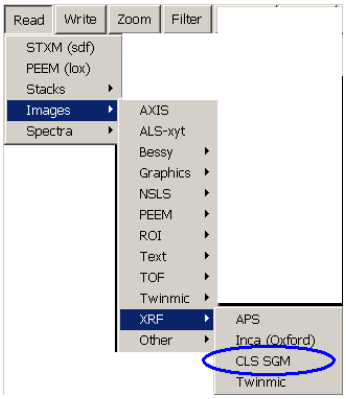
Reading CLS SGM X-ray fluorescence (XRF) excitation maps into aXis2000

GOAL: read data from CLS SGM; PGT SDD detector recorded at a sequence of incident photon energies into an axis2000 "image" for further processing

Test data: FH_AsV_B_Fe_20.dat - energies and detector spectra
FH_AsV_B_Fe_20_spectra.dat - set of XRF spectra

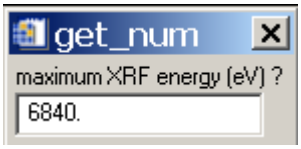
Command: Read~images~XRF~CLS SGM

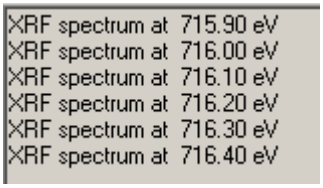


Example:

1. select **data file** (name filter is "*_spectra.dat")

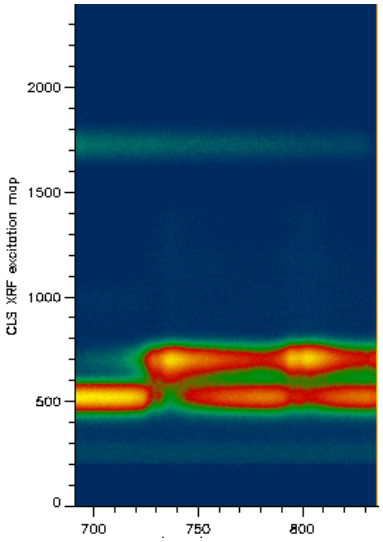
2. define **upper XRF energy** of interest (3 * highest excitation E perhaps)





File read-in occurs with progress indicated by primary E's

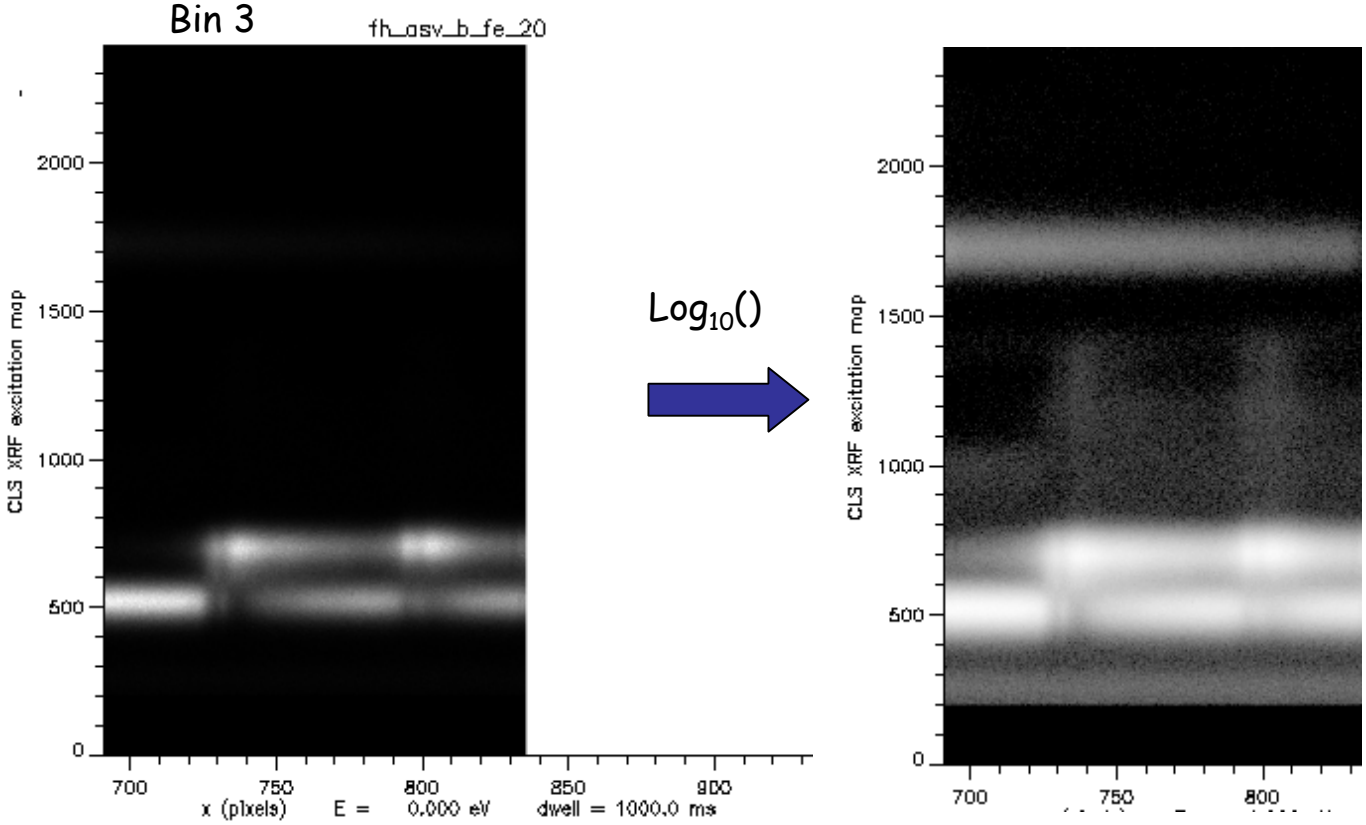
3. select **extent of binning of XRF** - generally the XRF spectra are oversampled relative to the energy resolution of the SDD



Data is now in the aXis2000 buffer that was active prior to executing the command (so select a buffer that is empty or one you are willing to overwrite BEFORE read-in)

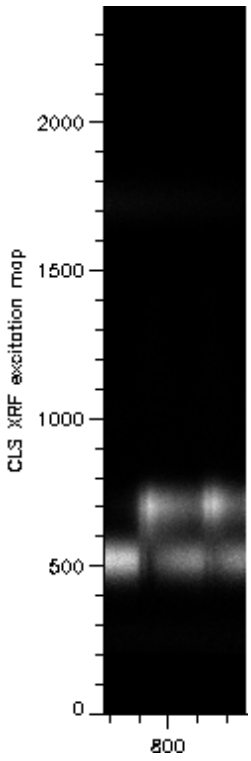
Example of XRF-excitation processing

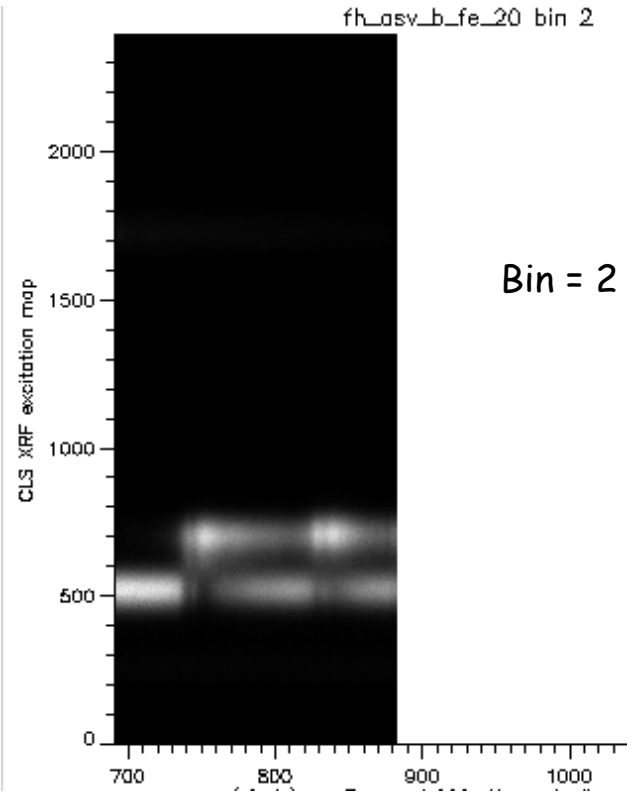
Bin 3



$Log_{10}()$

Bin = 1





Bin = 2

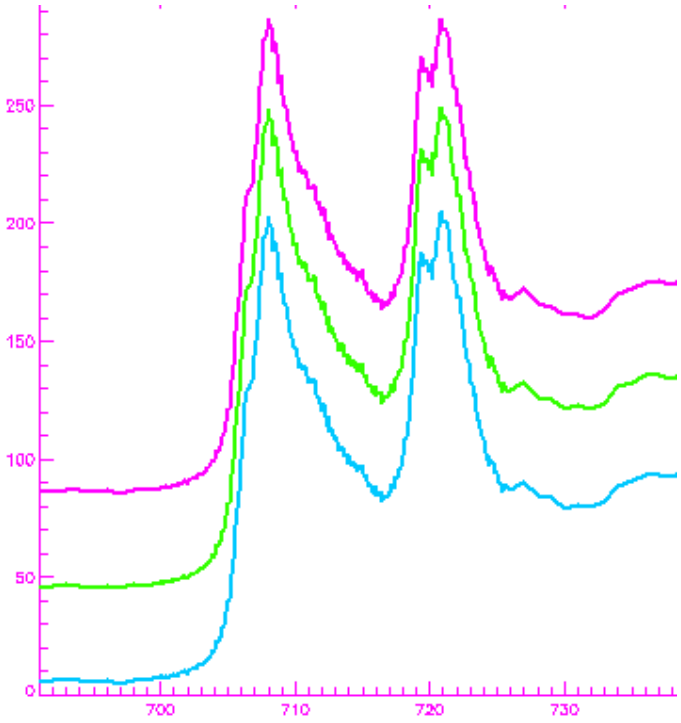
Example of XRF-excitation processing

Extract yield spectra from
Linescans~add lines~horizontal

Fe 2p spectra measured with Fe Kα yield

Offset added

NB no change since integrate over same signal



No bin

Bin = 2

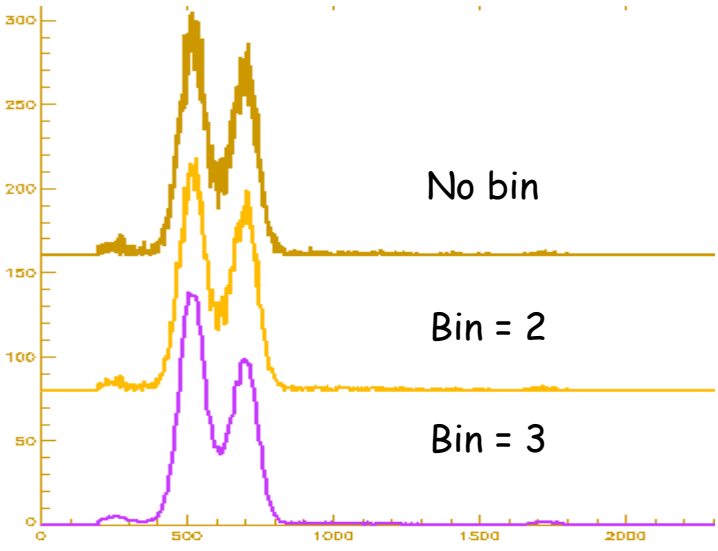
Bin = 3

Extract XRF spectra from
Linescans~add lines~vertical

XRF spectra at Fe L3 peak

Offset added

Binning greatly improves visibility, reduces processing time, increases precision / accuracy of any fitting



No bin

Bin = 2

Bin = 3

Issues with read-in routine

Assumptions

XRF data in *_spectra.dat

* LINEAR spacing of the XRF energies.
* the files are 4096 in length (in fact it may be useful to BIN the PGT output, either in their software, or in the CLS SGM acquisition software; if the XRf spectra are less than 4096 long, some code changes would be needed (but are anticipated)
* entries are at least comma separated
* header lines beginning with # are ignored

Excitation energy from *.dat

* Right now the routine only reads the incident photon energies - could extend to read Io and normalize the XRF spectra to that

* If that is needed a spectrum with x and y from any 2 columns in the *.dat file can be extracted using **read~spectra~multi-column** and the XRF-excitation image can be normalized using **linescan~normalize~vertical**