XOP tutorial at ESRF - Session 2
Data analysis with XOP

Data analysis with XOP

- Data visualization
- Working with SPEC files
- Data analysis
- Modeling data: Curve Fitting
- Advanced manipulation of SPEC data

1. Data visualization

You will learn to:

- start Xplot
- load a simple ASCII file
- prepar your plot for printing
- basic editing and cosmetics

Follow the 10-minutes tour to XPLOT (Chapter 1 in Xop/Xplot user's guide)

2. Working with SPEC data files

You will learn to:

- understand the SPEC data file syntax
- navigate through scans
- display titles
- clean SPEC files
- visualize MCA and MESH scans

1) Create a simple SPEC data file (see chapter 4 in Xop/Xplor user's manual, use the file `tmp_spec.dat`). Load it in Xplot. Navigate through SCANS.
2) Load a real file (`mica15mm20kev.dat`). Navigate trough scans. Experiment modifying the titles with Xplot|Edit|Titles… (see on-line help)
3) Clean the file. Create a new file with the following scans only:
   Scan 2 – Cols 1&8 – All interval
   Scan 5 – Cols 1&8 – [-, 37]
   Scan 10 (0,0,6 reflection)– Cols 1&7 – All interval
   Scan 12 (0,0,8 reflection)– Cols 1&7 – select peak
   Scan 14 –(0,0,10 reflection) Cols 1&7 – All interval (use Redraw button)
   Scan 16 (0,0,14 reflection)– Cols 1&7 – select peak
   Scan 18 (0,0,16 reflection)– Cols 1&7 – select peak
   Scan 20 (0,0,20 reflection)– Cols 1&7 – select peak
   Scan 22 (0,0,22 reflection)– Cols 1&7 – select peak
4) MCA: open the file `data.chungo` and then `mcf7c.spec.fixed`
   See the MCA scans. Visualize the different columns in the case of multi-column MCA. Observe that a SCAN may hold "counter" and "MCA" data simultaneously.
5) MESH: `mi428.4` scan 17, `mi428.2` scan 103, `mi428.8` scan 10. Set index column to 2 or –2. Play with surface/shade/contour/lines options. Add optional keywords.

3. Data analysis

You will learn to:

- overplot two and more graphs
- use Zoom and set Limits
- operate with columns
- make calculations on your data (statistics, derivatives, interpolation, peak finding, Fourier filtering, convolution and correlation, histogramming)
- operate with sets.
- mask data for fit

1) Operations with columns:

Scan normalization. Comparison with Xop: Use file `mi420.2` scan 84 col10. This is the Rocking Curve of monochromator in arcsec of Si 111 at 50 keV. FWHM=1.67 arcsec. Normalize it using Xplot|Calculations|Operations with columns…(set max Y to one and shift the max at X=zero). Then compare with Xop/Xcrystal calculation (rocking curve, i.e., autoconvolution of Si111 at 50 keV).

Statistics: calculate averaged I0/SRcurrent from a scan (Hints: use the file `mi428.2` scan 91, calculate I0/Srcurr at the direct beam zone (by selecting limits to this zone), obtain the averaged value using Xplot|Calculations|Moments) (Answer: 54.1984)

Normalize the scan 96 to reflectivity. (Answer: Peak=0.03, FWHM=0.40)

Try the operators > (floor), <(ceil)

Try also Reverse(), Sort(), alog()

2) Basic data analysis

Apply derivative and then CDF to a knife-edge scan (Hint: use the file `mi428.2` scan 93, Apply set limits to select the wanted data)

Interpolation/Smooth: calculate X values where Y is 10%, 20%, etc of the peak value. Use an experimental rock curve (`mi428.2` scan 96), normalize it to the maximum using operations with columns, interpolate it to get more points, list the points using Xplot|View|Data

Find Peaks: Use a diffraction spectrum `mica15mm20keV.dat`, scan 2, columns 1 and 8. Read the on-line help. Play with the cutoff parameter in order to obtain the wanted peaks (0.01)

Fourier Filtering. Filter a diffraction profile of a thin (e.g., 10 μm) Bragg crystal calculated with Xop|Xcrystal. Play with the controls.

Convolution/Correlation (Already seen with Xop/Xcrystal rocking curves)

Histograms: Use Xplot|Calculations|Histogram… to make histograms of the data in `histo.dat`. Fit the result to a Gaussian using Xplot|Calculations|Fit-Polynomial&Gaussian

3) Operations with sets:

Play with Xplot|Calculations|Create data sets…

Use Xplot|Calculations|Operations with sets…(See Chapter 2 in Xop/Xplot user's guide)

You can create a new abscissas data array using Cx=MergeArrays(Ax,Bx)

Masking data for fit. Use file `mica15mm20kev.dat,` first scan. Fit the background to a lorentzian and substract it from the data.

Hints: Use operations with sets to create a data set where the peaks are removed. For that use Cx=Ax[Where(Ay LE 4000)] and Cy=Ay[Where(Ay LE 4000)]. Then use Xplot|Calculations|Non linear fit to obtain the Lorentzian fit. Write the result to file. Then go back to your original data, and using operations with sets, substract from the main data the data in the newly created file.

Hints: Read Chapter 2 in Xop/Xplot user's guide.

4. Modeling data: Curve fitting

You will learn to:

- Multiple Peak fitting.
- Non linear fitting

a) Using the file, `data.chungo` MCA scan 100, make a fit with 5 peaks.
Hint: start fitting peaks one by one

b) Using Xplot|Calculations|Fit-Non linear, make a fit of the two peaks on the left with i) two Gaussians, and ii) two Lorentzians

5. Advanced SPEC

- On line display (demo) – How to visualize on-line SPEC data using the SPEC shared memory
- EXODUS (demo) – How to visualize and operate with data from several scans . EXODUS is an application of the XOP/XAID extension (see EXODUS documentation)
- MACROS: XOP macros are powerful scripts that allow to manipulate spec data using the SPEC_ACCESS IDL library. For example, open Xop|Tools|XOP Macro, load the file `splitspec.mac` and run it. Load, for instance, the file `mica15mm20keV.dat.cleaned`. This macro will create new files, containing the individual scans in `mica15mm20keV.dat.cleaned`