On-the-fly Scanning with EPICS and Spec

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Newport Diffractometer and MM4005 controller

- 5 installed at APS (GSECARS, MHATT, SRI, UNI(2))
- Other equipment uses MM4005
- Large goniometers have long setting times (>.5 sec) for short moves
- On-axis encoders and MM4005 permit rapid on-the-fly scanning with <.001 degree position errors

MM4005 controller

- Capable of complex coordinated motions
- Move up to 8 axes through a complex trajectory in 8-space
- Put out synchronization pulses at specified intervals along the trajectory
  - Used for multi-channel scaler channel advance signal for data collection
- Can read back from MM4005 the actual positions of every encoder when each pulse was output

EPICS Software

- Define the total number of trajectory elements.
  - Controller does linear moves between trajectory elements. Simple linear motion thus requires only 2 trajectory elements, no matter how many “points” are being measured.
- Define the absolute or relative position of each axis for each point in the trajectory.
- Define the time for each element of the trajectory, or alternatively the total execution time with equal time per trajectory element.
- Define the total number of output synchronization pulses.

EPICS Software (continued)

- Define the trajectory elements where pulse outputs begin and end.
- Define detector triggers to start detectors at the beginning of the trajectory and stop them at the end of the trajectory.
- Build the trajectory, checking for completion and errors.
- Define a total time scaling factor from .01 to 100 which will speed up or slow down the trajectory execution relative to its original definition.
- Execute the trajectory, checking for completion and errors. This can be done repeatedly without rebuilding if the only changes are in the start position or the execution time scale factor.

EPICS Software (continued)

  - Read back the actual position of each axis when each synchronization pulse was output.
  - Read back the following error (actual-theoretical positions) when each synchronization pulse was output.
- All documented at
  - http://cars.uchicago.edu/software/trajectoryScan.html

EPICS Implementation

- A database file, *trajectoryScan.db*.
  - Contains almost no “logic” with no links between records in the database. The records are simply variables which channel access clients and the State Notation Language (SNL) program use.
- An SNL program, *trajectoryScan.st*.
  - Implements all of the logic for communicating with the MM4005 and with channel access clients via the database.
- MEDM screens, *trajectoryScan.adl, trajectoryScanDebug.adl, trajectoryPlot.adl*.
  - Used to control the building, execution, readback, debugging and plotting of trajectory scans.

SPEC Interface

- SPEC macros have been written to allow SPEC to utilize trajectory scanning via EPICS interface
- Low level interface, all of SPEC's standard scans can be done "on-the-fly" with trajectory scanning software. Replacement macros for:
  - _ascan # Used by all ascan and dscan macros
  - Mesh
  - hklscan # Used by hscan, kscan and lscan
  - _hklmesh
  - _hkllline # Used by hkcircle, hlcircle, klcircle, hkradial, hlradial and klradial
  - _scanabort resume
  - _loop

SPEC Interface

- traj_index # Converts a SPEC motor index to an MM4005 motor index
- traj_build # Builds a trajectory
- traj_exec # Executes a trajectory
- traj_read_counts # Reads the data from the multi-channel scaler
- traj_read_actual # Reads back the actual MM4005 motor positions
- traj_scans_on # Enables trajectory scanning
- traj_scans_off # Disables trajectory scanning, uses step scanning
- Global variable TRAJ_USE_ACTUAL=(0,1)

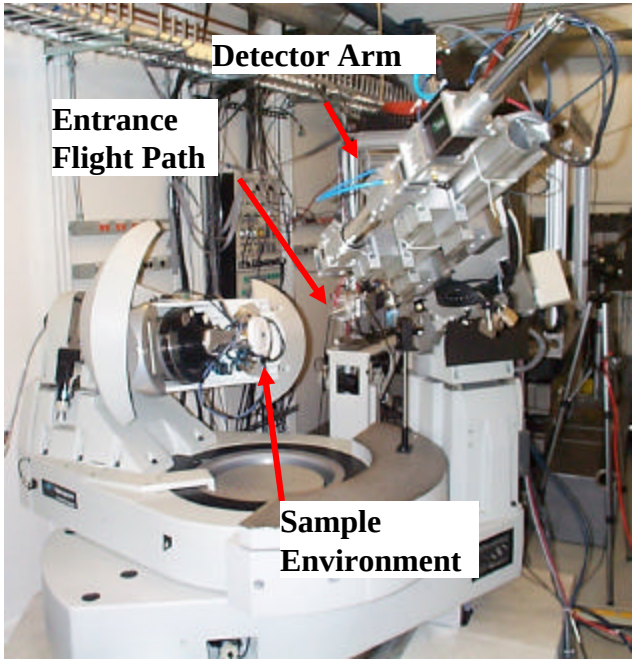
General Purpose Diffractometer (APS sector 13)

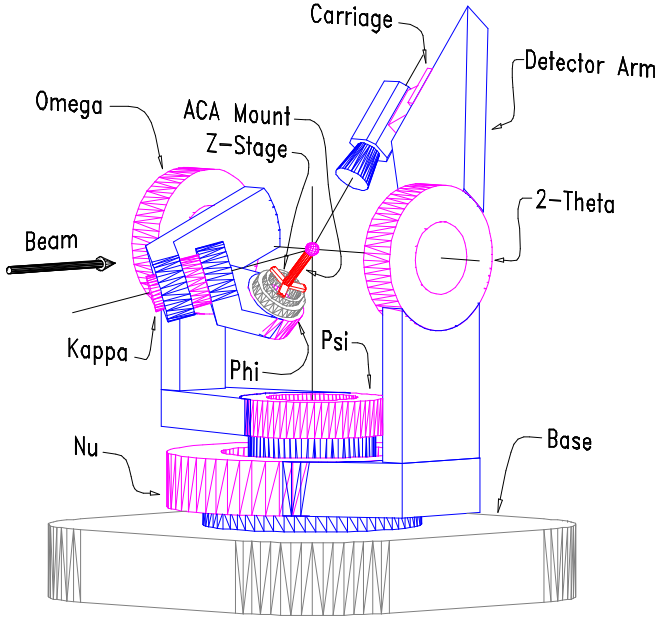
- Large Kappa-geometry six circle diffractometer
  - Leveling table with 5-degrees of freedom
  - High angular velocity (up to 8 deg/sec)
  - Small sphere of confusion (< 50 microns)
  - On the fly scanning

- Open sample cradle, capable of supporting large sample environments weighting up to 10kg.
  - Liquid/solid environment cells.
  - Diamond Anvil Cell (DAC)
  - Small UHV Chamber
  - High temperature furnace

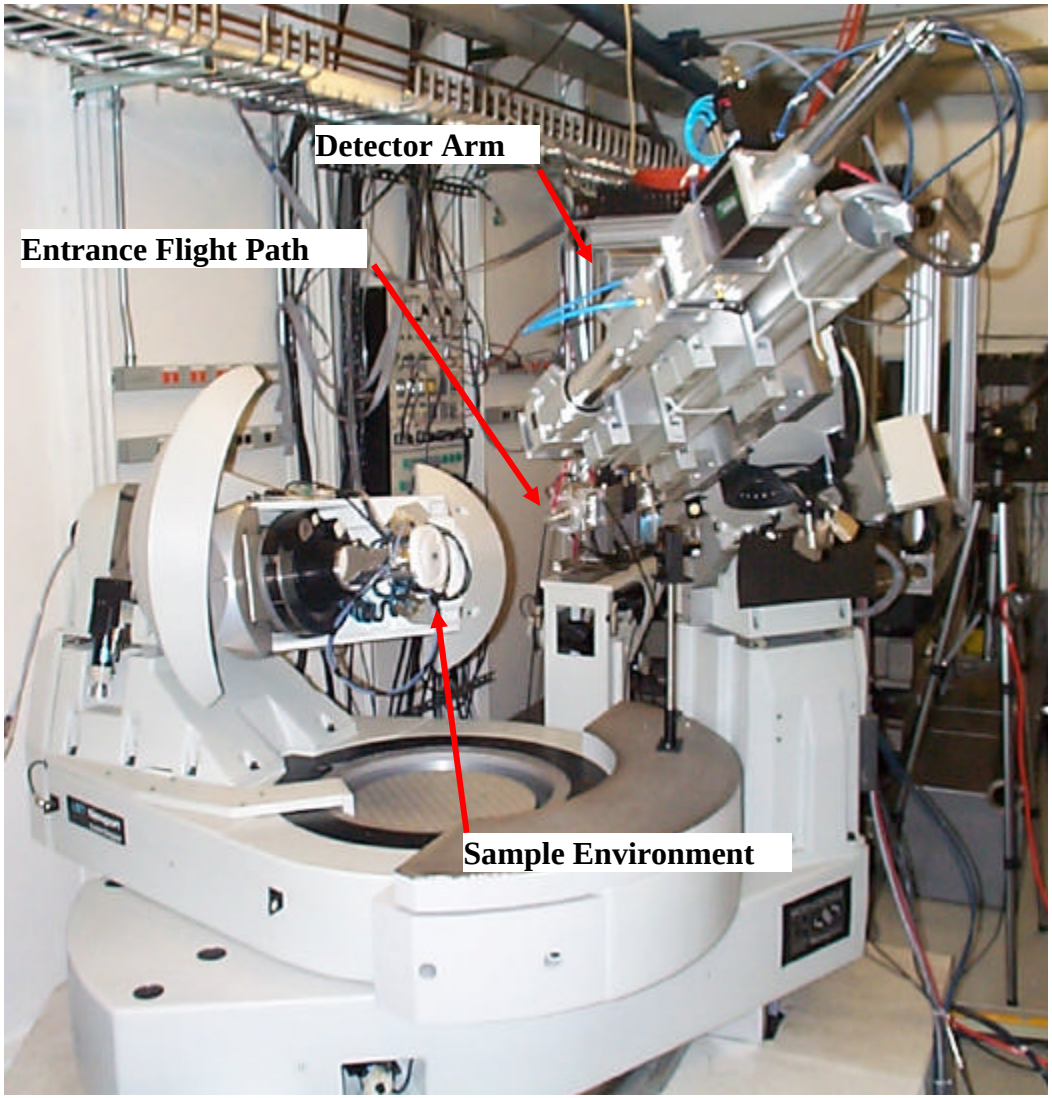
- Open geometry also allows for mounting solid state fluorescence detectors and beam/sample viewing optics on the Psi axis bench

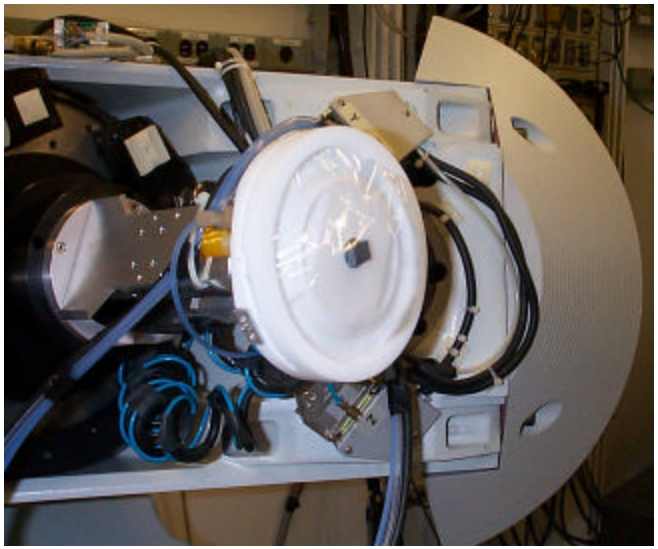
- High load capacity detector arm supports a variety of detectors
  - Point detectors
  - CCD based area detectors
  - Analyzer crystal for high resolution diffraction and inelastic scattering

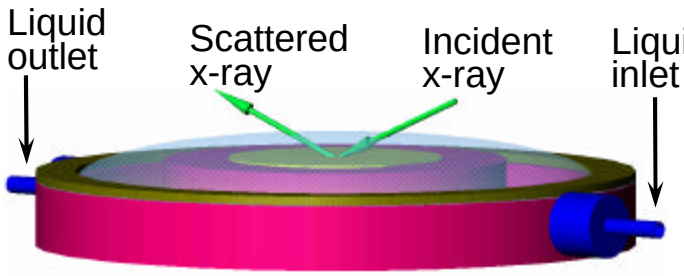




General Purpose Diffractometer (APS sector 13)

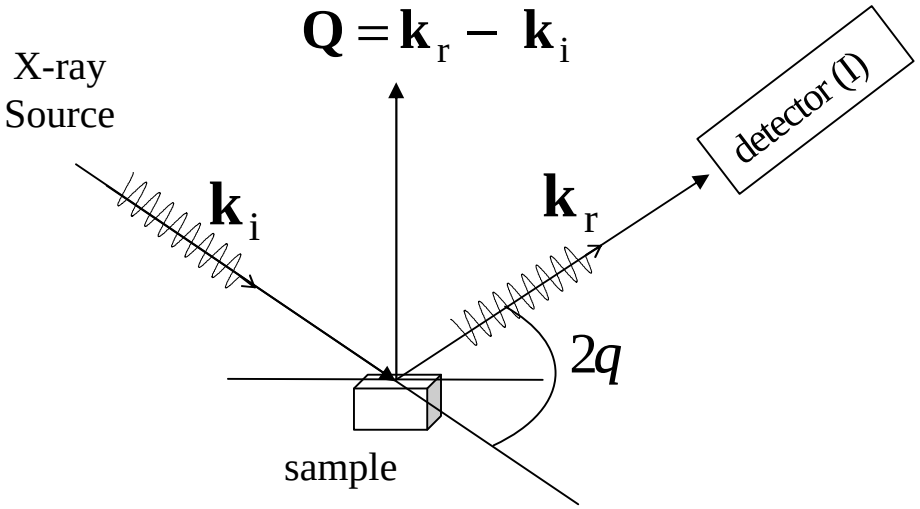


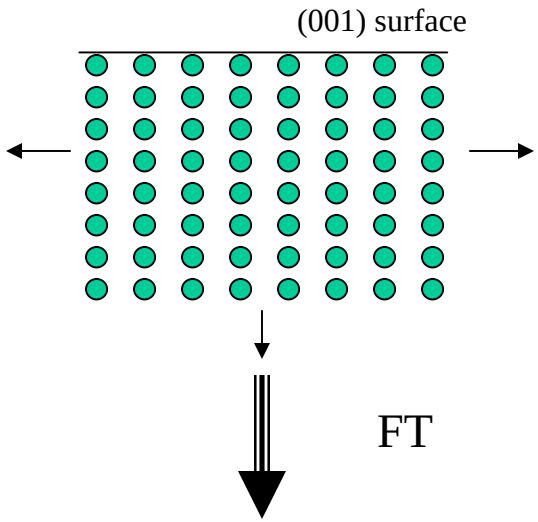


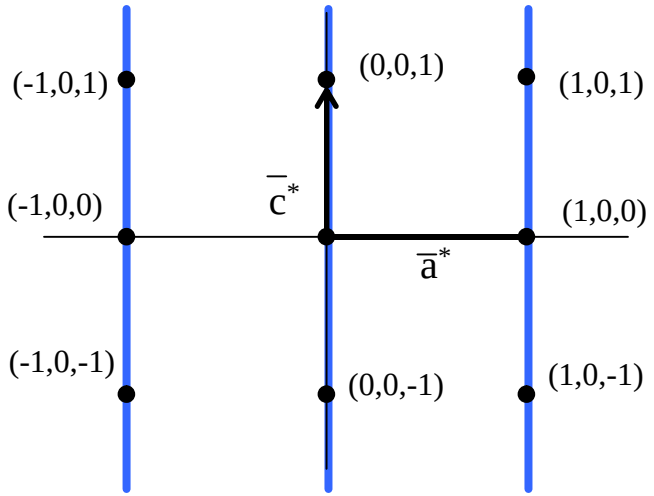


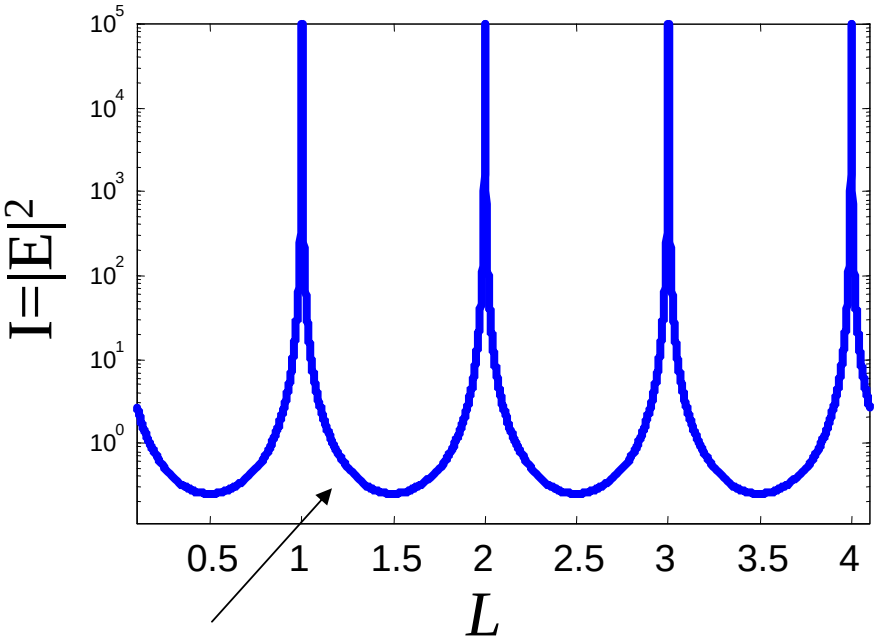
In-Situ Liquid/Controlled Atmosphere Cell

Surface Structure Determination: Crystal Truncation Rods



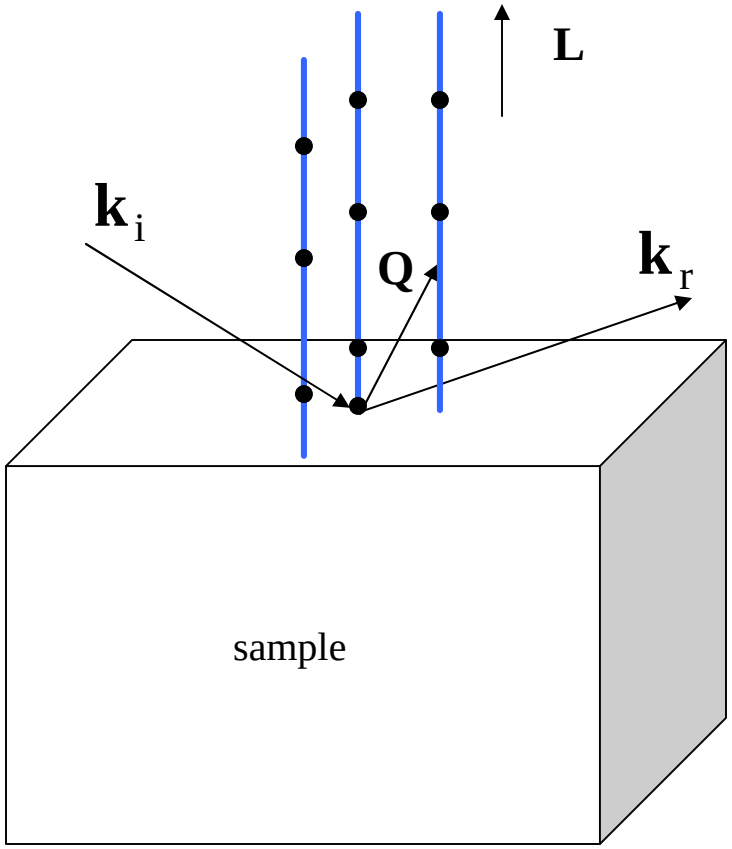


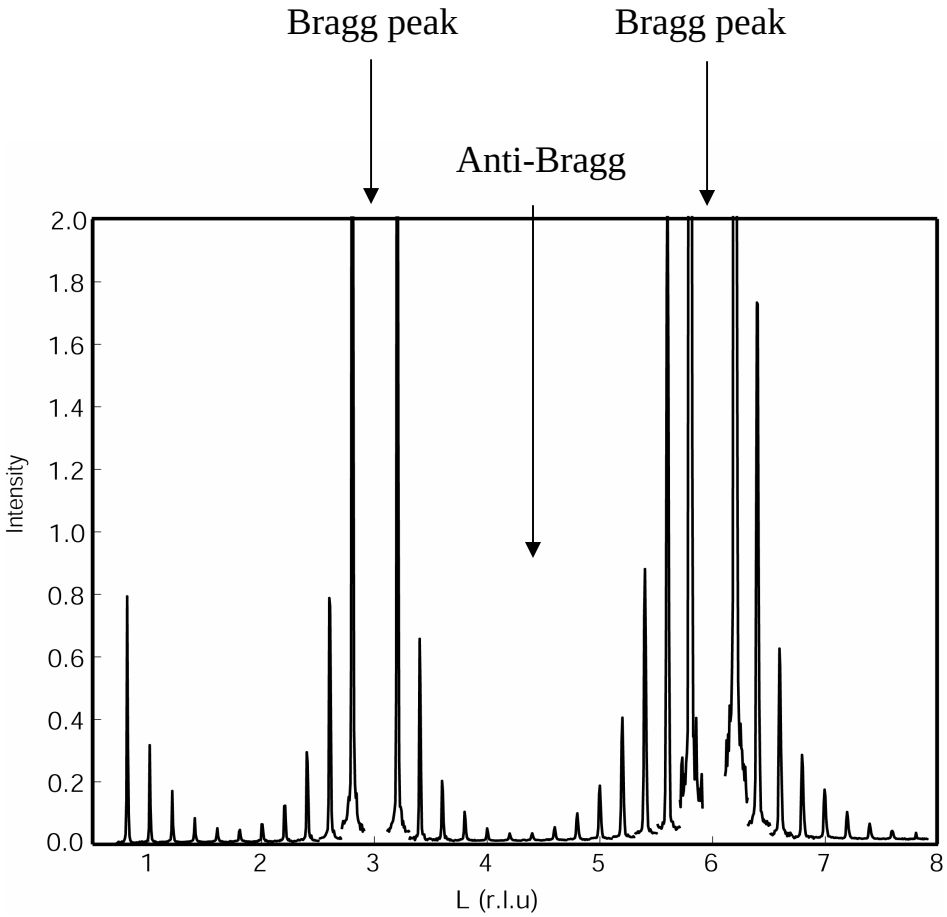




$$E \propto FT[\, r(\bar{r})] = \sum_n f_n e^{i\,\bar{Q}\bullet\bar{r}_n}$$

Measuring Crystal Truncation Rods

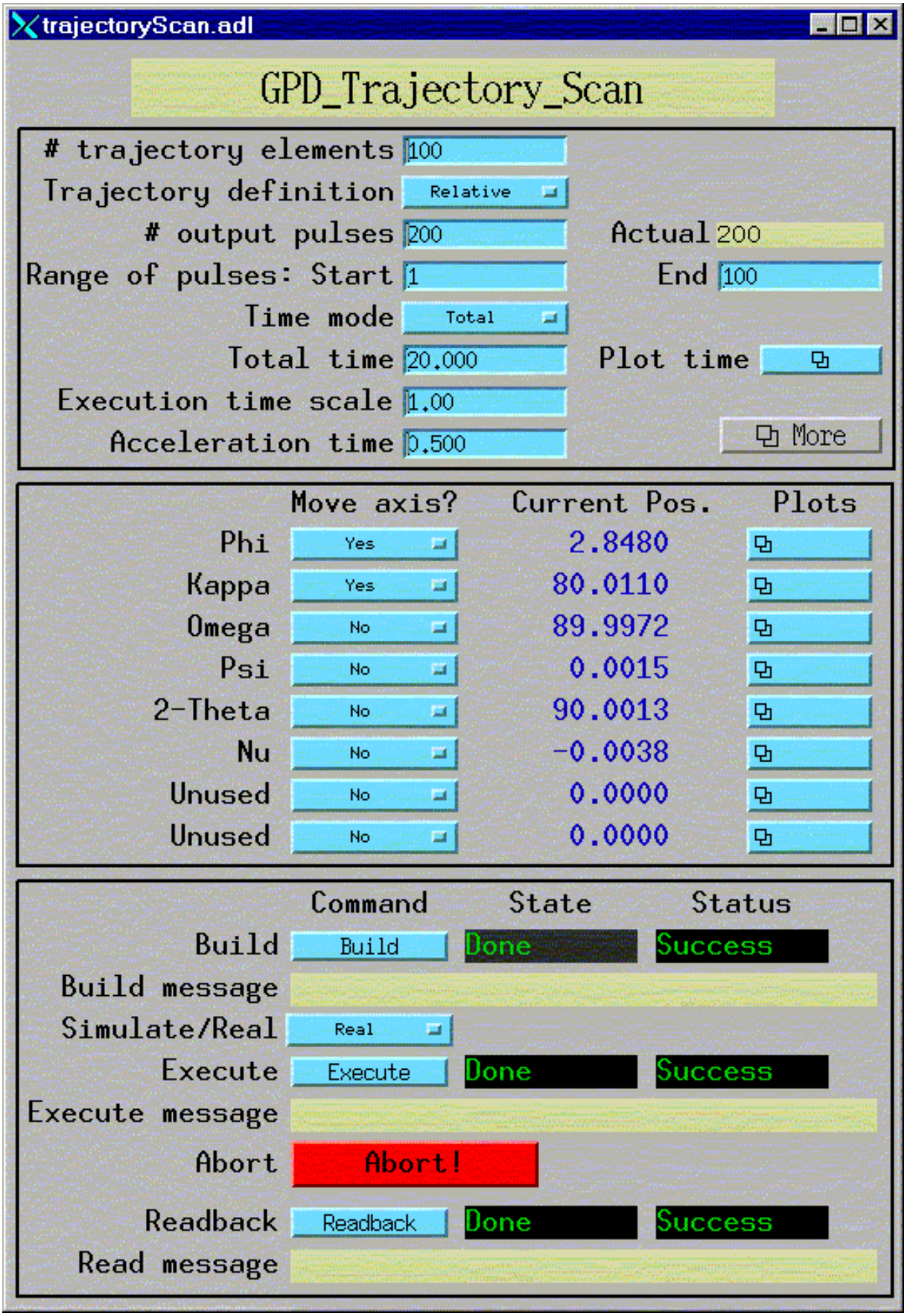


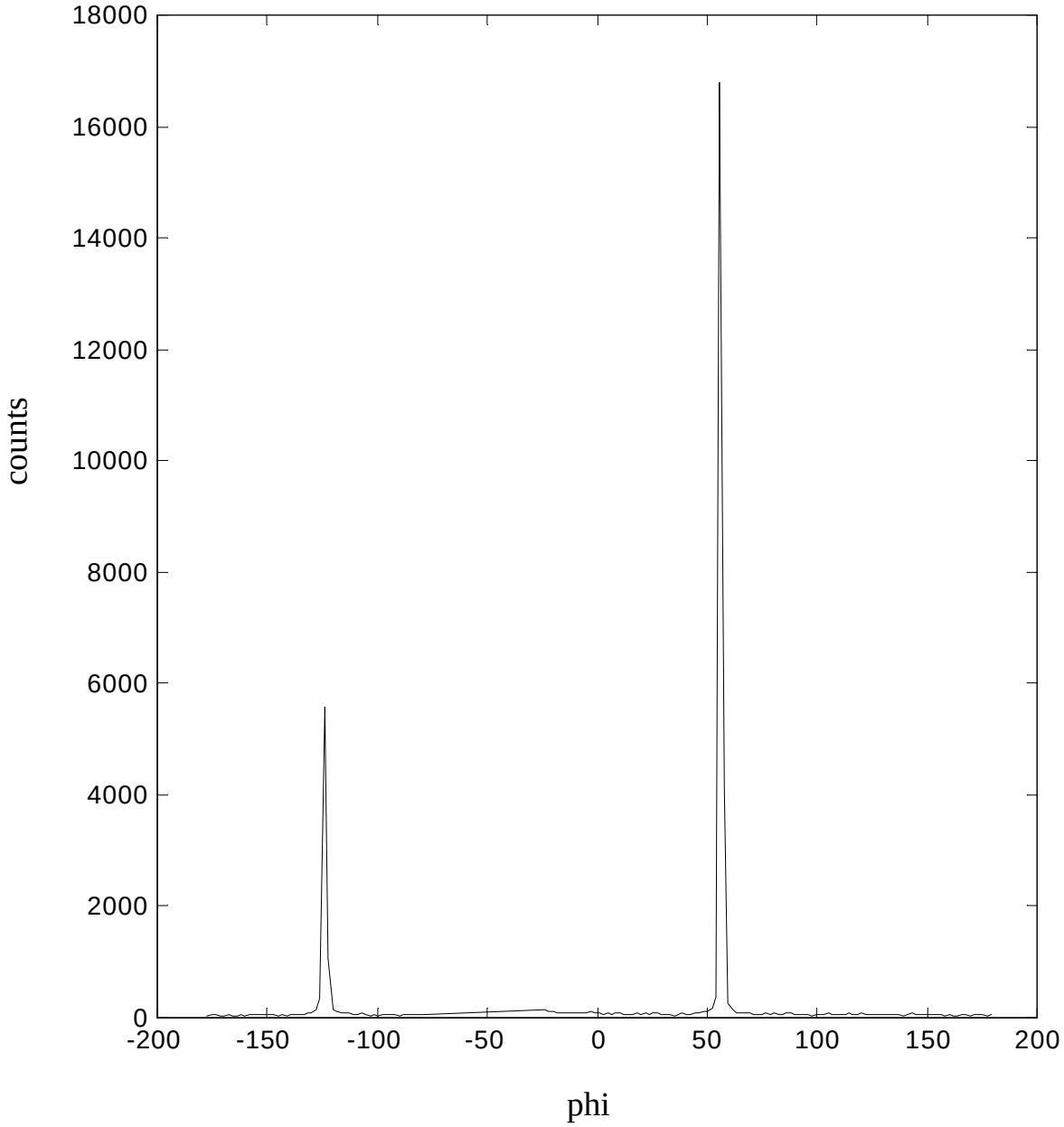


-Rocking curves are measured along the Bragg-rods

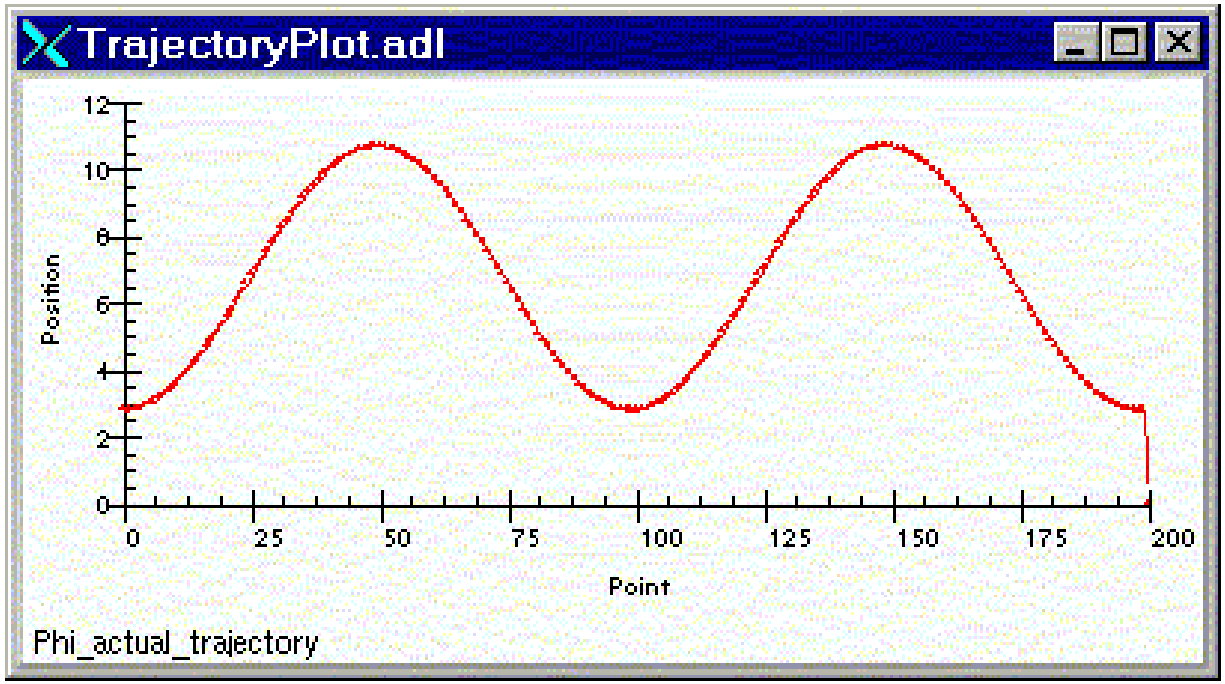
- Integrated intensity is background subtracted and correction for geometric factors

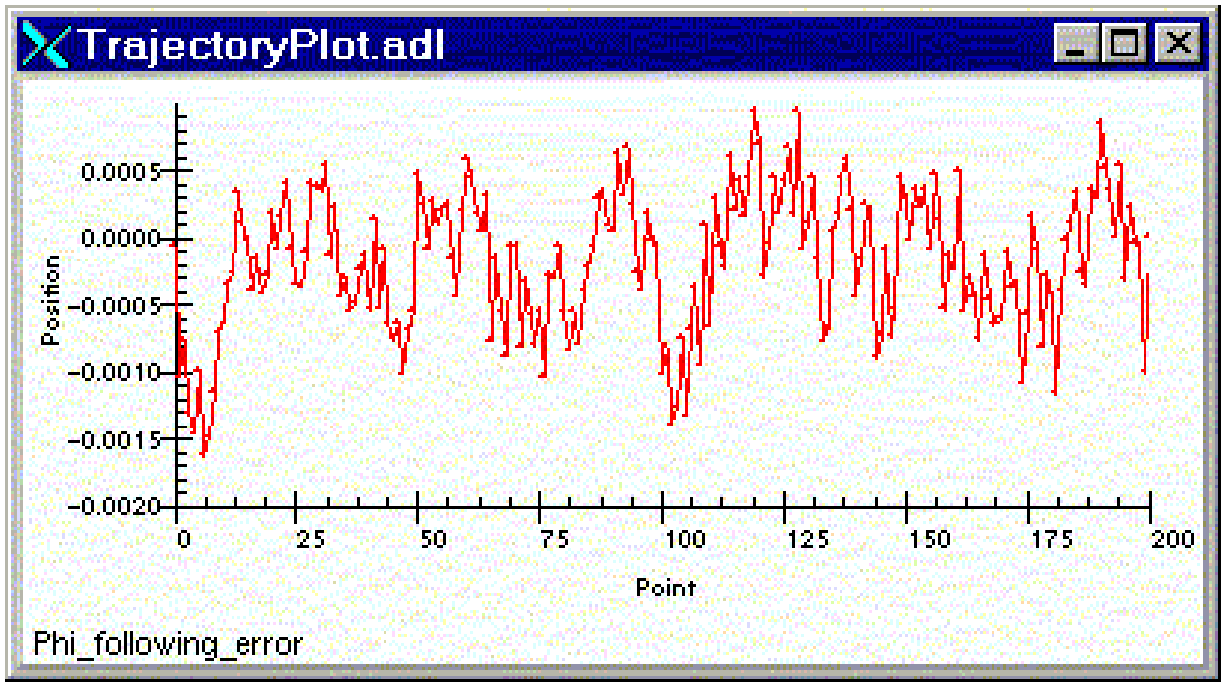
→ Experimental Structure Factor (F_T)

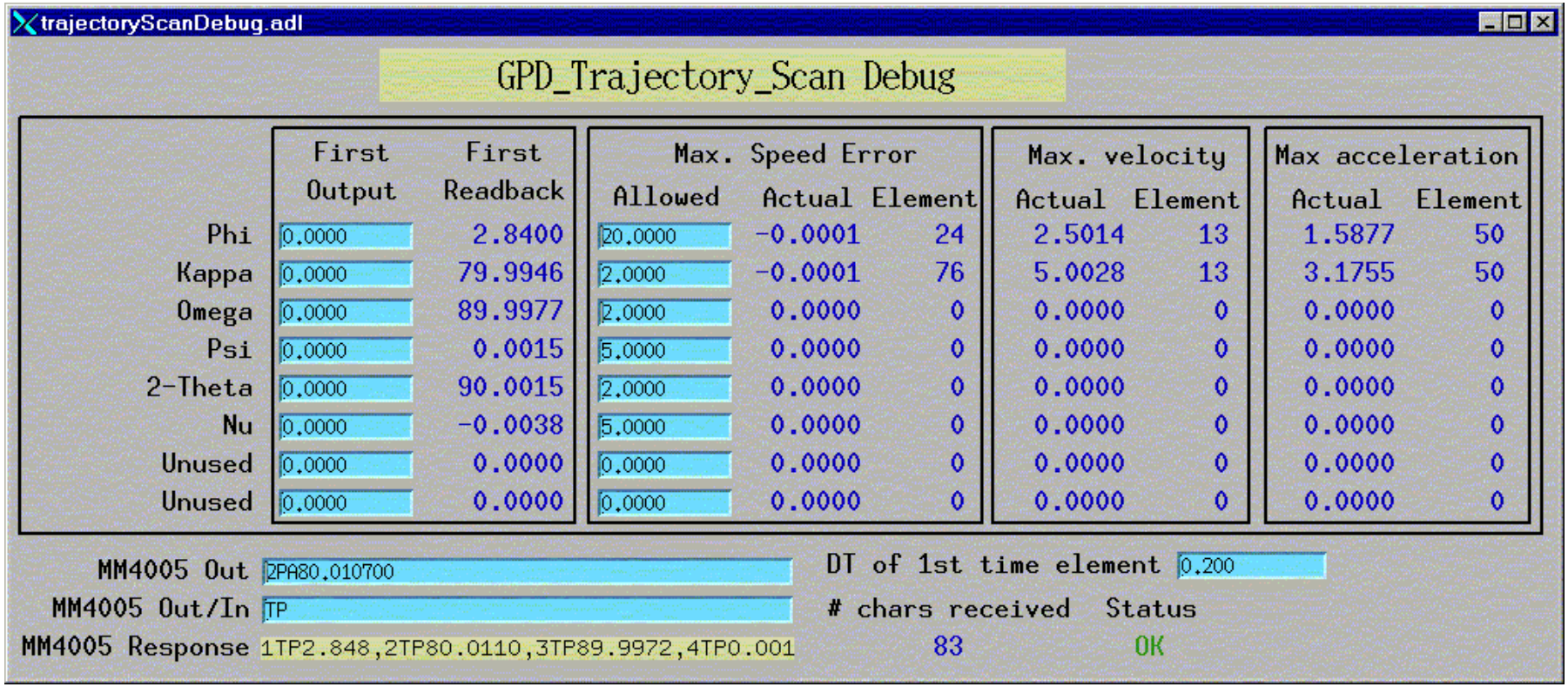

trajectoryScan.adl
GPD_Trajectory_Scan
trajectory elements
100
Trajectory definition
Relative
output pulses
200
Actual
200
Range of pulses: Start
1
End
100
Time mode
Total
Total time
20.000
Plot time
Execution time scale
1.00
Acceleration time
0.500
More
Move axis?
Current Pos.
Plots
Phi
Yes
2.8480
Kappa
Yes
80.0110
Omega
No
89.9972
Psi
No
0.0015
2-Theta
No
90.0013
Nu
No
-0.0038
Unused
No
0.0000
Unused
No
0.0000
Command
State
Status
Build
Build
Done
Success
Build message
Simulate/Real
Real
Execute
Execute
Done
Success
Execute message
Abort
Abort!
Readback
Readback
Done
Success
Read message



Example of a trajectory scan during crystal orientation. Phi scan looking for in-plane diffraction peaks. Scan is run at about 2 deg/sec.


TrajectoryPlot.adl
12
10
8
6
4
2
0
Position
0
25
50
75
100
125
150
175
200
Point
Phi_actual_trajectory


TrajectoryPlot.adl
0.0005
0.0000
-0.0005
-0.0010
-0.0015
-0.0020
Position
0
25
50
75
100
125
150
175
200
Point
Phi_following_error


trajectoryScanDebug.adl
GPD_Trajectory_Scan Debug
First Output
First Readback
Max. Speed Error
Allowed
Actual
Element
Max. velocity
Actual
Element
Max acceleration
Actual
Element
Phi 0.0000 2.8400 20.0000 -0.0001 24 2.5014 13 1.5877 50
Kappa 0.0000 79.9946 2.0000 -0.0001 76 5.0028 13 3.1755 50
Omega 0.0000 89.9977 2.0000 0.0000 0 0.0000 0 0.0000 0
Psi 0.0000 0.0015 5.0000 0.0000 0 0.0000 0 0.0000 0
2-Theta 0.0000 90.0015 2.0000 0.0000 0 0.0000 0 0.0000 0
Nu 0.0000 -0.0038 5.0000 0.0000 0 0.0000 0 0.0000 0
Unused 0.0000 0.0000 0.0000 0.0000 0 0.0000 0 0.0000 0
Unused 0.0000 0.0000 0.0000 0.0000 0 0.0000 0 0.0000 0
MM4005 Out 2PA80.010700
MM4005 Out/In TP
MM4005 Response 1TP2.848,2TP80.0110,3TP89.9972,4TP0.001
DT of 1st time element 0.200
chars received
Status
83
OK

Future Work

- Make motor record and trajectory scanning work with less possibility of interference
  - Almost done
- Support other controllers
  - e.g Galil, OMS58
- Improve performance
  - New MM4005 firmware or model