

SEQUOIA Operations Manual for Users

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Abstract

The SEQUOIA Operations Manual for Users presents a description of the SEQUOIA spectrometer located at beamline 17 (BL17) of the Spallation Neutron Source (SNS). It is the intent of this manual to inform the user regarding the SEQUOIA spectrometer and available sample environment, to run experiments, to access and analyze the collected data, and to provide the user with other potentially useful information. The first section serves to describe the components of which the instrument is comprised. The next section describes how to operate the data acquisition system and includes scripting commands necessary for automating data acquisition. Though documentation of the data reduction and analysis software which covers all of the Direct Geometry Spectrometers (DGS) exists separately, instrument specific information regarding data access and software packages is covered in the third section of this manual. Users are encouraged to contact members of the instrument staff with any questions that arise and to avail themselves of the beamline staff and other support personnel when on site. Additionally, constructive feedback is always welcome and will be taken into consideration when making improvements.

Precautions

Failure to follow the policies, procedures, and work practices described in this document may result in the unintentional release of activated samples to non-designated areas, may expose users or personnel to unsafe conditions, could damage equipment, and could potentially result in the cancellation of an experiment or the loss of beam time.

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1) Introduction

This user manual is a living document to help the user understand the SEQUOIA instrument and to remind them of things shown in the training. It is not intended to replace or supersede the instrument training. If you have any questions, please contact your local contact or the Instrument Hall Coordinators.

Accessing the SEQUOIA Instrument

From the Central Laboratory Office (CLO), there is a bridge connecting the CLO and the target building, which is accessible via the second floor of the CLO. In order to cross the bridge, a user must possess current target building training, as a proximity card reader controls access to the bridge. The door to this bridge is located near the User Office, as shown in the map below. The route to the bridge is shown with arrows in Figure 1.

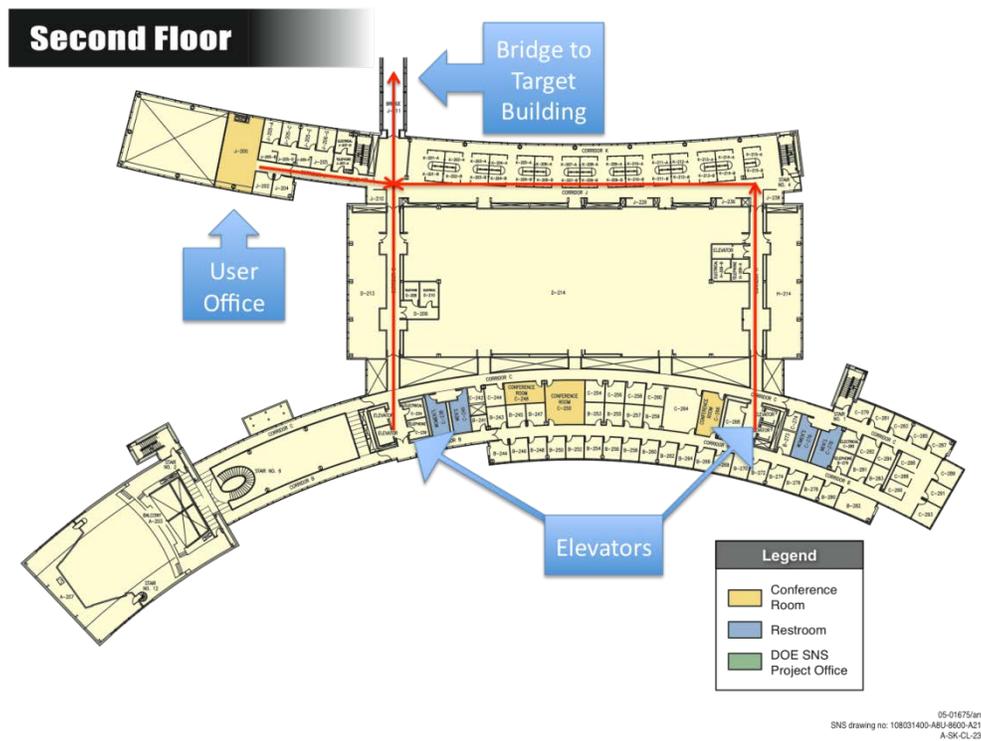


Figure 1 Accessing the Experiment Building

After crossing the target building bridge, turn right and continue along the north side of the mezzanine toward the west side of the target building. The SEQUOIA spectrometer and control cabin is placed at the north-west corner of the target building.



Figure 2 The Spallation Neutron Source Facility: The Central Lab and Office (CLO) building to the south contain office spaces, lecture halls, and the Central Control Room; at the end of the accelerator (in red) the Target building contains the suite of instrument.

SEQUOIA Control Cabin

The SEQUOIA control cabin has the terminals of the SEQUOIA control computer and SEQUOIA data analysis computers. Users of the current experiment may sit there. If you would like to use the hutch before or after your experiment, please contact the instrument staff to check if it is available. The SEQUOIA Vacuum System display (controlled by push buttons on the manual screens) is also located in the control cabin. The cabin is equipped with a wireless access point, providing wireless networking access to both the ORNL-visitor network and the secured WPA network. None of the Ethernet ports in Cabin provide outside access for users and should not be used by users. The cabin has its own air conditioning system. Feel free to adjust it for your comfort while using SEQUOIA.

Training

To ensure that all work is completed safely, SNS instrument users are required to be trained on laboratory policies, and instrument specific requirements.

The User Office will present you with your general ORNL training requirements. In order to ensure you are able to maximize your time on site working at the instrument, **please** complete this training as much as possible ahead of time.

At the SEQUOIA, the instrument specific training modules are:

- User orientation at the SEQUOIA (walkthrough of the instrument with local contact, including introduction to data acquisition and analysis)
- Responding to Alarms and Emergency Situations at the SEQUOIA
- User Operation of the SEQUOIA Instrument Personnel Protection System (IPPS).
- Sample handling at the SEQUOIA

When you arrive at the instrument, a member of the instrument staff will provide training on these instrument specific modules. There will be a checklist of these required modules given to you by the Instrument Hall coordinators (IHCs), which the SEQUOIA Instrument staff member will fill out and return to the training/user office.

User Portal

The new user portal found at the following link:

<https://user.ornl.gov> .

Everything you need for a successful experiment at SEQUOIA can be found here. There is a section for training, proposals, data and travel accommodations as seen in Figure 3.

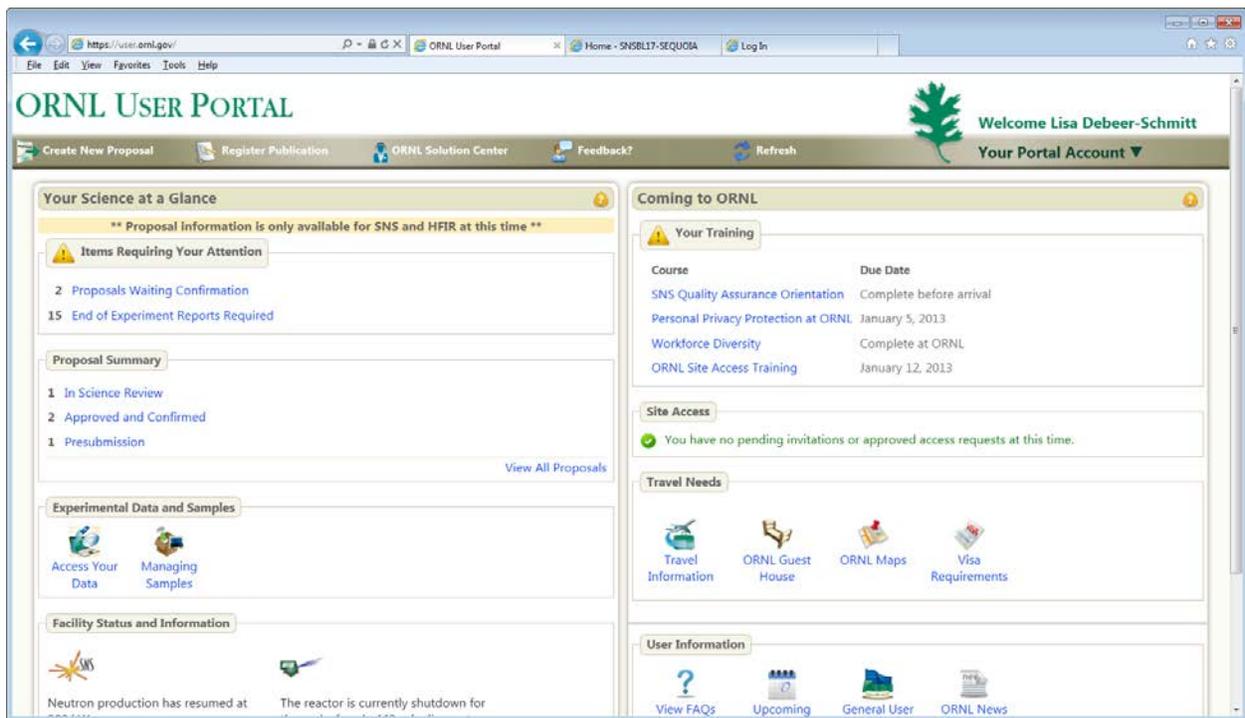


Figure 3 User portal main page

2) Instrument components

SEQUOIA is a fine resolution thermal - epithermal spectrometer located on SEQUOIA, Beamline 17, at the SNS. Figure 4 shows the overall layout of the spectrometer and points out major components many of which will be described shortly.

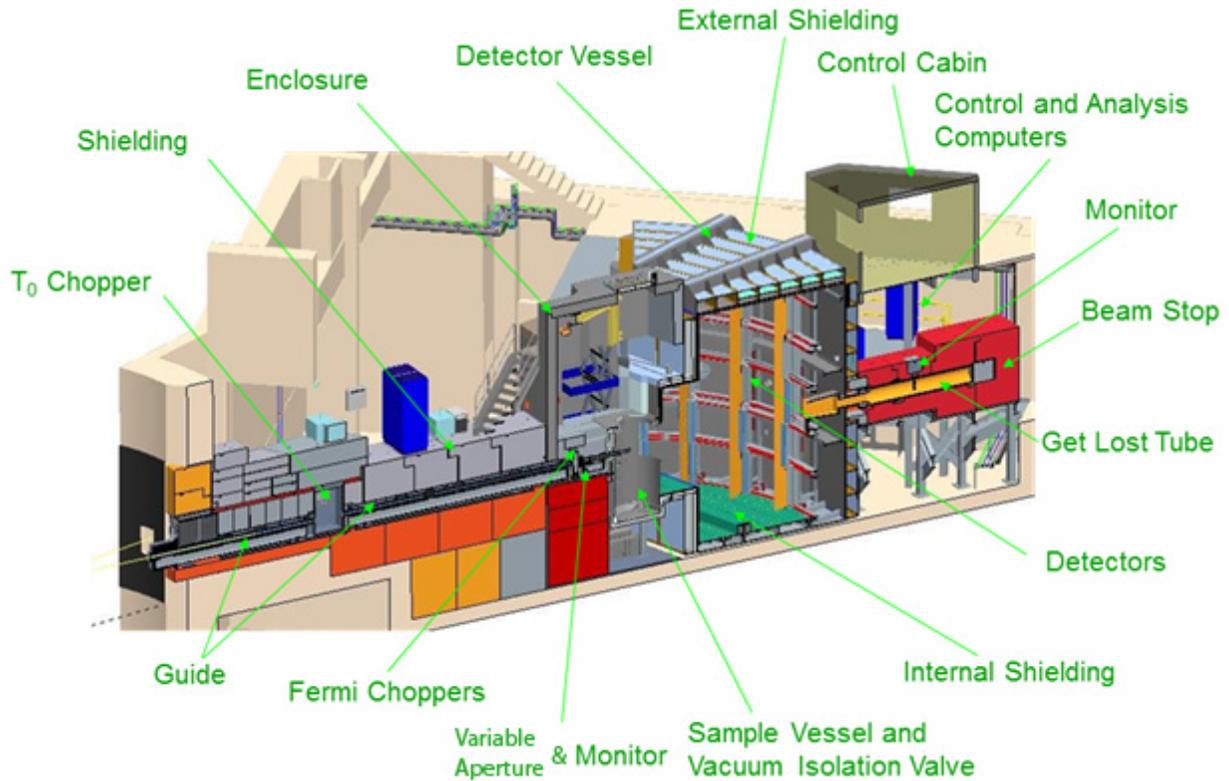


Figure 4 Schematic view of the SEQUOIA spectrometer indicating all of the major instrument components.

Though full details of the instrument geometry can be pulled from you data file, as described in Data Format, Table 1 summarizes several useful distances.

Description	Distance (m)
Moderator to T0 chopper	9.5
Moderator to Fermi chopper	18.2
Moderator to Monitor 1	18.2
Moderator to Sample	20.0
Sample to horizontal plane detector pixels	5.5
Moderator to Monitor 2	29.0

Table 1 Approximate distances to major instrument components

SEQUOIA is a direct geometry time-of-flight chopper spectrometer that can utilize incident neutron energies E_i between 10 meV and 2 eV. It is being used to conduct forefront research on dynamical processes in materials. In particular, SEQUOIA enables very high-resolution inelastic neutron scattering studies of magnetic excitations and fluctuations along with lattice vibrations. With its capability to acquire data quickly and relate them to three-dimensional momentum transfers, SEQUOIA applications span a wide cross-section of important research areas in condensed matter and materials science such as the following: strongly correlated electrons systems, high-temperature superconductors, colossal magnetoresistive materials, quantum and molecular magnetism, itinerant magnets and multilayers, alloys, ferroelectric, piezoelectric and thermoelectric materials, excitations in quantum fluids, quantum critical phenomena, and soft condensed matter.

SEQUOIA is also an outstanding tool for the investigations of novel systems and materials that are unknown today. In general, SEQUOIA is the instrument of choice for experiments that require fine Q and ω resolution and large solid angle at low to intermediate scattering angles.

Moderator

SEQUOIA is located on BL17 and thus has a direct view of the bottom upstream decoupled poisoned ambient water moderator (bu_17). This moderator has a poisoning depth of 25mm. Detailed calculations of the moderator performance are given elsewhere and compare well with respect to any measurements that have been performedⁱ. The peak flux as a function of energy from the reference [i] is given in Figure 5.

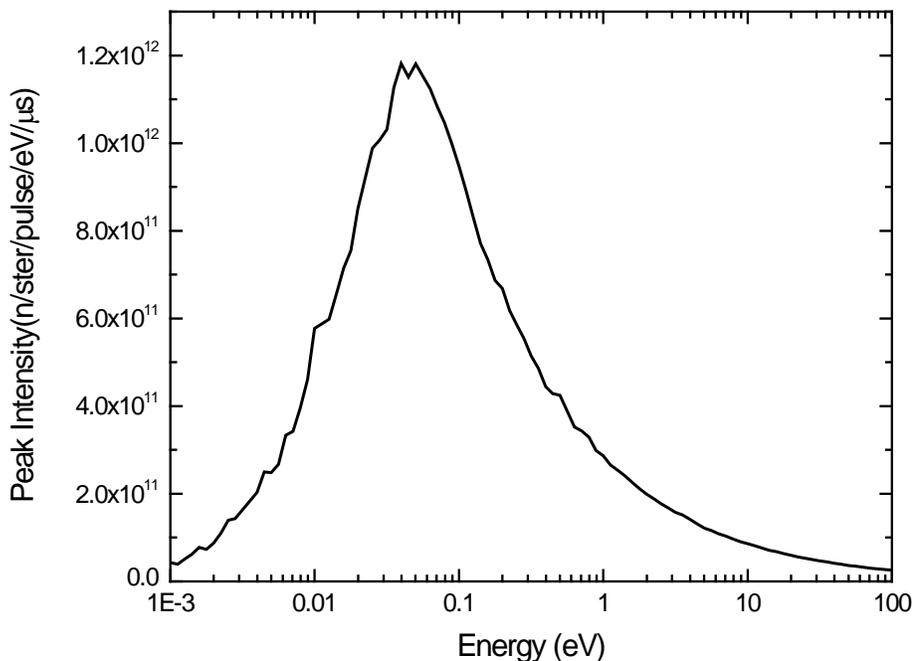


Figure 5 Output of the moderator as a function of energy.

Neutron Guide

There are five sections of neutron guide installed on SEQUOIA. Three of these sections are permanently mounted. The fourth section may consist of either an open rectangular guide, similar to the three permanent sections, or it may be replaced by a collimating guide section. The fifth section of guide, which is mounted inside the sample vessel and is closest to the sample position, may be removed to decrease beam divergence at the expense of flux. It must be removed to accommodate sample environment equipment bigger than 16" in diameter. With all 5 sections of guide in place, the guide approximates an elliptical shape with the upstream focal point at $-\infty$ and the downstream focal point at 6.3m and 5m past the sample in the horizontal and vertical directions, respectively. The choice of placing the focal point beyond the sample ensures the maximum flux on sample at energies where the guide gain is negligible while providing significant gain in the low energy range. Guide gain works by increasing the divergence on the sample. Figure 6 shows the net divergence at the sample position produced by the guide system.

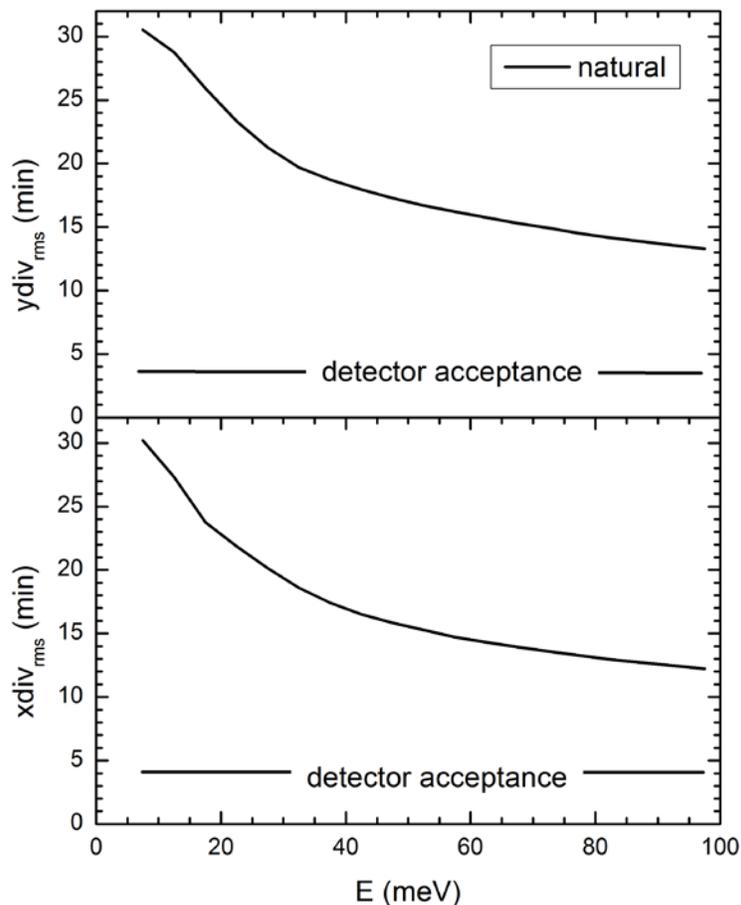


Figure 6 The vertical (top) and horizontal (bottom) divergence as a function of incident energy at the sample position with all guide sections included.

T₀ Chopper

The purpose of the T₀ chopper, which is located 9.861 m from the moderator, is to suppress the prompt pulse of fast neutrons produced when the proton beam strikes the target. This suppression is accomplished by having an approximately 0.20-m-thick piece of the alloy Inconel X-718 in the beam when the proton pulse hits the target. The material works by scattering neutrons into the neighboring shielding. This piece of inconel must be out of the beam in sufficient time for the 0.01 - 2 eV neutrons to pass. It only turns counter clockwise and can operate at rotational speeds between 30 Hz and 180 Hz in multiples of 30 Hz. The following table provides many standard T₀ configurations. Since the T₀ chopper transmits a much wider bandwidth than the Fermi chopper, it may let multiple Fermi chopper pulses through. Sometimes we adjust the phase of the T₀ chopper to block or allow specific additional openings of the Fermi chopper. Many common configurations are available in the following table. If the configuration you need is not on the table, please consult with instrument staff about the appropriate T₀ chopper frequency and phase for your experiment.

Fermi Chopper

Two Fermi choppers, which are mounted on a translation table so that either can be chosen independently, are installed on SEQUOIA. In the in-beam position the Fermi chopper is 18.0085 m from the moderator. Its purpose is to select a monochromatic pulse of neutrons. A Fermi chopper is a series of closely spaced neutron-absorbing blades (slit package) held together by a rotor that spins about a vertical axis in the path of the beam. All slit packages are 100 mm in length. Each Fermi Chopper can be spun from 0 to 600 Hz in increments of 60 Hz. Table 2 provides the parameters of the Fermi choppers. Only one Fermi chopper may be spinning at full speed at a time. When ramping down the chopper, go in increments of 60 Hz down to 360 Hz. Otherwise the chopper will fault and needs to be reset by the instrument staff or Hall coordinators. Figure 7 and Figure 8 provide the resolution and transmission for the two Fermi choppers. Your local contact can assist you in choosing the appropriate chopper and rotational speed for your experiment.

Incident Energy Range	FC ₁	T ₀ ₁	Ph ₁	FC ₂	T ₀ ₂
8				180	30
25				300	60
30	120	30		300	60
30				360	60
40				360	60
50	120	60		420	90
50	180	90			
60	180	60		480	90
60	240	60			
100	240	60		600	90
100	300	90			
150*				600	90

Incident Energy Range	FC ₁	T0 ₁	Ph ₁	FC ₂	T0 ₂
150	300	90		600	120
200*	300	120		600	90
200	360	120		600	120
250				600	120
300	300	120			
500	600	150			
700*	600	150			
800	600	180			
1000	600	180			

Table 2 Suggested T0 and Fermi chopper rotational frequencies for given incident neutron energy. A quick run should be made while observing monitor 1 to verify that there is no contamination by other energies

*Maybe better to shift phase.

Translation table position number	Chopper number	Number of slats	Channel width (mm)	Slat thickness (mm)	Radius of curvature (m)	Optimum E _i (meV) at 600 Hz
3	2	27	2.03	0.35	0.58	100
1	1	16	3.56	0.35	1.53	700

Table 3 Properties of the slit packages available on SEQUOIA

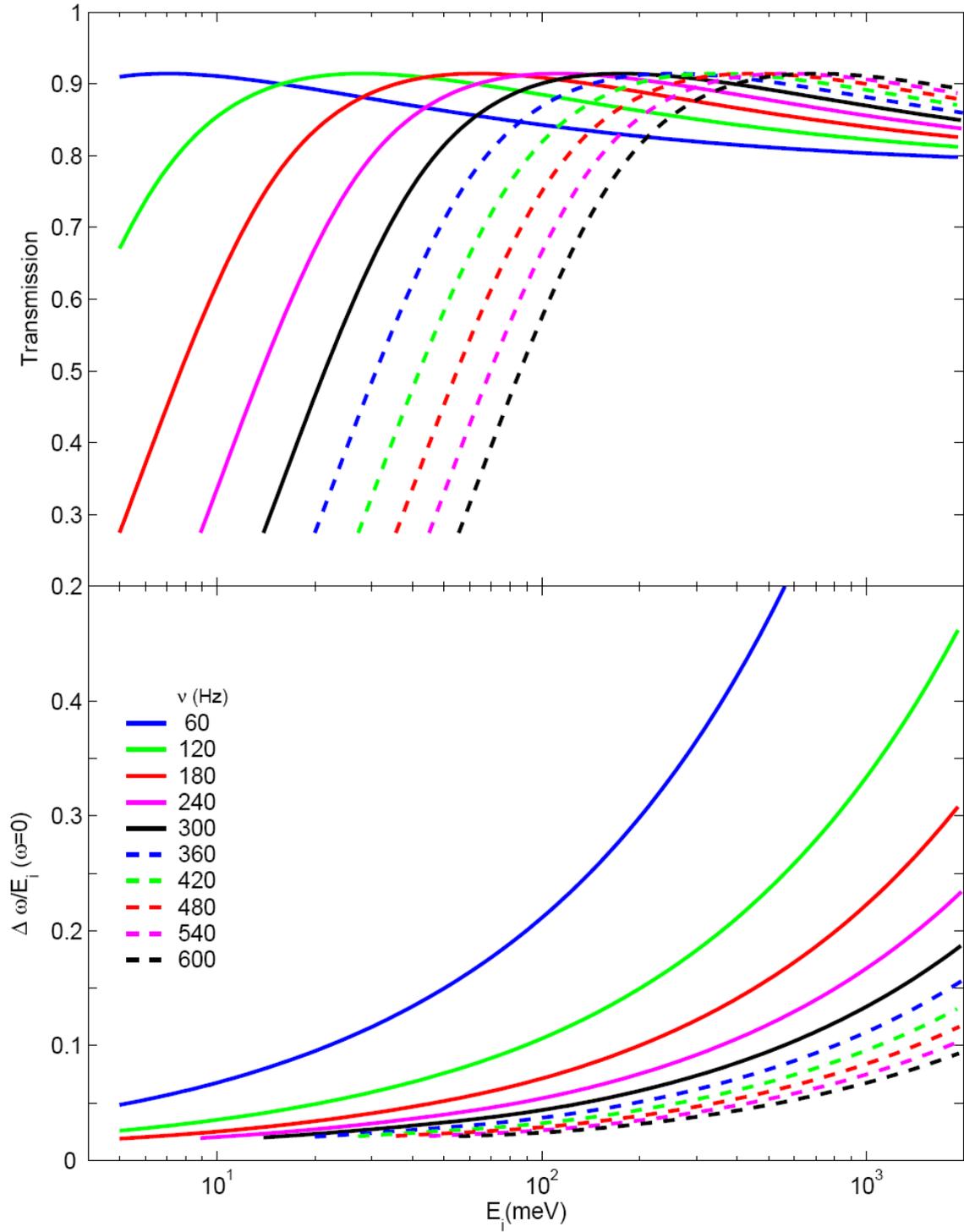


Figure 7 Transmission through the slit package and elastic energy resolution for Fermi chopper 1

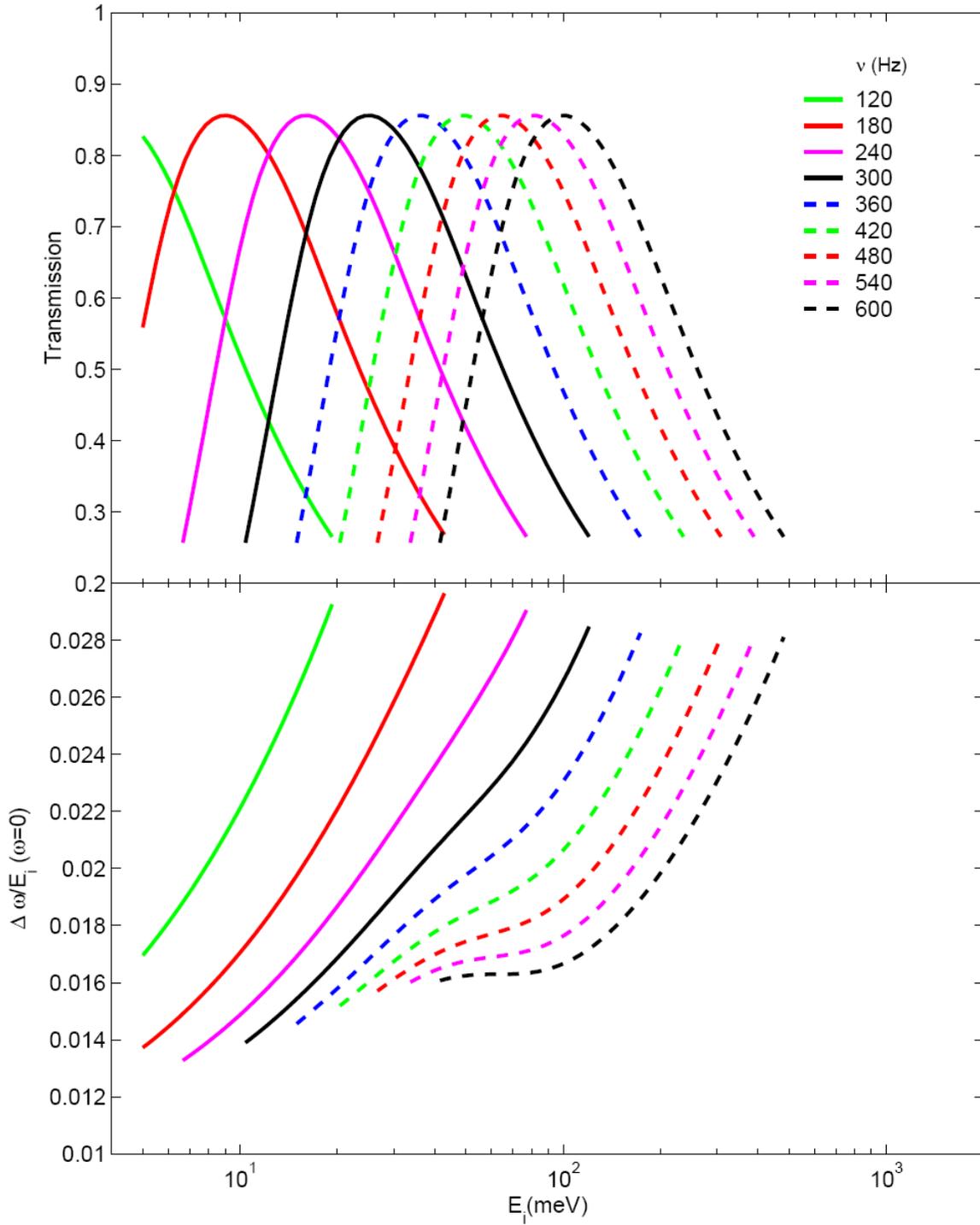


Figure 8 Transmission through the slit package and elastic energy resolution for Fermi chopper 2

Detectors

The detector array on SEQUOIA is an assembly of 1.2 m long by 25 mm diameter Linear Position Sensitive Detectors (LPSDs). The array has space for 1440 detectors grouped into packs of 8 and located on a vertical cylinder with a radius of ~5.5 m (which is the distance between the sample position and the detectors in the horizontal plane). The LPSDs are filled with He3 at a pressure of 10 Atmospheres (1.0 MPa). To reduce background there are no windows between the sample and the detectors; the detectors are located inside a detector chamber that is evacuated to a high vacuum (below 10^{-6} atm) and is contiguous with the sample vessel.

An incoming neutron is converted through the nuclear reaction $n + {}^3\text{He} \rightarrow {}^3\text{H} + {}^1\text{H} + 0.764 \text{ MeV}$ into charged particles tritium (T or ${}^3\text{H}$) and protium (p or ${}^1\text{H}$) which then are detected by creating a charge cloud in the stopping surrounding gas. The electrons from the ionized gas are collected at an anode wire running down the center of the detector tube. This wire is at 1870 V above ground and has a high resistance so the proportion of charge seen at each end allows one to determine the position of the neutron detection event. The length of the detectors is divided into 128 pixels of ~10 mm length by the electronics. Each pixel subtends an angle of $\sim 0.26^\circ$ perpendicular to the length of the tube and $\sim 0.16^\circ$ along the length of the tube. The overall solid angle of the whole detector is 0.83 Sr. Each pixel has a timing resolution of 1 μs and saturates at no less than 70,000 n/s. After saturation a tube is ready for measurement within 10 μs . Saturation is indicated by lack of response even if the signal is increased. In extreme saturation cases the charge cloud grows up and down the tube and position sensitivity is lost as well. This case usually occurs when a Bragg peak from a large single crystal is incident on the pack in white beam mode. An example of such a saturation condition is shown in Figure 9.

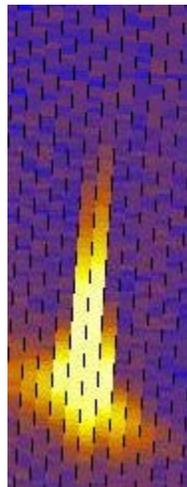


Figure 9 Example of tube saturation to the point of expansion of the charge cloud in the detector tube

If the Bragg peaks need to be used, for crystal alignment for example, one or more attenuators should be inserted into the beam. For inelastic measurements, the attenuators should be out of the beam and the 10 μs worth of data after the elastic line are contaminated. If data in an energy transfer range that corresponds to within these 10 μs is necessary of analysis, one can slightly change the orientation of a single crystal so the Bragg peak is not in the same detector as the inelastic signal. One of the reasons

non continuous detectors were used for the detector array is to reduce the amount of detector coverage lost in a saturation event.

Detector packs are variously labeled by their number or name in different places. The table below is a mapping between the two.

Number	Name	Number	Name	Number	Name
38	B1	75	C1	114	D1
39	B2	76	C2	115	D2
40	B3	77	C3	116	D3
41	B4	78	C4	117	D4
42	B5	79	C5	118	D5
43	B6	80	C6	119	D6
44	B7	81	C7	120	D7
45	B8	82	C8	121	D8
46	B9	83	C9	122	D9
47	B10	84	C10	123	D10
48	B11	85	C11	124	D11
49	B12	86	C12	125	D12
50	B13	87	C13	126	D13
51	B14	88	C14	127	D14
52	B15	89	C15	128	D15
53	B16	90	C16	129	D16
54	B17	91	C17	130	D17
55	B18	92	C18	131	D18
56	B19	93	C19	132	D19
57	B20	94	C20	133	D20
58	B21	95	C21	134	D21
59	B22	96	C22	135	D22
60	B23	97	C23	136	D23
61	B24	98	C24	137	D24
62	B25	99	C25T	138	D25
63	B26	100	C26T	139	D26
64	B27	101	C25B	140	D27
65	B28	102	C26B	141	D28
66	B29	103	C27	142	D29
67	B30	104	C28	143	D30
68	B31	105	C29	144	D31
69	B32	106	C30	145	D32
70	B33	107	C31	146	D33
71	B34	108	C32	147	D34
72	B35	109	C33	148	D35
73	B36	110	C34	149	D36
74	B37	111	C35	150	D37
		112	C36		
		113	C37		

Table 4 Mapping between detector pack number and name.

Detector Position Calibration

The instrument staff regularly performs detector calibration runs and ensures that the instrument geometry that is included with the user’s data is up to date. Nevertheless the procedure used for the

calibration procedure is outlined here for the interested user. The detectors positions are calibrated using several standard samples. It is a two-step process that involves using a Monochromatic V run to determine the distance from the sample to the detector and white beam powder diffraction runs to determine the angle of the detectors away from the scattered beam. Geometrical constraints on given the shape of the detector pack allow the full determination of each pixel position.

Monitors

There are two neutron beam monitors located along the direct beam, one located just downstream of the Fermi chopper (Beam monitor 1) and variable aperture and a second located farther downstream of the sample near the beamstop (Beam monitor 2). The positions of each monitor with respect to the moderator are 18.2331 m and 29.0033 m, respectively. If the upstream monitor has been removed a remounted, a new position is recorded. Please check the position tag in the NeXus file for the most current detection information. These two monitors are primarily used to determine the speed of the incident neutrons, but can also be used to normalize the intensity. Currently monitors are stored as histograms by the DAS.

The detection media is ^3He , just as in the detectors. However they have a relatively low gas pressure to detect a small portion of neutrons without saturating. More specifically their detection efficiency is 1×10^{-6} for $E_i=2$ eV neutrons. The detection area is 76.2 mm wide by 114.3 mm high and 12.7 mm deep. The gas is contained in an Al box. Both the ingoing and outgoing windows are 1.3mm thick. Note that if the prompt pulse hits the monitor without being stopped by the T0 chopper, (ie if the instrument energy is set above 6 eV) the upstream monitor will saturate. It is worth running a test run at this energy to see if you can analyze the data without the upstream monitor, before committing to a long run at Energies above 4 eV)

Apertures

A set of variable apertures are installed just downstream of the Fermi chopper. It consists of four 99% isotopically enriched hot pressed $^{10}\text{B}_4\text{C}$ plates (74 – 77% B, 23 – 26% C) having the dimensions 2.99" x 3.30" x 0.50". Two of the plates move vertically and two move horizontally. The limiting positions of each blade are given in the Table 5 and the transmission of the variable apertures as a function of the blades position is shown in Figure 10.

Blade	In Beam (mm)	Out of Beam (mm)
Left	75.26	0.00
Right	0.00	75.66
Bottom	0.00	75.92
Top	76.13	0.00

Table 5 Limiting positions for each variable attenuator blade. Left and right are defined when facing downstream.

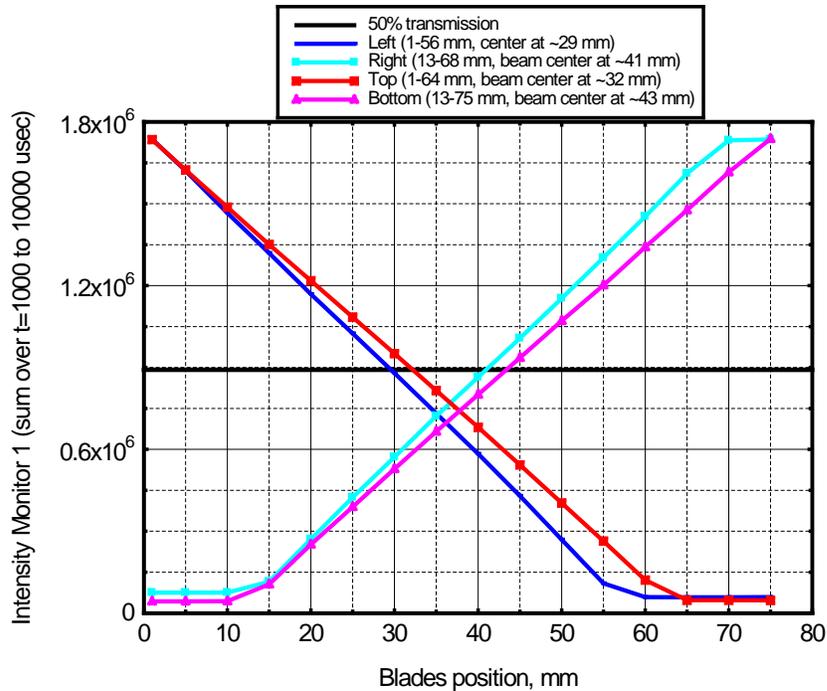


Figure 10 Monitor 1 Intensity versus the absorbing blades opening (50% transmission corresponds to the position of the corresponding blade edge in the center of the neutron beam).

Some standard slits settings:

Si powder – Ashfia’s cell: w = 12 mm, h = 32 mm, should be centered. L=23, r=47, b=60.

V plate (3x3) – w = 35 mm, h = 35 mm: should be centered.

Attenuators

Two attenuator plates, located between the Fermi chopper and the variable aperture, may be independently placed in the incident beam. Each plate is 1 mm thick and consists of 2% borated aluminum plates. Limiting positions for the plates are given in Table 6.

Attenuator	In Beam (mm)	Out of Beam (mm)
Attenuator 1	89.65	0.00
Attenuator 2	0.00	93.43

Table 6 Limiting positions for each of the attenuator plates.

These attenuators are primarily used during sample alignment to keep single crystal Bragg peaks from saturating the detectors during alignment.

Sample Environment (SE)

The sample environment equipment available for general use at the SNS is catalogued on the [SNS Sample Environment Equipment Inventory](#) site. A sample orienting displax is the workhorse SE at SEQUOIA and is described in further detail below. Additionally, a room temperature, cryostat, magnet and a furnace are available to use at SEQUOIA

Standard Flanges

The flanges at the SNS have been standardized in the attempt to accommodate all SE equipment. Flange specifications are detailed in SNS Interface Control Document: 107030501-IC001-R01. For sample environments requiring a 16" flange, there is the possibility of using a neutron camera for sample alignment, aperture adjustment, etc.

Neutron Camera

A neutron camera is available for real-time imaging of the beam as viewed from 13.485" downstream of the sample position. The neutron camera can be mounted in conjunction with any standard 16" sample environment. Installation of the camera will be performed by beamline staff.

Operation of the Control Unit

1. Make sure the red "freeze" button is off by toggling the red button.
2. Turn the exposure control to slow-5 which should cause the green light to blink at about 1 Hz.
3. Turn the gain and gamma to "HI" if necessary to maximize efficiency.
4. Turn IRIS control off since this is not used.
5. Adjust shutter speed, gain, and gamma as appropriate using the guide on the back of the control unit
6. "LO" gamma should be used to maximize dynamic range as long as a clear image is still attained.
7. For unlimited exposure, set the shutter position to "START" (top), expose for the required time, then press the red button to "STOP" and obtain the readout

Sample orienting displax

SEQUOIA has a closed cycle refrigerator, CCR, which capable to provide temperatures from 325 K down to 6 K with cooling time to the base temperature is about 45 min (Figure 11). A differentially pumped room temperature rotating seal provides the feed through of the rotation about a vertical axis. This rotary flange is connected to a motor that through the motion controller is run by the sample environment computer. The application is CCRV13Rot and a corresponding client application must be run on the control computer. To change the soft limits right click on the angle image and then change the limits. If the limits need to be changed outside of the limits given, then the soft limits need to be set. Contact your instrument staff to help you make this change.

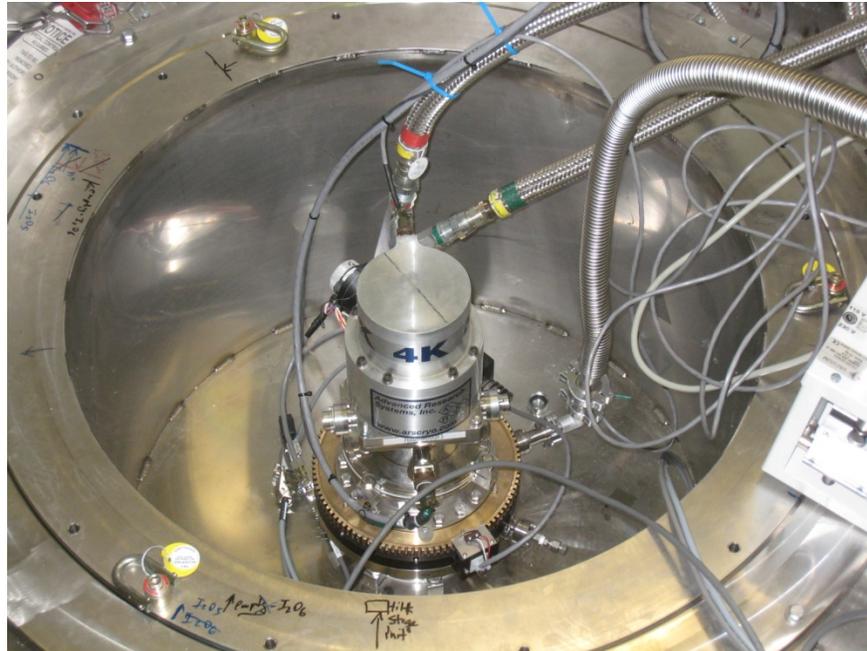


Figure 11 Top view of CCR at SEQUOIA sample position. The scribed line across the cold head is used for aligning the flat cells used for powder experiments discussed in later section.

Thermometry and Temperature Control

Two Si diode thermometers are provided; one on the CCR cold head and another on the sample container. Temperature readout and control is governed by a Lakeshore Model 336.

PID Parameters

PID parameters vary according to temperature and positions of the heaters and thermometers. Relevant parameters in assessing the appropriateness of these parameters are the initial and final temperatures, the temperature overshoot, the time it takes to settle to within about 1 K, and the fluctuation in temperature after setting.

Tests of the thermal performance when the heater is mounted on the CCR second stage cold head and the thermometer is on the exchange gas can are shown in Table 7. Initial warming shows that the PID = [110, 10, 10] are appropriate from base temperature to 70 K, but not up to 100 K. These values are marginal at 70 K if the overshoot is considered. From 30 K to 100 K, the same PID = [110, 5, 25] are suitable. The latter values have yet to be tested at base temperature.

T _{init} [K]	T _{final} [K]	T _{over} [K]	t _{settle} [min]	ΔT [K]	P	I	D
Base	30	0.1	1	0.05	110	10	10
Base	70	3.6	9	0.05	110	10	10
63	70	4	3	0.05	110	10	10
70	100	4	10	3.5	110	10	10
100	100	N/A	4 min osc.	<0.2	110	5	25
100	30	- 1	20	<0.01	110	2	25

Table 7 Heater is mounted on the CCR cold head and thermometer is mounted on the Cu upper flange of the exchange gas can. (Note: Parameters give significant overshoot at 70 K, but the fluctuations are small. Parameters for 100 K must be further tuned. Since

There are a couple of different ways for mounting samples on the CCR it depends on what kind of sample you are interested in running.

Single Crystals:

There are two ways of mounting single crystal samples. The preferred method is using a “soda” can described in Figure 12. This is a thin walled exchange gas can that produces the lowest background at SEQUOIA. It has a double indium seal to keep the helium gas pressure inside while the can is under vacuum.

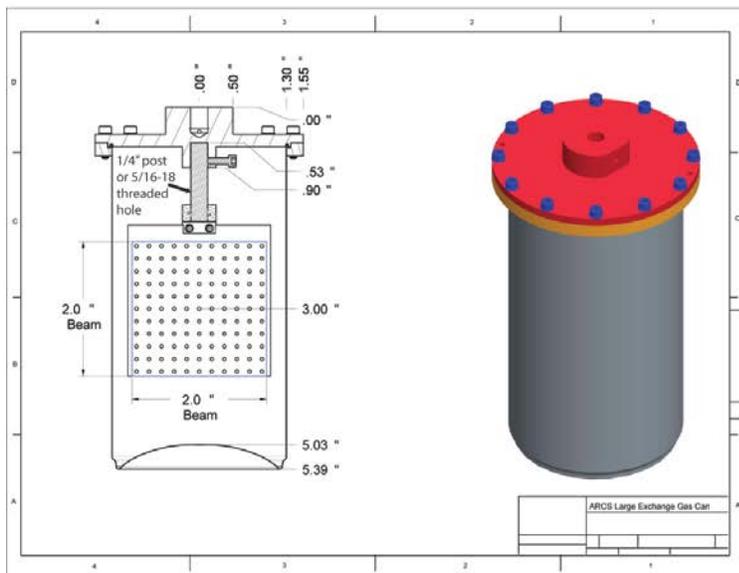


Figure 12 Dimensions for the "soda" can (left) and one installed on the bottom of CCR-13. The foil on the left side of the photo is the heat shield commonly used on CCR-13

The other can for single crystals is another exchange gas can but it has thicker walls shown in Figure 13. This can is sealed with indium but is mostly used for samples that will not fit into the soda cans.

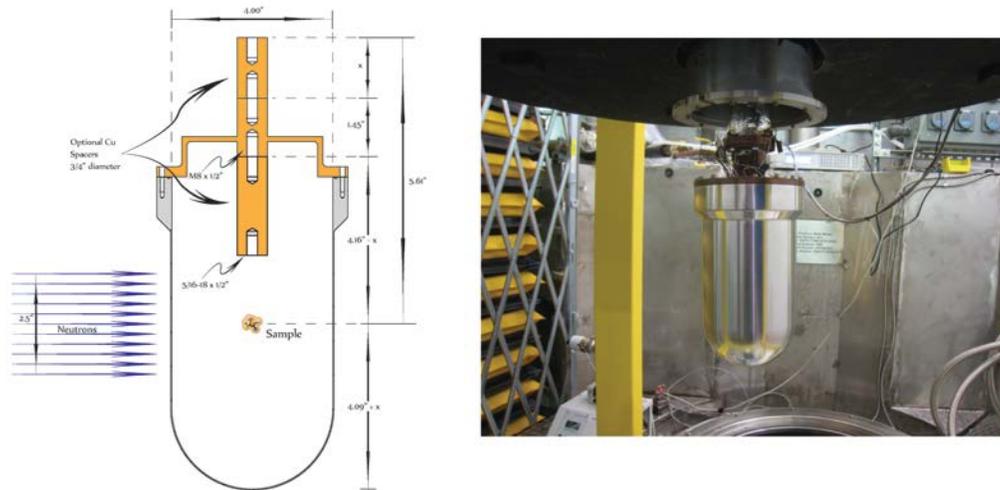


Figure 13 Exchange gas can use when samples will not fit into the “soda” cans. Orange represents copper while grey indicates aluminum.

The desired crystal axis may be easily translated to the side of the Cu flange just after mounting the crystal to the flange and before sealing the exchange gas can. After installing the can on the CCR, the mark may be translated to the 2.20” CCR flange and the arc distance from this mark to one of the blank bolt holes should be measured. The orientation of the blank holes has been translated to the top of the CCR (diameter 4.9”) and permanently marked. Multiply the arc length found on the CCR flange by $4.88/2.20 = 2.22$ and make a mark on the top of the CCR that distance from the permanent mark.

Powder Samples:

For powder samples, a flat cell design is used at SEQUOIA. Typical powder samples are loaded into a 50 x 50 mm² flat square indium-sealed cells as shown in Figure 14. Sample thicknesses of 0.1 mm, 0.5 mm, 1 mm, 2 mm, 4 mm, and 6 mm are available. As a rule of thumb, sample thickness is chosen such that the total scattering probability is approximately 10% or less. To calculate the thickness required, see the section entitled “Experiment Setup.” Typically, the powder is wrapped in a thin Al foil before inserting into the sealed cell. For low-temperature experiments in which the sample temperature is an important consideration or the sample requires an inert environment, the cell will be sealed within a He filled glove box and subsequently leak checked.

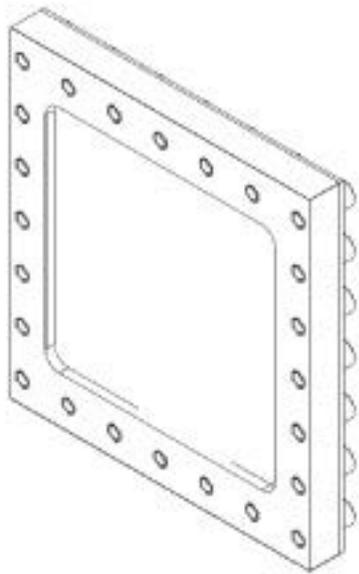


Figure 14 Flat cell schematic (left) and installed on CCR-13 (right) with a boron nitride mask.

Sample equipment lift

A lift is provided to transport most equipment from the mezzanine level to inside the sample room. When in the up position, the expandable gate in the sample area must be in closed position. This lift is for equipment only. No personnel should ride the lift. Before the sweep procedure of the sample vessel the sample equipment lift should be in up position. If the lift is not in the appropriate place to perform the sweep, contact the instrument staff or the Instrument Hall coordinators for assistance.

Orange Crush Cryostat

More details here about this in future revision.

3) GUI Control of the Instrument Components

The instrument components may be controlled via several shortcuts found on the desktop of the control computer.

- 1) The Motors App window
 - a. Slit11
 - b. Positions

- c. Select Chopper
 - d. Attenuators
- 2) Motors App has four sub-windows
 - a. Slit 1
 - b. Positions
 - c. Select Chopper
 - d. Attenuator
- 3) Chopper Control App
- 4) CCR13VRot
- 5) Lakeshore App

The Motors App Window

Positioning of several instrument components including the variable apertures (slit1), the Fermi choppers, and the attenuator blades is controlled by motors. The Motors App window is started from the “Motors” desktop shortcut. Within this window, shown in Figure 15, four sub-windows may be opened by clicking on the appropriate button. The settings in the sub-windows serve to adjust the variable aperture (“Slit 1”), to move the Fermi-chopper translation table or either of the attenuator blades (“Positions”), to choose fixed positions of the Fermi-choppers (“Select Chopper”), or to move either of two beam attenuators fully in or fully out of the beam. **Any movement may be immediately terminated at any time by pressing the “Stop Moves in Progress” button.**

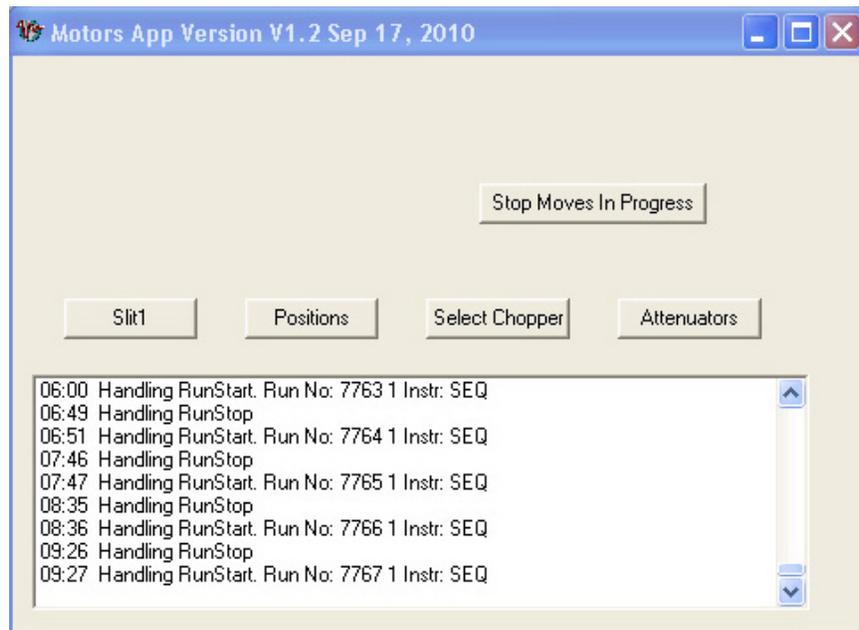


Figure 15 Motors App window

Slit1

The Slit1 window, shown in Figure 16, appears when the Slit1 button is pressed within the Motors App GUI (Figure 15). The slits may be adjusted either using absolute positions or virtual positions. The absolute positions are determined using the information presented in the transmission plot of Figure 10. When new values are entered into any of the four “Target Position” fields, the background color will turn yellow. To initiate movement of the corresponding slit blade the enter key must be pressed, at which time the background will return to white and the value shown in the “Current Position” field will begin to change.

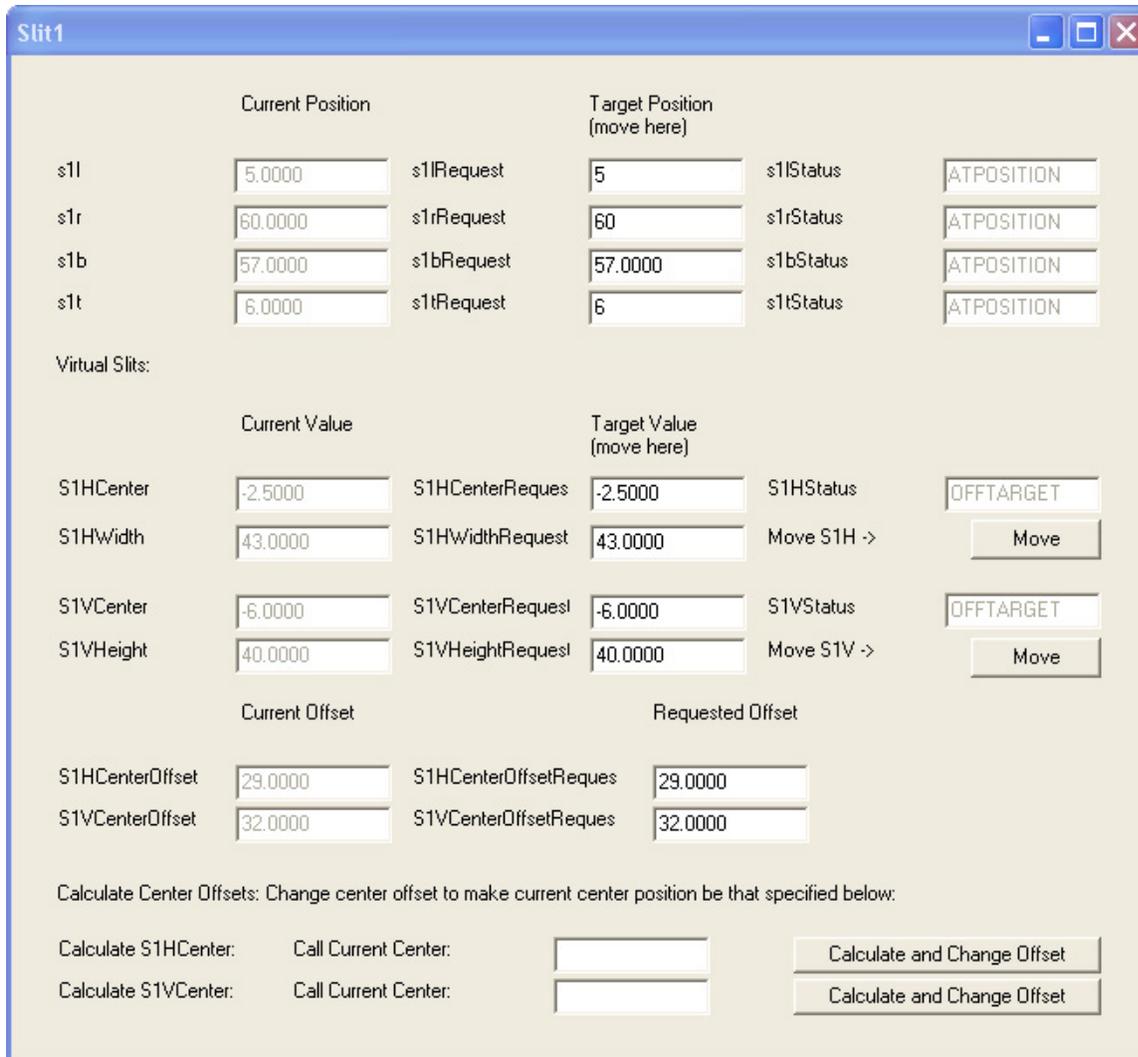


Figure 16 Example of “Slit1” App window.

More intuitive is to use the virtual slits. The horizontal center, width, vertical center, and height of the aperture opening are adjusted by setting “S1HCenterRequest”, “S1HWidthRequest”, “S1VCenterRequest”, and “S1VHeightRequest” values, respectively. The values are set by entering a number into the respective field. While entering the desired value, the background will turn yellow. Upon pressing the enter key, the background changes to blue, but no motion is yet initiated. To do so, the “Move” button must be pressed. The values in the “Target Positions” field above will change concurrently with the virtual slit settings and the “Current Position” and “Current Value” fields will update simultaneously.

Offsets should only have to be changed when the physical position of the slit package is moved. Hence the user will not need to use these remaining controls.

Positions

The position of the Fermi chopper translation table or either of the attenuators may be moved to arbitrary positions within set limits by setting the values in the “Other Positions” window. Though the translation table may be moved while the Fermi choppers are spinning, remember that it should never be the case that both Fermi choppers are simultaneously rotating with a frequency greater than 60 Hz. This window, shown in Figure 17, is opened by pressing the “Positions” button in the Motors App window (Figure 15). When values are being entered into the “Target Position” field for a given motor, the background will change to yellow. When the enter key is pressed, the background returns to white and movement is initiated. The status of the three motors is shown on the right.

Recall that all motions may be stopped by pressing the “Stop Moves in Progress” button in the Motors App window. Note that if these values do not correspond to predetermined values corresponding to, eg. the desired Fermi chopper to be centered on the beam or the attenuator to be fully in or out of the beam, then the instrument is not in a desirable operating state and the outcome will likely not be favorable.

	Current Position	Target Position (move here)		
chtrans	8.5008	chtransRequest: 8.5000	chtransStatus	ATPOSITION
attenuator1	0.0000	attenuator1Reque: 0.0000	attenuator1Status	ATPOSITION
attenuator2	93.1192	attenuator2Reque: 93.1192	attenuator2Status	ATPOSITION

Figure 17 The Other Positions window controls the Fermi chopper translation table and either of the two attenuators.

Select Chopper

Normally, the position of the translation table will take one of three values corresponding to either Fermi chopper 1 or Fermi chopper 2 centered on the beam, or else an open tube may be centered on the beam. The “Select Chopper” button, found on the Motors App window (Figure 15), opens the window displayed in Figure 18, within which the choice may be made by activating the desired radio button. The status of the translation table is displayed below.

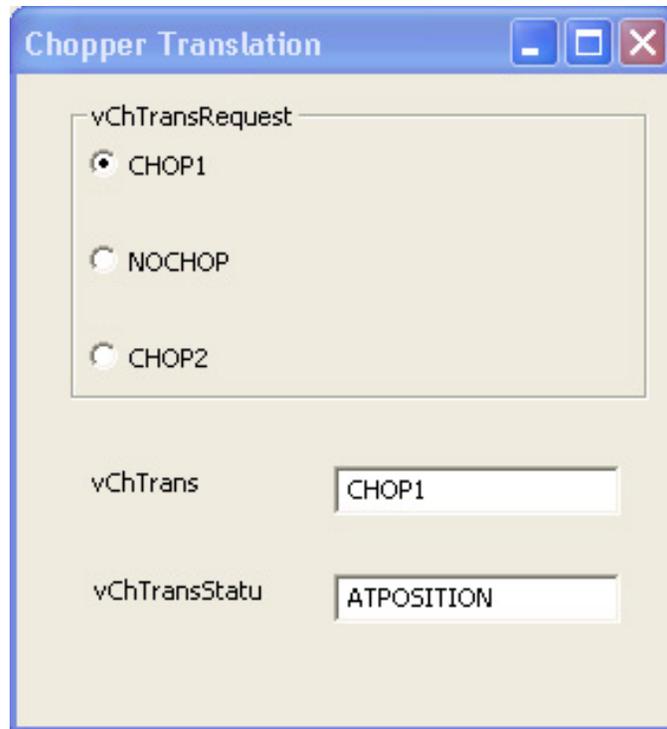


Figure 18 The Chopper Translation window allows the choice of Fermi chopper 1, Fermi chopper 2, or no chopper.

Attenuators

The two available attenuators may be requested to move to their fully in or fully out of beam positions by selecting the appropriate radio buttons in the Attenuators window. This window, shown in Figure 19, is opened by pressing the “Attenuators” button in the Motors App window (Figure 15). While the motors are changing the attenuator positions, the motor status will change to “MOVING.” When the motion is completed, the status will return to “ATPOSITION.” The current position of either blade is displayed below.

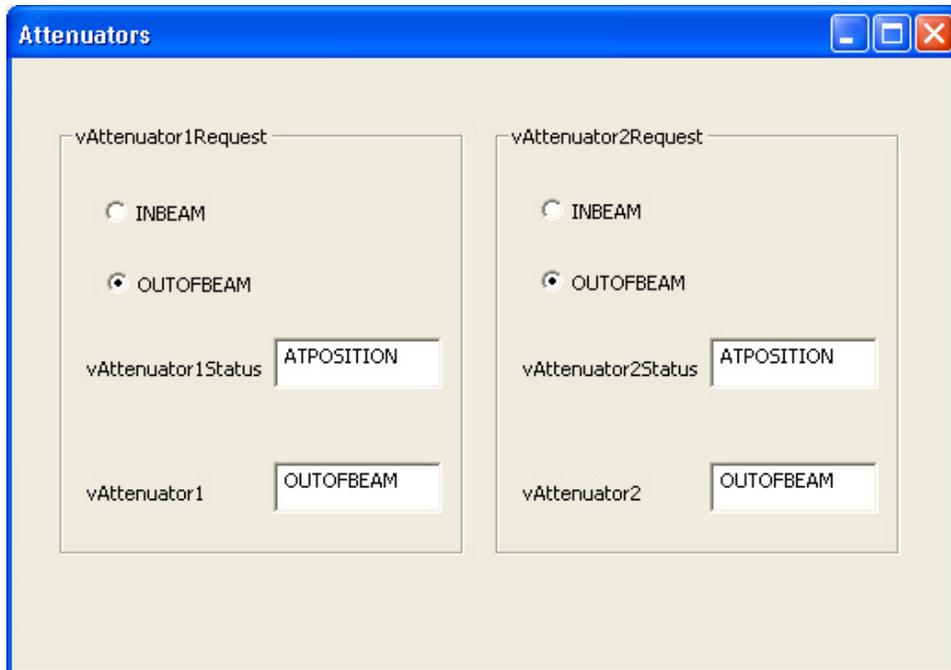


Figure 19 The Attenuator window controls the position of the attenuator blades.

The Chopper Control App

The Fermi chopper control application is available as a shortcut (Shortcut to cc_BL17.exe) on the instrument control computer's desktop. The corresponding window is shown in Figure 20. From this window, one can choose the frequency in Hz, the energy in meV, and the phase of each of the two installed Fermi choppers and background T₀ chopper. Note that when decelerating any of the three choppers, the frequency should be stepped down in single increments (60 Hz for the Fermi Choppers and 30 Hz for the T₀ chopper) else a hardware error may occur. It is not necessary to wait for the chopper status to return to "LOCKED", but only to wait for "ATSPEED." This window also provides feedback as to the actual chopper speed and status. If the Chopper control app shows an error, an Instrument Hall Coordinator will be notified and will attempt to manage the error. If this is not possible, a member of the chopper team of instrument staff will be contacted.

When a new value for the energy is entered, the field background will turn yellow. The enter key must be pressed in order for the DAS to accept the new value. Nominal values for the phase of each of the three choppers are then automatically entered as the Target phase. However, a circumstance may arise in which it may be desirable to adjust the phase of an individual chopper. In this case, the value of the phase may be entered as the target phase for that chopper. Please work with your instrument scientist or local contact to determine the appropriate Fermi chopper, frequency, energy, and possible unique phase settings suitable for the needs of the experiment. Due to excessive demands of the Fermi chopper cooling system, no more than one Fermi chopper may spin at more than 60 Hz simultaneously. However, it is permissible to accelerate one chopper to its desired frequency while the second is decelerating to 60 Hz.

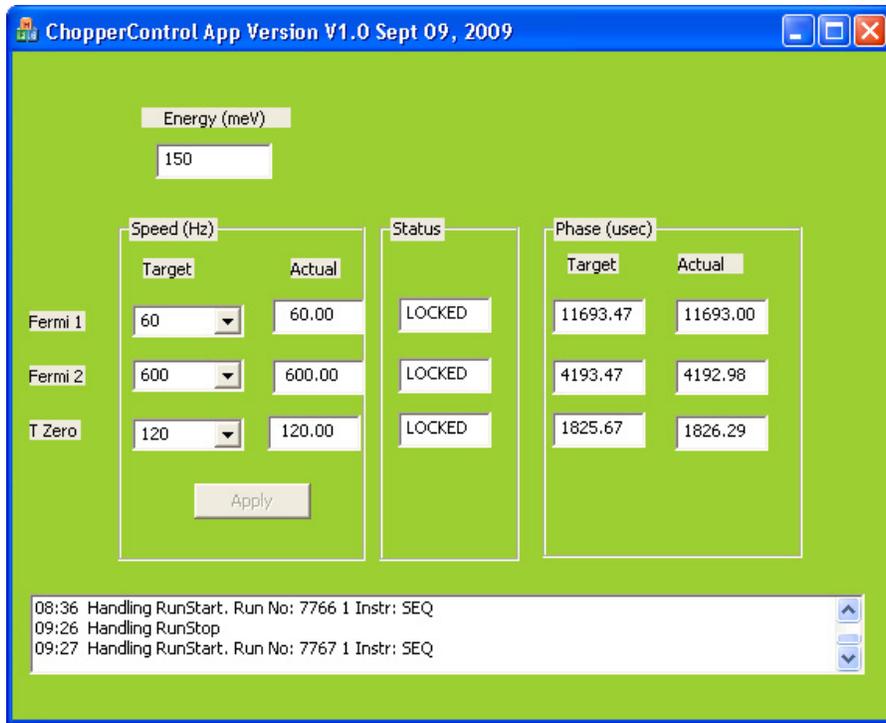


Figure 20 Chopper control App window.

Lakeshore App Window

The Lakeshore App window is initiated by running the shortcut (LakeShoreControl) on the desktop of the instrument control computer. The Lakeshore App Window is shown in Figure 21. This application is used with most of the variable temperature sample environments available at SEQUOIA. One can enter a requested temperature (“SampleTempRequest”) and set a tolerance window (“TolRequest”) around the requested temperature. The current actual sample temperature (“SampleTemp”), the current status of this temperature (“SampleTemp_Status”) and the current setpoint (“CurrentSP”) are also shown in this window. The temperature may be ramped by entering a ramp rate value (“LKSRampRate”), whose units are K/min. A plot of the temperature as a function of measurement time is also shown in the bottom portion of the window, along with a dialog of recent DAS events.

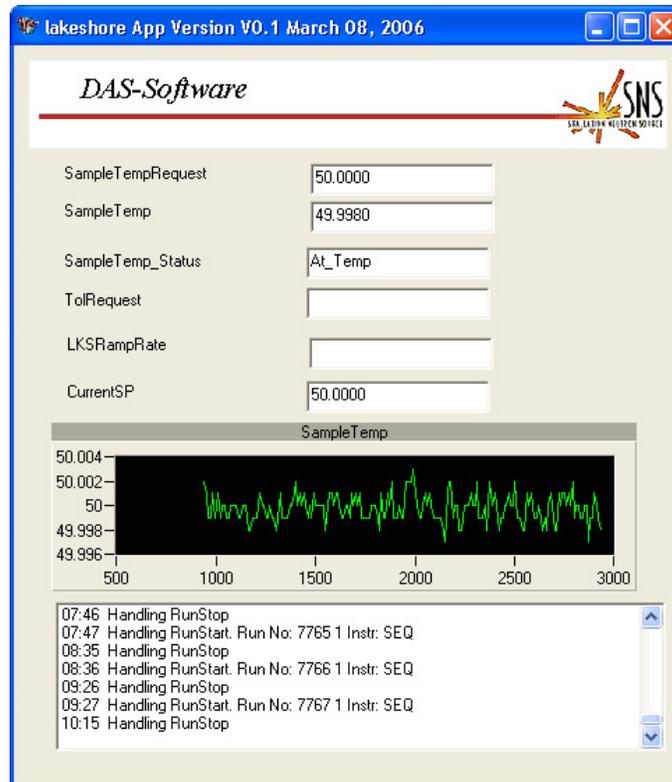


Figure 21 Lakeshore App window.

4) Data Acquisition System

The data acquisition system (DAS) controls the instrument parameters, data acquisition (DAQ), and recording of the acquired data via several satellite computers and a control computer. The control computer interfaces with these for a centralized point instrument operation. Only a small number of operations require direct access to any of the satellite computers. Operation of the instrument is performed from the control computer via a set of GUIs or a Python based scripting interface. Use of the DAS GUIs to adjust instrument parameters and acquire data will be explained followed by instructions on the use of the Python based scripting interface. Each GUI has a shortcut on the desktop of the instrument control computer. Please work with the local contact to implement either method of instrument control.

Viewing instrument status off site

The status of the experiment can be monitored offsite by going to the following link:
<http://neutrons.ornl.gov/sequoia/status/>

Accessing Satellite Computers

Accessing any of the satellite computers in situations other than those mentioned below is restricted to SNS staff.

Instances in which direct use of a satellite computer may be required include the control and viewing of the video images captured by either of the two cameras installed on the instrument, direct interface with sample environment software not yet fully integrated with the control computer, and use of the neutron camera. The software used with the cameras is installed on the remote services computer and the software for the temperature controller is found on the sample environment computer. **Note that only the temperature control application on the sample environment computer should be used since other applications may negatively affect DAS operations.** The appropriate satellite computer is accessed on either of two terminals labeled “KVM” installed in the instrument hutch and may be chosen by double tapping the CTRL key, choosing the desired satellite computer, and pressing enter. Operation of the software will be explained by instrument staff.

Use of DAS computers for any other purpose (web browsing, calculating, email, etc.) may adversely affect the DAS system and is not allowed.

Operation of the Cameras

Two internet explorer shortcuts are found on the desktop of the remote services computer. One will enable control and viewing the main IPPS panel and chopper rack. The second will enable control and viewing inside of the sample room. Double-clicking either shortcut will open an intuitive interface for panning, tilting, and zooming the camera. In the case that credentials are requested, both the username and password are ‘user’.

Operation of the Temperature Control Software

The sample environment computer enables direct interaction with the temperature control software.

Initiating the DAS

The DAS is initiated by running several shortcuts found on the desktop of the control computer.

- 1) NewPyDAS opens four separate windows
 - a. PyDAS: SEQ window
 - b. Dcomclient window
 - c. SEQUOIA Physical Histogram window
 - d. NewPython window
- 2) Motors App has four sub-windows
 - a. Slit 1
 - b. Positions
 - c. Select Chopper
 - d. Attenuator
- 3) Chopper Control App

- 4) CCR13VRot
- 5) Lakeshore App

PyDAS: SEQ

The PyDas “Welcome” window, as shown in Figure 22, is that which is initially opened. By choosing the “Chopper” or “Shell” tab, the display changes to that of Figure 23 or Figure 24, respectively. At the top of all three screens the IPTS number, author IDs, run number, experiment title, run time, run status, total detector counts, total counts in the upstream monitor, and total accumulated proton charge are displayed. At the bottom of each screen, the most current messages from the DAS system, which are additionally recorded in a log file, are displayed.

The chopper screen is useful to display and control the configuration of the T₀ chopper and the two Fermi choppers. Typically, the chopper parameters are controlled using the chopper GUI, as described later.

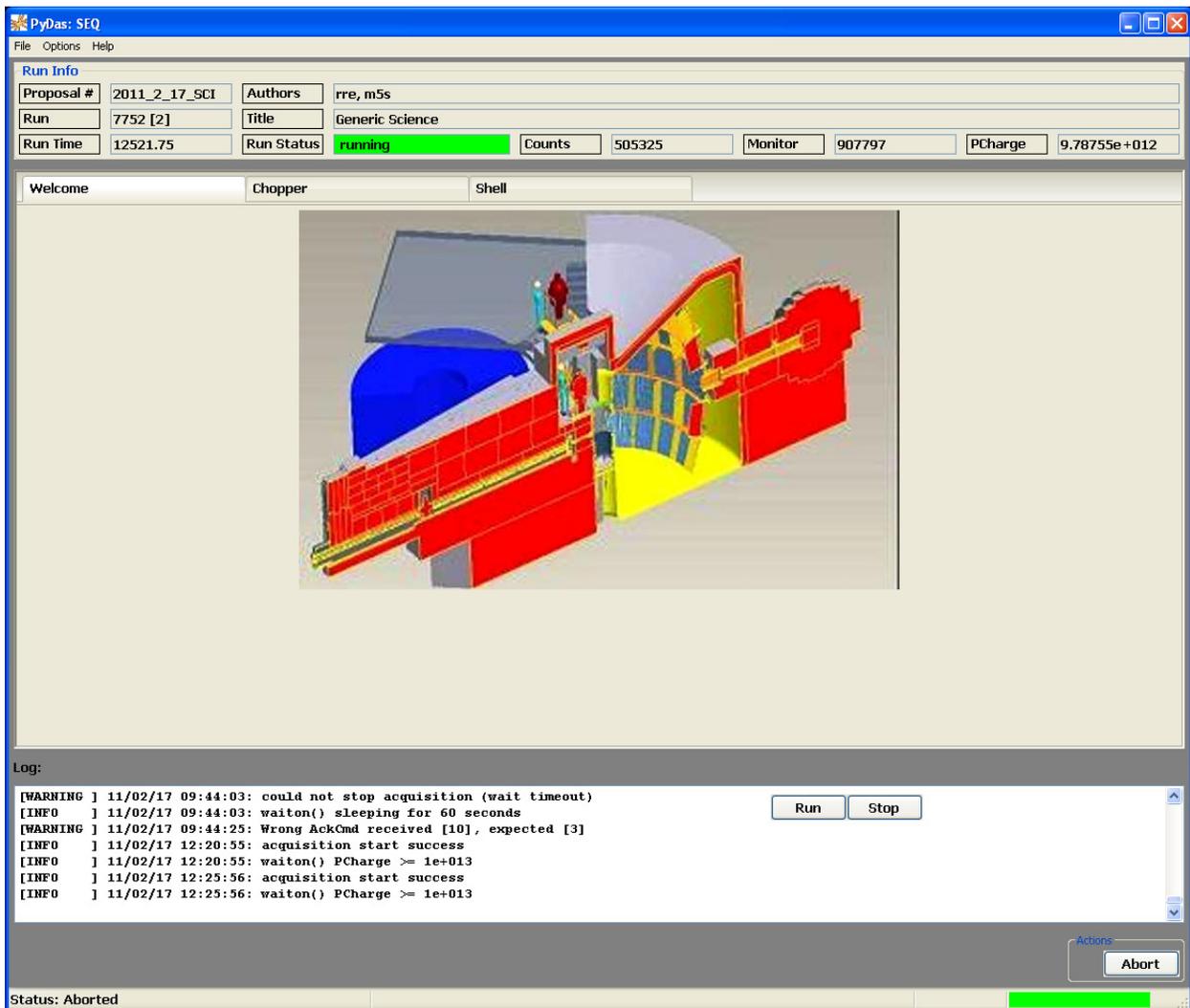


Figure 22 PyDAS "Welcome" screen.

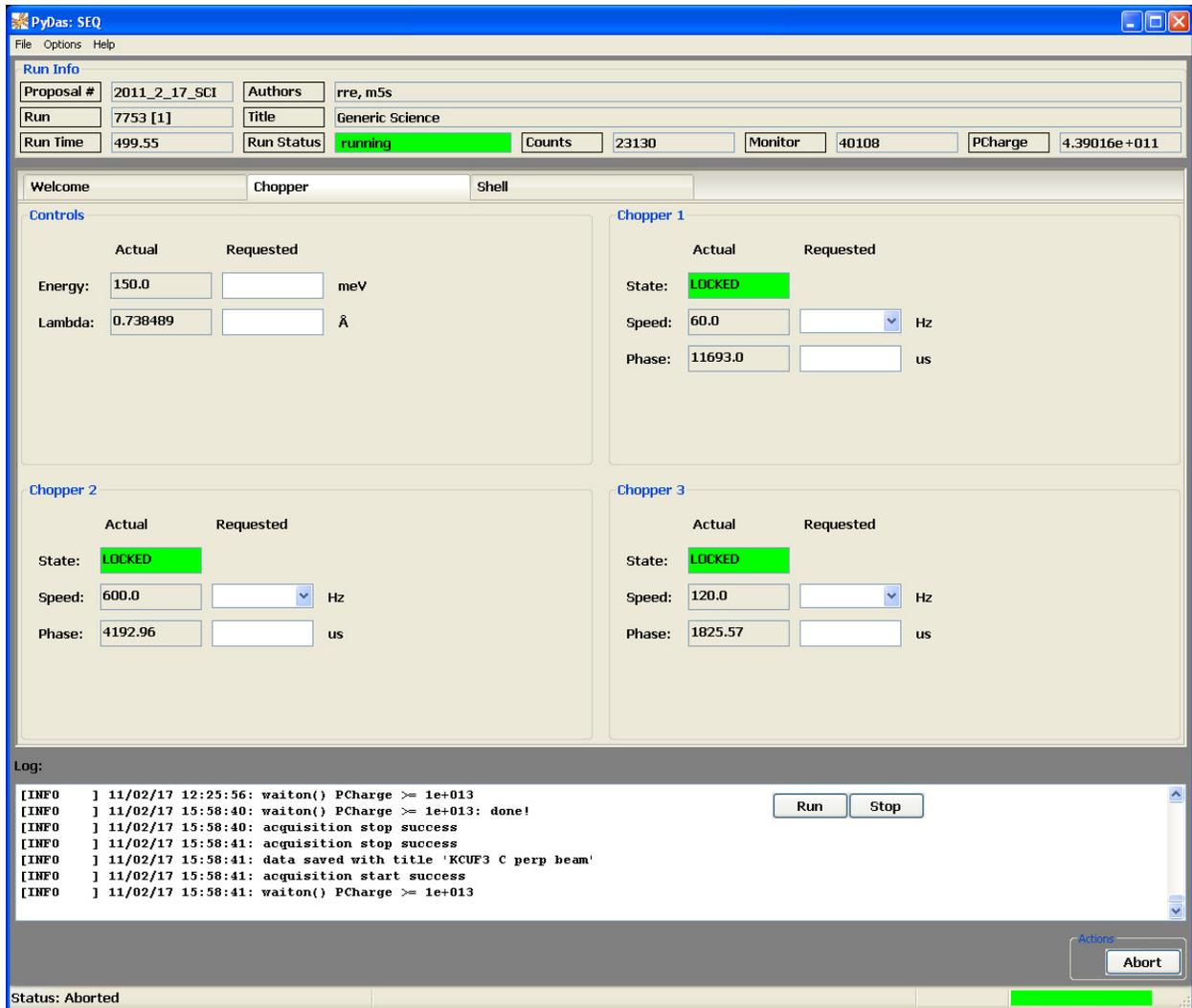


Figure 23 PyDAS "Chopper" Screen.

The most useful window in the PyDAS GUI is the "Shell" window, shown in Figure 24. The shell is the wrapping of an ipython shell and has most of the features of ipythonⁱⁱ, like tab completion, %bookmark and UNIX like file system navigation. It may be used to navigate through the file system, execute Python scripts or individual Python commands, etc. Details on Using the PyDAS "Shell" window are presented below in Chapter 5: Scripting Control of the Instrument.

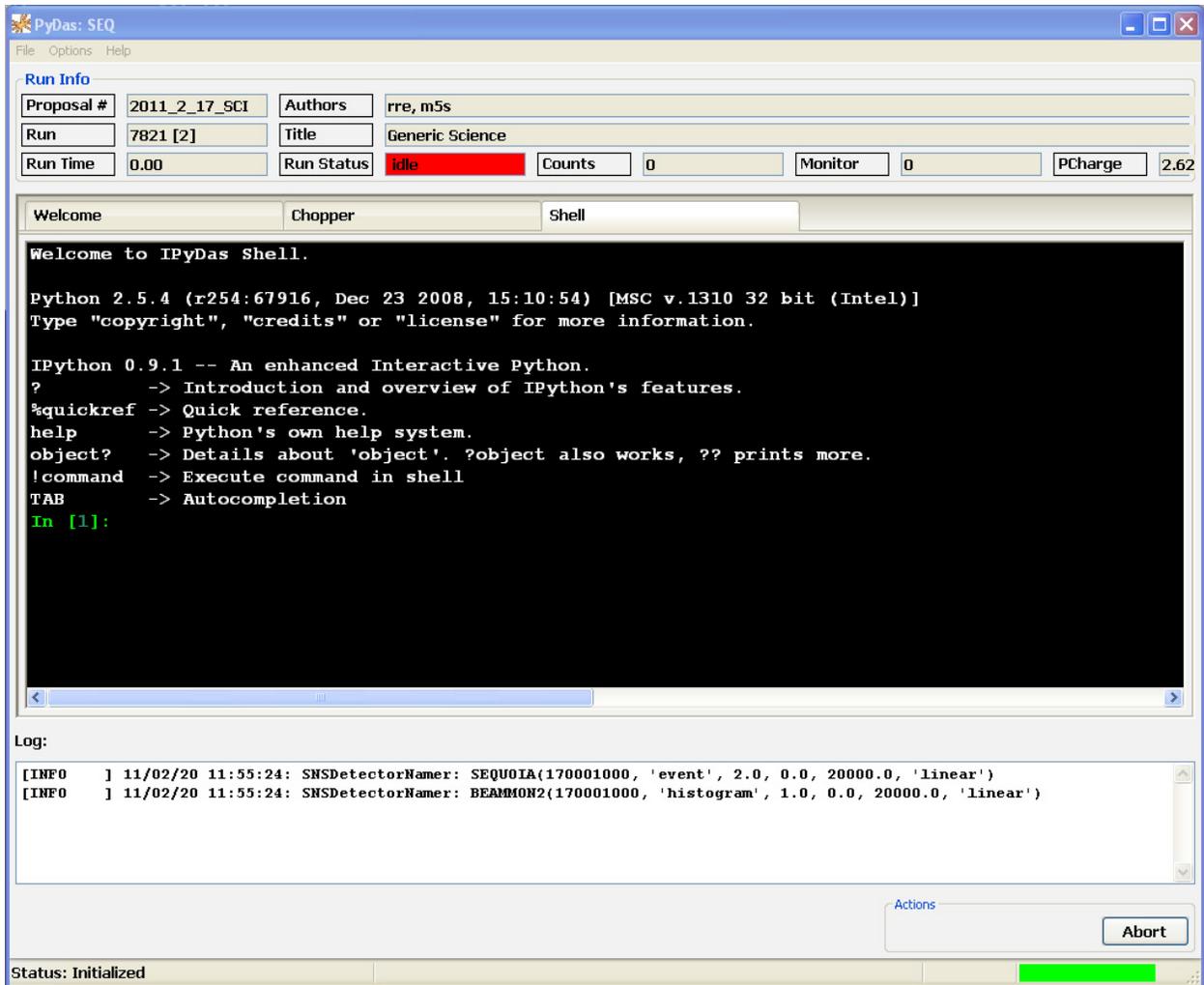


Figure 24 PyDAS "Shell" screen.

The dcomclient window

The dcomclient window (Figure 25) is used for starting, stopping, saving, and pausing measurements (buttons on upper-right side of window) manually. Additional buttons may be present depending on the state of the DAS, such as Cancel WaitOn which appears when the DAS is waiting for some condition to be satisfied. The DAQ window may be opened from the DCOMClient shortcut on the instrument computer desktop.

In the top three rows of the DAQ window, information regarding the current proposal, title, sample number and name, run number, and experiment number are displayed. If the proposal number is not correct please contact the instrument staff to change the proposal number. **If the proposal number is not correct, you will not be able to see your data.** The experiment number may be changed, for instance if the sample or some other instrumental variable is changed, and the data will be saved in a separate subdirectory. The fourth row shows the total counts in all detectors, the time elapsed in the current run, the current count rate, and the current state of the run.

The current time-integrated counts for either monitor are displayed in the plot below. The drop-down menu on the right enables the choice of the displayed monitor, while the check box indicates if the y-axis is linear or logarithmic. Regions of the plot may be zoomed in on by dragging a marquee window over the desired region. The restore button on the right will reset the axes based on the settings in the three Display Binning fields. The total beam monitor counts and accumulated proton charge are presented below the plot.

Parameters governing the binning of the Nexus Metadata may be entered in the fields within the TOF binning box. The minimum TOF, maximum TOF, and bin size may be specified for the main detector bank or either of the two monitors, the choice of which is governed by the drop-down menu to the right. To affect any changes, the Accept button must be pressed. **For the main SEQUOIA detectors, the bin size must be at least 2 for the data to be properly translated.**

Finally, in the lowest portion of the dcomclient window, feedback regarding the progress of which runs were saved, the motion of motors, or other DAS activities is shown. These messages are stored in a log file in the DAS.

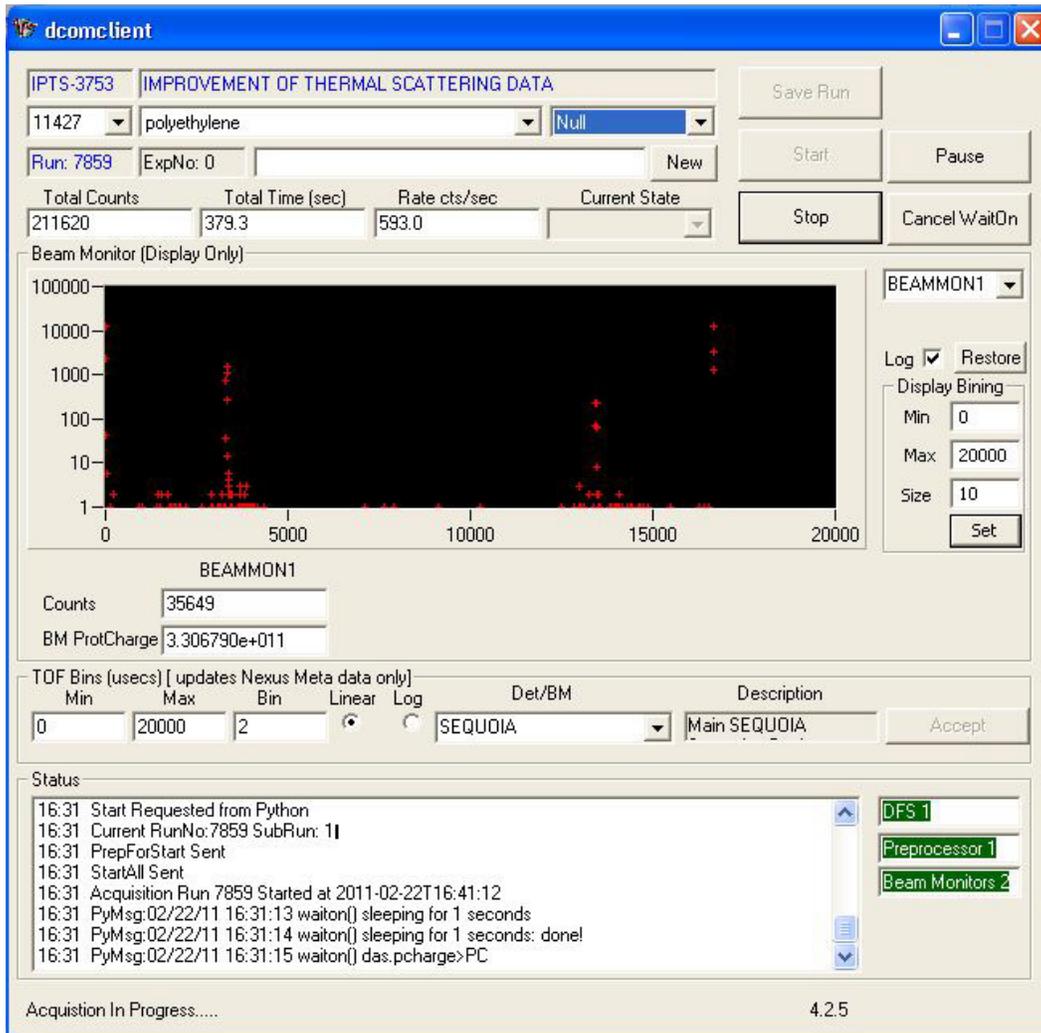


Figure 25 The dcomclient window.

Performing a Simple Measurement Run

Very simply, one can manually perform a measurement via the dcomclient GUI by pressing “Start”, waiting for a given time, accumulated proton charge or monitor counts, and then pressing “Stop”. A dialog box will appear for saving the run. Two fields should be filled out; title and comments. After entering an appropriate title, the comments should include the incident energy, T_0 chopper frequency, Fermi chopper number and frequency, temperature, and any other relevant instrument parameters unique to this run.

The SEQUOIA Physical Histogram window

The SEQUOIA Physical Histogram window also appears whenever the DCOMClient is opened. This window, shown in Figure 26, provides immediate visual feedback regarding the progress of the measurement. The two-dimensional contour plot shows the accumulated scattering intensity measured by the SEQUOIA detector array integrated over all time-of-flight. The default view is directly long the z-axis as if viewed as from the sample position. The beamstop is plotted at approximately (195, 318) in the (x, y) coordinates of the figure. These data may be used to determine detector packs which are not operating properly, to identify the presence of Bragg peaks, etc.

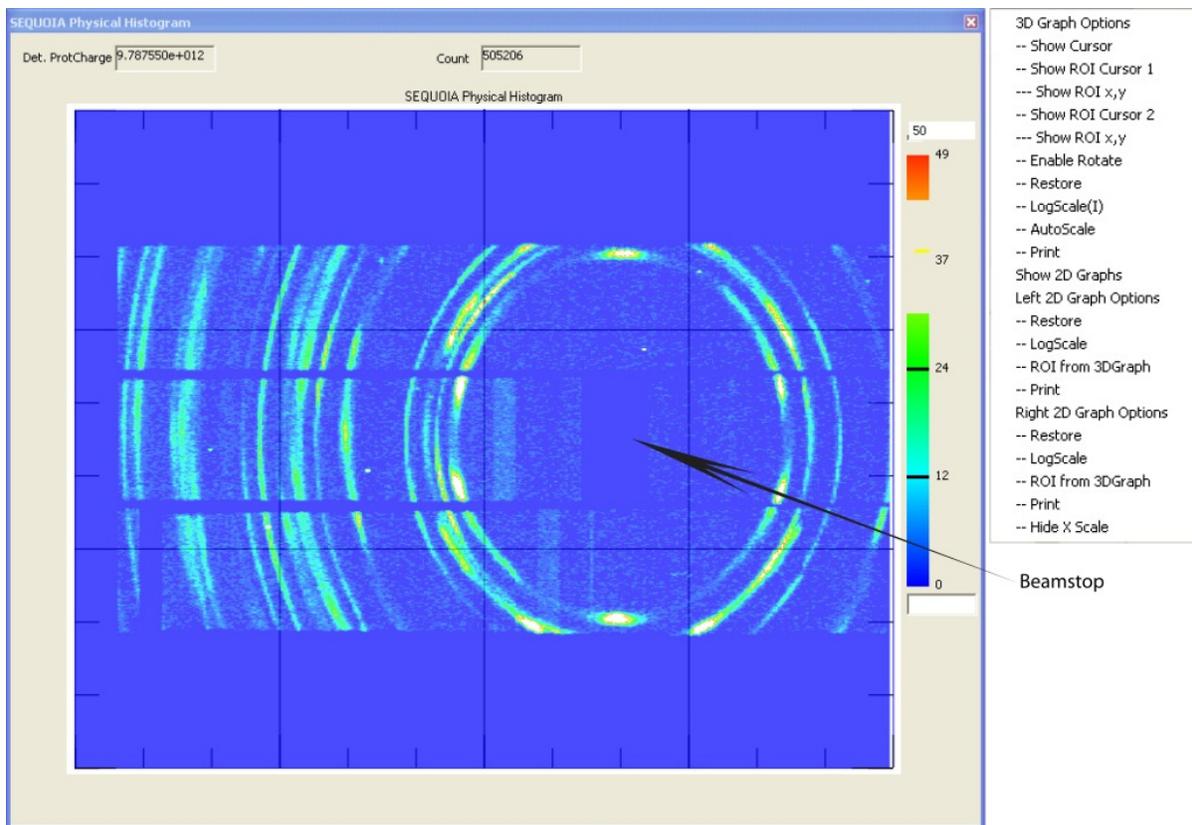


Figure 26 The SEQUOIA Physical Histogram window.

By right-clicking in the upper right portion of the window, a menu appears which presents several options for affecting the information displayed. By choosing “Show Cursor” and “Show 2D Graphs”, the Physical Histogram window will show a crosshair and two additional graphs, as shown in Figure 27. This

will place a cursor on the detector array image plot, and show the corresponding cross-sections in the two one-dimensional plots. The bottom two plots, X cross-section and Y cross-section, show the intensity across the horizontal or vertical dimension of the detector array. By left-clicking and dragging the cross hairs, the cursor will move and the two lower plots will update accordingly. The option to show either of the plots on a logarithmic scale may additionally be enabled.

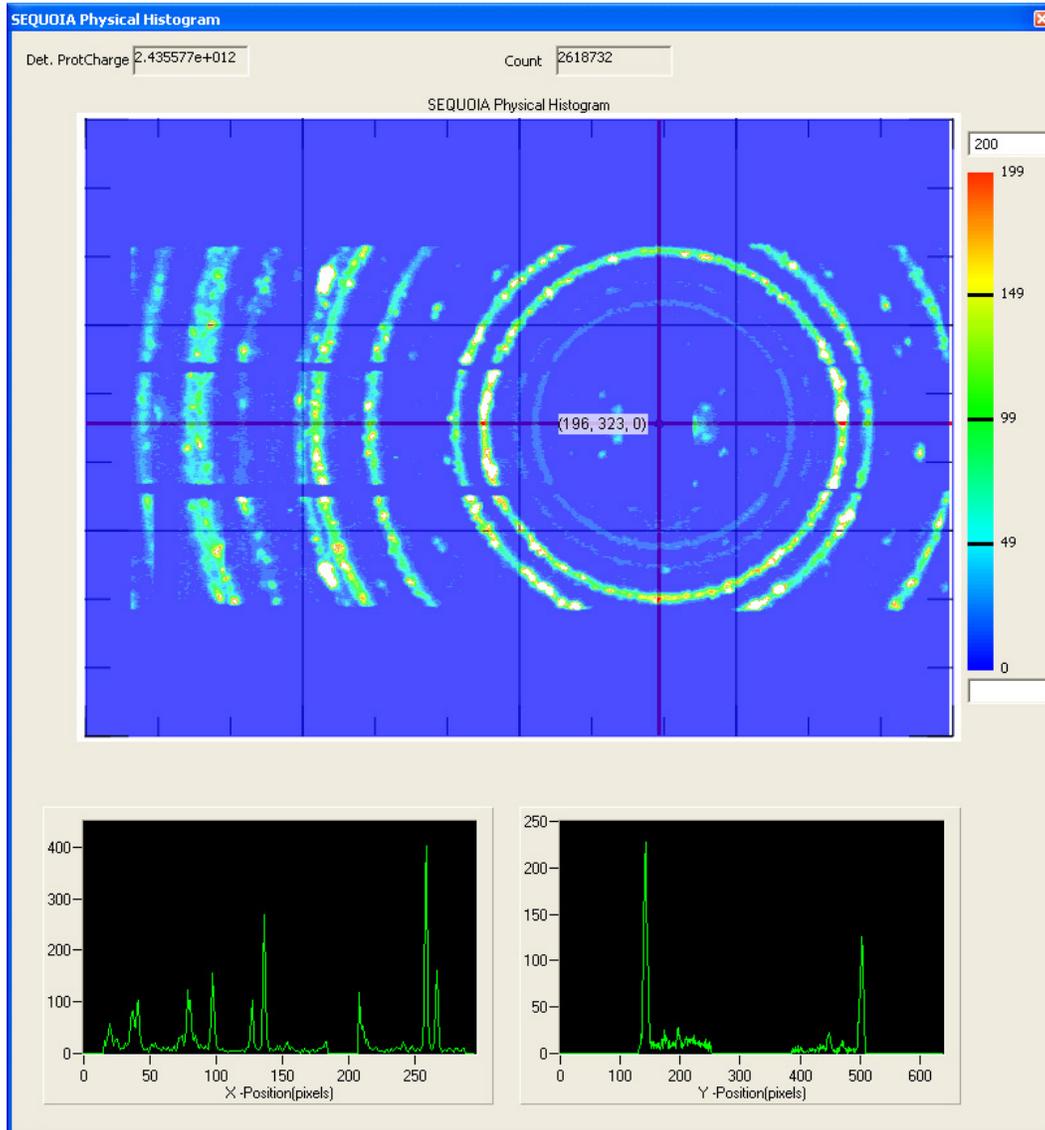


Figure 27 The physical Histogram window showing a cursor and intensities along the horizontal and vertical directions.

Two regions of interest (ROIs) can be defined using by selecting either “Show ROI Cursor 1” or “Show ROI Cursor 2”. Note that the plotted region of interest in the X and Y-cross section does not update every time a new region is chosen. To have the region of interest cross sections update when they are changed, one must start a new acquisition. The resultant window is shown in Figure 28. The regions of interest are particularly useful for aligning single crystals and comparing signal to noise. For instance, the integrated intensity within a region of interest may be plotted as a single crystal is rotated, thus the

optimal crystal alignment may be found. In another instance, the second ROI may be placed in a region where only background signal is observed while the first remains in a region where a strong signal is observed. Thus as instrumental parameters are adjusted; the signal-to-noise ratio may be determined and optimized. Further details of these procedures follows later in this document.

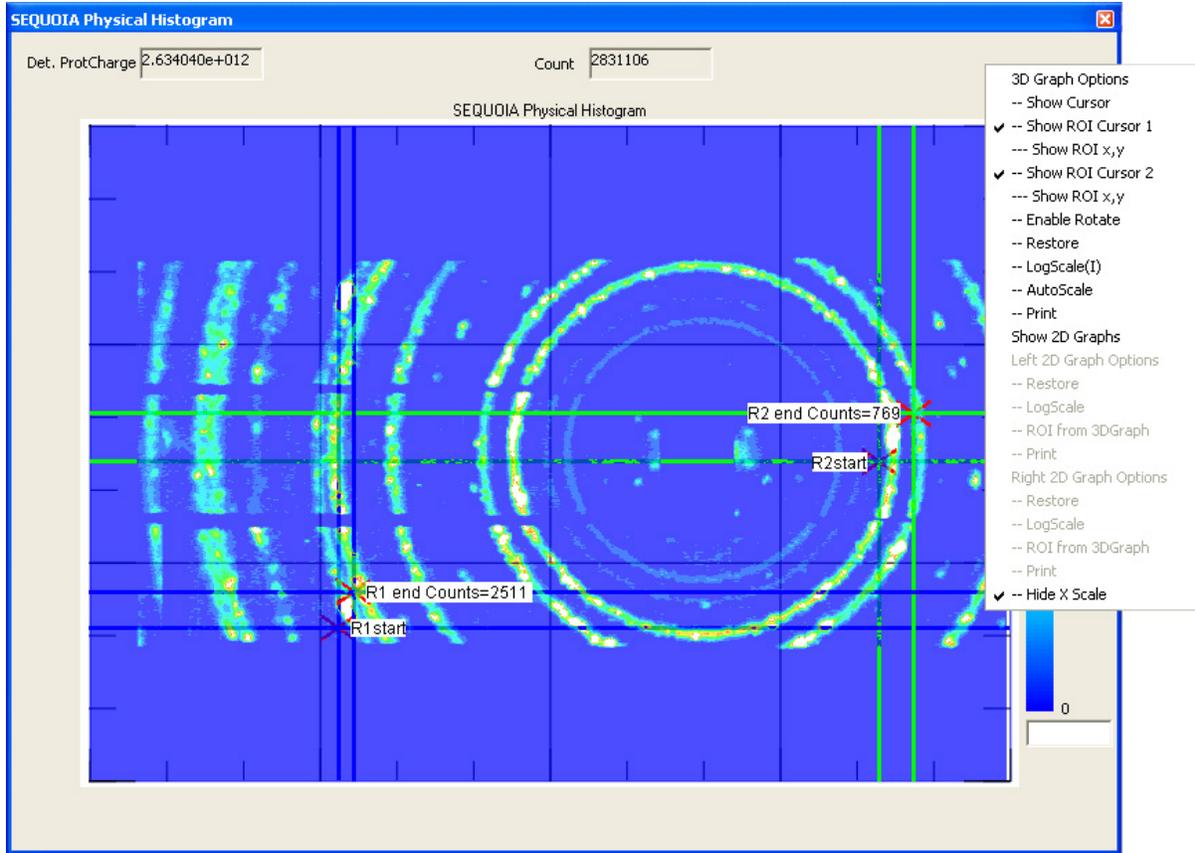


Figure 28 The Physical Histogram window showing two regions of interest centered around two different Bragg peaks.

The Sum Over All Space window

The Sum Over All Space window also appears when the DCOMClient shortcut is chosen from the desktop. This window is shown in Figure 29. The total integrated detector counts or counts within the defined ROI (see features of the Physical Histogram window) as a function of time-of-flight may be plotted. The total integrated detector counts versus d-spacing may also be plotted by activating the corresponding radio button. The “Restore” button resets the plotting limits and the default options of the window. These data may be saved to a text file using the “Save” button.

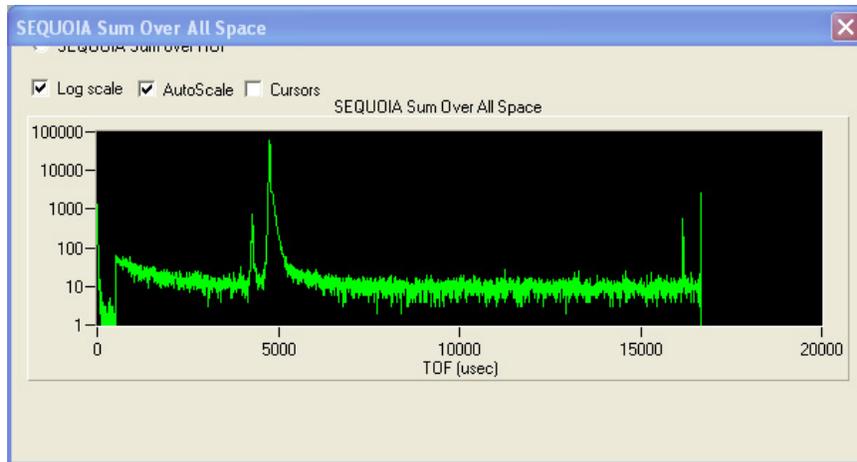


Figure 29 The Sum Over All Space window.

5) Scripting Control of the Instrument

The scripting interface is in python. So for variable manipulation, looping and other standard language constructions please refer to a standard Python textⁱⁱⁱ.

Scripts are placed in the following directory:

C:\Python25\Scripts\src\IPTS-xxxx

and can be edited with your favorite python or text editor.

To get a listing of devices (variable names which correspond to instrument settings) type “print get_device()” at the Python command prompt.

To execute scripts run “NewPyDas” from the shortcut on the main screen, which results in opening of two windows “Shortcut to dasstart.bat” (Figure 30) and “IPyDas” (Figure 24). Single lines can be tested from the python interface illustrated in Figure 31.

```

c:\ Shortcut to dasstart.bat
TARGET', 5: 'POSLIM', 6: 'NEGLIM', 7: 'PROBSTOP', 8: 'ABORTED', 9: 'OVERRIDDEN',
10: 'UETOED', 11: 'COMERR', 12: 'DRUERR', 13: 'REQERR', 14: 'MOVEERR'}
imported pypassing
executed c:/python23/Lib/ancillary_91031passing.py

>>> Chopper1State.getvalue()
'Locked'
>>> SpeedRequest1.setvalue(0)
new value assigned to SpeedRequest1: 0
>>> Chopper1State.getvalue()
'Seeking'
>>> vChTransStatus.getvalue()
'ATPOSITION'
>>> vChTrans.getvalue()
'NOCHOP'
>>> -

```

Figure 30 DCOMClient's command window

To run a script, change the directory in the “IPyDas” window to the directory where the desired script file is stored (e.g. C:\Python25\Scripts\src) and run

>>> run -i script_name.py

Please work with the instrument scientist to implement scripting of the DAS specific to your experiment.

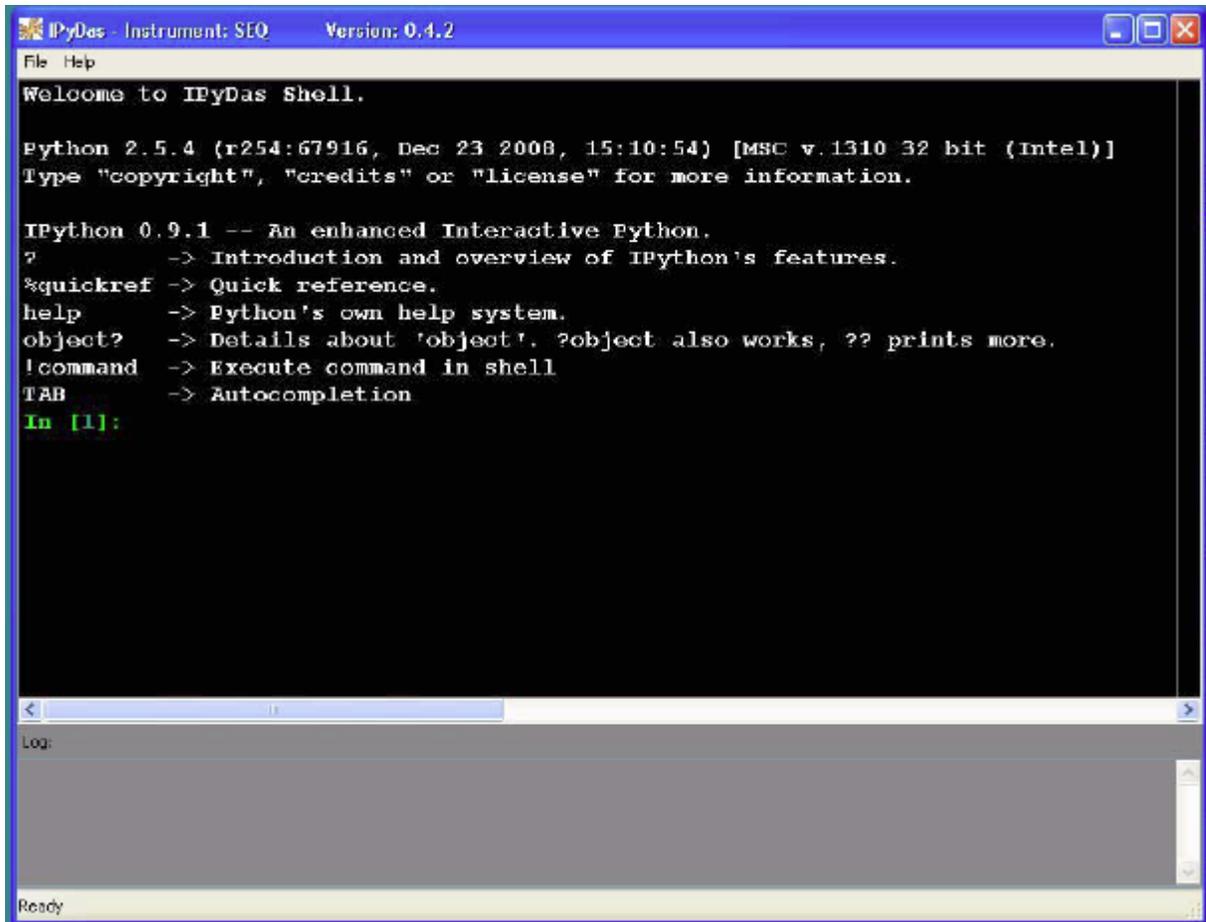


Figure 31 Python testing window

Scanning a motor

Often one wants to scan a motor and look at the integrated counts either over the entire detector array or over a region of interest. The command to do this is `scan` and the syntax is:

```
scan('<motor>,<list of values>,<what to count against>,<how long to count>,<plot=><what to plot>')
```

For example to scan the rotation angle of CCR13 and plot a region of interest:

```
Scan('CCR13vRot', arange(10.,20.,0.1),PCHARGE,1e10,plot='roi')
```

System commands

`das.waiton(string)`

waits until the condition given in *string* is true

Examples of *string*:

```
'Chopper1State.getvalue()=='\Locked\''
```

```
'das.runtime>10.0'
```

```
'das.pcharge>1e9'
```

```
'das.counts>100'
```

`das.start()`

starts the run

`das.stop()`

stops the run

`das.save(string,string,string)`

saves the data

The first *string* is a title, the second *string* is some notes, the third *string* is more notes

Fermi chopper commands

EnergyRequest.setvalue(*double*)

sets the phase of all choppers based on a given incident energy.

double = incident energy in meV

SpeedRequest1.setvalue(*double*)

sets the frequency of Fermi Chopper 1

double = an increment of 60 Hz

Chopper1State.getvalue()

reads the state of Fermi chopper1

possible values

0: 'Stopped'

1: 'Seeking'

2: 'Locked'

SpeedRequest2.setvalue(*double*)

sets the frequency of chopper 2

double = an increment of 60 Hz

Chopper2State.getvalue()

Reads the state of Fermi chopper1

Possible values

0: 'Stopped'

1: 'Seeking'

2: 'Locked'

Fermi chopper translation table

chtransStatus.getvalue()

vChTrans.getvalue()

get position of the chopper translation table

possible values

0: 'UNDEFINED'

1: 'CHOP1'

2: 'NOCHOP'

3: 'CHOP2'

vChTransRequest.setvalue()

set position of the chopper translation table to a predefined value

possible values

1: 'CHOP1'

2: 'NOCHOP'

3: 'CHOP2'

vChTransStatus.getvalue()

Slits

s1l
s1lRequest.setValue(*double*)
instance created for s1lStatus.getValue()
s1r
s1rRequest.setValue(*double*)
s1rStatus.getValue()
s1t
s1tRequest.setValue(*double*)
s1tStatus.getValue()
s1b
s1bRequest.setValue(*double*)
s1bStatus.getValue()

Sample script

```

#SNSpyScript
#<
#Simple Scan
#>

import time

def definite_stop():
    das.stop()
    time.sleep(10)
    if das.status!='idle':
        time.sleep(60)
        das.stop()
# set up experiment
das.beginscript()
das.start()
time.sleep(10)
das.waiton('das.pcharge>3.6e12')
definite_stop()
das.save('Vanadium rod, T=base', 'white beam T0@30 phased to 100 meV', '')

vChTransRequest.setvalue(1)
time.sleep(5.0)
das.waiton('vChTransStatus.getvalue()=='ATPOSITION')

EnergyRequest.setvalue(500.0)
time.sleep(10.0)
SpeedRequest1.setvalue(600.0)
time.sleep(10.0)
das.waiton('ChopperStatus1.getvalue()=='LOCKED')
time.sleep(10.0)
SpeedRequest3.setvalue(120.0)
time.sleep(10.0)
das.waiton('ChopperStatus3.getvalue()=='LOCKED')

for idx in range(2):
    das.start()
    time.sleep(10)
    das.waiton('das.pcharge>3.6e12')
    definite_stop()
    das.save('Vanadium rod', 'Ei=500 F1@600 T0@120 T=base', '')

EnergyRequest.setvalue(100.0)
time.sleep(10.0)
SpeedRequest1.setvalue(240.0)
time.sleep(10.0)

```

```
das.waiton('ChopperStatus1.getvalue()==\'LOCKED\')
time.sleep(10.0)
SpeedRequest3.setvalue(90.0)
time.sleep(10.0)
das.waiton('ChopperStatus3.getvalue()==\'LOCKED\')

for idx in range(2):
    das.start()
    time.sleep(10)
    das.waiton('das.pcharge>3.6e12')
    definite_stop()
    das.save('Vanadium rod','Ei=100 F1@240 T0@90 T=base,')

das.endscript()
```

6) Experiment setup.

Designing your sample

The success or failure of a neutron scattering experiment is largely determined by how one designs their sample. For the dimensions perpendicular to the beam you want your sample to fill the beam as much as possible. For the other two dimensions there are two philosophies depending on the scientific community. 1) The Rule of Thumb and 2) you want your sample to be no more than a 10% scatterer. The Rule of Thumb is that your sample should be about the size of your thumb. This applies when you are looking at relatively weak scattering (usually magnetic) and multiple scattering is not a concern. The 10% scattering idea applies to strong scatterers ie anything with H in it. The idea here is that if you sample is a 10% scatterer then 1% of your observed signal is double scattering events. For example users that are interested in water usually want a thickness of 0.1 mm to avoid multiple scattering. There are several intermediate cases that one can consider. In all cases one should consider the potential amount of multiple scatter when planning an experiment. An example calculation will be given shortly. Nevertheless here are a few examples of systems where careful thought is required.

1) Weak diffuse magnetic scattering.

Here one usually wants to maximize the sample size to make counting times reasonable. However one does need to consider multiple scattering when examining background features.

2) Metal-organics for magnetism

Here one should recognize that the organic frame work will be the largest scatter of neutrons in the system. One can reduce this scattering by an order of magnitude by deuterating the sample. However the magnetic framework may still be only a fraction of the sample so one may need a much larger sample to get enough spins to see a signal.

3) Metal-organics for molecular vibrations

In general the magnetism is much weaker than the lattice vibrations and can be ignored. But in the case of rare earth magnetic ions this may not be the case. One should remember to consider the magnetic excitations as well.

Example: Designing a C₆₀ powder sample that is less than a 10% scatterer

The density of C₆₀ is $\rho = 1.65 \text{ gm/cm}^3$ it is all Carbon so the number density is

$$\rho_N = \rho/12 \text{ (gm/Mol)} * 6.02 \times 10^{23} \text{ (atoms/Mol)} = 0.828 \times 10^{23} \text{ atoms/cm}^3$$

The transmission through a sample that is l with a total scattering cross section of σ thick is

$$T = e^{-\sigma \rho_N l}$$

Therefore the total scattering is

$$1 - T = 1 - e^{-\sigma \rho_N l}$$

$$0.1 = 1 - e^{-\sigma \rho_N l}$$

$$0.9 = e^{-\sigma \rho_N l}$$

$$l = -\ln(0.9) / \sigma_p = 0.105 / 8.28 \times 10^{22} (\text{atoms/cm}^3) / 5.551 \times 10^{-24} (\text{cm}^2) = 0.228 \text{ cm}$$

therefore, one would choose a 2 mm thick sample.

Vanadium Normalization

We use two different types of V measurements on SEQUOIA 1) A white beam measurement to determine the relative efficiency of each pixel and 2) Monochromatic V to determine the absolute flux of the incident beam for the purpose of measuring the scattering intensity in absolute units. For both measurements we use flat plate V samples.

White Beam V

The white beam measurements are performed each time the detector system is turned on. So the user should not have to do a V measurement themselves and can obtain the current V run from their local contact. However if the user wants to review the procedure or use some of their beam time for their own white beam measurement the standard procedure is outlined here.

For the white beam V measurements the following instrument configuration should be used:

- T₀ chopper at 150 Hz
- Chopper Translation at "NOCHOP" on control computer
- Incident energy set to 110 meV
- 1 attenuator in the beam
- Slits wide open (50 mm x 50 mm)

A 2 hour acquisition is sufficient for these purposes With the T₀ chopper spinning at 150 Hz there is more than one burst of neutrons per frame that occurs during a 60Hz frame. Guide effects on the normalization are minimized by only using the highest energy of these pulses.

Monochromatic V

Absolute units can be obtained in several ways. Using a phonon from your sample is the most precise and such a procedure is documented in^{iv}. Using V is the most generally applicable as it does not rely on one knowing the phonon modes of the sample.

The general idea for the V is to make sure one is fully illuminating a known mass of V. Then a flat beam profile will be assumed across the sample. Therefore the V must be smaller than the beam. We use a 3cm x 3cm x 2.12mm plate which has a mass of ~11.5 g. For this measurement use the identical chopper configuration as used in the measurement, but make the slits wide open. Since SEQUOIA has a neutron guide, the assumption of a flat beam profile is coarse approximation of the true profile for E_i < 150 meV. Either the neutron camera can be used to measure the profile or McStas simulations can be used to determine the profile.

Crystal Alignment

Crystal alignment is accomplished using either white beam measurements or by continuously rotating the sample to determine the angle of rotation where the Bragg condition for known peaks is satisfied. As samples are commonly sized to maximize inelastic scattering, the Bragg peaks can be quite

intense and may saturate the detectors. Detectors that are just over saturation are usually noticed during a monochromatic angular scan over a Bragg peak. Specifically the Bragg peak will be flat topped rather than peaked if the tube is saturating. If a Bragg peak has pushed a detector far into the saturation regime, pixels up and down the tube will be indicating counts, as described in the Detectors section. This is readily observed in the Physical Histogram window of Dcom client. If the detectors are saturating, use one or both of the attenuators to reduce the signal on the detectors, and retry your measurement.

Choosing a single E_i

SEQUOIA is usually operated so a single narrow bandwidth of neutrons is present on the sample and the chopper settings are discussed in section “Fermi Choppers.”

Choosing multiple E_i s (Repetition Rate Multiplication)

SEQUOIA can be operated in a multi incident energy mode, commonly known as repetition rate multiplication^v. This is accomplished by careful choice of the T_0 and Fermi chopper speeds and phases. Ask your local contact for details on which configurations are right for your experiment.

Eis	FC	FC speed	FC phase	T0 speed	T0 phase
120,20	1	300	Phase for 120	180	Phase for 120
2000,48	1	600	Phase for 2000	180	Phase for 2000
1000,42.8	1	600	Phase for 1000	180	Phase for 1000
900,41.8	1	600	Phase for 900	180	Phase for 900
800,40.8	1	600	Phase for 800	180	Phase for 800
700,39.6	1	600	Phase for 700	180	Phase for 700
600,38.0	1	600	Phase for 600	180	Phase for 600
500,36.3	1	600	Phase for 500	180	Phase for 500
400,34.0	1	600	Phase for 400	180	Phase for 400
300,31.7	1	600	Phase for 300	180	Phase for 300

Table 8 Tested multiple E_i settings

7) Data Access

To access and perform reduction of SEQUOIA data, one needs access to both the Neutron Scattering Portal and the SEQUOIA analysis machines (SEQUOIA and SEQUOIA 2). Your data will be available via

the Neutron Scattering Portal, the SEQUOIA analysis machines, while on site, and the analysis cluster (analysis.sns.gov) for offsite access. The path to your data is /SNS/SEQ/<iptsnumber>/data and is organized by facility, instrument and your proposal number (IPTS number). We outline here the steps which you should proceed through in order to access your data. More information is available at <http://neutrons.ornl.gov/portal/> and the respective FAQ page for Portal users <https://neutrons.ornl.gov/help/FAQ/user/>.

Data Format

The data from the experiments is stored in the event Nexus format. The details of this format can be found on [the NeXus website](#). The file format is an hdf5 format that can be browsed using either the neutron portal or any hdf5 reader.

8) Data Reduction

Data reduction

Data reduction is performed via Mantid. A full description of Mantid is beyond the scope of this document. Details and help can be accessed at http://www.mantidproject.org/Main_Page

After a run is saved, at the end of the translation process, a reduction script is automatically started. The script is called `reduce_SEQ.py` and can be found in /SNS/SEQ/shared/autoreduce directory. Users cannot modify this file, but they can read this script and use it as a template for more complicated reduction processes. The outputs of the autoreduction process are saved in the /SNS/SEQ/IPTS-YYYY/shared/autoreduce folder. The output consists of the following files:

- `van.nx5` is the processed vanadium file used in normalization
- `experiment_summary.csv` is a comma separated values file (you can read it with Excel or OpenOffice) containing several parameters for each run, including the rotation angle, sample temperature, and calculated incident energy
- for every run (XXXXX), if not white beam, there should be two saved files `SEQ_XXXXX_autoreduced.nxs` (an intermediately processed Mantid workspace), and `SEQ_XXXXX_autoreduced.nxspe`. The `nxspe` file can be read with DAVE Mslice and/or Horace for further visualization and analysis.

Users do not have permissions to delete or write files in the /SNS/SEQ/IPTS-YYYY/shared/autoreduce folder.

The autoreduction consists in the following steps:

1. White beam vanadium reduction

- 1.1. The file is loaded into a workspace, integrated in a certain wavelength range (usually 0.3 to 1.2 \AA^{-1}) and divided by the range
- 1.2. The workspace is normalized by the proton charge.
- 1.3. A hard mask is applied, usually banks that are off, and the top and bottom 8 pixels in each tube.
- 1.4. A diagnostic is run on the remaining pixels, using the default parameters in MedianDetectorTest (see <http://www.mantidproject.org/MedianDetectorTest>)
- 1.5. The output is masked, then saved as van.nx5. For the subsequent times the autoreduce script is run, it will just load this file. If you need to re-reduce a vanadium file, ask the instrument team to remove the van.nx5 file from your autoreduce folder.

2. Data reduction

- 2.1. Incident energy and time offset are calculated from the monitors. If this step fails, the script stops, and there is no further output. This behavior is expected if the file is a white beam run, or if the file saving has some errors. Inform your local contact if this happens.
- 2.2. The data file is loaded, corrected for the time offset, and bad events are filtered out
- 2.3. A correction for He3 tube energy efficiency is applied
- 2.4. Data is converted to units of energy transfer
- 2.5. A k_i/k_f factor is applied (to get data proportional to the dynamical structure factor instead of differential cross section)
- 2.6. Data is put on a regular energy transfer grid, from -0.5 times the requested incident energy, to 0.95 times the requested incident energy, with a step of 0.005 of E_i .
- 2.7. The workspace at this point is saved as the intermediate processed file
- 2.8. Data is then normalized by the proton charge, and divided by the energy bin width. This way longer runs, or runs with different energy bins will have similar intensity scales
- 2.9. Data is divided by the vanadium, to eliminate any detector efficiency effects
- 2.10. Data is saved in the NXSPE format

For more complicated reduction processes, like adding runs together, subtracting empty cans, etc., your local contact or the instrument team can provide you with Mantid scripts.

9) Data Analysis

There are two current packages that are routine used for analysis of SEQUOIA data: Dave and Horace. Both of these can be accessed from the SEQUOIA analysis computers or the SNS analysis cluster.

Dave

From the command line type dave. This is the recommended tool for powder data or if you have a small number of angle runs to co-analyze. You can obtain dave for your own computer from <http://www.ncnr.nist.gov/dave/>. This location also has the documentation. Nevertheless here are a couple of notes. When using angle scans the data sets can eat up a lot of memory. For example 50 angles can take in excess of 64GB of memory. Therefore we suggest using the SNS analysis clusters for all data that is not powder data and if you are analyzing more than a few multiple angle runs we recommend Horace.

Horace

Horace requires the use of Matlab. If you have not configured Horace before, talk to your local contact. Once it is configured, switch to your home directory. (`cd ~`) and type `matlab` to start a matlab session. Then from the matlab window you can run a script, provided by your local contact, that will produce the `sqw` file for use in Horace. `Sqw` files may take several hours to run. The most frequently useful commands are the `cut_sqw` and `plot`. More information on Horace can be obtained from the website http://horace.isis.rl.ac.uk/Main_Page.

SEQUOIA python tools

A small set of useful tools has been written in python to assist users with selecting instrument parameters and to identify some spurious features in their data. (In most cases ARCS has also been configured in these tools, however use with ARCS is untested.) They are located at `/SNS/SEQ/shared/python/plan_tools/`. There are two python scripts that are described here: namely `chop_tools.py` and `res_ints_4.py` `chop_tools` provides an interface to test a repetition rate multiplication configuration or to test for spurious from an additional opening of the Fermi chopper during the measurement frame. `Res_ints` calculates the energy resolution and an approximate intensity for various chopper configurations. These tools have been written in python within the `ipython` interface. So the recommended way to run them on the analysis clusters is to type

```
ipython --pylab
```

```
cd /SNS/SEQ/shared/python/plan_tools/
```

then type either

```
run -i chop_tools.py
```

or

```
run -i res_ints4.py
```

depending on which utility you want to use.

For `res_ints4.py` if you want to plot flux and resolution vs Fermi chopper speed, type

```
plot_flux(<nu>,<Ei>,<Ef>,<spectrometer configuration>)
```

where `nu` is a numpy array of frequencies (usually `arange(60,660,60)`), `Ei` is the desired incident energy, `Ef` is the desired final energy, and `spectrometer configuration` is an object defining some parameters of the instrument (usually `SEQUOIA` or `SEQUOIA_sloppy`). If you want to plot resolution as a function of energy transfer, type

```
plot_res_omega(<nu>,<Ei>,<omega>,<spectrometer configuration>)
```

where `nu` is the frequency of the Fermi chopper, `Ei` is the incident energy, `omega` is an array of energy transfer values and `spectrometer configuration` is an object defining some parameters of the instrument.

For `chop_tools.py` if you want to check if a particular chopper configuration is appropriate for RRM, type

```
RRM_check_diff((Ei, fc_nu, T0_nu, fc_sloppy_chopper=True, source_nu=60.0, Lfci=18.20,  
LT0=9.78, T0_shift=0.0, slit_pack=SEQ_700)
```

The defaults are set for the sloppy chopper on `SEQUOIA`, you can change to a different slit package by using `slit_pack=SEQ_100` or one of the `ARCS` slit packs, if they are available. The `Fc_sloppy_chopper` flag determines if `Ei`s that go backward through the chopper should be considered. `Ei` is the maximum `Ei` to be used, `fc_nu` is the Fermi chopper speed and `T0_nu` is the `T0` chopper speed. `T0_shift` is an optional parameter to figure out how much to phase shift the chopper to get an additional `Ei` of a slower value. It is best to run the tool with this set to zero and then use the output from the initial run to determine how to run subsequent runs.

SEQUOIA and SEQUOIA 2 Analysis Machine Access

SEQUOIA and SEQUOIA 2 are the Linux analysis machines available to users for transforming raw data, data reduction, and data visualization. These machines are available at the SEQUOIA instrument cabin. One must apply for use of these resources: go to <https://neutronsrl.us/accounts/request.html>, and choose SNS user, then choose the SEQUOIA instrument and provide the IPTS number of your experiment. This approval requires action on the part of an instrument scientist or a member of the computing staff.

Nxsummarytable

Typing `nxsummarytable -i SEQ <runnumber>-<runnumber> [-o <filename>]`

Will give you a comma separated list of run information. Adding the `-o <filename>` flag to the end will dump the list to a csv file for easy import into your favorite spreadsheet. (Open office is available on the analysis machines.)

10) Background and spurious features

This section describes various background or spurious features that have been seen before. It provides ideas for identifying them and a discussion for reducing them.

Al

Aluminum is used in sample mounts and sample cans, because it is the most transparent material to neutrons. However it will still contribute the to the background two ways.

Bragg peaks

Al has an F m -3 m and a lattice parameter of 4.0497. Therefore the two longest dspacing Bragg peaks are the 111 and 200.

Table 9 Aluminum peaks in d and q spacings

index	d (Å)	Q (Å ⁻¹)
111	2.338	2.687
200	2.0249	3.103
220	1.4318	4.390
311	1.222	5.140
222	1.169	5.374

Al Density of States

The following plots show the results from an empty Al powder can, the Incident energy is 120meV.

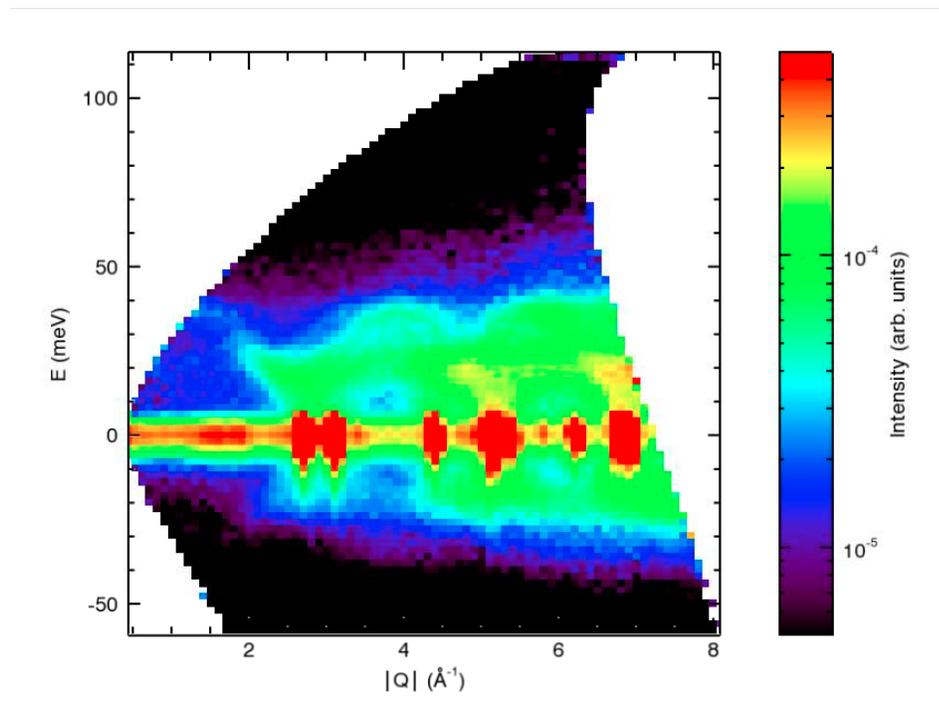


Figure 32 A measurements from an Empty Al can

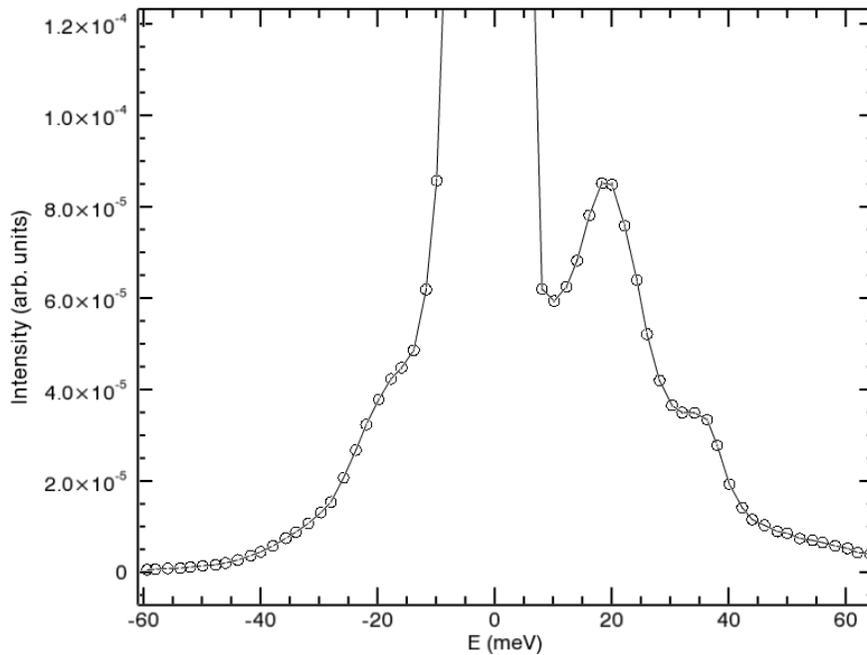


Figure 33 The data from the above figure summed over all Q. Note the prominent peak near 20 meV.

Recoil from Gases

There are several potential causes for gas to be in the beam near your sample. Namely we routinely use 1 Atmosphere of He for exchange gas, there could be an air leak (predominantly N₂) into the area near the sample (rare), or there may be adsorbed H in your sample. The first is only observed for very weakly scattering samples the latter is quite common for powders. Fortunately recoil is straight forward to identify. For a free particle it is straight forward to show^{vi} that the energy lost is related to the momentum transferred by

$$E = \frac{\hbar^2 Q^2}{2m} = 2.075(\text{meV}\cdot\text{amu}\cdot\text{\AA}^2) \frac{Q^2}{m}$$

where m is the mass of the particle. Usually energy is given in meV, Q is in \AA^{-1} and m is in amu. Therefore the second expression is there for convenience.

Usually if you see a quadratic dependence and the above equation give you an integer mass, you know the background feature is from the specific gas. If you suspect a specific gas, operating the instrument at 1eV for a few minutes will usually provide enough recoil data to compare to the above formula.

Molecular vibrations from bonded H

Coming soon.

New User Data Analysis Checklist – to be completed by instrument staff member when registering new user.

Done	Action
	Obtain XCAMS account, or recover old username and password if already registered: https://xcams.ornl.gov/xcams/regStep1.shtml
	Register for access to instrument computing resources (do this on a Windows machine). Go to: https://neutrons.ornl.gov/accounts/request.html Select SNS user (on-site and off-site) Select appropriate instrument, and enter proposal ID or other reason requiring access. Press submit. Enter UCAMS/XCAMS user name and password. Instrument staff or member of scientific computing must approve access request before proceeding.
	Verify user can log onto analysis machine – log in with XCAMS username and password.
	If using DGSreduction hard mask, copy appropriate mask files into user home area.

Table 10 New user data analysis checklist

11) Appendix A – Phone Numbers

Instrument Hall Coordinators	241-4432
Radiological Protection (RCT)	574-6588 (office) 274-8658 (mobile)
SEQUOIA Cabin	574-4818
Instrument Staff:	
SEQUOIA Lead Instrument Scientist - G.E. Granroth	805-0631 (mobile)
SEQUOIA Instrument Scientist - A.I. Kolesnikov	576-9145 (office) (630) 903-5428 (mobile)
SEQUOIA Scientific Associate - L. DeBeer-Schmitt	574-252-6060 (mobile)
Instrument Infrastructure:	
Data Acquisition Group (DAS)	574-0753
Detector Group	705-3650
Sample Environment Group	719-0656
Chopper Group	241-6351 (lab) 417-6352 (pager)

Note – these numbers are provided for reference – **ALWAYS contact the Instrument Hall Coordinators or your local contact if problems arise with equipment.*

Other Contacts:	
User Office	241-3675
NSSD Operations Manager - Greg Rowland	806-5481

(the area code prefix from external regions or phones is 1-865)

ⁱ Iverson E B, Ferguson P D, Gallmeier F X, and Popova I I 2002 Detailed SNS Neutronics Calculations for Scattering Instrument Design: SCT Configuration, Spallation Neutron Source Report SNS 110040300-DA0001-R00.

ⁱⁱ <http://ipython.org/>

ⁱⁱⁱ David M. Beazley, "Python Essential Reference", New Riders Publishing 2001

^{iv} I. A. Zaliznyak, A. T. Savici, V. O. Garlea, Rongwei Hu, and C. Petrovic, Phys. Rev. B **83**, 184414 (2011)

^v M. Russina and F. Mezei, Nucl. Instrum. Methods A **604**,624 (2009);M. Nakamura et al., J. Phys. Soc. Jpn. **78** 093002 (2009). G. E. Granroth J. Phys. Soc. Jpn **80** SB016 (2011)

^{vi} A. Messiah, "Quantum Mechanics"