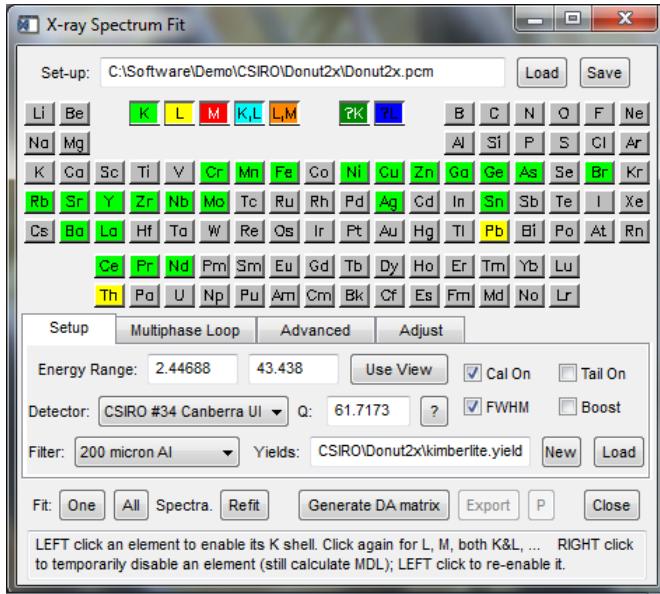
*Tip:* You can open two copies of the X-ray Identification window and set one in “Identify” mode and the other in “Mark Element” mode. To identify a line, click in the “Identify” mode window list (which will set the Identify marker), and then click and drag the cursor on the spectrum, or click a line to mark. To mark an element, click its symbol in the periodic table in the “Mark Element” mode window.

Once the spectrum is calibrated, save it to a GeoPIXE native spectrum file (.SPEC) using the "File→Save SPEC" menu in *Spectrum Display*. This saves the calibration, all spectra, and any fit overlays.

## Fitting a PIXE or SXRF Spectrum

### X-ray Spectrum Fit Window

Open the *X-ray Spectrum Fit* window using the "Windows→X-ray Spectrum Fit" menu of *Spectrum Display*. This shows a periodic table of elements to select for the fit, and entry for filters, detector calibration parameters and PIXE/SXRF yield calculation. Initially, the fit energy range is set to 4 to 38 keV and uses the SNIP background algorithm. This appears on the spectrum as a violet overlay. (NOTE: For clarity, use the *Spectrum Select* window to hide all other spectra in the file, except the one you're interested in fitting; e.g. using “Prev”.). Use the View markers in the spectrum to select a fitting range. Back in the *X-ray Spectrum Fit* window, select "Use View" to set the fit range to this view range.



The background shown is affected by the selection of detector, filter and yields. These should now be set-up. See below for information on calculating yields and setting up detector and filter files. Use the drop-lists for detector and filter to select the correct ones for your experimental set-up. To calculate yields, use the "New" button beside "Yields:" (see below), or "Load" to load an existing yield set.

**Follow worked examples in GeoPIXE Worked Examples PDF in the Help dir using demo data from the FTP site.**

New detector and filter specifications can be assembled using the *Edit Detectors* and *Edit Filters* window (see the later section in this manual) accessed via the "Windows" menu. The detector drop-list may be ghosted out and desensitized if a full detector array has been used in the yield calculation (see the discussion below under *Yield Calculation and Detector Arrays*).

If your spectrum does not already contain integrated charge ( $\mu\text{C}$ ) data, then enter this in the "Q" field. For SXRF "charge" is the photon fluence in units of  $6.242 \cdot 10^{12}$  photons. See the scenarios chapter for a discussion of setting the conversion from ion chamber counts to flux in these units (using the "?" button).

Now you can select elements to fit. (Use the *Identify* features mentioned above to identify lines in the spectrum.) One click on an element in the periodic table selects K X-ray lines only (the button is now green). One more click selects L lines (yellow button). Successive clicks select: M lines (red), both K and L lines (pale blue) and both L and M lines (orange). (See the legend at the top of the periodic table in *X-ray Spectrum Fit*.) You can disable an element by right-mouse clicking on it. Left-click it to enable it again. Shift-left-mouse click (left mouse click while holding down "shift" key) will clear an element setting completely.

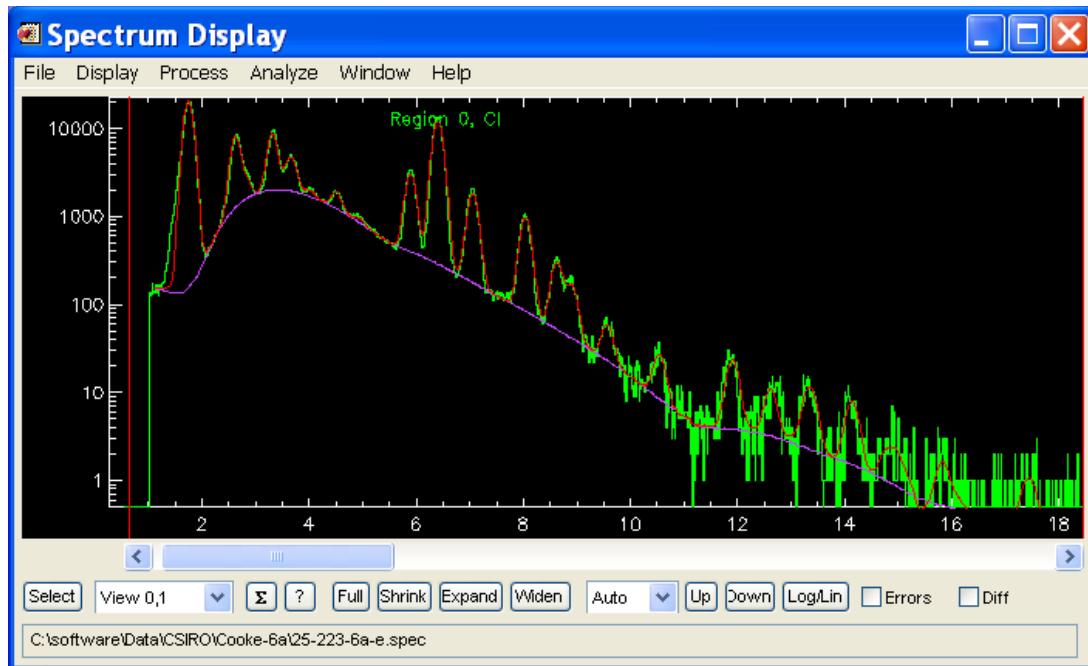
As each element is selected, an initial estimate for it is displayed on the spectrum as a guide, using the default detector resolution set-up in the detector file. This is not a fit yet. With all elements selected, click "Fit One" to perform the fit. The fit to the spectrum is overlaid on the data (in red) in *Spectrum Display*, along with the background estimate (in violet).

Two background options exist at present: SNIP, with or without Boost, and the Bauer algorithm (or a combination of both, which is good for lab XRF). SNIP uses the SNIP non-linear iterative peak-clipping algorithm. SNIP is appropriate for most spectra involving fairly strong filters. Boost is a modified SNIP where absorption effects are removed before application of SNIP. This is recommended for spectra with strong absorption features, such as a strongly rolling-over bremsstrahlung peak at low energy in PIXE. See details below under "Advanced Fitting Parameters".

This overlay can be hidden by selecting the spectrum in *Spectrum Select* and hitting the "Fit/Overlays" button to toggle its visibility. The "F" in the row label indicates the visibility of the overlay.

*Advanced fitting parameters that may need to be adjusted from time to time for added control on fitting are discussed*

below.



## Fitting Multiple Spectra

Note that the operation of the “Fit All” button of *X-ray Spectrum Fit* has changed in GeoPIXE 3.3.

To fit multiple spectra using the “Fit: All” button in *X-ray Spectrum Fit*, start by removing any undesired spectra if necessary. Cycle through the spectra using the “Next” button of the *Spectrum Select* window (“Prev” to begin with to display just the first spectrum). Any undesired spectra can be deleted using the “Delete Spec” button.

To delete all XY spectra (e.g. that may be there if the spectra have come from an Extract from list-mode operation) using the “No XY” button. Similarly, you might want to delete all spectra with “No Valid Energy Calibration”.

If it is not already present, set the charge/flux for a spectrum in the Q box in *X-ray Spectrum Fit*. If all the spectra do not initially contain Q information, then the “Fit All” operation will use the same Q for all spectra. If spectra have individual charge values, then these will be used in each fit.

Then click the “Fit: All” button in *X-ray Spectrum Fit*. The results of fitting all spectra will be appended to the *Fit Results* table.

## Fit Results Window

If any misfits indicate a missing element, add this element and perform the fit again. You can also use the “Refit” button for this. However, in order to use “Refit” you need the *Fit Results* window open, and you need to make sure a row of *Fit Results* is selected first (see *Fit Results* below).

*Fit Results* shows the results of fits to spectra and displays various result quantities given by the drop-list on the left (default is “conc” for concentration). The second drop-list allow the units of “conc” to be selected. The default is “ppm (wt)” for ppm by weight. “mmol/l” requires a valid density to be specified for the unknown layer of the sample (see *Yield Calculation* set-up elsewhere). “ng/cm<sup>2</sup>” is appropriate for a layered target and gives the mass density for the unknown layer.

The “Properties” button brings up a pop-up panel to refine parameters used in the Yield calculation and to specify fluid inclusions parameters for modelling yields from a buried fluid inclusion. See the section later on Fluid Inclusions for

details.

	File	Cr	Mn	Fe	Ni	Cu	Zn	Ga
0	donut2x-2-whole	<0.003%	0.175%	4.47%	464.	12.6	30.9	
1	fiji-2x			23.5%		0.370%	108.	
2	bc2pt14		0.38%	4.33%	0.241%	40.	0.328%	

Buttons at the bottom include Conc, ppm (wt), Load, Save, Export, Properties, Veto, Delete, and Clear.

Calibration parameters, peak width parameters, and tails can be enabled or disabled in the fit using the checkmarks to the right in *X-ray Spectrum Fit*.

If there are problematic detector artefacts in the spectrum that need to be ignored during fitting, specify the regions of the spectrum to excise using Cuts. Setting up Cuts is discussed below. Input these into *X-ray Spectrum Fit* using the "load" buttons beside "Cuts:" on the "Advanced/General" tab. These cuts will define ranges of energy in the spectrum that will be ignored by the fitting procedure.

As each fit is performed, the results (as well as all parameters) are added to the *Fit Results* table. This can be viewed via the "Windows→Fit Results" menu in *Spectrum Display*. The *Fit Results* window is described below.

The present *X-ray Spectrum Fit* parameters and element selection should be saved to a file (.PCM) using the "Save" button at the top of *X-ray Spectrum Fit*. New ones can be loaded with "Load".

Use the context-sensitive help field at the bottom to learn about each widget in *X-ray Spectrum Fit*.

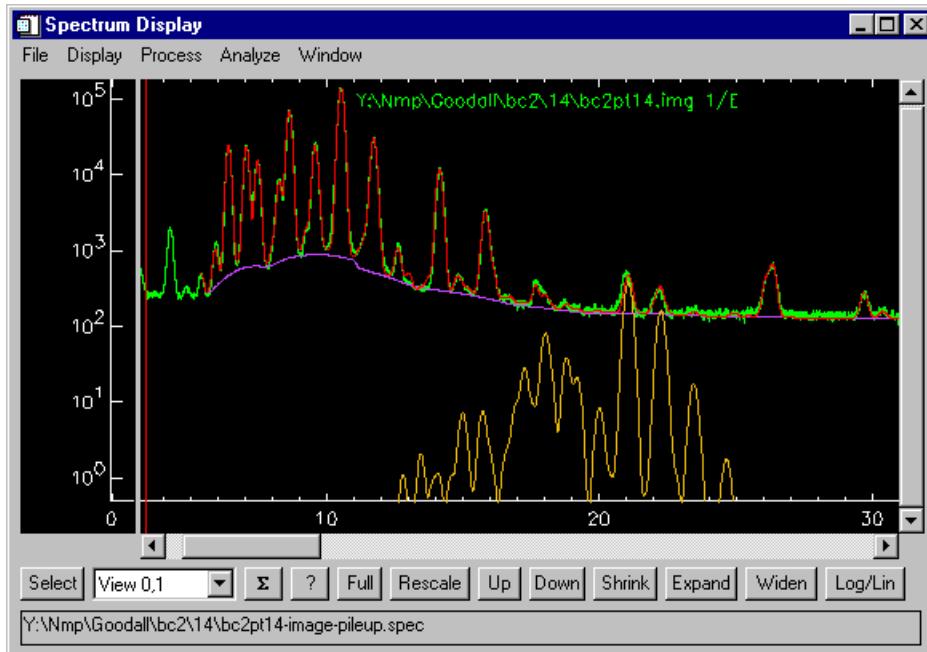
## Pile-up Models

The type of pile-up modelling can be selected using the "Pileup" drop-list. Normally, a "pile-up element" is used in PIXE or SXRF spectrum fitting; select this with the "from Spectrum" option. In this mode, the relative intensities of the pile-up element lines are calculated automatically from the intense lines in the spectrum being fitted, which will normally be from a selected region or the total PIXE/SXRF spectrum for the entire image area. Use this option for relatively uniform regions, or for images where a single element dominates the spectrum over all pixels. GeoPIXE calculates pile-up lines to second order (3 pulses pile-up) with up to 50 lines.

However, if the PIXE/SXRF spectrum corresponds to a whole scanned image area with spatially changing major elements then the nature of the pile-up will have changed with position across the image. In other words, the major intense X-ray lines and the resulting pile-up relative intensities will have changed with pixel. A better approach in this case is to calculate pile-up relative intensities using direct products of image pixel counts. This can be done using the "Display→Pileup→using Image products" menu in *Spectrum Display*; remember to load the corresponding images into the *Image Display* window first.

*Note: Use the calculation "Display→Pileup→using Image products" for a spectrum corresponding to the whole scan area.*

*Note: Don't confuse pileup modelling in *X-ray Spectrum Fit*, as discussed here, with pileup correction used during sorting of Maia list-mode data formats (see Sort EVT window and the section "Correction of Images for Pulse Pile-up Effects" below).*



*X-ray Spectrum Fit* can make use of this prior calculation of ‘Image Pileup’ by selecting the “Image pixel product pileup” option in the “Pileup” drop-list on the “Advanced/General” tab. Make sure to calculate this pile-up first before trying to fit, and it may be helpful to save the spectrum with this pile-up simulation for later reference.

*Note that this routine requires that images have been projected already, and makes use of products of elemental images, on a pixel-by-pixel basis. You will need to complete the stages given below on building a DA matrix and sorting elemental images first. Also, take care in fitting to make sure that cuts are not used that remove a major element line that is important for pile-up simulation. This is illustrated with worked examples in the GeoPIXE Scenarios and Data Flow section.*

## Example

Load the sample spectrum “25-223-6a.spec” from the “data\csiro\cooke-6a” directory. Select the View markers (normally set when window is opened) and click on the HIGH and LOW ends of the main part of the spectrum. Click on “Widen” to expand between these markers. Open the Spectrum Select window (click on “Select”) and click on “Prev”, to display just the PIXE energy spectrum.

Open the fitting window using the “Window→X-ray Spectrum Fit” menu. In *X-ray Spectrum Fit*, click on “Load” at the top to load fitting parameters from a saved PCM file (“25-223-6a.pcm” in the same directory). This will display the SNIP background (in Boost mode in this case) and the initial estimate of the spectrum. To fit the spectrum click on “Fit One”. The results of the fit can be viewed in the *Fit Results* window (“Window→Fit Results” menu).

There are also examples in the *GeoPIXE Scenarios and Data Flow* section and in the *GeoPIXE Worked Examples* PDF.

## Fit Results and Adjusting Properties

The *Fit Results* table can be opened using the "Windows→Fit Results" menu in *Spectrum Display*. The results show concentration calculated using the yields and parameters set-up in *X-ray Spectrum Fit*. The various parameters can be viewed using the drop-list at the bottom-left of *Fit Results*. These include concentrations, error estimates, minimum detection limits and all fitting, experimental and yield parameters. The *Fit Results* window can be resized and scrolled.

Buttons on the *Fit Results* window provide these functions: “Load” load previous results (stored in files with extension “.pfr”) and append them to the table; “Save” save results to a PFR file; “Export” to export selected data and parameters to a CSV file for import into a spreadsheet program; “Properties” to make adjustments to various sample properties (see below); “Veto” to veto selected element results columns; “Delete” to delete selected rows; and “Clear” to clear the

entire table.

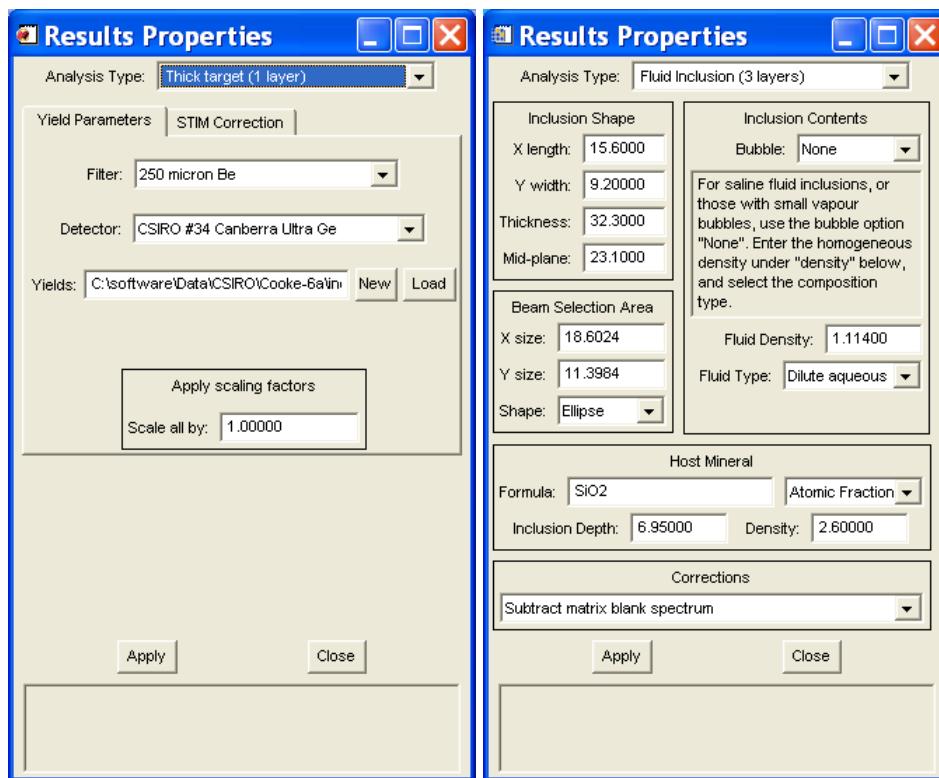
To correct a row of *Fit Results*, to add an extra element to the fit, for example, use the "Refit" button in *X-ray Spectrum Fit*. This will replace/update the first row selected in *Fit Results*. But the row must be selected first for this to work. To select a row, click in the left row label, or click and drag a range of rows within the table.

**Note that a row of the table must be selected for "Refit" to work.**

Selected rows can be deleted with the "Delete" button, or the whole table can be cleared with "Clear".

## Result Properties Window

Specific properties of each analysis can be adjusted using the "Properties" button, which opens the *Results Properties* window. For thick targets this enables filters, detector and yields to be changed or an overall scaling factor to be applied. Select a row, or range of rows, to effect. After making a change, hit "Apply" in *Results Properties* to apply the change. This will apply just the changes you made to all rows selected. Coming soon will be a "Tie" feature similar to the original GeoPIXE. For fluid inclusions, a number of parameters can be set governing the 3D modelling of the geometry of a fluid inclusion and subtraction of blank contributions (see the Scenarios section on fluid inclusion analysis).

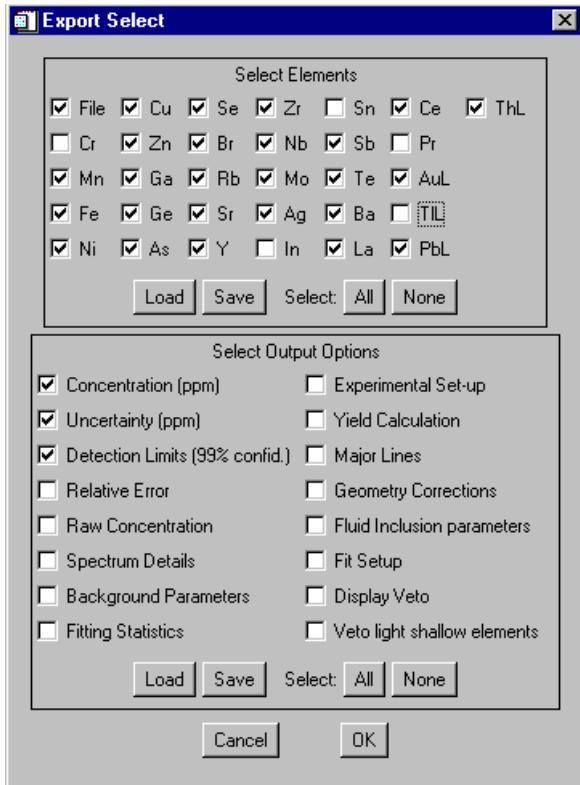


*Fit results* can be loaded or saved to a file (.PFR) using "Load" and "Save". The currently displayed results or parameters can be exported to a comma-separated ASCII file (.CSV) using "Export". This brings up a pop-up panel to select which categories of parameters and results to export, and to select elements. These files can be loaded into a spreadsheet program.

## Export Selection Requester

To export fitting results from *Fit Results* use the "Export" button. The following requester gathers information for the export. The top area selects the elements to export. This selection can be loaded from a SELECT file or saved for later use. The button section selects what to export from the tables available (see drop-list on left in *Fit Results*). The selection "Veto light shallow elements" selects a criterion to veto the export of error-prone light element results from

fluid inclusions where the lines have suffered excessive self-absorption in the sample matrix. These selections can also be loaded or saved to a file.



## Advanced Fitting Parameters

The “Advanced” tab on the X-ray Spectrum Fit window contains a number of parameters and options for refining the treatment of background, peak-tailing and detector parameters for spectrum fitting under the following tabs:

### 1. General:

- i. **Cuts:** A file of spectrum CUTs or regions-of-interest (ROI) can be loaded to specify regions of the spectrum to exclude ranges of spectrum channels from the fit.
- ii. **Pileup:** Enables selection of the pileup calculation mode, selecting between normal calculation of pileup based on line intensities in the spectrum being fitted, and advanced pileup based on pixel-by-pixel products of elemental images.
- iii. **Deficit(%):** Sets the % loss in the sum peak amplitude for a pile-up peak due to the finite timing resolution of the system and the shaping time of the amplifier.

### 2. Back1:

- i. **Background algorithm:** Chose the algorithm used for background estimation between the built-in “SNIP” and “Bauer” background algorithms and background plug-ins.
- ii. **Passes:** Select the number of passes through the background algorithm. SNIP uses 8 passes by default.
- iii. **Boost mode enable:** Enables “Boost” mode, which removes strong absorption related curvature in the background before applying the background algorithm. This is useful with PIXE spectra collected using filters that produce a strong roll-off towards low energies in the spectrum.

### 3. Back2:

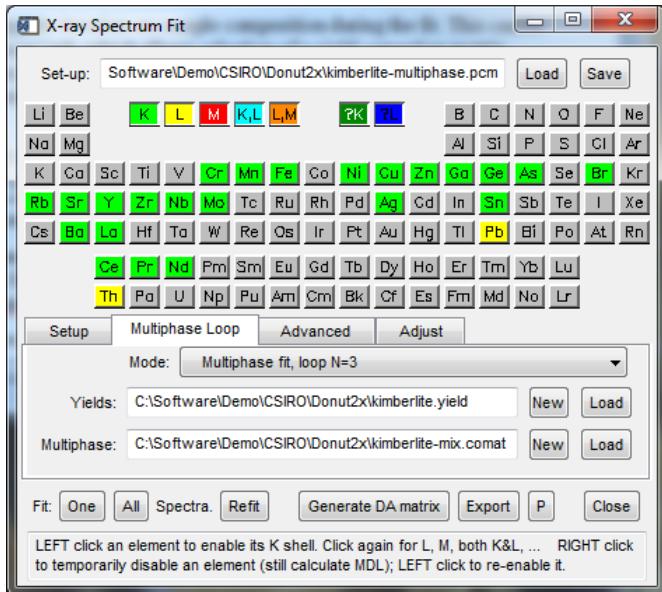
- i. **Multiple Background mode:** Off uses a single selected background component, while “Split Back” will split this background into two components, with a smooth transition from one to the other at the “Split Energy”.

- ii. **Split Energy:** Define the energy (keV) of the transition from one Back component to the other. This is used for lab XRF spectra to separate light element background from the broad continuum of a filtered lab XRF source spectrum.
4. **Cal:**
- i. **Cal fit parameters:** Free or fix Cal parameters (reflects radio button on “Setup” tab).
  - ii. **Free Gain term:** Optionally fix or free (default) the gain energy calibration term alone.
5. **Widths:**
- i. **Width Parameters:** Controls peak width fitting parameters, to be “Free” or “Fixed” in the fit, or return them to defaults. Only the Noise parameter is varied in the fit.
  - ii. **Free Fano factor:** Occasionally, for ultimate fitting accuracy, you may need to free the Fano factor, which controls the energy dependence of fitted peak widths. The default works well in most cases.
  - iii. **Mn K FWHM:** Text entry and slider to manually change peak width noise parameter, when width parameters are fixed in the fit. This parameter is refined when “Free” in the fit.
6. **Tails 1:**
- i. **Tail Fit Parameters:** Controls peak tail fitting parameters, to be “Free” or “Fixed” in the fit, or return them to defaults or disable tails altogether.
  - ii. **Tail Amplitude:** Text entry and slider to manually change tail amplitudes, when tail parameters are fixed in the fit. This parameter is refined when “Free” in the fit.
  - iii. **Write detector parameters:** Write the modified detector parameters (tail amplitude on this panel, and the parameters on the “Tail 2” panel) to a selected detector file.
7. **Tails 2:**
- i. **Amplitude: F, B:** Thickness ( $\mu\text{m}$ ) of regions of incomplete charge collection at the front (F) and back (B) of the detector crystal. These parameters help to shape the dependence of tail strength on X-ray energy.
  - ii. **Length: L, S:** Parameterization of the X-ray energy dependence of the exponential tail lengths ( $\text{lengths} = \text{L} + \text{S}^*(\text{energy}-6.4)$ ).
8. **PIXE:**
- i. **Curvature:** Parameter to fine-adjust the curvature of the background, particularly at lower X-ray energies in PIXE spectra (<7 keV), which is useful to refine curved background when Boost is active.
  - ii. **Secondary electron bremsstrahlung removal:** An alternate approach to shaping low-energy background (superseded by “curvature” and “boost” options).
9. **XRF:**
- i. **Compton Tail:** Amplitude of the exponential tail on the Compton inelastic scattering peak (and also high-energy tailing). This parameter is refined when “Free” in the fit (see 3(i) above). This term approximates the strength or amplitude of the multiple scattering tail of the scattering peak.
  - ii. **Tail Length:** Length of the Compton tail. This parameter is refined when “Free” in the fit (see 3(i) above). This term approximates the slope or length of the multiple scattering tail of the scattering peak.
  - iii. **Shift:** Slider and text entry field to adjust the energy of the Compton peak(s), to account for matrix effects and changing mean electron momentum.
  - iv. **Spread:** Slider and text entry field to adjust the width of the Compton peak(s), to account for multiple-scattering effects, sample layout, detector solid-angle and electron momentum distribution.

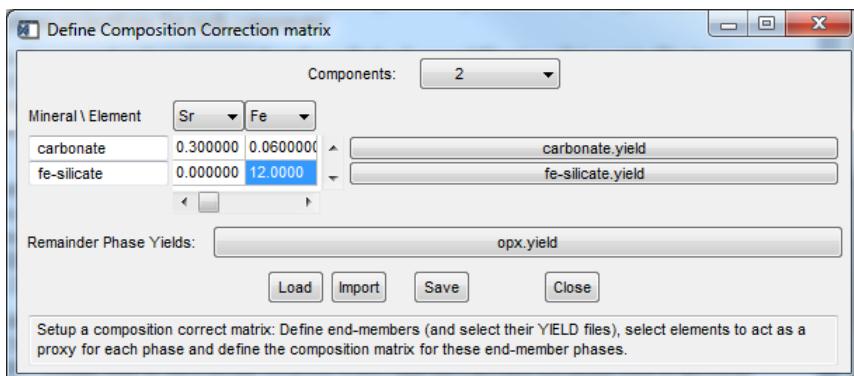
## **Multiphase Loop**

In the same way as the Correct Yields method can be used to perform a pixel-by-pixel sample composition correction of images (see “Correction of Images for Sample Composition Effect on Yields” section), the fit can be iterated to converge on the major element composition with the sample expressed as a mixture of end-member terms plus a remainder component. The results of a fitting iteration determines the end-member components, which is used to form a

weighted average of the (inverse) X-ray yields and line intensities for a further iteration. This converges on an improved estimate of sample composition and uses better X-ray relative intensities that reflect the major element composition.



First, select “Multiphase Fit” in the drop-list and the number of iterations (3 is usually ample). The end-member matrix needs to be defined in the *Define Composition Correction Matrix* window (open it using the “New” button opposite “Multiphase”). Identify the main end-member components (phases) in the sample and perform a yield calculation for each. Then identify elements that are observed well in the spectrum and provide some distinction between phases. Then define a mixing matrix, which defines the concentration of each of these distinguishing elements in each phase and select the pre-calculated yields files for each phase. The remainder, not accounted for by these components, uses a “Remainder” yield model. Save this to a COMAT file.



*A simple matrix defined to assume a mixture of a carbonate (largely identified by Sr concentration) and an Fe-silicate (characterized by Fe)*

In the *X-ray Spectrum Fit* window, select one of the “Multiphase fit, Loop N=n” modes for selected number of composition iterations. Seldom will you need more than N=2,3 iterations. Then click “Fit: One”, which will do the fit and iterate on major element composition and the inferred end-member phase mixture. The final concentrations should better correspond to the actual composition as sampled by the spectrum.

*NOTE: The model assumes uniform mixing of end-member component phases. If the region contains dramatically different areas in terms of composition, then the full MPDA imaging approach may be more appropriate.*

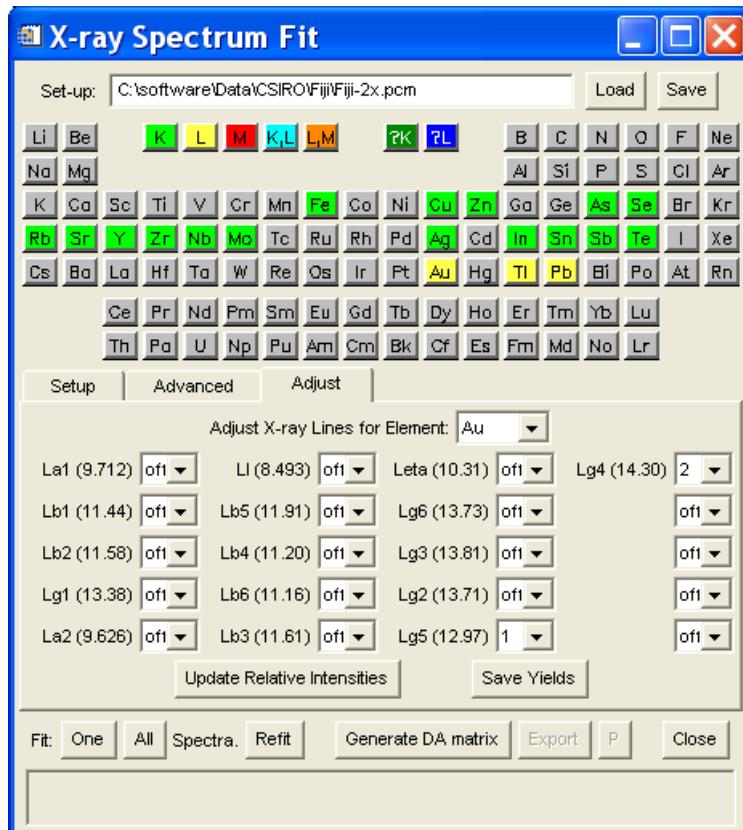
## Adjustment of X-ray relative-intensities

The “Adjust” tab on the X-ray Spectrum Fit window opens a panel to allow adjustment of the X-ray relative-intensities for a selected element. For a single element, the intensities of selected lines and groups of lines can be freed in the fit to

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help refine their relative intensities. This is intended for database refinement and to adjust minor line intensities that are known to be sensitive to chemical effects and atomic environment.

Select the element of interest with the top drop-list. Then select the lines to be adjusted. Always leave at least the alpha(1) peak fixed ("off"). Use the drop-list beside each line to select a free parameter to be used to scale this line intensity in the fit. Lines close in energy should be grouped and associated with the same free parameter number. In the example below, just the L $\gamma$ 4 and L $\gamma$ 5 lines of Au are being adjusted to account for chemical effects.



Once line intensities have been adjusted, the new values can be updated, which updates the yield calculation results in memory, using the "Update relative intensities" button. Once updated, these refinements could be used in general fitting using the current yield and relative intensity data in memory (select adjust element to "off"). To save these to disk, use the "Save Yields" button and give the new file a distinctive name that says that this element has been adjusted.

*N.B. These changes do not change the X-ray database values for relative intensities, or the fundamental parameters on which they are based. It only makes local changes, which are saved to the specified yield file.*

## Fitting Background User Plug-ins

The *X-ray Spectrum Fit* window has a user plug-in facility to cater for user derived background estimation. You can write background operations in IDL. These are loaded when GeoPIXE runs, and appear on the Background selection drop-list (on the "Advanced/Background" tab)

You need IDLDE to be able to compile your own plug-in procedures. However, once you have built the SAV file, you can run them through GeoPIXE using IDL run-time.

User plug-ins are designed at present for operations that change the spectrum data or add an overlay (e.g. background), for the currently selected spectra, but do not change the spectra names, the number of spectra, or their sizes. Extension in these areas may come later.

The file "template\_back\_plugin" is provided with the GeoPIXE distribution. It provides a template for writing

spectrum background plug-ins. It performs a simple median smooth as an example, with the option of removing absorption using Boost. See the file for a description of the arguments.

All Background template routines MUST be named with "\_back\_plugin.pro" at the end of the file name. For a new "Fred" plug-in, copy and rename the template file to "fred\_back\_plugin.pro" and edit the first line to the new name.

Plug-ins should be compiled in IDLDE and saved as a SAV file. Only compile routines for ONE plug-in and save it using the command:

```
SAVE, /routines, filename='fred_back_plugin.sav'
```

for a "fred\_back\_plugin" plug-in. To ensure this, exit IDLDE and start it again to compile and save another plug-in (or use the command .FULL\_RESET\_SESSION, ".f" for short, in IDLDE).

NOTE: It is very important to ensure that ONLY routines for ONE plug-in are saved in each SAV file. Otherwise, unexpected results may result when the SAV files are restored at run-time. The plug-in SAV files will then be loaded automatically when GeoPIXE.sav runs, if the plug-in SAV files are located in the "plugins" sub-directory of GeoPIXE.

## **Spectrum User Plug-ins**

The *Spectrum Display* window has a user plug-in facility. You can write spectrum processing and other user spectrum operations in IDL. These are loaded when GeoPIXE runs, and appear on the "Process→User Plug-ins" menu.

You need IDLDE to be able to compile your own plug-in procedures. However, once you have built the SAV file, you can run them through GeoPIXE using IDL run-time.

User plug-ins are designed at present for operations that change the spectrum data or add an overlay (e.g. fit), for the currently selected spectra, but do not change the spectra names, the number of spectra, or their sizes. Extension in these areas may come later.

The file "template\_spectrum\_plugin.pro" is provided with the GeoPIXE distribution. It provides a template for writing spectrum processing plug-ins. It performs a simple smooth as an example. See the file for a description of the arguments.

All Spectrum template routines MUST be named with "\_spectrum\_plugin.pro" at the end of the file name. For a new "Fred" plug-in, copy and rename the template file to "fred\_spectrum\_plugin.pro" and edit the first line to:

```
pro fred_spectrum_plugin, p, i, title=title, history=history
```

Plug-ins should be compiled in IDLDE and saved as a SAV file. Only compile routines for ONE plug-in and save it using the command:

```
SAVE, /routines, filename='fred_spectrum_plugin.sav'
```

for a "fred\_spectrum\_plugin" plug-in. To ensure this, exit IDLDE and start it again to compile and save another plug-in (or use the command .FULL\_RESET\_SESSION, ".f" for short, in IDLDE).

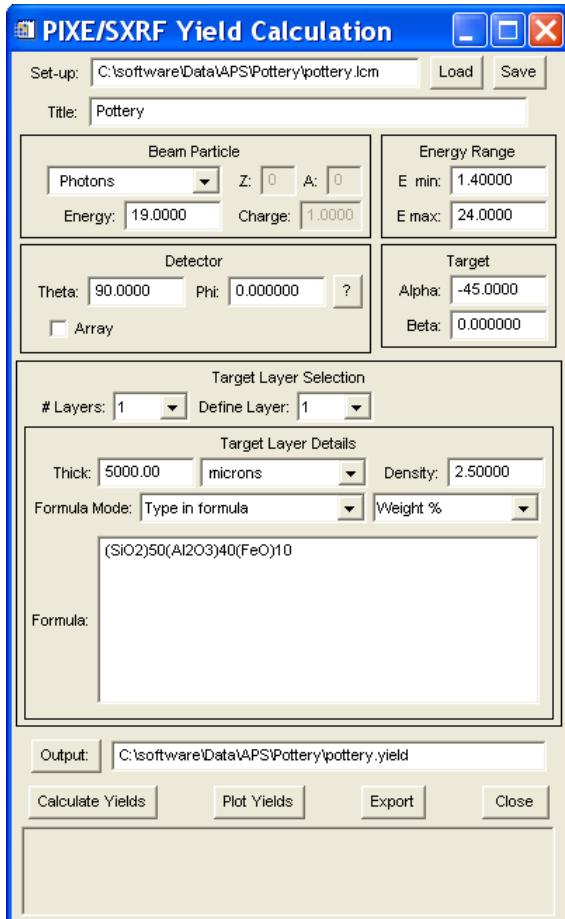
NOTE: It is very important to ensure that ONLY routines for ONE plug-in are saved in each SAV file. Otherwise, unexpected results may result when the SAV files are restored at run-time. The plug-in SAV files will then be loaded automatically when GeoPIXE.sav runs, if the plug-in SAV files are located in the "plugins" sub-directory of GeoPIXE.

## **Calculating Thick, or Multi-layered, X-ray Yields**

### **PIXE/SXRF Yield Calculation Window**

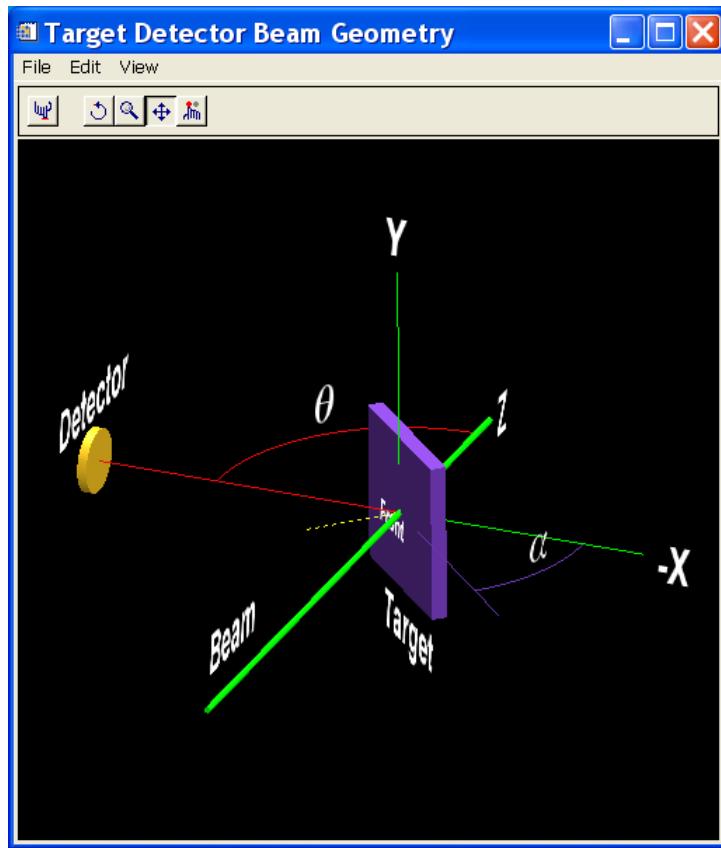
From the *X-ray Spectrum Fit* window, select "New" beside "Yields:" to open the *PIXE/SXRF Yield Calculation* window for multi-layered X-ray yield calculation. The groups of parameter fields include beam species, detector geometry and

target tilt, X-ray line energy range, the number of layers in the target and the set-up for each layer. The target can be thin, multi-layered or thick. With parameters set-up, use "Calculate Yields" to perform the calculation and open a file requester for the destination YIELD file name. The yields for all X-rays lines (K, L and M) within the energy range ( $E_{\min}, E_{\max}$ ) will be integrated throughout the layered structure, including secondary fluorescence contributions. Relative intensities determined this way are used in fitting the spectrum. In this way, we have accurate relative intensities for all lines, even from a layered structure.



Detector angle is specified in terms of "Theta" relative to the forward direction (i.e. back-angles are greater than 90°), and "Phi" which is the orthogonal out-of-plane angle. Theta angles less than 90° correspond to a transmission geometry, which is supported (in this case the target thickness is important to model the transmission absorption of fluoresced lines). Target angles are "Alpha" - a rotation about a vertical axis through the target (use Alpha= 0 for normal incidence); and "Beta" - a tilt about a horizontal axis across the face of the target (use Beta= 0 for normal incidence).

*For detector angles around 90° degrees or more, if the target is facing the detector, then Alpha must be negative (e.g. Theta = 90° and Alpha = -45° is a typical synchrotron geometry). Use the "?" button to bring up the 3D geometry viewer to check the layout in detail. Click and drag in this window to rotate the model view.*



Beam species are selected with the drop-list in the top-left of *PIXE/SXRF Yield Calculation*. These include protons, molecular hydrogen, photons, helium and heavy ions (general), as well as monochromatic X-rays and a continuum lab source (with the continuum plugin). At present, all ions use ECPSSR proton cross-sections at an equivalent velocity and scaling. This is accurate for protons and molecular hydrogen, but increasingly approximate for heavier species. (Helium cross-sections will be added soon.) Photons use the recent compilations of Ebel *et al.*, 2002.

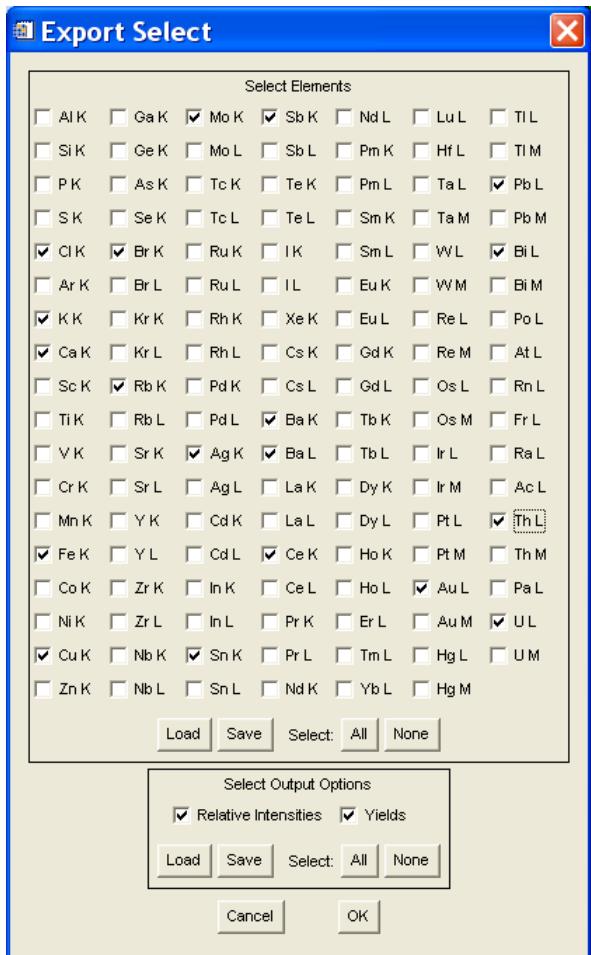
The number of layers in the target is set with "# Layers", and the layer in the editor below is selected using the "Define Layer" drop-list. A further drop-list selects the "Unknown Layer". This the layer in which detected elements, unaccounted for in the composition of any layer, are assumed to reside. The returned concentrations reflect their location in this layer.

For each layer, you can specify thickness (in mg/cm<sup>2</sup> or microns) and chemical formula. For micron thickness you need to enter density (unless it's a pure element layer; then density is extracted for you from the database). Formulae can be entered as text, or using a table of oxides, selected using the "Formula Mode" drop-list. For formulae, the action of any weighting factors (outside of brackets "()") can be set using the drop-list on the right. Formulae can take various forms (e.g. "Al", "Al<sub>2</sub>O<sub>3</sub>", "C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>", "(CH<sub>2</sub>)<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub>", "(Al<sub>2</sub>O<sub>3</sub>)<sub>70</sub>(SiO<sub>2</sub>)<sub>30</sub>"). When brackets are used "()", then the function of the multipliers outside the brackets is set with the drop-list on the right. It selects between "Atomic Fractions" for atomic weighing (e.g. "(CH<sub>2</sub>)<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub>") and "Weight %" for weight % proportions (e.g. "(Al<sub>2</sub>O<sub>3</sub>)<sub>70</sub>(SiO<sub>2</sub>)<sub>30</sub>"). This also defines what the numbers in an oxide table represent if used. See the context-sensitive help for details and examples.

With all parameters set-up, enter a title for this yield calculation and hit "Calculate Yields" to perform the integration. A file requester will prompt you for a file-name, which defaults to the "Output" (.YIELD) file specified in the set-up. You should also save all these set-up parameters to a file (.LCM) using the "Save" button at the top of the window. "Load" will load parameters from an existing .LCM file.

### Export of Yield Results

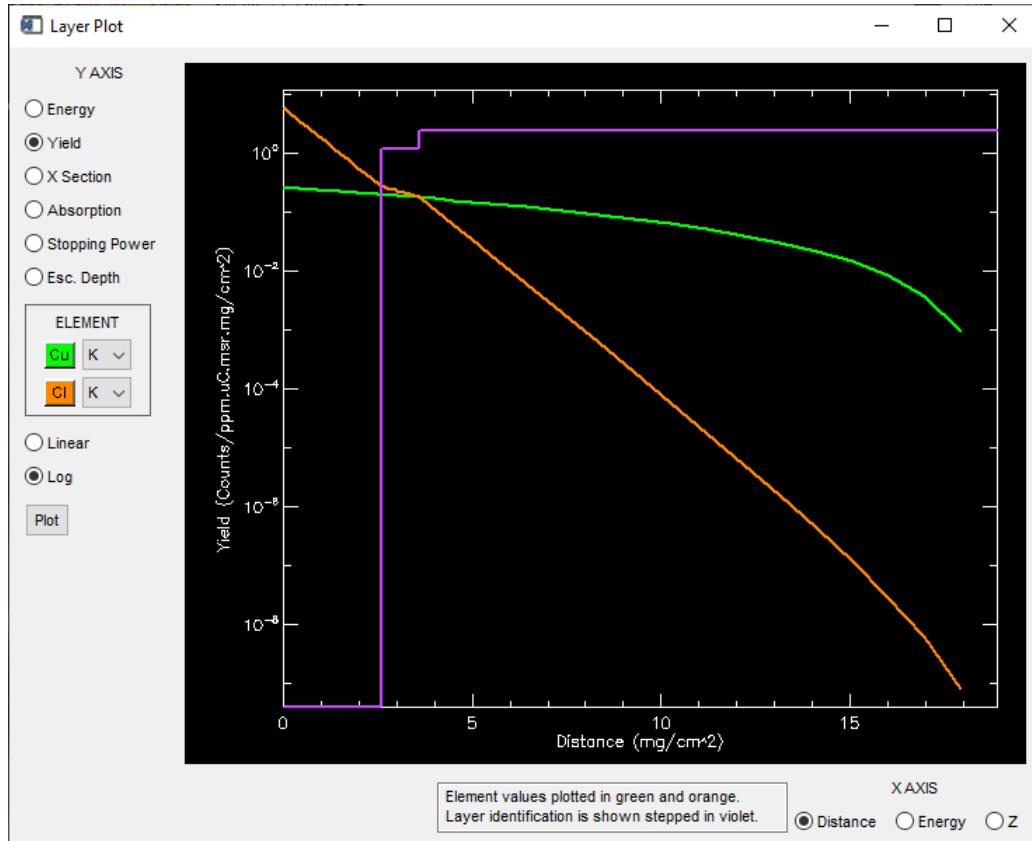
"Export" outputs selected results for relative-intensities and yields to a CSV file. A pop-up window enables the selection of elements and output options.



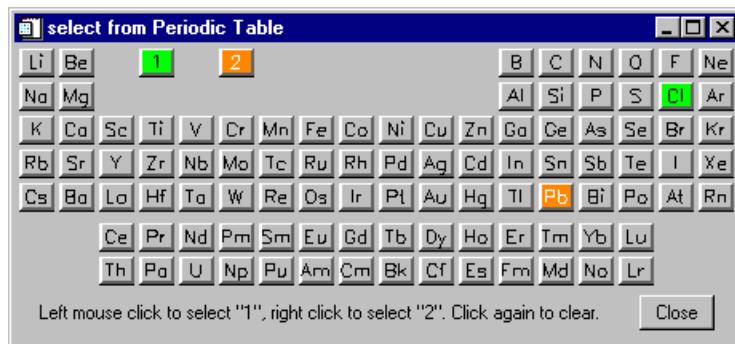
See the context-sensitive help information on each widget for more details and tips.

### Layer Plot Window

The variation of many calculated parameters and results, versus depth into a sample or versus the slowing down beam energy, can be displayed via the “Plot Yields” button, which brings up the *Layer Plot* window.



The *Layer Plot* window selects parameters for the X and Y axes. Some also require the selection of elements to plot. This is done via the green and orange buttons, and drop-lists to select between K, L and M shell results (if present within the *Layer Setup* energy range). Clicking on a coloured button brings up a periodic table to select up to 2 elements, plotted in green and orange. The steps in target layers are shown in violet. To select the green element, click on the element in the table with the **LEFT** mouse button. To select the orange one, click using the **RIGHT** mouse button.

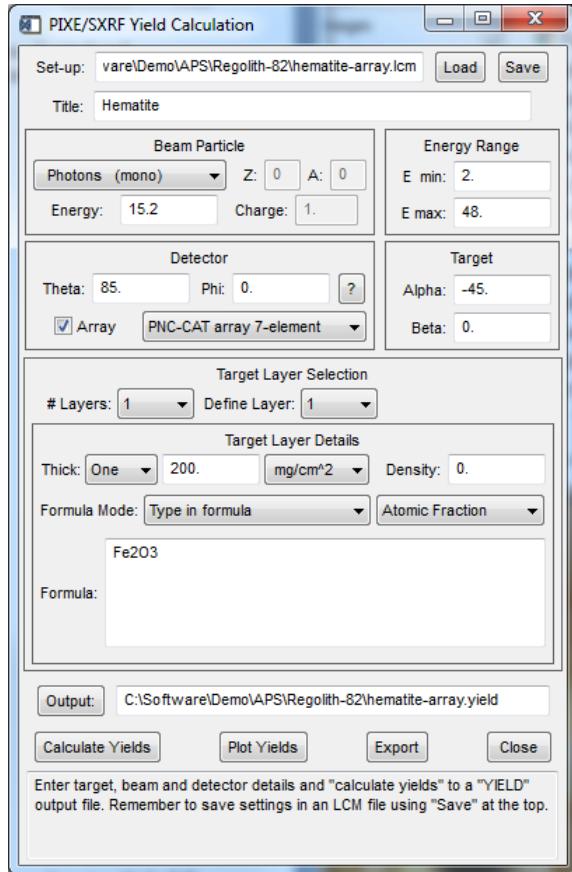


## Detector Arrays and the Yield Calculation

Detector arrays come in two flavours in GeoPIXE: (i) simple arrays, where all detector elements are regarded as identical and span a small range of take-off angle at the target, and (ii) full arrays, where the take-off angles cover a significant range, which effects self-absorption and the calculation of yields across the array. See the discussion in the section on Editing Detector Files later in this manual.

Simple arrays have been supported for some time in GeoPIXE. For this mode, leave the “Array” check-mark unchecked. In this mode the yield calculation is quite decoupled from the choice of detector (single or simple array) and produces ‘generic’ yields that can be combined with any choice of detector. If this detector is an array, then all detector elements are regarded as identical and contribute equally to the generation of images.

Full arrays require the yield calculation to calculate the take-off angles to each element in the array, as these change enough to affect the yields. This breaks the simple ‘generic’ yield model, and now the *PIXE/SXRF Yield Calculation* must consider the detailed layout and distance to the detector. When these yields are transferred to the *X-ray Spectrum fit* window, the detector drop-list will become ghosted and desensitized, as the detector has been specified in the yield calculation and cannot be changed in the fit window.



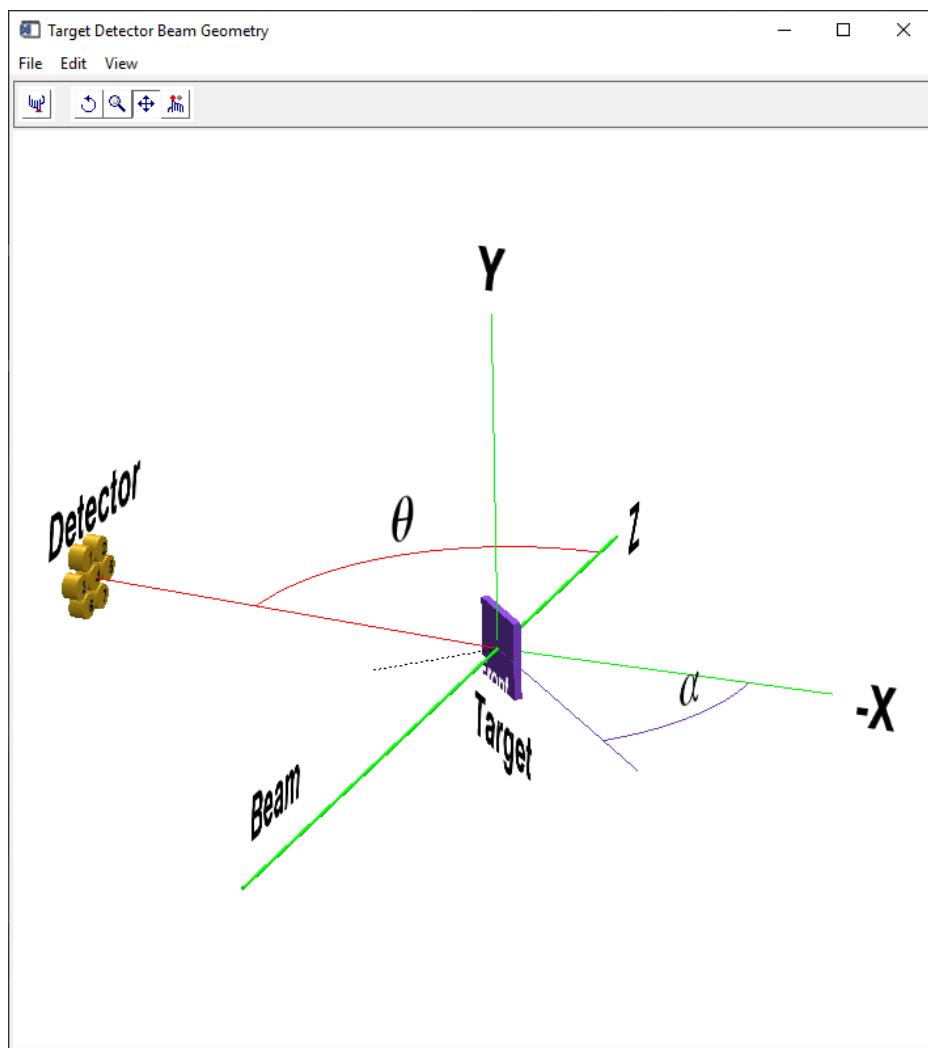
Checking the “Array” check-box brings-up another drop-list for selecting an array detector. Only full array detectors are listed. The “?” button opens a window to provide a full 3D view of the detector array in the beam-target-detector geometry as specified here. This is useful to check that the detector is positioned as desired (see below).

In full array mode, the calculation of yields has two passes: (i) The first pass calculates yields as for a generic detector, placing an ideal detector in the centre of the array at the specified Theta and Phi angles. (ii) The second pass calculates yields relative to the “central” one, for every element, target layer and detector pad, but without secondary fluorescence. Secondary fluorescence enhancement is calculated once for the ‘generic’ set and applied to all subsequent calculations. The result is a set of relative yields relating the sensitivity of each detector element to the ‘central’ one.

These relative yields are stored in the yield file and used to correct images (and fits to spectra that combine several detector spectra) for the actual detector elements enabled to project the images (or included in a sum spectrum).

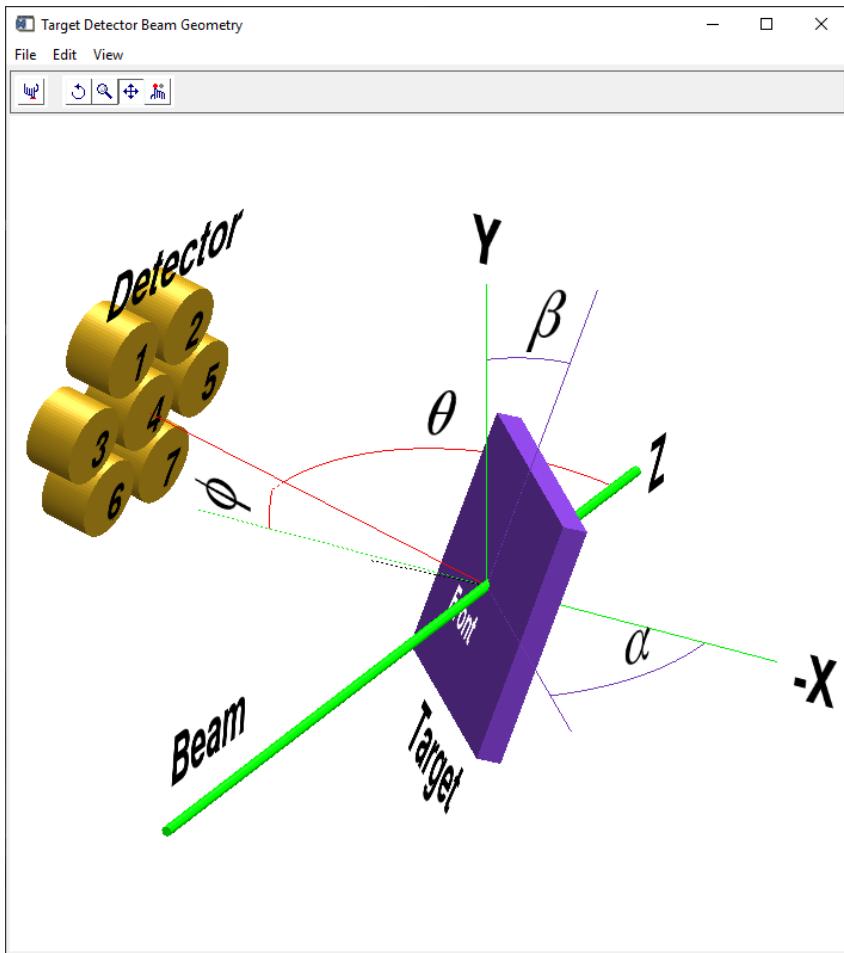
### 3D Geometry Viewer

The “?” button on the *Yield Calculation* window opens a window to provide a full 3D view of the detector array in the beam-target-detector geometry as specified here. This is useful to check that the detector is positioned as desired (you can zoom in on the detector to read the detector number labels; see below).



Geometry display for Theta=85°, Alpha=-45 °, and a 7-element array detector.

Note that the front of the sample is labelled “Front” and should be facing the beam and normally angled towards the detector (unless a transmission geometry is sought with fluoresced X-rays passing back through the sample to the detector, which is seldom used).



Example showing a close-geometry 7-element detector array with detector angles: Theta=85° (in plane detector angle), Phi=10° (out-of-plane, azimuthal detector angle), target tilt angles: Alpha=-45° (rotation of target about Y axis), Beta=20° (tilt of target about a horizontal axis across the face of the target).

## ***Creating a Dynamic Analysis Matrix for Image Projection***

Immediately after performing the fit in *X-ray Spectrum Fit*, click on "Generate DA Matrix" to calculate the Dynamic Analysis matrix, and write it to a file (.DAM for PIXE or .DAMX for XRF). This matrix contains all the information necessary to project a PIXE or SXRF list-mode data-file to quantitative elemental images, including a complete list of all observed elements identified in the spectrum during fitting. See details about sorting list-mode data below.

After clicking on the "Generate DA Matrix" button, a pop-up enables selection between "Normal "Simple single energy DA matrix", "Single DA matrix (w/ Master Weights)" and "XANES energy series DA matrix". The former calculates a single DA matrix for normal PIXE/SXRF imaging applications.

The "Master Weights" spectrum is an optional spectrum that is more representative of the average spectral data for a sample/region. It improves DA matrix construction for simple regions that focus on compositions approaching end-member phases. Use this for building DA matrices for Yield Correction or MPDA image analysis.

The latter is used to calculate a series of DA matrices, one for each energy in the XANES spectrum. A new "Energies" file field appears allowing you to load the name of your XANES energies file. There is also a field to select when to merge Compton and elastic peaks and treat them as a single "Scatter" peak. This is best done for energies below about 10 keV. XANES energy files can be (i) extracted from raw list-mode data using the *Spectrum Display* "File→Import→Energies from list-mode" menu or exported from an existing XANES image stack using the "File→Export→XANES energy list" menu from the *XANES Image* window.

## **Exporting a Dynamic Analysis Matrix for External Data Acquisition Use**

Immediately after performing the fit in *X-ray Spectrum Fit*, and saving the Dynamic Analysis matrix using "Generate DA Matrix", hit the button "Export" to export a binary or ASCII format matrix file for use in an external data acquisition system. The binary export mode at present defaults to IEEE floating-point and is Big-Endian, and hence has a different byte order to PCs, but the same as Unix and VME processors. See further information in the Help directory.

Note that "Export" is not needed for Maia data acquisition as the associated *Maia Control* program utilizes normal GeoPIXE DA matrix files directly.

Export brings up a pop-up window with some options. Select between binary and ASCII formats. In binary mode, you can select "big endian" format, or uncheck this option for PC platforms. There are fields to select the pileup limits file, linearization and throttle factors files, as used with the Maia data acquisition system. These data files are incorporated into the ASCII output export file only at present.

## **Sorting List-Mode Data using the Dynamic Analysis Matrix**

### **Sort EVT Window**

To open the *Sort EVT* window for sorting list-mode data-files, use the "Windows→Sort EVT" menu in the *Image Display* window (main *GeoPIXE* window). Here we need to specify the format of list-mode data, the type and dimensions of scanning used, the ADC number to sort and the Dynamic Analysis matrix to use for PIXE imaging (for other data, see Sorting using Spectrum Cuts below). For sorting images, make sure the radio button at the top is set to "Image".

*To have Sort EVT open each time GeoPIXE is run, make sure it is enabled in the config file "geopixe.conf". The default device for the device drop-list can also be set in the config file.*

**TIP:** Often the Sort EVT window is setup initially by loading a previous DA image file (.DAI), which contains all set-up parameters discussed here. Then simply change the ones you need to (e.g. raw data input files).

Near the top of the window there is a drop-list for selection of the list-mode data device. These devices vary in terms of event-data format, byte-ordering and floating-point format. GeoPIXE internal design means that a number of list-mode formats from various computer platforms can be processed and will aid migration of GeoPIXE to other platforms in future. All devices are set-up using Device Object SAV files in the "interface" directory. Current devices include:

- 1) **MARC MPsys Linux Data Acquisition:** List-mode files (.EVT) collected using the new Linux/PC based MicroDAS data acquisition system and MPsys (MARC) software for PC.
- 2) **Lund Kmax MAC Data Acquisition:** Multiple list-mode files collected using the Lund Kmax (Sparrow) CAMAC data acquisition system on Macintosh.
- 3) **iThemba XSYS VAX Data Acquisition:** List-mode files (.EVT) collected using the XSYS VAX-based data acquisition system at iThemba Labs.
- 4) **MARC MPsys Unix Data Acquisition:** List-mode files (.EVT) collected using the older Unix/workstation based data acquisition system and MPsys (MARC) software for Unix.
- 5) **OM DAQ Data Acquisition for PC:** List-mode files (.LMF) collected using the PC based OM DAQ data acquisition system of Oxford Microbeams.
- 6) **Sandia EVT Data Acquisition for PC:** The original data-cube files at Sandia National Labs.
- 7) **Sandia MPAWIN Data Acquisition for PC:** Older Fastcom list-mode files at Sandia.
- 8) **Fastcom MPA3 Data Acquisition for PC:** Fastcom Tec MPA3 format list-mode files.
- 9) **APS Data Cube:** APS SXRF data cube files, reformatted to LST format on a PC.
- 10) **Sandia BD12 Data Acquisition for PC:** Local list-mode to support the Rontec BD12 12 element Si-drift detector array.

- 11) **NSLS MCA VME Data Acquisition:** MED/MCA image pixel spectra files from the NSLS.
- 12) **Tohoku Labo Data Acquisition for PC:** Labo list-mode files (.LST) generated by Laboratory Equipment Co. multiparameter data acquisition software.
- 13) **Sandia Primecore U48** – Support by Primecore for the Rontec BD12 12 element Si-drift detector array.
- 14) **LIBI Data Acquisition for PC:** List-mode data collected by the LIBI group of the Ruder Bošković Institute, Zagreb.
- 15) **GSE-CARS Unix data Acquisition:** Image pixel spectra files (Epics generated ASCII files) from GSE-CARS, APS.
- 16) **Hasylab FIO data acquisition:** ASCII pixel spectra files, generated at Hasylab.
- 17) **Maia-384 data acquisition:** Event files generated by the CSIRO Blog event server for the Maia 32, 96 and 384 detector arrays.
- 18) **CSIRO MicroDAQ and MDAQ2 listmode data.**
- 19) **NSLS HDF format SXRF image files:** Scan full-spectral data files in HDF format.
- 20) **SLS MCA data acquisition:** Pixel spectra files in MCA format collected at the Swiss Light Source (preliminary support).
- 21) **ESRF EDF files:** ESRF EDF format image spectra files (preliminary support).
- 22) **Wakasa UniDAQ data acquisition:** List-mode data from the Wakasa Wan Energy Research Centre.
- 23) **Horiba Raw:** Horiba bench-top XRF raw full-spectral image files.
- 24) **NSLS Net CDF line format:** Line oriented NSLS NetCDF format full-spectral image data.
- 25) **FalconX:** initial support for the new FalconX list-mode data from XIA-Southern Innovation.
- 26) **iThemba Midas:** initial support for the new Midas list-mode data at iThemba Labs.
- 27) **Ruder Boskovic:** Support for list-mode data acquired at the Ruder Boskovic Insitute, Zagreb.
- 28) **CSIRO Maia detector array:** Blog event mode data.
- 29) **Fastcom MPA4 Data Acquisition for PC:** Fastcom Tec MPA4 format list-mode files.
- 30) **Spring8 37U:** Image raw data from beamline 37U at the Spring8 synchrotron.
- 31) **UQ iXRF:** List-mode data from the Atlas iXRF mapper at UQ.

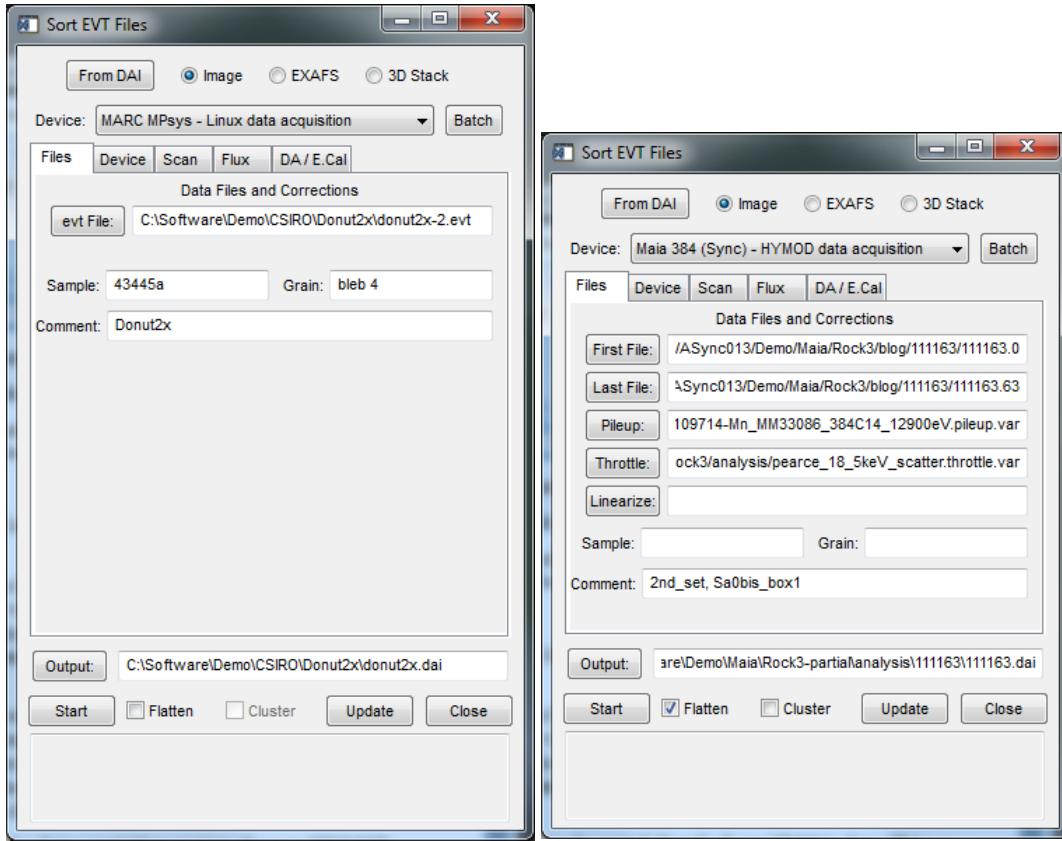
Next to the device drop-list is a “Batch” button, which accesses Batch Mode operation of *Sort EVT*.

The Sort EVT window is divided into several panels for setting up necessary parameters and selecting input files.

#### *Files*

The files tab allows selection of the source list-mode file to process. The file types (and the name on the button on the left) will change with the device type selected on the drop-list above. For most devices, only a single list-mode file is used. In the case of the Lund Kmax system and the NSLS MED, GSE-CARS, Hasylab and Maia files, for example, a range of list-mode spectra is used. In this case two file entry fields appear, one for the first file, one for the last file to sort. *You can leave the last file field blank in order to sort all files numerically after the first one.*

*The working directory tree for input of raw list-mode data can be different to the output images and other files. If you want to output images into a different directory tree, then you will need to select the new output directory by clicking on the “Output:” button.*



For Maia event files, three more fields appear. One allows the selection of a **Throttle** file that contains the throttle factors used to tame intense peak input data rates during data acquisition. Select the file here in order to correct for throttle losses during sorting. A second selects a **Pileup** file for pile-up rejection, which contains the time-over-threshold limits for each pulse-height. These files are generated from the *Time Amplitude Display*, which can be accessed via the *Spectrum Display* Windows menu. A third selects a **Linearize** file for linearization of gain corrections during processing of list-mode data. This option is only used to apply a second order correction when needed or for older data that was not corrected in real-time by the HYMOD processor in Maia (pre-2010 data).

*The “cluster” check-box enables parallel processing of certain types of data where the raw event data is contained in a series of files with numeric file extensions. These files can then be dispersed to a number of parallel IDL sessions to process parts of the image, which is reconstructed after processing. This option works well for Maia data, which can amount to >100 Gb per image. An IDL run-time license is needed in this case.*

The “Flatten” option enables normalization images to flux per pixel. All images are normalized, as well as the Flux map itself. The original flux map is also stored as “Raw Flux”. A plugin is available to view this.

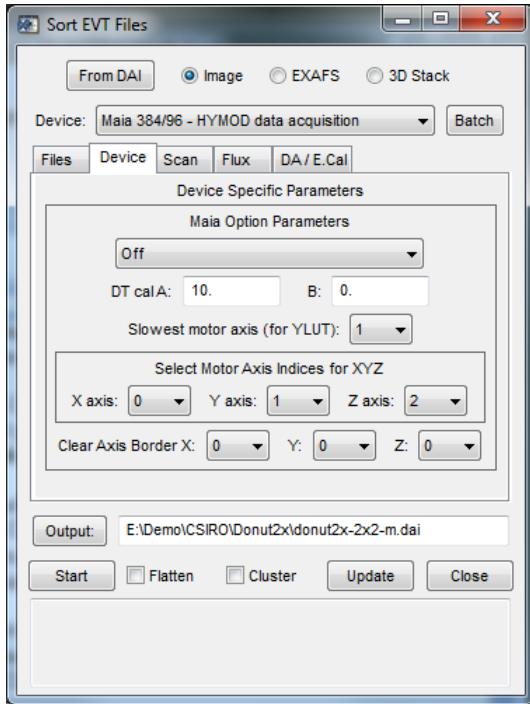
When the list-mode file is selected, any associated header information is read, and many of the Sort EVT widgets are updated (e.g. X range, Y range, energy calibration coefficients, and perhaps X size and Y size).

Below this are fields for sample details and a comment area.

### Device

This panel controls device specific parameters, with the GUI elements set-up and drawn from the device object plugin. Device parameters are internal to the drivers and defined in the device object plugins.

A typical control for some device drivers (e.g. Maia) is to allow a level of re-direction between encoder input channels (motor axis indices: denoted 0, 1, 2, ...) and the X, Y and Z axes used by GeoPIXE. The “slowest axis” (e.g. used for the Y lookup table and cluster processing mode) can be selected as well. For cluster mode processing, this must be the same as for the Y axis for now.

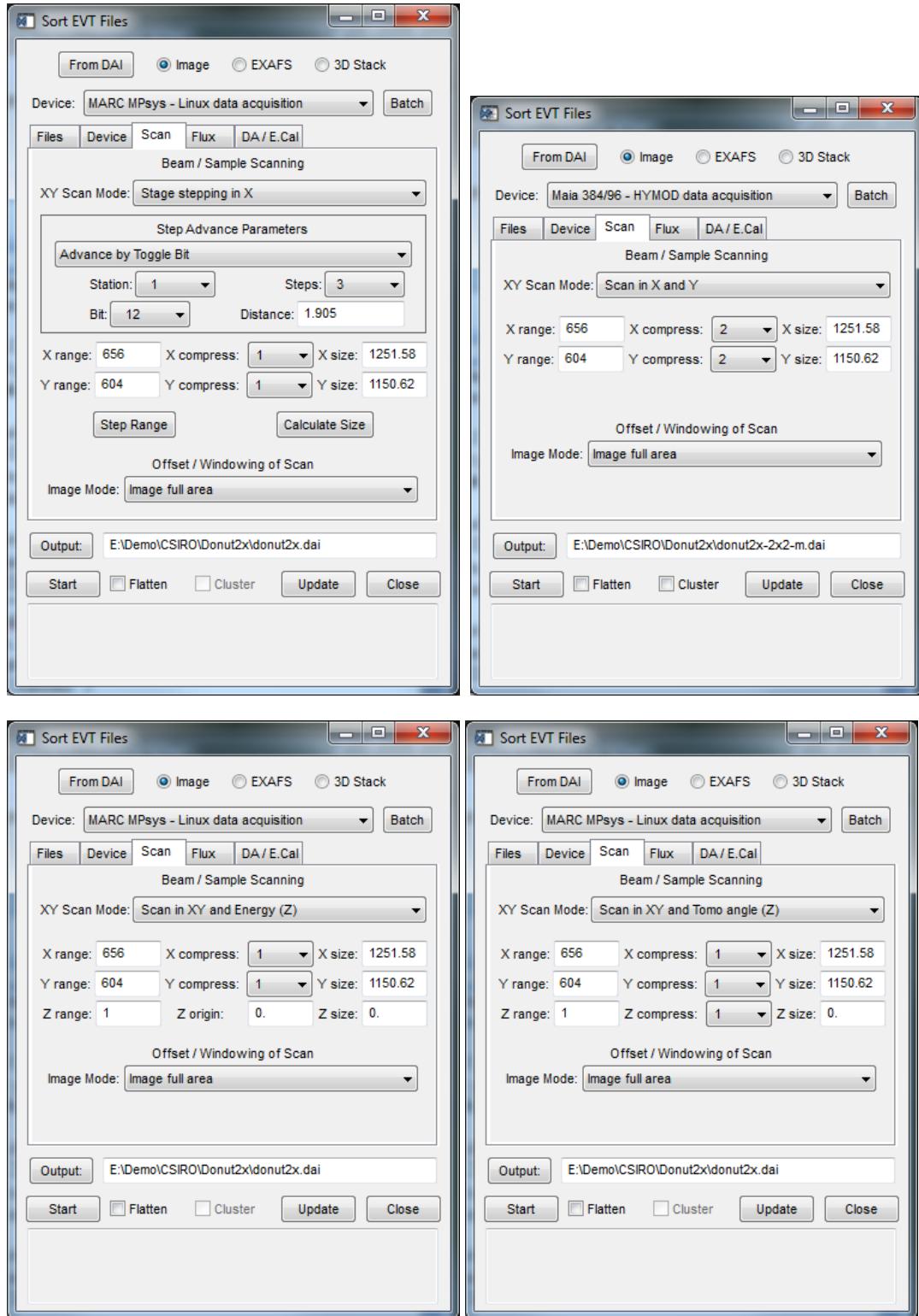


Some Device Objects will add some controls specific to the device driver. For the Maia detector array (as illustrated above right), there are various scan corrections, the option to clear borders and the dead-time calibration coefficients DTcalA (slope) and DTcalB (offset).

## Scan

This panel has a drop-list selecting the type of "XY Scan Mode" used. Choices currently include (see also the context help window):

- 1) **Beam Scan in X and Y:** Normal raster, triangle or random scan in both X and Y, with both X and Y data in each event. All devices support this mode; PIXE data uses beam-scanning and SXRF data uses stage scanning/stepping.
- 2) **Stage Stepping in X:** Raster scanning in Y only, with X advanced using the sample stage. X moves are encoded into the list-mode data using various approaches (see below).
- 3) **Linear Traverse in XY:** Both X and Y are not scanned but moved using the stage along a line (this uses the same stepping options as for X stepping).
- 4) **Stage Stepping in Y:** Raster scanning in X only, with Y advanced using the sample stage. Y moves are encoded into the list-mode data using various approaches (see below).
- 5) **Scan in XY and Energy (Z):** 3D scan where 3 axes define X,Y and E (Z axis), where the Z axis is used for monochromator angle, which is related to energy using the table loaded on the DA/E.Cal tab. The 3D modes display further controls for the Z axis. The mapping from axes to X, Y and Z can often be controlled on the Device tab.
- 6) **Scan in XY and Tomo angle (Z):** 3D scan where 3 axes define X,Y and Tomo angle (Z axis), where the Z axis is used for tomography rotation angle. The 3D modes display further controls for the Z axis. The mapping from axes to X, Y and Z can often be controlled on the Device tab.



In the case of stepping mode, there are additional fields to set-up how the stepping advance is encoded into the event stream. This is set-up using another drop-list under "Step Advance Parameters". Options include:

- 1) **Advance by Toggle Bit:** Fields appear to specify which bit of which ADC encodes the step advance. This bit is assumed to be toggled at each step. Bit 12 on Station/ADC 1 is used with old CSIRO NMP data.
- 2) **Advance by ADC count:** In this case, a specified ADC is used solely to register step advance events. Any event on this ADC is used to advance the position.

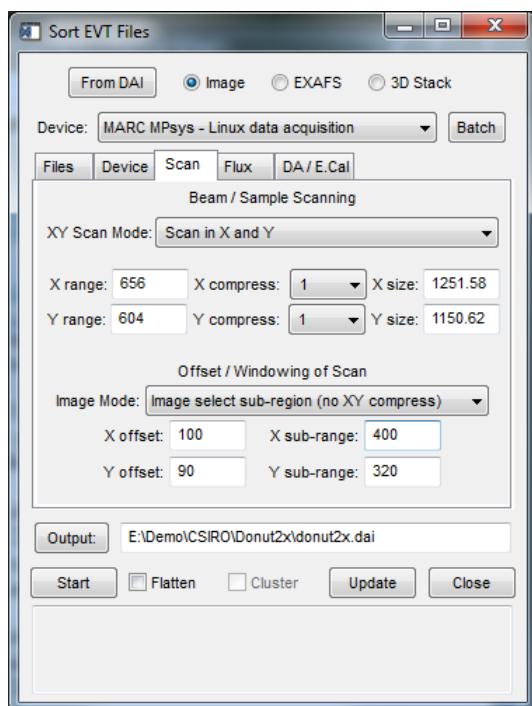
3) **Advance by Event Count:** A specified count accumulated in a specified ADC indicates advance of the stage.

In each mode, a drop-list selects the number of steps and distance moved in each step. This is used to set the stepping axis micron scale. There is a fixed pitch per step at present (this will be updated on demand).

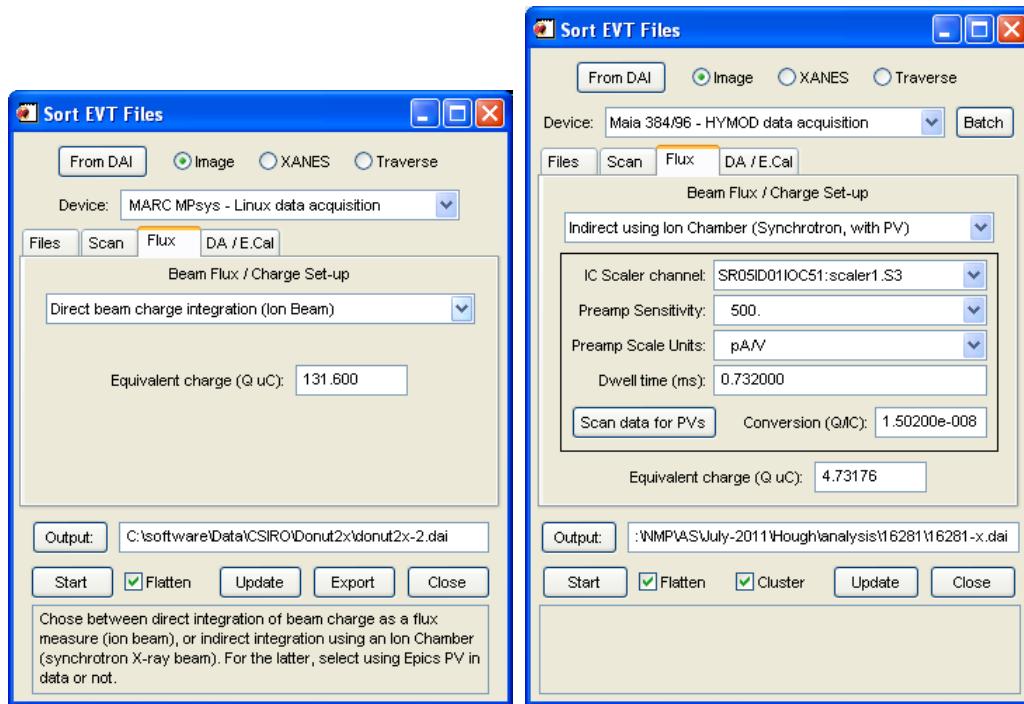
The next group of fields set the size of the X and Y data in pixel units (X Range and Y Range) and provides the option of compressing X and/or Y data, by integral factors, into smaller images during sorting of the list-mode data. On the right, the full X and Y size of the scan area can be entered in microns. Some devices may supply these values when the EVT file is selected. The 3D modes add details for the Z axis.

The “image mode” allows selection of full image sorting or a sub-region with options:

- 1) **Image full area:** Process the full XY pixel range selected above under X and Y range and using selected X,Y compress..
- 2) **Image selected sub-region:** Form the image of only a sub-region specified by the X,Y offset and X,Y sub-range sizes, both specified in non-compressed units. Note this mode forces X,Y compress = 1 on the output image.

*Flux*

Ion beam systems commonly measure beam flux directly by integrating beam current. Synchrotron X-ray beams are monitored indirectly using current recorded in an ion chamber (IC), which produces a current proportional to the absorbed fraction of the beam passing through it. In many systems this signal is converted to a pulse train using a voltage to frequency converter and integrated as a pulse count. In this case we need to establish a conversion factor from IC count to equivalence beam charge ( $\mu\text{C}$ ;  $6.242 \cdot 10^{12}$  photons). This is done by selecting one of the “Indirect” flux measurement options, with or without specification of Epics/ Tango PVs for encoding IC count and preamplifier sensitivity and range (unit selector).



For indirect with the availability of Epics/ Tango PVs for IC count in the list-mode data stream (or header file), a button appears (“Scan data for PVs”) that allows the data to be scanned to collect PV information. This populates the PV drop-list allowing selection of the desired PV for IC count. Other drop-lists allow selection of the sensitivity. Once selected, this data will be saved in the Image DAI file header.

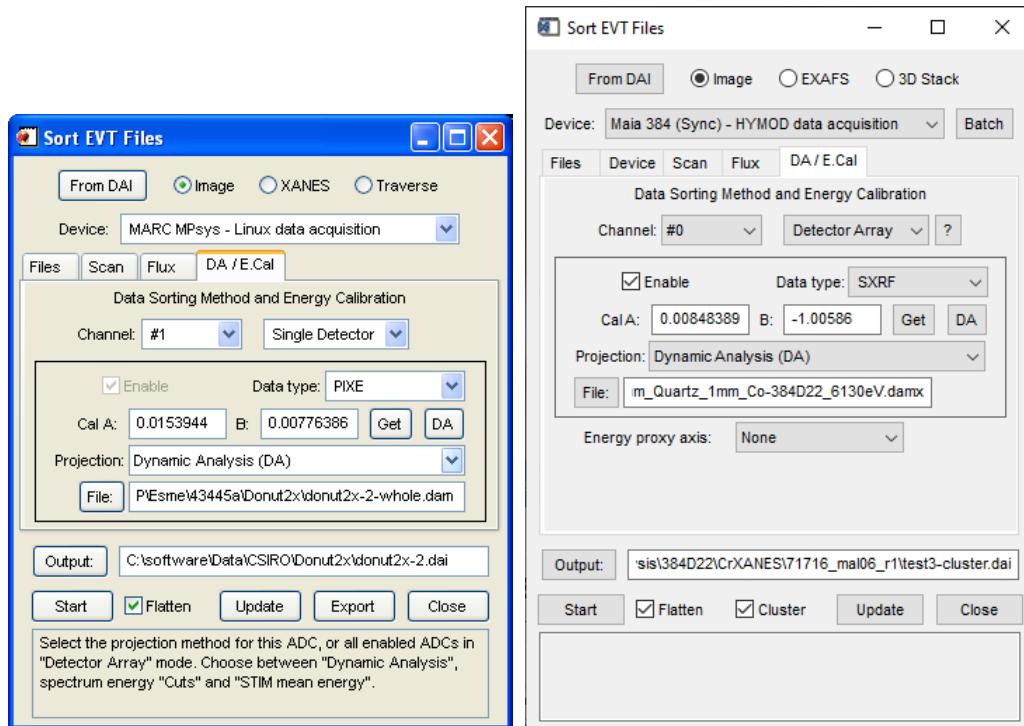
#### *Dynamic Analysis, ADC Selection and Detector Arrays*

The “DA / E.Cal” panel allows selection of the sorting mode. Normally, for PIXE and SXRF analysis and imaging, the Dynamic Analysis (DA) method is used for spectral deconvolution and image projection.

The first widget (“Channel”) is a drop-list widget to select which ADC to consider. The next widget selects between sorting data for a single detector or an array of detectors. For “Single detectors”, the Channel widgets select the ADC to sort data for. Images reflecting the data from this ADC only will be produced. The parameters for this ADC are displayed and can be selected in the area below.

In “Detector Array” mode, the Channel widgets select which ADC’s parameters are displayed and edited in the frame below, but the ADCs included in the sort are selected using the “Enable” check marks, one on each ADC panel.

Note: Detector array parameters (cal and enable) *can be set all at once using the “Get” function described below, and indirectly from the Detector-Layout window.*



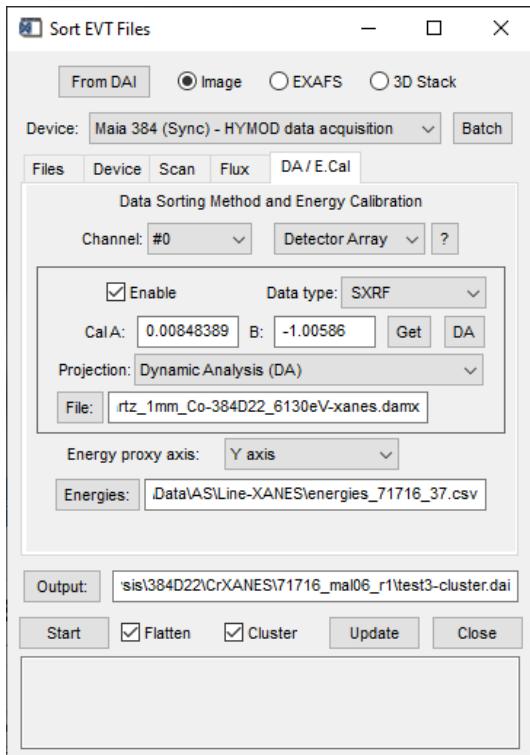
For each ADC, there is a set of parameters, which specify the projection mode, spectrum energy calibration and the file-name of the Dynamic Analysis matrix or Cuts file. There are fields to enter the data type ("PIXE", "RBS", "PIGE", "SXRF", etc.), energy calibration, projection method and associated projection data file. Each of these relate to the selected ADC channel. Projection methods currently supported include:

- 1) **Dynamic Analysis:** Use the DA method to project quantitative PIXE/SXRF elemental images. The associated file is the DA matrix file (.DAM or .DAMX). The DAM file contains the list of element images to project and all PIXE/SXRF yield data.
- 2) **Spectrum Cuts:** Use spectrum energy cuts to define the windows for each image. The associated file is a cuts file (.CUTS) containing energy window definitions or regions-of interest (ROIs). Cuts are discussed more below under sorting using cuts.
- 3) **CUT Mean Energy (STIM):** Use a spectrum cut to define a region of the spectrum to average to determine the mean energy of a transmitted beam in STIM.
- 4) **Multiphase DA (MPDA):** Use the new Multiphase extension to DA (MPDA) specified in the associated file (.MPDAM). The MPDAM file contains pointers to the phase map and yield correction files (see “Multiphase DA imaging (MPDA)” below).

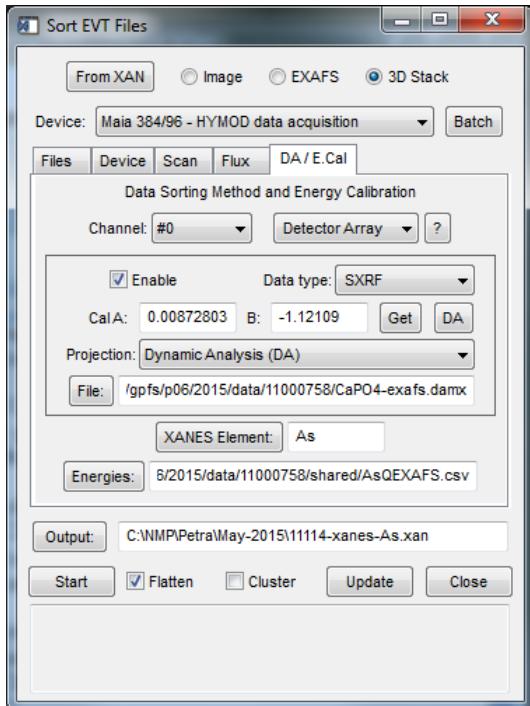
In “Detector Array” mode, the data type and projection method and file are set globally, once for all detectors in the array.

The energy calibration corresponds to the ADC being displayed. It is used to map energy of each event onto the correct column of the DA matrix, or to correct energy for cuts. It can be loaded from an existing SPEC file (e.g. saved after fitting the spectrum) using the "Get" button. In “Single Detector” mode, “Get” will retrieve the calibration from a SPEC file for the selected ADC #.

In the case of Line XANES (2D scan mode), where one of XY is a spatial axis along a scan line and the other provides an index that tracks changing beam energy, we select the “energy proxy axis” using a new dropdown, else use “None” for normal XY spatial axes. This example shows the case of stage scanning along the X axis with the Y axis pixel value (the “energy proxy axis”) providing an index into a table of energies, one for each Y value.



In the case of the 3D XANES imaging mode, extra controls are provided to select the XANES Element (corresponding to the edge being scanned over) and the XANES energy table corresponding to each monochromator angle Z pixel.

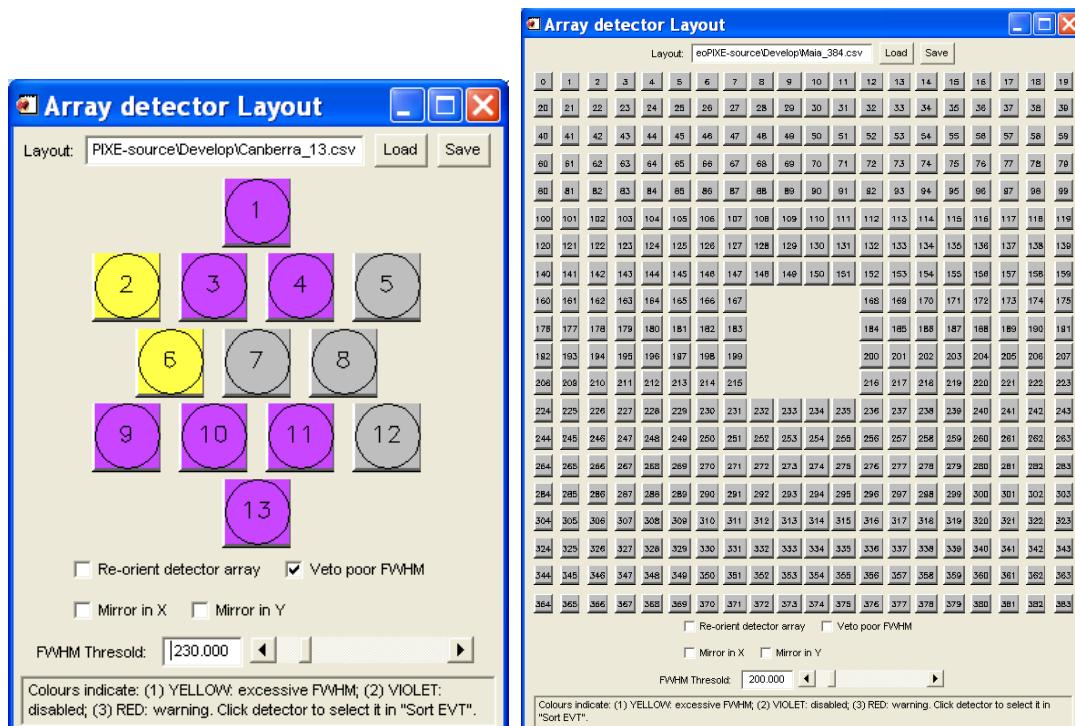


## Energy Calibration – Array Detectors

In “Detector Array” mode, the “Get” button will retrieve the energy calibrations for all ADCs/ detector channels from the SPEC file. To make best use of this feature, construct a file of all good detectors in the array in *Spectrum Display*. Use the “Delete” and “No XY”, “No T” buttons in *Spectrum Select* to remove any bad detector channels, and the X, Y, T spectra. Then fit all good spectra using the *X-ray Spectrum Fit* “Fit All” button to generate accurate energy

calibrations for all detectors. Delete any bad detector channel spectra, and save to a file tagged as “-cal.spec”. Then when you use the “Get” button in *Sort EVT*, it will not only load all the energy calibrations but also “Enable” only all good detectors.

Click on “?” to view the layout in a pop-up window. The *Detector Layout* window has a FWHM Threshold slider, which sets the limit of usable detector resolution. You can slide this to reject detectors with poor resolution (if the “Veto poor FWHM” check-box is selected). These are shown in Yellow. Dead detector channels can be specified in the layout file (bad=2); these are shown in Violet and are disabled. *This feature is seldom used these days.*



This rejection can be used in *Sort EVT* to veto poor detectors in an array while sorting raw data to build images. FWHM values are saved in SPEC file after a fit to all spectra (GeoPIXE v4). When the “Get” button is used in Sort EVT (to retrieve energy calibration for all valid detectors) the FWHM values are transferred to the *Detector Layout* window; any missing detector spectra flags a dead channel. These can be saved to the Layout file, using the Save button.

### Energy Calibration – Single Detectors

In the case of DA projection, if the DA matrix was built using a fit to a spectrum extract from this same list-mode file, then the DA matrix contains the fitted refined energy calibration. In “Single Detector” mode, you can click on the “DA” button to use this calibration here.

*However, if the DA matrix was built from a different data set, or on another day where the calibration may have been different, then don't use this option. Similarly, don't use it with detector arrays. Instead, use the “Get” button to load energy calibration information from up-to-date fitted spectra. Alternatively, the calibration coefficients can be typed in (A is gain, B is offset).*

Note for MPsys users: *In the case of MPsys data, if an MP file of the same name as the EVT file is found, then various set-up parameters are extracted from this file to set scan size, stepping parameters, integrated charge and scan resolution in pixels. Note: This will reset the energy calibration to the values contained in the MP file. If using Dynamic Analysis, then after selecting a new list-mode file you may need to press the “DA” button to copy the fitted energy calibration from the dynamic analysis matrix, or use “Get”. In stepping mode, a button “Step Range” brings up a panel to calculate the pixel count along the stepping direction and the integrated charge.*

Note for APS users: *The LST files generated from the APS MDA files do not all contain energy calibration information.*

*In this case, the A and B parameters will be reset to 1 and 0. You will need to load these using the “DA” button to copy the fitted energy calibration from the dynamic analysis matrix, or for detector arrays use “Get” to load all calibrations from a SPEC file for good detector elements and set the Enable flags. Use a file that only contains ‘good’ detector channels.*

Similar parameters are retrieved from file headers when using Maia, MPA3, OM DAQ, Sandia EVT and some APS format list files.

## Output and Start Sort

The final field is the name of the "Output" file. This will be set-up by default using the (first) list-mode file name, but can be changed here. ***In particular, make sure the output directory is correct.***

Optionally, any variation in flux or beam charge across the image can be used to normalize all images. The “Flatten” checkbox selects this option to remove flux variation from images.

For device types that support it, the “Cluster” option will be available, which uses parallel processing to speed up sorting of event data. This option requires an IDL RT license at least.

*Remember to view the context-sensitive help on the various fields in this window. Just move your pointer over widgets and view the help at the bottom of the window.*

Once all parameters are set-up, the list mode data can be sorted by clicking on "Start". A progress bar appears to chart the progress through the list-mode file, or the set of files. It also shows time remaining and some statistics regarding bad events, those clipped outside of the DA matrix range, and the X position in stepping modes.

After the sort finishes, *Sort EVT* writes an image file (.DAI), as specified under Output, and sends the images to the parent *Image Display* window (main *GeoPIXE* window). The DAI file contains all concentration images as well as variance images (at half the pixel resolution to conserve memory), PIXE/SXRF yields and detection limits.

Note: The header of the DAI file also contains all the set-up parameters specified here. Therefore, if you need to re-sort, or to sort another ADC or another list-mode file with similar settings, load these parameters from the DAI file using the "From DAI" button at the top of the window.

## Sort EVT Widgets

This list summarises the functions of all widgets on the *Sort EVT* window, including buttons, sliders, drop-lists and text entry widgets. These are listed from left to right, top to bottom.

### *In all XY Scan Modes:*

- From DAI Button Load set-up parameters from an existing DAI image file.
- Mode Radio Buttons Select between sorting “Image” data and 1D “EXAFS” and “3D Stack” data (XANES or Tomography).
- Device Drop-list Select data acquisition source of the event file(s) (see details above).
- “Batch” Button Brings up the Batch Processing window.
- EVT File Select event data file. This is labelled “First File” for event file formats that use individual pixel files; another field appears for the “Last File”.
- Last File Last event file to process. Only used for pixel-file format data types.
- Sample Name of the sample.
- Grain Name for this image area on sample.
- Comment A free text comment string.

### *Only in Stepping Modes:*

- Step Advance Mode Select the way stage stepping is encoded into the event data stream.
- Station ADC number that contains step data.
- Bit ADC Bit number that flags a step advance.
- Steps Number of sample stage steps per line.

- Distance Width of a line in microns.
  - Count Advance to next line after this number of counts in the selected ADC.
  - Step Range Pop-up an input calculator to convert stepping total range and pre-scaler counts to pixels and integrated charge.
  - Calculate Size Calculate image size from step size and pixels, assuming square pixels.

*In all XY Scan Modes:*

- XY Scan Mode Select between scanning and stage stepping modes (see details above).
  - X range Number of pixels in source data in X.
  - X compress Compress data by this factor before mapping to image X.
  - X size Size of image in X in microns.
  - Y range Number of pixels in source data in Y.
  - Y compress Compress data by this factor before mapping to image Y.
  - Y size Size of image in Y in microns.
  - Image mode: Select between full image and a sub-region (no XY compress).

### *In 3D Scan Modes:*

- Z range Number of pixels in source data in X.
  - Z origin Origin of Z axis in device units (e.g. angle).
  - Z compress Compress data by this factor before mapping to image Z.
  - Z size Size of total scan range in Z in device units (e.g. angle).

In “Image sub-region” scan mode:

- X, Y offset Pixel offsets in X, Y to start image.
  - X, Y sub-range Pixel size in X, Y for sub-region image.
  - Get Get offset and size from last Box region selection on *Image*.

### *In all XY Scan Modes:*

- Charge Total charge for image in  $\mu\text{C}$ .
  - ADC Channel/Station Selects which ADC channel(s) to edit or sort from.
  - Detector Mode Selects between single and array detectors.
  - Layout pop-up “?” button to invoke the Layout pop-up window
  - Data Type Flags the type of spectral data (PIXE, PIGE, RBS, SXRF, ...).
  - Enable Enable this ADC, in detector array mode (better to use “Get”).
  - Cal A The calibration gain (keV) for the source data.
  - Cal B Calibration offset (keV).
  - Get Button Retrieve the energy calibration(s) (and set the Enable flags in detector array mode) from a selected SPEC file.
  - DA Button Retrieve the energy calibration from the DA matrix selected below under Dynamic Analysis projection. Do not use in “detector array” mode.
  - Projection Select between Dynamic Analysis and the use of spectrum energy Cuts (with or without background subtraction), or Cuts used for STIM, or Multiphase DA (MPDA).
  - File Select the DA matrix file, Cuts file or MPDA .mpdam file.
  - New button Opens a popup to select phase maps and yields correction file and enable the creating of a .mpdam file.

*Only in XANES 3D mode*

- XANES Element Select the element name for the edge being scanned.
  - Energies The name of the XANES energies lookup table.

*Only in Line XANES (2D) mode:*

- Energy proxy axis Select the stage axis that provides the index into an energies table.
  - Energies The name of the XANES energies lookup table.

### *Only with Indirect Beam Flux Modes:*

- IC Scaler channel drop-list to select Epics PV for flux ion chamber.
  - Preamp sensitivity select preamplifier sensitivity multiplier
  - Preamp Scale Units select preamp sensitivity scale range
  - Dwell time (ms) dwell time per pixel (ms), using when IC is a count rate and a time is needed to

- Scan data for PVs
- Conversion (Q/IC)

determine IC count per pixel.

scan data (or headers) for PV information and pop-up a selector to select Epics PV and preamp sensitivity.

the conversion factor between IC count and equivalent charge in  $\mu\text{C}$ .

**Bottom row:**

- Output
- Start
- Flatten
- Cluster
- Update
- Close
- Help Text

Select the image DAI output file name (usually the default, set after using the EVT Button, is correct).

start processing. Results will be stored in the Output file and displayed in the Image window.

optionally, correct images for flux variation across image.

enable parallel processing on a computer cluster or multi-cores.

write header information back to the DAI file. Use this to update non-critical parameters (e.g. sample name, comment, charge [can also double click on Charge details in *Image Properties & History* window] ...)

Close the window. Parameters remain stored in parent window.

Context-sensitive help area, shows help prompts for widgets as the mouse pointer moves over them.

**Only in all Maia Scan Modes (or for devices that enable these):**

- Throttle
- Pileup
- Linearize

File of throttle factors to correct throttle losses. Only used with Maia format event files.

File of pileup rejection limits for each pulse-height. Only used with Maia format event files.

File of gain linearization function parameters and lookup table. Only used with Maia format event files.

**Only in all Maia Scan Modes:**

- Encoder XY correction
- X margin
- Clear X borders
- Clear Y borders
- DTcalA, B

A drop-list to select between: (i) enable an algorithm to correct noisy Y encoder effects. It deduces an advance in Y only when X is within a margin width on the left and right of the scan. Normally, this is not needed. (ii) Filter out spurious XY position glitches that produce shifts of small portions of the image by 16 pixels).

selects the width of the margin for use with Encoder Y correction.

clear the X border pixels (2).

clear the Y border pixels (1).

dead-time calibration parameters, which depend on Maia shaping times.

## Multiphase DA imaging (MPDA)

MPDA is a new approach to quantitative imaging that solves: (i) quantitative per pixel concentrations (equivalent to the older "Correct Yields" matrix method), (ii) better X-ray relative intensities that evolve spatially with composition (which enable better spectral deconvolution), and (iii) improved background shapes that adapt with composition changes.

It is triggered by selecting the "Multiphase DA (MPDA)" mode and supplying a new .mpdam file on the *Sort EVT* window DA/Cal tab. The .mpdam file is created by clicking "New" and selecting in the popup window:

1. path to a 'phase map'.dai file (specific to this image area)
2. path to the "Correct Yields" setup (.correct) file (more general phase description)

To use it, you need the following (later we'll have a Wizard to orchestrate these steps):

### 1) Identify end-members

- Identify end-members components, and elements that provide a measure of each.
- Fit regions that sample the end-members as much as possible, using a yield calculation with composition for the end-member, and make a DA matrix for each.
- Also fit a region that samples a background component that will be used as a remainder component called "Rest".

**Correct images using the "Correct Yields" method**

- Open the "Correct Yields" window and select components, elements that distinguish each end-member component or phase and their matching DA matrices from above and fill in the composition matrix that relates end-members to their elements.
- Also select the DA matrix to be used as the remainder "Rest" component.
- Open the .dai image for your sample, and click "Correct" to correct concentrations based on the end-member (phase) proportions. Typically, this correction needs 2-3 iterations (press button again).
- Save the setup as a .correct file (this path will be referenced from the .mpdam file).

**Project end-member or phase maps**

- Click in "Mineral" to project the end-member or phase maps.
- Save this as your 'phase map' .dai file (this path will be referenced from the .mpdam file).

**Load an existing .mpdam file using "Load"**

- If you have an .mpdam file for this image data-set/scan, load it here.
- If GeoPIXE detects that the .mpdam file, and the referenced phase maps, are for a different run/data-set, it will endeavour to generate new phase maps for this data. This may entail the following steps:
  - Perform and normal DA analysis
  - Correct yields for spatially varying composition.
  - Project end-member phase maps and save these to a file.
  - Generate a new .mpdam file referencing these new phase maps and the Correct file.
  - Perform the MPDA analysis.

**Create your .mpdam file from the "New" button.**

- Select the 'phase map' and 'Correct setup' file paths from above. Note that the .mpdam file is specific to this data-set/scan area as it contains the specific phase maps.

**Select this .mpdam file in the *Sort EVT* window (DA/Cal tab)**

- This will happen automatically if you use "New".

**Start the sort (you can use "cluster" mode for parallel processing when available)**

- Normal GeoPIXE functions work the same from there, but you should see better concentrations in images, and better region spectra reconstruction overlays.

**Warnings:**

- 1) Phase maps only work if the data is quantitative so you get realistic phase proportions for each component. There fore take care with standards and refinement of the detector settings and calibration of the Conversion factor (for SXRF).
- 2) Select component compositions that produce good separation between phases and elements that dominantly point to each phase.

**Automated MPDA imaging**

MPDA requires phase maps for a particular data-set or run. To project phase maps requires processing Normal DA maps first and then using the *Correct Yields* process to correct for composition effects on yields in these images and project phase maps. These steps are now automated.

Hence, if an MPDAM file, used to process one data-set using MPDA, is selected to process some new image data-set "xxxx", it is checked to see if the MPDAM file contains the correct phase maps for the new data. Normally, it won't, as the MPDAM file was for an earlier run. In this case, a few automated steps are performed:

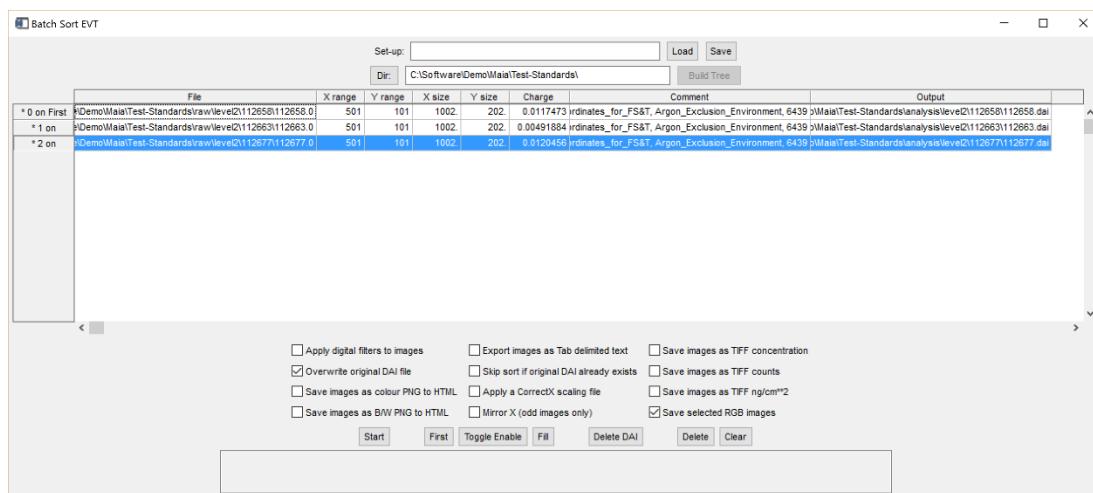
- A Normal DA sort is done first, using the original DA matrix used for the earlier data-set to generate the images "xxxx.dai".
- These images are corrected using the *Correct Yields* method, using the CORRECT file referenced in the MPDAM file. Three iterations of the yield correction are performed.
- The corrected images are projected onto end-member proportion phase maps and saved with the name "xxxx-phases.dai".
- A new MPDAM file "xxxx.mpdam" is created that points to the original CORRECT file and the new phase maps.
- The MPDA processing begins using the new MPDAM file and generates MPDA images file "xxxx-MPDA.dai".

Hence, the method to process a series of new data-sets is to simply select the new raw data files, answer "no" to the questions about E.cal and Pileup/Throttle, which probably will not change between runs in a series like this, and click "Start". This should also work within the Batch Sort process.

## Batch Processing of List-mode Files

The “Batch” button adjacent to the “EVT File:” button in the *Sort EVT* window brings up the *Batch Sort EVT* window for editing parameters and controlling batch sorting of entire directory trees of list-mode files.

**NOTE: Before opening Batch Sort, load Sort EVT with the settings for the first image to sort. Typically, the first in a series is processed first. Then the Batch Sort window is opened to continue processing more data with the same method.**



Select the root directory using the “Dir.” button. A pop-up allows a restricted range of run numbers to be selected, for device types that use numeric run-number based file-names.

*Batch Sort* will then scan this directory for all list-mode files (select the device type first in *Sort EVT*). Any information on each list-mode that can be found (in headers or parameter files) will be included in the table along with each file name. Edit these parameters by clicking in a cell and hitting <return> to get into edit mode.

Before starting sorting of all these files, valid global parameters (those not changed between list-mode files) must be set-up in *Sort EVT*. The best way to do this is to sort the first file normally in *Sort EVT*. **This is also the only way to establish different directory tree paths for input raw data and output image data, if that is desired.** Note that if a new output path is selected, then a pop-up will give you the option to apply this new remapping to all files in the table.

Now make sure there are valid entries for Xrange, Yrange (pixel size), Xsize, Ysize (micron size) and Charge for each run (if a fixed charge is appropriate). Some device will collect the charge/flux as the data are processed, and the charge is only known after processing. Alternatively disable these using row selections and the “Toggle Enable” button.

Use “Fill” to duplicate an entry down a set of selected rows, over the range of selected columns. Use “First” to select which run is sorted first. For indirect charge devices, such as many synchrotron devices, the Charge is set automatically during processing based on the “conv” calibration factor (set this on the “Flux” tab in the *Sort EVT* window) and the total flux extracted from the raw data.

After each sort is completed, the images are automatically sent to *Image Display* and saved to disk as DAI files. Optionally, digital filtering can be applied to these images according to history information in a prior filtered image file. *Batch Sort* will prompt you for an appropriate selection of file name and element selection after the first sort in the table. To enable digital filters, check the option below the table. By default, after filtering the file will be saved with an amended file name with “-m.DAI” or “-x.DAI” appended. This can be vetoed to save disk space by checking the “Overwrite initial DAI file” option.

Other options enable the generation of PNG images, HTML files of thumbnail images, in colour and/or black and white and the output of RGB image sets based on the RGB list generated using “Learn” in the *RGB Image* window.

This table, directory details and options parameters can be saved, or restored, from a SBATCH file with the “Load” and “Save” buttons, respectively.

### **Building and Populating Directory Trees (not available at present)**

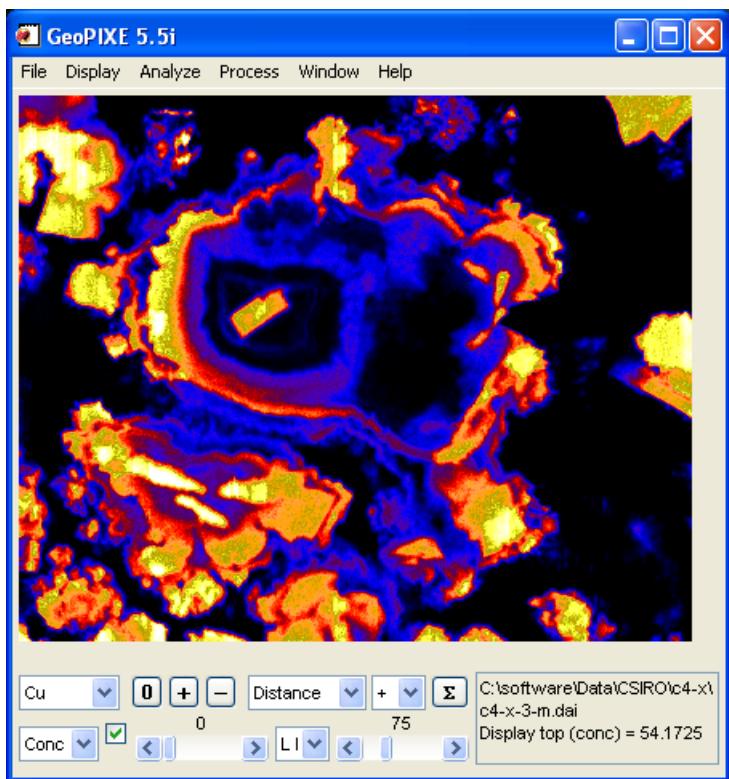
After transfer of list-mode files from the data acquisition system, initially all list-mode files will sit in one directory. This is the directory selected with the “Dir:” button. The “Build Tree” button can be used to automatically build a directory tree based on the structure of the file names. The use of special characters (“-“, “\_”, “\$”, etc.) will denote a level of sub-directory, provided there are more than one list-mode file at each level. The final directory levels will contain one list-mode file each (and accompanying parameter files).

*Important Note:* At present, these operations apply to single-file list-mode data. Multi-file formats (e.g. Lund KMax, NSLS, GSE-CARS, Hasylab, Maia), which use multiple files for each image scan, are not catered for as yet.

The table will be updated after the tree building process. Hit the “Start” button to sort all files and apply the selected optional operations.

### **Image Display (main GeoPIXE window)**

The *Image Display* window displays elemental images, sent from the *Sort EVT* window, or loaded from a DAI file using the “File→Load Image” menu. The element displayed is set using the drop-list on the left below the image. Use the context-sensitive help to view help information about each control widget. Next to the element drop-list is a series of zoom buttons labelled “0”, “+” and “-”. These set full resolution display, zoom in and out, respectively. Next comes two drop-lists which select region selection shapes and include/exclude mode, and finally a “Σ” button. These are discussed below.



On the next row is another drop-list, which selects between concentration display ("Conc") and variance images ("Var"). Next to it is a small check-box that enables bilinear interpolation of images when zoomed in. Then there are two sliders, which control the minimum and maximum values (as % of the maximum image pixel value) that map onto the bottom and top of the colour map. All concentrations between these values are mapped onto the current colour map, using a linear scale by default. Use the small drop-list between the bottom and top sliders to select between Linear (L), Log (G) and Sqrt (S) scales for the Z axis. The Sqrt and Log scales have the effect of compressing dynamic range, which can be useful for images with strong hot-spots and low-level traces. (Colour maps can be selected under the "Display→Colours" menu.) The maximum displayed value (usually in ppm) is shown in the help window (when not used for context-sensitive information).

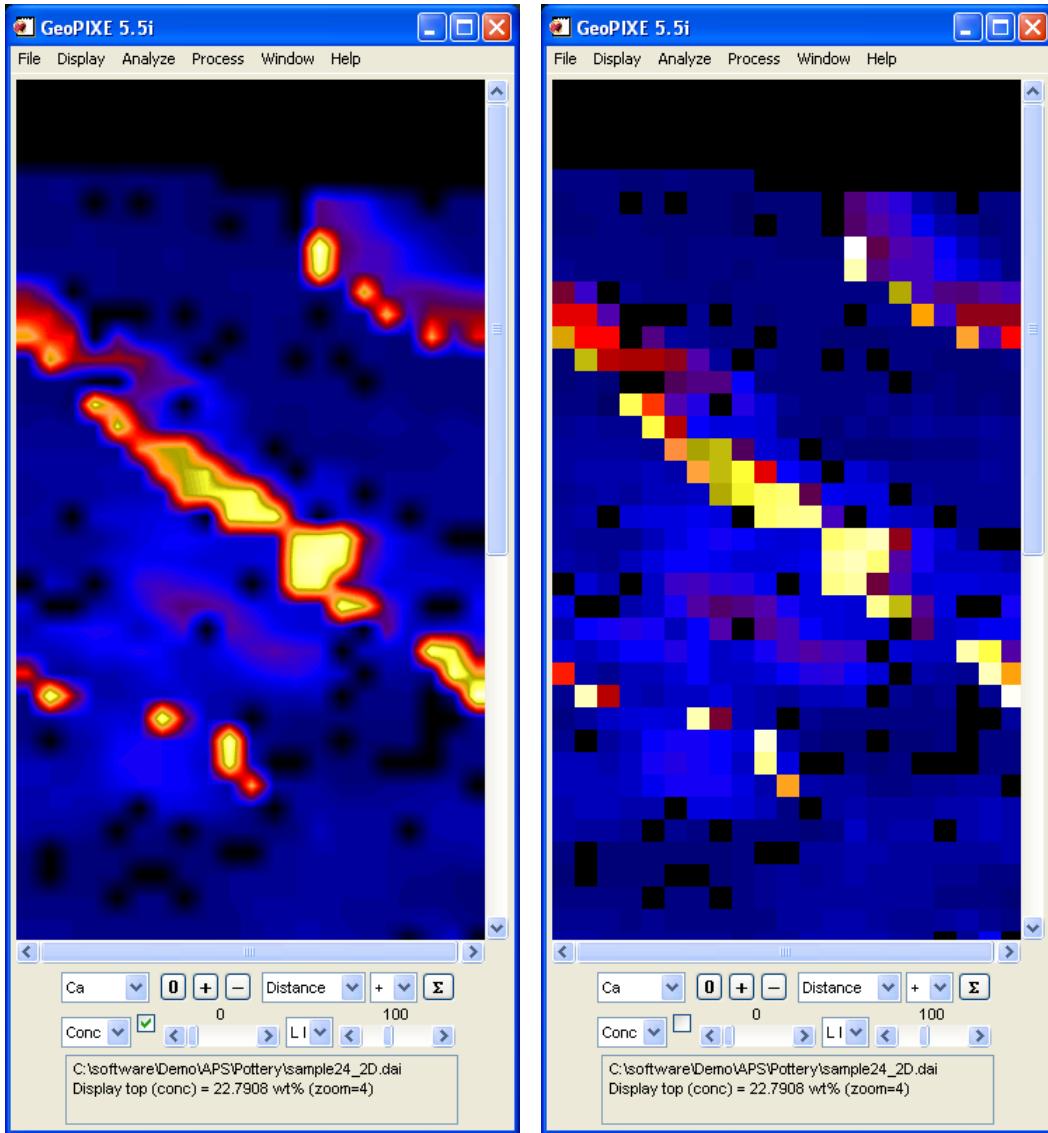


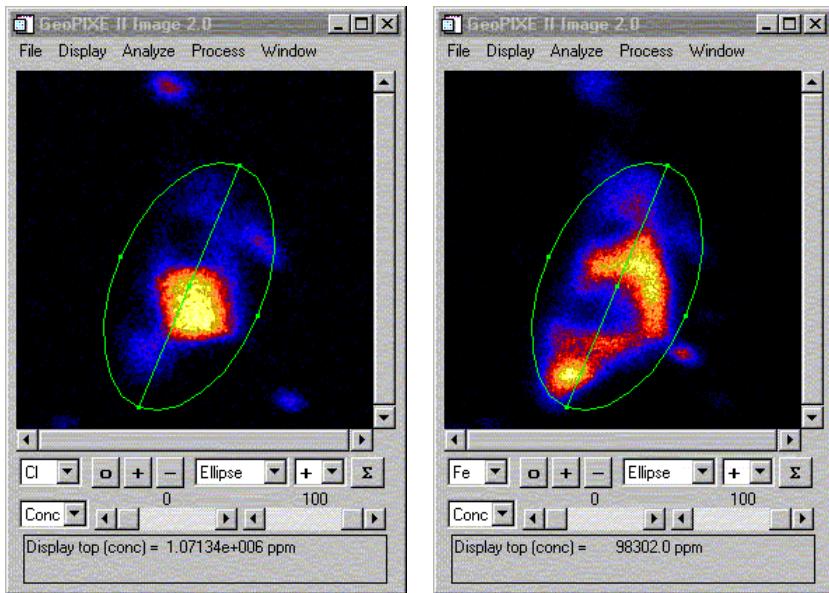
Image window zoomed in on a small image area with Interpolation (left) on and (right) off.

Using the zoom buttons, you can repeatedly zoom further in and out on an image. When zoomed in, the image is displayed using linear interpolation between pixels. Particularly when zoomed in, you can resize the window and use the scroll bars to move smoothly throughout the image.

Elemental images can be exported to PNG files, referenced by a HTML file using the "File → Save ALL as HTML (PNG)" menu. This creates a HTML file that can be opened, or printed, from a browser. Each image appears as a thumbnail scaled down to 200x200 pixels with an element label and any shape overlaid in green. These are hyperlinked to the full version of each image. (Your browser may need a plug-in to view PNG images.) (Note: Under IDL 5.3, GIF images will be produced. However, GIF is not supported beyond version 5.3.1).

## Image Clones

Clones of the current *Image Display* window can be created using the "Display → Clone ..." menus. You can create from 1 to 11 clones in a regular grid using the "Display → Clone → ..." menu. The clones act in unison. When you move a region on one Clone, it is redrawn moved on all related clones (i.e. all clones from the same parent *Image Display* window). Similarly, you can hit "Σ" in any clone and the results will be sent to the related *Image Regions* window. Each row of results in the *Image Regions* table are labelled by the name of the element image displayed when the "Σ" button was pressed.



*Note:* To open an independent Image Display window, to display unrelated image data without affecting the current images or the default path, use the menu “Window→Image Display (**unlinked**)”.

## Image Display Menus

### File Menu:

- Load Load images from a GeoPIXE native DAI image file.
- Save Save images to a DAI file.
- Clear Clear image memory.
- Load (ignore null) Loads some old corrupt images with null matrix data.
- Save All as HTML Save all images as PNG and imbed them in a HTML web page.
- Black and White HTML Save all as HTML, but in black and white format images.
- Import→ ... Import image grey-scale files for limited manipulation and display.
- Convert→ ... File format conversion programs.
- Export→Simple Images Exports the image as a simple PNG or TIFF file (including the shape), or the current pixels selected, using a shape or Association highlights, as a transparent PNG image file. TIFF export uses either (i) ppm, (ii) counts (all detectors), or (iii) ng/cm<sup>2</sup> units.
- Export→Image Plot Export selected images in a plot saved in various image formats (typically use JPEG). Formats supported include: Computer Graphics Metafile (CGM) and Windows Metafile. Opens the *Plot Image Select* pop-up panel to select various options for creating an output plot.
- Export→Image Data Export selected images as CSV (comma or tab separated) text files, one for each element selected (filename contains element name) for either the whole image or the currently selected region. Optionally, export selected images in Chimage native format (Chimage is the CSIRO electron microprobe image analysis package).
- Retry cluster image ... If the reconstruction of a cluster mode parallel processing *Sort EVT* run is interrupted, often the reconstruction can be continued here. The results from each process have names ending in .dai.0, .dai.1, ...
- Print Opens the *Plot Image Select* pop-up panel to select various options for printing the current image to the default printer.
- Print All As above, but prints all images, two to a page.
- Image Properties Open the *Image History* window to show and edit (some) image properties.
- Image Properties & Stats Open the *Image History* as above but includes some per pixel statistics (may take some time on images above 10M pixels).
- Exit Close this instance of the Image Display window (if this is the main parent

window for GeoPIXE, then close all child windows and exit GeoPIXE).

Export of regions of type “ProjectX” or “ProjectY” in XY format first collapses the region onto the central axis, averaging across the region width, and then exports this average along the projection line.

#### Display:

- Clone→... Clone various numbers of copies of this *Image Display* windows in a grid.
- Multi Image Display a simple grid of element images.
- 3D Stack Image Opens the 3D Image (XANES, tomography, ...) window.
- Colours→Colour Table Opens the colour table requester to change the colour table used for images.
- Colours→Default Sets the default colour table, Standard Gamma II.
- Colours→10 Step A ten colour step table, based on Standard Gamma II.
- Colours→Grey Scale Sets the colour table to grey scale, with black as zero.
- Colours→Invert Table Inverts the order of the colour table.
- Colours→Linear Luminance Remaps the colour table onto a linearly increasing luminance.
- Clear All Shapes Clears any shape displayed on the image.
- Clear Assoc. Highlights Clears any highlighted areas set from the *Associations* window.
- Reset display min/max Re-calculate the min and max values for display of each element. The min and max controls are relative to these in %. May be needed after some processing or plugins.

#### Analyze:

- Mode→Include Set the shape or regions mode to “Include”, just like “+” on the drop-list.
- Mode→Exclude Set the shape or regions mode to “Exclude”, just like “-” on the drop-list.
- Type→... Sets the current region shape, like the shape drop-list.
- Region Analyze the contents of the current selected region; like using the “ $\Sigma$ ” button.
- Throttle Use the current images to derive a spectrum of Throttle factors to be used to reduce Maia data acquisition data-rates with minimal loss of quality.

“Throttle” uses a pop-up panel of parameters to derive a ‘factor’ by which the count-rate must be reduced, while minimising loss of image quality and trace element statistics. Once this factor is derived interactively, the routine uses the current set of images to sample the variation in elemental intensity in order to construct a model spectrum to calculate a spectrum of factors to reduce each channel count-rate by. This derived model spectrum replaces the current spectrum displayed in *Spectrum Display*. The throttle factors spectrum is saved to a TXT file for use with the Maia data acquisition system and also for replay and correction of Throttled event file collected in this way. (See also the *Spectrum Display* Analyze→Throttle menu for a simpler method, and *Sort EVT* for the use of Throttle files on play-back.)

#### Process:

- Clear→Border Clear a selected range of pixels on the image border.
- Clear→Kill Region Zeros image data for selected element within region.
- Clear→Kill Region all planes Zeros image data for all element planes within region.
- Clear→Kill all Regions all planes Zeros image data for all element planes within all regions.
- Filter→Smooth→... Apply a smoothing digital filter to the current image, in various strengths (pixel widths), using Boxcar or Gaussian kernel weights or a Median filter.
- Filter→Edge Enhance→... Apply a Sobel or Roberts edge enhancement digital filter.
- Filter→Erode Apply the erosion operator to this image in various widths.
- Filter→Dilate Apply the dilation image operator.
- Scale Scale ALL images by various factors
- Rotate Rotate ALL images by 90 degree increments, or mirror them.
- Shift Shift either odd or all image rows by selected pixels left or right.
- Clip→ ... Clip all images to either Right or Top.
- Correct→Xstep Current Correct all images for current integration problems in X-step mode (see examples in the next chapter).
- Correct→Ystep Current Correct all images for current integration problems in Y-step mode.
- Correct→Suppress Region Attenuates image data for selected element within region or Association highlighted area.
- Correct→Image Pileup Subtract pileup artefacts from Images making use of Image Pileup simulation loaded in Spectrum Display (see Spectrum Display “Display→Pileup→using

- Correct→Missing rows      “Images” menu).  
Eliminates missing row data, selected using a Box shape, replacing it with the average on either side.
- Correct→Double-counted rows      Row portions, selected using a Box shape, that contain double-counted data are corrected (halved).
- Correct→Missing columns      Eliminates missing column data, selected using a Box shape, replacing it with the average on either side.
- Correct→Double-counted columns      Column portions, selected using a Box shape, that contain double-counted data are corrected (halved).
- Correct→Zero pixels      Eliminate isolated zero pixels in all images. “Zero” pixels are defined as those that are surrounded by at least 6 non-zero pixels. It uses a threshold of 3% of the display maximum of the currently displayed element to determine which pixels contain anomalous zero data. GeoPIXE then replaces these zero pixels in all element images with the average of surrounding non-zero pixel data.
- Correct→Ghost      Eliminate a “ghost” or “echo” feature in an image, corresponding to second displaced beam at a fixed offset. The menu offers relative intensities of the ghost feature in 10% and 1% increments. Use these in combination to correct ghost features; the operation is applied to all images. Beforehand, use the “Distance” shape tool to drag out a vector giving the offset to the ghost or echo features.
- Undo Operation      Undo the last operation (except for rotation, scale, clip).
- User Plugins→...      Apply one of the loaded user plug-ins for user-defined image processing.
- Reload user plugins      Reload all plugin SAV files (e.g. if any have been added).

***Window:***

- Image Regions      Open the Image Regions window to display region integration results.
- Image Operations      Open the Image Operations window for single click image processing steps.
- Image History      Open the Image History window to display a history of all image processing steps on the current image and to edit selected image properties (double click to edit).
- Element Associations      Open the Associations window to display 2-element associations in the current image.
- PCA, Cluster      Use for PCA and cluster analysis of XANES 3D stacks.
- 3 Element RGB Images      Open the Image RGB window to overlay 3 elements as Red, Green and Blue components.
- Spectrum Display      Open the Spectrum Display window for spectra display and fitting.
- Sort EVT      Open the Sort EVT window to sort event files to project images.
- XANES Image      Opens the 3D Stack image window.
- Correct Yields (N=6)      Open the Correct Yields window for correction of spatial variation of yields, up to 6 components.
- Correct Yields (N=16)      Open the Correct Yields window for correction of spatial variation of yields, up to 16 components.
- Project Minerals      Open the Correct Yields window as well, to project onto end-member mineral components.
- Edit Filters      Open the Filter Setup & Edit window to create of edit X-ray absorber files.
- Edit Detectors      Open the Detector Setup & Edit window to create or edit detector specification files.
- Image (unlinked)      Open a new Image Display window that is independent and not linked to the parent image window and its progeny.
- Spectrum (unlinked)      Open the Spectrum Display window that is independent and not linked to the parent image window and its progeny.
- PIXE/SXRF Simulator      Open the PIXE/SXRF Simulator window to simulate anticipated count-rates for specified beam, sample, and detector arrangements.
- Blog Browser      Open the Maia blog raw list-mode data browser.

***Help:***

- GeoPIXE User's Guide      Points to documentation and diagnostics.
- Maia Users Guide      Points to the Maia users guide \*.
- Query IDL Environment      Displays details of the current IDL operating environment.
- Update GeoPIXE      Run “geopixe\_update” to connect to the CSIRO FTP site to update the software.  
NOTE: This does not update the Maia specific extensions of GeoPIXE for run-

- About GeoPIXE time operation of a Maia detector (use “maia\_update”).  
Shows GeoPIXE version.

**NOTE:** There are PDF versions of the manuals in the GeoPIXE Help directory.

## Image Display Widgets

This list summarises the functions of all widgets on the *Image Display* window, including buttons, sliders, drop-lists and text entry widgets. These are listed from left to right, top to bottom.

### First row below image:

- X Scroll Bar Control to scroll image in X, similar one for Y on the right side of the image.

### Second row:

- |                         |  |
|-------------------------|--|
| • Element Drop-list     | Select element image to display.   |
| • “0” Button            | Return to no zoom (full resolution) display.   |
| • “+” Button            | Zoom in by a factor of 2.  |
| • “-“ Button            | Zoom out by 2.   |
| • Shape Drop-list       | Select the region shape to be used to select or integrate various regions of the image area.                           |
| • Region Mode Drop-list | Select between “+” for inclusive selection (default) and “-“ to exclude selections from the currently selected region. |
| • “Σ”                   | Analyze the current region; results appear in the <i>Image Regions</i> window.   |

### Third row:

- |                         |   |
|-------------------------|---|
| • Quantity Drop-list    | Selects between the concentration image and the variance image.                         |
| • Interpolate check-box | Enables bilinear interpolation of image data when zoomed in.                            |
| • Low Limit Slider      | Sets the lowest concentration visible, as a percentage of the maximum.                  |
| • Z axis display scale  | Select the Z axis (colour axis) display scale between L (linear), G (log) and S (sqrt). |
| • High Limit Slider     | Sets the highest concentration visible, as a percentage of the maximum.                 |

### Bottom row (or to right for larger images):

- Help Context-sensitive help area, shows help prompts for widgets as the mouse pointer moves over them.

## Image Region Selection Shapes

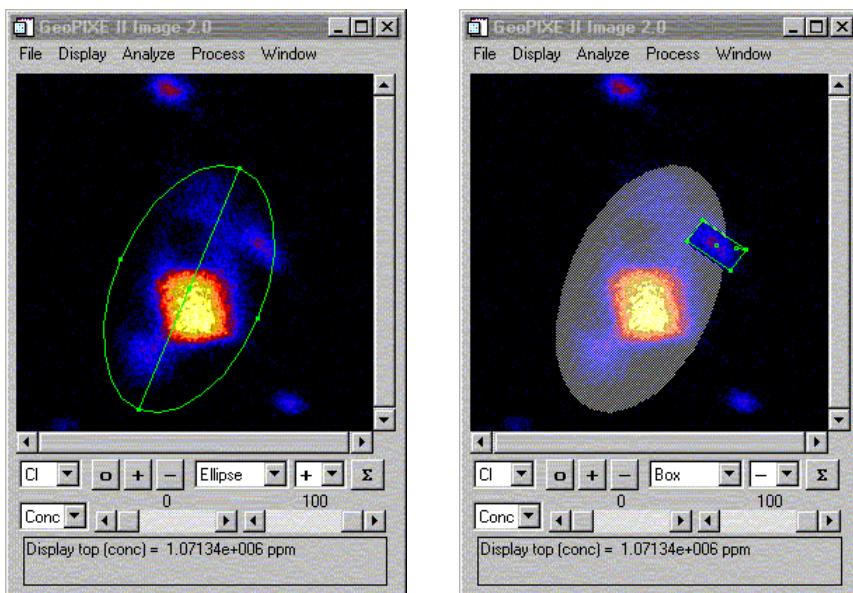
The region selection drop-list selects between the following shapes. Apart from the first, used to measure distance only, these shapes are used to define an area of the image. Clicking on "Σ" will then measure the average concentrations of all elements in this region. The results can be viewed using the *Image Regions* window ("Windows→Image Regions" menu). More on this below.

- 1) **Distance:** Used simply to draw and measure distance between selected points on an image. (This will show in microns if the X and Y scan sizes were entered into the Sort EVT set-up.) Simply left-click on a point and hold and drag to the second point and release.
- 2) **Box:** With this you can click and drag out a box to surround a feature. The box has handles in the corner that can be used to resize the box. There is also an extra handle on a short diagonal line that can be used to rotate the box. A final control point in the centre can be used to move the box.
- 3) **Circle:** Click and drag a circle based on control points on a diameter. There is also a central control point used to move the circle.
- 4) **Ellipse:** Like circle, but with control points on the minor axis as well to set the width of the ellipse.
- 5) **Traverse:** This drags out a line projection area. It is used to form a line profile or traverse across a selected rectangular area of the image. Handles at each end set the projection line. Handles on the sides of the rectangle set the projection width (left mouse button) or the shear (right mouse button); all points are projected back onto the central line. (Traverses and line projections are discussed later.)

- 6) **Curve 8:** A spline curve shape to define traverses along non-linear paths. Click and drag out the line as usual for Traverse. Adjust width using side handles and adjust the shape using spline control points. To move the spline curve *en masse*, click on the central spline control point using the right mouse button.
- 7) **Spline 10:** Initially, this drags out a circle with 10 control points, and central move handle. Each point on the circle is a spline control point. Move them independently to form arbitrary shapes.
- 8) **Spine 32:** Like Spline 10, but with 32 control points for greater control.
- 9) **Spine 100:** Like Spline 10, but with 100 control points for greater control.
- 10) **ProjectX:** Like Traverse, but the (long) projection axis is constrained to lie in the horizontal X axis only.
- 11) **ProjectY:** Like Traverse, but the (long) projection axis is constrained to lie in the vertical Y axis only.
- 12) **S Pixel:** Selects a single pixel only (shown as a small box).

To view the results of the " $\Sigma$ " operation using regions you need to have the *Image Regions* window open. This is discussed below.

*An alternative approach to selecting regions of pixels on images is to use the Associations window. This selects pixels based on value and the correlations between elements.*



### Image Selection Modes

If the include/exclude drop-list (to the right of the regions/shape drop-list) is set to include "+", then the operation includes all pixels within the region in the concentration average. The exclude mode "-" can be used to exclude shapes from a previous include area.

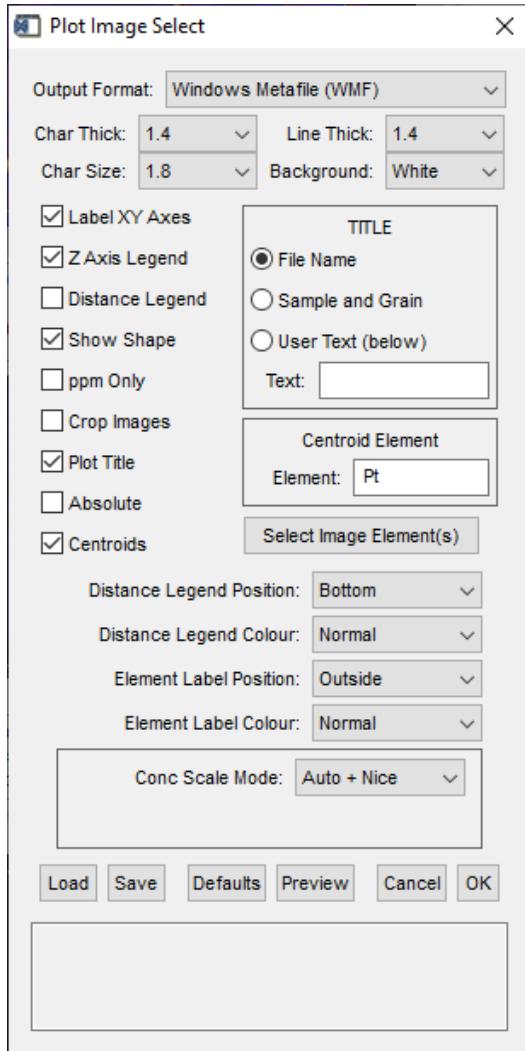
As an example, use include mode "+" and an ellipse region to select an area of an image (as shown above) and hit " $\Sigma$ ". The *Image Regions* window shows the average concentrations within this ellipse region. Now, select exclude "-". The ellipse changes to a shaded area showing all pixels included in the average (if no shading appears, you may not have clicked on " $\Sigma$ " first). Now, select a box exclude shape. Drag out a small box within (or partly within) the shaded ellipse area; move handles or rotate as needed. Now when you hit " $\Sigma$ ", this box is excluded or removed from the shaded area. The row in *Image Regions* window now shows the average concentrations within the ellipse, excluding the box area. This exclude operation can be repeated with more boxes or different exclude shapes to remove unwanted cracks, pits, inclusions, etc. from a desired area. Exclude works with all shape types, including traverses/line projections.

*If a region is selected and highlighted based on element Associations, then the exclude operation can be used to remove*

*pixels from the Association highlighted area.*

## Image Plotting and Exporting

Other format output, which includes optional distance scales and a Z axis concentration legend, can be exported using the “File→Export” menu. This brings up a pop-up panel that enables various plotting parameters to be selected.

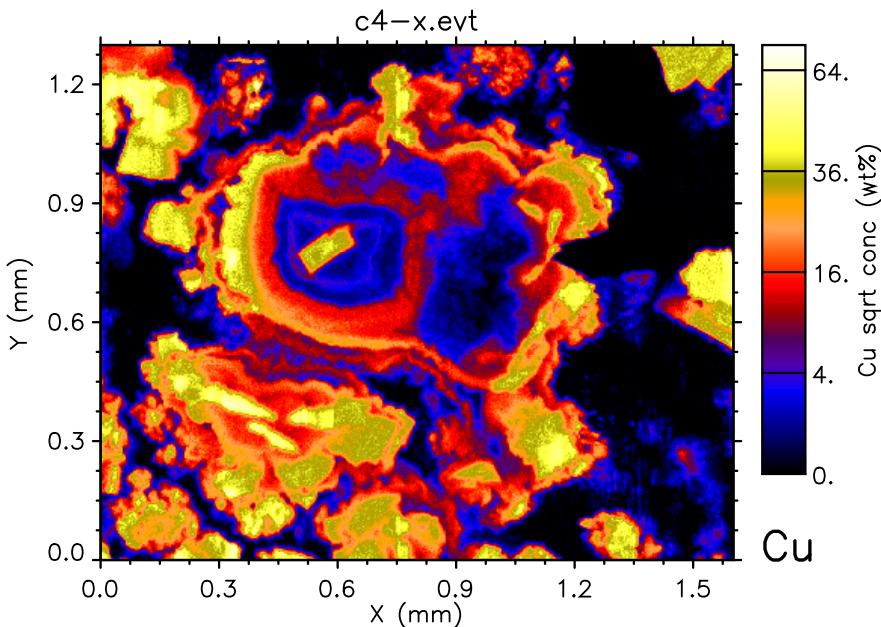


Plotting parameters that can be controlled include:

- 1) **Output format:** Select between Computer Graphics Metafile (CGM), Windows Metafile (WMF), Encapsulated PostScript (EPS) and Printer output.
- 2) **Char Thick:** Character line thickness (default 1.6).
- 3) **Char Size:** Character Size (default 2.0).
- 4) **Line Thick:** Line thickness for axes, etc. (default 1.6).
- 5) **Background:** Background colour (default is black).
- 6) **Label XY Axes:** Label X and Y axes and draw distance tick-marks in “mm” or “microns”, if the image was sorted with a known size specified, or “pixels” otherwise.
- 7) **Z Axis Legend:** Add a colour bar legend with a concentration scale.
- 8) **Distance Legend:** Add a scale bar on the plot. The position is specified with the “Distance Legend Position” drop-list. Note that you probably don’t need this as well as axis tick marks.

- 9) **Show Shape:** Overlay the current region selection shape in green.
- 10) **ppm Only:** Use only ppm values in the concentration legend.
- 11) **Crop Images:** Use the current shape on the image to crop the image for output.
- 12) **Plot Title:** Add a title to the top of the plot, in addition to the element name label. The choice of title options is selected on the right, between using the source list-mode file name, the sample and grain codes, or user supplied text in the text box.
- 13) **Absolute:** Show the absolute stage coordinates for the scan area, based on the stored scan origin.
- 14) **Centroids:** Enabled the use of XY centroids for the presently loaded *Image Regions*. This uses the XY centroids for each region for the element selected under “Centroid Element” and plots a circle around each centroid. This is intended to help locate small hot-spots.
- 15) **Distance Legend Position:** Choose the position of the scale bar between top and bottom of the image.
- 16) **Distance Legend Colour:** Choose the colour of the distance bar to normal (same as the axes and text) or reversed.
- 17) **Element Label Position:** Choose between outside the image on the bottom right, or inside the image area in the various corners.
- 18) **Element Label Colour:** Choose the colour of the element label text to normal (same as the axes and text) or reversed.
- 19) **Conc Scale Max:** Choose the mode for selecting the concentration legend range: “Auto” means select the maximum concentration range automatically, “Nice” means use only ranges based on a logarithmic 1-2-5 sequence, and “Manual” to enter a concentration maximum manually.
- 20) **Manual Scale Max:** If “Manual” is selected for Conc Scale Max, then enter the maximum value here.

These selections can be saved and restored (.PLOT files) using “Save” and “Load” or set to default values using the “Defaults” button. Once parameters are selected, click “OK” to complete the export. The CGM and WMF formats can be imported into PowerPoint as Pictures.



The export panel (from “Export→Image Plot “ menu) is used to produce figures in CGM, WMF, EPS formats or in very large format, high resolution JPEG image files or to output to your default printer device. It provides options to set background colour, character size and line widths and options for the placement of distance and Z axis (e.g. concentration) legends. Further options can be used to crop the image to the current shape in the *Image* window, show the axes in “absolute” coordinates, which are the stage coordinates used for the scan and to show the location of “hot-

spots". The latter show the pixels selected in the current region selected in the *Image Region* window in green, with enclosing circles to show where they are located. Hover the mouse pointer over each option and widget to get more help on each.

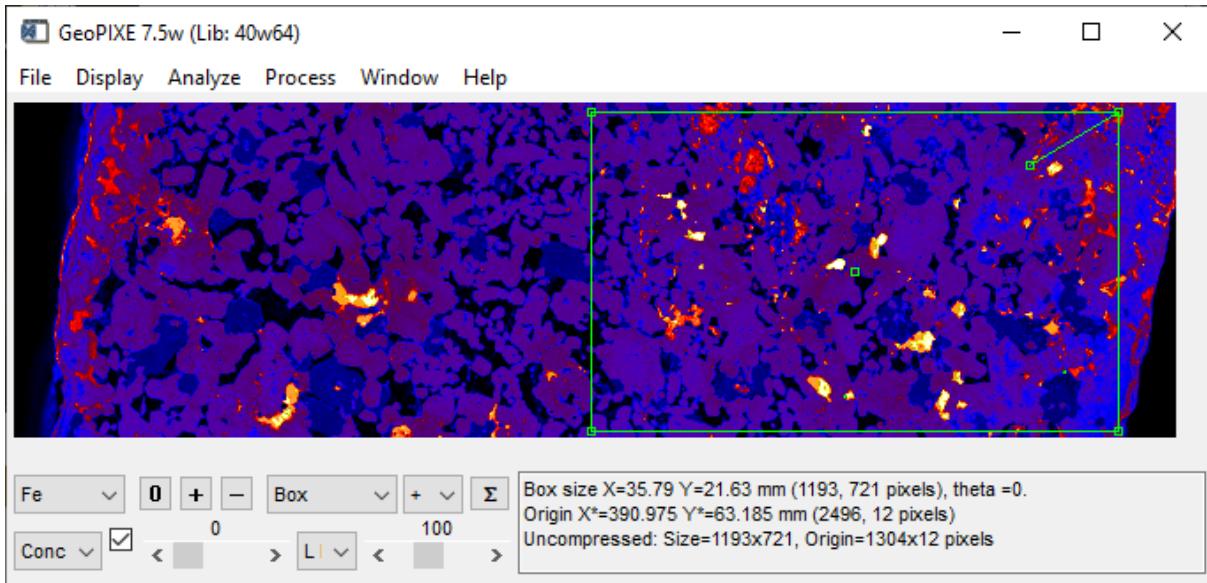


Image window (demo example MM/925) showing a Box region shape selected

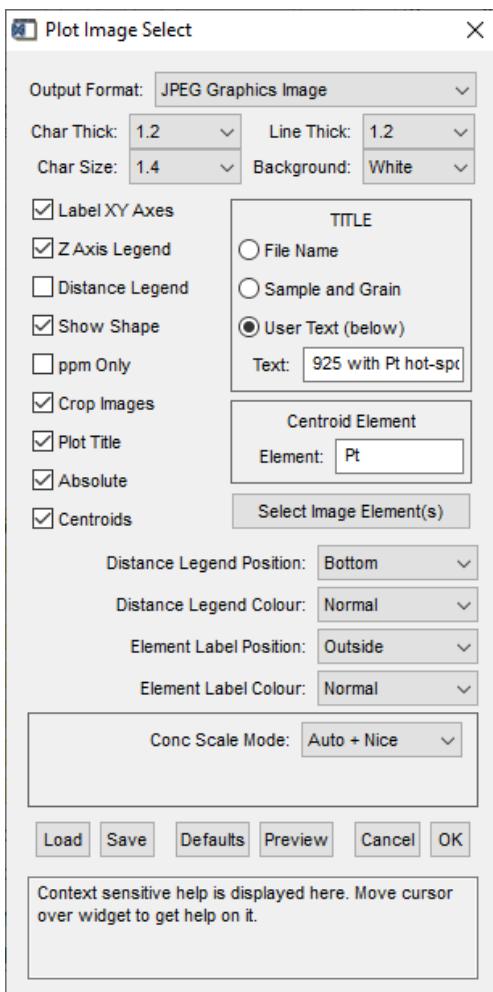
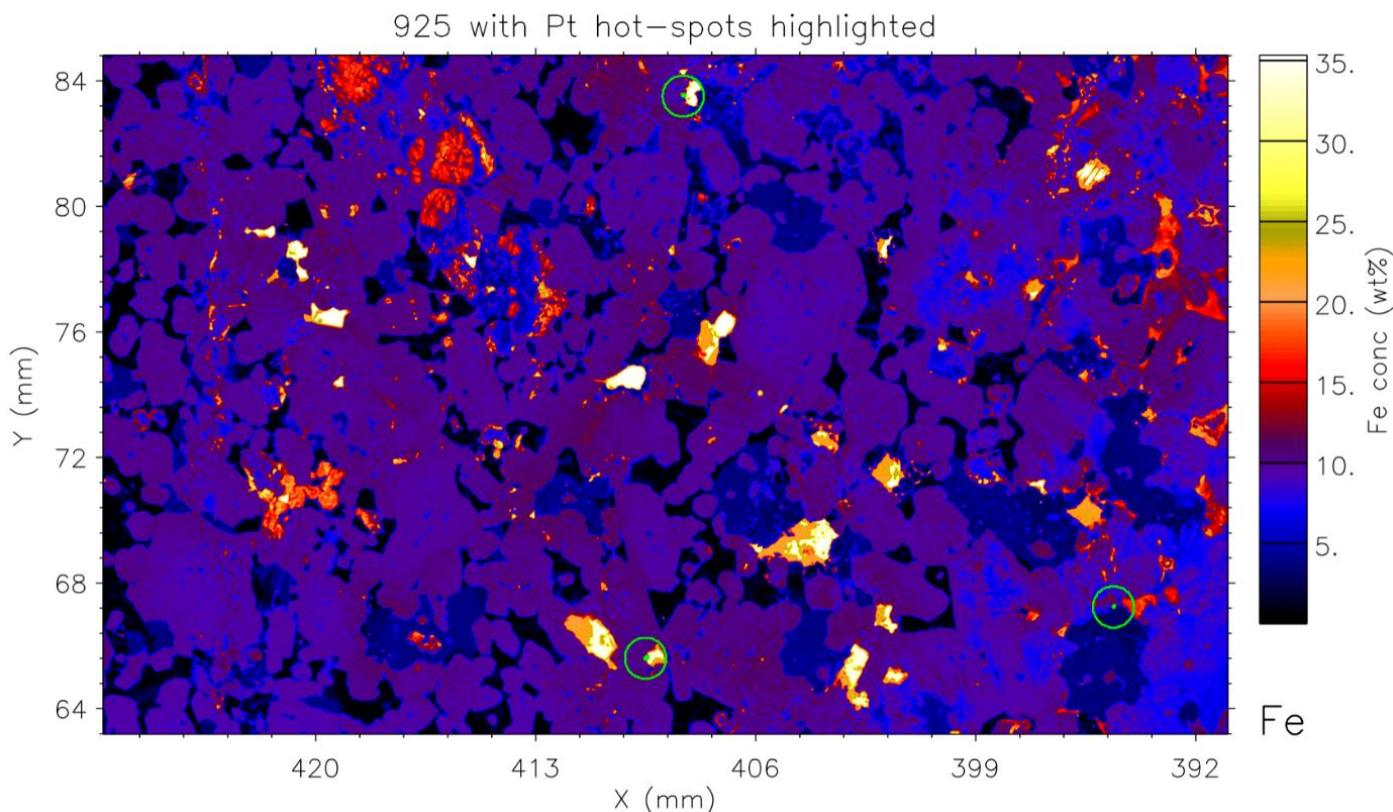


Image Export pop-up selecting JPEG plot output, crop to shape and overlay of hot-spots circled



*Image Export to a JPEG file, cropped to shape bounds, plotted in absolute stage coordinates and showing hot-spots in green, enclosed in circles*

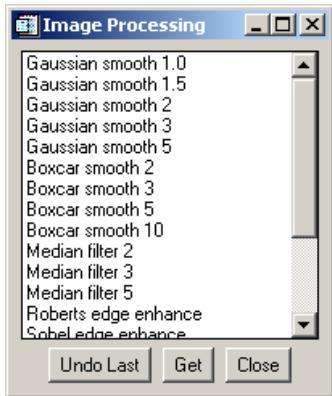
## Image Operations

### Image Operations Window

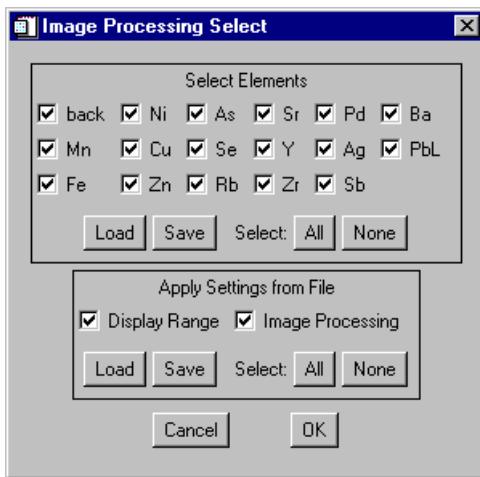
Low statistics images can suffer from large statistical fluctuations within individual pixels. These can be averaged or smoothed using various operations under the "Process→Filter→..." menus. There are also functions for edge enhancement and other image processing operations. Alternatively, open the *Image Operations* window using the "Windows→Image Operations" menu. Now a single click on a selected digital filter in the *Image Operations* list will perform that operation on the currently displayed elemental image. If the image is a "Conc" image, then the "Var" image is filtered as well.

Existing Image Plugins are also added to the Operations window list.

Simple, single element operations can be undone using the "Undo Last" button on the *Image Operations* window, or using the "Process→Undo Operation" menu on the *Image Display* window. Only a single level of undo on the current element is supported. Operations that apply to all elements (e.g. Scale, Clip, Y charge correct) cannot be undone; save the images first to enable a restore.



The “Get” button permits another image file to be read and the image-processing operations used for that image, and stored in the history records in its image header, to be applied selectively to the current image(s). The Get button pops-up the following requester:



Select which elements to apply operations to. These selection options can be restored from a file using the “Load” button and saved with the “Save” button. This selection and the image file-name remain as the defaults for further invocations of the “Get” button.

Use this feature to apply standard image processing steps, such as various smoothing passes and also user plug-in operations, to a series of image data sets. View processing history records in the *Image History* window.

## Image Processing Operations

The digital filters and operations currently available include the following. These are available on the *Image Display* “Process” menu, and many (that apply to a single element image) can be accessed at a single click in the *Image Operations* window. The current Image Plugins are also available in the window list. Operations that apply to a single element can be undone.

Most operations relate to the entire image displayed (e.g. Boxcar smooth), or all element images (e.g. Scale). Some operate on a selected region of an image (e.g. Correct Current, Kill Region). In these cases the function will use the current region shape selection for the operation. If one is not set, then it will use an Association highlighted region, if set. Use the *Associations* window to establish these pixel selections.

*Simple operations, that do not require the use of a selection Region, are logged to the Image History window and can be “re-played” from existing modified image DAI files (e.g. to apply the same operations to a new image file), using the “Get” button on the Image Operations window.*

- 1) **Boxcar n:** Simple 'n' x 'n' pixel average. Quite a severe smoothing effect.

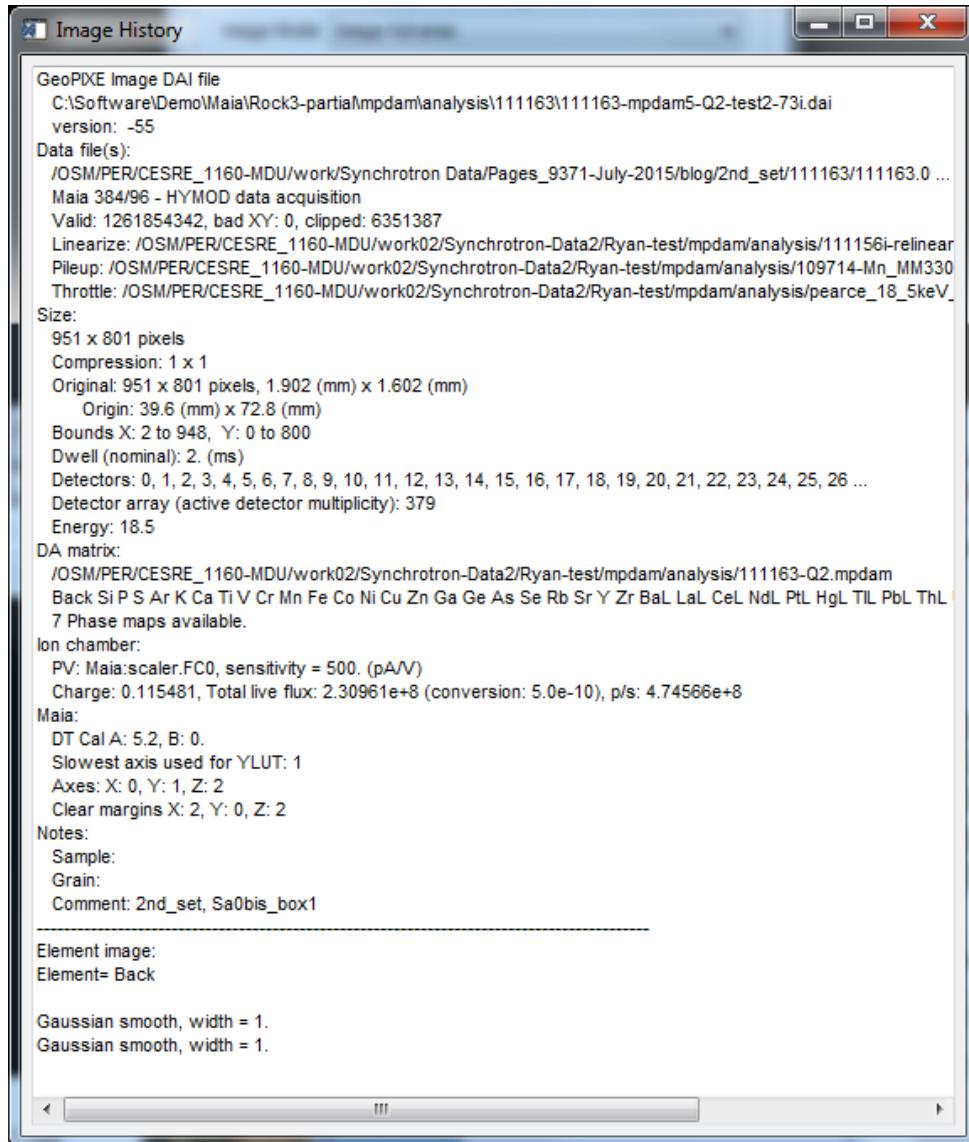
- 2) **Gaussian n:** Uses a rotated Gaussian digital filter kernel with a FWHM equal to 'n'. These are softer smoothing filters. The Gaussian 1.0 is a very subtle filter with a FWHM of just 1 pixel.
- 3) **Median n:** A median filter using an 'n' x 'n' pixel area. It is best to use one of the other smoothing filters first to avoid loss of counts or biasing concentration.
- 4) **Roberts n:** Applies the Roberts edge enhancement digital filter.
- 5) **Sobel n:** Applies the Sobel edge enhancement digital filter. Works better for noisy data.
- 6) **Erode n:** Thins or erodes features using a 'n'x'n' structure element. Uses the middle of the intensity scale as a threshold, so adjust the maximum display concentration slider to adjust the desired effect.
- 7) **Dilate n:** Opposite of the Erode operation.
- 8) **Scale:** Applies various scaling factors to ALL elemental images (this cannot be undone).
- 9) **\*Rotate:** Rotates or mirrors ALL elemental images (can not be undone). Note that you cannot extract spectra from regions applied to rotated images.
- 10) **Clip:** Clip all element images to either Right or Top (to preserve origin for Region validity).
- 11) **Correct Step Current:** Corrects for fluctuations in current integration during X or Y step scanning. By using a region selection, using the include and exclude features of regions to exclude cracks, etc., include what should be areas of constant composition in a selected element, that span the image from one side to the other. Then use this feature to flatten this distribution, thereby correcting for current fluctuation in ALL elements. If a region shape is not selected, then this function will use an Association highlight if set. (This cannot be undone.)
- 12) **Correct Image Pile-up:** Correct the images for the effects of complex pile-up, using the current spectrum, complete with modelled pile-up and fitted intensity parameters. See the description of pile-up correction below.
- 13) **Correct Missing Rows:** Correct all images for a missing scan line or part of one. Select the missing row portion by dragging a Box shape around the missing area and then use this menu, or its equivalent in the *Image Operations* Window. (This cannot be undone.)
- 14) **Correct Double Rows:** Correct all images for a scan line or part of one that is double counted. Select the missing row portion by dragging a Box shape around the missing area and then use this menu, or its equivalent in the *Image Operations* Window. (This cannot be undone.)
- 15) **Correct Missing Columns:** Correct all images for a missing vertical scan line or part of one. Select the missing row portion by dragging a Box shape around the missing area and then use this menu, or its equivalent in the *Image Operations* Window. (This cannot be undone.)
- 16) **Correct Double Columns:** Correct all images for a vertical scan line or part of one that is double counted. Select the missing row portion by dragging a Box shape around the missing area and then use this menu, or its equivalent in the *Image Operations* Window. (This cannot be undone.)
- 17) **Suppress Region:** Attenuates image for selected element within the current region area. If a region shape is not selected, then this function will use an Association highlight if set.
- 18) **Kill Region:** Zeroes the image for selected element within the current region area. If a region shape is not selected, then this function will use an Association highlight if set.
- 19) **Correct Zero pixels:** Eliminate isolated zero pixels in all images. "Zero" pixels are defined as those that are surrounded by at least 6 non-zero pixels. It uses a threshold of 3% of the display maximum of the currently displayed element to determine which pixels contain anomalous zero data. GeoPIXE then replaces these zero pixels in all element images with the average of surrounding non-zero pixel data. (This cannot be undone.)
- 20) **Correct Ghosts:** Eliminate a "ghost" or "echo" feature in an image, corresponding to a second displaced beam at a fixed offset. The menu offers relative intensities of the ghost feature in 10% and 1% increments. Use these in combination to correct ghost features; the operation is applied to all images. Beforehand, use the "Distance" shape tool to drag out a vector giving the offset to the ghost or echo features. (This cannot be undone.)
- 21) **Undo Operation:** Any single element operation (e.g. Smooth) can be undone.

The scaling and clipping operations will change the size of all element images. Information is saved in the image header that still enables the position of any regions set on this scaled image to be related back to the original XY coordinates in the EVT file. This means that you can still use the "EVT" button in the *Image Regions* window to

extract spectra from within regions, even if the images have been scaled. However, some other operations (e.g. Rotate) will render the regions invalid.

## Image History

All operations, such as this one, add history information to each image. This information is saved with the image file. An *Image History* window, invoked using the “Windows→Image Properties and History” menu in *Image Display*, allows viewing of this information and basic information about the image. A variant of the menu also displays per pixel statistics, such as mean and standard deviation for dwell time per pixel, count rates, dead-time and pile-up. This can be slow for images beyond ~10M pixels and take a few seconds to appear.



Some parameters can be changed in the *Image History* window, such as the Sample, Grain and Comments fields and the Charge and flux conversion factor fields. Double click on active rows to make changes.

If you open the window using the “Windows→Image Properties and Pixel Statistics” menu in *Image Display*, extra rows will be added providing various per pixel statistics. Note: this may take some time to compute (and each time the element drop-list is changed) for massive images of 10's M pixels, such as from the Maia detector array.

## Image User Plug-ins

The *Image Display* window has a user plug-in facility. You can write image processing and other user image operations in IDL. These are loaded when GeoPIXE runs, and appear on the “Process→User Plug-ins” menu. They are also appended to the bottom of the image operations list in the *Image Operations Window*. As with other image operations, these add an information line to the image history record. The “Undo” menu (or button on the *Image Operations* window) can be used to undo this user plug-in operation.

You need IDLDE to be able to compile your own plug-in procedures. However, once you have built the SAV file, you can run them through GeoPIXE using IDL run-time.

User plug-ins are designed at present for operations that change the image data, for the single, currently selected element, but do not change the element names, the number of elements, or the sizes of images. Extension in these areas may come later.

The file “template\_image\_plugin.pro” is provided with the GeoPIXE distribution. It provides a template for writing image processing plug-ins. It performs a simple smooth as an example. See the file for a description of the arguments.

All Image template routines MUST be named with “\_image\_plugin.pro” at the end of the file name. For a new “Fred” plug-in, copy and rename the template file to “fred\_image\_plugin.pro” and edit the first line to:

```
pro fred_image_plugin, p, i, title=title, history=history
```

Plug-ins should be compiled in IDLDE and saved as a SAV file. Only compile routines for ONE plug-in and save it using the command:

```
SAVE, /routines, filename='fred_image_plugin.sav'
```

for a “fred\_image\_plugin” plug-in. To ensure this, exit IDLDE and start it again to compile and save another plug-in.

*NOTE: It is very important to ensure that ONLY routines for ONE plug-in are saved in each SAV file. Otherwise, unexpected results may result when the SAV files are restored at run-time. The plug-in SAV files will then be loaded automatically when GeoPIXE.sav runs, if the plug-in SAV files are located in the “plugins” sub-directory of GeoPIXE.*

## **Image Regions**

### **Image Regions Window**

Regions are selected by dragging a Shape on the image window draw area. The Shape is selected using the Shape, or select area analyze type drop-list below the image. The shapes are listed above in the description of the *Image Display* window.

Each click on “ $\Sigma$ ” in *Image Display* window will produce a new row in the *Image Regions* window table, corresponding to the average concentrations within the selected region pixels. Each row is labelled with the element name displayed when the “ $\Sigma$ ” button was pressed, in the “Image” column. This provides a reminder of what you were looking at when you pressed “ $\Sigma$ ”. See the discussion above under *Image Display* for details of using the “ $\Sigma$ ” button, image regions and selection modes (include and exclude).

Using the Analyze menu in the *Associations* window will also produce a results row in the *Image Regions* window corresponding to all pixels selected using the spline shape on the selected element-element correlation. See the discussion of the *Associations* window below.

**Image Regions**

	Image	Si	P	S	Ar	K	Ca	Ti
0	Ti	67.%	28.%	10.%	2.3%	3.5%	5.6%	11 ^
1	V	48.%	14.6%	16.1%	0.86%	4.7%	3.24%	0.6
2	Fe	37.%	<4.%	52.%	<0.3%	1.0%	3.9%	
3	Fe	20.%	25.%	7.1%			15.4%	
4	Ni			49.%			5.3%	
5	Cu	28.%	21.%	24.%	<0.3%		34.4%	

Load/ Save/ Display    Modify    Delete    Extract    Hotspots

Conc    Load    Save    Update: One    All    Export (no centroids)

Table of concentrations in each region. Click on row to display the region shape (or highlighted pixels) on the image, and associated spectrum. Click on element column heading to sort and on "Image" heading to restore initial order.

If you click on the row label for a row, it redraws that shape in the parent *Image Display* window, and in all related clone *Image Display* windows. If an image is zoomed, the regions are also enlarged/ reduced as appropriate. If the *Spectrum Display* window is opened, and the spectra were extracted using the “EVT” button, then the spectrum appropriate to this region will be displayed along with the spectrum reconstruction overlay (see below).

If you click on a Column heading, it sorts the entire table into descending order for that column.

**Image Regions**

	Image	Si	P	S	Ar	K	Ca	Ti
0	Ti	67.%	28.%	10.%	2.3%	3.5%	5.6%	11 ^
1	V	48.%	14.6%	16.1%	0.86%	4.7%	3.24%	0.6
2	Fe	37.%	<4.%	52.%	<0.3%	1.0%	3.9%	
3	Fe	20.%	25.%	7.1%			15.4%	
4	Ni			49.%			5.3%	
5	Cu	28.%	21.%	24.%	<0.3%		34.4%	

Load/ Save/ Display    Modify    Delete    Extract    Hotspots

Detectors: array    Extract spectra     Cluster

Table of concentrations in each region. Click on row to display the region shape (or highlighted pixels) on the image, and associated spectrum. Click on element column heading to sort and on "Image" heading to restore initial order.

For devices that support cluster processing, the “Cluster” option becomes available to distribute processing over multiple cores, or members of a cluster.

The “Modify”, “Delete” and “Hotspots” tabs can be used to access additional operations that can be performed on regions or the regions table.

**Image Regions**

	Image	Si	P	S	Ar	K	Ca	Ti
0	Ti	67.%	28.%	10.%	2.3%	3.5%	5.6%	11 ^
1	V	48.%	14.6%	16.1%	0.86%	4.7%	3.24%	0.6
2	Fe	37.%	<4.%	52.%	<0.3%	1.0%	3.9%	
3	Fe	20.%	25.%	7.1%			15.4%	
4	Ni			49.%			5.3%	
5	Cu	28.%	21.%	24.%	<0.3%		34.4%	

Load/ Save/ Display    Modify    Delete    Extract    Hotspots

Modify: Erode 3    Undo

Table of concentrations in each region. Click on row to display the region shape (or highlighted pixels) on the image, and associated spectrum. Click on element column heading to sort and on "Image" heading to restore initial order.

**Image Regions**

	Image	Si	P	S	Ar	K	Ca	Ti
0	Ti	67.%	28.%	10.%	2.3%	3.5%	5.6%	11 ^
1	V	48.%	14.6%	16.1%	0.86%	4.7%	3.24%	0.6
2	Fe	37.%	<4.%	52.%	<0.3%	1.0%	3.9%	
3	Fe	20.%	25.%	7.1%			15.4%	
4	Ni			49.%			5.3%	
5	Cu	28.%	21.%	24.%	<0.3%		34.4%	

Load/ Save/ Display    Modify    Delete    Extract    Hotspots

Delete: Selected row(s)     Spectra too     Keep #0    Clear

Table of concentrations in each region. Click on row to display the region shape (or highlighted pixels) on the image, and associated spectrum. Click on element column heading to sort and on "Image" heading to restore initial order.

**Image Regions**

	Image	Si	P	S	Ar	K	Ca	Ti
0	Ti	67.%	28.%	10.%	2.3%	3.5%	5.6%	11 ^
1	V	48.%	14.6%	16.1%	0.86%	4.7%	3.24%	0.6
2	Fe	37.%	<4.%	52.%	<0.3%	1.0%	3.9%	
3	Fe	20.%	25.%	7.1%			15.4%	
4	Ni			49.%			5.3%	
5	Cu	28.%	21.%	24.%	<0.3%		34.4%	

Load/ Save/ Display    Modify    Delete    Extract    Hotspots

Element: Pt    Hotspot separation    Neighbourhoods    Export (w/ centroids)

Table of concentrations in each region. Click on row to display the region shape (or highlighted pixels) on the image, and associated spectrum. Click on element column heading to sort and on "Image" heading to restore initial order.

These include: (i) separate hot-spot pixels selected using the *Association* method into distinct ‘clusters’ of pixels, (ii) selecting the pixels in the spatial neighbourhood of hot-spot pixels, (iii) delete all regions, except #0 (used to delete separated hot-spot regions), (iv) export the hot-spot region table, including centroid XY and number of pixels, (v) delete the selected region, and its matching spectrum (must have *Spectrum Select* window open). If “Keep #0” is enabled, then region #0 will be updated to be the sum of all separated pixel regions as deletions are made (this is used for total hotspots maintenance).

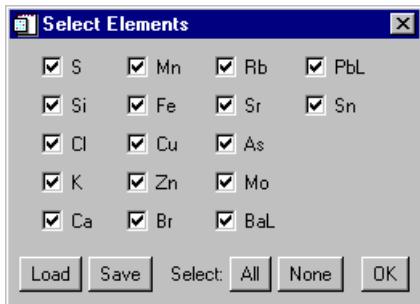
For example, using *Association* with both axes selecting the same element can be used to threshold one element. This will select pixels above a threshold concentration. These may be contiguous spatially or occurring in separate ‘objects’ distributed across the image area. Use the “Hotspot separation” button on the “Hotspots” tab, for a selected region row

(created using the *Association* threshold approach), to separate this selection of pixels into distinct spatial objects, such as hotspots. A pop-up will warn of how many objects have been found. Hit “Continue” to separate these into distinct regions of pixels, one for each cluster found. Note that this is time-consuming for object numbers beyond about 1000.

In large images, the location of a small number of pixels in a cluster may be hard to see. Use the drop-list on the *Image Regions* window to select “Centroid X” or “Centroid Y” to show the centroid position (X,Y in pixels) in the table.

### Export Selection Requester

These results can be exported to an ASCII (.CSV) file using the “Export” button. This brings up a panel to enable the selection of elements to export.



The image regions, along with the average concentrations, etc., can be save to a file (.REGION) using the "Save" button, or loaded using "Load". If the images have been updated (e.g. perhaps resorted after the addition of a missing element), use the "Update: All" button to redo the region averages to update the *Image Regions* table, and then Save the results again. If you need to adjust the position of a region, then select it by clicking on the row in the *Image Regions* window table. Then click on “Update: One” button to update the concentrations and region geometry for just this region.

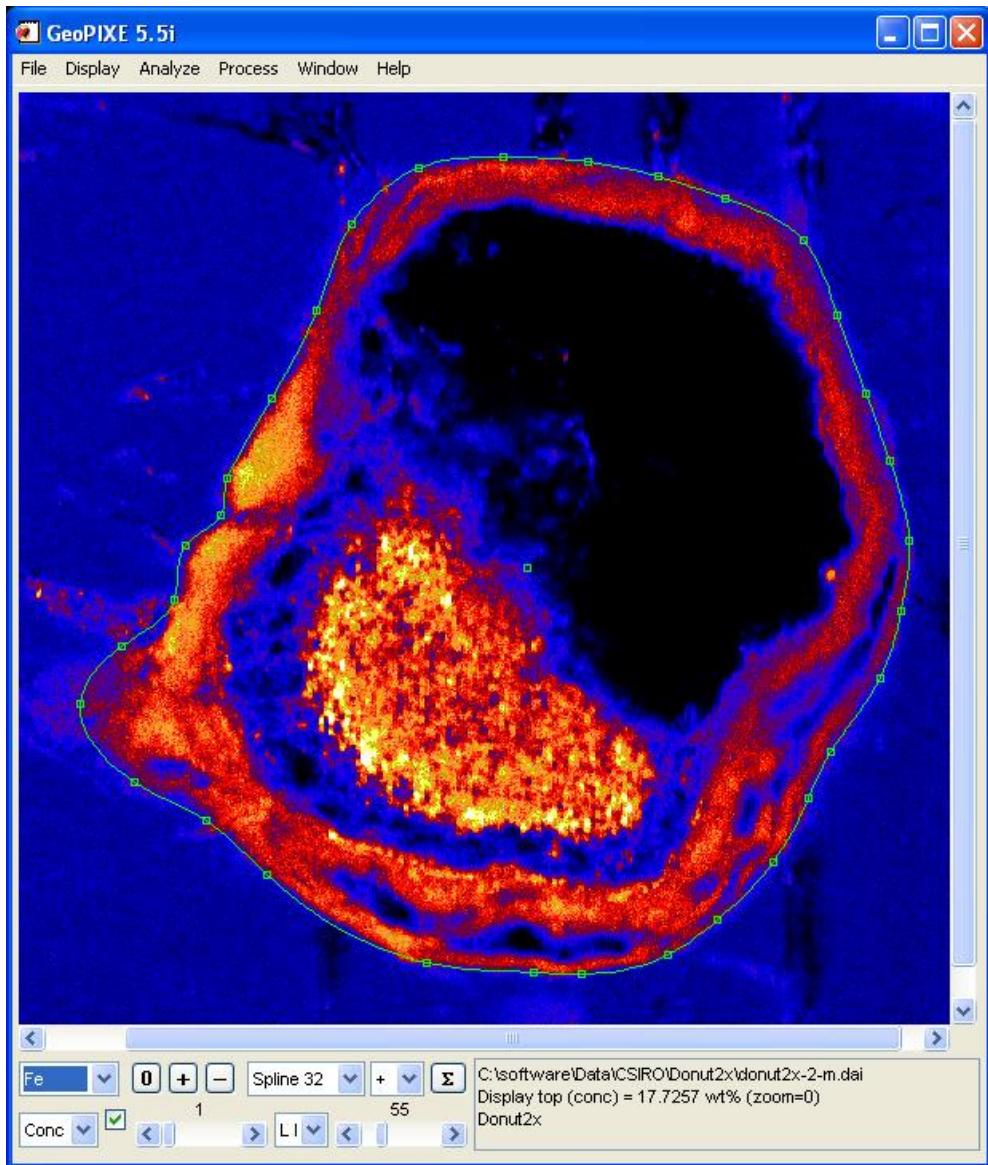
### Extracting Spectra from Image Regions

Spectra can be extracted from all the currently loaded regions by clicking on the "Extract spectra" button in the *Image Regions* window (“Extract” tab) (make sure you save the regions to a file using the “Save” button first). This will prompt for the name(s) of the source list-mode file(s) and the name of a destination SPEC file. Then the list-mode file(s) will be sorted and the ADC/ detector selected in the drop-list next to the Extract button will be extracted from the list-mode data. For each region specified, a separate spectrum will be created in the final SPEC file (with spectrum integrated charge proportional to region area).

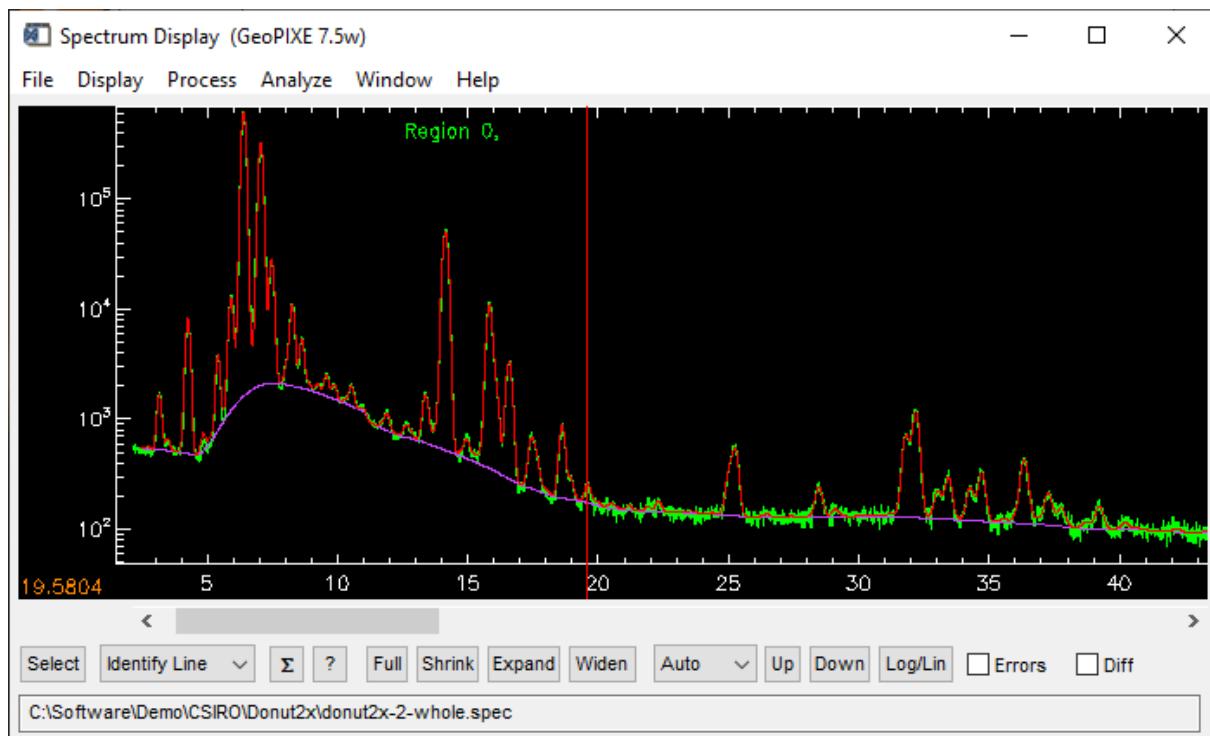
The ADC/ detector drop-list also has the entries: “individual” and “array”. Use “array” for an array detector in order to extract a sum spectrum across all active detector elements for each region. The individual energy calibration for each detector will be used to map the spectra summed onto a common energy calibration. The option “individual” is used to extract the separate spectra from each detector, but only for the first region in the list. See “Detector Arrays” below.

*NOTE: The name of the SPEC file is given by default based on the regions file name. For PIXE/SXRF data, it is best not to change these filenames. Then, when later you load a regions file into Image Regions, the corresponding spectrum file will be loaded into Spectrum Display automatically. Clicking on a row in Image Regions will display the corresponding spectrum in Spectrum Display.*

However, if you want to extract non-PIXE/SXRF data from a regions file that you set-up, as above, on PIXE images, then give the spectrum file a new name (e.g. append “-RBS” for RBS data). Select the correct ADC number for the RBS data, and hit “EVT”. Now, when prompted for a SPEC file-name, edit the name (append “-RBS” in the above example); this SPEC file will not overwrite your PIXE/SXRF spectrum file extracted previously from the same regions.



If a *Spectrum Display* window is open, it will be loaded with the resulting spectra (in addition to a SPEC file being written). Now, if you select a row of the *Image Regions* window (click in the row label at the left), the corresponding extracted spectrum will be displayed in the *Spectrum Display* window.



If the data is of type PIXE or SXRF, and the images use the DA method, then this spectrum will be overlaid with the spectral components scaled by the region concentrations. This “fit” gives a visual guide to the quality of the images in this region. For example, a missing element will usually mean a poor fit to overlapping elements, or an overestimate of background. This often shows up as a hot spot in the “Back” image or as a poor overlay on the extracted spectrum. These can be investigated in detail by extracting spectra from all suspicious regions in the elemental image and background. Any new missing elements can then be added to the fit to build a new revised DA matrix, and the image sort repeated, and regions Updated.

### Detector Arrays

The *Image Regions* window has a new feature for sorting all detectors of an array into merged spectra for regions. The spectra are mapped onto the energy calibration of the first spectrum before being accumulated into single spectra, one for each region. The ADC drop-list (next to “EVT” button) has the entry “array” which means sort all array detectors enabled for the image in *Sort EVT* when the list-mode file was sorted (assumes “Detector Array” type was selected in *Sort EVT*).

The option “individual” on the drop-list is used to extract the separate spectra from each active detector for which counts were recorded in the region, **but only for the first region in the list**. This option might be used together with a large region across a standard foil in order to check the relative sensitivity across an array.

An effective *multiplicity* internally keeps track of total collection sensitivity or the effective number of detectors merged together. This together with charge or flux Q is used to determine concentration from fits to these spectra. For the full array yield calculation, the relative sensitivity of each detector is also accounted for here.

## **Element – Element Associations**

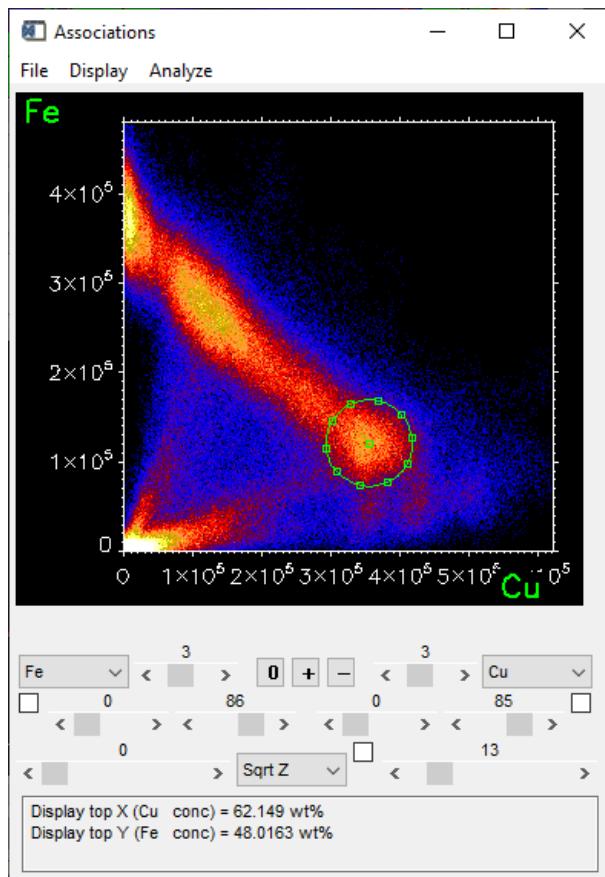
### Associations Window

A window *Associations* is used to plot associations of two elements in images. In other words, each pixel in a set of elemental images represents a data point in multi-element space. *Associations* displays two-element projections from this space. This can show up discrete phases in a sample, for example, which appear as discreet blobs that may be separated in some two-element views.

Open the *Associations* window using the “Window→Element Associations” menu on the *Image Display* window. This shows a window in which every pixel of the parent image is treated as a data point, and one element is plotted against another accumulated in a 2D histogram. Select the elements for the X and Y axes using the right and left element drop-lists, respectively. By default, each axis is a log scale showing about 5 cycles down from the maximum concentrations. To toggle the log/linear behaviour, use the small check-box below the element drop-lists (checked means log scale active).

The source element images may be noisy, which will adversely effect your associations. This can be remedied using a degree of pre-smoothing, applied to the X and Y elemental images prior to association. The pre-smooth is controlled using the slider next to each axis element drop-lists. A default of 3-point smooth is preset when the window opens.

By default the *Association* window opens with about a 300x300 pixel size with surrounding axes. This can be zoomed up or down, in factors of two, using the zoom buttons in the centre of the middle row (“+” makes bigger, “-”, smaller). Use the “o” button to return to normal size. Once zoomed larger, you can either use the scroll bars to move around in association space, or resize the window, or a combination of both.



The maximum intensity scale of the association, which is the Z histogram count for each element-element concentration pair, can be controlled using the two sliders at the bottom, maximum on the right, minimum on the left. The drop-list in the centre can select between a Linear Z histogram scale SQRT and Log to compress the dynamic range.

The minimum and maximum concentration displayed on each axis is controlled by the sliders in the middle row, Y on the left (low and high) and X on the right. The check box beneath the element drop-lists select a log scale for that axis.

*TIP: Remember to use the context-sensitive help. Pass the cursor slowly over a widget and look at the help text at the bottom of the window. Many widgets in complex windows, such as this, are not labelled to save space. Use this help to remind you of what each widget does.*

## Spline Tool Shape Selection and the Image Regions Window

A spline tool is available in the *Associations* window to select arbitrary areas in two-element space. These selections can be used to highlight all pixels in the element images that represent this area in two-element composition space. Click and drag out a circle, using the left mouse button. This sets the initial shape. Click and drag each control point to form the desired shape. Move the spline using the centre handle. The concentration coordinates of the centre are shown in the help area at the bottom while you move the spline curve around.

*You can clear the spline curve to start again by either a ‘right click’ on the mouse in the window or using the “Display→Clear Spline” menu.*

To highlight all pixels in the source images that have concentration values that fall within the spline curve, use the “Analyze→Within Spline” menu in the *Associations* window. All relevant pixels in the spatial images will be highlighted in green.

To remove pixels from the current Associations highlighted area, back in the *Image* window use the exclude “-“ mode of region select shape. Select exclude, drag out a shape and use the “ $\Sigma$ ” button to remove pixels within this region from the current *Associations* selection. Note for this to work, no include region should be set. To make sure, use the main GeoPIXE *Image* window menu “Display→Clear ALL Shapes” and then select the exclude region.

*Tip: To temporarily hide the green pixel highlighting, click within the Image Display window, away from all region handles, using the right mouse button. The green highlighted area will hide while the right mouse button is held down.*

These pixel selections, plus the average concentrations within these highlighted pixels, are saved in the *Image Regions* table. To view these open the *Image Region* window. The “image” column will now show the two elements viewed in the *Associations* window. If you click on a row in the *Image Regions* window, then the association spline will be displayed in the *Associations* window as well as the matching pixel highlights in the *Image Display* windows.

As with normal image region selections, the spectra from any ADCs within these selected areas (all pixels highlighted green) can be extracted. First save the regions using the “Save” button on the *Image Regions* window and make sure a *Spectrum Display* window is open. Now select the desired ADC to sort out spectra from (or “array” to combine all detectors of an array), using the drop-list beside the “EVT” button on the *Image Regions* window. Now click on “EVT” to select the list-mode file(s) and the output spectra file. The sort will start and on completion the spectra will appear in the *Spectrum Display* window.

*Apart from the file extension, the region and spectra files should have the same name for PIXE and SXRF data, for later auto loading of spectra (this is the default anyway). Hence, for PIXE/SXRF data, if you use the default name for the spectrum file, then the spectra are located and loaded automatically when the corresponding regions file is ever loaded later. This is recommended. However, for this to work, you must save the regions to a file first.*

*For non-PIXE/SXRF data, it is best to give the extracted spectra file an extra label in the file name that distinguishes it from normal PIXE/SXRF data (e.g. “Fred-RBS-q1.spec”).*

## Associations within a Sub-region

If a normal image shape region is used to select a spatial area within an image, in an *Image Display* window, then the element associations shown in the *Associations* window only show data from within this spatial sub-area of the image. For example, this can be used to learn about specific phases in a region of an image, exclude a dominant phase, or to separate subtle intergrowth compositions. Form a normal region in one of the *Image Display* windows. Click on “ $\Sigma$ ” button. This will add this entry to the *Image Regions* table, and also tells the *Associations* window(s) to only consider associations between elements within this region’s pixels.

Alternatively, if you already have regions saved in REGION files. These can be loaded into *Image Regions* window. Click on a row to display the associations. If it is a normal shape region, then you see the associations between elements for just these selected spatial image pixels. If it is an association spline region (shown with two element names in the “Image” column), then these elements are displayed on the axes of the *Association* window(s) and the association scatter plot will cover ALL spatial image pixels. The spatial image pixels corresponding to compositions within the spline curve will be highlighted on all *Image Display* windows.

## Operations on Pixels selected by Association

Several operations on images that make use of a region selection will use regions highlighted using the Association method, if no shape region is selected. Use this to select the pixels to operate on for “Correct→Current” operations and “Suppress” and “Kill region”. You may need to use the menu “Display→Clear All shapes” to make sure the highlighted pixels are used instead of a simple shape.

The selected pixels can be edited using the Exclude “-“ region mode. Select a shape (e.g. Circle) and then select the exclude mode. Each time you position the circle and click in “Σ”, any highlighted pixels in the circle will be removed from the highlight selection.

## Associations Widgets

This list summarises the functions of all widgets on the *Associations* window, including buttons, sliders, drop-lists and text entry widgets. These are listed from left to right, top to bottom.

### *First row below image:*

- X Scroll Bar

Control to scroll image in X, similar one for Y on the right side of the image.

### *Second row:*

- Y Element Drop-list
- Y Smooth Slider
- “0” Button
- “+” Button
- “-“ Button
- X Smooth Slider
- X Element Drop-list

Select element to display on Y axis.

Controls a pre-smooth to Y element image data before association plotting.

Sets zoom back to original size.

Zoom in by 2.

Zoom out by 2.

Controls a pre-smooth to X element image data before association plotting.

Select element to display on Y axis.

### *Third row:*

- Y Log Checkmark
- Y Minimum Slider
- Y Maximum Slider
- X Minimum Slider
- X Maximum Slider
- X Log Checkmark

Enables log Y axis.

Sets the lowest concentration visible, relative to max.

Sets the highest concentration visible, relative to max.

Sets the lowest concentration visible, relative to max.

Sets the highest concentration visible, relative to max.

Enables log X axis.

### *Fourth row:*

- Low Z Slider
- Z scale drop-list
- Green highlight
- High Z Slider

Sets the lowest Z histogram score displayed in the colour map.

Select a Linear, Log or Sqrt Z histogram scale.

Enable showing currently selected points in green (used with PCA/Clusters)

Sets the highest Z histogram score displayed as a colour.

### *Bottom row:*

- Help Text

Context-sensitive help area, shows help prompts for widgets as the mouse pointer moves over them.

## RGB Three Element Images

### Image RGB Window

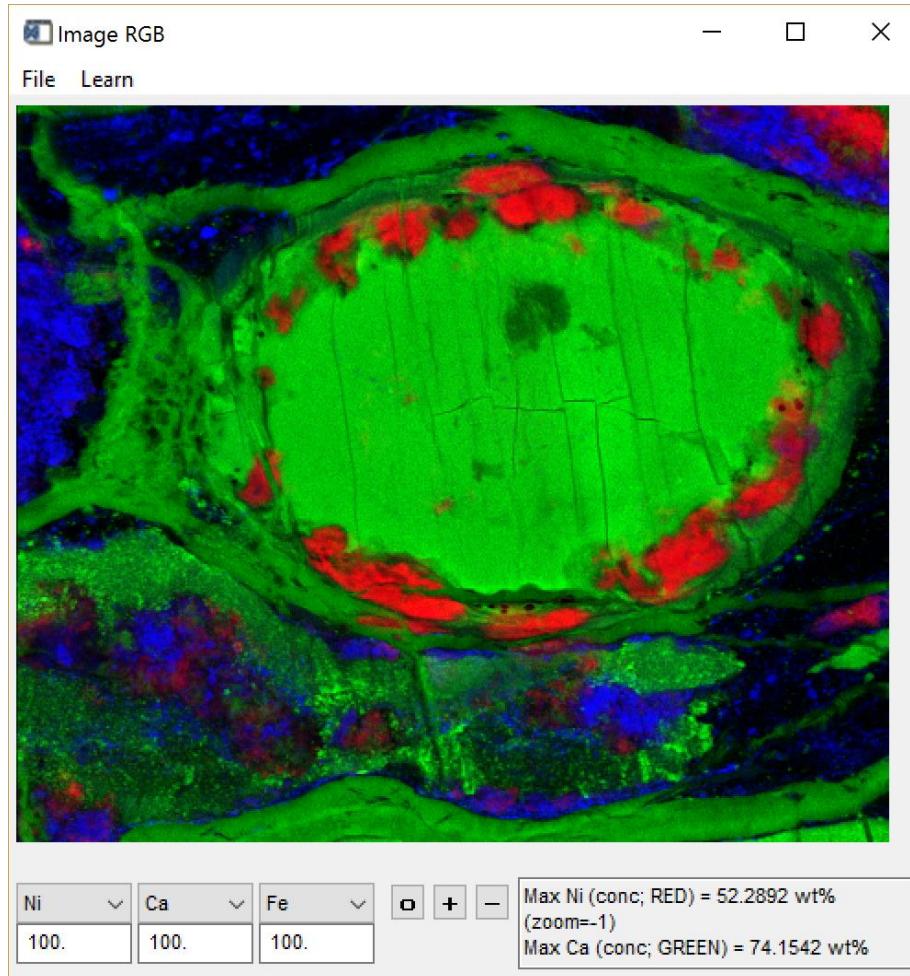
True colour images (24/32-bit) can be generated that use three elements as the Red, Green and Blue axes, using the *Image RGB* window (“Windows→3 Element RGB Images” menu on *Image Display*). It has drop-lists to select the three elements for red, green and blue. All other controls come from the linked *Image Display* Windows.

Control the minimum and maximum display values using the sliders in the *Image Display* windows and clones, or select display scale type (Linear, Sqrt, Log); any changes will be dynamically displayed on the RBS display. The maximum display % is also provided as a text widget below the RGB element drop-lists to manually set the display

maximum. Control of display zoom follows the same scheme as the main Image window, using the “0”, “+” and “-“ buttons.

The result can be exported as 24-bit PNG or JPEG files, using the current zoom level. *Note that the lossless PNG files are about 10x larger than the JPEG. For JPEG, GeoPIXE uses maximum quality, and so these are generally very good.*

A “Learn” menu allows selections of elements for RGB to be learnt, as a list, and saved to a file to be later restored and executed to provide a standard set of RGB images saved for a particular project. These are always saved at original (full) size (zoom=0).



## Image RGB Widgets

This list summarises the functions of all widgets on the *Image RGB* window, including buttons, sliders, drop-lists and text entry widgets. These are listed from left to right, top to bottom.

### *First row below image:*

- X Scroll Bar Control to scroll image in X, similar one for Y on the right side of the image.

### *Second row:*

- |                       |                                     |
|-----------------------|-------------------------------------|
| • R Element Drop-list | Select element to display in Red.   |
| • G Element Drop-list | Select element to display in Green. |
| • B Element Drop-list | Select element to display in Blue.  |
| • “0” Button          | Sets zoom back to full resolution.  |
| • “+” Button          | Zoom in by 2.                       |
| • “-“ Button          | Zoom out by 2.                      |

***Third row:***

- R display max Set the display maximum as a %
- G display max Set the display maximum as a %
- B display max Set the display maximum as a %

***Bottom row:***

- Help Text Context-sensitive help area, shows help prompts for widgets as the mouse pointer moves over them. By default it shows the maximum concentration displayed for each element.

**Image RGB Menus*****Files***

Mostly, image data is made available to *Image RGB* via a notification from the main *GeoPIXE Image* windows when new data are loaded. However, the “Compare Images” menu offers a way to load another data-set (e.g. to compare PIGE with PIXE images); the new elements are added to the *Image RGB* element drop-lists. Select any of the original elements (as in the associated *Image* window) or the new “Compare” elements in the drop-lists.

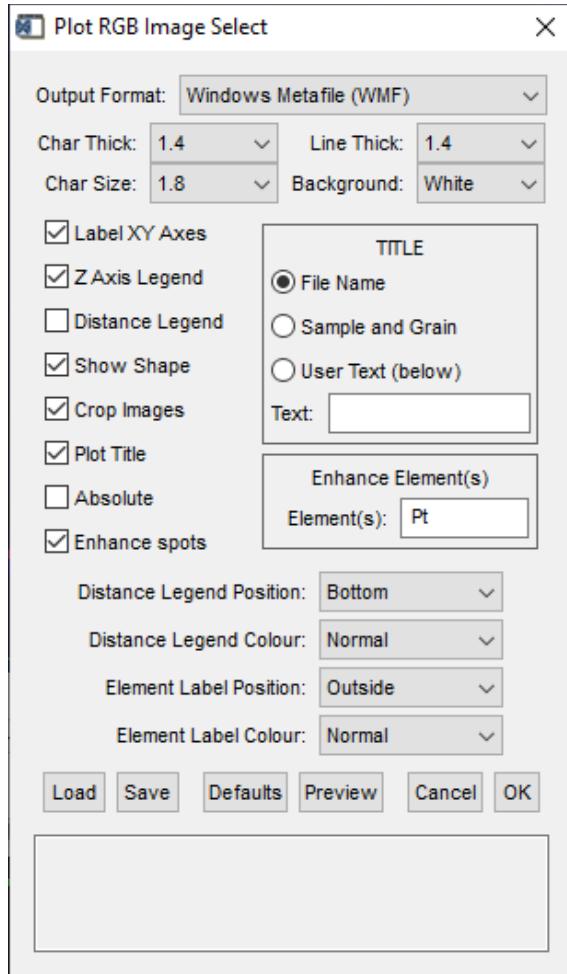
- Compare images Load image .DAI file to compare (assumed for same scan area).
- Export → Simple Image Export as a JPEG or PNG image file.
- Export → Image Plot Export selected images on a plot with axes and legends in image (JPEG, PNG) or vector formats (Computer Graphics Metafile (CGM) or Windows Metafile (WMF) format). Opens the *Plot RGB Image Select* pop-up panel to select various options for creating an output file.
- Print Opens the *Plot RGB Image Select* pop-up panel to select various options for plotting to the default printer.

***Learn***

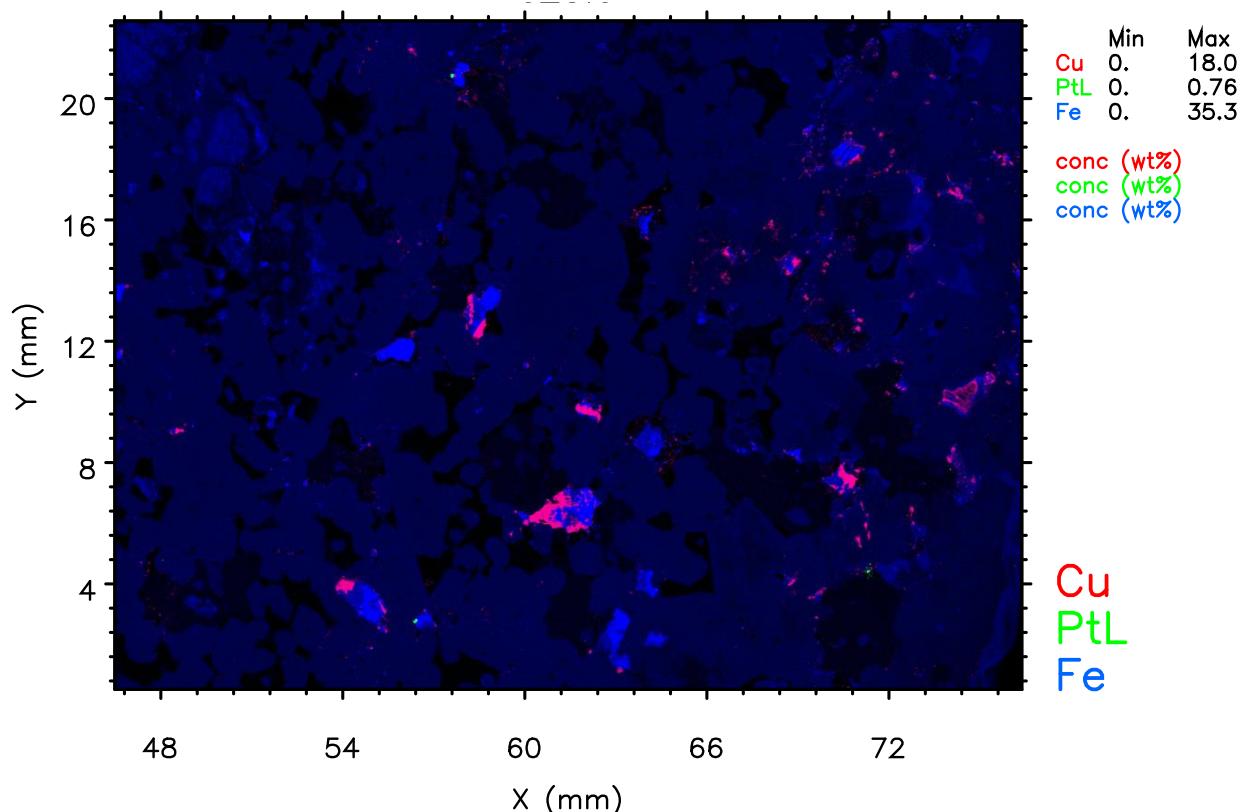
The Learn menu allows RGB element selections to be added to a list to be executed later. Hence, use “First” to start a new list, “Next” to add the current RGB element selection to the list, “Save” and “Restore” to save/restore the list to a file and “Execute” to execute it, which is always at ‘full’ zoom. This output list can also be triggered from the *Batch Sort* window.

**Image RGB Export**

The export panel is used to produce figures in CGM, WMF, EPS formats or in very large format, high resolution JPEG image files or to output to your default printer device. It provides options to set background colour, character size and line widths and options for the placement of distance and Z axis (e.g. concentration) legends. Further options can be used to crop the image to the current shape in the Image window, show the axes in “absolute” coordinates, which are the stage coordinates used for the scan and to enhance hot-spots in a selected image plane. The latter uses a Dilation operator to prevent small hot-spots from disappearing on output. Hover the mouse pointer over each option and widget to get more help on each.



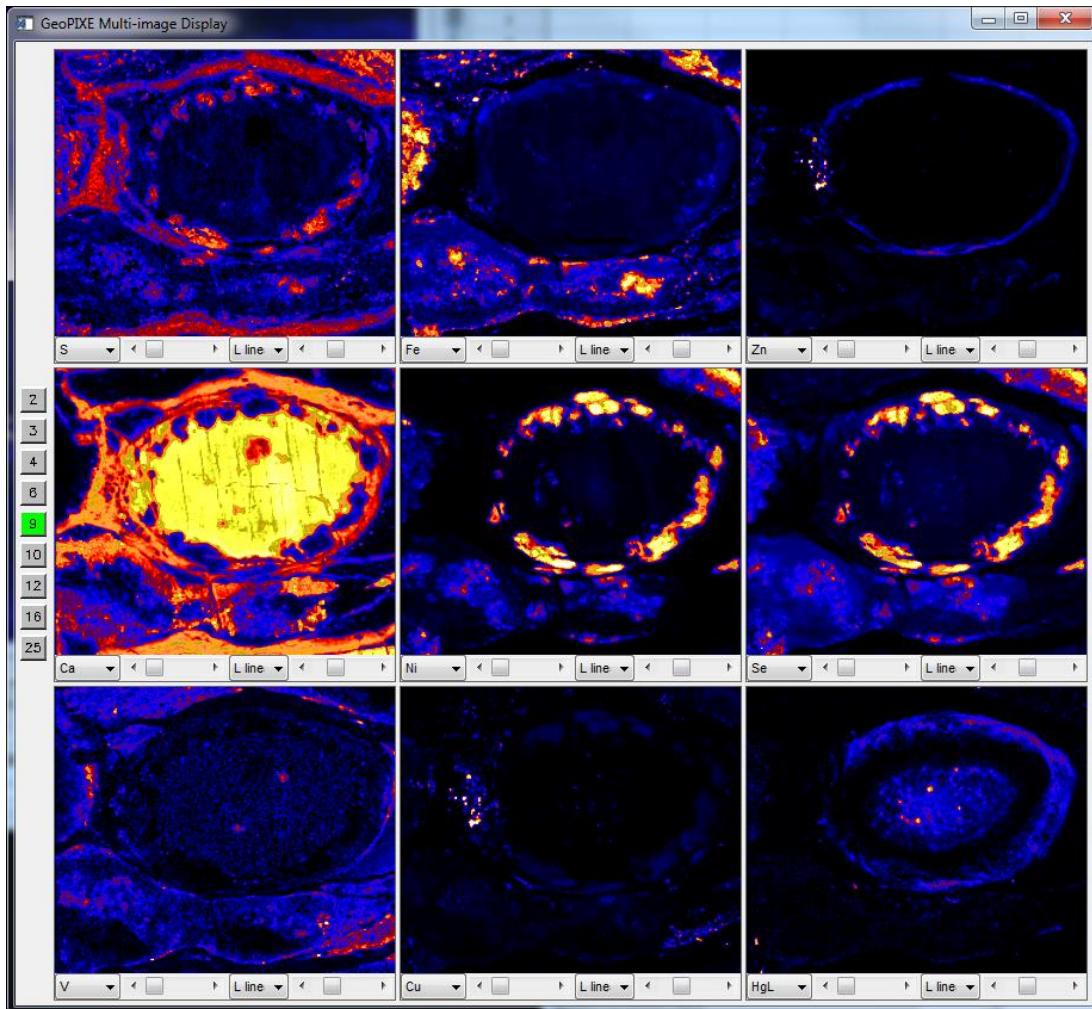
*Export RGB image options to plot a selected (crop) sub-area and enhance the Pt hot-spots output*



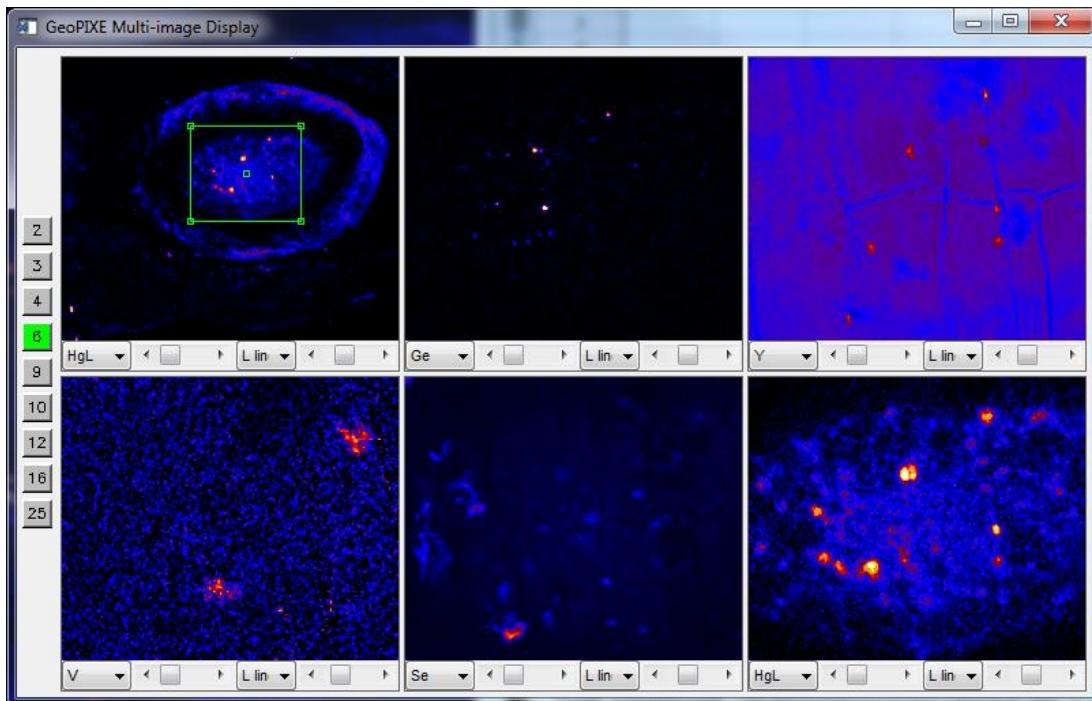
## Multi Image Display Window

### Multi Image Window

A tiled group of small image windows can be displayed in a *Multi Image Display* window (“Display→Multi Image” menu on *Image Display*). It has buttons to select the number of tiled images to display (2-25). Resize the window to change the shape and arrangement of window, and the element drop-lists on each to select elements to display. Each window has controls for display min/max (%) and Z scale type, that are all linked to these controls on the attached *Image Display* window.



The top-left image has a special function: Click and drag out a rectangular region on this image and this area is magnified and displayed in the other windows. Right-click in this window to cancel this magnify function.



## Multi Image Widgets

This list summarises the functions of all widgets on the *Multi Image* window, including buttons, sliders, drop-lists and text entry widgets. These are listed from left to right, top to bottom.

### *Left of main window:*

- Tiled number Select the number of images to display tiled.

### *First row, below each image:*

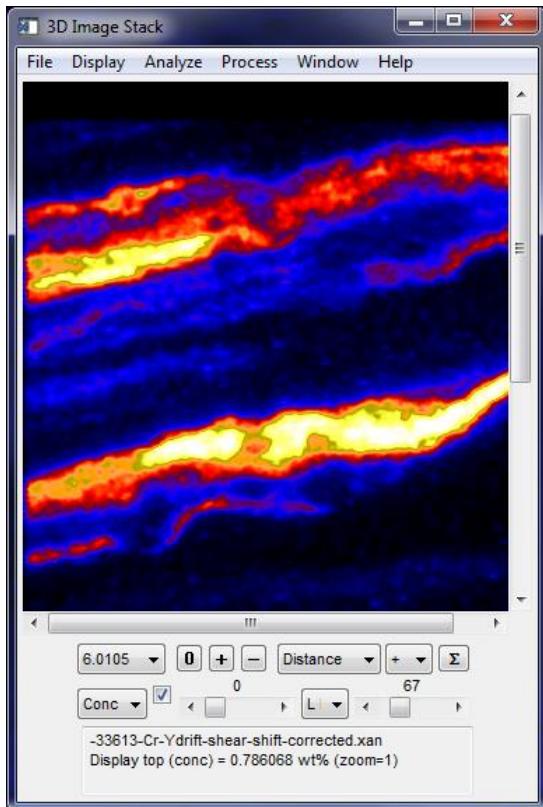
- Element Drop-list Select element to display in this window tile.
- Low Limit Slider Sets the lowest concentration visible, as a percentage of the maximum.
- Z axis display scale Select the Z axis (colour axis) display scale between L (linear), G (log) and S (sqrt).
- High Limit Slider Sets the highest concentration visible, as a percentage of the maximum.

## 3D Image Stack Display Window

### 3D Image Stack Window

Various 3D image stack data-sets can be displayed (and assembled) using the *3D Image Stack* window (open it from the *Image Display* window *Display* menu). It operates much like the *Image Display* window, but instead of having an element list, it has a drop-list for the Z axis, which is energy for XANES and tomo angle for tomography. Image stack files (extension .xan) are constructed and loaded in two ways, depending on the data organization:

- 1) **2D stacks:** Stacks of normal 2D images can be imported into the *3D Image Stack* window using the *File*→*Import* menus. It accommodates image stack planes organized as .dai files in a single directory, or spread over a series of directories, with one frame per directory.
- 2) **3D data:** Full 3D raw data can be processed using the Sort EVT window directly into a .xan output file, and displayed in an attached 3D Image Stack window.



### 3D Image Stack Menus

These largely parallel the Image Display window, with the following differences.

*File Menu:*

- Import→ XANES ...      Import 2D image stacks from .dai files within one directory or in one directory for each .dai file.
- Export→XANES Energies    Export the energies of each stack frame to an energies file.

### 3D Image Stack Widgets

These are similar to the Image Display window, with the following differences.

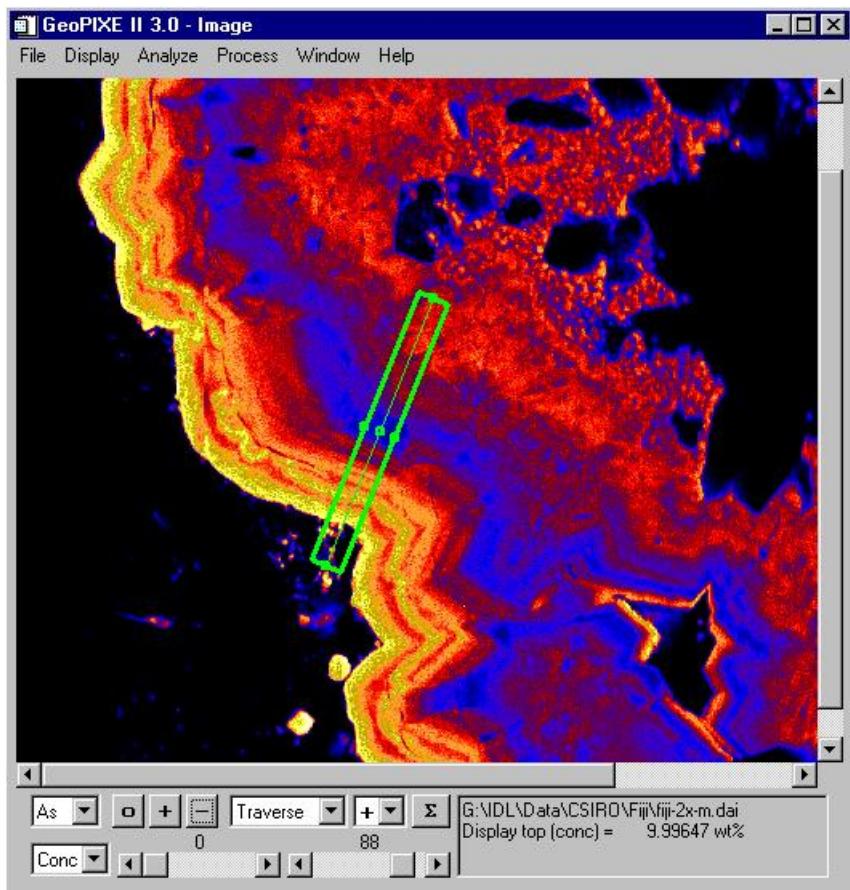
*Second row:*

- Energy Drop-list      Select energy stack plane to display. Use the arrow keys on the keyboard to scroll through planes.

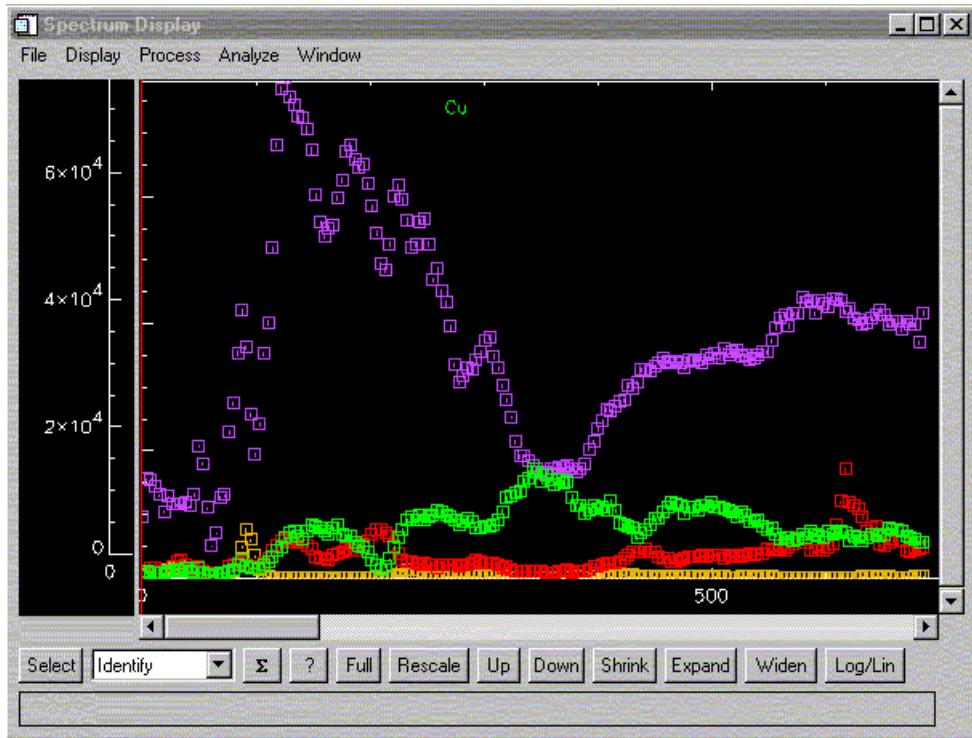
### Linear Traverses and Line Projections

Using the "Traverse" region in the *Image Display* window, a traverse or line projection can be defined across an interesting area of zonation. Then spectra representing the concentration variation of all elements projected along this traverse line can be extracted. For curved traverse paths, use the "Curve 8" region tool. To constrain the projection to just the X or Y axis, use the "ProjectX" or "ProjectY" tools, respectively.

Select the "Traverse" region type from the drop-list. Click (left mouse button) on the starting position and drag out the traverse region to the end position. Handles on the ends of the traverse line can be used to move these end-points (using the left mouse button). Now use the handles on the sides of the traverse region to tailor the width of the rectangular integration area (using the left mouse button). All points in the rectangle will be projected onto the traverse axis in a direction parallel to the ends of the box. To change the shear on the box, to change from normal projection perpendicular to the traverse line, select and drag these side handles using the right mouse button.



When the " $\Sigma$ " button is pressed, two things happen. Firstly, as discussed above, the line details and representative concentrations within the rectangle are appended to the *Image Regions* table. These definitions can be saved for later to record the position of your traverses. Secondly, if a *Spectrum Display* window is opened, spectra corresponding to the concentration profile along the projection line are sent to *Spectrum Display*. These show concentration as a function of distance (microns if the image sizes were defined in *Sort EVT*) for all elements, with error bars determined using the variance images.

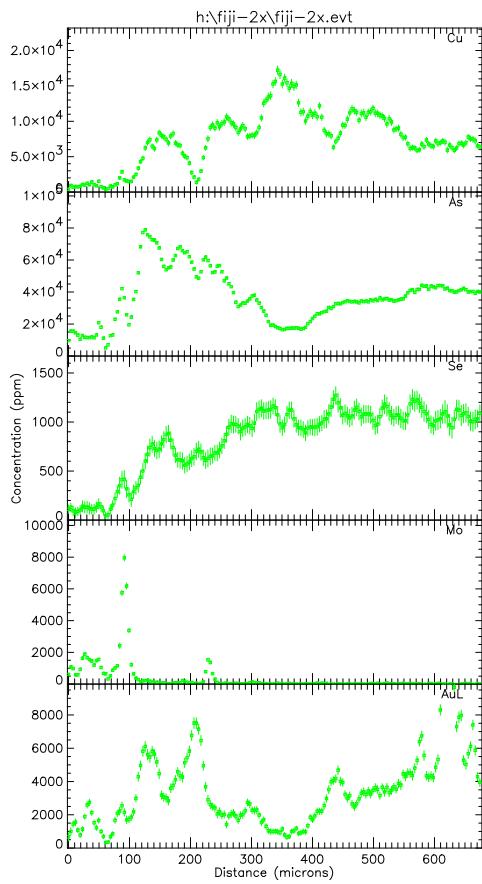


The estimated minimum detection limit in each distance step bin (99% confidence) is plotted as a dashed curve overlaid on the data points for each element.

To step through these profiles, one at a time, use the *Spectrum Select* window. First, hit "Prev". This will display the profile for just the first element, or "Back". Then hit "Next" to advance to the next profile.

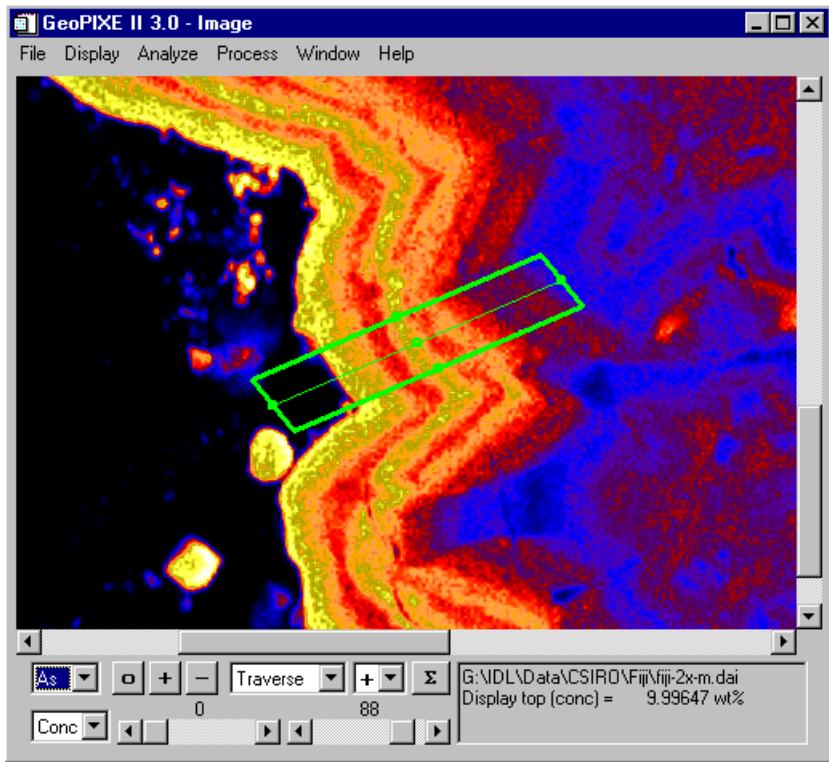
Alternatively, you can select "Highlight" mode, using the left drop-list at the bottom of the *Spectrum Select* window. This highlights, or draws in green, the spectrum selected in *Spectrum Select*. To select a spectrum, simply click on that row label.

*Spectrum Select* can also be used to hide or show a selection of elemental profiles, by selecting rows (or ranges of rows) and toggling their visibility using the "Display" button. A composite plot of all these profiles can be exported in Computer Graphics Metafile format (CGM) using the "Export→CGM Plot" menu in *Spectrum Display*. These CGM pictures can be inserted into PowerPoint to create figures and add annotations. Similar export options in Windows Metafile Format (WMF) and encapsulated PostScript (EPS) are also available. There are also Print menu options. Use the Preview button on the pop-up panel to preview the plot on the screen.

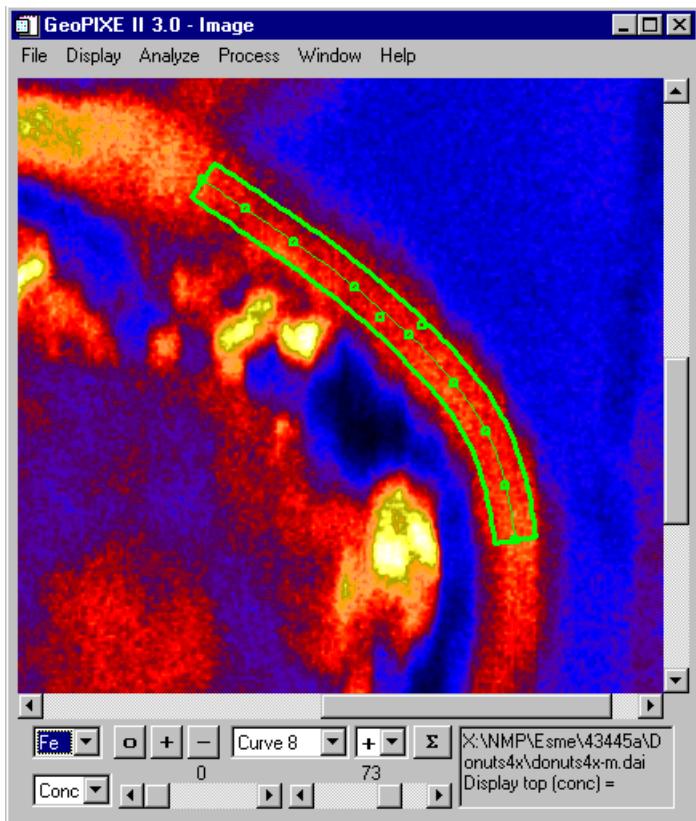


### Tailoring Traverse Projection in More Detail

Using the “Traverse” shape tool you can adjust the angle on the projection back to the centre line by adjusting the shear on the traverse shape. To do this click on the side handles that normally adjust width, but now using the right mouse button. This allows you to shear the traverse shape. Use this to adjust the projection direction for non-perpendicular projection.



For non-linear traverses, use the “Curve 8” shape tool. This initially provides a linear traverse, but with extra spline control points. Use these to adjust the shape of the curve (click and move them with the left mouse button). The side handles control the width. To move the whole spline curve *en masse*, click on the central spline control point using the right mouse button. Take care not to make the curve area too wide, or extremely curved. This will induce ambiguities in the projection function, back to the centre line. This ambiguity will be evident as cusps in the sides of the projection area. If these are seen, reduce the width or the curvature of the area.



## Correction of Images for Sample Composition Effect on Yields

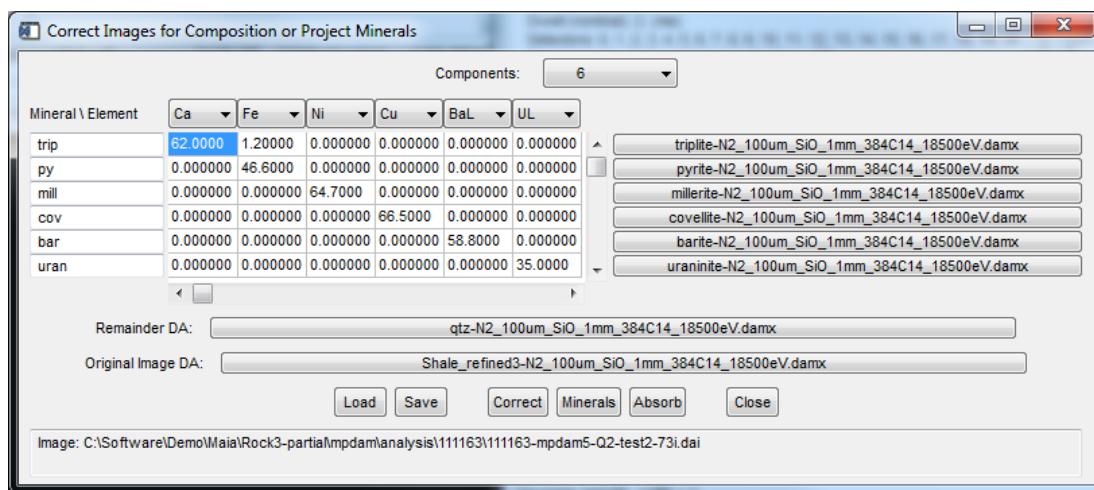
Sample composition varies generally across an image area. This means that the yield model assumed in projecting the images using the DA method will only be an approximation to any given pixel. This section describes a method to correct model yields on a pixel-by-pixel basis based on an end-member analysis of the image using a set of end-members that adequately describe the range of variation in composition (at least for the heavy elements that strongly affect self-absorption and secondary fluorescence) (see C.G. Ryan, "Quantitative Trace Element Imaging using PIXE and the Nuclear Microprobe", International Journal of Imaging Systems and Technology [Special issue on Quantitative Imaging] 11 (2000) 219-230 and C.G. Ryan, E. van Achterbergh, C.J. Yeats, Tin Tin Win and G. Cripps, "Quantitative PIXE trace element imaging of minerals using the new CSIRO-GEMOC Nuclear Microprobe", Nucl. Instr. Meth. B189 (2002) 400-407).

Firstly, identify the important chemical phases in an image area that can be distinguished on the basis of measured PIXE/SXRF elemental concentration. You will also need to have an idea of the background (or *remainder*) composition, where these phases are not present. Create separate yield files for these phases using *PIXE/SXRF Yield Calculation* (access this via the "New" button adjacent to "Yields:" in the *X-ray Spectrum Fit* window). Now return to *X-ray Spectrum Fit* and the spectrum fitted to make the DA matrix file. Now, using each of these yield calculations in turn (i.e. "Load" it into "Yields:"), refit the spectrum and generate a new DA matrix for each; name each separately.

*NOTE: There is now a better (but a little more involved) method for the correction of images that also improves reconstructed spectra overlays on extracted region spectra (see "Multiphase DA imaging (MPDA)").*

### Correct Yields Window

Now return to the *Image Display* window and open the *Correct Yields* window ("Windows→Correct Yields" menu). → Select the number of components (phases) to use and the elements to use to define these phases (in the drop-lists at the top of the table). (For the moment, the number of elements must equal the number of phases.) Select these elements as column headings and fill in the phase names as row headings. Now in the table, enter the concentrations (in wt%) of each element in these phases (each row corresponds to a phase). (These don't need to add up to 100% as there are usually missing elements, such as oxygen.) The matrix created in this way must define independent phases. i.e. No row can be a linear combination of other rows. If the program warns you of an ill-conditioned matrix, or a zero determinant, then this matrix contains non-independent phases.



To enter values into a table, click in a cell (or move around using the arrow keys) and then hit the <return> key. This activates a selected cell for editing. Once you're happy with the cell's contents, hit <return> again to keep the changes. Now move to the next cell using the arrow keys and continue.

Now, on the far right side of each row, click to bring up a file requester to load the DA matrix files created above in *X-ray Spectrum Fit*, one for each phase. Load the correct one for each row. Now load the DAM file corresponding to the "Remainder" unaccounted for by the other phases, using the "Remainder DA" button. Also, load the DA matrix used

to make the initial images using the "Original Image DA" button at the bottom of the window.

All is now ready. Hit "Correct" to start the process. Watch out for errors regarding the nature of your matrix. When this process finishes, you have corrected all elemental images based on the proportions of the end-member phases in each pixel. This process may need ~2-3 iterations to converge. Simply click on "Correct" again to do another iteration. Save the images after correction (using the "File→Save" menu in the *Image Display* window).

The "Save" button on the *Correct Yields* window will save your correction details to a file (.CORRECT). Use "Load" to load correction details.

## ***Projection of Elemental Images onto End-member Proportion Images***

Using the same control panel as *Correct Yields* above (or use the "Windows→Project Minerals" menu on *Image Display*), you can project elemental concentration images onto images of end-member proportion, by hitting the "Minerals" button in the *Correct Yields* window. This produces a reduced set of images in the *Image Display* window, one for each end-member phase, and one for the *remainder* between phases. (The current elemental images are lost; save these first.)

## ***Correction of Images for the Effects of Differential Absorption***

This is a new method for correction of artefacts caused by absorption of X-rays through neighbouring pixels, of different composition, on their way to the detector. Set-up as for yield correction, but now click on "Absorb". It will now correct for absorption, assuming a detector of 45° take-off angle, located to the right in images. These parameters are fixed at the moment; more control will be added later. As with other corrections, two or more iterations can be performed. However, most correction happens in the first iteration and the process converges quickly.

*NOTE: This does not as yet use the relevant detector model or array, only a 45° assumed take-off angle.*

## ***Correction of Images for Pulse Pile-up Effects***

The nature of pile-up in a given pixel is related to the most intense lines in that pixel. In other words, the energies and relative intensities of all pile-up lines, in the 'pile-up element', will vary from pixel to pixel in general. GeoPIXE can model the nature of pile-up on a pixel-by-pixel basis to build a more accurate pile-up contribution to the spectrum. This can be used for more accurate fitting of a PIXE spectrum extracted from the entire image area that spans different phases, or ultimately for correcting images for pile-up related artefacts.

The process, which is detailed in an example in the analysis scenarios chapter, follows these steps:

- 1) Generate elemental images by the normal method, using a *X-ray Spectrum Fit* with the "using Spectra" pile-up option.

Load the total PIXE spectrum for the entire image area again in *Spectrum Display* and execute the "Display→Pileup→using Image products" menu. Select the major elements to consider in the pop-up list. (Remember that the calculation may be slow with a large number of elements selected. However, in some cases relatively minor elements may be significant if they occur spatially in close association with strong major elements or concentrated in small phases.) This builds a new pileup overlay to the spectrum using products of images. You may like to save the spectrum to preserve this pile-up model for later use.

Fit the spectrum in *X-ray Spectrum Fit*, using the "Image pixel product pileup" pile-up option. This option requires that you have already modelled the pile-up, as above. Fitting the spectrum now uses this pile-up overlay. Save this fitted spectrum for later reference. The fit, and this file, now contain some data giving the intensity of pile-up in this spectrum, which is related to timing resolution and count-rates.

Click on "Generate DA Matrix" to build a new DA matrix file. Save it with a name that tells you that this matrix is for use in pile-up correction (e.g. append "-pu" to the name). This DA matrix will not have a matrix row for pile-up. Any images generated using this matrix will include all pile-up related artefacts. These will need to be removed

using the steps below.

Open *Sort EVT* and sort the event data again using this new DA matrix file. You may notice some elements that overlap with pile-up lines may now show artefacts due to pile-up.

In *Image Display*, use the “Process→Correct→Image Pile-up” menu to now subtract pile-up. This step requires that the fitted spectrum from step 3 be loaded into *Spectrum Display*. This step calculates pile-up on a pixel-by-pixel basis, using the intensity deduced from the spectrum fit (and stored with the spectrum data), to subtract pile-up contributions from all images. i.e. This spectrum fit effectively constrains the product of count-rate times pulse-pair resolution of the system, which sets the rate of pileup.

To go on and produce pile-up corrected images of image areas elsewhere on this sample and similar ones, you only need to repeat these steps:

- 1) Open *Sort EVT* and sort the new image area event data using the new “-pu” DA matrix file from above.

Load the total PIXE spectrum for the new image area in *Spectrum Display* and execute the “Display→Pileup→using Image products” menu. Select the major elements to consider in the pop-up list.

Fit the spectrum in *X-ray Spectrum Fit*, using the “Image pixel product pileup” pile-up option.

In *Image Display*, use the “Process→Correct→Image Pile-up” menu to now subtract pile-up. This step calculates pile-up on a pixel-by-pixel basis, using the intensity deduced from the spectrum fit, to subtract pile-up contributions from all images.

See the analysis scenarios chapter for more examples.

## **Sorting List-Mode Data using Spectrum Cuts**

Using the *Sort EVT* window is covered above under "Sorting List-Mode Data using the Dynamic Analysis Matrix". Just a few things change to use spectrum energy Cuts. In the parameter area at the bottom, you now select "Spectrum Cuts" as the projection method. Now enter the name of a suitable Cuts file (.CUTS) in the field below (or hit the "File" button to bring up a file requestor).

Cuts specify energy windows to use to produce images, with optional background subtraction. Each is labelled with a name, and these are set-up interactively in the *Spectrum Display* window, and using the *Cuts Setup* window, as discussed below.

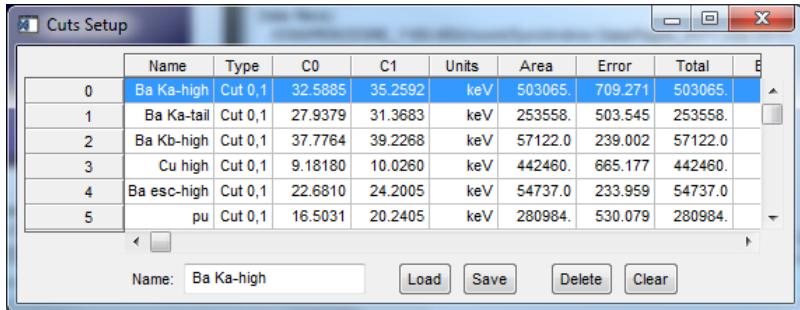
Now just start the sort as before ("Start" button). The resulting images are sent to *Image Display*. They are now in simple counts units, with simple Poisson variance. Extracted averages in *Image Regions* (using the "Σ" button) are not in ppm units now, but simply counts.

If the set of cuts includes multiple cuts for a particular element (e.g. multiple γ-ray lines in a PIGE spectrum), you can merge these into a single image for each element, after the sort has finished, using the menu “Process→Merge PIGE” in the *Image Display* window. This will combine any images with a common first part of the name (before a space character) (e.g. combine “F 1”, “F 2” and “F 3” into a single “F” image). Note that this test is case-sensitive.

## **Setting-up Spectrum Cuts Files**

### **Cuts Setup Window**

Start with a suitable spectrum in *Spectrum Display* and open the *Cuts Setup* window using the "Window→Cuts Setup" menu. This will also switch the marker mode in *Spectrum Display* to "Cut 0,1". You can also use the drop-list to do this (bottom left in *Spectrum Display*). To set a cut on the spectrum, left click at the position of the HIGH energy end of the cut, and then click at the LOW energy end. If there is already a cut on the spectrum, then click and drag the markers with the pointer. Press the "Σ" button in *Spectrum Display* (not the one in *Image Display*) to make the cut. The parameters for this cut are appended to the list in *Cut Setup*. Edit the name for this cut in the text field at the bottom of the *Cuts Setup* window and hit “enter”. Note that the energy window (C0, C1) appears in the table, using the current energy units for the spectrum.



This defines a simple (Cut 0,1) type cut. This is just an energy window, with no background subtraction. To use background subtraction, you need to use 6 markers, called X0-X5. These can be selected using the drop-list (bottom left) in *Spectrum Display*. Now you need to click on the marker positions (starting at the HIGH energy end) for X5, X4, which define the high energy background energy window, X3, X2, which defines the peak energy window, and X1, X0, which defines the low energy background energy window. Now there are more columns in *Cut Setup* to show the extra marker energies. The background regions of interest will define a linear background under the ROI used for the peak.

The *Cut Setup* window also shows "total", the integral of the spectrum between the C0, C1 markers (or X2, X3 in background subtraction mode), "Area", this integral after background subtraction, "Error", the statistical error in Area, "Back", the background under the peak (using linear interpolation between the left and right background windows), the sums in the "Left" (X0-X1) and "Right" (X4-X5) windows, and the spectrum energy calibration coefficients. These results can be saved to a file (.CUTS) using the "Save" button or restored using "Load". Load will append loaded cuts to the current list. Use "Clear" to clear the table, or "Delete" to delete selected rows (rows are selected by drag selection).

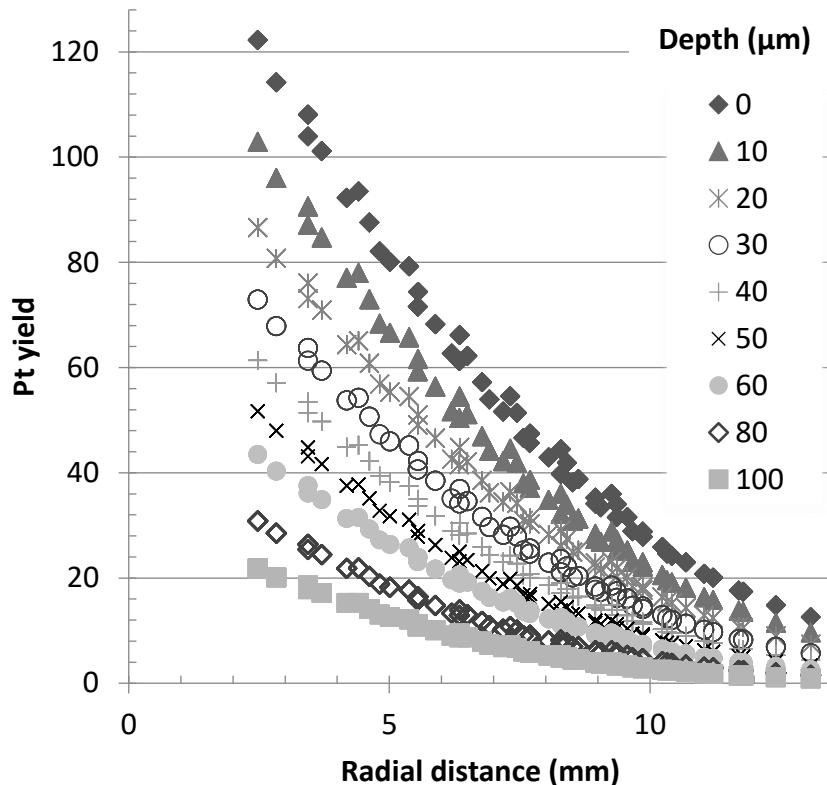
## **Wizard Plugins**

Wizards are another form of plugin that can orchestrate GeoPIXE operations. A formal interface is under development. Presently, it is being used to develop custom interfaces for specific laboratory specific analysis work-flows. See the doc "Wizard Hooks in GeoPIXE" in the Help directory.

## **Depth Wizard**

The large size of the detector array, located just 10 mm from the beam spot on the sample, provides a large range of take-off angles at the sample surface, with the angle between sample normal and rays to masked detector element centre varying between 13.9° and 52.6°. This makes the outer detector elements much more sensitive to self-absorption for X-rays from a particle at depth in a sample than the inner detectors. Such a difference can be harnessed to provide an imaging contrast based on particle depth and also a quantitative measure of depth for discrete identified particles.

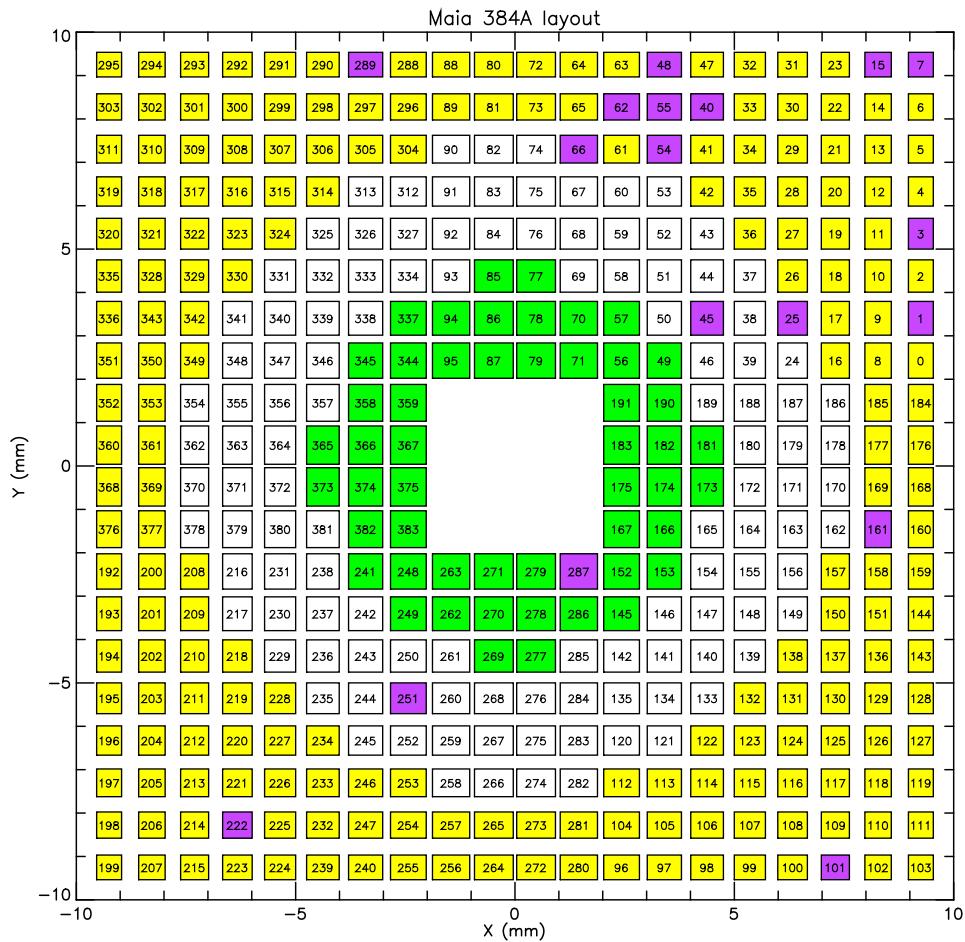
The variation in model yields across the array is illustrated below, which shows the yield (counts/ppm/μC) of Pt L $\alpha$  X-rays from a buried particle for individual detector elements plotted as a function of the radial distance of each detector from the centre of the array (beam axis). Each symbol type represents the yield from a 1 μm layer of Pt at various depths within an olivine sample matrix. Subtle absorption-related effects of particle shape versus a simple layer have been ignored in this discussion. The interesting apparent scatter in these points reflects the non-equivalent positions and orientations of detectors around the square array. Masking, distance and angle gradually reduces the efficiency of the more peripheral detector elements. Depth to the Pt layer has a marked effect on yields, with stronger attenuation seen in the more peripheral detectors.



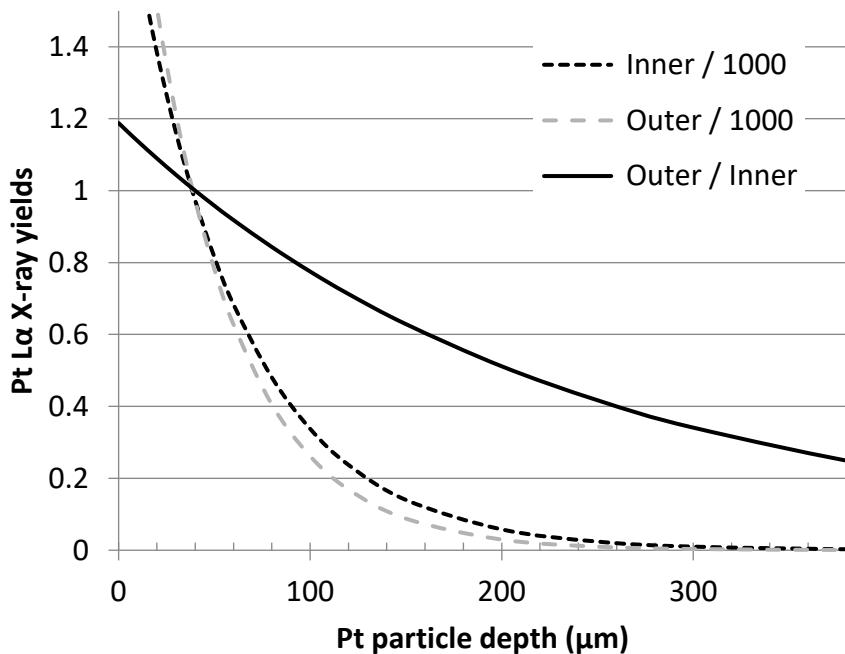
*Yield (counts/ppm/ $\mu\text{C}$ ) of Pt La X-rays from a small Pt particle (modelled as a 1  $\mu\text{m}$  buried Pt layer in olivine) versus radial position of individual Maia detector elements for various depths ( $\mu\text{m}$ ) to the particle.*

If the two-layer sample model is correct, i.e. has the correct depth to the PGM, then both inner and outer detectors will “measure” the same effective concentration of Pt in the buried or “unknown” layer. Hence, since conc = area/yield, then  $(\text{area}/\text{yield})_{\text{inner}} = (\text{area}/\text{yield})_{\text{outer}}$ . Or, we can relate  $(\text{area}_{\text{inner}}/\text{area}_{\text{outer}}) = (\text{yield}_{\text{inner}}/\text{yield}_{\text{outer}})$ . Therefore, we can relate the Ratio =  $(\text{yield}_{\text{inner}}/\text{yield}_{\text{outer}})$  to the measured ratio  $(\text{area}_{\text{inner}}/\text{area}_{\text{outer}})$ . They should be equal at the correct depth.

Combining yields for 51 “inner” and 199 “outer” detectors as shown in the Layout below, chosen to give a roughly total yield for a surface feature, produces the inner/outer yield ratio curves below. The ratio of “outer”/“inner” yields produces a good contrast with the depth of the particle. This can be applied to estimate the depth of a small particle feature, given the assumption that the host mineral composition is uniform above it.



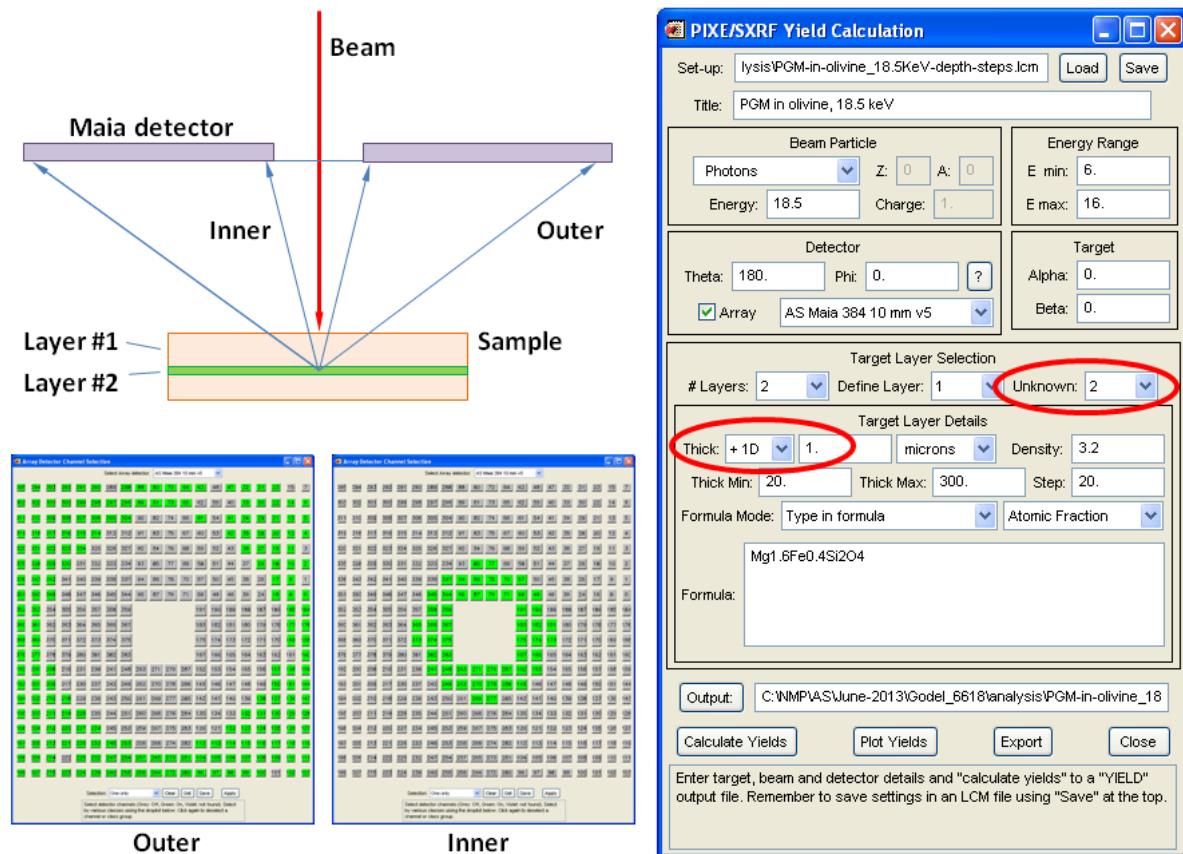
Layout of Maia detector array (old model A) showing detector index and the masked effective size of detectors. Shaded detectors for 51 "inner" (green), 199 "outer" (yellow) and 18 disabled (violet) detector elements.



Yields of Pt La X-rays (counts/ppm/ $\mu\text{C}$ ) summed over "inner" and "outer" rings of detectors scaled by 0.001, as a function of Pt particle depth ( $\mu\text{m}$ ) in olivine, and the ratio of "outer" to "inner" yields.

**Calculate a Depth Curve**

Start the *Depth Wizard* using the *Image* window menu “Process→Wizards→Wizard\_Depth”. Read the information provided and follow the steps described in the Wizard. Also, move your mouse pointer over widgets to get more information on what each one does.

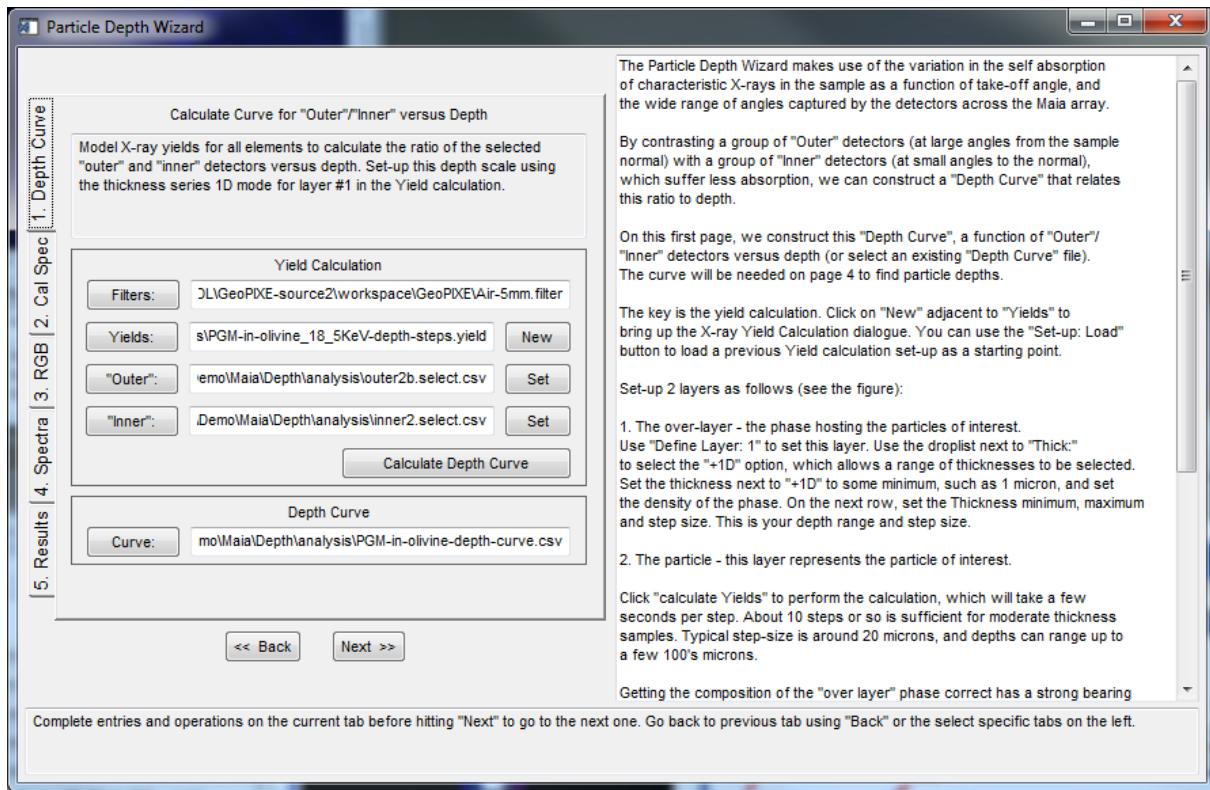


*Help information displayed by Depth Wizard on its starting tab*

Follow this procedure (as taken from the “GeoPIXE Worked Examples” notes):

- 2) On the **first page** (tab “**1. Depth Curve**”), set the Filter as relevant for the data (“Air 5 mm” in this case).
- 3) Open the X-ray Yield Calculation window by clicking on “New” adjacent to “Yields:” and load the LCM file “Demo/Maia/Depth/analysis/PGM-in-olivine\_18.5KeV.lcm”.
- 4) For layer #1 (the top olivine over-layer), change the “Thick:” mode to “+ 1D” to allow a range of thicknesses to be modelled, set initial Thick to 1  $\mu\text{m}$ , Min to 20  $\mu\text{m}$ , Max to 300  $\mu\text{m}$  and Step to 20  $\mu\text{m}$ , and change the output file name to something like “PGM-in-olivine\_18\_5KeV-depth-steps.yield”.
- 5) Click “Calculate Yields” to start the modelling for all layer #1 thickness steps (15 depth steps for 384 detectors, including secondary fluorescence will take some time). The output file-name will appear in the “Yields” field.  
In future you can just load this file using the “Yields” button.
- 6) Select the “Outer” detectors by clicking on “Set” opposite “Outer”. Select the detector layout for the old Maia 384A detector array (“AS Maia 384 10 mm v5”) from the dropdown.
- 7) Try setting the detector pad selection mode to “Radial” and clicking on detectors in different radial position to toggle the selection on/off of detectors at this radius from the centre. Once done, click “Save” to save this selection to a “select.csv” file (e.g. “test.select.csv”).
- 8) Back on the *Depth Wizard* panel, click “Outer” and load the file “outer2b.select.csv”, which shows our Outer

detector selection. Also load the “Inner” detector selection from file “inner2.select.csv”.



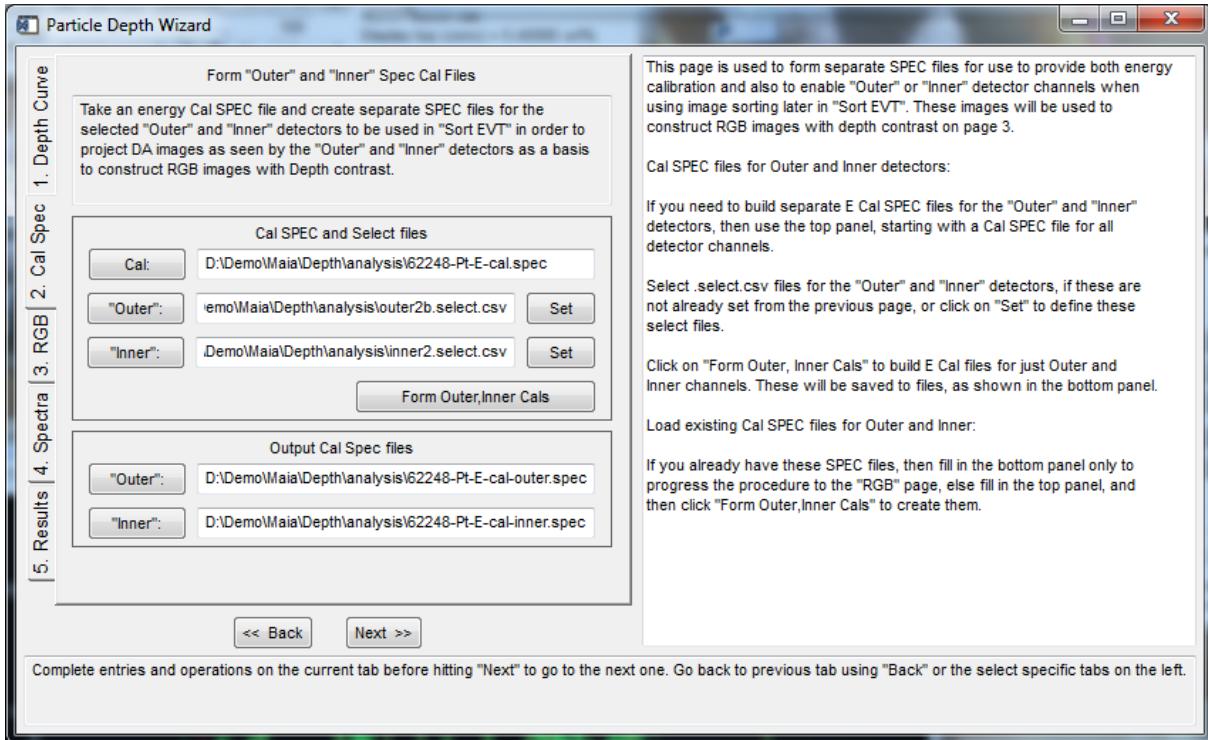
- 9) Click on “Calculate Depth Curve” on the *Depth Wizard* panel, to form a model curve that relates the ratio of “outer/inner” to depth”. It will be prompt for a filename. This will be needed on later tabs.

In future, for this sample matrix, you may only need to load this depth curve file.

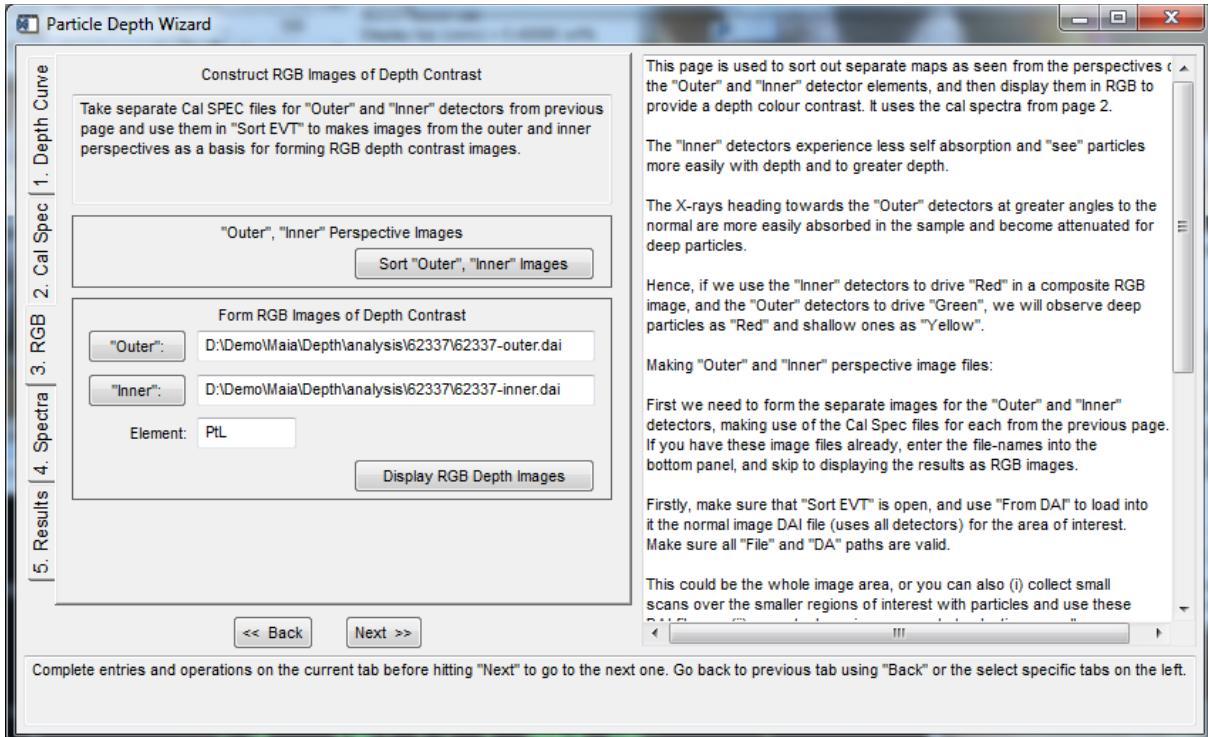
#### *Form “Inner” and “Outer” detector calibration files*

- 10) Advance to the next tab (“**2. Cal Spec**”). Here we load the per detector channel energy calibration file “62248-Pt-E-cal.spec” and click on “Form Outer, Inner Cals” to derive separate energy cal files for generating images for just Outer or Inner detectors (remember how the “Get” button on the DA tab of *Sort EVT* also selects the detector channels to use).

In future, just load the inner, outer cal files if you have done this before.

***Form “RGB” depth images***

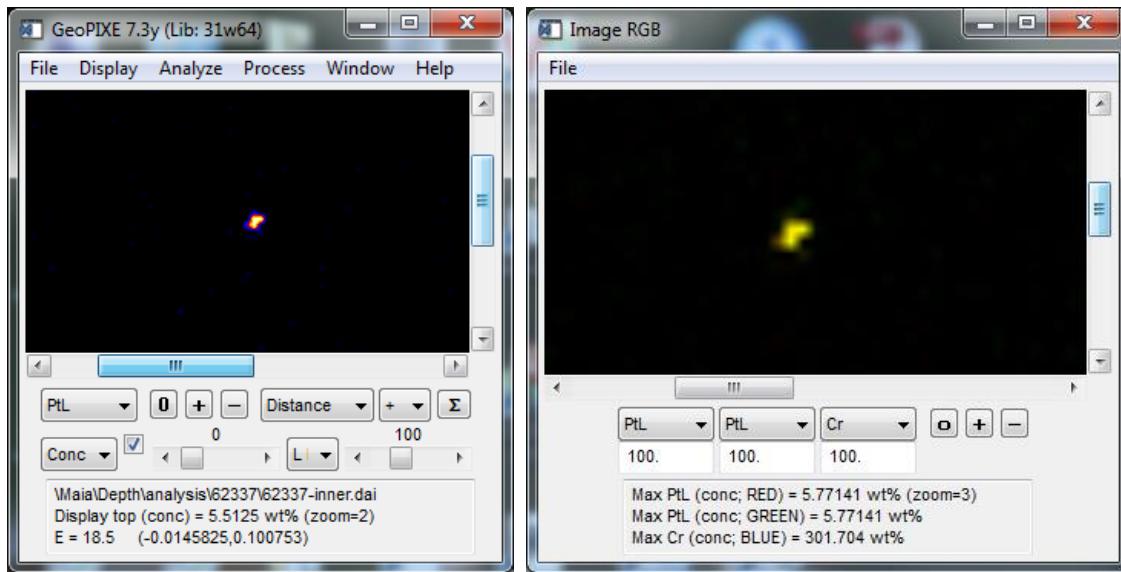
- 11) Advance to the next tab (“**3. RGB**”), load the DAI file “62337.dai” into the Sort EVT window and make sure the paths to all “Files” and the DA matrix are correct.



- 12) Click on “Sort Outer, Inner images” to sort images for Inner and Outer detectors.

In future, you can just load them if they have been previously sorted.

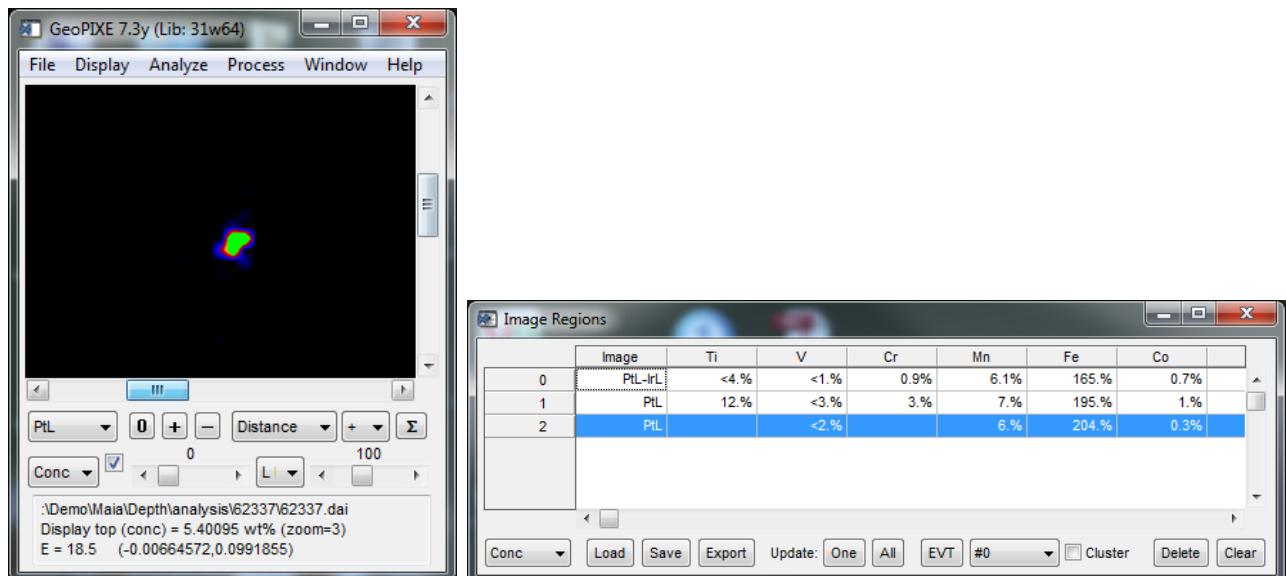
- 13) Open the *RGB Image* window and select the element “PtL” on tab “3. RGB”. Click on “Display RGB Depth Images” to form RGB images colour-coded for depth. RED is loaded with the inner detector images, while GREEN is driven by the Outer detector images. Shallow particles will appear Yellow, while deep ones will appear Red and intermediate depth particles will appear Orange. Zoom in a couple of clicks ...



Pt image (left) and depth coded Pt image (right), which compares the Outer and Inner detector Pt images. Pt is yellow, which indicates quite a shallow inclusion depth.

#### *Fit Region spectra for particles to determine depth*

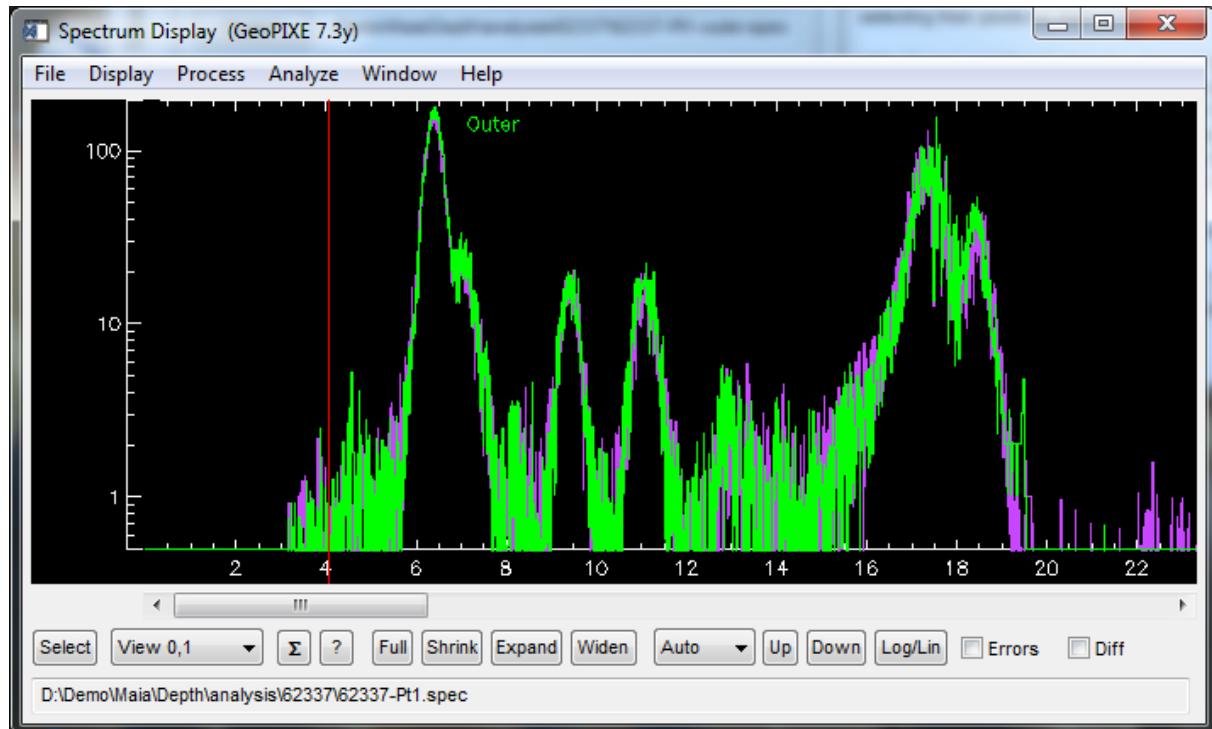
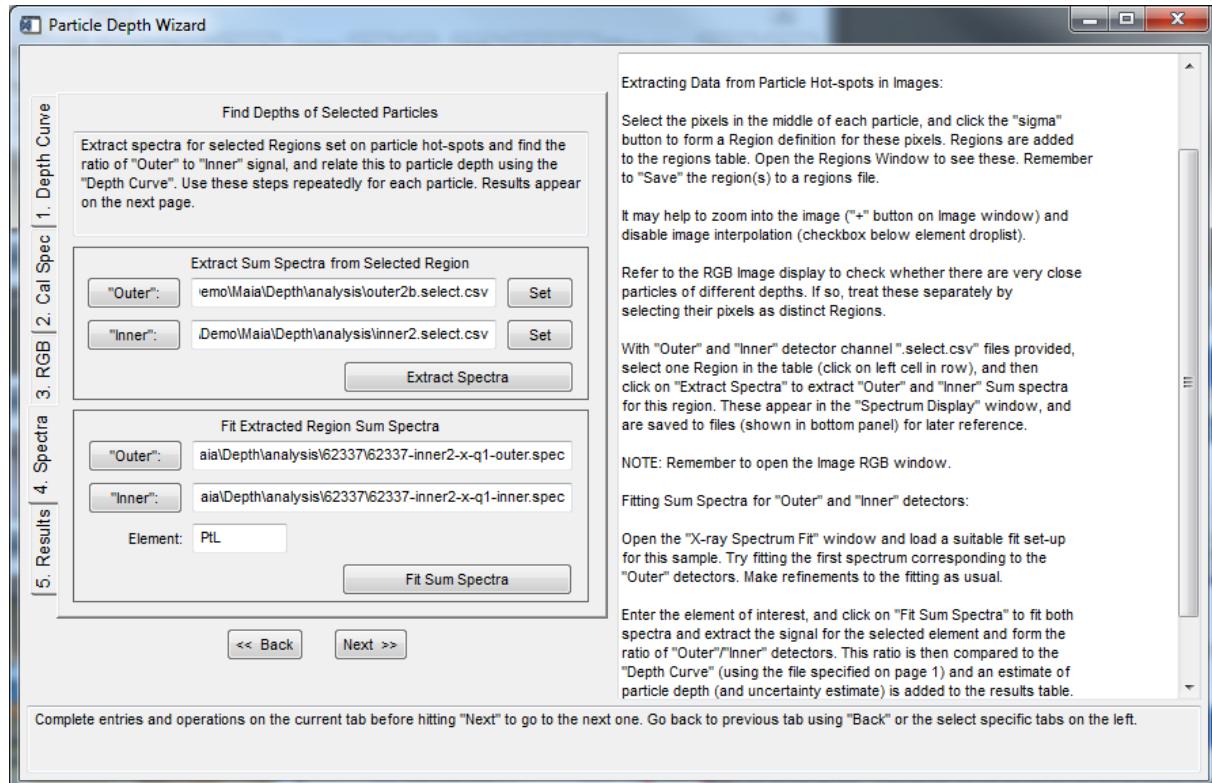
- 14) Advance to the next tab (“4. Spectra”). Load the original image DAI file (“Demo/Maia/Depth/62337.dai”, for all detector channels) that shows your buried particle and open the *Image Regions* window. As noted in the help text for this tab, select pixels on the particle (tip: use *Associations* window to ‘threshold’) and click on “Σ”. Repeat this for other particles, and then “Save” the regions to a file. See example file “62337-Pt1.region”, which has 3 regions defined.



Zoom in (+3 zoom) on a PGM particle, showing just 3 pixels selected on the grain using Ir-Pt in Association window

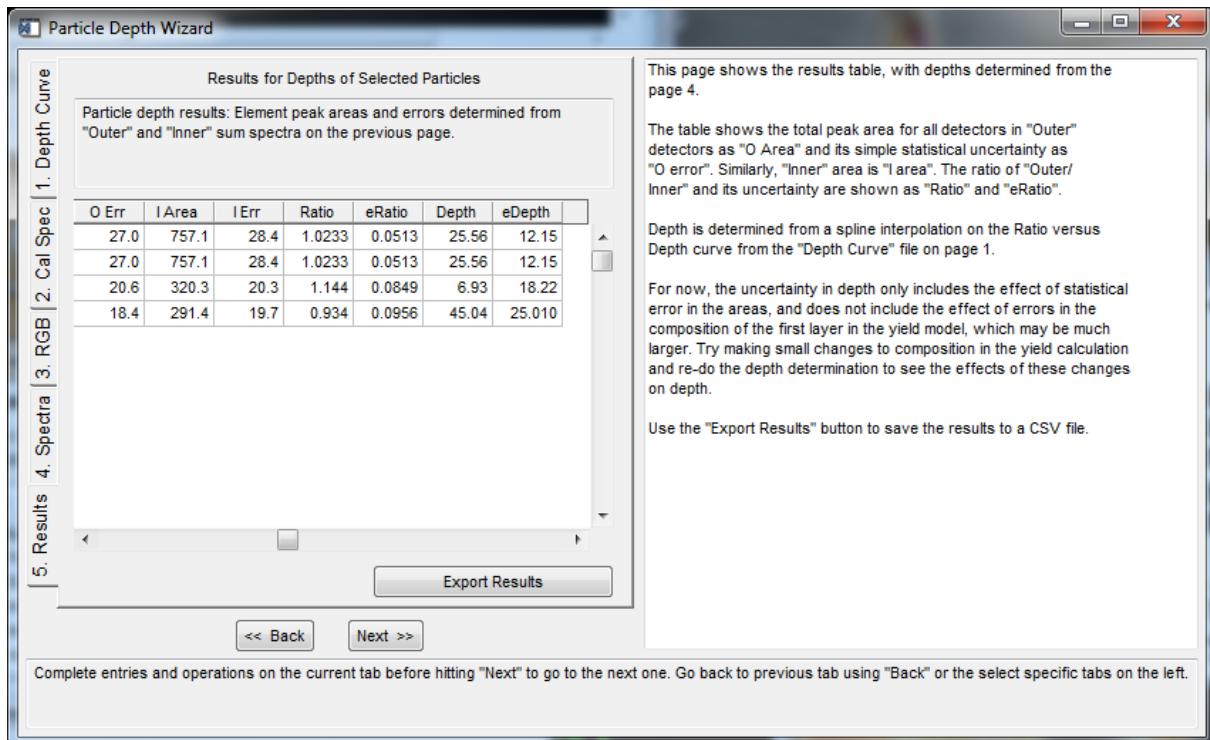
- 15) Open the *X-ray Spectrum Fit* window and load a suitable PCM set-up file for fitting your particles (“PGM-in-olivine-18\_5keV.pcm”).

- 16) Click on the row title for a selected particle region and then "Extract Spectra", which will apply your Outer and Inner detector channel selections and extract a sum spectrum for each (accept the initial file-name for individual detector spectra). The resulting file-names are entered into the spectra fields.
- 17) Enter the element of interest ("PtL" in this example) and click on "Fit Sum Spectra" on the Wizard to fit both spectra and extract the signal for the selected element and form the ratio of "Outer"/"Inner" detectors.



Sum spectra for Outer (green) and Inner (violet) detector channels

- 18) The ratio of "Outer"/"Inner" detectors is then compared to the "Depth Curve" (using the file specified on page/tab 1) and an estimate of particle depth (and uncertainty estimate) is added to the results table.
- 19) Repeat steps 20-22 for regions #1,2 in the example file “62337-Pt1.region”, which select just a ~single pixel each.
- 20) The results (e.g. 25  $\mu\text{m}$  for the 3 pixels selected in region #0) will appear on the final tab. Note how different the two single pixel results are for regions 1,2; evidently we have two particles at different depths here (7, 45  $\mu\text{m}$ ).
- 21) Use the Export button to export the results to a CSV file.



## Standards Wizard

The Wizard is designed to automate the standard foil analysis process at the Australian Synchrotron. It makes use of metadata variables set in the Maia control socket and passed into the Maia raw blog data files. The steps for semi-automated analysis are:

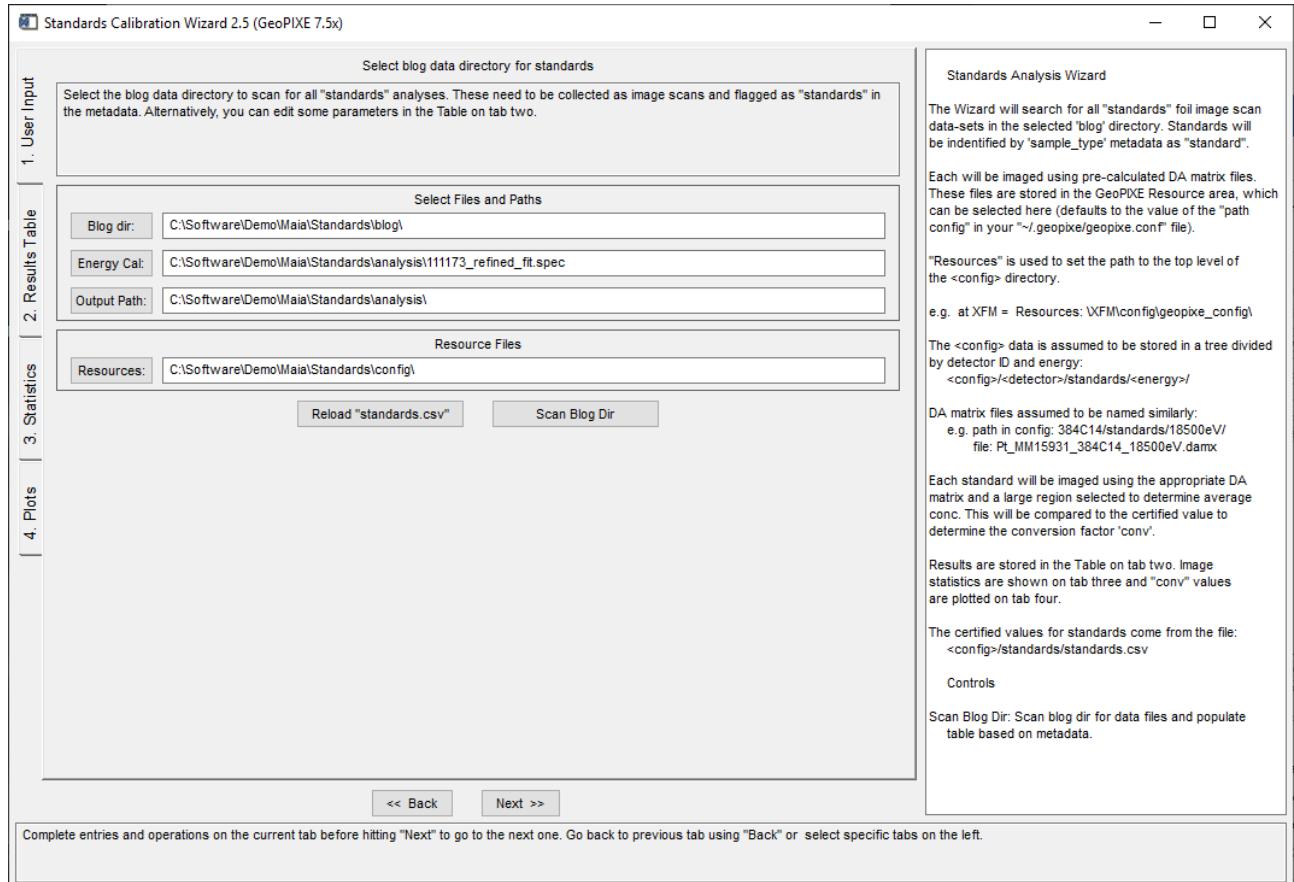
- Scan selected dir for all blog files.
- Applying energy calibrations to all detectors.
- Building a DA image for each.
- Use a large Box Region to sample foil concentration.
- Set the “Conv” factor to reproduce the desired foil composition (e.g. Mn = 100% in this example).

It reads a “standards.csv” file from “**Demo/Maia/Standard/config/**”, which contains the details of each foil at each energy (on Linux, use “**more ~/Demo/Maia/Standard/config/standards.csv**” to view this file).

Follow this procedure (as taken from the “*GeoPIXE Worked Examples*” notes):

### Set-up the Wizard

- 1) Run the Wizard using menu “Process→Wizards→Standards Wizard”.
  - a) See the Info panel on the right for detailed information and view context sensitive help at the bottom of the window as you move the mouse cursor over widgets.

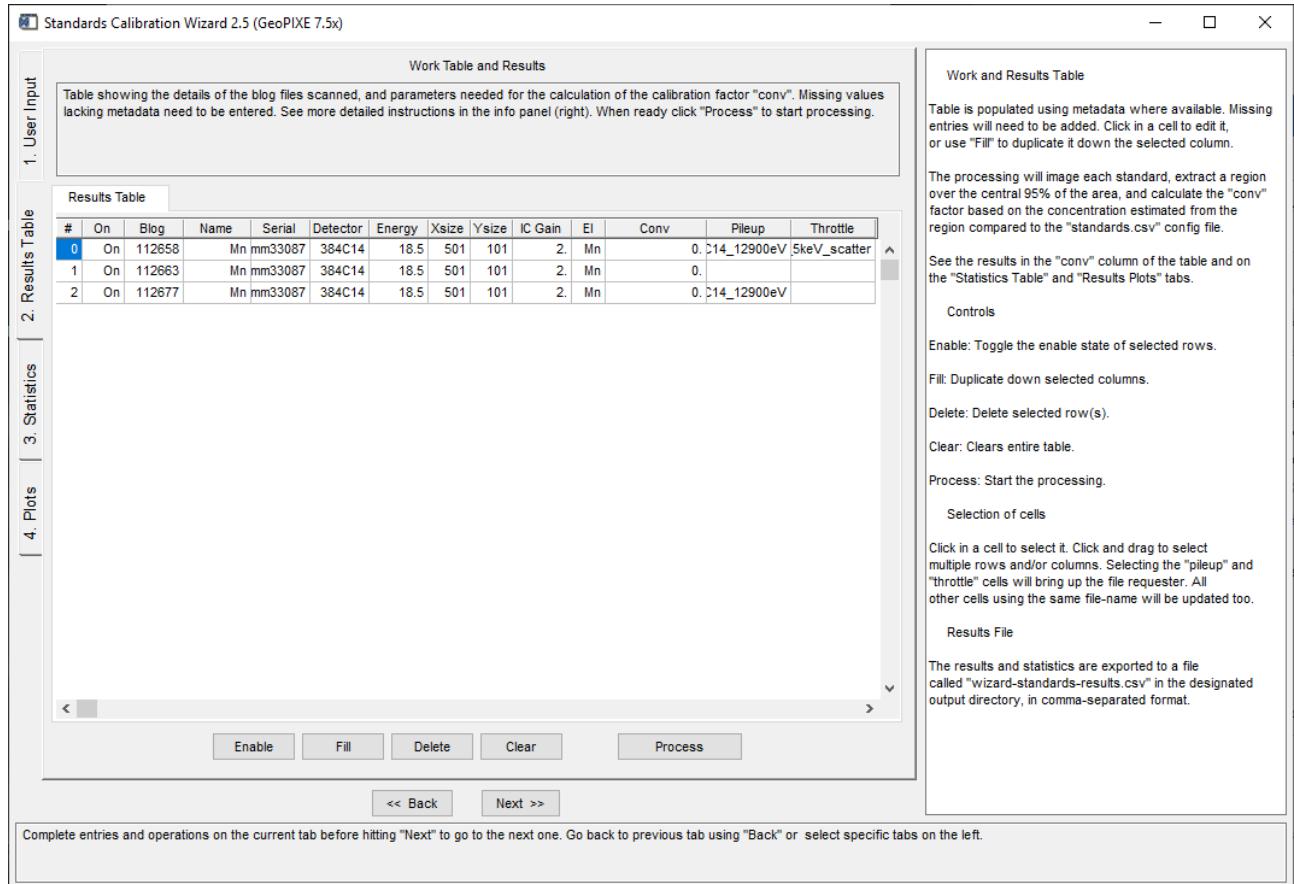


## 2) Select dir and energy cal:

- Select the blog dir for the standard foil raw Maia data: "Demo/Maia/Standard/blog".
- Select the energy calibration file: "Demo/Maia/Standard/analysis/111173\_refined\_fit.spec"
- Select the output path (defaults to neighbouring "analysis" dir tree).
- Select the Resources path: "Demo/Maia/Standard/config/"
  - Defaults to the "path config" in your ".geopixe/geopixe.conf" file.

## 3) Scan the blog dir tree.

- Click on "Scan Blog Dir" to scan the selected blog dir tree for all raw Maia data.
- This operation takes a couple of minutes and populates the Results Table.



#### 4) Check settings:

- For raw data with metadata (created after 1-Aug-2015), most columns will be populated for you.
- Missing entries can be entered. Use "Fill" to duplicate down from a selected cell.

#### Process the data

#### 5) Click on "Process" to process data, which does the following:

- Forms DA image for each in Sort EVT.
- Draws a large Box region on image for selected element (e.g. "Mn").
  - Avoids null areas.
- Integrates the Region and calculates "Conv"
- Updates Results Table (and Plots on later page) with "Conv".

#### 6) Results:

- See "Conv" column in Results Table.
- The "statistics" table shows a column "SD/Error". If all is well, this should be close to 1, which means the variation between pixels is just Poisson statistics.
  - Much larger than 1 suggests a non-uniform image; should not be the case for a standard foil.
  - In this case, open the image DAI file and check it out. There is a problem.
- Plots of "Conv" versus run number on "Plots" page.

# OFFICIAL

GeoPIXE - Quantitative PIXE / SXRF Imaging and Analysis  
Open Source release

Version 8 User's Guide  
February 11, 2026

**Standards Calibration Wizard 2.5 (GeoPIXE 7.5x)**

Work Table and Results

Table showing the details of the blog files scanned, and parameters needed for the calculation of the calibration factor "conv". Missing values lacking metadata need to be entered. See more detailed instructions in the info panel (right). When ready click "Process" to start processing.

1. User Input

Results Table

#	On	Blog	Name	Serial	Detector	Energy	Xsize	Ysize	IC Gain	EI	Conv	Pileup	Throttle
0	On	112658	Mn mm33087	384C14	18.5	501	101	2.	Mn	1.95069e-10	C14_12900eV_5keV_scatter		
1	On	112663	Mn mm33087	384C14	18.5	501	101	2.	Mn	1.63177e-10			
2	On	112677	Mn mm33087	384C14	18.5	501	101	2.	Mn	1.9143e-10	C14_12900eV		

2. Results Table

3. Statistics

4. Plots

Enable Fill Delete Clear Process

<< Back Next >>

Complete entries and operations on the current tab before hitting "Next!" to go to the next one. Go back to previous tab using "Back" or select specific tabs on the left.

Work and Results Table

Table is populated using metadata where available. Missing entries will need to be added. Click in a cell to edit it, or use "Fill" to duplicate it down the selected column.

The processing will image each standard, extract a region over the central 95% of the area, and calculate the "conv" factor based on the concentration estimated from the region compared to the "standards.csv" config file.

See the results in the "conv" column of the table and on the "Statistics Table" and "Results Plots" tabs.

Controls

Enable: Toggle the enable state of selected rows.

Fill: Duplicate down selected columns.

Delete: Delete selected row(s).

Clear: Clears entire table.

Process: Start the processing.

Selection of cells

Click in a cell to select it. Click and drag to select multiple rows and/or columns. Selecting the "pileup" and "throttle" cells will bring up the file requester. All other cells using the same file-name will be updated too.

Results File

The results and statistics are exported to a file called "wizard-standards-results.csv" in the designated output directory, in comma-separated format.

**Standards Calibration Wizard 2.5 (GeoPIXE 7.5x)**

Image Statistics

Table showing statistics for the region selected on the image. See more detailed instructions in the info panel (right).

1. User Input

Statistics Table

#	Blog	Name	Serial	Energy	EI	Mean	Error	Std.Dev	SD/Error
0	112658	Mn	mm33087	18.5	Mn	1000000.	660.141	148541.	1.05262
1	112663	Mn	mm33087	18.5	Mn	1000000.	1183.59	174732.	1.03189
2	112677	Mn	mm33087	18.5	Mn	1000000.	661.471	147093.	1.04026

2. Results Table

3. Statistics

4. Plots

<< Back Next >>

Complete entries and operations on the current tab before hitting "Next!" to go to the next one. Go back to previous tab using "Back" or select specific tabs on the left.

Image Statistics Table

Table of basic image statistics for each data-set. These are calculated after normalization to determine "conv". These include:

Mean: Average region concentration (ppm), which should now equal the nominal value for the standard.

Error: The 1-sigma error estimate for "Mean" over region.

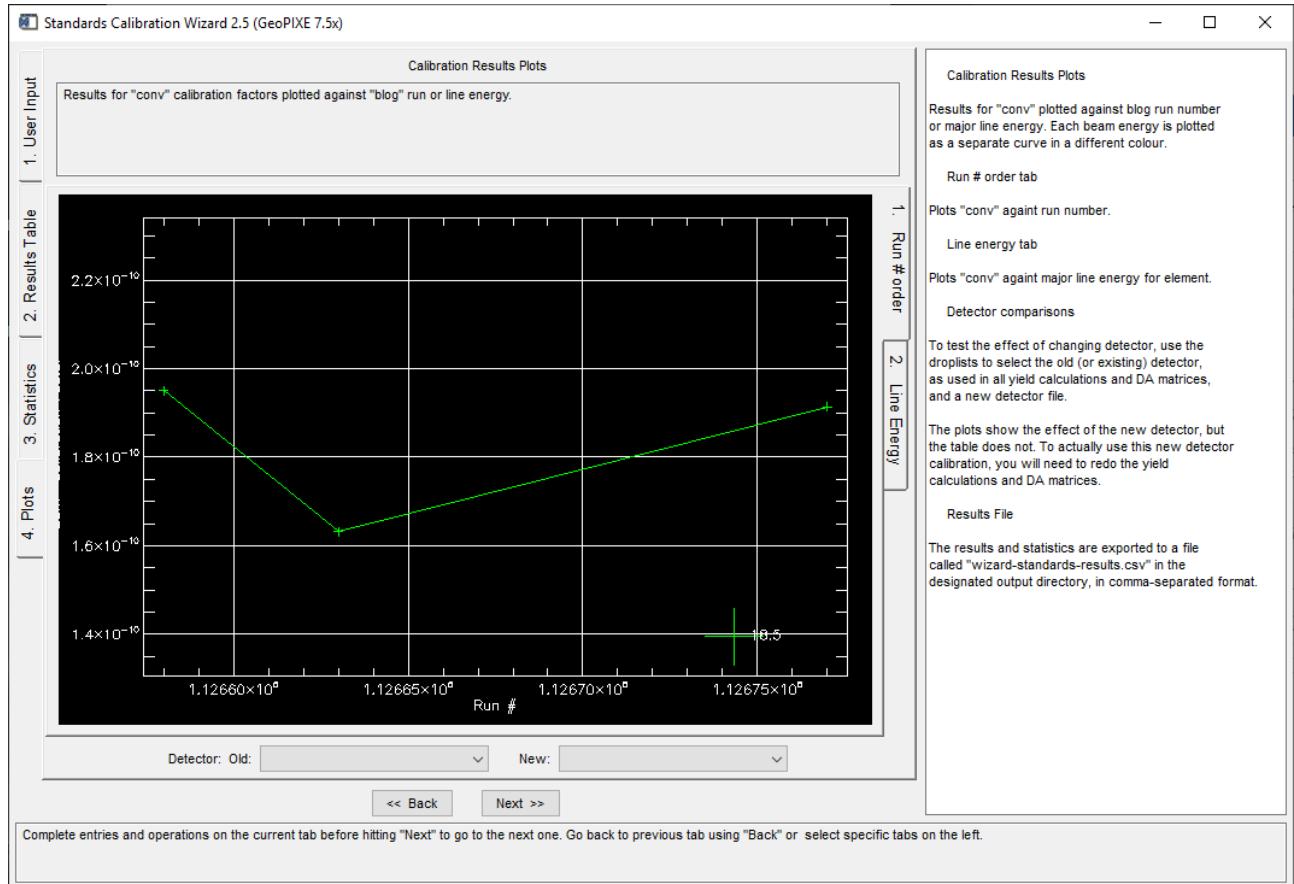
Std.Dev: The standard deviation (ppm) of the per pixel concentration values over the region.

SD/Error: The ratio of the per pixel standard deviation to that expected from Poisson statistics.

A value of "SD/Error" that departs significantly from unity indicates unwanted structure in the image beyond simple counting statistics. This may indicate damage, a hole, contamination or misalignment of the scan (e.g. so it hits the sample frame).

Results File

The results and statistics are exported to a file called "wizard-standards-results.csv" in the designated output directory, in comma-separated format.



## 7) Notes:

- a) If the pileup or throttle file is not found, you will be prompted (just for first occurrence of each file). In this example, the files are located in the “Demo/Maia/Standards/analysis” directory.

## MPDA Wizard

Under development ...

## GeoPIXE Analysis Scenarios, Data Flow and Worked Examples

This chapter illustrates GeoPIXE data analysis using various worked examples and provides a working knowledge of data flow between windows elements of GeoPIXE, and how changes made in one window affects others or update their displays. This will be done for several data analysis scenarios.

*A very good starting point also is to work through the worked examples (with sample data from Demo/ on the FTP site) found in the GeoPIXE Worked examples PDF, located in the Help directory.*

*See the /Demo directory and the “GeoPIXE Worked examples” PDF.*

### Raw PIXE Data to Elemental Images

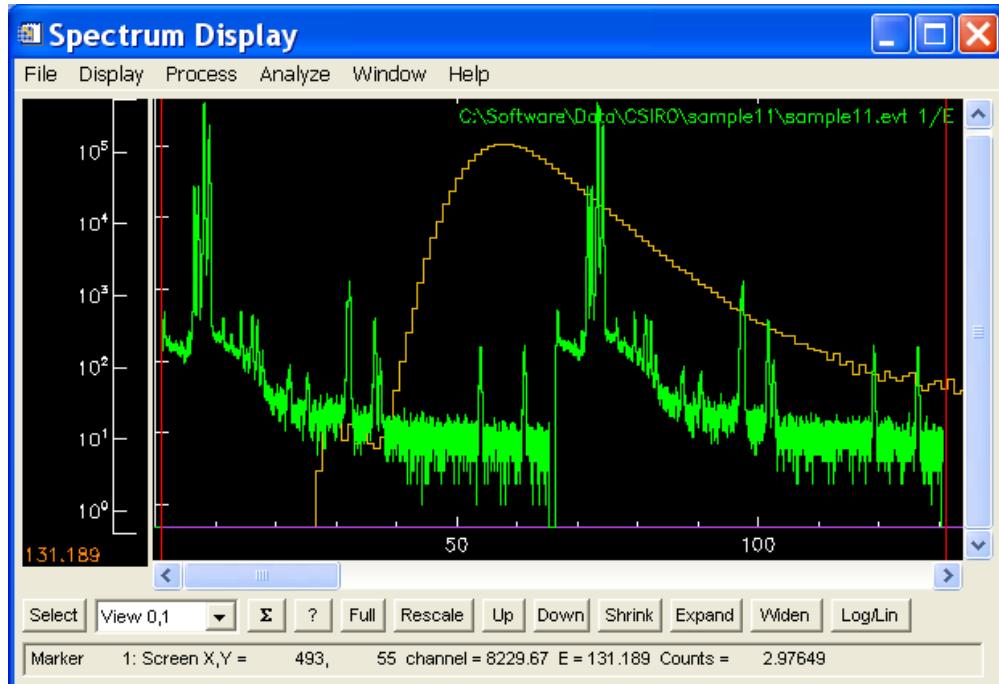
This scenario follows workflow from raw PIXE data, as spectra and event data, through to quantitative elemental images using the *Dynamic Analysis* method. The example data used is stored in the “Data\CSIRO\Sample11” directory.

This worked example illustrates the following processing steps.

1. Extraction of total spectra from an EVT file.
2. Fitting a total X-ray spectrum
3. Generation of the Dynamic Analysis matrix for image projection.
4. Sorting the EVT file and image generation.
5. Verification of images and Identification of missing elements discussed elsewhere (p. 126).
6. Generating a DA matrix for a detector array.
7. Digital filtering techniques.

### Spectrum Display and Selection

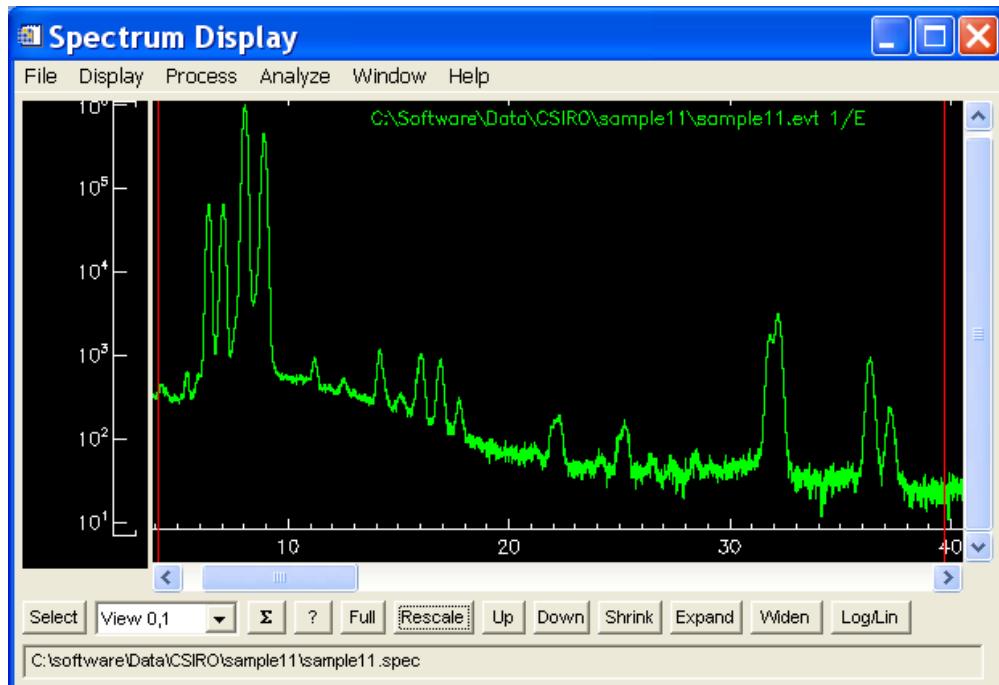
Load spectrum data using the *Spectrum Display* window menu “File→Load SPEC” to load “Sample11.spec”.



The spectrum data we need to start with is the total spectra over the entire image area. Hit the “Select” button to bring up the *Spectrum Select* window and click on “Prev”. This will display only the first spectrum from the file, the PIXE spectrum. You can now close the *Spectrum Select* window.

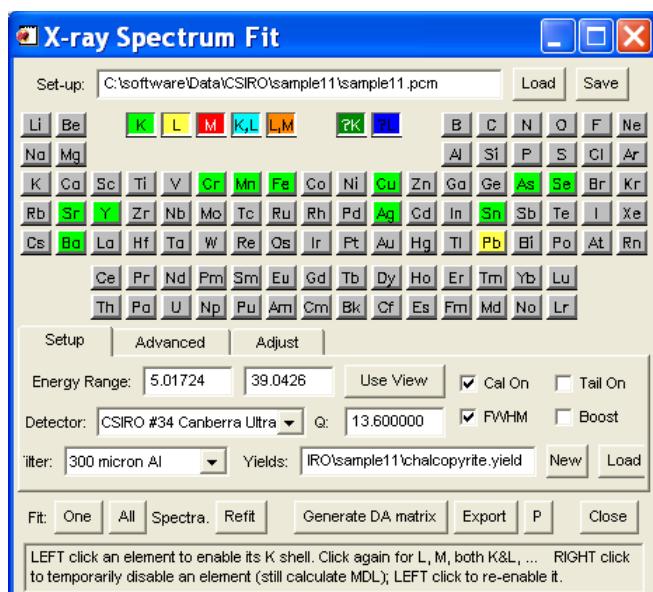
This spectrum comes from a list-mode file that uses the top ADC bit to tag X-stepping in X-step mode images. This produces twin spectra, one in each 4K half of the spectrum. Use the menu “Process→Fold (bit #12)” to combine these into a single 4K spectrum. Click on “Full” to see the full spectrum.

Select the View markers, using the drop-list on the left of the *Spectrum Display* window (these may be set already, by default), and click to position the right, then left markers to define an energy range that covers all interesting parts of the PIXE spectrum (i.e. 5 – 39 keV). You can left-click and drag these markers into position. Click on “Widen” to display just this range (select “Auto” on the vertical scale drop-list to automatically rescale the display to the best vertical scale).



### Fitting the PIXE Spectrum

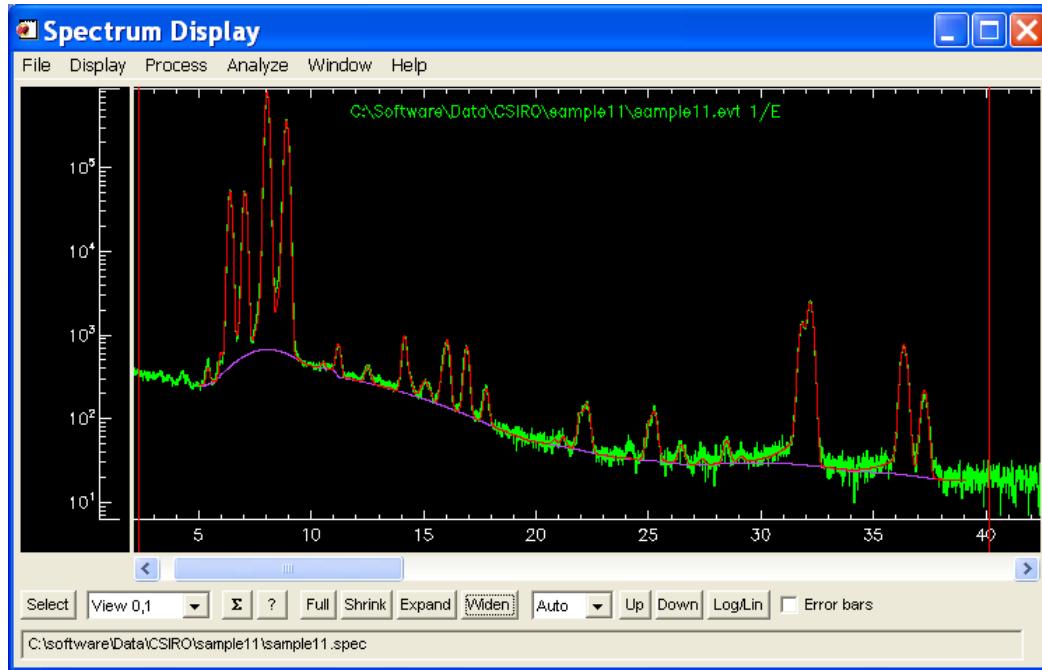
Open the *X-ray Spectrum Fit* window using the “Window→X-ray Spectrum Fit” menu of *Spectrum Display* and load fit settings from the PCM file “Sample11.pcm”. Details of the *X-ray Spectrum Fit* window options are given above (*Fitting a PIXE or SXRF Spectrum*, p. 26).



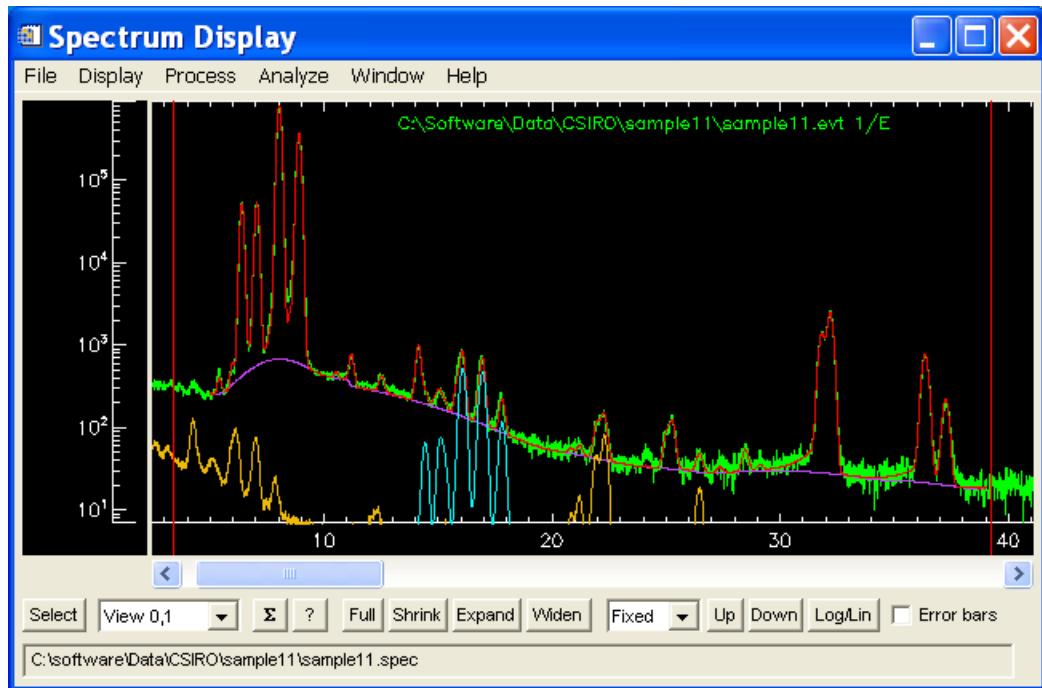
If an error message is encountered for the yield file, dismiss the message, and click on the “Load” button to the right of “Yields:” and locate the file “chalcopyrite.yield” in the Demo/CSIRO/Sample11 directory. Save back to the PCM file “Sample11.pcm” using the “Save” button. Yields use absolute paths, which will be different on your system.

This spectrum file does not contain a charge Q. Enter 13.6 in the “Q” field in *X-ray Spectrum Fit*.

Click on “Fit: One” to fit the spectrum. The results shown in a *Fit Results* window, if open, will correspond to the full image area.



Many of these features in the spectrum are due to Ge escapes and pile-up. To view these use the menus: “Display→Ge escapes” and “Display→Pileup→from single spectrum”.



## Generate the Dynamic Analysis Matrix

Now click on “Generate DA Matrix” to build the Dynamic Analysis matrix and save it as “Sample11.dam” (use the default single DA matrix option). The generated DA matrix contains the list of all elements fitted, as well as the matrix transformation that maps each PIXE event onto quantitative elemental images.

## Sorting the Event Data to Project Images

Open the *Sort EVT* window using the “Window→Sort EVT” menu on the *Image Display* window. Load the settings for imaging from the DAI file (“Sample11-chalco.dai”) using the “From DAI” button on *Sort EVT*. Click on the EVT file” button and locate the file “Sample11.evt” in the Sample11 directory. Now load the DA matrix that you generated (“Sample11.dam”), by clicking on the “File” button below the Projection drop-list showing “Dynamic Analysis”. This matrix contains all the information needed to project event data onto elemental images. The only critical extra piece of information needed is the integrated beam charge, which is provided in this example.

When the EVT file was loaded, the accompanying energy calibration from the data acquisition file was also set (in the Cal A and B entries above Projection). Once the DA matrix has been loaded, a better energy calibration is available. Included in the DA matrix file is the refined energy calibration from the least squares fit to the spectrum. To make use of this calibration, click on the “DA” button alongside the Cal parameters.

This particular EVT file contains data collected at the CSIRO using a single detector and a hybrid scanning-stage stepping mode, with stage steps encoded into the top bit of ADC/station 1. Don’t worry about the details of this. This sorting and DA projection process works the same for simple XY scanning data.

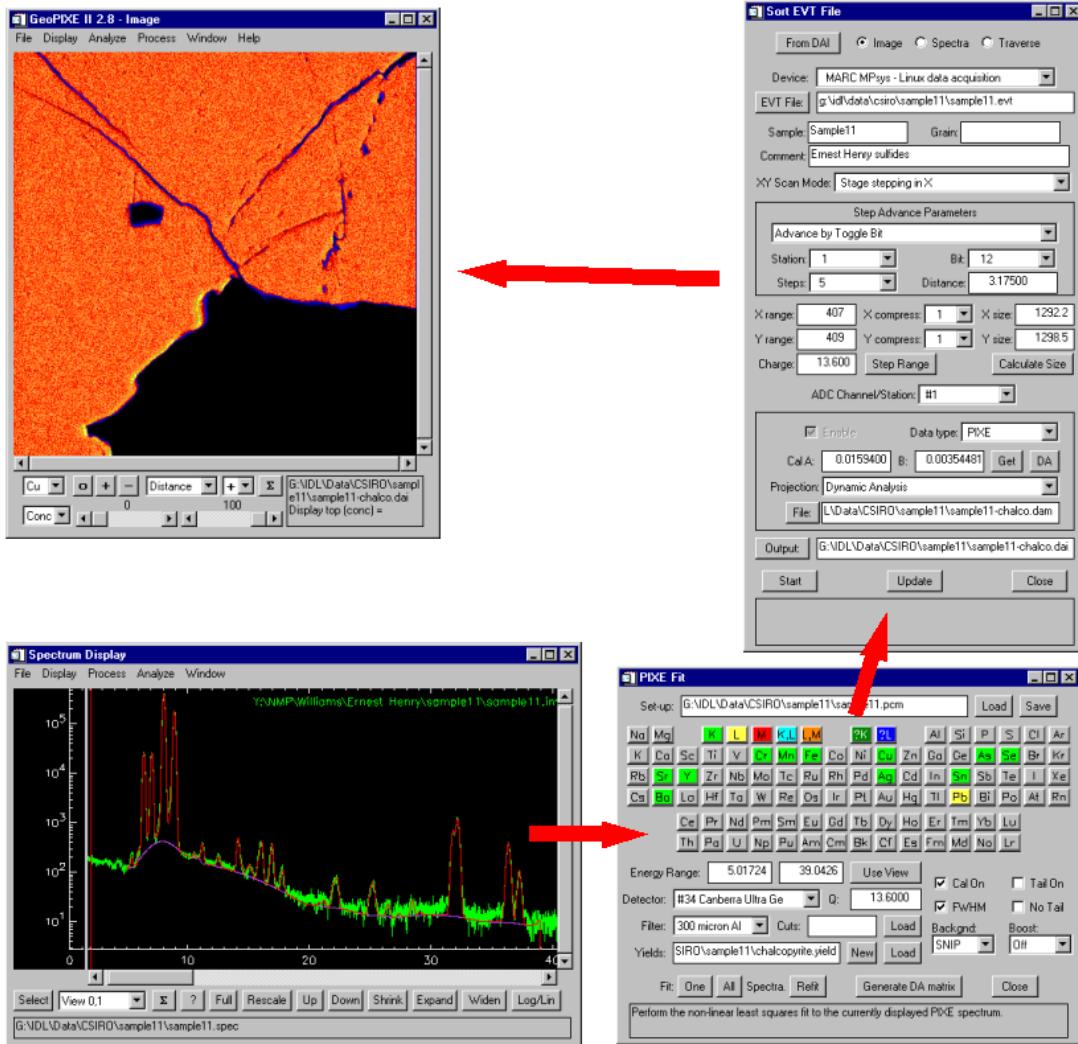
Click on “Start” to start sorting the EVT file. The resulting images are sent to the ‘connected’ *Image Display* window for display, and they are stored in the output DAI file, specified at the bottom of the *Sort EVT* window. Use the element drop-list in the *Image Display* window to switch between element images (the arrow keys on the keyboard can be used to change the drop-list selection after the first one has been selected). See the section “Image Display (main GeoPIXE window)” above for more details.

*Note:* By default all images and clones, spectra, regions, X-ray Spectrum Fit and sort windows are all connected and function in concert. However, if you need to load image or spectra data from an unrelated project, then use the “Unlinked Image” and “Unlinked Spectrum Display” menus on the *Image Display* window.

## Notes on Data Flow

The process of generating a DA matrix from a least-squares fit to a representative spectrum, and the use of this matrix for image projection, is illustrated below. Once a DA matrix has been generated, it can be used to project out image data for any sample data set with similar constituents (same element list) and collected using the same experimental conditions (same filters, detector efficiency, and detector resolution).

If the new data-set does not have the same energy calibration as the DA matrix (or its original fitted spectrum), then do not use the DA button. In this case, load the correct energy calibration into the “Cal A” and “Cal B” fields, or use the “Get” button approach to retrieve an energy calibration from a new calibrated spectrum.



## Verification of Images

Exploration and verification of image data is the next important step in image projection. This is outlined in a following section (*Verification of Images using Regions*, p. 126).

## Generating a DA Matrix for a Detector Array and Sorting Images

To sort event data from an array detector select “Detector Array” from the drop-list adjacent to the “ADC/Station” drop-list; for single detectors select “Single Detector”. Then “Enable” all used detector channels (or use the “Get” button, see below). The *Sort EVT* procedure also needs to know the energy calibration of all detector elements. To accomplish this, all detector spectra need to be fitted to obtain a refined energy calibration.

Load a spectrum file containing spectra from all detector elements into *Spectrum Display*. This can be obtained, for example, using the “Import” menu pop-up on the *Spectrum Display* “File” menu to extract spectra from a list-mode file. Delete any spectra files not needed, such as X and Y spectra (e.g. use “No XY” in *Spectrum Select*), bad detector channels or non-array detector channels (use “Delete”). Then click on “Fit: All” in *X-ray Spectrum Fit*. This will fit all spectra and update them with their refined energy calibrations. Examine the “Fitting” parameters in the *Fit Results* window to check for convergence of each fit. Bad fits may need some individual attention. Save the spectra to a SPEC file.

In *Sort EVT*, after selecting “Detector Array”, load a spectrum file that has all good detector elements fitted, using the “Get” button. You can cycle through ADCs to check that this was done. Note that while the “DA” button only loads an energy calibration into the currently displayed ADC, the “Get” button loads all calibrations, provided that “Detector

Array” is selected first. It also enables the detector elements for the good spectra found.

Sort the images as usual by hitting “Start” in *Sort EVT*. Processing may be a little slower as it collects data for all detectors now. The process uses each detector’s calibration to map event energies onto the correct column of the DA matrix for image projection.

### Digital Filtering of Images

Many images, particularly of trace elements, will contain a lot of noise. The amount of beam charge (flux) deposited in a single pixel is quite small, typically less than 1 nC ( $10^9$  photons). Therefore, the counting statistics in each pixel will be quite poor. For these noisy images, averaging between pixels can be used to increase the effective charge per pixel, at the expense of smoothing out spatial detail.

To apply digital filters, open the *Image Operations* window (or use the Process menu of *Image Display*). The *Image Operations* window provides a palette of digital filters that can be applied to the current image using a single mouse click. You can view all operations applied to images in the *Image History* window.

Select the Cr image, and smooth it by clicking on “Gaussian smooth 2” in the Image Operations window. The Fe image is quite good, so just use a small degree of smoothing (e.g. “Gaussian smooth 1.0”). The Gaussian smooth uses an averaging structure element of 1.0 pixels full width at half maximum.

To re-apply all the digital filtering operations contained in the history records of another file, click on the “Get” button on the *Image Operations* window. Load the previously filtered file (e.g. “Sample11-chalco.dai”). Then select “All” elements and “OK”. It will apply the same filtering and set the display range as well.

## Raw SXRF Data to Elemental Images

This example follows a similar data-flow through an SXRF data-set collected on the PNC-CAT 20-ID beamline of the APS. The example APS\PNC-CAT\82, is an image of a geological sample (144 x 130 pixels) across a small (~1000  $\mu\text{m}$ ) area of regolith (weathered earth) sample imaged at PNC-CAT at 15.2 keV (Hough *et al.*, 2005). It was collected on the 20-ID X-ray microprobe using a 230  $\mu\text{m}$  Al filter in front of a 7-element Ge detector at an angle of 85° to the beam, with the target rotated -45° (i.e. towards the detector).

This example illustrates the following processing steps, including steps specific to PNC-CAT and synchrotron data more generally.

1. Conversion from the APS MDA format to the GeoPIXE LST format.
2. Extraction of total spectra from an LST file.
3. X-ray peak identification.
4. Fitting a total X-ray spectrum and generation of the Dynamic Analysis (DA) matrix for image projection.
5. Sorting the LST file and image generation using DA.
6. Analyzing features directly from images.
7. Extraction of spectra for selected or all detectors from regions on images.
8. Identification of missing elements.
9. Regeneration of images after adding extra elements.

See also the section on “Verification of Images using Regions”.

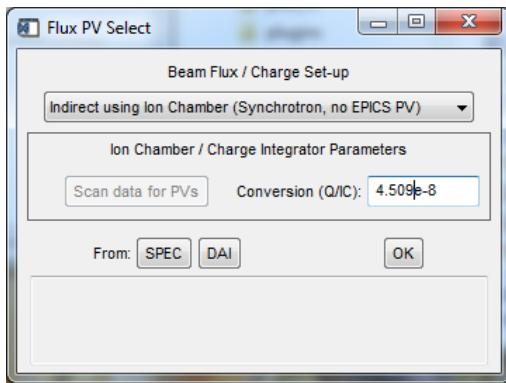
### Extract total spectra

To extract the raw total spectra for all detectors, use the “File→Import” menu in *Spectrum Display* to pop-up the *Import* requester and select “Synchrotron (SXRF)” data from the “APS” of format “Extract from APS LST” and then select the LST data file (“pncid\_0082.lst”). Select the output path to this same directory.

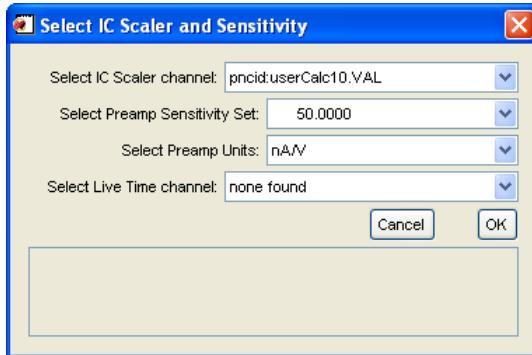
Next the Flux PV select pop-up appears. This enables you to enter a conversion factor from ion chamber (IC) count to equivalent charge as a measure of beam flux. Select “Indirect using Ion Chamber (synchrotron, no EPICS PV)” and enter the conversion factor  $4.509 \cdot 10^{-8}$ . For the IC count of  $3.25 \cdot 10^{10}$ , this corresponds to an equivalent charge of 1464.6.

The “charge” nomenclature comes from PIXE analysis and is the integrated proton beam charge in  $\mu\text{C}$ . For synchrotron applications it represents the integrated flux in units of  $6.242 \cdot 10^{12}$  photons. The conversion from total IC count, as stored in the LST file (as converted from the original MDA file “pncid\_0082.mda”) can be established using a standard at the same photon beam energy (this is discussed elsewhere).

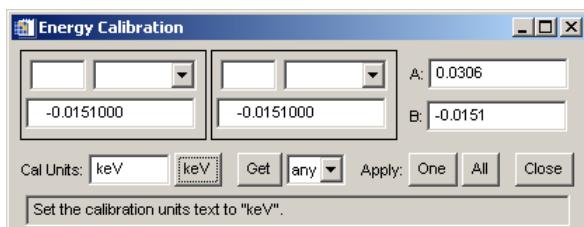
Once this conversion from IC count to Charge is established, it is maintained internally for the duration of the session (or can be changed on the pop-up requester or using the “?” button next to “Q” charge on the X-ray Spectrum Fit window).



The LST event file has been built from a source APS data acquisition MDA data file using the “File→Convert→APS MDA to LST” menu in Spectrum Display of the main GeoPIXE Image window. If you try this you will need to select the correct Epics PV for the IC used and the range on the current pre-amplifier (in this case “pncid\_0082.mda”, a PV of “pncid:UserCalc10.VAL” for dead-time corrected I0, and a Sensitivity of 50 nA/V). Note that MDA files from other beamlines may contain details of ion-chamber PVs and preamplifier settings as PVs. In these cases drop-lists may appear in this window to permit selection of the correct PVs for both IC and preamplifier settings.

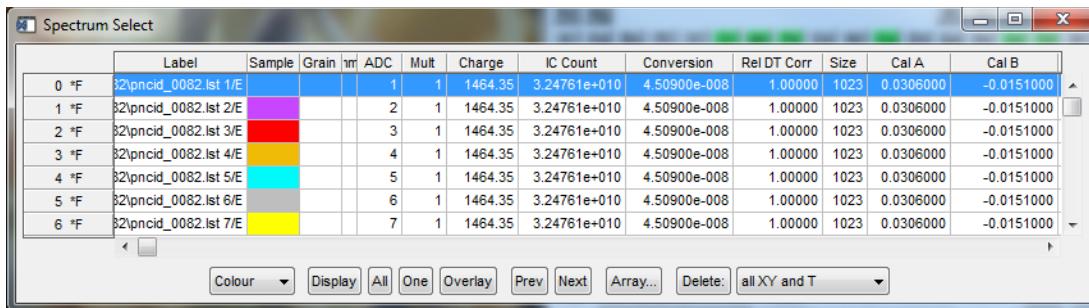


The spectra are not calibrated for energy. For now, open the *Energy Calibration* window (“Display→Calibrate Energy” menu) and set A= 0.0306 and B= -0.0151 (A is slope, B is offset), click on “keV” and hit the “Apply: All” button. This will apply this Cal to all spectra.





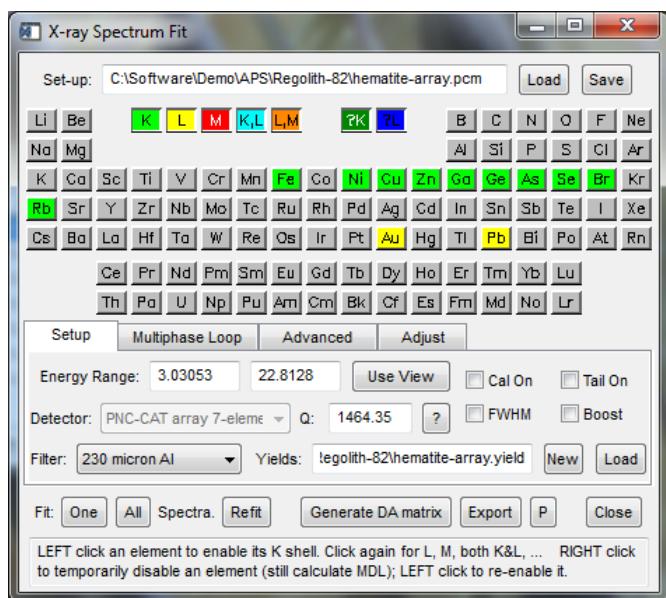
The Cals (energy calibration coefficients A,B, where  $E=Ax+B$  and  $x$  is channel number) can be viewed in the *Spectrum Select* window (click on “Select” button, bottom-left of the *Spectrum Display* window). Scroll right to see the Cal parameters. We don’t need the X,Y spectra (total projections of all data onto X, Y axes), so select “No XY and T” and delete them. Save these spectra as “pncid\_0082-raw.spec” using the “File→Save Spec” menu.



All energy calibration parameters for all detector channels can be set from a previous spectrum with all detectors calibrated using the menu “Display→Get ALL energy Cals”. You can load these in this case from spectrum file “pncid\_0082-cal.spec”.

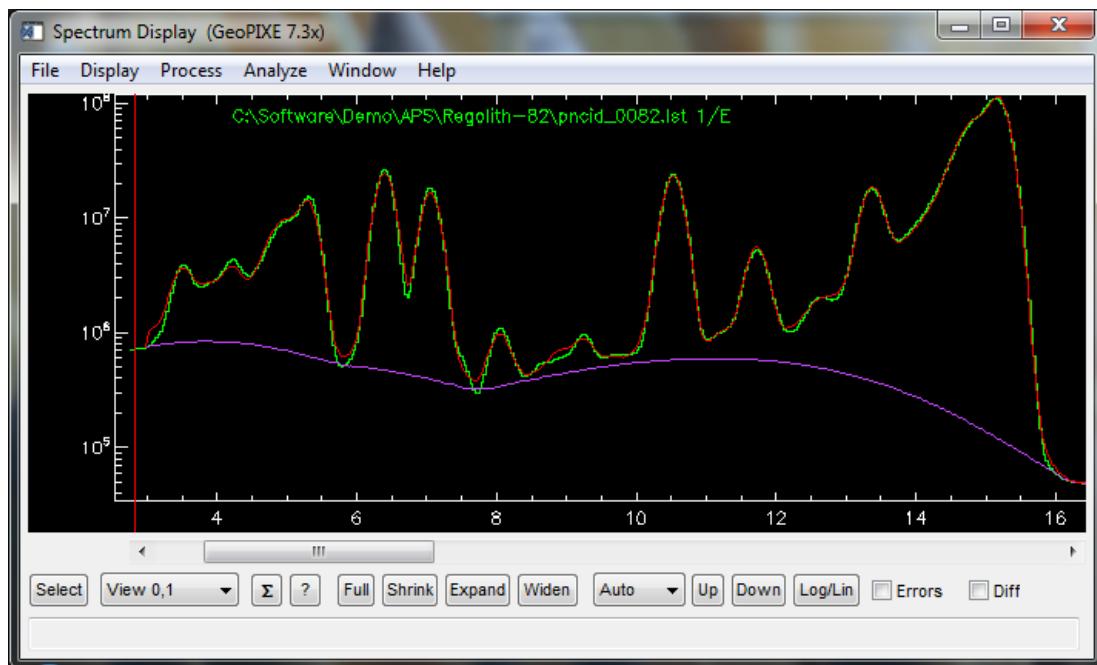
### Fit the X-ray spectrum and generate DA matrix

Now open the *X-ray Spectrum Fit* window using the “Window→X-ray Spectrum Fit” menu. Load the fit parameters from file “hematite-array.pcm”. The charge “Q” will be set to the charge already in the spectrum data header. The yields have been pre-calculated for a photon energy of 15.2 keV. Click on “Fit:One” in *X-ray Spectrum Fit* and see if it fits the spectrum. If the fit fails to converge (a message to this effect may appear) use the fitting strategy discussed below.



Now click on “Fit: All” to fit all 7 spectra. You may need to enable energy cal fitting using “Cal” and peak width fitting using “FWHM” check-boxes. Save the fitted spectra in file “pncid\_0082-fit.spec”. *These fitted spectra now contain adjusted energy calibrations for all 7 spectra. This will come in handy later. (All detector channels are also calibrated in file “pncid\_0082-cal.spec”).*

If a good fit is obtained, select the menu “Process→Add (remap Cal)” to add the spectra together (after mapping to a common energy calibration), repeat “Fit One” and then click on the “Generate DA matrix” button (select default single DA matrix option) to build and save a DA matrix file; save it as DAM file “hematite-array.damx”.



## SXRF Spectrum Fitting Strategy

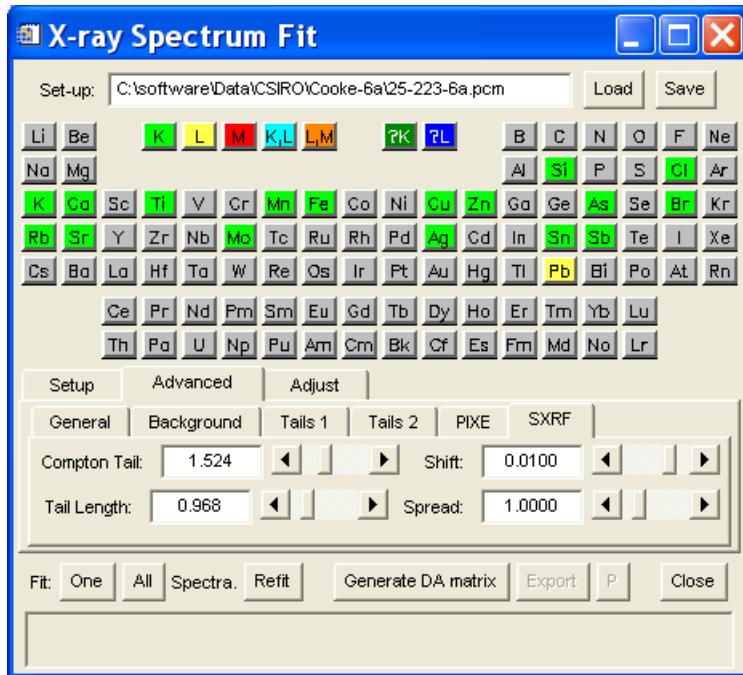
The non-linear least-squares fit to a spectrum can become unstable for a number of reasons. In the case of SXRF spectra, the dominance of the scatter peaks in the spectrum can be a particular problem for a couple of reasons. Firstly, the beam energy may not be known precisely. Even an error of 10 eV can have a strong effect on the fit. If the energy Cal parameters are left free in the fit, GeoPIXE will adjust the Cal to best fit all peaks including the poorly positioned

scatter peaks. This will introduce a bias error into the Cal parameters and make the fit less stable and perhaps affect the fitting of peak tailing. For this reason, we normally do not enable “Tail” fitting for SXRF data.

Even with the elastic peak energy well known, the energy and shape of the Compton peak will vary reflecting factors including sample composition, through the bound electron momentum distribution, and multiple scattering, which becomes sensitive to sample layout and structure. Parameters to adjust the position and width of the Compton peak can be found under the “Advanced” → “XRF” tab. Use these to manually improve a fit to the Compton peak (click on “Fit: One” after each [small] adjustment of these parameters) (see below).

Therefore, the following approach proves helpful to isolate some problems associated with the energy and details of the scatter peaks:

1. Choose a range of energy in the spectrum that includes most X-ray lines but excludes the Compton and elastic scatter peaks (and their escape peaks, if they are prominent [e.g. at ~10 keV lower energy in the case of a Ge detector]). Drag the View markers to bracket this range and hit the “Use View” button in the *X-ray Spectrum Fit* window.
2. Fit this range with Cal and FWHM parameters ON, or free to vary. Add any additional elements as needed, until the fit is looking good.
3. Expand the fitting range to include the scatter peaks and their escapes. Also include pileup peaks at higher energy.
4. Disable variation of the Cal and FWHM parameters in the fit (un-check “Cal” and “FWHM” in the *X-ray Spectrum Fit* window).
5. Fit the spectrum again. How does the position of the elastic peak look now? Does the fit match the data? If not, this may indicate that the beam energy is in error. Perhaps adjust the Compton peak parameters.
6. If necessary, use the peak in the spectrum now to determine a better estimate of the actual beam energy (expand the spectrum around the elastic peak and drag a marker to probe its centroid energy).
7. Open the *PIXE/SXRF Yield Calculation* window (“Yields: New” button in the *X-ray Spectrum Fit* window) and re-calculate yields using this new beam energy (you will need to load the Set-up file, “Hematite-array.lcm” in the present case, into *PIXE/SXRF Yield Calculation*).
8. Re-fit the spectrum now. Does the elastic peak fit look better?



9. How does the fit to the Compton peak look now? There may still be errors arising from assumed electron momentum distribution and multiple-scattering. These can be adjusted manually using the “Shift” and “Spread” parameters on the “Advanced/XRF” tab panel. Make small changes and repeat the fit to see how these changes affect the final fit. Avoid large excursions of these parameters.

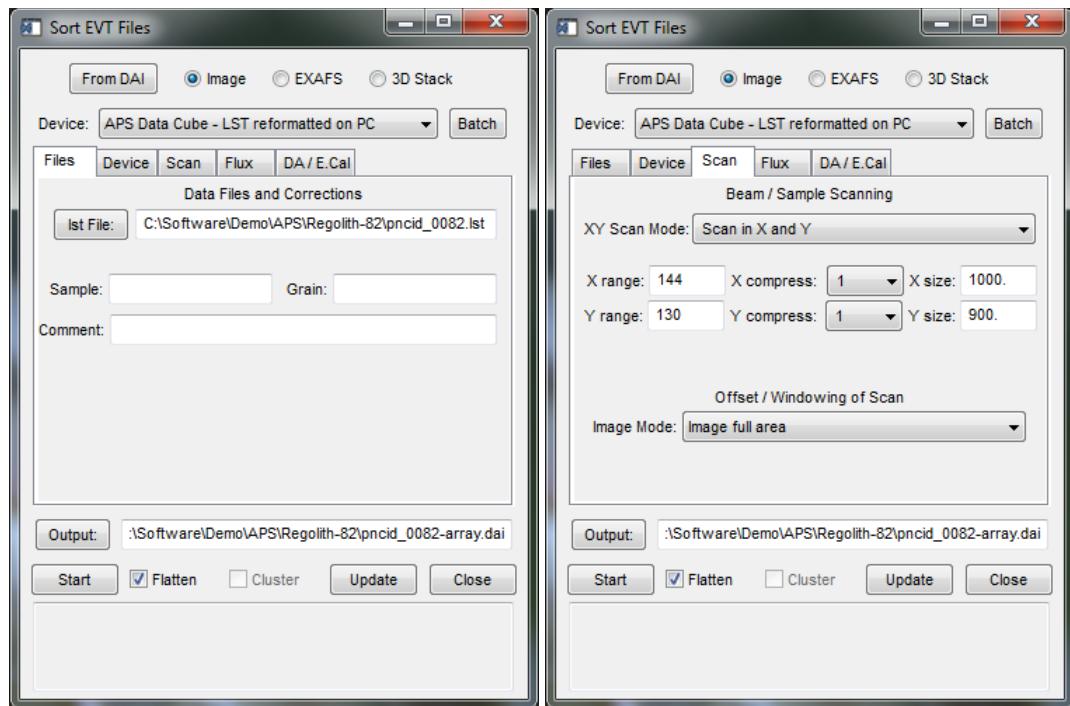
10. If the fit to the Compton peak remains very poor (e.g. there are prominent multiple-scattering peaks present), and effects detrimentally the fitting of incomplete charge-collection tails on all peaks, it may be more effective to move the upper View marker to sit on the exponential tail of the Compton peak, just above X-ray lines of interest (e.g. around 12.2 or 14 keV in the example above). Note that GeoPIXE will still include the scatter escape peaks in the fit.
11. Typically for SXRF data, disable the fitting of Tail parameters in the fit, if this combined with the scatter peak fitting makes the fit unstable. “Fixed” or “default” tail parameters can be used.

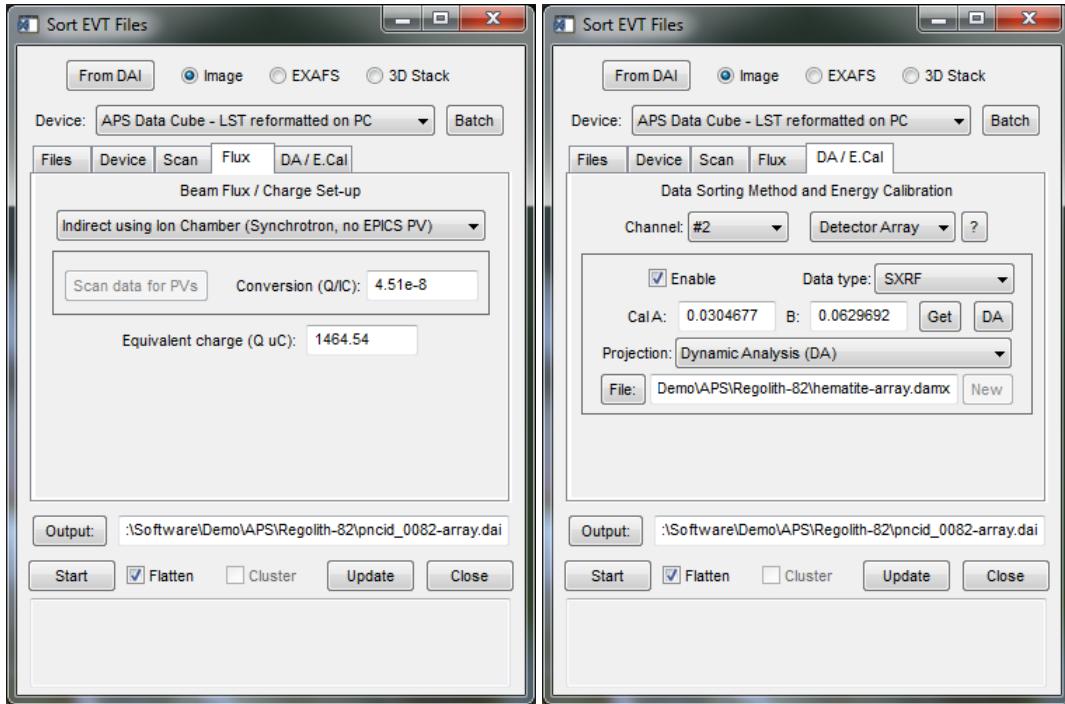
### Sort the LST file to project images

In the *Sort EVT* window select the “APS Data Cube” device and load the LST file “pncid\_0082.lst” using the “LST file” button. On the Flux tab make sure the conversion factor is set as previously. The scan dimensions are loaded from the LST file (see “Scan” tab). But the file does not contain energy calibration information, so the Cal parameters A,B are left at defaults (see “DA/E.cal” tab).

An array detector was used, so on the “DA/E.cal” tab select “Detector Array” in the drop-list labelled “Channel”. In order to enter the energy calibration for all detector elements make use of the file you saved before, which contains all fitted energy Cal parameters. Click on “Get” and load energy calibrations from file “pncid\_0082-fit.spec”.

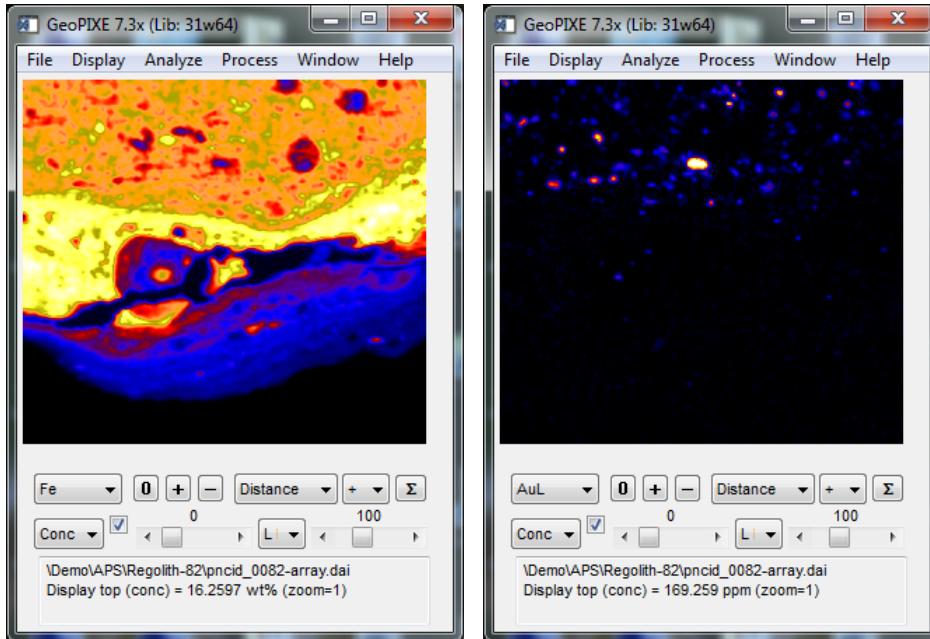
*See more detail about this example in the Workshop notes and worked examples.*





“Get” also enables/selects all detectors found in the spec file. If you had found a detector that was bad, deleted it from the array spectrum data before Adding spectra (select a spectrum by clicking on its row number and use the “Delete:” button in Spectrum Select after selecting “selected spectra” in the drop-list). Save these remaining array spectra without this detector for use with “Get” in future.

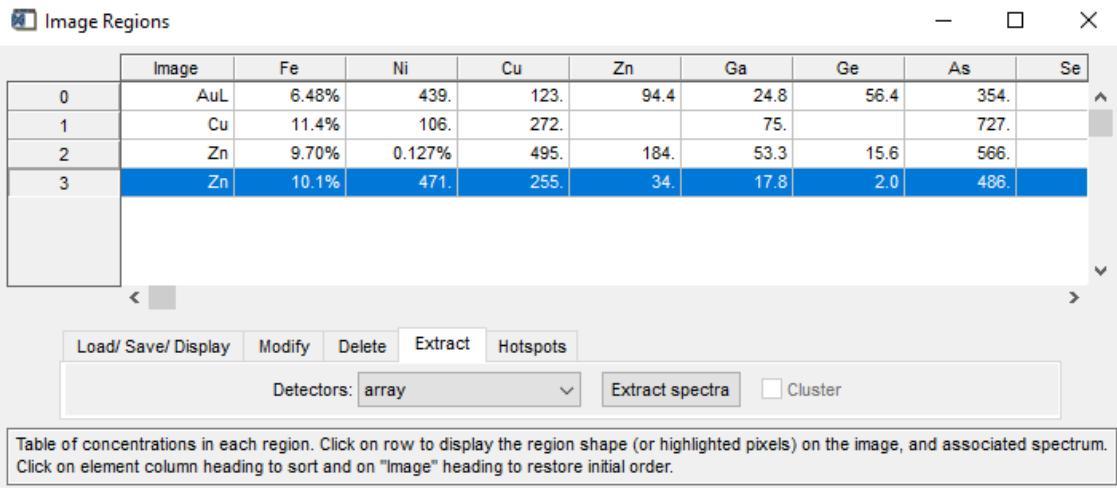
Now load the DA matrix file “hematite-array.damx”, and click on “Start” to start sorting events and projecting them into elemental images using the supplied DA matrix. The images appear in the main GeoPIXE *Image* window. Zoom (“+” button) these out to view them better.



## Image regions

In the image window, cycle through the elements using the drop-list on the left (and the mouse thumbwheel or

keyboard arrow keys). Of interest are hot-spots in Zn and Au. Select a “circle” or “ellipse” shape using the Shape drop-list in the centre and click and drag it out over each of these hot-spots (select using the left mouse button and move control points), first on the Au image and then on the hotspot in the Zn image. Click on the “ $\Sigma$ ” button for each to extract the average concentration of all elements in these regions directly from these quantitative images. The region analysis appears in the *Image Regions* window.



**Image Regions**

	Image	Fe	Ni	Cu	Zn	Ga	Ge	As	Se
0	AuL	6.48%	439.	123.	94.4	24.8	56.4	354.	
1	Cu	11.4%	106.	272.		75.		727.	
2	Zn	9.70%	0.127%	495.	184.	53.3	15.6	566.	
3	Zn	10.1%	471.	255.	34.	17.8	2.0	486.	

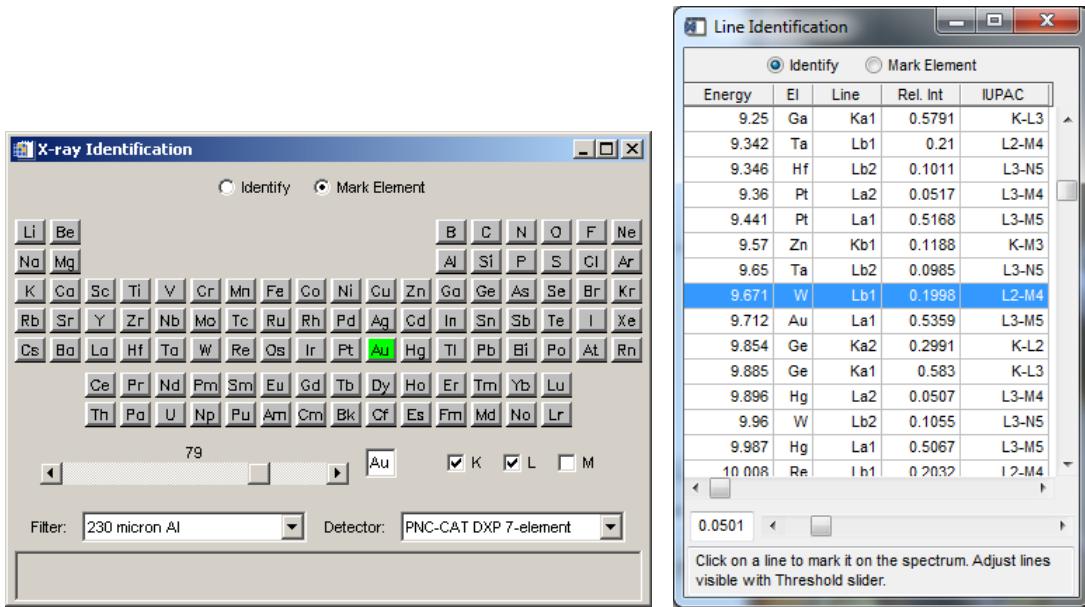
Table of concentrations in each region. Click on row to display the region shape (or highlighted pixels) on the image, and associated spectrum. Click on element column heading to sort and on "Image" heading to restore initial order.

Region (#0) would suggest an average concentration of ~100 ppm for Au in the hot-spot (scroll to the right to see the average for Au). We will need to test if this is correct. Save these regions as “pncid\_0082-q1.region”.

Close the *X-ray Spectrum Fit* window for now. Replay the LST file to extract spectra from these shapes using the “Extract spectra” button on the *Image Regions* window “Extract” tab. But first, select “array” from the detector channel drop-list to the right of “Extract” so that the spectral data from all detectors are combined together (corrected for Cal). This generates a set of spectra, one for each region. Click on a region row in the *Image Regions* window to see the shape on the image and the corresponding spectrum for that region in *Spectrum Display*.



Click on the first, which was set-up on the hotspot in the Au image. The red overlay on the spectrum shows the peak contributions plus background (shown in violet) ‘predicted’ using the DA images for all elements. Open the *X-ray Identification* window using the “?” button below the spectrum in the *Spectrum Display* window. Click on Au; there appear to be prominent Au L lines in this extracted spectrum. However, the ‘fit’ seems very poor at some energies (e.g. around 8.4 keV).



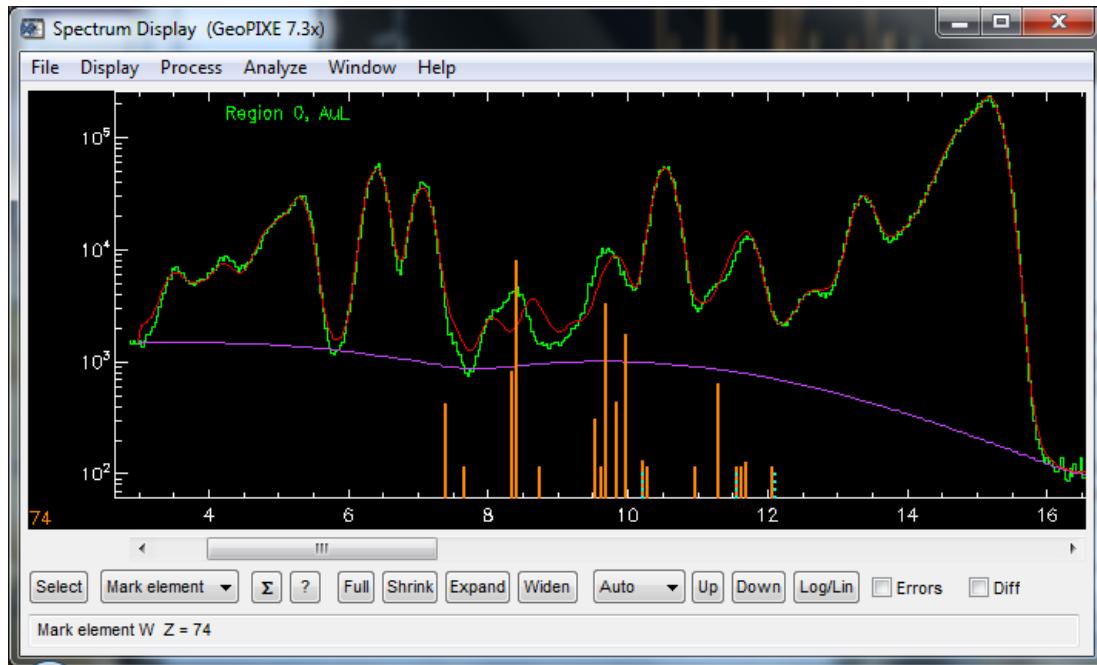
Now click on the Au row in *Image Regions*, and on “Au” in *X-ray Identification*. There is a very plausible Au L $\alpha$  peak shown in the spectrum. Note that the peak at 13.4 keV is Rb K $\alpha$ , not the Au L $\gamma$ 1. But, is the Au real?

Put the *X-ray Identification* window in “Identify” mode and click within the line list (this sets the marker type to “Identify” in *Spectrum Display*). Now click and drag the marker on the spectrum to 9.7 keV, over the Au L $\alpha$  peak. The *X-ray Identification* window shows other plausible line possibilities.

Click to the right of the relative intensity slider at the bottom to increment the relative intensity threshold to hide very minor lines. Near to Au L $\alpha$  are the lines for W L and Ge K. You can also stay in “Mark Element” mode and scan the atomic number by clicking on the arrows beside the atomic number slider. Click on “W” to display the W lines. There does appear to be a W L $\alpha$  line as well in the spectrum. So is the 9.7 keV peak due to Au L $\alpha$  or W L $\beta$ ? We need to add W to our analysis.



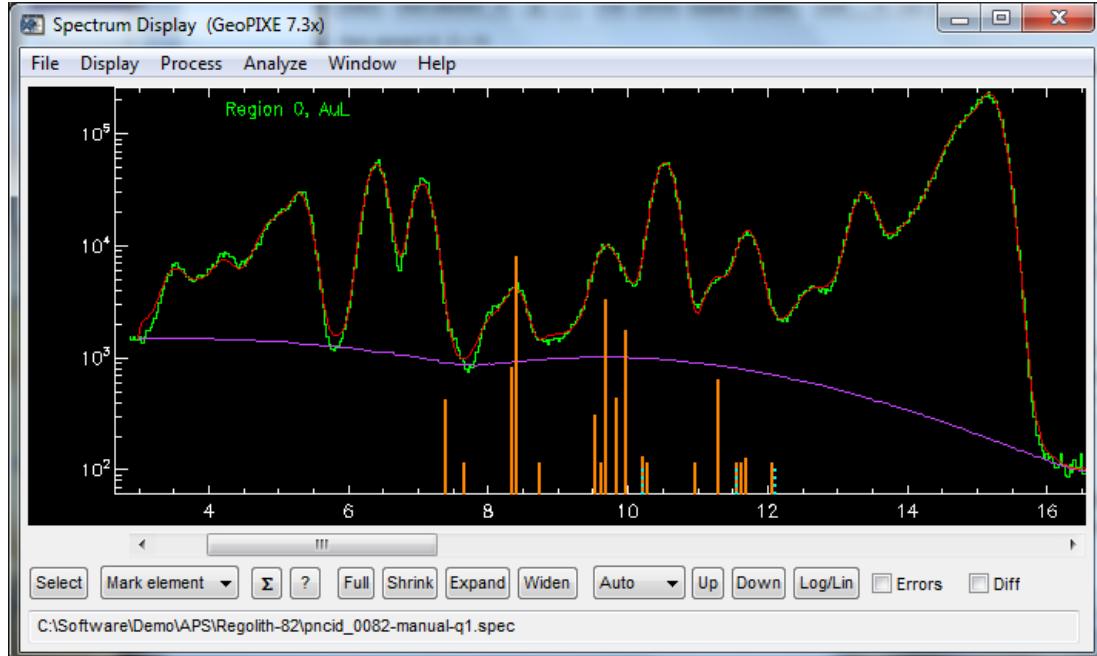
Fitting this spectrum using “Hematite-array.pcm” results in this fit, which clearly shows a misfit at the position of the W L $\alpha$  peak.



### Regenerate images after adding extra elements

Load the “pncid\_0082-fit.spec” spectrum file again, select “Prev” in *Spectrum Select* to display just the first spectrum, and open the *X-ray Spectrum Fit* window again. You might set View markers in *Spectrum Display* (select “View” from drop-list at the bottom on the left, and then click first to the right of the spectrum to set the high marker and then to the left to set to low marker; click and drag to move markers) and click on “Widen” to display a portion of the spectrum.

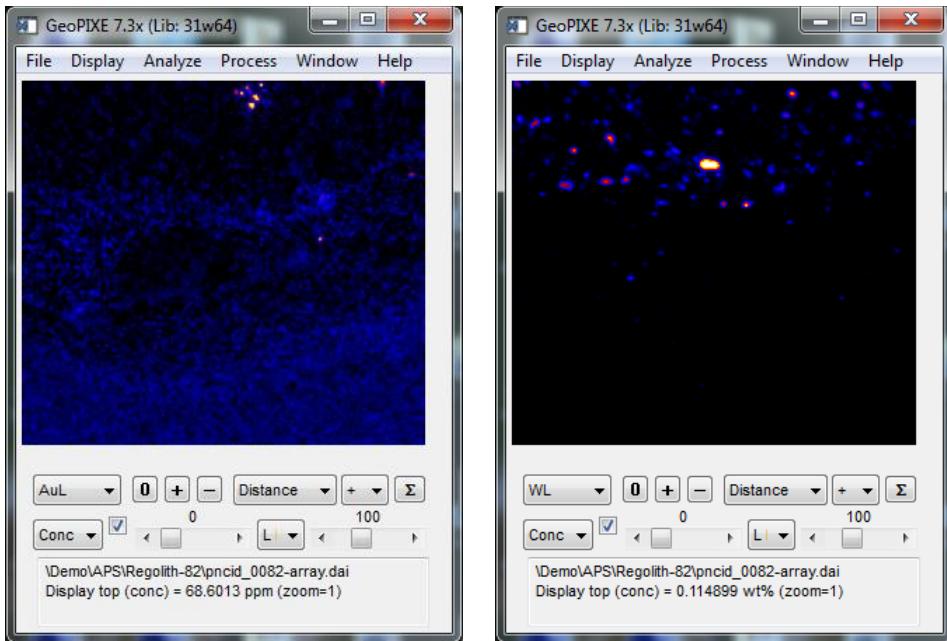
Now click on “W” twice in *X-ray Spectrum Fit* (first to green for K lines, next to yellow for L lines) and hit “Fit: One” to fit the spectrum again, this time including W (you may need to enable fitting energy calibration the “Cal” and peak widths using the “FWHM” checkbox controls). Save the new fit-setup as “hematite-with-W.pcm”.



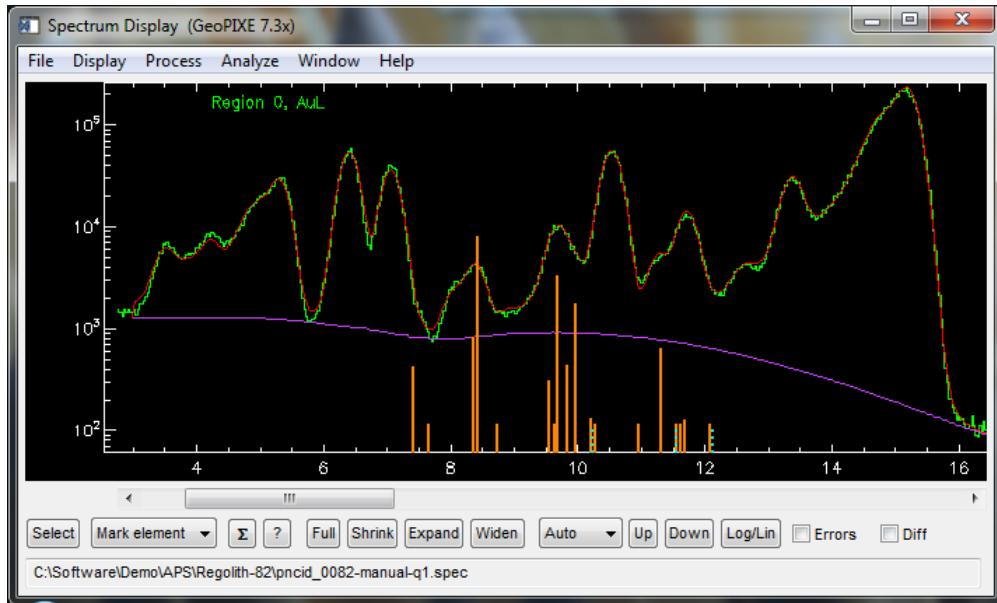
Then generate the DAM matrix (“Generate DA matrix” button) and save it as “hematite-with-W.damx”. In the *Sort*

EVT window, select the new DAM file and Start it sorting again. Save these images as “pncid\_0082-x.dai”.

The Images will now include W. Now the hotspot appears in the W image, as were most of the hotspots in Au. Evidently, this image area contains only a little gold, and the peak at 9.7 keV was due predominantly to W L $\beta$ . However, there are some real gold particles in the top of the field.



Let's confirm this by loading the “pncid\_0082-q1.region” file again into *Image Regions*, and clicking “Update: All”, which applies these regions to the new images. Now the Au analysis disappears. Yes, evidently the main hotspot was tungsten not gold. Save the regions again in file “pncid\_0082-q1.region”.



Now select region #0 again and fit it (“Fit: One”) using this new fit set-up with W included. The quality of the fit is very good, which tends to confirm that we have included all important elements. Try removing W from the fit (right-click on “W” in X-ray Spectrum Fit to temporarily disable W; you can left-click it again later to re-enable it) and fit the region #0 spectrum again. Clearly, this fit quality is inferior, indicating that W is essential.

## Summary

This example illustrates the main data flow from initial total spectra, fitting, DA matrix generation and image projection.

It then showed how these images can be probed and tested for accuracy. In this case, we found that an extra element (W) was needed, which was not really noticed in the initial total spectrum fit, probably due to its minor nature in the overall image area. However, it showed up clearly in the “Au” image, which could be tested by spectrum extraction from a small region.

*TIP: Often missing elements will appear in the “Back” background image, which mainly reflects the spatial variation of the continuum components of the spectrum if this element does not strongly overlap with an included element such as in the present case. Always probe significant features in the “Back” image and check the fit to the extracted spectra for signs of missing elements.*

This example illustrates that any feature for any element that is regarded as important to an investigation can be probed in detail and the quality of the fitted spectrum checked with and without an element of interest. Hence, full-spectral data collection and the DA method in GeoPIXE enables full testing, or quality control, on all inferred images.

## Verification of Images using Regions

Once images are projected using Dynamic Analysis, they can be interrogated for concentration within features seen in images. Load the image file “data\CSIRO\Sample11\Sample11-chalco.dai”, which shows areas of chalcopyrite ( $\text{CuFeS}_2$ ) and quartz ( $\text{SiO}_2$ ) and veins of Fe oxide and barite ( $\text{BaSO}_4$ ). Open the *Image Regions* window (“Windows→Image Regions” menu). Select a shape, to define an area of the image, using the drop-list in the centre of the *Image Display* window, below the image. Select “Spline 10” and drag out the spline, first as a circle (click left mouse button, hold and drag), then by selecting and moving individual control points. Click on the “ $\Sigma$ ” button to integrate the region defined. The results are shown as a new row in the *Image Regions* window.

Load the file “Sample11-chalco-q1.regions” into *Image Regions*, which shows several regions selected on features seen in the images. The “Image” column labels the image that was displayed when the “ $\Sigma$ ” button was pressed; this is most likely the image with the feature. For example, note the hot spot in As, as seen in the As image and region 2 (click on row 2 of the table to display the shape on the image, or images if several image clones are open).

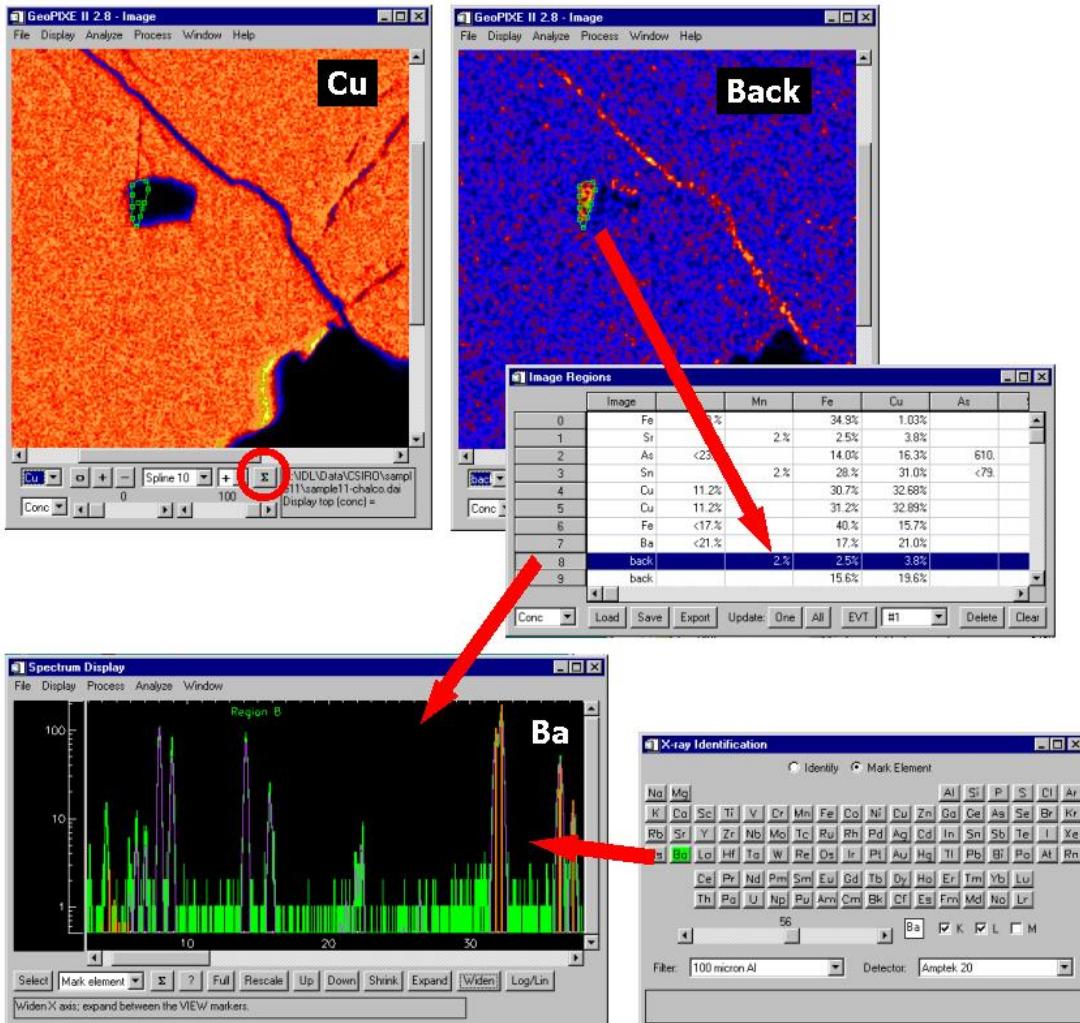
## Extraction of Spectra from Regions

The spectra associated with each region can be extracted from the event data by using the EVT button in the *Image Regions* window. Before using this feature make sure that the regions have been saved to a file (or read from a file, as in this example). Use the drop-list to the right of the EVT button to select which ADC to extract spectra for. If you have a *Spectrum Display* window open, the results of the region extraction will be displayed in this window.

Open *Spectrum Display* now, if it is not open. Select ADC #1 from the drop-list in *Image Regions* and click on the EVT button and select the EVT file (“Sample11.evt”) and spectrum file name (the defaults are usually what you want, so just click on “Save”). A progress bar appears as the EVT file is scanned for all events within the selected shapes. The resulting spectra, one for each region, are automatically loaded into *Spectrum Display*, and the first one displayed.

## Linked Display of Spectra from Regions

Click on a row in the *Image Regions* table to show the shape on the image, and the corresponding extracted spectrum will be displayed in *Spectrum Display*, with a DA reconstruction overlay in red and background in violet. The overlay is constructed by taking the elemental concentrations integrated from the image and using these to scale the pure element spectral components (which were calculated in the *X-ray Spectrum Fit* and stored in the DA matrix file). The result can be compared with the PIXE/XRF spectrum to verify the accuracy of the images in this region. A missing element for example, not in the original element fit list, would produce a bad “overlay” here (green peaks not accounted for by the red overlay).

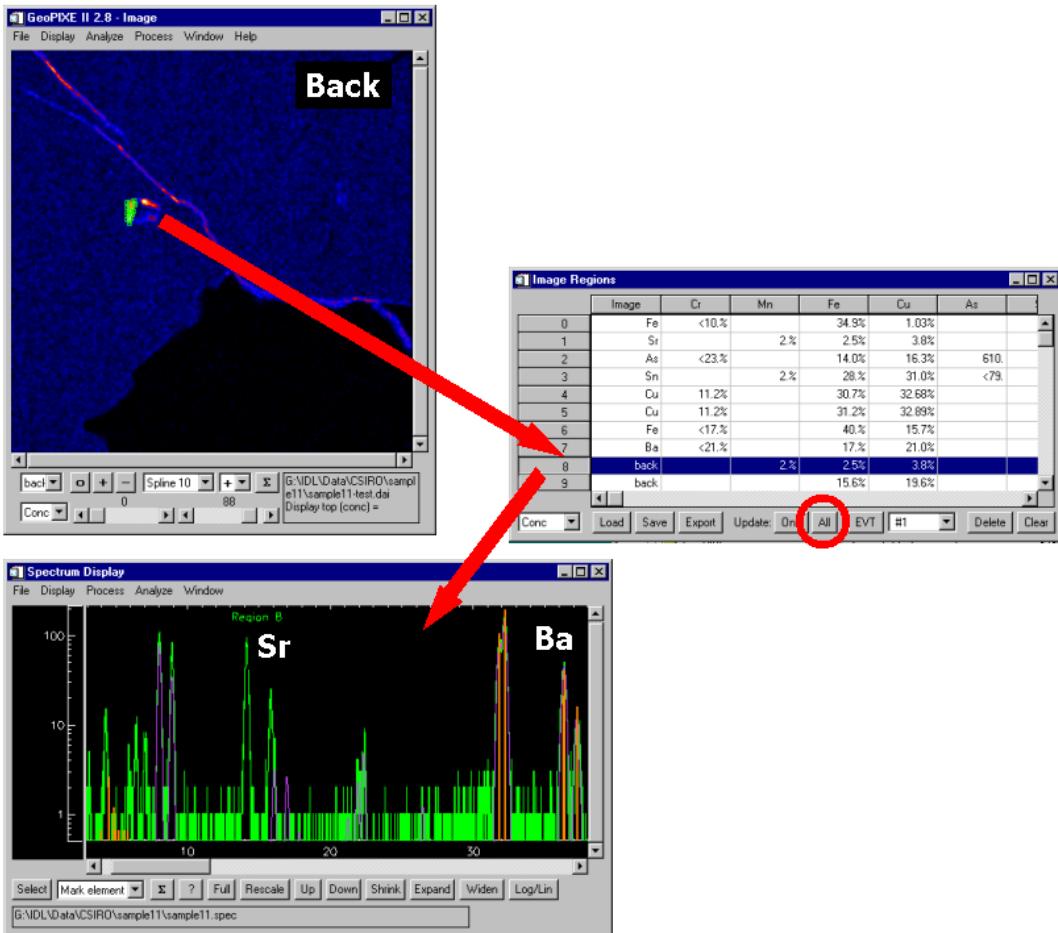


### Diagnosis of Missing Elements

One image called “Back” is projected to track background intensity. The intensity largely reflects bremsstrahlung intensity and mean atomic number. However, any elements that were not included in the fit, but occur in the image area, may produce features in Back as well. Hence, it is a good idea to always check the Back image for hot spots, etc. The example above shows the spectrum extracted from a hot spot in Back. However, in this case it’s just caused by barite, as indicated by the good “fit” and strong Ba K lines.

Try this test: Load the original total PIXE spectrum for Sample11 again (“sample11.spec” as before, use the *Spectrum Display* “Select” button, and the *Spectrum Select* “Prev” button, and the *Spectrum Display* “Process→Fold” menu), and open *X-ray Spectrum Fit*. Load the fit set-up file “Sample11.pcm”. Now remove the element Sr from the fit (shift left-click to remove entirely, or right-click on Sr to disable it). Now fit the spectrum without Sr (note the misfit on the Sr K $\alpha$  peak at 14.14 keV) and then generate a DA matrix and save it as “test.dam”.

Open *Sort EVT*, if it is not open, and use the “From DAI” button to load sort set-up parameters from “Sample11.dai” that was made previously (see section above). Now load the “test.dam” file that you just created as the Dynamic Analysis projection file and change the output file name to “sample11-test.dai”. Click on “Start” to sort using this ‘incomplete’ DAM file.



Look at the “Back” image now. It contains much stronger features along the vein and in the inclusions that used to show Sr. In the *Image Regions* window, load the file “Sample11-chalco-q1.region”, and click on “Update All” to tell *Image Display* to re-integrate all regions for the newly projected images. Save these as “Sample11-test-q1.region”, and click on the “EVT” button to extract spectra as before (now the default output file will be “Sample11-test-q1.spec”).

*Spectrum Display* now shows these projected spectra with overlays. Click on row 8, which was the high Sr inclusion area as seen in the Back image. Now the spectrum shows large Sr peaks ( $K\alpha$  at 14.14 keV) without a corresponding “fit” in red (see figure above). Row 9, corresponding to the vein shows a similar effect in the spectrum. This would indicate that Sr is missing from the fit.

Normally, when this behaviour is encountered the extra element would be added to the fit to the original total spectrum, a new DA matrix would be generated, and the sort of the EVT file to project images repeated (load the previous settings using the “From DAI” button). Any old regions file could then be updated (“Update: All”), and resaved.

## PIXE Fluid Inclusion Analysis

In brief, the procedure for analysis of fluid inclusions follows these basic steps:

1. Extract the fluid inclusion spectrum using an ellipse shape surrounding the inclusion.
2. Create a 3-layer yield model comprising layers for the host mineral, the fluid layer, and the host. Use layer thicknesses of d, T, 200 microns, where “d” and “T” are the depth and thickness of the inclusion.
3. Fit this spectrum in *X-ray Spectrum Fit* using a fit set-up that incorporates this 3-layer yield model.
4. Open the *Fit Results* window and select the fit results row for this fit (click on row label).
5. Open the *Results Property* window, using the “Properties” button in *Fit Results*.
6. Enter the fluid inclusion geometry parameters into the entry fields and hit “Apply” to update the results in the

- selected row of *Fit Results*.
7. Save the results from *Fit Results* into a pfr file, including the input parameters.
  8. The results can be exported following the “Export” button prompts.

The ellipse shape is used to select all signal associated with the inclusion. The selection is used to improve signal-to-background. Use it to also exclude any signal in the image due to nearby objects (e.g. surface cracks, solid-phases, etc.) and other inclusions.

In creating the 3-layer yield model, do not worry too much about the specifics of the thickness of the first 2 layers (i.e. inclusion depth d and thickness T) as these will be refined via the *Result Properties* window dialogue later in the procedure.

Typically, in the fit set-up, set the “View 0,1” markers on the spectrum to about 36 keV (for View marker 1) down to just below the Si peak (for a quartz host, using the left marker: View 0) (select View markers in Spectrum Display and click and drag them into position, starting with the right marker). This range encompasses all elements from Si through to Ba (K lines). Use the “Use View” button in *X-ray Spectrum Fit* to transfer the View marker energies into *X-ray Spectrum Fit*. For data collected with a thin filter such as Be, will use the “Boost” background algorithm option, to better track the shape of the background caused by filter absorption.

Click on a row of the *Fit Results* window and use the “Properties” button to open the *Results Properties* window to manipulate properties of the selected fit. Context sensitive help in the *Results Properties* window give details of the various parameters. View the help in the box at the bottom of the window, as you move the cursor over various fields and options.

The “Inclusion Shape” parameters in the *Results Properties* window define the physical dimensions of the fluid inclusion. “X length” and “Y width” are the length and width of an ellipse that has the same area as the fluid inclusion, as observed under the optical microscope (make sure the microscope graticule is calibrated to determine dimensions in microns). For irregular shaped inclusions, try to estimate the dimensions of an ellipse with the same area as the inclusion cavity. For a somewhat square inclusion, the equivalent ellipse may be slightly longer and slightly narrower to achieve equal area. Equal area means we are in a better position to estimate inclusion volume, which affects the total mass of contained fluid, which is necessary to relate measured signal to concentration.

“Mid-plane” is the depth of the mid-plane of the inclusions as observed under the microscope by racking the focus up and down (the scale on the focus range or Z axis of the microscope will need to be calibrated – e.g. using cover-slip thickness). For most inclusions, the measurement of the mid-plane depth can provide a reasonable average inclusion depth. “Thickness” is an estimate of the thickness of the equivalent ellipsoidal inclusion volume in the vertical “Z” direction, out of the image plane of the microscope. This is best determined directly using a spindle stage, which enables the sample to be rotated and viewed side-on. “Mid-plane” and “Thickness” are coupled to “Inclusion Depth” in the “Host Mineral” parameter section. Read the context-sensitive help on each for details. “Mid-plane” is assumed to be the most accurate, by default. Hence, a change to “Thickness” will modify “Inclusion Depth”. Similarly, changing “Inclusion Depth” will modify “Thickness”. If a spindle stage is used, it may be necessary to change “Mid-plane” until the desired “Inclusion Depth” is achieved.

The “Beam Selection Area” parameters refer to the region sub-set of the image area used to select the signal associated with the inclusion. Typically, an ellipse shape is used on the image to select signal from the inclusion. This ellipse is usually a little larger than the inclusion to encompass all signal. Optionally, use the exclude mode (“-“ on the drop-list) to exclude any nearby cracks or solids that overlap with the selection ellipse. If the ellipse shape is used, the “X size” and “Y size” parameters will be set in *Results Properties* from the ellipse dimensions. The “Shape” parameter will then be set to “Ellipse”, referring to the shape of the ellipse selection region. Other options here refer to “XY scan” for a rectangular selection area (e.g. entire area), or to “Gaussian”, which refers to a defocused beam used to bathe the inclusion in beam. The latter is seldom used now as a finely focussed beam, and fast raster scanning to evenly illuminate the inclusion is preferred.

The “Inclusion Contents” parameter section refers to how the inclusion should be modelled in order to calculate X-ray yields. There are 3 “Bubble” options. “None” means no bubble, in which case it is assumed that we are dealing with a small bubble, such as in a brine inclusion, and we wish to enter the density as the homogeneous density of the inclusion (see the context-sensitive help, and the notes under the drop-list). “Large dilute” is used for dilute aqueous inclusions where it can be assumed that the fluid shell or meniscus at room temperature has a density of 1. Again, we enter the homogeneous density (which will be less than 1 in this case), but the modelling then calculates the size of a central

vapour bubble surrounded by a density 1 fluid shell that yields this overall density. “Fluid type” is a drop-list that selects the broad composition band for the inclusion, as input to the yield calculation.

If it is necessary to modify the choice of detector or filter for some fluid inclusion results, this can be done using these steps:

1. Select the fluid inclusion results in Fit Results (drag select a range or rows).
2. Open *Results Properties*, if is not open, and select “Thick Target (1 layer)” using the “Analysis Type” drop-list at the top of the *Results Properties* window.
3. Select the new detector using the detector drop-list.
4. Return to the “Fluid Inclusion (3 layers)” setting of the top drop-list.
5. Click on “Apply”. The changed detector will now be applied to all selected fluid inclusion results, preserving all other settings for each.

## Refitting the Spectrum Keeping Geometry Parameters

If you need to refit the spectrum, to add an element for example, but would like to keep the existing fluid inclusion geometry parameters, then follow this procedure:

1. Load the spectrum for the fluid inclusion. This is usually the ellipse region, and the file usually have a name ending in ‘-q1.spec’ or ‘-e.spec’.
2. Open the *Fit Results* window and load the saved fit results (extension .PFR and mostly likely the same name as the region and spectra files).
3. Open the *X-ray Spectrum Fit* window and load the fit set-up (PCM) file (e.g. ‘inc-d10-T10.pcm’) and make any changes to it as required (e.g. adding a new element).
4. Now select the row of the *Fit Results* for this spectrum, by clicking in the row.
5. Hit “Refit” in the *X-ray Spectrum Fit* window. This will refit the spectrum but preserve all geometry parameters. You can view these settings by opening the *Results Properties* window.
6. Save the results back to the PFR file, and export as needed.
7. To repeat for the next spectrum, clear the *Fit Results* window, load the new ellipse spectrum and the results file, select row of *Fit Results* and hit “Refit”.

## Subtraction of Scattered Beam Contributions

Beam scattering from slits gives rise to a wide diffuse beam extending for several mm, which can excite X-rays from surrounding phases containing major elements of interest. To subtract contributions due to beam scattering, also collect data on a blank area near to the fluid inclusions of interest and follow these steps. (Use the example in Data\CSIRO\Scatter\.)

1. Fit the fluid inclusion as usual (see above).
2. Fit the blank spectrum using the same fit set-up.
3. *Fit Results* should now contain 2 rows; select the first row by clicking on it.
4. Open *Results Properties* and set all fluid inclusion parameters and click on “Apply”.
5. The first row should show the results for the fluid inclusion, ignoring scattering. Note that it is not necessary to correct the blank for geometry as only the peak areas and integrated charges are used.
6. Save these results to a PFR file. These results still enable re-fitting to be done later.
7. Now use the drop-list in *Results Properties* under Corrections to select “Subtract Scatter blank spectrum” and click on “Apply”.
8. The results table now shows one row for the fluid inclusion with the scattered contributions, measured in the blank, subtracted.

*Note: Once the subtraction has been done, it cannot be reversed or changed. This is why it is best to save the results before this step and save the final (subtracted) results to a separate file, suitably named.*

## Subtraction of Host Mineral Contributions

X-rays from elements excited in the host mineral can be subtracted with this procedure:

1. Fit the fluid inclusion and the host mineral spectra, and enter fluid inclusion parameters for both, as above for subtraction of scattered beam.
2. Also, refit the host spectrum using an appropriate thick-target fit set-up and yield calculation.
3. There should now be 3 rows in *Fit Results*, two with fluid inclusion parameters set, and one thick target.
4. Save these results to a PFR file. These results still enable re-fitting to be done later.
5. Now use the drop-list in *Results Properties* under Corrections to select “Subtract Matrix blank spectrum”, and click on “Apply”.
6. The results table now shows one row for the fluid inclusion with the matrix or host contributions, measured in the blank, subtracted. Note that it is not necessary to correct the blank for geometry as only the peak areas and integrated charges are used.

*Note: Once the subtraction has been done, it cannot be reversed or changed. This is why it is best to save the results before this step, and save the final (subtracted) results to a separate file, suitably named.*

### Refitting Fluid Inclusion Spectra

If you need to alter the fit to a fluid inclusion spectrum, to add an element for example, where you have already set-up inclusion parameters in *Results Properties*, then follow these steps:

1. Select the results row in *Fit Results* corresponding to the fluid inclusion spectrum.
2. Click “Refit” in the *X-ray Spectrum Fit* window. This refits the spectrum and updates *Fit Results* using the same *Results Properties* as before.

### Fitting Spectra using Cuts

Close the *X-ray Spectrum Fit* window, if it is still open. Load this example spectrum from “data\CSIRO\Fiji\Fiji-2x.m.spec”. Then use the *Spectrum Select* window (“Select” button, then “Prev”) to display just the first spectrum.

This spectrum comes from a list-mode file that uses the top ADC bit to tag X-stepping in X-step mode images. This produces twin spectra, one in each 4K half of the spectrum. Use the menu “Process→Fold” to combine these into a single 4K spectrum.

Sometimes there are problems with detectors that result in distortions of the spectrum, such as excessive, distorted un-rejected pile-up or in the example below, satellites to peaks. The spectrum below was collected using a Canberra Ultra LE Ge X-ray detector (optical reset) and a Canberra 2060 digital signal processor (DSP). The default inhibit period following a reset is just ~300 µs. With the 2060, this caused satellite peaks on the right, *high-energy* side, of peaks. This can be seen clearly for Ag K $\alpha$  (22.1 keV) and Te K $\alpha$  (27.5 keV) as a hump on the high-energy side. Lengthening the reset period to 2.5 ms cured this problem. However, this data remained with the distorted peaks.

This spectrum was analyzed by excluding portions of the spectrum from the fit, and the DA matrix projection, by using Cuts. Open the *Cut Setup* window, using the *Spectrum Display* “Window→Cuts Setup” menu. This switches the marker mode in *Spectrum Display* to Cuts.

### Types of Spectrum Cuts

There are two types of cuts. One uses 2 markers (“Cuts” on the marker drop-list) to define a simple region based on an energy range between these two markers. Position the high-energy marker first, then the low energy, and hit the “Σ” button in *Spectrum Display* to define a simple cut (with marker drop-list still on “Cut 0,1”).

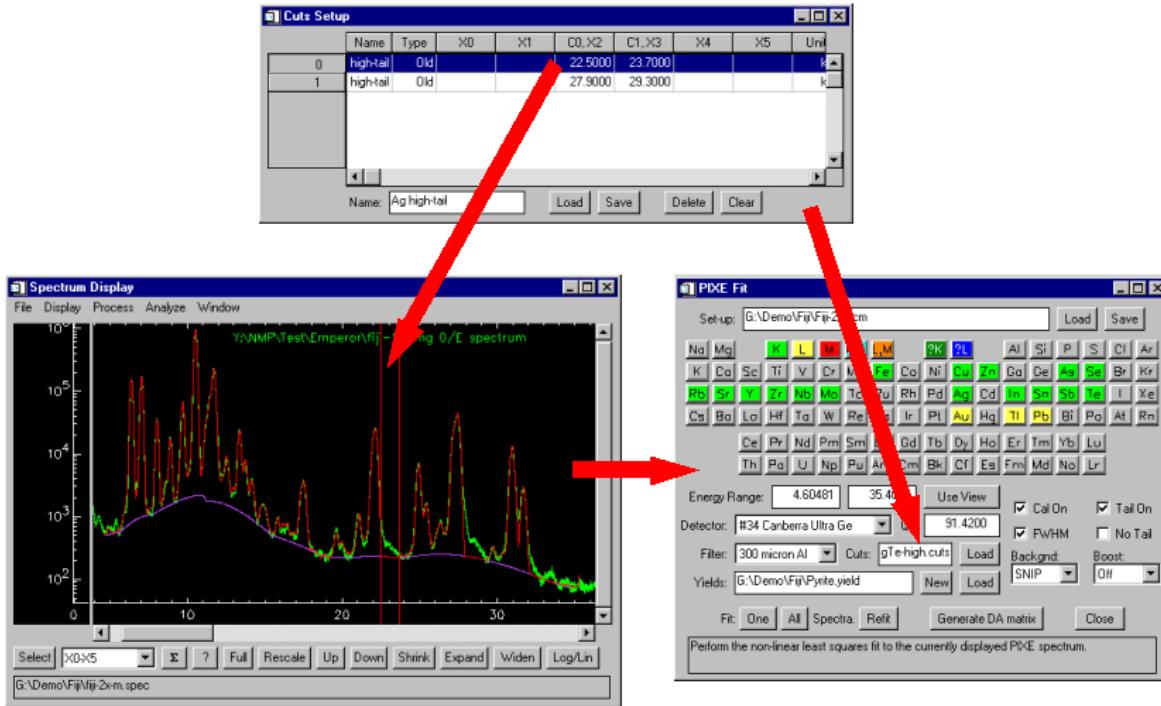
*If the same HIGH marker is “grabbed” by the cursor, then move further to the left to position the LOW marker. You can reposition markers by left-clicking and dragging.*

The *Cuts Setup* window now shows a new row with the cut energy range, plus the integrated counts in the spectrum in the range. You can give this cut a name by typing in the “Name” entry box at the bottom of the *Cuts Setup* window and hitting carriage-return or “Enter”. This “name” will appear on the ‘element’ drop-list in the output *Image Display*.

Another type of cut uses 6 markers (X0-X5) to define an energy range (X2-X3), plus two background areas on each

side (X0-X1, X4-X5). These are used to do background subtracted area extraction from peaks, or to sort event data using cuts on peaks to project images based on simple peak counts after background subtraction; more on these later.

The simple 2 marker cuts are used to define regions of spectra to exclude from the fit. “Clear” any cuts you have made, and “Load” previous cuts from the file “AgTe-high.cuts” in the “Fiji” directory. Click on a row in the *Cuts Setup* table to display the corresponding cut on the spectrum. They are positioned on these problematic high satellites.



## Fitting Using Cuts

Now open the *X-ray Spectrum Fit* window (“Windows→ “X-ray Spectrum Fit” menu) and load the PCM file “Fiji-2x.pcm”. This fit set-up file makes use of these cuts.

*Now the absolute file paths may be wrong for your system, so if any errors are encountered, click on the “Load” button opposite “Cuts:” and navigate to the file “AgTe-high-cuts”. Similarly, click on “Load” opposite “Yield:” and load the PIXE yields from “Pyrite.yield”. Save the PCM back again with these updated paths.*

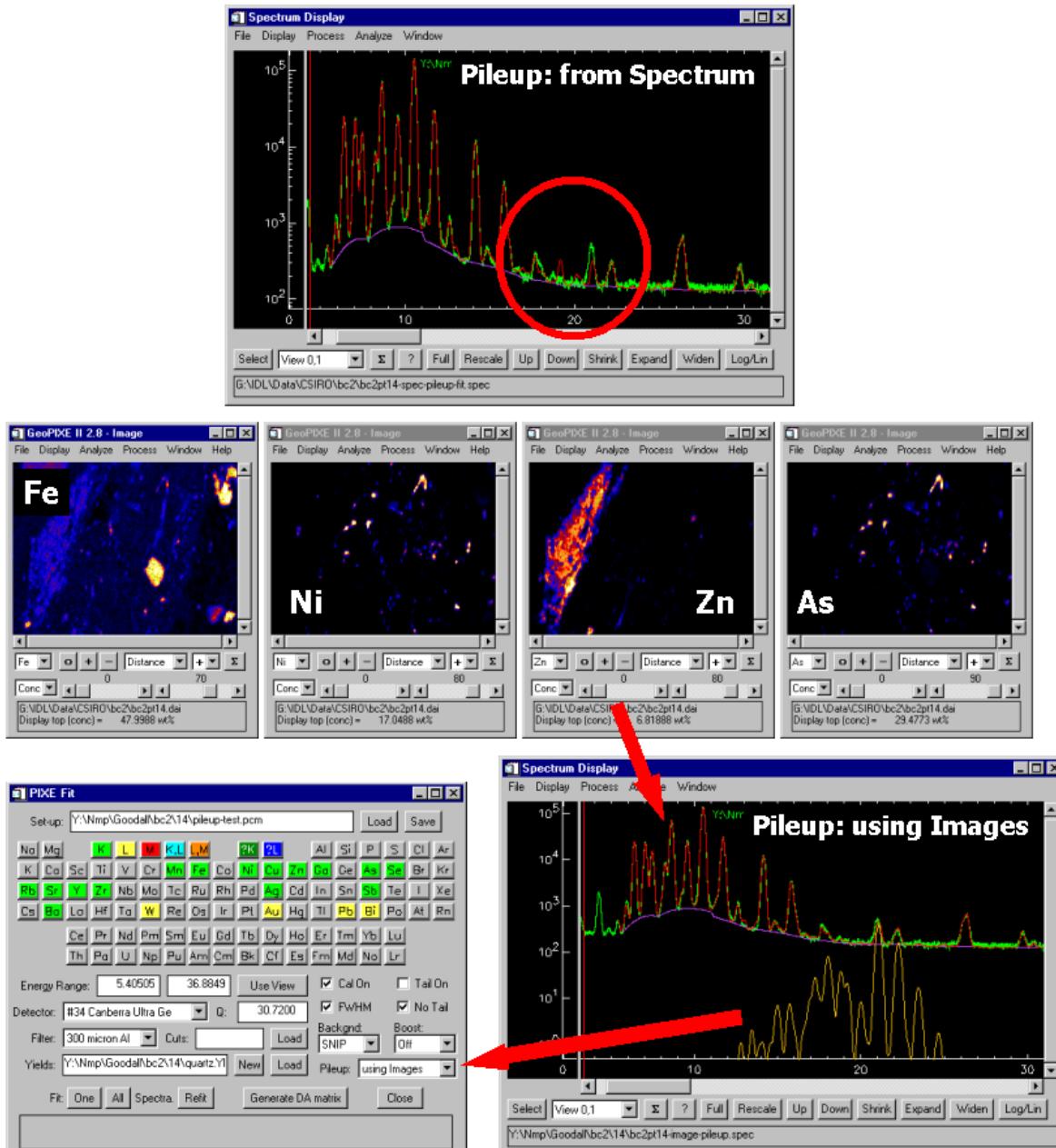
Click on “Fit One” to fit the spectrum. The fit now considers all channels in the selected energy range but excludes all cuts. This is why the fit (shown in red) dives down to the right of the Ag and Te K $\alpha$  peaks. Similarly, the DA matrix excludes these cuts and can be used to project accurate elemental images that reject the effects of this particular spectral distortion.

## Fitting Spectra for Images with Complex Pile-up

The type of pile-up modelling can be selected using the “Pileup” drop-list in *X-ray Spectrum Fit*. Normally, a pile-up element is used in PIXE/XRF spectrum fitting; select this with the “from Spectrum” option. In this mode, the relative intensities of the pile-up element lines are calculated from the intense lines in the spectrum being fitted. GeoPIXE calculates pile-up lines to second order (3 pulse pile-up).

However, if the PIXE/XRF spectrum corresponds to a scanned image area using a microbeam then the nature of the pile-up will have changed with position across the image. In other words, the major intense X-ray lines and the resulting pile-up relative intensities will have changed with pixel.

The following example illustrates this effect. Load the spectrum file: "data\csiro\bc2\bc2pt14.spec" and open *X-ray Spectrum Fit* and load the PCM file: "pileup-spec.pcm" from the "bc2" directory. Fit the spectrum and notice the quality of the fit around energies 17-22 keV. The poor fit is because the pile-up relative intensities have been calculated from this spectrum, and hence conclude that As and Zn are the dominant elements and should pile-up together. However, it is clear from the spectrum that there is little As K $\alpha$  + Zn K $\alpha$  pile-up at 19.14 keV (red overlay, but no green raw data). This is because As and Zn do not occur together spatially anywhere in the image area (see the images below). This can be seen by loading the associated images from image file "data\csiro\bc2\bc2pt14-m.dai".



A better approach in this case is to calculate pile-up relative intensities using direct products of image pixel counts. This can be done using the "Display→Pileup→using Image products" menu in *Spectrum Display*. This calculates intensities of pile-up components from products of image intensities on a pixel-by-pixel basis.

Choose the dominant elements in the pop-up requester (Fe, Ni, Zn, As and Sr in this case; you can choose "Load" from the pop-up requester and load the file "pileup.select"). Now the peak at 19 keV is weak, reflecting the lack of spatial

association of Zn and As. However, the relative intensities now show a strong peak at about 18 keV, apart from the strong As K $\alpha$  + As K $\alpha$  pile-up at 21 keV. This 18 keV has a strong component from Ni K $\alpha$  + As K $\alpha$  pile-up. This is because these elements occur together, spatially in the image. So, although Ni is not a strong element overall in the spectrum, it makes a very significant contribution to the pile-up.

Now, in *X-ray Spectrum Fit*, select the “using Images” pile-up option and fit the spectrum again (“Fit: One”). Now *X-ray Spectrum Fit* uses the pile-up model as calculated above, and currently stored with the spectrum, to provide a much improved fit to the spectrum.

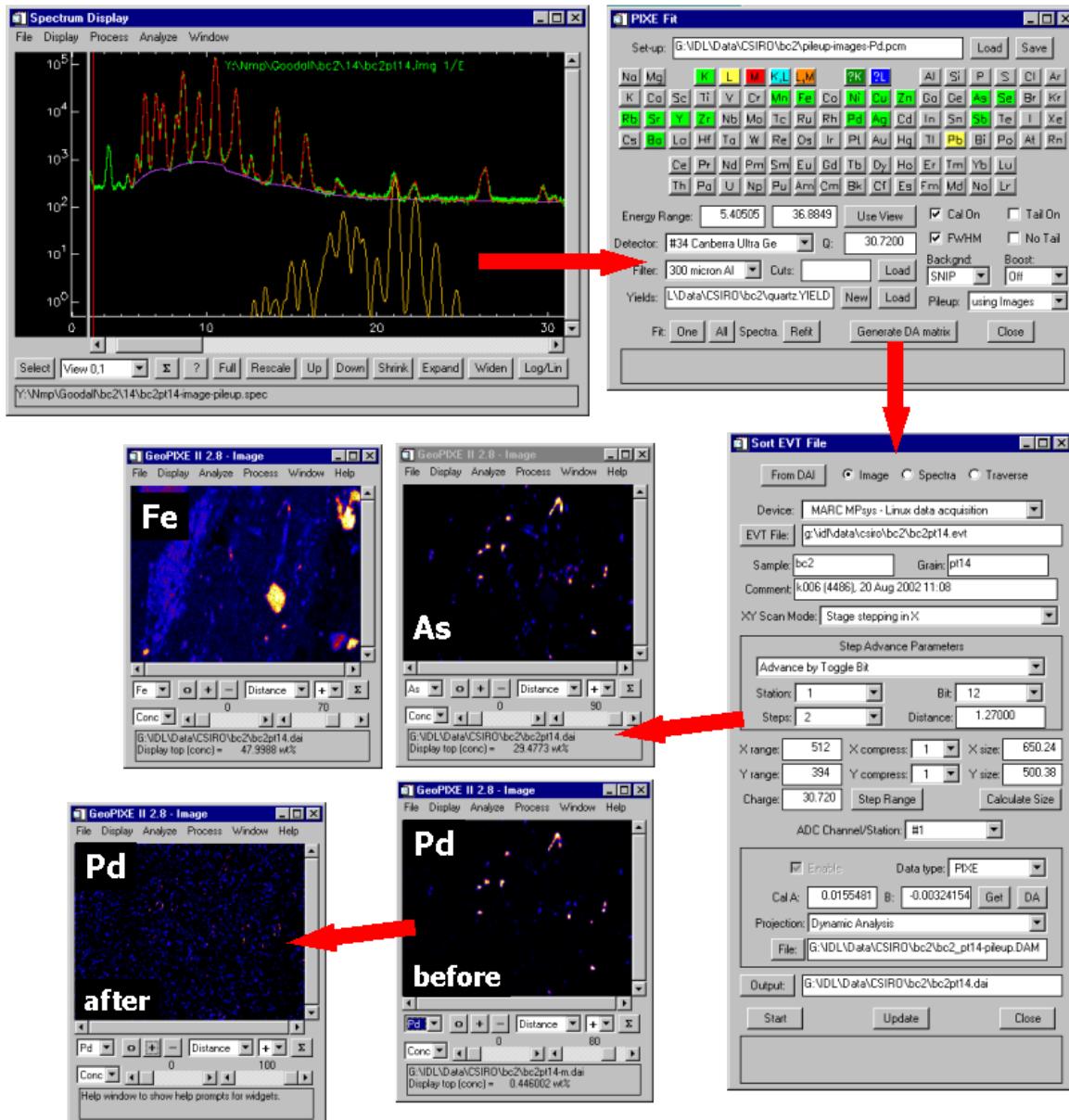
*Note that the Spectrum Display, X-ray Spectrum Fit and Image Display windows are all coordinated for these calculations, and all need to have the appropriate data loaded and operations performed, as outlined above.*

## Correction of Images for Complex Pile-up Effects

We can continue this example (“data\csiro\bc2\bc2pt14”) to build pile-up corrected images by first following the steps listed above under “Correction of Images for Pulse Pile-up Effects”.

Now, fit the spectrum (it should still include the image pile-up calculation overlay) in *X-ray Spectrum Fit* including “Pd” in the fit (left-click on “Pd” to select it for K lines; it appears green), and using the “using Images” pile-up option. (You can load these parameters from the file “pileup-images-Pd.pcm”. ) Now, fit the spectrum again, and then generate a Dynamic Analysis matrix using the “Generate DA Matrix” button. This builds a DA matrix that does NOT include any pile-up element rows, because these will be treated in a separate step described below. Save it with the name “bc2\_pt14-pileup.DAM”.

Open *Sort EVT* and reload the image set-up parameters from “bc2pt14.dai” using the “From DAI” button and locate the EVT file. Now, under the projection file entry load the file “bc2\_pt14-pileup.DAM” and click on the “DA” button to use the energy calibration as fitted and contained in the DAM file. Now click on “Start” to sort the event data using this matrix.



To apply some image smoothing to the lower statistics images, open the *Image Operations* window and click on “Get”. Then select the image file “bc2pt14-m.dai”, and select all elements in the pop-up requester, and click on “OK”. This applies all the same digital filter operations to all images that were performed to this file and are stored as history records in the image file header.

The images generated will include the element Pd. This was chosen as it is not present in these samples but has lines that overlap with the As K + As K pile-up. Due to the strong As pile-up, the Pd image contains strong artefacts due to pile-up, up to an apparent maximum of about 0.5%. Ag shows artefacts as well.

Now invoke the *Image Display* menu item “Process→Correct→Image Pileup” to subtract pile-up contributions. Load the file “pileup.select” in the pop-up requester, and click on “OK”. This process corrects all images for pile-up contributions.

*Note: this makes use of the loaded images and also intensity data contained with the spectrum and image pile-up model in Spectrum Display. So, Spectrum Display must contain the spectrum and Image Pileup model overlay.*

The Pd image now shows no significant pile-up artefacts, only subtraction noise, and shows an average (over whole

area) or less than 1.4 ppm (drag out a large Box region and click “ $\Sigma$ ” to see). All other elements have been corrected as well (e.g. try Ag now).

*Note that the Spectrum Display, X-ray Spectrum Fit and Image Display windows are all coordinated for these calculations, and all need to have the appropriate data loaded and operations performed, as outlined above.*

## Correction of Images for Sample Composition Effects on Yields

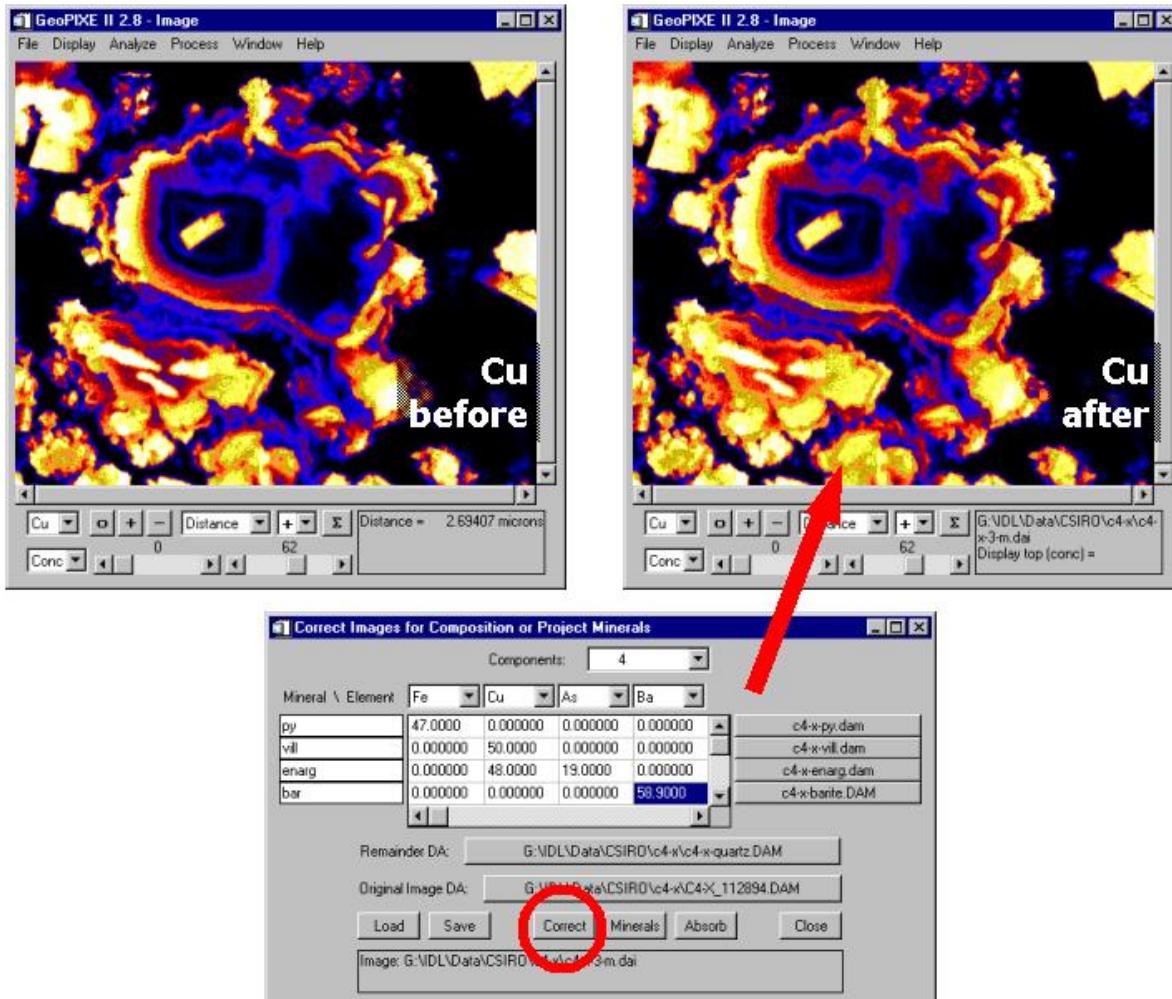
Load the image file ‘data\csiro\c4-x\c4-x-3-b.dai’. Click on the “-“ button to zoom the display out, and select the Cu image. It contains regions spanning a solid solution series from pyrite ( $\text{FeS}_2$ ; high Fe) to villamaninite ( $\text{CuS}_2$ ; high Cu), plus areas of enargite ( $\text{Cu}_3\text{AsS}_4$ ; high As) and barite ( $\text{BaSO}_4$ ; high Ba). View the various images to see Fe, Cu, As and Ba. Our aim here is to correct for the variation in calculated PIXE yields as the composition varies across the image area.

*See the more detailed worked example notes in the “GeoPIXE Worked Examples” PDF located in the Help directory.*

### Correct Yields Window

Open the *Correct Yields* window (menu “Windows→Correct Yields”), and load the file “py-vill-enarg-bar.correct” from the same directory into *Correct Yields*. This shows a matrix to project onto pyrite (py), villamaninite (vill), enargite (enarg) and barite (bar), assuming the remainder to be quartz. The matrix table shows values entered for the composition of each end-member component, in wt%. The columns show the main elements visible to PIXE that distinguish between these phases (Fe, Cu, As and Ba). The buttons to the right of the matrix table show the names of the DAM files that were created in *X-ray Spectrum Fit* using these pure end-member compositions. The DAM file used to project the images in the first place (Original Image DA) assumed a pure chalcopyrite matrix. Everything else (the “Remainder”) will be assumed to be quartz.

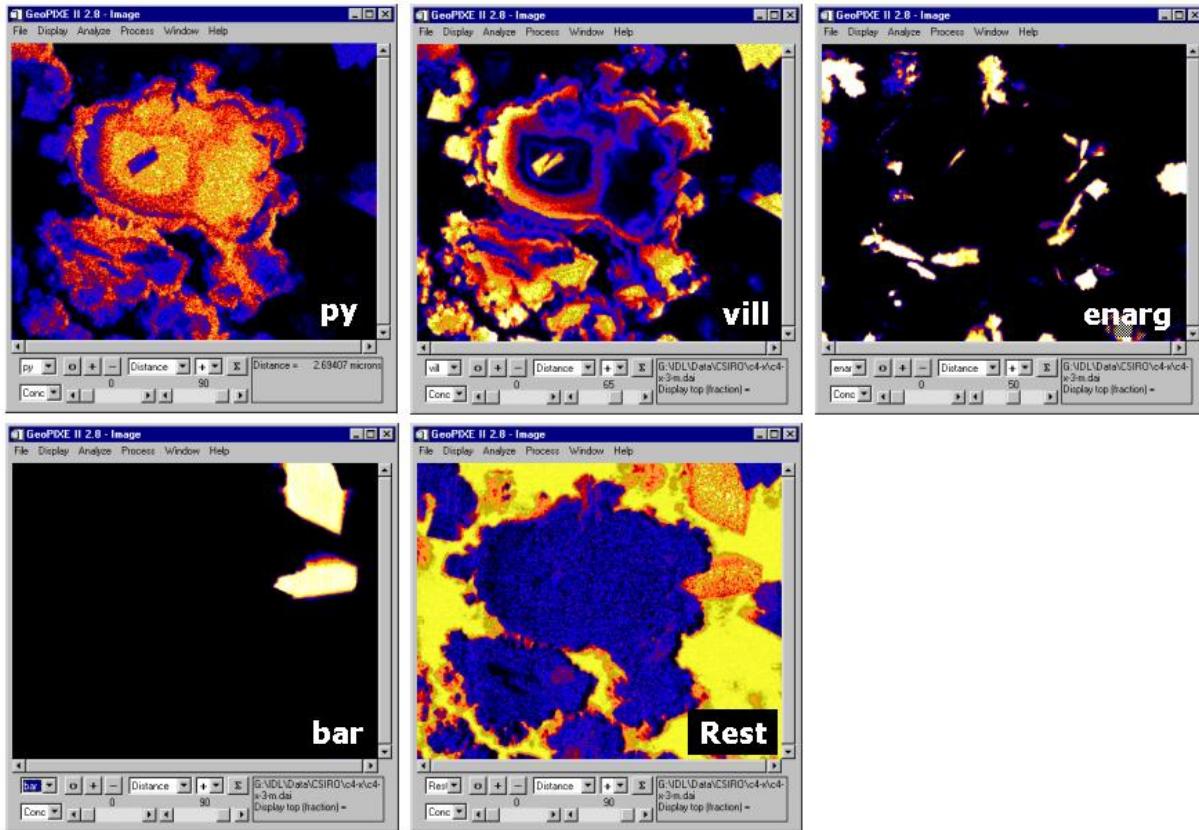
*The paths in this window to the DAM files may be different on your system. If you encounter errors in the steps that follow, you will need to click on these in turn to locate the files named on the buttons, from within the “c4-x” directory. i.e. Click on the DAM file buttons to the right (e.g. “c4-x-py.dam”), and also the DAM file buttons for “Remainder DA” and “Original Image DA”. For each, locate the directory “data\csiro\c4-x” and select the DAM file with the same name as displayed now on each button. After this is done, save the corrected set-up again using the “Save” button. These steps are not usually necessary if a directory is not moved around to a new location.*



Now you are ready. Click on "Correct" to start the correction. This will take a minute as it internally projects onto end-member proportions and calculates a better estimate for the PIXE yield in each pixel for every element. It then corrects every element for the ratio of these yields to the ones assumed originally. A second iteration can be performed by clicking on "Correct" again. Note the changes, particularly seen in the Cu image. The process typically converges quickly in 2-3 iterations.

### ***Projection of Elemental Images onto End-member Proportion Images***

Continuing the example started above for *Correction of Images for Sample Composition Effect on Yields*, click on "Minerals" to project onto the end-member proportions. The result will be images for pyrite (py), villamaninite (vill), enargite (enarg), barite (bar), as well as an image for the remainder assumed to be quartz (Rest). The images display proportion in wt%. The images show clearly the areas corresponding to enargite and barite, and the solid solution gradient between pyrite and enargite, and the gangue assumed to be quartz. Note that the high Cu areas in enargite appear as low proportions in the villamaninite image.



### **Correction of Images for the Effects of Differential Absorption**

If we return to “Sample11” (load image file “data\CSIRO\Sample11\Sample11-chalco.dai”), it shows an interesting feature. On the right of the chalcopyrite areas (high Cu) near the quartz areas (black on the Cu image) there appears to be an enhanced Cu concentration as a rim on the chalcopyrite. This is just an artefact of reduced absorption of X-rays, generated beneath the surface, on their way to the detector (located on the right) as they pass through quartz. GeoPIXE can correct for this 3D absorption effect, which results from contrasting composition within a pixel’s neighbourhood.

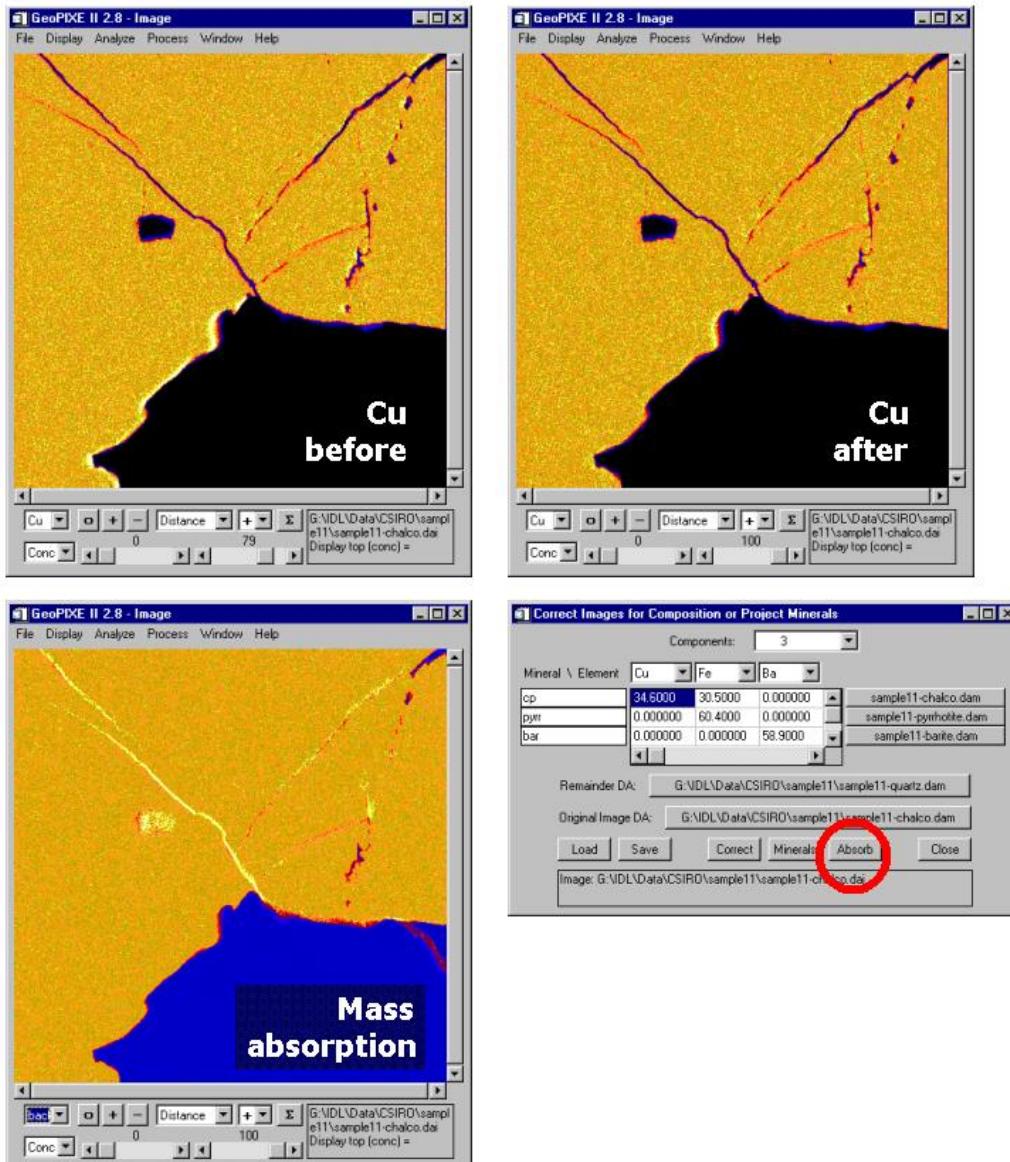
*Note: This correction is limited to normal incidence and 45 take-off angle at the moment.*

Open the *Correct Yields* window, and load the file “chalco-pyrr-barite-on-quartz.correct”. This specifies a projection onto the end-member components, as discussed in the *Verification of Images using Regions* example above. Click on “Absorb” to start the correction of absorption. This will take a minute as it corrects every element image for an assumed detector at a take-off angle of 45° degrees, located to the right.

*Note: If the detector is located at another cardinal direction, then rotate the images first (using the “Process→Rotate→+90 degrees” menu of Image Display) before correction to place the detector on the right. Then rotate them back afterwards.*

On completion, the “Back” image is replaced with an image of the spatial variation of mass absorption coefficient. All other elemental images are now corrected for absorption. Note that the edge effect in the Cu image is now largely corrected.

This process assumes vertical boundaries between contrasting areas of composition, but still does a remarkably good job of correcting these effects. Remaining artefacts probably reflect non-vertical phase boundaries.



### Correction of Images for Charge Variation

You may have noticed that the previous examples in which “Sample11” was re-sorted showed some faint vertical streaks on the Cu image. This resulted from a problem with charge integration in this measurement, in time as the stage stepped across in X. These effects can be removed by using the constraint that the Cu content of the chalcopyrite in this case is uniform, which aside from the streaks appears to be valid.

The approach is to renormalize all elemental images so that the integral of one image is constant as a function of X (there is a similar function for Y). However, seldom do we want to integrate the whole image. Usually, only parts of the image are deemed uniform, and there are often cracks and inclusions, etc. that should be avoided. Therefore, the approach is to select just those parts of the image that are uniform in this element.

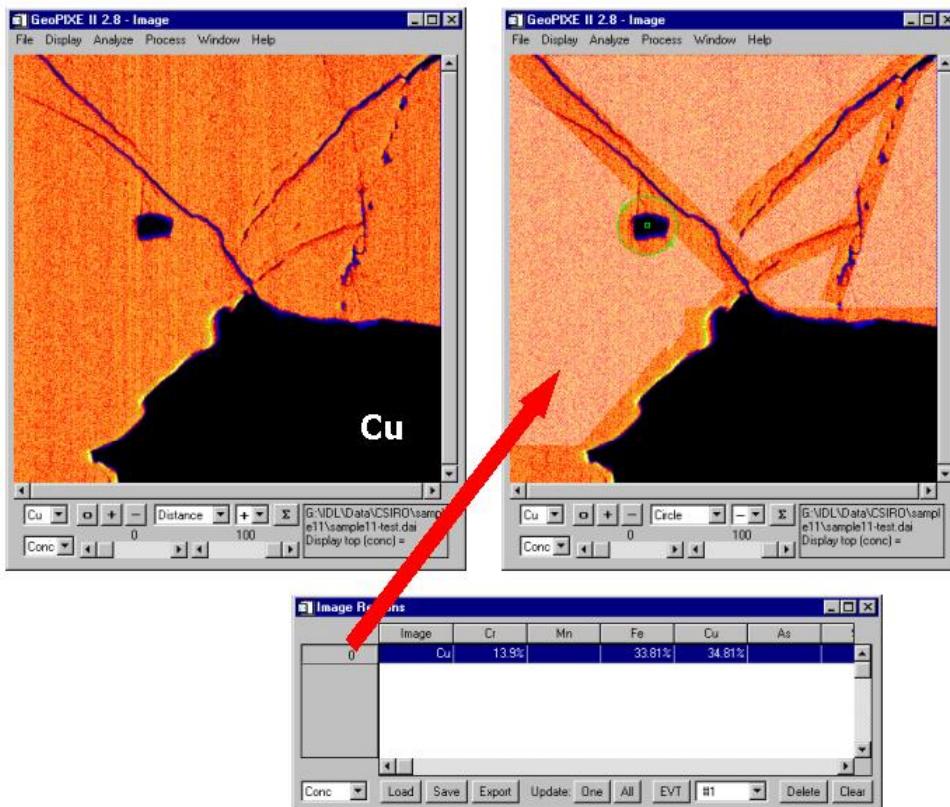
There are two approaches to selecting the ‘uniform’ pixels using: (i) the shape tool on the *Image Display* window to select a region, or (ii) pixels selected based on element-element associations and a selection in the *Associations* window.

## Using the Shape Tool for Region Selection

Load images from “Sample11.dai” in the “csiro\Sample11” directory, and display Cu. Open the *Image Regions* window and load the file “Sample11-charge.region”, which contains just one region that selects all uniform chalcopyrite parts of the image area.

### Exclude Mode of Region Selection

This region uses the exclude mode. It was built by first using a “Box” shape to select the whole area. Then, the selection mode was switched into exclude (“-”) using the drop-list immediately to the right of the shape drop-list in the *Image Display* window. Then various parts of the image (cracks, veins, inclusions) were outlined using various shapes in turn in order to remove them from the Box selection. Outline an area with a shape and click on “Σ” to remove that area. The shaded part of the image shows the areas that remain selected. They provide a discontinuous sampling of pixels across **all X values**.



Using this image region selection, use the menu item “Process→Correct→Xstep Current” in *Image Display* to renormalize all images. Clear the region shading using the “Display→Clear All Shapes” menu. Now Cu appears smooth and uniform.

### Charge Correction using Element Association Pixel selection

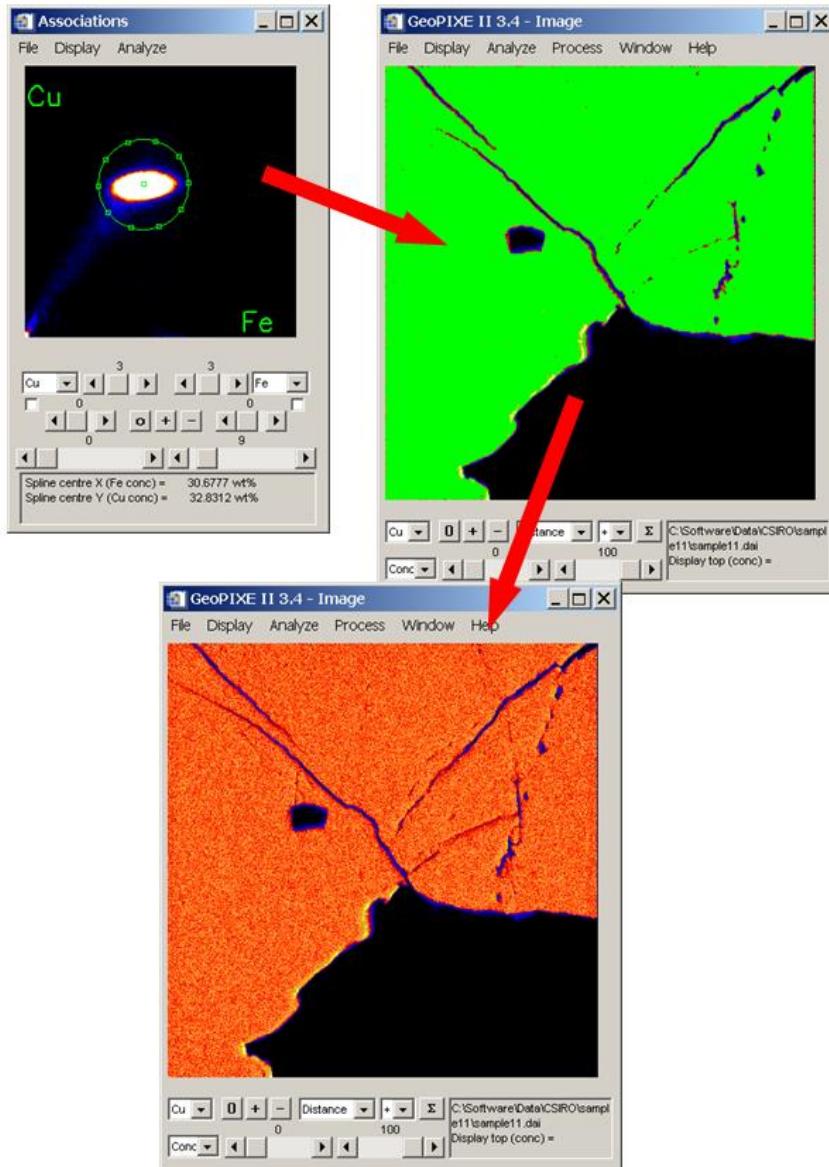
Continuing with the Sample11 example, re-load the original images from “Sample11.dai” in the “csiro\Sample11” directory, and open an *Associations* window (“Windows→Element Associations” menu) and select correlations between Cu and Fe on linear scales (un-check the Log check-marks); you may need to reduce the display maximum slider to see more of this distribution.

Now click and drag a spline curve around the knot of nearly fixed Cu-Fe composition in the centre of the window corresponding to chalcopyrite.

You can clear the spline curve to start again using a mouse 'right click' with the cursor in the window.

Now use the “Analyze→Within Spline” menu to select all image pixels within this Cu-Fe field; these are highlighted on the *Image* window in green (right click in the *Image* window to temporarily hide this selection to view the full image). This has selected all pixels with this close Cu-Fe relationship. If the selection looks a little noisy, try applying some pre-smoothing of the Cu and Fe images first. To do this, increase the sliders next to the element drop-lists by one click to 4. Then use “Analyze→Within Spline” again.

Now use the “Process→Correct→XStep Current” menu in the *Image* window to apply the charge correction based on the selected ‘green’ pixels. Right click to hide the green selection and see the result briefly or use the “Display→Clear Association Highlights” menu to clear them entirely from the display.



## Notes on IDL and GeoPIXE Installation

GeoPIXE is written in the IDL language (by Research Systems Inc. and later owned by Harris Geospatial) in modular form. Each window is effectively a separate program that communicates with the others using some message notification services designed for GeoPIXE. This structure has many benefits. If a window crashes with a bug, for example, you can usually close it (using the "X" widget in the top-right of the window) or close its parent window (to close both windows; often a windows data is stored in the parent) in order to clear the problem and try again, often without loss of data. The contents of other window and data remain intact. There is no practical limit on the number of windows, or image clones for example, subject to available computer memory.

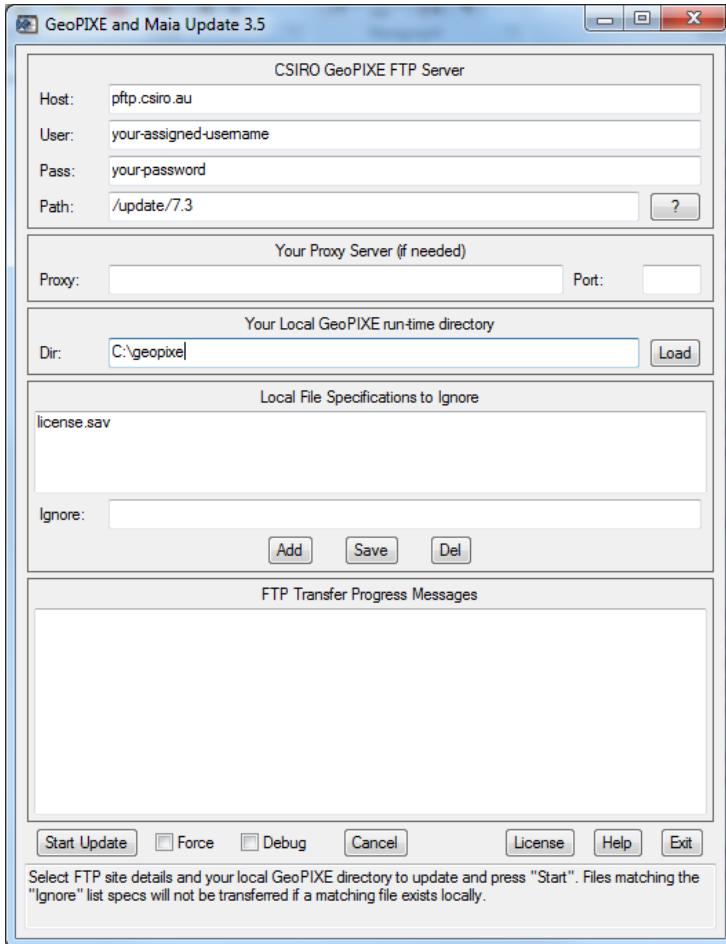
### Installation Notes

GeoPIXE is downloaded from the GeoPIXE FTP site. The entire **GeoPIXE** directory tree (e.g. in “/update/7.4” on the FTP site) should be copied to disk for a complete installation using the **geopixe\_update** tool. Demo data, as used in the Scenarios section and the Workshop notes, can also be downloaded with this tool from “/Demo”. Make a shortcut to the “GeoPIXE.sav” file in your new geopixe directory, and place this in a handy place (e.g. on your Desktop). Make sure that the shortcut starts in the same directory as GeoPIXE.sav. GeoPIXE runs under IDL and needs IDL run-time, Virtual Machine or full development system support, and at least IDL version 8.5. GeoPIXE has been tested under PC (XP/W7/W10) and Linux.

Install IDL on your system. GeoPIXE can run under the IDL Virtual Machine (VM), but for parallel processing options (e.g. as used to speed up processing of large Maia data-sets, using “Cluster” mode) it is best to purchase the RT (run-time) license. Contact Harris Geospatial for details. Download IDL from Harris Geospatial, and for VM mode select the “Virtual Machine” option during installation or skip the license step. For a full IDLDE or RT system, follow the instructions provided to you by Harris Geospatial.

With IDL installed, download the “geopixe\_update.sav” file from the FTP site in the “/update” directory (also download the instructions text file). Run it by double clicking on it. Set the FTP “Host” to “pftp.csiro.au” and enter the Username and password assigned to you by CSIRO. The main path for updates is “/update; click on the “?” to view a list of available versions. Usually you will select the latest one (or the “beta” directory). If you do step up to a new version, it is best to make a fresh geopixe directory for it (the “Dir” field is the path to your geopixe directory on your system).

*NOTE: It is not necessary to install GeoPIXE in a “Program Files” directory tree, which may require special administrator privileges.*



To obtain a license key (file: “license.sav” in main geopixe dir), run the license tool by clicking on “License” in geopixe\_update. Fill in all fields, agree to license terms and save the result to a license request file (“geopixe-request.txt” saved in your home .geopixe directory). Send this file to [geopixe@csiro.au](mailto:geopixe@csiro.au) to request your license key.

To run GeoPIXE, double click on the shortcut for GeoPIXE.sav. If it fails to open, check the shortcut properties for the correct path to the GeoPIXE directory. ***Make sure that the shortcut starts in the same directory as GeoPIXE.sav.***

The manual and other help documents (e.g. Workshop notes) are available in the “Help” directory in your new GeoPIXE installation.

## Preferences

GeoPIXE will read preferences on start-up from the config file “geopixe.conf” in the “.geopixe” sub-directory to your home directory (if not found it will create a default file). The file can be edited to select the following options:

- 1) **path data:** select the default path for raw data when the file-requester is opened.
- 2) **path analysis:** select the default path for analysis results, such as images when the file-requester is opened.
- 3) **path config:** default standards config directory (e.g. for Standards Wizard).
- 4) **default device:** sets the name of the default device (e.g. MAIA\_DEVICE). Valid devices have SAV files with names ending in “\_define.sav” in the directory “<geopixe>/interface”.
- 5) **cluster type:** select between “cores” and “CWS” to select between parallel processing using multiple IDL sessions running on multiple cores or using the CSIRO CWS cluster processing services. Note that a full IDL (runtime) license is needed.

- 6) **cluster nodes:** select the number of nodes to use in a cluster or the number of IDL sessions in “cores” mode.
- 7) **startup:** enables automatic opening of various windows when GeoPIXE is first started.
- 8) **origin auto:** the absolute coordinates of the origin (lower left corner) of the current image is normally obtained from the data stream, if an origin is supported. If no origin is supported in the device data, set this to “0”.
- 9) **origin x, y:** if no auto origin is available, then set a manual coordinate origin (mm) for X and Y. With an origin set, dragging a box shape on a window will show the boxes origin in the context sensitive help frame.

Similarly, file path bookmarks, as used in the file requester, are stored in the “.geopixe” sub-directory to your home directory (if not found it will read initial default bookmarks from the GeoPIXE directory). It will save paths back to the .geopixe directory. The token “\$HOME” in the bookmark list translates to your home directory (as pointed to by the HOME environment variable).

## **Setting Up Filter Definition Files**

Filter definitions reside in individual files within the main GeoPIXE directory or in the “config/filters” path, using ‘config’ as defined in your “geopixe.conf” file. Add new local filter files to this config path.

All filter (.FILTER) files are loaded when *GeoPIXE* is started, and appear in drop-lists throughout the program. These files can be edited or created using the *Filter Setup* window, accessed via the "Windows→Edit Filters" menu item in *Image Display* and *Spectrum Display*. If a detector is edited or added, it is typically immediately accessible to the various windows that use filters.

*If a DETECTOR or FILTER file is not found for one of the examples, try looking for it in the “Storage” directories.*

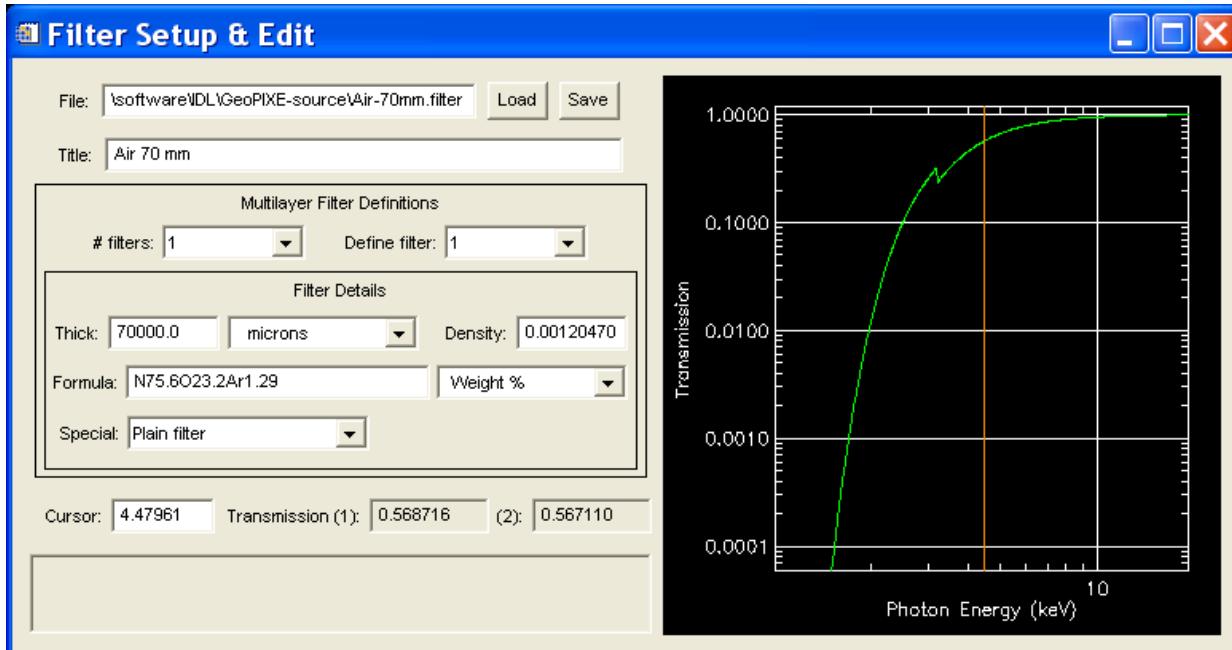
### **Note:**

An energy cursor and energy entry field have been added to the *Edit Filters* windows. Enter photon energy (keV), or drag a cursor on the plot, to determine the transmission or efficiency at the cursor energy for filters and detectors, respectively.

If an X-ray line is selected in the *X-ray Identification* window (click on a line in the list), the filter and detector window cursors will be set to this energy.

## **Filter Setup**

Use the "Load" and "Save" buttons to edit or create filter files. The "Title" will appear on all drop-lists for this filter; it should no longer than about 16-20 characters. Each filter file can contain a number of filters, which form a composite X-ray filter. The number of filters is specified using the "# Filters" drop-list, and the "Define Filter" drop-list selects a filter for editing.



Filter thickness can be in  $\text{mg/cm}^2$ , microns or Gas (mm NPT). The latter specifies mm of gas at normal pressure and temperature (20 °C, 1013.25 mbar). This is selected using the drop-list beside thickness. If microns are used, then a density is required. For pure element filters, this will be provided automatically by the program. For a gas filter, density is calculated from the composition assuming an ideal gas. Next, the chemical formula of the filter is entered beside "Formula". This can take various forms (e.g. "N2", "CO2", "(CH<sub>2</sub>)<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub>", "(N<sub>2</sub>)<sub>70</sub>(O<sub>2</sub>)<sub>29</sub>(CO<sub>2</sub>)<sub>1</sub>"). When brackets are used "()", then the function of the multipliers outside the brackets is set by the drop-list on the right. It selects between "Atomic Fractions" for atomic weighing (e.g. "(CH<sub>2</sub>)<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub>") and "Weight %" for weight % proportions (e.g. "(N<sub>2</sub>)<sub>70</sub>(O<sub>2</sub>)<sub>29</sub>(CO<sub>2</sub>)<sub>1</sub>"). For a Gas filter, make sure the "()" contain the main gaseous molecular components.

The bottom line defines special filter properties. This is used for pinhole and Bragg filters. When a pinhole filter is selected by the drop-list, then a new field appears on the right for the entry of the solid-angle ratio. This is the ratio of the detector solid angle to the pinhole solid angle, and hence is always larger than one. Note that a Gas filter cannot use the "pin-hole" mode.

In Bragg filter mode, in addition to the absorber foil, the filter adds a Bragg filter transfer function. A Bragg filter is an X-ray lens, shaped to a rotated log-spiral, that focuses one narrow energy band into the X-ray detector. An extra button appears to enter Bragg filter parameters for centre energy, curve width, height (enhancement) and base-line (from scattering). A small window shows the current shape of the transfer function. *Make sure you hit return when entering parameters to have them shown in the display.*

*View the context-sensitive help at any time for a reminder of the function of these fields. The transmission through this complete list of absorbers is dynamically updated in the plot on the right as changes are made.*

Remember to save changes.

## Setting Up Detector Definition Files

Detector definitions reside in individual files within the main GeoPIXE directory or in the "config/detectors" path, using 'config' as defined in your "geopixe.conf" file. Add new local detector files to this config path.

All detector (.DETECTOR) files are loaded when *GeoPIXE* is started, and appear in drop-lists throughout the program. These files can be edited or created using the *Detector Setup* windows, accessed via the "Windows→Edit Detectors" menu item in *Image Display* and *Spectrum Display*.

If a DETECTOR or FILTER file is not found for one of the examples, try looking for it in the "Storage" directories.

#### Note:

An energy cursor and energy entry field have been added to the *Edit Detectors* windows. Enter photon energy (keV), or drag a cursor on the plot, to determine the transmission or efficiency at the cursor energy for filters and detectors, respectively.

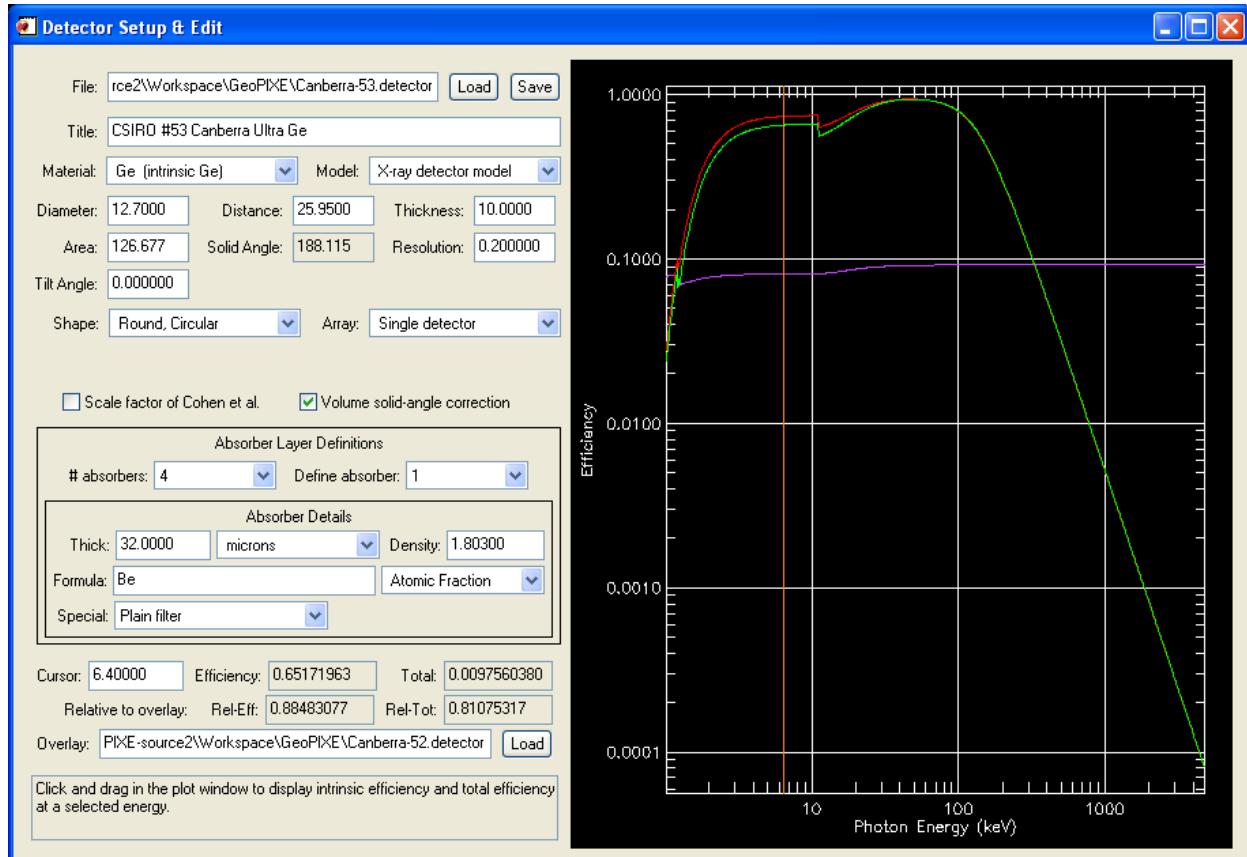
If an X-ray line is selected in the *X-ray Identification* window (click on a line in the list), the filter and detector window cursors will be set to this energy.

### Detector Set-up

Use the "Load" and "Save" buttons to edit or create detector files. The "Title" will appear on all drop-lists for this detector; it should be no longer than about 16-20 characters. Each detector file contains various parameters about the crystal and geometry and a number of absorbers which form a composite X-ray filter. Select the crystal from the "Material" drop-list, and enter all geometry parameters in the text fields.

"Diameter" and "Area" are linked, so you only need to enter one of these. Units are mm, and keV for resolution (see the context sensitive help information). The shape of the detector can be selected between round and rectangular/square. "Distance" is measured directly from target to the centre of the face of the detector crystal, which is points directly at the target position unless a non-zero "Tilt angle" is used. "Solid-angle" reflects area, distance and also tilt angle. A tilt angle will increase the effective thickness of the active volume.

An optional scaling factor of 0.717 can be selected to be consistent with the detector efficiency function of Cohen (Nucl. Instr. Meth. 178 (1980) 481). By default, the volume solid-angle correction of Cohen et al. is used, to account for the effective reduction of solid-angle for X-rays that penetrate through the volume of the detector and hence experience a slightly smaller solid-angle. Strongly collimated detectors, such as Maia with an inclined Mo mask, should not use this correction, as the solid angle is completely controlled by the mask/apertures.



The number of X-ray absorbers is specified using the "# Absorbers" drop-list, and the "Define Absorber" drop-list selects an absorber for editing. Absorber thickness can be in mg/cm<sup>2</sup>, microns or Gas (mm NPT). This is selected using the drop-list beside thickness. If microns is used, then a density is required. For pure element filters, this will be provided automatically by the program. For a gas filter, density is calculated from the composition. Next, the chemical formula of the absorber is entered beside "Formula". This can take various forms (e.g. "N2", "CO2", "(CH2)4(NH2)2", "(N2)70(O2)29(CO2)1"). When brackets are used "()", then the function of the multipliers outside the brackets is set by the drop-list on the right. It selects between "Atomic Fractions" for atomic weighing (e.g. "(CH2)4(NH2)2") and "Weight %" for weight % proportions (e.g. "(N2)70(O2)29(CO2)1"). For a Gas filter, make sure the "()" contain the main gaseous molecular components.

The bottom line defines special filter properties. This is used for pin-hole filters. When a pin-hole filter is selected by the drop-list, then a new field appears on the right for the entry of the solid-angle ratio. This is the ratio of the detector solid-angle to the pin-hole solid-angle. View the context-sensitive help at any time for a reminder of the function of these fields.

The intrinsic efficiency, including transmission through this complete list of absorbers, is dynamically updated in the plot on the right as changes are made.

Position a cursor on the plot by left-clicking and dragging. The intrinsic efficiency and total efficiency (including the ratio of solid-angle to  $4\pi$ ) is shown for the current cursor position. If the *X-ray Identification* window is open, the cursor here will track the energy of lines selected in the *X-ray Identification* window.

An existing detector file can be loaded and ‘overlaid’ in “red” on the current detector efficiency, shown in “green”. The ratio of the new total efficiency to the overlay’s total efficiency is also displayed offset in “violet” (scaled down by 10).

Remember to save changes. Once saved, the new detector will appear in the detector drop-lists in the *X-ray Spectrum Fit* and *X-ray Identification* windows.

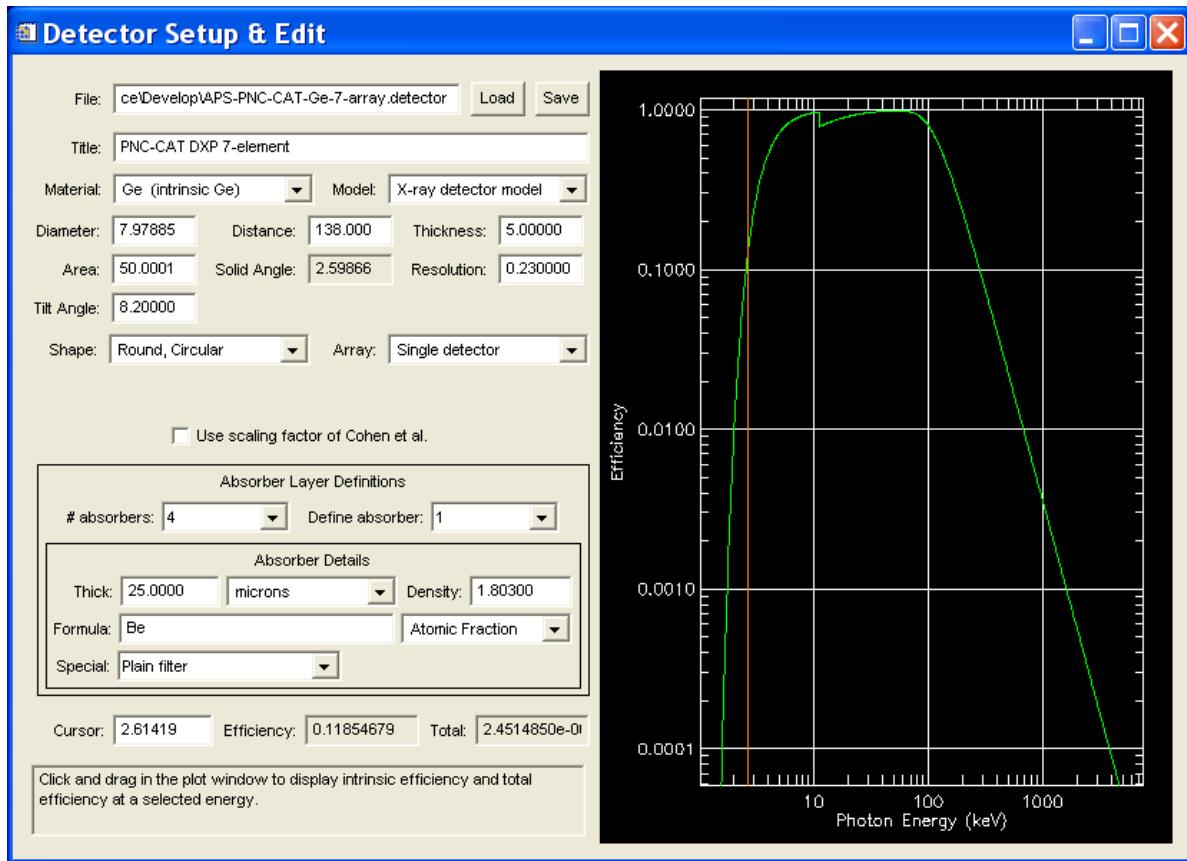
## Detector Arrays

Two approaches to detector arrays are supported:

1. **Simple arrays** – Select “Array: Single detector” and specify the detector parameters for one (central) detector element and assume that all others have the same solid-angle and efficiency and span a negligible range of take-off angles at the target. All detectors will be assumed to have the same Diameter, Distance, Thickness, etc. This works fine for a small array, located at some distance from the sample where the take-off angles across the array vary little. The solid-angle shown is for just one of the detectors.

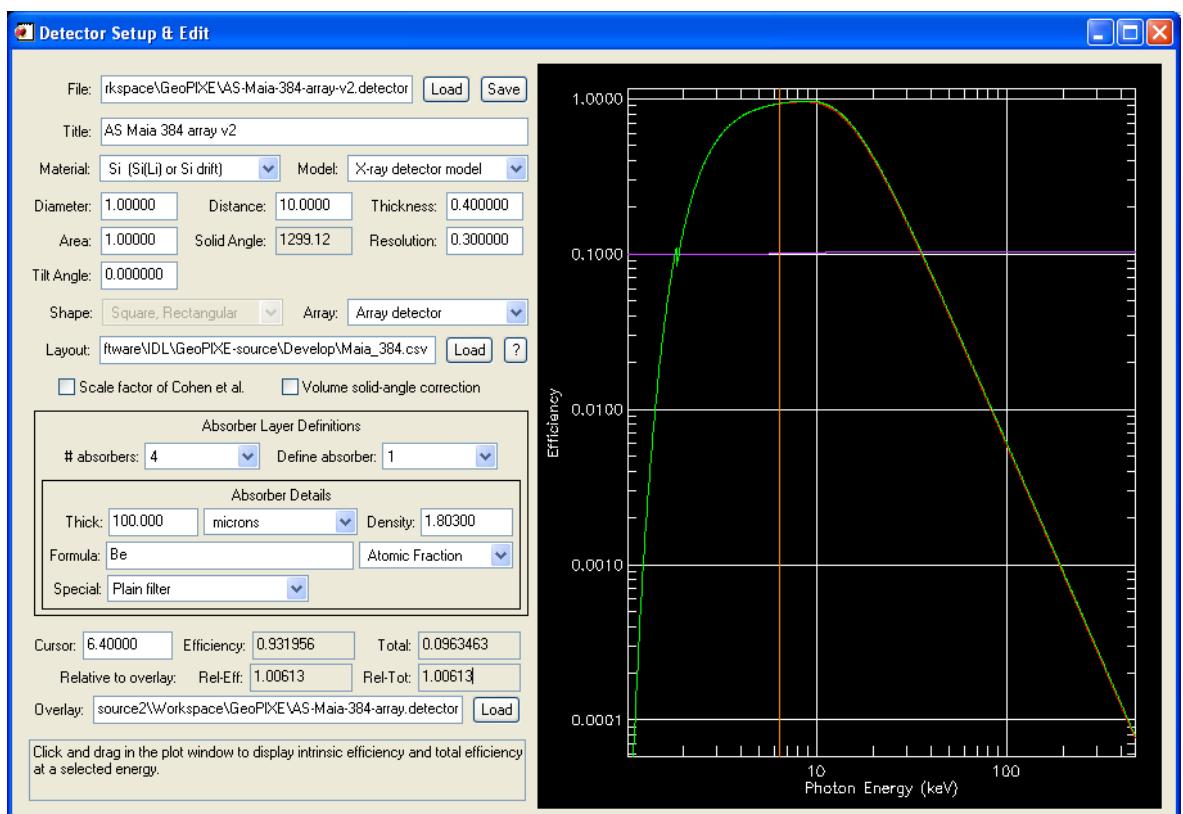
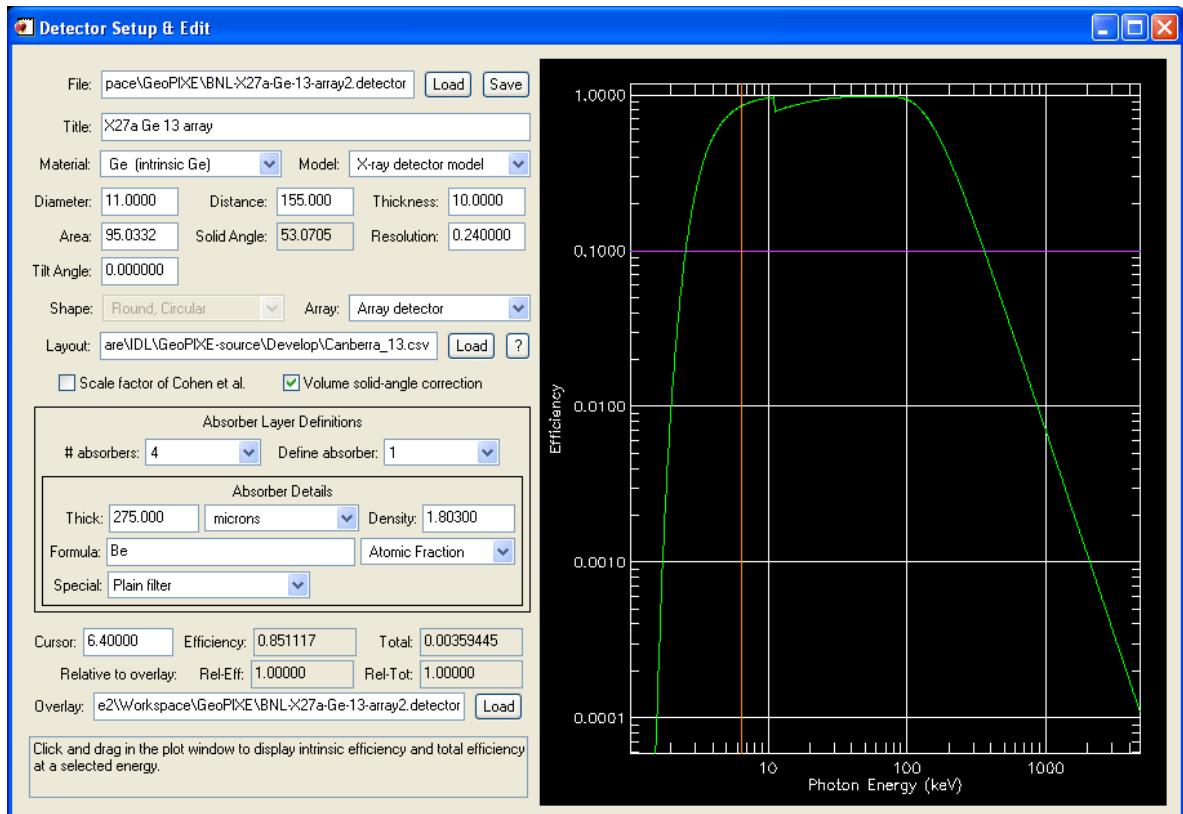
This approach assumes that X-ray yields are the same for each element of the array, which only applies for more distant arrays. For close geometry, or where some detector element have a more glancing take-off angle, use the Full array approach below.

When the data for all detector elements are merged into quantitative images, the number, or multiplicity, of active detector elements (enabled in *Sort EVT*) will be accounted for in correcting both the concentration and variance images.

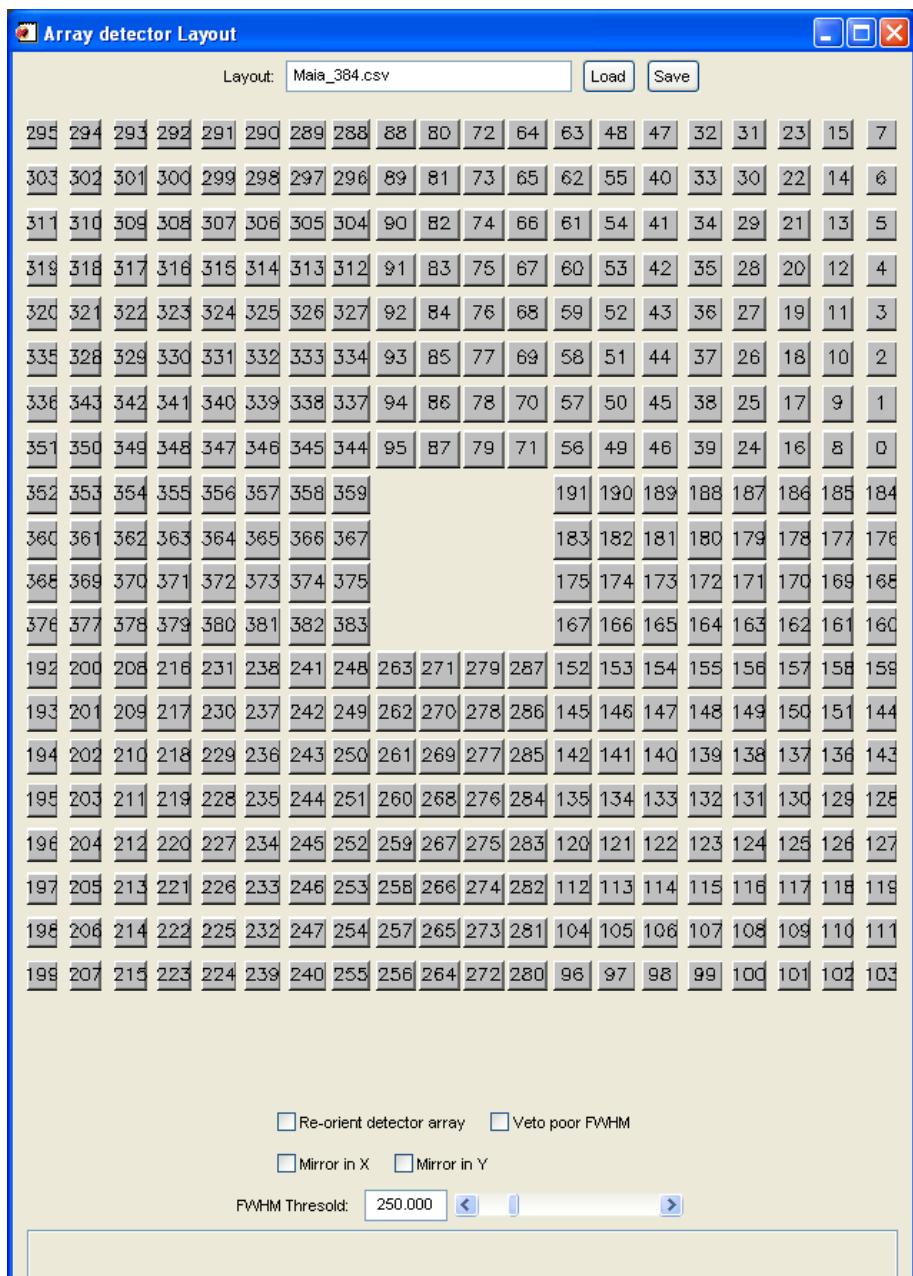


2. **Full arrays** – Select “Array: **Array detector**” and specify the layout of elements in the detector array in a Layout file. The values for Thickness and Absorbers now apply to every detector in the array. The Tilt is now the tilt of the **array as a whole** (individual detector tilts can also be accommodated in the layout file, e.g. for a hemi-spherical array).

Solid-angle is calculated for the whole array, taking into account relative solid-angle, tilts and variation in distance. The Diameter and Area value now are for a notional “central” detector – the yield calculation will relate all yields as ratios to this “central” detector. Normally, this is set by the user to an area typical of the central detector elements as specified in the layout file.



Click on the “?” button next to the detector layout “Load” button to display the detector layout.



Maia 384 detector layout mimic display.

### Detector Array Layout File

The layout file lists a number of parameters and the coordinates and dimensions of the detector elements, relative to the centre of the detector array. It's a commented Comma-Separated Text (CSV) file, so you can view it in a text editor or Excel.

```
# This file produced by program: "detector_layout_save.pro"
title      Canberra 7 Ge array
N          7 Number of detectors
Start      1 Start at this # (default: detector numbers start at 0)
Shape      0 Shape of d 1=square)
Symmetry   4 Detector array symmetry steps for 360 degree (default is 4)
Reorient   0 Re-orient or rotate by "reorient*360/symmetry" degrees
MirrorX    0 Mirror the layout in X
MirrorY    0 Mirror the layout in Y
Veto       0 Veto channels with excessive FWHM
Threshold  300 FWHM threshold (eV)
# Data: X Y offsets fr Z offset frc Width Height (mr Tilt (degree bad (0=go 1=poor 2=dead) FWHM (eV
Data      X           Y           Z           width        height       tilt      bad      0
Data      X           Y           Z           width        height       tilt      bad      1
Data      X           Y           Z           width        height       tilt      bad      0
Data      X           Y           Z           width        height       tilt      bad      0
Data      X           Y           Z           width        height       tilt      bad      0
Data      X           Y           Z           width        height       tilt      bad      0
Data      X           Y           Z           width        height       tilt      bad      1
Data      X           Y           Z           width        height       tilt      bad      0
Data      X           Y           Z           width        height       tilt      bad      0
```

A typical layout file, for a 7-element Ge detector array. The X,Y,Z coordinates position each detector relative to the centre of the array (mm). Width, height are the size of each (mm), and tilt is a tilt angle (degrees) for each element (positive angles are towards the centre of the array).

#### Detector Layout file parameters:

1. N              Number of detector pads
2. Shape          Choose between 0=round, 1=square/rectangular, [2=hexagonal (later?)]
3. Start          The number for the first detector (usually either 0 or 1)
4. Symmetry      Rotational symmetry for array, or number of rotational reorientation steps for 360° (default is 4)
5. Reorient       Re-orient (rotate) the detector layout by this many symmetry steps
6. MirrorX       Mirror the layout in X, before applying re-orientation
7. MirrorY       Mirror the layout in Y, before applying re-orientation
8. Veto           Enable vetoing (disabling) of detector channels based on FWHM
9. Threshold     FWHM threshold (eV)

#### Detector Layout Pad parameters (one row for each detector pad):

1. Index          Unique index number tag for this detector pad (can be in any order)
2. X              X coordinate (mm) from centre of array
3. Y              Y coordinate (mm) from centre of array
4. Z              Z coordinate (mm) of pad out of plane, towards target
5. Width          width of pad (mm)
6. Height        Height of pad (mm)
7. Tilt           Tilt angle of pad (degrees) (positive is towards the centre of the array)
8. Bad           Flags a bad detector element (0=good, 1=poor FWHM, 2=bad and deactivated)
9. FWHM          optional FWHM (eV) for element (see *Sort EVT* “Get”)

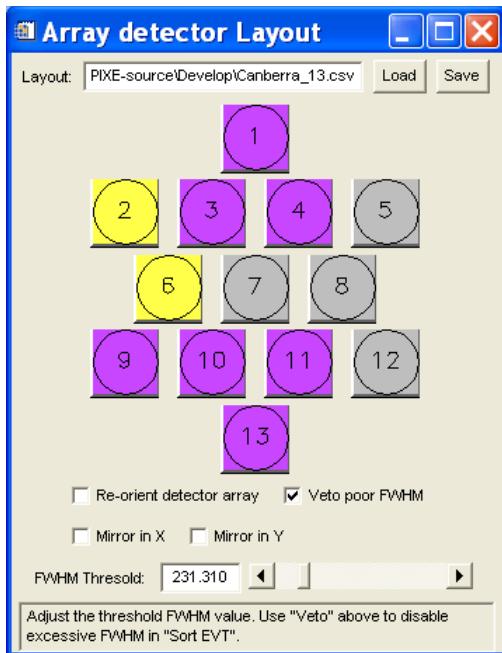
The Maia detector layout files have additional columns to encode:

10. HERMES      Readout chip group of 32 channels (one of 12)
11. Quadrant     One of 4 quadrants of Maia
12. Radial       Detectors grouped by radius from centre into 12 groups
13. Column       Grouped by column (in the 20x20 square array)
14. Row           Grouped by row.

The options for “Mirror in X”, “Mirror in Y” and “Re-orient array” are there to rotate or reflect the arrangement to match the organization of detector numbers as set-up at the beam-line, if necessary. View the layout and numbering in 3D as part of the beam-target-detector geometry using the “?” button on the *Yield Calculation* window. This can be used to verify that the correct numbering and position of detector pads relative to the sample plane and take-off angles.

Click on “?” to view the layout in a pop-up window. The Layout window has a FWHM Threshold slider, which sets the limit of usable detector resolution. You can slide this to reject detectors with poor resolution in the Sort EVT window (if the “Veto poor FWHM” check-box is selected; see below). These are shown in Yellow. Dead detector channels can be specified in the layout file (bad=2); these are shown in Violet and are disabled.

*Note: This feature of channel veto is seldom used. Use a SPEC file to include only good, energy calibrated detector channels as a method to select channels to use (e.g. “Get” button on “DA/E.cal” tab of the Sort EVT window).*



This rejection can be used in *Sort EVT* (which also has a “?” button to invoke a pop-up like this) to veto poor detectors in an array while sorting raw data to build images. FWHM values are saved in SPEC file after a fit to all spectra. When the “Get” button is used in *Sort EVT* (to retrieve energy calibration for all valid detectors) the FWHM values are transferred to the *Layout* window; any missing detector spectra flags a dead channel. These can be saved to the Layout file, using the Save button. The dead channels are shown in Violet, and the poor FWHM channels are shown in Yellow.

### Platforms Supported:

The supported workstation OS at present is Windows Win10, under IDL 8.5 (8.6, 8.7, 8.8) and Linux. GeoPIXE has been ported to the Mac, but there is limited support for that mode. Enquire if this is needed.

GeoPIXE can sort list-mode data written using various data acquisition, operating systems and byte order (Endian type), including Linux (MPsys, Maia-384), Unix (MPsys, APS MDA, GSE-CARS, Hasylab, NSLS HDF), MacOS (KMax), PC Windows (OM DAQ, FastcomTec, MPAWIN, MPA3, MPA4, Labo, and Primecore) and embedded systems (CSIRO Maia/Hymod). IDL support for VAX/VMS (XSYS) has been discontinued.

Quality spectroscopy, including good fits to PIXE and SXRF spectra, are best achieved using electronic pile-up rejection or digital signal processing. The lack of pile-up rejection produces pile-up tailing, which degrades detection sensitivity and should be avoided. It is not treated in GeoPIXE; the pile-up model assumes that some form of pile-up rejection is active.

Using a 64-bit PC with 8-16 Gbyte RAM, gives good performance. 32-bit operating systems, such as Windows suffer from memory limits per process and should be avoided unless your image sizes are not large. On Linux this means a 4 Gb limit. On Windows the limit becomes effectively 1.2 Gb or less due to system limitations, which limits image sizes to about 2500 x 2500 pixels. 64-bit operating systems are essential for large data-sets and resulting image sizes, such as generated by the CSIRO Maia detector system (images up to 1 G pixel have been acquired). A large monitor, or better still dual LCD monitors, and the use of high resolution (1600 x 1200 minimum) are recommended. Plenty of disk space

is also recommended. Processing speed (e.g. using parallel processing and IDL RT) is directly linked to disk throughput and so fast disks or SSD are recommended.

Large Maia detector data-sets benefit from parallel processing using multiple processes across a multi-core processor. To make use of this you need a run-time IDL or higher license and enable the “cluster” mode where it appears. Data throughput is then limited by the total disk bandwidth of your system. However, data throughput of between 100-400 Mbytes/second can be achieved.

## New Features in Each GeoPIXE Release

(also see the “Update Notes.pdf” file in the Help directory)

### **New Features in 8.8:**

- 1) GeoPIXE open source
  1. Changes made to the directory structure and organization and the building approach for GeoPIXE has been assigned a new version 8.8.
  2. This assumes the latest IDL 8.8.3.
  3. For now, this is assumed to be built against py3.8 if any python extension is needed.

### **New Features in 8.6:**

- 2) GeoPIXE python extensions
  1. Extensions to GeoPIXE, which make use of the python bridge in IDL, need to be compiled for the version of python being used. To handle py2.7 versus py3.8, a simple branch of GeoPIXE has been defined. Version 7.6 continues to assume py2.7, while v8.6 is compiled against py3.8. The source code remains the same, but the SAV files are created against the respective python.
  2. Version 8.6 supports export in ZARR format, which requires py3.

### **New Features in 7.6:**

- 1) GeoPIXE is a workflow
  1. GeoPIXE can be launched passing it arguments so it will do processing triggered within a data workflow.
  2. Buttons labelled “C\*” on various windows are used to output GeoPIXE Command Files (.gcf), which provide templates of parameters to use for workflow processing.
  3. See the GeoPIXE Software Organization PDF.
- 2) MPDA analysis
  1. If an .mpdam file references the wrong phase maps (not for the current image data), it will generate these (perhaps doing a normal DA process first and correcting for composition effects on yields).
  2. A new “Master Weights” spectrum is recommended when generating DA matrices for Yield Correction and MPDA. This spectrum should be more representative of the major elements seen across your sample.
- 3) Line XANES
  1. Use the pixel values from an “energy proxy axis” as an index into a supplied energies table to allow changing energy to be tracked during event processing. This flags “Line XANES” mode.
  2. A DA matrix stack is expected, calculated for each value of the energy table along the XANES beam energy scan. These do not need to be equally spaced.
  3. Export of regions in XY, in Line XANES mode, treats the “ProjectX” and “ProjectY” regions differently. These are collapsed onto the projection axis, using an average across the line, and the average along the projection exported to tab or comma separated formats.
- 4) RGB image export script
  1. The export of RGB images as plots can make use of a “RGB Learn” script to output all RGB element combinations in the script in the selected export format.
- 5) Add ZARR image export
  1. The image data structure can now be exported in ZARR format for AWS Cloud service operations.
  2. The requires python 3.6+ support, and operating GeoPIXE under IDL 8.8+.

### **New Features in 7.5:**

- 1) Crop image data-sets
  1. Have a new menu item “Crop to shape”, which crops an image to the (XY extent of the) current shape, which creates attributes for the image consistent with a “windowed sort”.
  2. Dropped the menu items for “Clip to right” and “Clip to top”.
- 2) Spectrum plot export

1. Add export to PNG and JPEG formats to draw spectrum plots in a large bitmapped field, to avoid ongoing issues with Windows veto of the CGM standard for vector graphics and the unavailability of WMF on non-Windows platforms.
- 3) Export of images within regions
  1. Now has the option of setting the pixel values to zero for any pixels output outside (irregular) region boundaries.
- 6) Image “missing line” correction improved
  1. The correction of missing lines in images has been improved using bilinear interpolation.
- 7) Compare RGB images
  1. Now 2 additional image data-sets can be loaded into the RGB Image window, so that the RGB planes can be selected from 3 image data-sets (current one plus the 2 “compare” data-sets).
- 8) Correct image zeroes improved
  1. Now uses up to 3 passes to iteratively replace image zeroes with local neighbourhood interpolation.
- 9) Inter-element operations
  1. Pop-up window to control pixel-by-pixel operations between selected element planes. Save once desired correction is achieved.
  2. Use this to subtract identified artefacts in images, for example.
- 10) Region spectra extraction
  1. Extraction of a huge number of regions from large images can require huge allocation of temporary memory during processing. This is now detected, and the extraction of large numbers of regions (e.g. 2000 for hotspot analysis of huge images) will proceed in multiple passes. A pop-up message will alert the user to this.
- 4) File-Requester and finding files
  1. The File-Requester endeavours to find files provided by searching in the local directory tree, if they are not found where expected from their complete filename with path. Hence, if dir structure has been changed, or files moved to a new system, the File-Requester (called behind the scenes from various window, such as Sort EVT and Image Regions) will work to find them locally on the new system.
  2. You may see a progress bar appear when a search is underway. If it is taking too long, or clearly wandering into unwanted parts of a dir tree, you can “Cancel” it and navigate to the lost file.
- 5) Handling large data-sets
  1. Given enough computer memory, GeoPIXE handles images beyond 200 M pixels with no special methods. Images up to 1 G pixels have been handled by using a Windowed sort to handle them in 4 parts.
  2. Using very large number of Regions on large images becomes a challenge (e.g. 2000 regions on a 30 M pixel image). To deal with this, the extraction of spectra from these regions may be split automatically into a number of passes (e.g. example above uses about 4 passes).
- 6) Export of RGB images
  1. ‘Max area’ option to remove as much of the border trimming as possible.
- 7) Linearize spectrum plugin
  1. Now fitting to 13th order in double precision.
- 8) New device object driver for NSLS XFM beamline HDF5 (.h5) data
  1. Still needs work on dead-time correction.
- 9) New device object driver for EDS HMSA map data
  1. As used for files converted from Tornado BCF format to HMSA by the BCF2HMSA program.
  2. These files appear ~20x larger.
  3. Minimum of metadata is acquired, so we are missing dwell and pixel size in particular.
- 10) Update to device object driver for Oxford Microbeams OM DAQ (.lmf) data
  1. Cater for Header\_Version 14 (rundata 9, adcinfo 9, file-structure 2) and LMF-version 4.
  2. Add ‘eqn’ struct to sample in rundata, and QscalerCount to end of rundata.
  3. Expand adcinfo, and add ‘timing’ struct.
  4. For LMF version >= 4, also now read pixel address lookup table.
  5. Events now has PixelIndex and Composite E,channel,multiplicity Long word.
- 11) Layer plot

1. Plotting of yields now has a plot of Escape depth (depth at which yields drop to 1/e).
2. Use the new X axis display for “Z” and Y axis “Escape Depth”.

## 12) Associations

1. Added new menus to be able to further refine an element-element selection. Now you analyze the spline selection using "Include points within spline" menu. Then on different element axes, you can further trim down this selection using two menus: (i) "further refine within spline": using a new spline on the new two-element plot, only the points from the first selection that also are contained within the new spline are kept, and (ii) "reject selection within spline": use new spline as a tool to edit the selected points, deleting any points within the new spline curve.
2. Added a check-box (next to Z scale drop-list) to enable display of current pixel selection on Cluster plots, highlighted in green. This shows the current selection, after any multiple 2D field ‘include’ or any ‘exclude’ edits.

## 13) New device object driver for XRF mapping data from iXRF Atlas.

1. Does not handle 16-bit characters in header JSON. Data format now uses 8-bit ASCII only.

## 14) Background in X-ray fit can now be split into two components.

1. This is useful for continuum XRF spectra, such as from Maia Mapper, to split the lower background under major element peaks from the large hump from filtered continuum from the source.

## 15) New alternate storage for detector and filter files.

1. Looks for detector files in geopixe main directory, but also ‘config/detectors’, with config defined in ‘geopixe.conf’.
2. Looks for filter files in geopixe main directory, but also ‘config/filters’, with config defined in ‘geopixe.conf’.

## 16) File Requester will now often try searching neighbouring directories, or down directory trees.

1. If this is failing to find a match, just select “Cancel” to bring up the file requester browser.

## 17) Revised Export plots from Image and RGB Image windows.

1. These now offer more options, such as hot-spot analysis indication/highlighting.
2. Output is now from the IDL Z buffer to high resolution image files (e.g. JPEG), which preserves resolution of images to well beyond 10,000 pixels across when imported into PowerPoint, etc.
3. Option of using absolute stage coordinates in plots.

## 18) Batch sorts

3. Added an RGB output images option. The RGB Images window will be opened (if not open) and the names of an export Learn list will be prompted for. This will generate full resolution RGB images for all combinations in the Learn list.

## 19) Hot-spot analysis

1. Add new tabs and controls to the *Image Regions* window to decompose a region into isolated hot-spots, which then appear as separate regions.
2. Use this on regions constructed for Thresholds of selected elements and field selected in the Association window.
3. Can also for regions of the immediate “Neighbourhood” of each hot-spot.
4. Spectra for region hot-spots can be extracted, as for normal regions.
5. Deletion options allow matching spectra to be deleted, and the sum hot-spot region updated as regions are deleted.
6. Exported Regions table will include the X,Y centroids for the centre of gravity of each hot-spot.

## 20) Image Regions

1. New organization of the buttons into tabs (Load, Modify, Delete, Extract, Hotspots), and add new feature (modify highlight pixel selections, with Erode, Dilate operators).
2. Image Regions table can be sorted by clicking on the heading for each column.
3. Can now drag select multiple rows (e.g. for deletion). Click and drag down in any column (except the row label).

4. The EVT button will now go searching in the directory tree in neighbourhood of the current directory to find the raw data. This is useful for full file-names with paths saved in files from different computer systems.
5. Regions table now has a “Pixels” column, which shows the number of pixels selected in a region (shape or from Associations spline selection).
6. A new “Modify” tab allows operations on region pixel selection to “Erode” or “Dilate” these pixel groups.

## 21) Sort EVT window

1. File requesters now go searching in directory tree in neighbourhood of a given file name. This is useful for full file-names with paths saved in files from different computer systems. These search up the directory tree and down looking for the file (especially for raw data files). If this is failing to find the selected filename locally, just click on “Cancel” to cancel the search and revert to the file browser.
2. Cluster processing progress bar now shows the number of remaining background processes. These count down as the background processes complete their part of the sort.

## 22) New IDL version 8.7/8.8 support

1. IDL 8.6 introduced a whole new licensing scheme and removed some features that GeoPIXE was using.
2. In GeoPIXE 7.5, workarounds have been developed to use IDL 8.6.1 and 8.7/8.8. But these require the generation of new license keys (“license.sav” files).
3. IDL is needed for Python bridge support after Anaconda python introduced various features that broke the usual bridge operations. This is only needed for extensions to GeoPIXE for Maia Mapper support.

**New Features in 7.4:**

- 1) 3D detector geometry display
  1. Each detector is offset by thick/2 in Z so that the front face appears at the correct distance.
  2. Local detector pad tilt added to 3D modelling.
- 2) Window placement in GeoPIXE
  1. Worked around issue under Linux where windows would jump to original position.
- 3) New device object driver for FalconX from XIA:
  1. Cater for merged data-streams from multi-detector arrays, as handled by Australian Synchrotron daemon.
  2. To cater for long headers, if no Y found in first read, reread 6 MB of data.
  3. Handle up to 6 stage axes and 4 FC channels.
- 4) Fixed bug in continuum source spectrum modelling of attenuation.
  1. Only effected continuum source spectral modelling, as used in Maia Mapper.
- 5) Batch processing of event data to images, and image operations.
  1. Allow for a limited range of run numbers to process.
  2. Better updating of paths after a change in Sort EVT window.
- 6) Added option to output RGB Images based on a selected Learn list,
  1. The RGB images will be output at full resolution, by default, with options to reduce the image size.
- 7) Maia data processing for Maia Mapper
  1. Allow “ms” to be a new charge/flux unit to use simple dwell time as a flux weight.
- 8) Maia device improvements
  1. Allow for flipping of the X (and Y) axis to cater for the reversal of stage X axis on Maia Mapper on the Left stage of each system.
- 9) Kill/ blank pixel values
  1. Image processing menus to kill pixel values within current pixel (and optionally to this is all element planes).
- 10) NSLS\_MARS\_Ge device

1. New device NSLS\_MARS\_Ge device for binary data from MARS Ge system.
  2. Two long words per event: First is E,T,adr in Maia event\_1 format, Second: long word time stamp.
- 11) Sort EVT
1. Permit the final data file (in a data file series) to be in the next numerical (run) directory.
  2. This still has problems with the YLUTs, so do not use Cluster mode for now.
- 12) New image plugin: Raw Count Rate image display.
1. Plot a histogram of detector count rates.
- 13) Image Regions table:
1. Add "Centroid X" and "Centroid Y" to display mode drop-list.
- 14) Continuum XRF source model
1. Allow alloy anode composition
  2. With polycapillary transmission function.
- 15) Filter and detector setup
1. Allow Gas layers under NPT conditions.
- 16) OM DAQ device: Header read:
1. Added support for header-versions 12, 13.
  2. Problem has emerged in the live-time values returned. Needs to be fixed.
- 17) Sort EVT
1. Add a "Get" button to Scan tab to retrieve Box offset/range for windowed sort.

### New Features in 7.3:

- 1) MPDA is a new approach to quantitative imaging that solves: (i) quantitative per pixel concentrations (equivalent to the older "Correct Yields" matrix method), (ii) better X-ray relative intensities that evolve spatially with composition, and (iii) improved background shapes that adapt with composition changes.

It is triggered by selecting the "Multiphase DA (MPDA)" mode and supplying a new .mpdam file on the Sort EVT window DA/Cal tab. The .mpdam file is created by clicking "New" and selecting in the popup window:

1. path to 'phase map' .dai file
2. path to the "Correct Yields" setup .correct file

To use it, you need the following (later we'll have a Wizard to orchestrate these steps):

1. Identify end-members
  - a. Identify end-members components, and elements that provide a measure of each.
  - b. Fit regions that sample the end-members as much as possible, using a yield calculation with composition for the end-member, and make a DA matrix for each.
  - c. Also fit a region that samples a background component that will be used as a remainder component called "Rest".
2. Correct images using the "Correct Yields" method
  - a. Open the "Correct Yields" window and select components, elements that sample each and their matching DA matrices from above, and fill in the composition matrix that relates end-members to their elements.
  - b. Also select the DA matrix to be used as the remainder "Rest" component.
  - c. Open the .dai image for your sample, and click "Correct" to correct concentrations based on the end-member (phase) proportions. Typically, this needs 2-3 iterations (press button again).
  - d. Save the setup as a .correct file.
3. Project end-member or phase maps

- a. Click in "Mineral" to project the end-member or phase maps.
- b. Save this as your 'phase map' .dai file.
- 4. Create your .mpdam file as discussed above
  - a. Use the popup window, and select the 'phase map' and 'Correct setup' file paths from above.
- 5. Select "Multiphase DA (MPDA)" projection mode.
  - a. On Sort EVT DA/Cal tab.
- 6. Select this .mpdam file in Sort EVT (DA/Cal tab)
  - a. Change the file filter to "\*.\*" and select the .mpdam file.
- 7. Start the sort (you can use "cluster" mode for Maia data).
  - a. Normal GeoPIXE functions work the same from there, but you should see better concentrations in images, and better region spectra overlays.

Warnings:

1. Phase maps only work if the (corrected) image data is quantitative so you get realistic phase proportions for each component.
- 2) The File-Requester has been improved, and can find referenced files (e.g. DA matrix files in a range of places in the current directory tree, or via the translation tables, where it will look up those alternative trees as well. Use the Translation tables to translate from path roots (the first part of a path, which is local to a computer/file system) to the matching root on the new computer/file-system.
- 3) The 'Sort EVT' window now supports XANES stacks sorted directly from 3D Maia data. This requires spatial information for X,Y as well as energy Z (or mono angle) to be captured by Maia encoders and selected for position output as axes 0,1,2. Re-direction from the 0,1,2 axes onto GeoPIXE X,Y,Z is done in the Maia device. The re-direction also allows sorting 3D data into normal 2D maps with selection of the 2 axes to display as X,Y.
- 4) Added device drivers for the iThemba Labs Midas data acquisition system, the new HYMOD-based CSIRO DAQ 36-channel data acquisition system and the FalconX list-mode data acquisition system (XIA and Southern Innovation drivers) used by the CSIRO Nuclear Microprobe.
- 5) Improved Maia device drivers for new record tags and better error detection.
- 6) Parallel processing ('cluster' mode) has been improved, so that multiple instances of GeoPIXE can be run in cluster mode in parallel. However, avoid running EVT spectra extraction at the same time as Image sorting in the same GeoPIXE process, as this won't work.
- 7) The *X-ray Spectrum fit* now supports iteration on sample composition during the fit. This can be set-up using the "Multiphase Loop" tab, which allows selection of a yield correction matrix, which parallels the composition matrix in the correction of images using the *Correct Yields* window and makes use of an end-member decomposition approach to cater for major element terms and missing elements.
- 8) Filters and absorbing layers (e.g. in detectors) can include a new thickness mode ““Gas (mm NPT)” for mm of gas at normal pressure and temperature (20 °C, 1013.25 mbar). If spectrum data files include P,T, then this is used to adjust for ambient conditions in detectors and filters.
- 9) Shared memory scheme has changed (e.g. in parallel processing using the “cluster” mode). The change means that the log files for the background processes have a different unique name and so will accumulate in your `~/.geopixe` directory. Delete old ones occasionally.

## New Features in 7.2:

- 1) Improved the management of background processes in Maia\_Control for Maia detector real-time monitoring and real-time DA imaging.
- 2) Develop a work-around for Linux file-system not reporting write ability of directories through IDL correctly on some file-systems.
- 3) Developed a new *Import Fit Wizard* to import a series of raw data files and produce spectra.

- 4) Fixed bug that sometimes lost the top row in some frames of XANES image stacks.

## New Features in 7.1:

- 1) Some new metadata is read from Maia blog files, and these can populate the 'pileup' and 'throttle' fields in *Sort EVT* and in spectrum Import. When you start the sort, if the paths to these files is not correct, it will prompt for new paths; navigate to the new location, or perhaps use the 'translation table' in the file requester to translate from old paths (e.g. as they are used at XFM or on Massive) to your new path (e.g. on your laptop, lab computer or on Massive).
- 2) *Maia\_Control*: The main addition is catching the ion chamber details from Kandinski variables 'flux.chan[].coeff' and 'flux.chan[].unit' to set the sensitivity of the 'Maia:scaler.FC0' and 'Maia:scaler.FC1' PVs for the built-in Maia scalers for flux IC0, IC1. If these are being set by the beamline, then they will be flagged as 'remote' in *Maia\_Control*, and you will not be able to change them on the "Imaging" tab.
- 3) The dead-time calibration coefficients "DTcalA" and "DTcalB" are now set automatically from the Scepter slope parameter.
- 4) A new image file format reads header information quicker for faster file-requester preview.
- 5) A new menu "Image History and pixel statistics" on the *Image* window adds pixel statistics to the Properties for the image.
- 6) Added a new 'FalconX\_device' for the Southern Innovation-XIA FalconX tests done at XFM. This will change in future as the draft list-mode format is refined.
- 7) The 'Windowing' sort options in *Sort EVT* now allows negative offsets, if your list-mode data (accidentally) move into negative XY.
- 8) The *Sort EVT* window now supports XANES stacks sorted directly from 3D Maia data. This requires spatial information for X,Y as well as energy Z (or mono angle) to be captured by Maia encoders and selected for position output as axes 0,1,2. Re-direction from the 0,1,2 axes onto GeoPIXE X,Y,Z is done in the Maia device (and can be set on the *Sort EVT* "Device" tab). The re-direction also allows sorting 3D data into normal 2D maps with selection of the 2 axes to display as X,Y.
- 9) Added new scan modes to *Sort EVT* to cater for XYZ data-sets for XANES ("Scan in XY and Z (energy)") and for tomography ("Scan in XY and Tomo angle (Z)'), used with the "3D Stack" mode. The first generates a single XANES stack .XAN file, while the second builds a series of tomo stack .XAN files, one for each element, all in a single pass through the 3D data.
- 10) Added new escape modes in the *Cal* window to cater explicitly for Ge and Si detector escapes.
- 11) New image region modes: "Single pixel", "Project X" and "Project Y". The latter are like "Traverse" but constrained into the X or Y directions only.
- 12) A new *Standards Wizard* has been developed to automate processing of standards samples and the determination of the "conv" calibration factors across a run. These will use new metadata that will start to be seen in raw blog data from late August, 2015.
- 13) Corrected problems with stopping background processes in *Maia Control* and *GeoPIXE*.

## New Features in 7.0:

- 1) GeoPIXE device drivers have been changed and are incompatible with the older versions. To use v7.0 you need to use the new drivers, and correct any drivers you have written or modified. The key changes are (see the source pro files):
  - The keywords for the methods 'read\_setup' and 'read\_buffer' have changed. Check the new source files. A few obscure keywords are now optional, and a new keyword 'veto' has been added for a vector to flag rejected events to parallel the normal 'x1,y1,e,t' vectors.
  - 'n' is now the full return length of the 'x1'y1'e,t,veto' vectors.
  - 'good' is the number of good events in 'n', which is the same as 'n' if 'veto' are all zero.
  - 'veto' an optional return to show events for GeoPIXE to ignore (veto[i]=1).

- 2) This will make it necessary to modify device drivers a little going from version 6.6 to 7.0. See the notes documents in file “GeoPIXE-device-devel.zip” in the Help dir.
- 3) The Maia 384 device driver has been updated to get rid of old test code. It can now provide a better template for stream directed list-mode devices.
- 4) Updated device object drivers for Maia, NSLS NetCDF, NSLS MCA, NSLS HDF, GSE-CARS, Hasylab, ESRF EDF and NSLS NetCDF.
- 5) Now each load of a spectrum or image will use a new instance of the device object relevant to the data, and so the device specific parameters (e.g. in Sort EVT window “Device” tab) will be independent and not ‘global’ to the session.
- 6) Added a “Wizard” plugin approach, and a wizard for depth profiling of particle hot-spots in images. This works for an array detector with detector elements that span a wide range of take-off angles, such as Maia. See the new “Wizard” menu under the image “process” menu. During development and debugging of a user written Wizard in IDLDE, the Wizard will automatically load GeoPIXE. More on Wizards later as the hooks into GeoPIXE are added.
- 7) IDL ‘file\_test(/write)’ does not work correctly on some Linux mounted drives, so a workaround was used using a test file creation.
- 8) The GeoPIXE file requester now has a “Find” field, which will (on <return>) search for a supplied file-name (with wild-cards) in the current directory tree, and if a file is found, set the dir in the file-list to the file’s directory.
- 9) A new option on the “Display” “Colour” menu allows an alternate spectrum colour palette that may help Red-Green colour visually challenged users.

**New Features in 6.6:**

- 1) The Fastcom MPA3 device has been extended to provide X,Y ADC selection widgets in the “Device” tab of the *Sort EVT* window, for the selection of X,Y ADCs for image data processing. New image DAI files will save this information.
- 2) Changed the way shapes are drawn on images. Now do not round on display as shape is moved. So movement is nice and smooth, even at large zoom and very pixelated images.
- 3) Fix bug in Sort EVT that forced global (post cluster stripes) flatten even if not set.
- 4) Align image plugin now compares all images to first one to get absolute X,Y shifts. This fixes occasional error creep that became an apparent drift of position.
- 5) Fix error in Plot Images with “absolute” so that switch to ‘microns’ below 0.3 mm range does not happen now, which upsets plot scales.
- 6) Correct edge behaviour in shift image rows to extend and not wrap/rotate.
- 7) New PIXE/SXRF Depth Profile Calculation added to window menu of Spectrum Display. This allows you to combine “inner” and “outer” detector selections to call the yield calculation to calculate ratio of yields for elements from grid yield calculation data to output spreadsheet compatible output for depth determination. A full implementation is underway.
- 8) The *Image History* window now shows image version number.
- 9) Add Bauer *et al.* AES (H.E. Bauer, "A fast and simple method for background removal in Auger electron spectroscopy", Fresenius J Anal Chem 353 (1995) 450-455) background algorithm as a plugin.
- 10) Fixed issues with Geopixe\_update on certain Linux systems.
- 11) Fixed a bug in Windowed image sort mode that offset the flux map incorrectly.

**New Features in 6.5:**

- 1) Maia Control has been extended to cater for both “Project” and “Group” directory specifications in the on-line acquisition path.
- 2) Added the Spine 100 region shape for very fine control of selected regions.

- 3) Added “Reload User Plugins” menu to search for all existing and new plugins and reload them. Use this if you recompile a plugin that is in use, or if you compile a new one that needs to be added to the “Process → User Plugins” menu.

### New Features in 6.4:

- 1) Geopixe\_update.sav extended to allow the use of a proxy server if this is required at a user site to access the GeoPIXE FTP server. Geopixe\_update also displays recent news of new features and changes during the update download, from the “news.txt” file in the Help directory.
- 2) Fixed a bug in the “Spectrum\_add” routine that affected the “Add (remap cal)” operation that adds spectra by energy after remapping by energy calibration. Some low counts channels were becoming zeroed.
- 3) Streamlined file selection using the “EVT” button for spectra extraction. It now does not prompt for named files that it can find. You will only get a file-requester to confirm the output .spec file-name (this should be the same as the .region file-name if you remembered to save it first) and any files not found (because the paths have changed).
- 4) Selective image sorting: The *Sort EVT* window “Scan” tab now has extra fields to select the sorting of a selected sub-region of the full image area. Use this to select a portion of the full image area (which may be huge for Maia data) and produce images for that sub-region without any compression. This is handy for producing full-resolution sub-region images from a huge scan that can’t be loaded into 32-bit machines. For the present, select sub-regions using a Box shape on the full-image and read off the offset and size (in uncompressed pixel units) from the context help field when you lift your mouse finger after moving/dragging the Box.
- 5) WARNING: The format of .dai and .region files has changed with this release and cannot be read with previous versions of GeoPIXE.
- 6) GeoPIXE keeps track of the offset into this sub-region, so that regions can be used interchangeably between the full-scan image (probably compressed) and the sub-region images for average concentration estimation and spectra extraction. Box shape coordinates in the Image window show both absolute and relative (to sub-region) pixel and XY coordinates in mm.
- 7) A new menu item in the File menu on the Image window called “retry cluster image combine” can be used to re-assemble image stripe image files (\*.DAI.n) if the cluster processing stops due to a lack of memory (e.g. on 32 Window systems). After regaining some memory, use this menu and select the \*.DAI.n files to combine.
- 8) The *Detector Select* window (opened from the “Array...” button on the *Spectrum Select* window), now has a “Get” button to set detector channel selection based on the detector channels found in a selected SPEC file.
- 9) The Spectrum Select window “Delete” drop-list now has new entries to delete “not selected spectra”, “not displayed spectra” and “spectra with invalid energy calibration”.
- 10) Added XANES spectra (non image data) sorting from directories, such as for Maia data acquired with a new energy step in each dir. Use the XANES radio button on the top of the Sort EVT window.

### New Features in 6.3:

- 1) New record header information for data from the Maia detector enables per pixel and per detector accounting for dead-time and pile-up losses and the use of the 2 Maia hardware flux counter inputs. New features in GeoPIXE 6.3 use this data to provide: (i) correction for dead-time in images and spectra, (ii) correction for pile-up losses, (iii) use of the hardware counters for accurate pixel-locked integration of flux using pulse streams from V-to-F preamplifiers. A new calibration (DTcal A, B) is included to convert time-over-threshold T to ns for dead-time measurement.
- 2) A number of new plugins enable display if (i) raw flux map, (ii) dead-time map, (iii) pile-up loss map, (iv) dwell map, and (v) detector channel dead-time and pile-up histograms.
- 3) Consistent use of parallel processing options for multi-core acceleration of imaging, spectra import and spectra extraction from regions. Core number is configured in the “geopixe.conf” file, which is normally read from your home .geopixe directory (if not found a copy will copied there from the main geopixe dir).
- 4) The *Spectrum Select* window has been revamped for more flexible selection of spectra based on detector channel, especially for detector arrays. The new “Array...” button opens the *Array Detector Channel Selection* window, which provides a mimic display of the detector array on which to select desired channels. Selection class options

allow selection in groups based on row, column, radial position, odd, even and underlying hardware (chip, quadrant) relevant to the Maia detector array. Groups of detectors can be deleted using these selection classes and other groupings, or by drag-selection in the *Spectrum Select* table.

- 5) A new updater program has been added to GeoPIXE (standalone as “geopixe.update.sav” and spawned from *GeoPIXE Image* Help menu) to manage updates of software and support files for registered users from the GeoPIXE FTP site. See the file “Help/GeoPIXE-update.txt” for details.
- 6) Spectra can be selected by clicking on them in *Spectrum Display* when in Highlight mode. This is useful to select one spectrum feature of interest from hundreds of overlaid spectra when displaying up to 384 spectra from the Maia detector array. Click on the spectrum data for one channel to make it the highlighted channel. Avoid clicking on markers to select the spectral data.
- 7) The *XANES Image Stack* window has been extended to provide (i) importing image frames to build a XANES image stack, (ii) normalization of frames to flux, (iii) coupled display scale auto-scaling to maintain the relativity between frames, (iv) the determination of selected feature centroids for region shapes, and (v) shifting of image frames to match centroids across a stack (“Match Centroid” feature of *XANES Image Regions* window). To support XANES, image frames now contain beam energy and a Z (energy) axis coordinate list to permit irregular energy steps across the XANES spectrum.
- 8) Support for the Maia detector hardware counter inputs FC0, FC1 has been extended. These counters are tightly registered to pixel address in hardware. Now they can be selected and used as ion-chamber or beam charge integrators and images from both inputs are projected along with elemental images, normalized to the currently selected flux/charge map, during DA and ROI image generation. They appear as the images “Flux0” and “Flux1”.
- 9) New Process→Shift menus have been added to the *XANES Image* window to allow added correction functionality for backlash removal. If the sense of backlash changes between XANES frames, due to a reversal in stage direction (a problem occurring for a time using XFM scripts for XANES stacks with an odd number of Y rows), then a new set of menus allow ‘toggling’ or reversal of the sense between frames.
- 10) A stage movement problem at XFM that resulted in a drift in apparent Y coordinate in images between *XANES Image* stack frames, can now be corrected using the new menu “Process→Correct→Correct Y drift”. This detects zero/blank rows at the bottom of subsequent image frames to remove the drift. Use this in conjunction with the “Match Centroids” feature of the *XANES Image Regions* window to correct for position jitter or drift between frames in a *XANES Image* stack.
- 11) The detector model (see “Edit detector” menus) has been extended to make a distinction between normal detectors that may have a volume effect on effective solid-angle (higher energy X-rays penetrate deeper into a detector and hence “see” a smaller solid-angle) and those that use highly absorbing collimation that prevents this volume effect, such as Maia. Use the “volume solid-angle correction” check-box to select this (or disable it for Maia). The layout arrangement of a detector array can now be viewed using the “?” button next to the Layout file name field.
- 12) The DA matrix can now be generated for an entire XANES energy series. Options on the “Generate DA matrix” button in *X-ray Spectrum Fit* allow the selection of a normal DA matrix or a XANES series DA matrix, and there are new facilities for generating the XANES energies files (*Spectrum Display* window menu “Import → Energies from list-mode” and *XANES Image* window menu “Export→XANES energy list”). The XANES series DA matrix can then be used for imaging frames in the XANES image stack using Sort EVT as before. However, the correct energy matrix is used for each step in the XANES stack series and spectra overlays on extracted spectra from regions on single frame images will use the correct beam energy for the “DA Fit” overlay. For edge energies below 6.5 keV, the Compton and elastic peaks begin to merge and are combined in the DA matrix (element called “scatter”).

## New Features in 6.2:

- 1) While the effects of the varying sensitivity of detectors across a detector array has been used in GeoPIXE for some time to correct model calculated X-ray yields, the relative intensities needed for spectrum fitting have just used the integration through the multi-layered sample and correction for filters and detector efficiency for the ‘central’ detector element only. Now for each spectrum, the detector elements that were active in contributing to the spectrum are used to calculate a weighted average of relative intensities for each detector, including intrinsic efficiency and external filters across the array.
- 2) Certain Image parameters displayed in the *Image Properties & History* window (Windows and File menus) can now be edited. Just double-click on the text fields for Sample, Grain and Comment, the Scan Size or Origin, or the

Charge and Conversion factor fields to pop-up an edit window. Most parameters are fixed and reflect parameters used in the Sort or later image processing steps. To change fundamental parameters, such as DA Matrix and element list, Compression or flux PV selection, the data will need to be re-sorted in *Sort EVT*.

- 3) The *Association* window has been revamped to provide axes and better control over the displayed concentration ranges in X and Y. The 2D histogram Z scale can also be displayed using Sqrt of histogram frequency to compress dynamic range.
- 4) Version 6.2 includes a new window for *XANES Image Stack* construction and exploration, accessed via the *Image* window Display menu. More on this later ...
- 5) GeoPIXE preferences are now kept in a config file “geopixe.conf” in the “.geopixe” sub-directory to your home directory (if not found it will search in the GeoPIXE directory). It can be edited to set-up default paths, cluster and parallel processing parameters, window startup and image origin.
- 6) Similarly, file path bookmarks, as used in the file requester, are stored in the “.geopixe” sub-directory to your home directory (if not found it will read bookmarks from the GeoPIXE directory). It will save paths back to the .geopixe directory. The token “\$HOME” in the bookmark list translates to your home directory (as pointed to by the HOME environment variable).
- 7) Support for computer clusters and multiple cores on modern PCs has been added. The cluster mode is selected in the new config file “geopixe.conf”. When “cluster type cores” is selected, multiple IDL sessions are used to divide up the processing of raw data. This works for data streams in a series of files, with absolute XY coordinates contained within them and using numeric file extensions on the files. Select the number of cores to use in “cluster nodes n”, and enable cluster mode on the *Sort EVT* window. Log files are written to the “.geopixe” sub-directory to your home directory.

### New Features in 6.1:

- 1) Libraries for low-level processing code have been compiled for both 32 and 64 bit versions of Windows, Linux and Mac OS 10. GeoPIXE should now run on all these platforms, although it is only tested routinely on Windows 32 and Linux 32/64.
- 2) An interim version of these libraries was placed on the FTP site without optimization. The new versions are a factor of 2 faster and should be downloaded to replace any interim libraries.

### New Features in 6.0:

- 1) The major reorganization in GeoPIXE 6.0 is the development of Object Oriented Device driver plugins. All device specific code is now gathered together in a single PRO file that is loaded automatically from the “interface” directory as an IDL Object. Each file name has the form “XXX\_DEVICE\_\_DEFINE.PRO” for device “XXX” object code. Users can now view and modify their device-dependent IDL code and indeed write new drivers using these as templates. A new guide “Help\Object Oriented Device Driver Modules.doc” is provided to help with this.
- 2) Device objects may choose to read and write new device-specific parameters to Image (.DAI) and region files (.REGION). Older, Maia explicit parameters have been removed. Matching read and write methods need to be written in the object definition to do this consistently for each device that needs extra parameters. For this reason, extensions to DAI and REGION files now exist that will make them unreadable to older versions of GeoPIXE 5.
- 3) The following devices make good templates for writing driver code: (i) MPsys\_device – simple PIXE list-mode in a single file, (ii) NSLS\_MCA – SXRF raw data stored in pixel MCA spectra files that also scans for variables providing ion chamber count rates and sensitivity, and (iii) Maia\_device – uses all methods, including use of Y lookup tables and defining extra widgets and use (and read, write) of local device parameters.
- 4) The GeoPIXE directory has been reorganized. Now plugins are located in the “plugins” directory, the Maia config file (used with the Maia device) and the Maia background processes (used with the Maia\_Control program for detector monitoring and control) are located in the “maia” directory, the new device objects are in the “interface” directory and image files are located in “images”. Example setup files have been moved to the ‘setup’ directory.
- 5) The GeoPIXE PIXE database has been extended to include Np and Pu L lines, using an extension of the ECPSSR tables of Cohen and Harrigan for L cross-sections (At. Data Nucl. Data Tables 33 (1985) 255) and relative intensities (At. Data Nucl. Data Tables 34 (1986) 393) (D,D. Cohen, pers. Comms, 2011). The XRF database extends to Z=98 using the tables of Elam *et al.* 2001 (see v3.1).

**New Features in 5.5:**

- 1) An extra feature has been added to the *Image Table* EVT button called “individual”, which allows extracting individual spectra from each detector for the first region in the region list. This complements “array”, which forms a summed spectra of all detectors for each of the regions.
- 2) A new checkbox under the element drop-list in the main GeoPIXE *Image* window allows toggling the interpolation of image data when zoomed in. Uncheck the box to suppress bilinear interpolation.
- 3) Some errors have been corrected in the geometry corrections for large array detectors with non-monotonic detector number order, such as Maia. The correction means that the relative sensitivities across an array, and the accumulation of sensitivity when a sub-set of detectors is utilized, have been corrected. The impact of these corrections is that all **Maia Yield files** and **Maia DA matrix files** should be regenerated and IC count to charge conversion factors may need to be corrected. It is best to check all calibrations on Maia quantitative images.
- 4) A number of structural extensions have been made to accommodate 3D data-sets for XANES imaging. These include a XANES image stack window and extensions to RGB images, Associations and regions. Image DAI files now contain beam energy and X and Y pixel coordinate vectors. More on this later ...
- 5) Two new Region selection types or shapes have been added: “Project X” and “Project Y”. These work like “Traverse”, providing a method to produce linear traverse profiles across images, but are constrained to project only in X or Y. These are useful for pseudo 2D data-sets, such as XE XANES line scans, in which a line is scanned (in X) at each beam energy E and the data-set is built as an image with E as the Y axis. Then “Project Y” provides the XANES spectrum for a selected portion of the scan line. New additions to DAI files store non-uniform X and Y coordinate vectors if available from raw data source.

New TIFF export options have been added to the *Image* window to export in (i) concentration (ppm), (ii) counts (summed over all detectors), and (iii) ng/cm<sup>2</sup> loading per pixel. These options have been added to the *Batch Sort* window too.

New information is packed into the DA matrix files to allow images to be reported and exported in ng/cm<sup>2</sup> units. Older DA files will need to be regenerated to access this feature (e.g. TIFF export).

A new Image window File menu option “Load (ignore null)” has been introduced as an option to read certain poorly formatted files that fail to load normally. Try this if you get a load error using “Load”.

A “No Q” button has been added to the *Spectrum Select* window to zero all charge values in the table. If a charge is set for the first spectrum in the table, then a “Fit All” applied to the *X-ray Spectrum Fit* will apply this charge to all subsequent zero charge spectra. In the case of SXRF, the current conversion factor from IC count to charge will be applied to any valid IC count values in the subsequent spectra to calculate a charge before fitting. Click on “?” next to the charge (Q) field in the fit window to make sure the correct conversion is applied.

**New Features in 5.2-5.4:**

- 1) A number of structural changes have been made to accommodate new Maia 384 detector features, such as real-time spectra and DA image display, as well as underlying changes needed for using parallel processing on computer clusters. The parallel processing features are still under test.
- 2) The *Import* spectrum process looks quite different now. Selection of ion chamber sensitivity for synchrotron data and a button to “scan for Epics PVs” has been added. The flow of operations is more logical.
- 3) The *Sort EVT* window has been updated to incorporate ion chamber PV and sensitivity selection and the conversion factor between IC count and equivalent charge. Now input files, scan details, ion chamber settings and DA settings and energy cal are on separate tab panels.

**New Features in 5.1:**

- 1) A new image export has been added to output images in floating point TIFF format for use elsewhere, such as for tomographic reconstruction. It can be accessed on the “File→Export→selected Images as TIFF counts” menu of the main GeoPIXE *Image* window. The output is one TIFF file per selected element plus a summary HTML file, output to the TIFF subdirectory by default.

A new *Multi-image Display* window has been added that displays a grid of simple element windows (*Image Display* menu). These can be zoomed by dragging out a rectangle in the first window.

Maia detector array support has been extended to accommodate the new 384 detector array developed by CSIRO and BNL for the Australian Synchrotron and the NSLS.

### New Features in 5.0:

- 1) Flux handling for synchrotron XRF imaging has been improved. A new “?” button next to “Q” charge in the X-ray Spectrum Fit window provides a place to set ion-chamber count to flux conversion based on charge, or to set charge based on a prior conversion factor. See the Data Analysis Scenarios chapter on SXRF imaging.

Flux is tracked through image, spectra, region and results files. Hence, the format of these files has all changed in version 5. These new files cannot be read by older versions of GeoPIXE (v4).

### New Features in 4.9:

- 1) A new File Requester has been developed to provide better file selection, directory navigation, bookmarked paths, content previewing and to give better consistency across platforms.

The *Blog\_Browser* program is available from the Windows menus to browse and probe the details of records in Maia data files.

The saving of HTML files and new DAI output images has been improved to create subdirectories automatically.

Batch processing has been extended to include Maia-96 detector data files.

### New Features in 4.8:

- 1) Support for the CSIRO-BNL Maia-96 advanced fluorescence detector arrays has been extended to support flux measurement in images, and correction of images for flux variation, which has necessitated extension to libraries. This version requires the new “image\_dll.dll” file under Windows and “image\_lib.so” under Linux.

Support for detector arrays has been extended to “refit” in *X-ray Spectrum Fit* and adjustments made in *Result Properties*, which were inherently simple detector array functions before, to now include variation in sensitivity across detector arrays and the selection of an arbitrary subset of detectors in an array.

Extended Maia-96 support for linearization to work with either a single linearization table, or one for each detector, as stored in .linear files. These tables are constructed with plug-ins specific to the Maia-96 detectors.

### New Features in 4.7:

- 1) Support for the CSIRO-BNL Maia-96 advanced fluorescence detector arrays has been extended to support gain linearization, pileup rejection, rate throttling and increased number of detector elements up to 384. This has necessitated moving to Combobox widgets for detector selection throughout, which is also necessary to move towards Linux support. The linearization and throttling follow through to extracted spectra as well.

Support for Ortec Maestro spectra format and the Wakasa ACC UniDAQ list-mode data files has been added as well as preliminary support for SLS MCA and HASYLAB FIO image spectra files.

Fixed behaviour of the vertical scale drop-list in *Spectrum Display* for fit overlays and added the ability to normalize spectra within the Cut range. Fixed behaviour of the Shrink, Expand and Widen buttons when in Auto and Norm vertical modes.

Separated the working directory tree for raw input data from output images, spectra and other files. These can now be different allowing raw data to be stored in a separate directory tree for easier archival of raw data.

### New Features in 4.6:

- 1) Starting with GeoPIXE 4.6, IDL version 7.0 will be used for all code and new plugins. GeoPIXE will still be able to load v6 plugins.

The Cal window has a new button “RA” to ‘re-assign’ selected peaks to a new calibration. Use this when all spectra are calibrated relative to each other and you want to re-assign the element identity of the peaks marked for energy calibration. This will change energy calibrations for all spectra to assign the peaks to the new selected energies. RA is a form of global re-calibration adjustment for detector array support.

**New Features in 4.5:**

- 1) A new Y display scale mode drop-list has been added to *Spectrum Display* to control vertical scale normalization options. This replaces the “Rescale” button. There are now options for automatic scale setting and for re-normalization of multiple spectra to match the vertical range of the first. The *Spectrum Display* controls have been rearranged to group the X and Y controls together.

The X-ray line identification window has been enhanced. Now all lines for an element are highlighted if one of its lines is selected by clicking on a row. All lines for an element in the line list are selected similarly if an element is selected in the periodic table view.

The *X-ray Spectrum Fit* “Advanced/Widths” tab now has the ability to fix or adjust the Noise peak width parameter via setting the resolution, based on Mn K $\alpha$  FWHM. The resolution is still available in *Fit Results* as before. There is also a check-box to free the Fano factor in fitting peak widths. Use this sparingly as the default works well most of the time and increases fit stability.

A new “Export” menu option has been added to the *Associations* window. Use it to export to CGM, WMF and EPS, or to display the associations in a new window with detailed axes and axis tick-marks, etc.

Pile-up in GeoPIXE *X-ray Spectrum Fit* assumes the use of pile-up rejection strategies (electronic rejection or on-demand beam switching). However, finite timing resolution can still lead to a small deficit in the sum-peak amplitudes. A new “Deficit(%)” control has been added to the “Advanced/General” tab of *X-ray Spectrum Fit* to adjust for this deficit.

Support for list-mode data that does not fill out the specified pixel range completely. The actual bounds is detected and beam flux will be assumed to be spread evenly only within these bounds.

**New Features in 4.4:**

- 1) The scattered beam subtraction options, previously in the *Fit Results* drop-list, have now been moved to the Fluid Inclusion (3 layer) mode of the *Result Properties* window. Now these corrections are made once, which modifies the data, and stored as a property (see the section on “Fluid Inclusion Analysis” in the Data Scenarios section of the manual).
- 2) Version 4.4 is the first version of GeoPIXE to use the license key approach, and the FTP site. Hence, the main executable of GeoPIXE (geopixe.sav) needs to be used with the new versions of the files “geopixe2.sav”, “image\_dll.dll” and a valid license key “license.sav”, sent to you independently. Check the “ftp-read-me.txt” file for the location of files on the FTP site.

**New Features in 4.3:**

- 1) A second detector efficiency curve can now be overlaid in red on the detector efficiency being edited in the *Edit Detector* window. The ratio of the new detector efficiency to the overlay is also displayed in violet, scaled down to 10.

Spectra in *Spectrum Display* can be optionally displayed with points and errors bars for data, using a new check-box called “Error bars” next to the Log/Lin button.

**New Features in 4.2:**

- 1) The various colour/intensity scales in the main image window, introduced in version 4.0, have been extended to the 3 *Element RGB Image* window. Any scale settings for each element in the main image window are now reflected in the RGB colour scales in the *RGB Image* window.

A new *Import* pop-up window is available to import spectra files into *Spectrum Display*. This replaces the lengthy menus and enables the selection of PIXE versus SXRF laboratories and the selection of various file formats from each.

**New Features in 4.1:**

- 1) An extra tab on the *Results Properties* window for thick targets enables the calculation of target thickness from STIM transmission ion energy loss data. This updates the thickness of the target in the yield model, and upon “Apply” calculates the new yields based on this thickness and applies these to the selected results in *Fit Results*.

**New Features in 4.0:**

- 1) In the main GeoPIXE *Image* window, all concentrations between the bottom and top sliders are mapped onto the current colour map, using a linear scale by default. Use the new small drop-list between the bottom and top sliders to select between Linear (L), Log (G) and Sqrt (S) scales for the Z axis. The Sqrt and Log scales have the effect of compressing dynamic range, which can be useful for images with strong hot-spots and low-level traces.

The *X-ray Spectrum Fit* window has been re-vamped to place more subtle parameters and controls on an “Advanced” tab panel. In addition, a number of controls have been added to this panel to control background, tailing and parameters specific to PIXE and SXRF.

“Conc” units can now be specified in “ppm (wt)”, “mmol/l” and “ng/cm<sup>2</sup>”, the latter being appropriate for a layered sample such as a fluid inclusion.

Full detector array support has been added for yield calculation, image projection and spectrum fitting. Now the take-off angle variation across large arrays can be catered for, as well as arrays with non-planar geometries (e.g. hemispherical), round and square pads, and arbitrary tilt relative to the detector-target axis.

Support for the Maia series of detector system has been extended to support full-spectral SXRF (or PIXE) imaging using up to 384 detector elements.

**New Features in 3.9:**

- 1) Ghost features in images, corresponding to second displaced beam at a fixed offset can be corrected using the “Process→Correct→Ghost” menu. The menu offers relative intensities of the ghost feature in 10% and 1% increments. Use these in combination to correct ghost features; the operation is applied to all images. Beforehand, use the “Distance” shape tool to drag out a vector giving the offset to the ghost or echo features.

GeoPIXE can process the HDF format NSLS scan files now as a new device in *Sort EVT* and the *Spectrum Display Import* menu.

Fixed a bug related to *Fit Results* files (PFR) that contained fits that used multi-layer filters. The file format had an error in it. The fix now permits all old PFR files, which may contain the error, to be read and rectified. All new PFR files have the correct format.

If a region is selected and highlighted based on element *Associations*, then the exclude operation can now be used to remove pixels from the Association highlighted area.

To remove pixels from the current *Associations* highlighted area, use the exclude “-“ mode of region select shape.

Select exclude, drag out a shape and use the “Σ” button to remove pixels within this region from the current *Associations* selection. Note for this to work, no include region should be set. To make sure, use the menu “Display→Clear ALL Shapes” and then select the exclude region.

The Image Export options have been extended to permit export of whole images, or selected regions, for selected elements as tab or comma delimited ASCII files, or as *X,Y,concentration* files with multiple columns for multiple element image selection.

An energy cursor and energy entry field have been added to the *Edit Filters* and *Edit Detectors* windows. Enter photon energy (keV), or drag a cursor on the plot, to determine the transmission or efficiency at the cursor energy for filters and detectors, respectively.

If an X-ray line is selected in the *X-ray Identification* window, the filter and detector window cursors will be set to this value.

Loading filter files that use explicit density for compound filter layers will now display in the *Edit Filters* and *Edit Detectors* windows in “microns” mode with this density set.

Mostly, image data is made available to *Image RGB* via a notification from the main *GeoPIXE Image* windows when new data are loaded. However, the new “Compare Images” menu offers a way to load another data-set (e.g. to compare PIGE with PIXE images); the new elements are added to the *Image RGB* element drop-lists. Select any of the original elements (as in the associated *Image* window) or the new “Compare” elements in the drop-lists.

Zero pixel data can be removed using the “Process→Correct→Zero pixels” menu of the main *GeoPIXE Image* window. “Zero” pixels are defined as those that are surrounded by at least 6 non-zero pixels. It uses a threshold of 3% of the display maximum of the currently displayed element to determine which pixels contain anomalous zero data. GeoPIXE then replaces these zero pixels in all element images with the average of surrounding non-zero pixel

data.

Several parameters that can be used to adjust the behaviour of background, tailing and scatter peaks in the fit are now available on an “Advanced” tab on the *X-ray Spectrum Fit* window. Many features that were only occasionally used (such as CUTs background algorithm parameters) are also now on this Advanced panel.

### New Features in 3.8:

- 1) New features have been added to accommodate the Maia-32 event-file format produced by the CSIRO Blog server. In addition to this device being added to the device list in *Sort EVT* and to the Import list in *Spectrum Display*, data-rate throttling has been implemented.

Throttling is a method to reduce data rates by selectively scaling down parts of the spectrum to reduce total count rates while making little impact on image quality and trace element analysis. Throttle files can be produced in two ways: one from a source spectrum (in *Spectrum Display Analyze*→Throttle menu) and one taking into account image variation (in *Image Display Analyze*→Throttle menu). See the help on these menus for details.

For Maia-32 EVT files, *Sort EVT* includes a file specification entry for a pileup limits file, which specifies the range of valid time-over-threshold for each detector pulse-height. The Import menu of *Spectrum Display* also has options for sorting spectra with or without pileup removed by this approach. The EVT button on the *Image Regions* window sorts out spectra with pileup removed, if appropriate for the image data-set.

A new window (*Time Amplitude*) is available (in the *Spectrum Display* “Windows” menu) to plot the Time-over-threshold time versus pulse-height amplitude for Maia 32 events. Use the “File” menu to select EVT files to sort. If an image is loaded into *Image Display*, and a region is selected and the “Σ” button is pressed, then the *Time Amplitude* window will sort and display the Time-Amplitude points for all events that fall within the selected region.

If a region is selected on an image while *Time Amplitude* is open, then only the subset of Maia-32 events that fall within the region will be displayed in *Time Amplitude*. It will sort through as many files as needed to display the requested number of events.

### New Features in 3.7:

- 1) Entry of energy and A, B data into the Cal window text widgets is now a little smarter, and do not require a <return> to be properly registered.
- 2) Images can be corrected for missing scan lines, or portions of scan lines, in both the horizontal and vertical. Look under Image Operations in the Help for tips. Surround the missing line segment with a Box shape, and go to the “Process→Correct→Missing Rows” menu to replace the missing data with the average on either side. Similarly, “missing columns” works for vertical missing data. Use “Double-counted rows” to attenuate double-counted rows by two, and similarly for columns. These operations are applied to all elemental images, and cannot be undone; save the image file first.

### New Features in 3.6:

- 1) The “Convert→APS MDA to LST” operation, on the *Spectrum Display* File menu, can now use multiple file select to process a sequence of MDA files. These are assumed to use the same assignment for ion chamber PV, sensitivity and live-time correction.
- 2) Initial support for Hasylab FOI full-spectral pixel data files has been added.

### New Features in 3.5:

- 1) Several functions that use regions now will use Association highlighted areas on images, if no valid Region is selected (i.e. Shape tool on *Image* window is set to “Distance” or no shape has been drawn). These include Correct Current and Kill and Suppress Region.

In the *Association* window, a spline region can be cleared using a right mouse button click.

A new menu in Spectrum Display (“Display→Get ALL Energy Cals”) can be used to load all energy calibrations for multiple spectra corresponding to elements of an array from a selected spectrum file.

Support has been added for GSE-CARS full-spectral pixel data files.

### New Features in 3.4:

- 1) GeoPIXE now includes an improved elastic and inelastic scattering model for SXRF. The intensities of these, and the length of the inelastic and multiple-scattering tail, can be varied in the fit. However, at present there is not control or variation on the electron momentum distribution for inelastic scattering. These will appear later.

### New Features in 3.3:

- 1) The *Image Regions* window has a new feature for sorting all detectors of an array into merged spectra for regions. The spectra are mapped onto the energy calibration of the first spectrum before being accumulated into single spectra. The ADC drop-list now starts with “array” which means sort all array detector enabled for the image in *Sort EVT* when the list-mode file was sorted (assumes “Detector Array” type was selected in *Sort EVT*).

The *Detector Setup* window has been updated (access from “Edit Detector” menu). Now the solid-angle properly reflects detector tilt angle as well as detector dimensions and distance.

The *Filter Setup* window now has a new “Special” filter option for Bragg filters. These are log-spiral X-ray lenses tuned to Bragg diffract a certain energy. The centre, width, height (enhancement) and background (scattering) of this transfer function can be specified.

When fitting a series of spectra, using the “Fit All” button on the X-ray Spectrum Fit window, if only the first spectra has a Q value (e.g. entered into the Q box in the fit window) then all spectra will assume the same charge/flux.

Sometimes *Spectrum Select* was not being updated as spectrum properties were changing. This has been rectified.

Support for Tohoku Labo, NSLS MCA image pixel spectra and Sandia Primecore U48 list-mode formats has been added to GeoPIXE.

Association highlights on images can now be exported as Transparent PNG images using a new File→Export menu.

Results of yield calculations can be exported for examination using the new “Export” button on the *PIXE/SXRF Yield Calculation* window.

### New Features in 3.2:

- 1) A simple scheme has been added to enable determination of the conversion from Ion Chamber counts to flux or “charge” for APS generated data using a standard foil. Quantification is then straightforward for unknown samples.
- 2) The Image Export options have been enhanced to control the format of Exported output to the printer and various metafile formats. Also, a selected region of an image can be selected for export by dragging a shape on the image and checking the “Crop Image” option.
- 3) Export of images to CSV file now has the option to export only a selected region of the image. Use a shape and the new menu item for export of a region.

### New Features in 3.1:

- 1) The scene has been set for XRF imaging and analysis for synchrotron X-ray microprobe applications with the addition of XRF fundamental parameter databases for Z up to 98, making use of recent compilations by Elam *et al.*, 2002, Ebel *et al.*, 2002 and Campbell *et al.*, 2003. To select photons, select “Photons” in the beam particle drop-list in the yield calculation window (bring up with the “New” button in the *X-ray Spectrum Fit window*) or set Z1 and A1 to zero. Beam energies are then in keV.
- 2) Detector array handling has been improved, and a new section in the Scenarios chapter has been added.
- 3) A new button “Export” has been added to the *X-ray Spectrum Fit window* to export the Dynamic Analysis matrix to a binary file (extension DMX) for download into a data acquisition system for real-time generation of elemental images.
- 4) GeoPIXE has been ported to Linux; the same XDR portable SAV file will run on both Windows and Linux platforms. All binary files are in XDR format and can be used on either platform. *Note that while this manual tends to refer to file extensions in uppercase, they should all be lower case under Linux.*

- 5) GeoPIXE now assumes IDL version 6.0.

### New Features in 3.0:

- 1) GeoPIXE now has support for detector arrays. The *Sort EVT* window can process all detectors of an array simultaneously and project all data onto a common set of elemental images using a Dynamic Analysis matrix. *Sort EVT* has a drop-list to select the array option. Select a DA matrix as usual, and enable all ADCs that are part of the array. The “Get” button can be used to load the energy calibrations of all detectors from a spectrum SPEC file. Fit the spectra first in *X-ray Spectrum Fit* to refine the calibrations using “Fit: All”.

Many device drivers have been moved into external Fortran code to improve the speed of processing list-mode files. Some file formats show significant speed increases with throughput up to 20 Mb/sec (on a 2GHz P4).

A new curvilinear traverse shape “Curve 8” has been added to the GeoPIXE *Image Display* window. It provides a spline curve to tailor non-linear traverses in order to project changing concentration data along non-linear paths across images.

The “B” button adjacent to the “EVT File.” button in the *Sort EVT* window brings up the *Batch Sort* window for editing parameters and controlling batch sorting of entire directory trees of list-mode files. It also enables a tree directory structure to be generated and populated with list-mode and related files. Note that this function handles single-file list-mode data, but can not handle multiple-file list-mode data, as used at Lund and GSE-CARS, at this time.

Support for Sandia BD12 list-mode format, for use with the Rontec 12 element Si drift detector array, has been added to GeoPIXE.

### New Features in 2.9:

- 1) GeoPIXE now has Preferences selection (“Preferences” on the “File” menu of the main GeoPIXE *Image Display* window). These set options for launching various GeoPIXE windows on start-up, and parameters referring to XY stage ranges and stepper resolution. Preferences stored to the file “GeoPIXE.prefs” become the defaults for the next launch of GeoPIXE.

### New Features in 2.8:

- 1) Export of image plots to structured drawing formats, such as CGM, EPS and WMF has been improved, and now produce plots with concentration legend, labels, and axes in microns (if image size was supplied). The *Image Display* “File→Export→Save Images as CGM” and “File→Export→Save Images as WMF” menus, as well as the “File→Print” menu, pop-up a requester to tailor the size and weight of characters, line thickness, the placement of optional items, such as a distance bar, and the choice of output format (CGM, WMF, EPS, Printer).

Export of spectra plots to structured drawing formats, such as CGM, EPS and WMF has also been improved. The *Spectrum Display* “File→Export→CGM Plot” and “File→Export→WMF Plot” menus, as well as the “Print Plot” menu, pop-up a requester to tailor the size and weight of characters, line thickness, etc. and the choice of output format.

The way that user written image processing plug-ins are treated has changed a little. In particular, the format of the returned history record must contain the name of the routine. Please check the code in “template\_image\_plugin.pro” for details. Image processing plug-ins now appear in the *Image Operations* list for easy access.

A bug that effected the calculation and plotting of pileup spectrum overlay when there was a large energy calibration offset has been fixed.

A bug in OMDAQ produces an error offset in the energy calibration for spectra extracted from LMF files. Use the enclosed OMDAQ E Offset plug-in to correct for this.

A new menu “Process→“Fold” can be used to remove the toggle bit effect, which produces the effect of a double spectrum. This ‘folds’ a spectrum back on top of itself to half the length in channels adding contributions to channels as it goes.

An accurate pile-up spectrum can now be calculated using image pixel intensity products. Use the “Display→Pileup→from Images” menu in *Spectrum Display*. *X-ray Spectrum Fit* can now use these calculated image pileup spectra to obtain more accurate fits to spectra corresponding to total spectra from PIXE images with

wide variation in major element spatial distribution..

Images can now be corrected for pile-up related effects, based on pixel-by-pixel calculation of pile-up components. A new menu in *Image Display* called “Process→Correct→Image Pile-up” performs this task in concert with the *Spectrum Display* window. See the expanded manual sections for details.

Image processing operations that were applied to element images in one image file can now be applied selectively to element images in a new image file. This makes digital filtering and smoothing of images in a batch run of many analyses much quicker.

A ten-step colour table has been added to the *Image Display* “Display→Colours” menu, and the Export→CGM options will now adjust the Z legend tick marks to these colour transitions.

A new output option allows the image shapes to be export as transparent PNG files. See the “File→Export→Current Shape as PNG” menu in *Image Display*.

Support has been added for reading Fastcom MPAWIN and MPA3 list-mode files and Sandia EVT data-cube files.

## New Features in 2.7:

- 1) The *Edit Filters* and *Edit Detectors* windows now show plots of transmission and intrinsic efficiency, respectively. Both the HTML save format in *Image Display* (menu “File→Save All as HTML (PNG)”) and the Chimage format save operation (menu “File→Save as Chimage”) now use a pop-up to select elements. This pop-up also allows selection lists to be saved and restored to enable the use of standard element lists.
- The *X-ray Identification* window (“Display→Identify X-rays” menu, or the “?” button, from *Spectrum Display* window) now has drop-lists to select X-ray filters and the detector in “Mark Element” mode. All X-ray line relative intensities are now calculated assuming detector efficiency and absorption through these filters. These lines are shown on the *Spectrum Display* window as orange markers.
- The *Sort EVT* function now accumulates the total integrated charge for OM DAQ list-mode file during sorting. The charge field is updated AFTER the sort completes, and the charge is written into the image header. A new requester will pop-up to allow editing, or scaling the charge up or down by multiples of 10.
- The “File→Save ALL as HTML (PNG)” output menu operation of the *Image Display* window now pops up a requester for the entry of the desired elements to output. These element selection lists can also be saved and restored from this pop-up panel.
- The “Export” buttons on the *X-ray Spectrum Fit* and *Image Regions* windows now bring up pop-up panels to select options for export, including quantities to export and element selection.
- Menus under the *Image Display* “Window” menu can be used to bring up “unlinked” versions of the *Image Display* or *Spectrum Display* windows. Normally, all windows are linked together and reflect one dataset under study. By opening *unlinked* windows, you can load quite independent images or spectra without affecting the current images and spectra, or the current path.
- The *Layer II Setup* window now has a “Plot” button to bring up a plot window to display various calculation results, such as PIXE yields, as a function of depth or energy.
- Sort EVT*, as well as functions to read IMG spectra files or extract spectra from EVT files in *Spectrum Display*, all now look for an MP file of the same name. If one is found, relevant details, such as images sizes, energy calibration and integrated charge are retrieved from the MP file.

## New Features in 2.6:

- 1) GeoPIXE can now process list-mode files generated using the Oxford Microbeams OM DAQ data acquisition systems and software. Select “OM DAQ Data Acquisition for PC” on the input device drop-list in the *Sort EVT* window.
- Loading of all spectra, and import of spectra from files or extracted from list-mode files, can now use multiple file selection. Simply use multiple selection in the file requester (using control or shift keys) to select multiple files within a selected directory.
- Spectra (single or multiple) can now be appended to the spectra already in memory using the “File→Import→Append→ ...” menus. Use the “File→Import→New→ ...” menus to clear memory first.

The *X-ray Spectrum Fit* window now has a button to fit ALL spectra currently loaded into GeoPIXE. Coupled with the ability to load multiple files, this enables simple batch processing of series of spectra from multi-spectra SPEC files, or loaded from a series of single spectrum files.

The Cal window for energy calibration now has a button to set the calibration for all spectra loaded (“All”) or just the currently displayed spectrum (“One”), and a button to set the units to “keV”.

Improved the intensity of the Ge K<sub>β</sub> escape peak.

The *Spectrum Display* window now has a user plug-in facility. Now you can write spectrum processing and other user spectrum operations in IDL, such as custom fitting. These are loaded when GeoPIXE runs and appear on the “Process→User Plug-ins” menu.

Spectra import now available for ANSTO RPT format spectrum files.

### New Features in 2.5:

- 1) A new window *Image RGB* window displays three element images as the Red, Green and Blue components of a 24-bit colour image. The intensity of each element is set in the Image Display windows. The results can be exported as 24-bit PNG or JPEG files.

The *Image Display* window now has a user plug-in facility. Now you can write image processing and other user image operations in IDL. These are loaded when GeoPIXE runs and appear on the “Process→User Plug-ins” menu. As with other image operations, these add an information line to the image history record. The “Undo” menu (or button on the *Image Operations* window) can be used to undo this user plug-in operation.

Image processing operations have been added to the *Image Display* window (“Process” menu) for edge enhancement (Roberts and Sobel filters), erosion and dilation, and rotation and mirroring of images. Many of these are also in the *Image Operations* window list for quick access.

### New Features in 2.4:

- 1) A new window *Association* is used to plot associations of two elements in images. In other words, each pixel in a set of elemental images represents a data point in multi-element space. *Association* displays two-element projections from this space. This can show up discrete phases in a sample, for example, which appear as discreet blobs that may be separated in some two-element views.

A spline tool is available in the *Association* window to select arbitrary areas in two-element space. These selections can be used to highlight all pixels in the element images that represent this area in two-element composition space. These pixel selections, plus the average concentrations within these highlighted areas, are saved in the *Image Regions* window table. As with normal image region selections, the spectra from any ADCs within these selected areas can be extracted.

If a normal image region is used, to select a spatial area within an image, then the element associations shown in the *Association* window only show data from within this spatial area of the image. For example, this can be used to learn about specific phases in an image, exclude a dominant phase, or to separate subtle intergrowth compositions.

An *Image History* window is now available from the “Windows→Image History” menu of the *Image Display* window. It shows all image processing operations that have been performed on each elemental image. This will show all history for all existing image files as well.

The *Image Table* window now has a button to update just the currently selected region. To make an adjustment to a region, select it by clicking on the row in *Image Table*, and then click on the “Update: One” button. This will update the concentrations and store the new region shape and position in the selected table row.

The *Image Operations* window has been updated. It now includes an “Undo Last” button to undo the last image processing operation performed. This also updates the *Image History* window accordingly.

Line profiles generated using the “Traverse” region now include an overlaid plot of the detection limit (99% confidence) in each distance step, as a dashed curve.

### New Features in 2.3:

- 1) *Fit Results* now has an “Export All” button to export all results and parameter categories to the output ASCII .CSV

table.

The “Traverse” image region now has shear control. The side handles, moved using the left mouse button, usually control the width of the traverse region, perpendicular to the projection axis. Now you can shear this projection, so that it’s not perpendicular. Use the right mouse button to select these side handles and slide parallel to the main axis to change the shear.

### New Features in 2.2:

- 1) *Spectrum Display* now has two ASCII spectrum file import options. One reads spectra, one from each column, into consecutive spectra. The other reads ASCII spectra files that contain channel energy as the first column (e.g. as produced by the “File→Export→CSV Table” menu) and one or more spectra channel counts as the subsequent columns. These files can be white space, comma or tab delimited, or a combination of these.

More import options have been added for old format GeoPIXE VAX binary spectra files and for ASCII files. The ASCII import option can read files with multiple spectra as columns. There are two menus. One reads files where the first column is channel energy. The second reads all columns as spectra. Both assume that the first row contains column labels, and if energy mode is chosen, it uses the label for the first column as energy units. These functions can handle column separation using white-space (spaces, tabs) or commas, or a combinations of these.

*Spectrum Display* now has Windows Metafile export options. Go to menu “File→Export→WMF Plot on Black” for output for a dark background, or “File→Export→WMF Plot on White” for output for a light background. These files, like the CGM ones, can be imported into PowerPoint as pictures.

The detector efficiency function has generally followed the function of Cohen (Nucl. Instr. Meth 178 (1980) 481), as corrected by Ryan et al. (C.G. Ryan, D.R. Cousens, S.H. Sie and W.L. Griffin, "Quantitative Analysis of PIXE Spectra in Geoscience Applications", Nucl. Instr. Meth. B49 (1990), 271-276), which uses a multiplicative factor of 0.717. GeoPIXE has used this to be consistent with packages such as PIXAN. A new option in the *Detector\_Setup* window makes this factor optional. Use this to be consistent with other packages that do not follow Cohen.

The menus for display of calculated pileup and Si and Ge escape spectra are now active in *Spectrum Display*, under the Display menu.

### New Features in 2.1:

- 1) There is a new feature in the *Correct Yields* window for the correction of artefacts in images caused by the spatial variation of X-ray absorption across the image. At present it just assumes that the detector is to the right in the images, and at a take-off angle of 45°. Details of the process can be found in (C.G. Ryan, E. van Achterbergh, G. Mark, C.J. Yeats, S.L. Drieberg, B.M. McInnes, T.T. Win, G. Cripps and G.F. Suter, "Quantitative, High Sensitivity, High Resolution, Nuclear Microprobe Imaging of Fluids, Melts and Minerals", Nucl. Instr. Meth. B188 (2002) 18-27.).
- 2) The projection onto end-member phases now also produces an image corresponding to the *remainder*, i.e. the proportion not assigned to the end-member phases.
- 3) Support for 4 list-mode formats is provided: Mpsys on Linux and Unix, Sparrow Kmax on Macintosh, and XSYS on VAX/VMS.
- 4) Interactive set-up windows for filter and detector definitions are now provided. Go to the Windows menus on the *Image Display* or *Spectrum Display* windows.

### New Features in 2.0:

- 1) There is a new *Cuts Setup* window for the interactive set-up of energy cuts on spectra. The window also displays background-subtracted peak-areas deduced using cuts. Cuts can be named for use in sorting list-mode data, for example from non-PIXE ADC channels.

### New Features in 1.9:

- 1) There is a new feature for the correction of concentration due to the spatial variation of PIXE yields caused by changing sample composition across an image. The new *Correct Yields* window allows for this correction, using a

new approximation for combining PIXE yields calculated for end-member components (see C.G. Ryan, "Quantitative Trace Element Imaging using PIXE and the Nuclear Microprobe", International Journal of Imaging Systems and Technology [Special issue on Quantitative Imaging] 11 (2000) 219-230 and C.G. Ryan, E. van Achterbergh, C.J. Yeats, Tin Tin Win and G. Cripps, "Quantitative PIXE trace element imaging of minerals using the new CSIRO-GEMOC Nuclear Microprobe", Nucl. Instr. Meth. B189 (2002) 400-407).

- 2) The *Correct Yields* window also provides projection of element images onto images of end-member components.
- 3) GeoPIXE can sort list-mode data with up to 8 ADCs (extended to 384 detector channels in later versions).