Software for X-ray Scattering Measurement

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Software

- Software for SAXS
  - John Pople will talk about this

- Software for 2-D WAXS

- Software for point detector based scattering.
Software for 2-D WAXS

BluIce
Bluice – Scan tab
Preliminary Analysis
Software for Point Detector

• Architecture –
  • OS – VMS,
  • Super
    • Splot, Scal

• What it Looks Like?

• How to collect data And still get some sleep
  • Running Indirect (batch) files
Most beamlines have a “PC” and the beamline computer.

Beamline Computer runs OpenVMS.

- Command line driven. (Like MS-dos)
- easy to get online help
- Commands not case sensitive.
- Will recognize commands even if not fully written out.
- Never overwrites files.

Beamline computer has two “drives”

- $user1$: (default when you login) : indirect files
- $data1$: : data files.

Beamline computer has four “desktops”
Some VMS Commands

- `>command/modifier1(optional) argument`

- `>help` (if no argu → will display a menu – unlike unix.)

- `>dir` (e.g. `>dir/since=18-oct-2003 *.his`)

- `>set default` ↔ “cd” (`>set def $data1:`)

- `>ftp computer_name` (or IP address)
  - But most people use “reflection ftp” on the PC to transfer data.
Super

Moves motors

Reads detectors

Creates data files

Stores 20 scans

Plots data

Fits peaks

Takes derivatives

“Thinks” in Reciprocal space

Translates scans into “motor” space

Splot

Scal

Two Daughters
Command line structure

Structure similar to VMS

> command/modifier1(optional) argument
  > 2theta 42
  > >2th/relative 1

Extensive online help

> help command (if no argument gives the full menu)
More Super details

- Can scan by just writing out a scan
  - \( \text{Lineup 2theta 0.05 10 21} \)
  - \( \text{Scan m3, 2, 0.01, 10, 1} \)

- Or run a preprogrammed scan (20 stored)
  - \( \text{Scan 10} \) (run scan # 10)

- Three ways of counting
  - For a fixed time (count/time 1 - 1 sec)
  - Fixed Dose (count/dose 15 - 100000 monitor ct)
  - While moving a motor (count/rock theta; ct 21\(\rightarrow\) \(\theta\) 2deg once)
For Polycrystalline or amorphous samples, transformation to Q space is straightforward.

For a single crystal, Super has to know orientation of the crystal in diffractometer space.

- Need diffractometer settings for two non-collinear reflections.
- Need to know the diffraction geometry and restrictions.
  - E.g., 4-circle, kappa, GIXS, fixed omega. Etc
  - Restrictions imposed by a sample stage – cryostat, for example

More in the hands-on sessions
A few Examples of Super Scans

- Single motor scan
  - Scan m4 5 .1 10 1 (scan mtr# 4 from 5 to 6)

- Multiple motor scans
  - Scan s2 1 4 0.02 2 2 0.01 100 21 (scan mtr# 1 from 4 to 6 and mtr# 2 from 2 to 3 – $2\theta - \theta$ scan)
  - 5 motor scan if doing DAFS on single crystals

- Reciprocal Lattice Scans
  - Scan l1 2 2 0 3 1 0 100 23 (scan from 220 → 310)
  - Scan k0 8000 2 .001 10000 1 (scan from Q =2 → 12)

- Energy Scans, Time scans, 2D grid scan….
• What it Looks Like?
Modes of operation

- **Setup mode**
  - Interactive
  - “disposable” filenames (e.g. junk, align etc.)
  - Doesn’t look for beam in the hutch before starting a scan

- **Data Collection mode**
  - Batch -> Preprogrammed
  - “Real” filenames (e.g., FAP_t300_x12 etc)
  - Looks for beam before and during a scan
Batch files

- Can list a set of “super” commands in an ascii file (called indirect file).

- Executing the indirect file will execute the listed super commands sequentially.

- Note: the command to execute an indirect file is a super command too.
A Simple indirect file

- Optimize table
- Count/rock theta
- Filename Sample_16may06
- Scan s2 1 4 .1 2 2 0.05 500 21
Example of another Indirect file

File = rast1mm.ind

Optimize table

M3n 1
Ind apk 01
M3n 2
Ind apk 02
M3n 3
Ind apk 03
M3n 4
Ind apk 04

...........

File = apk.ind

Scan/beamdump
Count/rock theta
File FAP_t300_@x
Sample Fully ann. Plate T =300, x=@
Set 10 k0 8000 1 0.002 500 21
Scan 10
File align
Count/time
Scan/nobeamdump