These python scripts allow for:

1. Batch import and conversion of psmsa or emsa files (NORAN/NSS) to csv
2. Extraction of key header parameters which are stored in a comprehensive file index
3. Tweakable automated background fitting of the x-ray background
4. Adjustments for pathological overlap of adjacent peaks
5. Integration of peak counts after background subtraction
6. Batch plotting of all spectra including backgrounds to multipage PDF reports
7. Quantitative compositional analyses via Cliff-Lorimer k-factor technique (including error propagation)

These scripts are currently just run from an IDE (such as Spyder) usually section-by-section which allows examination of results as they are generated.

SEMEDX\_batch\_import\_main.py

An index called SEMparamlog.csv) is created and stored in each project folder and contains many key parameters extracted from the \*.\*msa header (beamkv, livetime, realtime, calculated deadtime fraction

If there are other header parameters you which to also store you can add them to the SEMparams template (which sets pandas columns for this log file, sets expected data type for each column, and has the flag string (e.g. #BEAMKV) that finds this quantity within the header).

Description of integquant results (for SEM-EDX quant scripts):

**Basename, filenumber, point, filename, filepath, sample, comments**:

*mostly* *self-explanatoryand from default spectrum naming scheme during collection*

*Point* - differs from 1 only when multiple spatial areas are defined in a point& shoot

Sample and comments - custom added by user

**Element** – name of elemental peak, one can have multiple lines per element such as Fe (K line at 6.4keV) and Fe2 (L line at 0.7 keV)

**Energy** – this is index # of center of the integration… if there are indications of peak shift (from the Gaussian fits) this can differ from the ideal index value; the typical conversion from index value to energy is (640 \*0.01)-.01

**Shift**: energy shift suggested by Gaussian fit… however shifts are limited to 0.03 KeV and actual shift applied is evident from above energy (again gives the center value of the integration and width is specified for each element in SEMquantparams

**Rawcounts** – integration of Counts column from center-halfwidth to center+ halfwidth (usually summing about 15 channels

**Backcounts:** integration over same region as above but of the backfit column

**Subtractedcounts**: Rawcounts – Backcounts

**Adjcounts:** adjustments made due to pathological overlap (i.e contribution to V-K from Ti-Kbeta; not needed for many elements

**% err:** relative/fractional error as percentage due to counting statistics for peak in question (2/sqrt(subtracted counts)) … if count adjustment is made, this value is changed to include counting stat error and error in adjustment ratio (so if adjcounts is not blank, % err refers to this value)

# error in adjcounts=

**Significance**: Ratio of subtracted counts to sqrt(background counts) in same region … often 2 sig of background used as criteria for inclusion in SEM basis

**Correctedcounts**: kfact\*integrated counts/mass for each element

**Errcorrcnts:** Includes kfactor error (element specific from table) and % err (from peak counting statistics)

*The final two can be modified/recalculated after changes in k-factors or k-factor errors, but others are typically not changed (unless background fits are redone for some reason); these are also adjusted if there is an unresolvable interference (adjusted counts);*

**Compositional Calculations**

**Elements=** subset of elements (w/ associated corrected counts) for inclusion

**Sigthreshold** – significance threshold below which element is excluded from calculation

For Al crater spectra it’s tricky to properly fit the small Si peak just to right… works fine with second fit cubic and then cross-faded into third parabolic fit

Regarding the mandatory minimum points between Al and Si… index range can move a lot depending on relative strengths of Al and Si peaks

Including cubic in raw projectile spectra not terrible but sometimes

Existing backfit problems:

Large Na peak can cause slightly high background at Mg

Big Ni-L line can screw up low energy region a bit (i.e. Alstubr2\_pt7 from Acfer projectile

Redo of integrations is possible while keeping existing background fits – just set newback and overwrite to false; also can set savegauss to false (doesn’t save new Gaussian peak centering fits)

Hacking SI file format?

Float are typically 4 bytes/8 bits in hex editor (i.e. flexHEX)

Big or little endian—

NSS CSV x-ray maps extracted from .si:

*Determination of units in the resulting files?*

*Most logical would be for the Si map to have Si counts above background for each pixel in the spectral image.*

**Spectral image processing scripts**:

Starting point is x-ray maps that can be generated/exported from .si data using Noran (no direct hack yet of underlying file struction;

X-ray map output format are csv files of specified resolution (e.g. 64x64);

Batchnssreader gets info for all SI files in folder:

.Siref – just a tif file with different extension

.sitif – thumbnail image

.csi- small file point to si, siref and sitif files

Stage coords … probably stored in binary .si somewhere