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# 1. Propose an experiment

- a. Choose an instrument
  - i. Basic decisions
    1. Elastic or spectroscopy?
    2. Energy resolution desired? (TAX, DGS / VISION, backscattering, NSE)
    3. Type of measurement (parameter in narrow Q is better for TAX)
    4. Energy transfer range & Q desired? (ARCS/SEQ or CNCS/HYSPEC)
  - ii. HYSPEC is NOT a typical Direct Geometry Spectrometer
    1. Our strength is NOT out-of-horizontal-plane scattering, so don't bother lining up on the c-axis to measure the AB-scattering.
    2. Instead, just like at a TAX, align any single crystal with the desired scattering plane in the horizontal plane.
    3. Yes, we also do powders.
    4. Vertical focusing washes out our vertical Q resolution. Most users prefer the flux.
  - iii. Recommended papers to read to understand HYSPEC's niche:
    1. "Recent progress on HYSPEC, and its polarization analysis capabilities", EPJ Web of Conferences, **83**, 03017(2015)
    2. "A comparison of four direct geometry time-of-flight spectrometers at the Spallation Neutron Source", Review of Scientific Instruments, **85**, 4, 045113 (2014).
  - iv. Communicate with instrument scientists about your experimental needs
    1. Ovi Garlea: [garleao@ornl.gov](mailto:garleao@ornl.gov)
    2. Barry Winn: [winnbl@ornl.gov](mailto:winnbl@ornl.gov)
- b. Consider instrument configuration (see section 7 below) in advance
  - i. NOW THAT'S THINKING AHEAD!
- c. IPTS 101
  - i. The links under 'Become a User' at <http://neutrons.ornl.gov/users> are helpful.
  - ii. Instructions on using IPTS in general???
  - iii. HYSPEC specific: Special questions for polarization analysis and for being considered for the HYSPEC IDT proposal review.

## 2. Before you travel to HYSPEC

a. Know your sample

i. ICSD 101 (for Bragg peak locations and neutron scattered intensities)

<https://icsd.fiz-karlsruhe.de/search/basic.xhtml>

Home | Contact Welcome to ICSD Web. IP authenticated (160.91.238.68). Oak Ridge Natl Laboratory Close session

**Basic Search & Retrieve**

**Search Action** Run Query Clear Query

**Search Summary**  
Basic Search: 25

**Query History**  
Number of queries: 1  
Clear Query History  
2016-01-27T22:04 25

**Navigation**  
Basic search & retrieve  
Advanced search & retrieve  
Bibliography  
Cell  
Chemistry  
Symmetry  
Crystal Chemistry  
Structure Type  
Experimental Information  
DB Info  
Query Management  
Manage Queries  
List Combined Queries  
Create Combined Query  
Customer Survey  
ICSD Customer Survey 2015

**Bibliography**  
Authors: \_\_\_\_\_ Year of Publication: \_\_\_\_\_  
Title of Journal: \_\_\_\_\_  
Title of Article: \_\_\_\_\_

**Chemistry**  
Composition: Al Number of Elements: 1

**Cell**  
Cell Parameters: \_\_\_\_\_  
Cell Volume: \_\_\_\_\_ Tolerance +/-: \_\_\_\_\_ %

**Symmetry**  
Space Group Symbol: \_\_\_\_\_ Space Group Number: \_\_\_\_\_  
Crystal System: \_\_\_\_\_ Centering: \_\_\_\_\_

**Exp. Info. & Ref. Data**  
New Data Only:   
PDF Number: \_\_\_\_\_ Temperature: \_\_\_\_\_ K  
ICSD Collection Code: \_\_\_\_\_ Pressure: \_\_\_\_\_ MPa

Clear Basic Search Count Basic Search

Home | Contact Welcome to ICSD Web. IP authenticated (160.91.238.68). Oak Ridge Natl Laboratory Report Print Close session

**Results: List View** # of Hits: 25

Select All Deselect All Show Detailed View Show Synoptic View Export Selected Data Back to Query

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference
<input checked="" type="checkbox"/> 43423	F m -3 m	Al	ccp-Cu	Precise lattice constants of germanium, aluminum, gallium arsenide, uranium, sulphur, quartz, and sapphire	Cooper, A.S.	Acta Crystallographica (1962) 15, p878-p882
<input type="checkbox"/> 43492	F m -3 m	Al	ccp-Cu	Lattice parameter determinations with an X-ray spectrogoniometer by the Debye-Scherrer method and the effect of specimen condition	Otto, H.M.	Journal of Applied Physics (1961) 32, p1536-p1546
<input type="checkbox"/> 44321	F m -3 m	Al	ccp-Cu	Absorption correction in precision determination of lattice parameters	Straumann, M.E.	Journal of Applied Physics (1959) 30, p1865-p1869
<input type="checkbox"/> 44713	F m -3 m	Al	ccp-Cu	The thermal expansion of aluminum at low temperatures as measured by an X-ray diffraction method	Figgim, B.F., Jones, G.O., Riley, D.P.	Philosophical Magazine, Serie 6 (1956-) (1956) 1, p747-p756
<input type="checkbox"/> 52255	F m -3 m	Al	ccp-Cu	Precision measurements of crystal parameters	Quinn, E.A., Yates, E.L.	Philosophical Magazine, Serie 7 (1926-48) (1935) 15, p472-p488
<input type="checkbox"/> 52611	F m -3 m	Al	ccp-Cu	X-ray diffractometer determination of the thermal expansion coefficient of aluminum near room temperature	Otto, H.M., Montagu, W.G., Welch, D.O.	Journal of Applied Physics (1963) 34, p3149-p3150
<input type="checkbox"/> 53772	F m -3 m	Al	ccp-Cu	Crystal structures of common elements	Hull, A.W.	Physical Review (1935-) 132, 1963/141, 1965-160, 1969 (1917) 10, p601-p606
<input type="checkbox"/> 53773	F m -3 m	Al	ccp-Cu	Determination of the crystal structures of regular alloys	Young, J.F.T.	Philosophical Magazine, Serie 6 (1901-1925) (1923) 46, 2091-p2095
<input type="checkbox"/> 53774	F m -3 m	Al	ccp-Cu	Precision measurements of the lattice constants of 12 single metals	Davey, W.P.	Physical Review (1893-132, 1963/141, 1965-160, 1969) (1925) 21, p733-p753
<input type="checkbox"/> 53775	F m -3 m	Al	ccp-Cu	Koerigen-spektroskopische Untersuchungen enger Metalllegierungen nach Siemens-Boden	Lange, H.	Annalen der Physik (Leipzig), Folge 4 (1825) 76, p455-p475

[1-10] [11-20] [21-25] [LastPage]

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ICSD  
 Home | Contact | Welcome to ICSDWeb. IP authenticated (168.91.238.66), Oak Ridge Natl Laboratory | Page 1 | Close session

Entry 1 of 1 | Back to List View | Back to Query

**Summary** Collection Code 43423

Struct formula	Al	Author	Cooper, A.S.
Space Group	Fm-3 m(225)	Title of Article	Precise lattice constants of germanium, aluminum, gallium arsenide, uranium, sulphur, quartz and isoprene
Unit Cell	4.048750(15) 4.04875 4.04875 90, 90, 90	Reference	Acta Crystallographica (1. 1940-23. 1967) (1962) 15, p676-p682
Cell Volume	66.42 Å <sup>3</sup>	Formula Units per Cell	4
Temperature	room temperature	Pressure	atmospheric
POF-numbers	01-088-2768 4.787	R-value	

Warnings & Comments: 2 Warnings / 2 Comments

Remark:

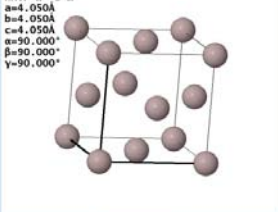
Export CIF File | MyBaseFilename | Show Synoptic View | Feedback to the ICSD Editor

**Details**

Expanded All Collapse All  
 Visualization

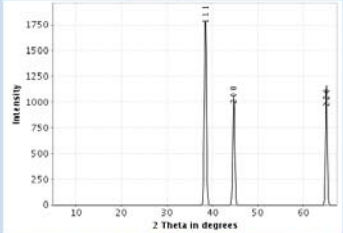
**Published Crystal Structure**

HKLF: F m -3 m  
 a=4.050Å  
 b=4.050Å  
 c=4.050Å  
 α=90.000°  
 β=90.000°  
 γ=90.000°



Interactive Visualization

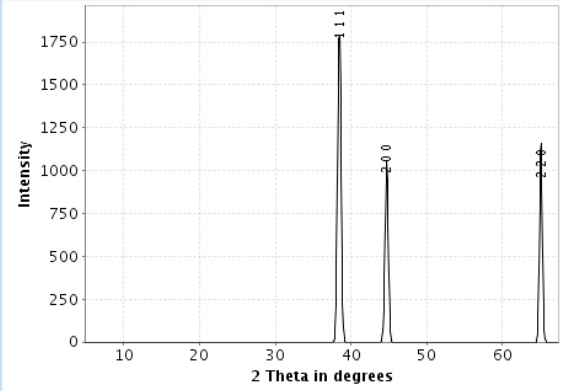
**Powder Pattern**



Display in Window | Export as x-y data | Export as table | Show as PDF

Configure Powder Pattern Calculation and Display

Chemistry | Published Crystal Structure Data



Display in Window | Export as x-y data | Export as table | Show as PDF

Configure Powder Pattern Calculation and Display

**Calculation Parameters**

Radiation Type: Neutron Diffractometer  
 Wave Length: Custom | Custom Wave Length: 1.54 Å  
 Include Dispersion

**Width Parameters**

u 0.1791 | v -0.4503 | w 0.4 |  Intensities only

**Visualization Parameters**

Plot Type: 2Theta  
 Xmin 5.0 | Xmax 67.312 | Xstep 0.1  
 Color Display |  Display Indices

Save As Default | Restore Default | Reset to System

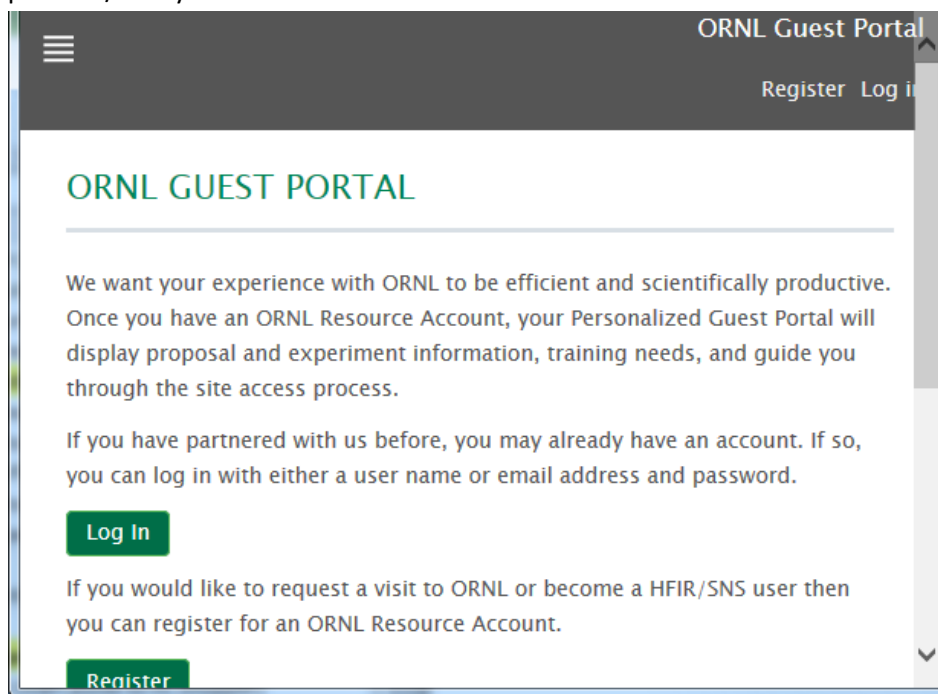
Redraw Display

ii. Users are expected to know the crystal lattice structure and dimensions prior to arriving. You need to know the basis cell dimensions and angles, and if it's a

single crystal you also need to know which scattering plane you intend to study, in terms of key symmetry directions in reciprocal lattice unit dimensions (r.l.u). These directions often correspond to Bragg peaks visible in that plane.

b. Preparing for data

- i. You must have an XCAMS account in order to do several things, including the web-based training required prior to entry. You also need this account in order to access your experimental data and to use ORNL's computing resources to process / analyze the data.



If you do not yet have an account, go to the guest portal at <https://user.ornl.gov/> to register.

ORNL Guest Portal

Register Log in

**LOG IN TO YOUR ACCOUNT**

User name or email address

Password

Log in

[Forgot your password?](#)

[Register](#) if you don't have an account.

Not to worry; there is a link at <https://user.ornl.gov/Account/Login> for those many users who have once again forgotten their passwords.

- ii. Information concerning data analysis for HYSPEC and other neutron scattering instruments at ORNL can be found at <http://neutrons.ornl.gov/users/data-mgmt>.

## Data Analysis and Management

### Monitor Experiments

Active experiments at HFIR instruments can be monitored using [neutron.ornl.gov/spice/](http://neutron.ornl.gov/spice/).  
Active experiments at SNS instruments can be monitored using [monitor.sns.gov](http://monitor.sns.gov).

### Analyze Experiment Data

Data from HFIR instrument experiments can be accessed using [neutron.ornl.gov/spice/](http://neutron.ornl.gov/spice/).  
Data from SNS instrument experiments can be accessed using [analysis.sns.gov](http://analysis.sns.gov).

### Data Analysis and Visualization Software

- Mantid
- Spice
- SasView
- Reslib
- GSAS & EXPGUI
- Fullprof
- Horace
- PDFgui
- DAVE

### Data Management Practices

If you are unfamiliar with analysis software for direct geometry spectrometers, we recommend you familiarize yourself in advance with DAVE and in particular its mslice application at

[http://www.ncnr.nist.gov/dave/documentation/dcs\\_mslice.pdf](http://www.ncnr.nist.gov/dave/documentation/dcs_mslice.pdf).

For users that require greater sophistication for their analysis, we recommend you familiarize yourself with Horace at

[http://horace.isis.rl.ac.uk/Main\\_Page](http://horace.isis.rl.ac.uk/Main_Page) .

- iii. If you have an XCAMS account, you should also have an account on the analysis cluster. Go to <https://analysis.sns.gov/> and inside the 'connection options' box you will see a variety of ways you can open terminals or move data to your

personal computers.

linux@support.sns.gov or call 865-309-4649 for urgent requests.'

- iv. From <https://analysis.sns.gov/>, click the 'launch session' button to begin a session on the Analysis Cluster, which uses Linux. It is using a web-based version of the ThinLinc client found in the 'connection options' box.
- v. Confirming your IPTS directory is ready (*not yet prior to first run*) involves launching a session as described above, opening a terminal, and attempting to move to the following directory from a terminal using the following command:

```
cd ~/data/SNS/HYS/IPTS-<#>
```

Where <#> corresponds to the number for the experiment about to begin. If this doesn't work please contact your Local Contact.

- vi. Sometimes this directory isn't yet available

```
~/data/SNS/HYS/IPTS-<your IPTS #>/
```

but you can access:



```
/SNS/HYS/IPTS-<your IPTS #>/
```

then type in the following either from the HYSPEC analysis machine or the ANALYSIS cluster:

```
/usr/local/sbin/create_symlinks
```

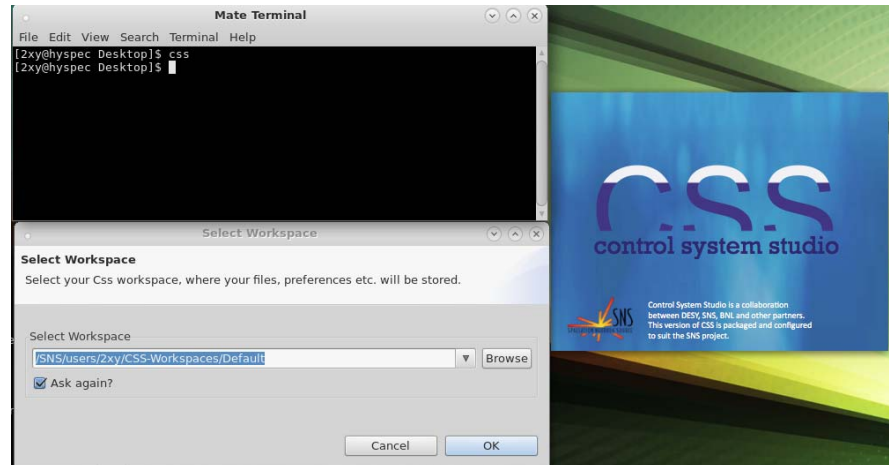
### 3. Navigating Control Systems Studio (CSS)

#### a. Starting CSS from DASUSER computer

##### i. From icon



##### ii. From terminal

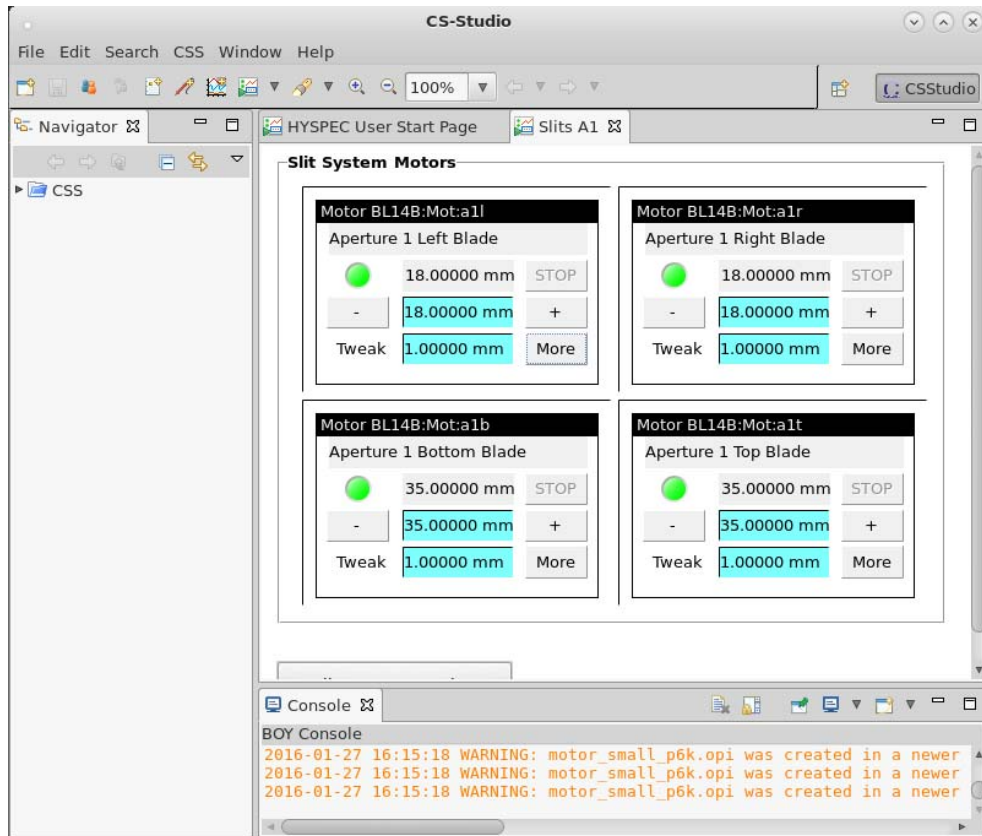


1. Start terminal
2. Type 'css' and enter
3. First window 'Select Workspace' has a question. Click the 'OK' radio button.

##### iii. Starts in previous configuration

1. You may have some tabs open that you don't need. Get rid of everything except the HYSPEC user page.

b. ECLIPSE-based Tab'd Graphical User Interface



c. Radio buttons

- i. Some drill down to other tab'd GUI's
- ii. Right click allows option to spawn another tab or window

d. Color coded

- i. Grey fields are read-back values: where devices actually are
- ii. Blue fields can be input fields. They are request fields.
  - 1. No 'Enter', no request!
  - 2. Compared to Advanced Photon Source, blue field doesn't turn yellow when editing field
- iii. Right click on field to
  - 1. Copy the PV name, useful for some scans

e. Colon anatomy: understanding the syntax of EPICS variables

- i. Not to worry. They are known as process variables (PV's)
- ii. Master prefix BL14B refers to the HYSPEC instrument (beamline 14-B)
- iii. Next field refers to type of PV: MOT for motors, SE for sample environment, etc.
- iv. Final fields are abbreviations that (at least for motors) follow the HFIR TAX naming standards.
- v. Needed for automated scans.

## 4. First day at HYSPEC: general setup

- Reading, understanding, acknowledging and signing off on the Experimental Safety Summary

Navigation: Home | All Processes | My Processes | My History | Help | Logout

Home

---

**Experiment Summary**

Proposed Run: **8020.2.1** Title: **Ultraviolet Photoelectron Analysis**

Instrument: **U-100** Run Dates: **01/12/2018**

Start Date: **01/09/18** End Date: **01/09/18**

Lead Contact: **David Carter (011 232 7145), Gary How (011 423 407), Brian Lee (011 423 407)**

**Tracker**

Generate PDF

---

**Attendance**

Print Attendance

Add Absent

---

**Sample Information**

Name	Description	State	Formula	Mass	Total	Form	Material	UHM Material	Container	Preparation	Approval Status	UHM Sample #	UHM Disposition
MSD	green powder	Solid	MSD	20g		Powder	None	None	Aluminum Sample Can	N	Sample approved after initial SAC approval	31026	0
UHMMSD	0.17g single crystal of UHM-MSD Sample in a dry air sensitive long term storage needs to be in a desiccator	Solid	UHM-MSD	0.17g		Single Crystal	None	None	Aluminum Sample Can	N	Sample approved after initial SAC approval	31027	0
T2P-rod	Solid cylinder tapered bottom	Solid	T2P	2g		Polypropylene	None	None	Cylinder	N	Sample approved after initial SAC approval	31028	0
Quartz-rod	Rod of Quartz	Solid	SiO2	2g		Polypropylene	None	None	Cylinder	N	Sample approved after initial SAC approval	31029	0
Quartz-rod	Rod of Quartz	Solid	SiO2	2g		Polypropylene	None	None	Cylinder	N	Sample approved after initial SAC approval	31030	0
vanadium	rod of vanadium	Solid	V	1g		Polypropylene	None	None	Bag	Y	Sample approved at time of SAC		
Hexane in can	single crystal	Solid	C6H14	1g		Single Crystal	None	None	Bag	Y	Sample approved at time of SAC		
LithiumCl	black powder	Solid	LithiumCl	1g		Powder	None	None	Aluminum Sample Can	Y	Sample approved after initial SAC approval		
MSD	MSD - being a UHM. This is an existing separate sample in a vanadium can	Solid	MSD	1g		Powder	None	None	Vanadium Sample Can	Y	Sample approved after initial SAC approval		
K2CO3	single crystal	Solid	K2CO3	1g		Single Crystal	None	None	Bag	Y	Sample approved at time of SAC		
vanadium	7mm disk of V ring	Solid	99% V, 0.02% Nb, 0.03% Si	2g		Polypropylene	None	None	Cylinder	N	Sample approved after initial SAC approval		

---

**Sample associated through UHM**

UHM Sample ID	Name	Description	State	Formula	Masses	UHM Material	Disposition
1117	MSD	powder sample	Powder	MSD	Mass 0.001-0.01 grams, less than 50 mg dry weight, but not more than 500 mg dry weight		
33475	LithiumCl	powder	Powder	LithiumCl	Mass available in the UHM (MSD, mg/100,000)		

---

**Classification History**

U-100-None

---

**Safety**

**Research Description:** Describe the tasks and procedures required for your experiment (i.e. what will be done and who will do it). What are the samples?

**Hazards and Precautions:** Describe your experiment and assess the potential hazards for identification. Major or gas release potential - check applicable to the work. Exposure to vapors or dust - identify any required precautions.

**Safety & Health Considerations:**

Have prepared a sign-out case (Number of samples to be analyzed)

MSD sample removal (after exposure to the UHM) needs to be completed by qualified individuals trained at UHM, or the process and location of the hazard is immediately obvious to those that perform the work. Removal of the sample from UHM or sample will require an inventory, which is coordinated with UHM (before and after) "location, condition, material" data.

**Save**

---

**Approvals**

The above safety information describes all known potential hazards associated with the experiment, not all the time on the active end of the procedures and equipment necessary for the task in a safe, healthful work environment unless at UHM Experimental Facility. Please be the user of the described equipment. Do not participate in the experiment and safety in the standard and emergency procedures relating to the hazards associated with this experiment process.

Instrument Team Comments:

Enter Personnel and Check Approvals \*

Approver: Instrument Team

---

**Team Members and Actual Dates**

Assignment #	Role	Name	Initials	Mobile Phone	User ID	UHM Signature	UHM Signature
1. Local Contact (Proposed)	Delta	David Carter	[Signature]	001-202-7145	DCD		
	Green Book	David Carter	[Signature]	001-202-4810	MSD	Agreed 08/08/18 14:20	
	White	David Carter	[Signature]	001-202-4810	DCD		
2. Instrument Team	Delta	Instrument Team Member	[Signature]	001-202-7145	DCD		
	Green Book	Instrument Team Member	[Signature]	001-202-4810	MSD	Agreed 08/08/18 14:20	
	White	Instrument Team Member	[Signature]	011-202-4810	MSD		
	Green	Instrument Team Member	[Signature]		MSD		
3. Proposal Team	Delta	Collaborator	[Signature]	001-202-7145	DCD		
	Green Book	Collaborator	[Signature]	001-202-4810	MSD	Agreed 08/08/18 14:20	
	White	Collaborator	[Signature]	001-202-7145	DCD		
	Green	Principal Investigator	[Signature]	001-202-4810	MSD		

\*The UHM has not been signed by Safety. Member Signatures not available.  
 \*The Proposed by User Submitted to Run within the UHM Signature. Member Signatures not available.

Home | Start Date: 01 Sep 2018 05:02 | Actual End Date: 02 Oct 2018 08:00

12

b. CSS User page

**Experiment**

IPTS 8020 Run 100851 Idle

Acquisition Start Stop Run Time 00:42:39

Title SrTiO3 4.5 K s2 -78 Ei 13 300 Hz vary s1, 8 min per r

Notes

Scan Idle

**Neutrons**

Energy 13.000 meV

Beam Power 0E0

PCharge 0.0000E0 C 0.000000E0 pC

**Shutters**

Primary

Secondary Status

Tertiary Status

**Motion Control**

s1 Upper Limit 100.00 Aperture 1 Aperture 2

s1 Lower Limit -110.00 Sample SE Stages

Detector Vessel

**Sample Environment**

Select Environment Vacuum Cube Dilfridge He Compressor

CRYO-09 AMI1800 Lakeshore Cryostat

**Equipment**

All OK

Equipment Status User Monitor Main

bl14b-user

c. Assigning the experiment and sample

- i. Why bother? Because only the instrument team tied to the assigned IPTS (and the local contacts) can view the data. It would be a shame to generate data without being able to access it!

ii. CSS IPTS page

The screenshot shows the CSS IPTS interface. On the left, a table lists experiments with columns for ID, Sub, Start, Title, and Members. On the right, a detailed view for 'Samples for IPTS-- 8020' is shown, including a table of sample details (ID, Name, Description, Mass, Container, Nature, Comments) and a form for sample information (ID, Name, Container, Mass, Description, Nature, Comment).

ID	Name	Description	Mass	Container	Nature	Comments
1	None	No sample	N/A	N/A	N/A	N/A
31427	YbBr-BI2	0.75g single crystal of green powder	759g	Aluminum Mo	Single Crystal	Sample has been in I
31225	MnO		25g	Aluminum Sar	Powder	-
31025	Quartz rod	Rod of Quartz.	10g	Cylinder	Polycrystal	-
31024	Quartz rod	Rod of Quartz.	10g	Cylinder	Polycrystal	-
31023	TiZ rod	Solid cylinder tapped	10g	Cylinder	Polycrystal	-
20475	LaFeAsO	powder	5g	Glass vial	Powder	-
1117	NiO	powder sample	15g	Vanadium Sar	Powder	Contact: Ovi Garlea a

d. Fresh slate

i. CSS Zero motors page

The screenshot shows the 'Zero Motors' interface with a dialog box titled 'Set and move to preset positions'. The dialog contains a table of motor positions and 'Move' buttons for each.

Preset Position	Current Position	Move
s1	0.00 / -0.00172 deg	Move
sgu	0.00 / 0.00754 deg	Move
sgl	0.00 / -0.00094 deg	Move
stu	0.00 / -0.00100 mm	Move
stl	0.00 / -0.00100 mm	Move
a1b	35.00 / 35.00000 mm	Move
a1t	35.00 / 35.00000 mm	Move
a1r	18.00 / 18.00000 mm	Move
a1l	18.00 / 18.00000 mm	Move
a2b	35.00 / 35.00000 mm	Move
a2t	35.00 / 35.00000 mm	Move
a2r	18.00 / 18.00000 mm	Move
a2l	18.00 / 18.00000 mm	Move

Buttons: Move All, Abort

e. Changing sample environments

- i. Local Contact to restart the associated software driver package
- ii. Local Contact to reconfigure software for any changes to rotation stages

f. Setting global's

- i. General

ii. What's rotating?

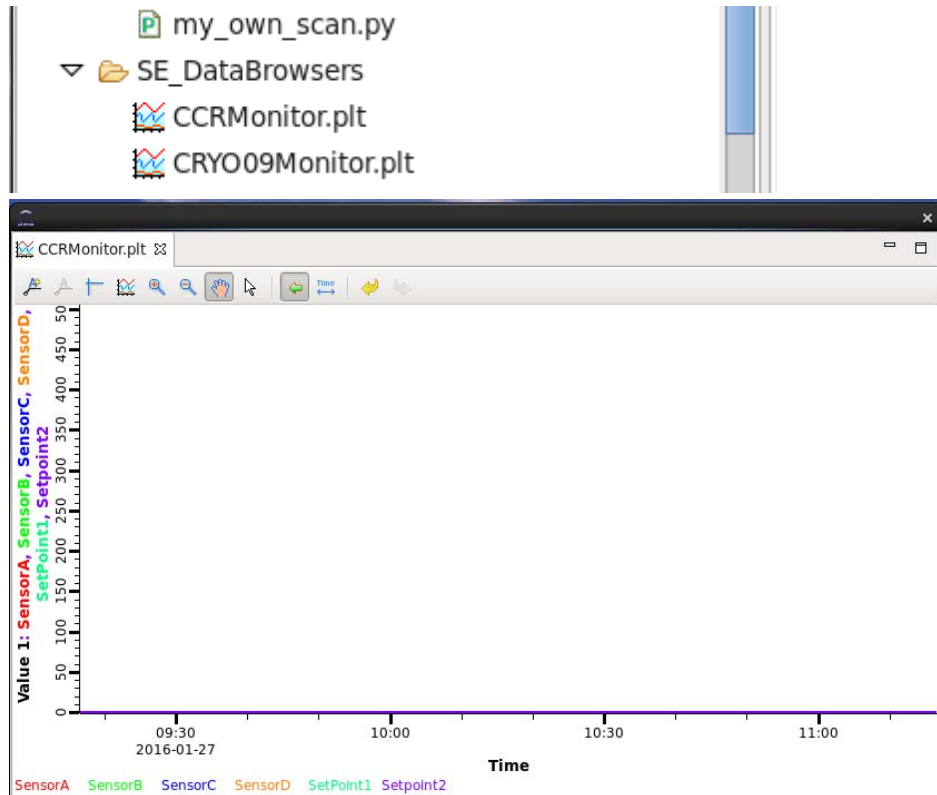


iii. Which sample environment to track? CSS \_ page

iv. How do I alarm the right sample environment? For now, go to the main page for a given sample environment. You will find a high-level radio button there to toggle between an alarm-sensitive state or not. This is important for enabling Instrument Hall Coordinators to be alerted to any bad situation.

g. Useful charts

i. Choose depending on sample environment





## 5. Aligning a single crystal

- a. Have a powder instead? See section 7.f. for preliminary planning, and then go straight to section 6. You may ignore the rest of this section.
- b. Starting with a good guess
  - i. Choose two symmetry directions in desired scatter plane
  - ii. Line up first direction with incident beam
  - iii. If the cyan tilt and translation stages beneath the sample environment don't look roughly square, you forgot to do step 5.c.
- c. Spaghetti in the way?
  - i. In the field, carefully determine the range of your rotator in advance. The range may be restricted by vacuum lines, compressor lines, cryogen lines, or other cables connecting to the sample environment. Although now rare, if you are rotating the 's1' stage it is also a good idea to look down at the rotation stages to ensure the motor cables are not catching on anything.

Sample Motion

<b>Motor BL14B:Mot:stl</b> Sample Translation Lower <input type="radio"/> -0.00100 mm <b>STOP</b> <input type="button" value="-"/> <input type="text" value="0.00000 mm"/> <input type="button" value="+"/> Tweak <input type="text" value="1.00000 mm"/> <input type="button" value="More"/>	<b>Motor BL14B:Mot:stu</b> Sample Translation Upper <input type="radio"/> -0.00100 mm <b>STOP</b> <input type="button" value="-"/> <input type="text" value="0.00000 mm"/> <input type="button" value="+"/> Tweak <input type="text" value="1.00000 mm"/> <input type="button" value="More"/>
<b>Motor BL14B:Mot:sgl</b> Sample Goniometer Lower <input type="radio"/> -0.00172 deg <b>STOP</b> <input type="button" value="-"/> <input type="text" value="0.00000 deg"/> <input type="button" value="+"/> Tweak <input type="text" value="0.10000 deg"/> <input type="button" value="More"/>	<b>Motor BL14B:Mot:sgu</b> Sample Goniometer Upper <input type="radio"/> 0.00323 deg <b>STOP</b> <input type="button" value="-"/> <input type="text" value="0.00000 deg"/> <input type="button" value="+"/> Tweak <input type="text" value="0.10000 deg"/> <input type="button" value="More"/>
<b>Motor BL14B:Mot:s1</b> Sample Vert Rotation <input type="radio"/> -0.00172 deg <b>STOP</b> <input type="button" value="-"/> <input type="text" value="0.00000 deg"/> <input type="button" value="+"/> Tweak <input type="text" value="1.00000 deg"/> <input type="button" value="More"/>	<b>Motor BL14B:Mot:bst</b> Beam Stop <input type="radio"/> 14.00000 mm <b>STOP</b> <input type="button" value="-"/> <input type="text" value="14.00000 mm"/> <input type="button" value="+"/> Tweak <input type="text" value="1.00000 mm"/> <input type="button" value="More"/>

**s1 Settings**

Speed

Position

Offset 0.00000 deg

**Mapping to phi and chi for Nexus 1**

phi	0.0000	BL14B:Mot:Du
chi	0.0000	BL14B:Mot:Du
omega	-0.0017	BL14B:Mot:s1.

**Motor BL14B:Mot:s1**

Sample Vert Rotation

-0.00172 deg **STOP**

Tweak

d. Slowing down your rotator

**s1 Settings**

Speed

Position

Offset 0.00000 deg

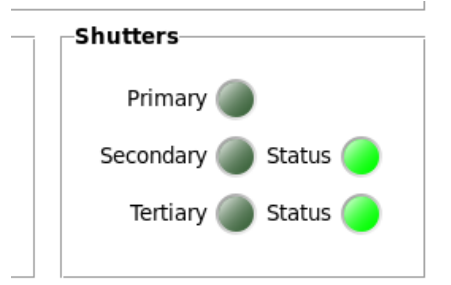
e. What am I looking for?

i. Determining Bragg peak scatter angle and guess of sample angle

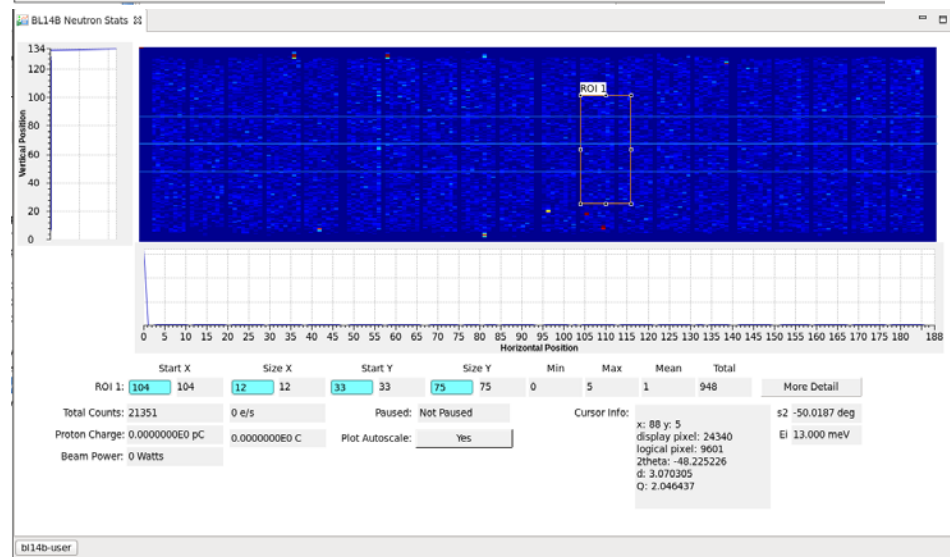
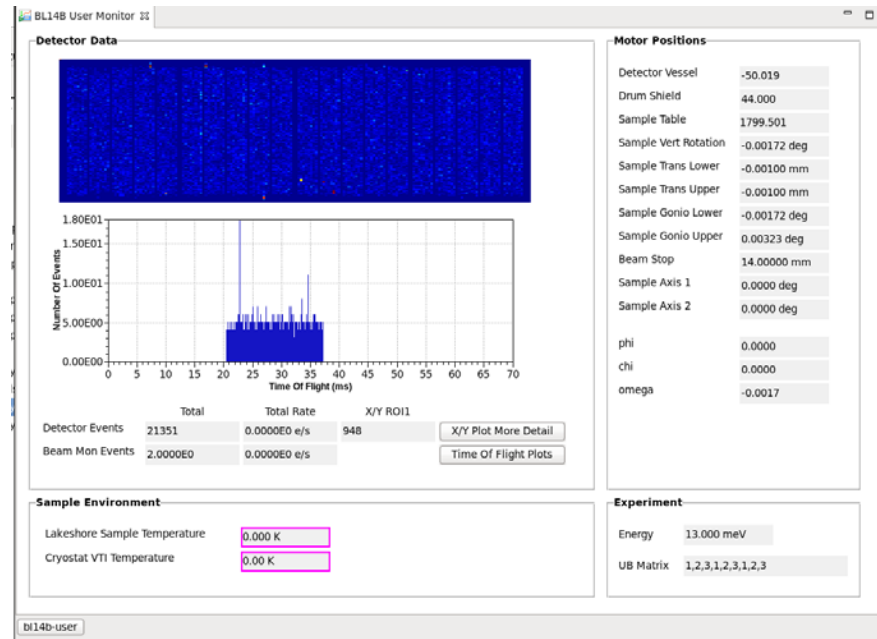
1. Use either the python planning tools (section 7.g.) and/or ICSD (section 2.a.i.) in order to determine scatter and sample angles. ICSD will also

provide relative intensity information useful to choose a good Bragg peak to search for.

2. General recommendation: low  $E_i$ 's mean fewer and more obvious Bragg peaks
  3. May need to modify instrument configuration (see section 8)
- ii. Confirming shutters are truly open



iii. CSS Monitor screen and/or xy view screen



iv. Where will the scatter be? The cursor has a hover feature that tells you all about where the cursor is in angle, elastic d and elastic Q. Note that due to vertical focusing the Bragg peaks are usually extended

- f. Keeping an eye out for your first Bragg peak!

HYSPEC User Start Page

**Experiment**

IPTS 8020 Run 100851 Idle

Acquisition Start Stop Run Time 00:42:39

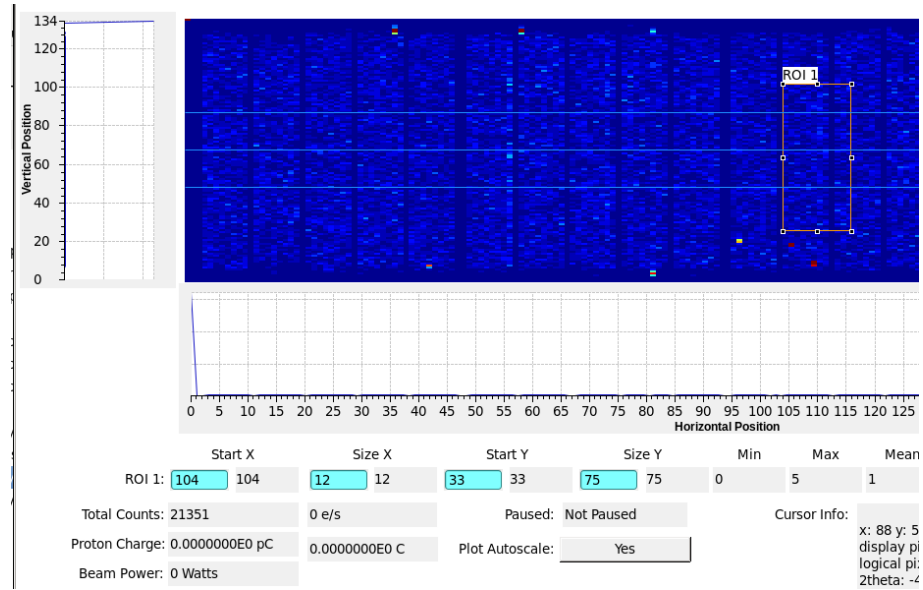
Title SrTiO3 4.5 K s2 -78 Ei 13 300 Hz vary s1, 8 min per r

Notes

Scan Idle

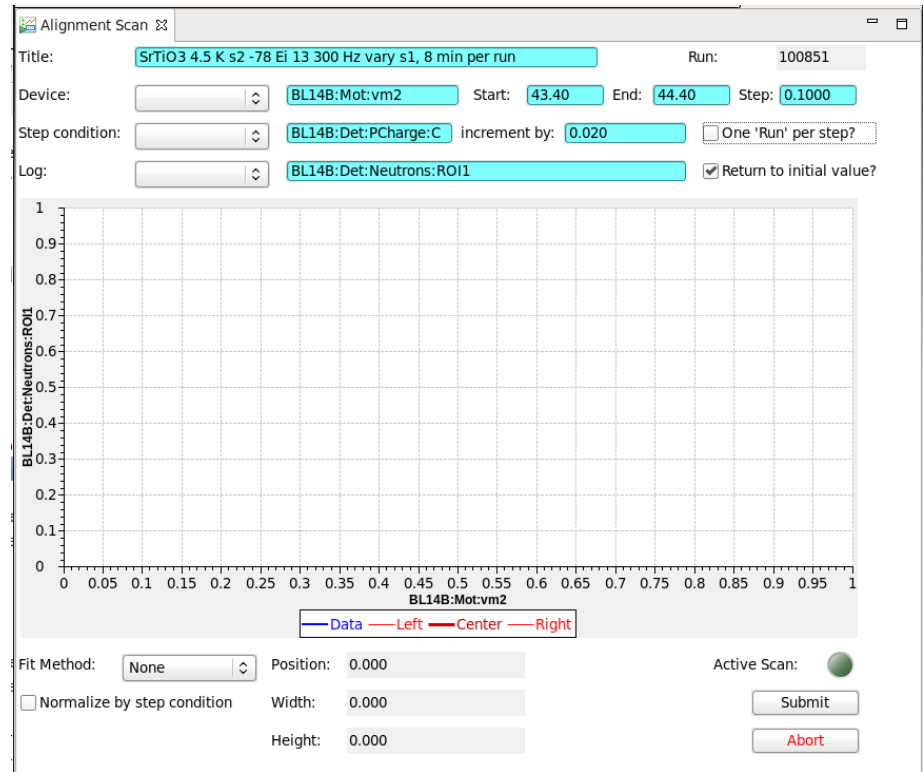
- i. Starting acquisition from HYSPEC User screen
  - ii. Start moving your rotation motor slowly by entering a desired destination value in the blue field.
  - iii. Hitting motor stop button once you've seen your peak
- g. Oh no! I cannot find the peak!
- i. Be patient. Breathe.
  - ii. Be willing to go 180 deg
  - iii. You may be seriously tilted, beyond about 7 degrees of misaligned tilt the Bragg peaks are no longer visible (they move above or below the position sensitive detectors)
  - iv. Contact Local Contact. You two probably have a long night ahead of you.
- h. Alignment scan, main rotation stage
- i. Fine tuning the location of the Bragg peak
    1. 0.5 to 1 deg steps are OK for the initial check
    2. 0.2 deg steps preferred for fine check.

ii. Choosing your Region of Interest (ROI)



1. CSS Instrument View Screen.

iii. CSS alignment scan screen



1. Pull-down makes choice of what's scanned fairly easy
2. Defaults
  - a. Return to original value when scan is done (beware because an abort doesn't cause a return)
  - b. One NeXus run for the whole scan
3. Recommend you have scanned variable's page in separate window

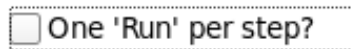
- a. Otherwise no clear way to confirm it's moving or have a good idea of desired range
- b. A strategy to view the as-stepped value on the alignment screen was proposed and rejected for now...

4. Fitting option selected PRIOR to scan

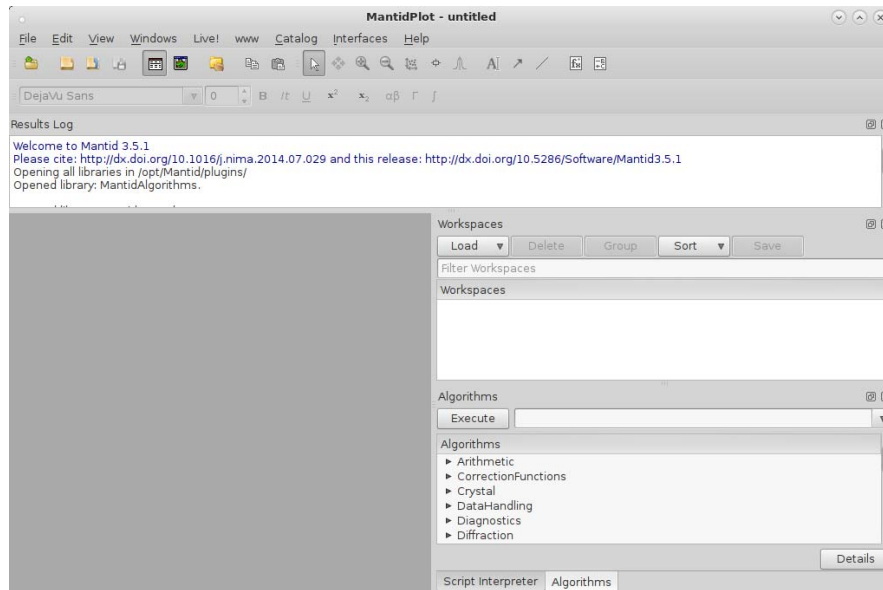


5. Plotting. Right click on the plot field to generate a paper plot of a given alignment scan. Plot before changing scan parameters for the next scan, because the plot axis changes before the data does.

- i. If you must work with error bars...
  - i. Although CSS is a state-of-the-art system using sophisticated code, it has yet to be able to estimate or to plot statistical errors, so MantidPlot provides an alternative.
  - ii. On the CSS alignment scan page, be sure that all steps are in the same run-file.

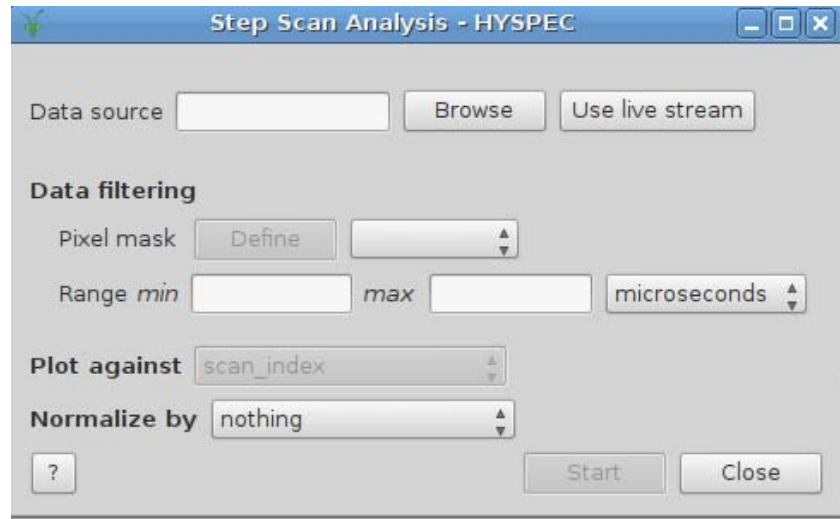


iii. Open MantidPlot from an analysis session (either HYSPEC or Analysis cluster).



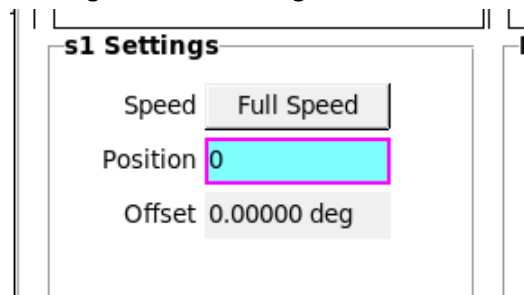
- iv. On 'Interfaces' pull-down menu, open under 'General' subsection the 'Step Scan Analysis' feature. Fill in features as needed and either use Live Stream or a

saved file.



- v. Until we have a way to communicate region of interest used on CSS to Mantid, you will need to independently choose your region of interest.

- j. Shifting the rotation stage value



- k. Complimentary Bragg Peak

- i. Typically parallel to the other symmetry direction
- ii. Usually OK to go directly to nominal rotation stage value and confirm peak is present
- iii. Why bother? In case you have a crazy tilt that wasn't clear at the first Bragg peak

- l. How much is too much?

- i. To avoid saturation, peak count-rate needs to be ~100-300 cps. Otherwise saturation will cause non-linear response (counts are no longer proportional to scattered neutron number messing up aperture width selection and rocking scans).
- ii. Attenuation strategy #1: Attenuate via a borated aluminum sheet
- iii. Attenuation strategy #2: Change the Fermi Frequency (see section 8.a.)

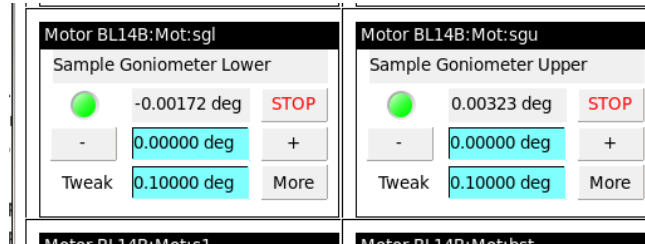
- m. Getting peaks on the level

- i. Most sample environments are mounted on a tilt and translation stage, and are rotated using the s1 stage. In this case it is fairly trivial to adjust the sample tilt by tilting the entire sample environment. If tilting when using a stick-rotation



mode, we're either unable or not yet ready to implement (tilt would change as a function of rotation angle).

- ii. When are they level? When the tall Bragg peaks are centered vertically in the instrument view! There are guides to the eye for normal focusing conditions, and if you're inside them you are probably just fine.
- iii. SGU and SGL motors and screen



- iv. A perk to a good guess (6.a.) is that the tilt stages are roughly aligned with the symmetry directions.
  - 1. If they are not aligned, there is significant cross-talk between tilt stages when optimizing tilts.
  - 2. If your guess was more than, say, 15 degrees off, it's worth your while to physically reorient the sample with respect to the tilt stages
- v. Although some prefer an alignment scan (~1 deg steps), we generally find that visual inspection of monitor screen is sufficient. If you do an alignment scan please remember to adjust the Region of Interest to be more or less in the center of the detector array vertically, and about the height of the lines that are guides to the eye.
- vi. If you must, we can change to no vertical focusing and you can check again. Most users don't bother.

- n. I cannot get my peaks on the level and don't intend to re-align
  - i. In this case you'll need to account for misalignment on the analysis side. Will need UB matrix formalism and 3D U and V vectors for different analysis software.

```

MantidPlot: Python Window
HYS_addPeaks_E.py X
1 from mantid.kernel import *
2 from mantid.api import *
3 import numpy as np
4 import math
5
6
7 class HYS_addPeak(PythonAlgorithm):
8
9     def PyInit(self):
10        # Declare properties simply
11        self.declareProperty(IntProperty("FileNumber", defaultValue=""))
12        self.declareProperty(FloatArrayProperty("a,b,c (Angstrom)", validator = FloatArrayLengthValidator(3)))
13        self.declareProperty(FloatArrayProperty("alpha, beta, gamma (deg)", validator = FloatArrayLengthValidator(3)))
14        self.declareProperty("u (r.l.u.)", defaultValue="")
15        self.declareProperty("v (r.l.u.)", defaultValue="")
16        self.declareProperty(GoniometerVerticalAxis, defaultValue="sl")
17        self.declareProperty("PeakPickAxis", defaultValue="E")
18
19     def PyExec(self):
20        # Run the algorithm
21        from mantid.simpleapi import Load, DeleteWorkspace, ConvertUnits, Rebin, SetGoniometer
22        _tmpws = Load("HVS" + self.getPropertyValue("FileNumber"))
23        _tmpws = ConvertUnits(_tmpws, Target = "dSpacing")
24        E1 = _tmpws.getRunID("EnergyRequest").value[0]
25        a = GETE1("tmpws")
26        ChangeBinOffset(InputWorkspace = "_tmpws", OutputWorkspace = "_tmpws", Offset = -a[3])
27        RunAndPostProcessSubAlgorithm(FindPeaks)

```

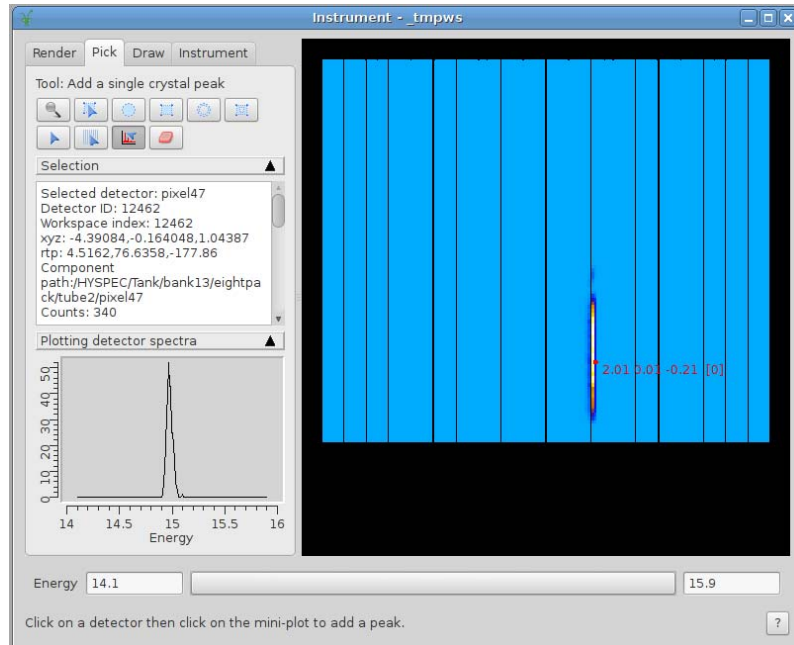
**HYS\_addPeak input dialog**

Filenumber	75637	⌵
a,b,c (Angstrom)	3.783,3.783,13.2	⌵
alpha, beta, gamma (deg)	90.0,90.0	⌵
u (r.l.u.)	1,1,0	⌵
v (r.l.u.)	1,-1,0	⌵
GoniometerVerticalAxis	Ox2WeldRot	⌵
PeakPickAxis	E	

?      Keep Open       Run      Close

Click on the instrument-view screen, then click on the peak position, to set the

peak and create the SingleCrystalPeakTable.



- ii. If you have more files with more peaks to tab, re-run HYS\_addPeak with the new run number.
- iii. When you are finished locating peaks, right-click on SingleCrystalPeakTable and edit the h, k and l fields as needed to make them integers you expect.

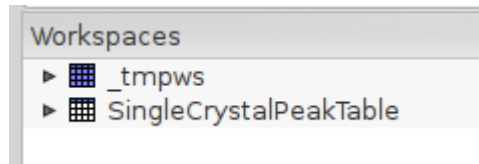


Table-1 - SingleCrystalPeakTable									
RunNumber	DetID[Y]	h[Y]	k[Y]	l[Y]	Wavelength	Energy[Y]	TOF[Y]	DSpacing	In
0	75637	12462	2.01	0.01	-0.21	2.33713	14.9765	26752.7	1.88471

Table-1 - SingleCrystalPeakTable									
RunNumber	DetID[Y]	h[Y]	k[Y]	l[Y]	Wavelength	Energy[Y]	TOF[Y]	DSpacing	In
0	75637	12462	2.00	0.00	0.00	2.33713	14.9765	26752.7	1.88471

- iv. You will then use the CalculateUMatrix Algorithm, with SingleCrystalPeakTable as input whose result will refine the \_tmpws workspace U matrix (I think) and will change the index values shown on the instrument view for \_tmpws
- v. If you then get a handle on the SingleCrystalPeakTable workspace in MantidPlot's screen interpreter screen by typing:  
`handle=mtd[<SingleCrystalPeakTable>]`  
you can then get the UB matrix by:  
`handle.sample().getOrientedLattice().getUB()`  
and the u or v vectors respectively by:

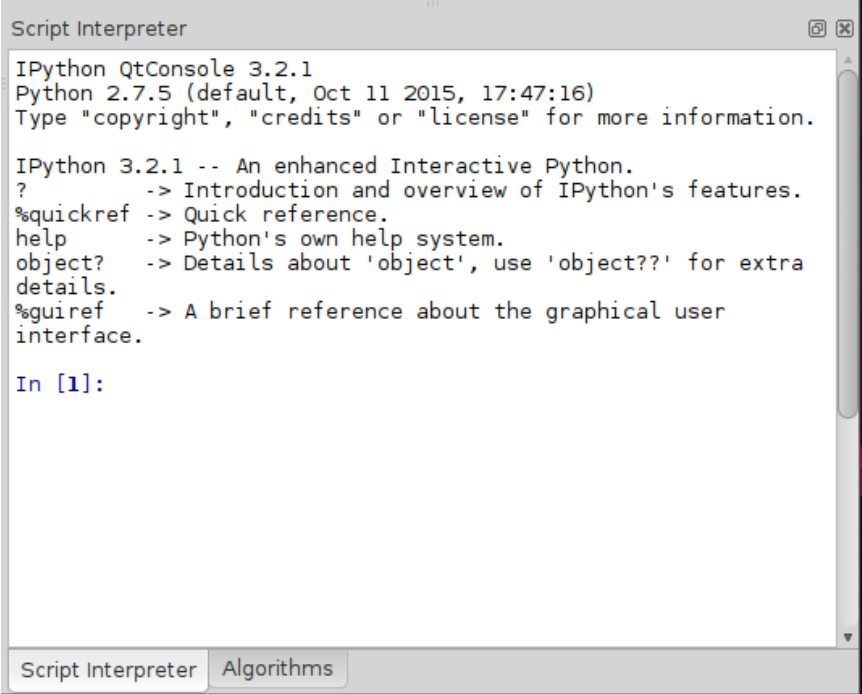
```
print handle.sample().getOrientedLattice().getuVector()
```

or

```
print handle.sample().getOrientedLattice().getvVector()
```

and of course the u and v vectors can be input into MSLICE. Finally, you can copy all UB matrix, u vector, v vector, etc over to an arbitrary SPE workspace using:

```
CopySample(InputWorkspace=<SingleCrystalPeakTable>,  
OutputWorkspace=<_tmpws>, CopyName=False, CopyMaterial=False,  
CopyEnvironment=False, CopyShape=False)
```

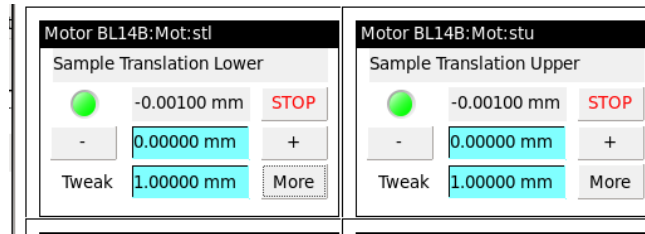


```
Script Interpreter
IPython QtConsole 3.2.1
Python 2.7.5 (default, Oct 11 2015, 17:47:16)
Type "copyright", "credits" or "license" for more information.

IPython 3.2.1 -- An enhanced Interactive Python.
?          -> Introduction and overview of IPython's features.
%quickref  -> Quick reference.
help       -> Python's own help system.
object?    -> Details about 'object', use 'object??' for extra
details.
%gui?ref   -> A brief reference about the graphical user
interface.

In [1]:
```

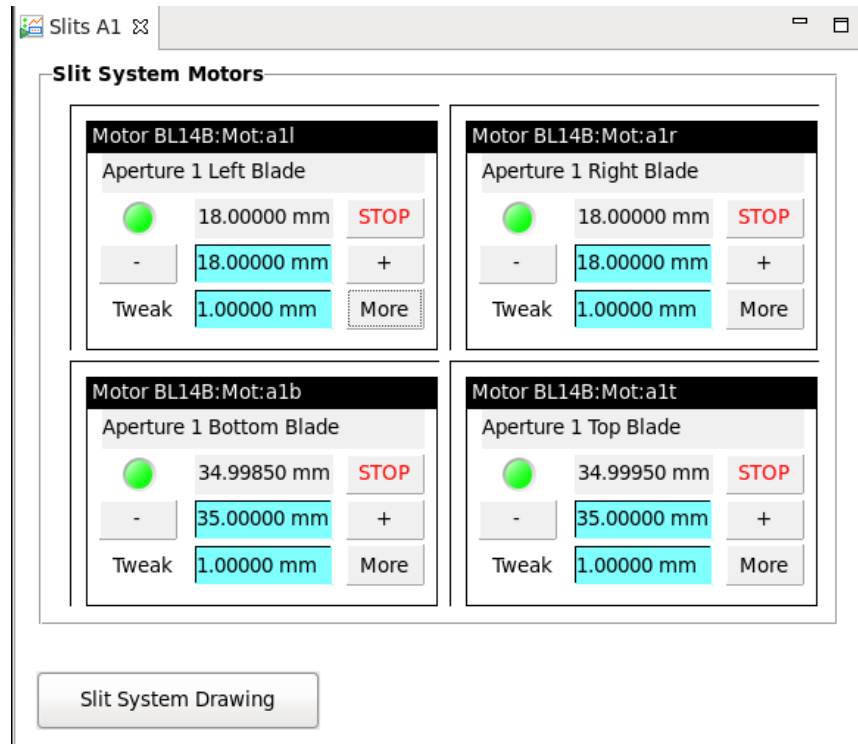
- o. Is my sample centered on the beam?
  - i. Has the potential to increase scattered intensity
  - ii. STU and STL, recommended step 2-5 mm.



- iii. Recommend that you scan the same translation stage as you did the goniometer stage (STU & SGU on same Bragg peak, for example)
    - iv. Rule of thumb: don't go much further than 5 mm in either direction
    - v. Needs to be done prior to aperture scans
  - p. Quirk of symmetry used: general crystallographic know-how
    - i. If you have a rhombic crystal, it's often easier to visualize and work with it using a hexagonal notation. HOWEVER, the mapping is only MOSTLY correct. Some Bragg peaks you might think are there are in fact not there. We recently had fun looking for a (1,1,4) peak, couldn't find it, and then went to a (-1,-1,4) peak and the Bragg peak 'appeared'. Since the system was rhombic, there was in fact no (1,1,4) peak to look for. So, word to the wise, if you're in a 'hexagonal' system, and you cannot find your bragg peak in one location, it might be wise to hunt for the other 'equivalent' peaks!

## 6. Remaining instrument setup tasks

- a. Aperture width selection
  - i. For polarization analysis and with strong cryo-magnets, we generally use manual apertures and have removed the motorized ones
  - ii. CSS Aperture 1 and Aperture 2 pages



Slits A2

### Slit System Motors

Motor BL14B:Mot:a2l	Motor BL14B:Mot:a2r
Aperture 2 Left Blade	Aperture 2 Right Blade
17.99950 mm STOP	18.00000 mm STOP
- 18.00000 mm +	- 18.00000 mm +
Tweak 1.00000 mm More	Tweak 1.00000 mm More

Motor BL14B:Mot:a2b	Motor BL14B:Mot:a2t
Aperture 2 Bottom Blade	Aperture 2 Top Blade
34.99996 mm STOP	35.00000 mm STOP
- 35.00000 mm +	- 35.00000 mm +
Tweak 1.00000 mm More	Tweak 1.00000 mm More

A1 Diagram

**Beam direction is OUT of screen.**

**Positive direction is away from the beam for all blades.**

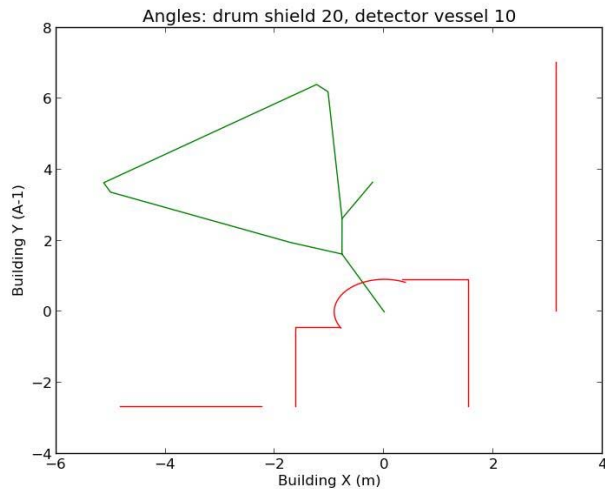
**Center and gap motors will move either Top and Bottom or Left and Right.**

- iii. Alignment scan parameters recommended
  1. A1T, A1B, A2T, A2B: range(35,-1,-5)
  2. A1L, A1R, A2L, A2R: range(18,-1,-3)
- b. REMOVE ANY BORATED ALUMINUM ATTENUATORS. Too many users have stories of forgetting to remove the attenuator until the next morning. As an inelastic instrument, we need every neutron we can get.
- c. Improving horizontal divergence?
  - i. Most users DON'T do this.
  - ii. Soeller collimators manually put in

## 7. Deciding on instrument configuration

- a. Don't hit the wall!

```
#Real_space_plot(M2_deg_try, S2_deg_try, MSD_m_try=1.8,  
SafetyRadius_m=0.25, FillStation3He=0 )
```



```
Real_space_plot(20,10)
```

```
Is_Position_Safe(15,15)
```

```
#Is_Position_Safe(M2_deg_try, S2_deg_try, MSD_m_try=1.8,  
SafetyRadius_m=0.25, FillStation3He=0 )
```

- b. HYSPEC's incident energy restrictions

```
#IsEiOverPromptPulse(Ei)
```

```
IsEiOverPromptPulse(20)
```

```
output: good Ei
```

- a. Energy resolution tools

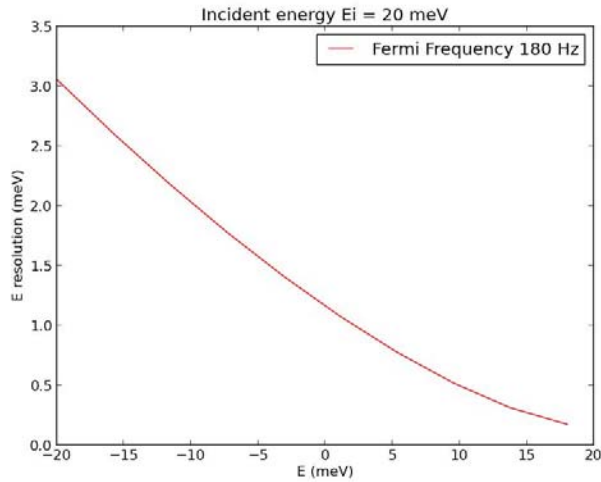
```
#Resolution_Calc_single(Ei,Ef,msd=1.8,FermiFreq=180.0)
```

```
Resolution_Calc_single(20,20)
```

```
output: energy resolution in FWHM is 1.16 meV
```

```
#Plot_Resolution_vs_E(Ei,EMin,EMax,nE,msd=1.8,FermiFreq=[18  
0.0])
```





Plot\_Resolution\_vs\_E(20,-20,18,10)

b. Momentum resolution tools

(development state. Not yet ready for prime time)

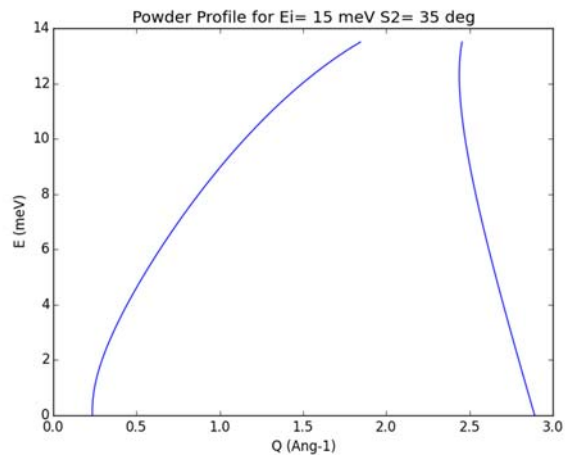
c. Flux tradeoff tools

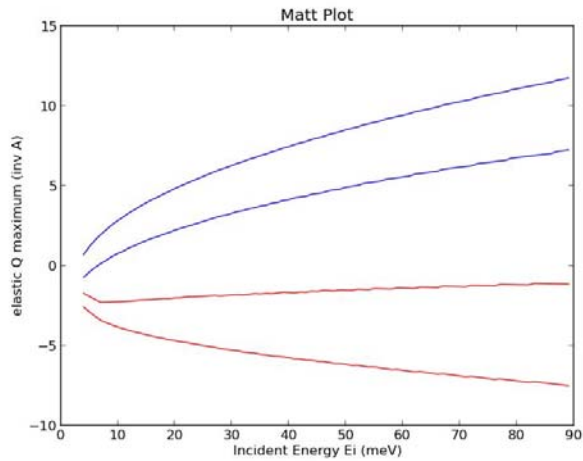
```
#relative_flux(Ei1_meV,Fermi1_Hz,Ei2_meV,Fermi2_Hz)
relative_flux(20,180,20,420)
output: relative flux ratio is 2.3
```

d. Powder planning tools

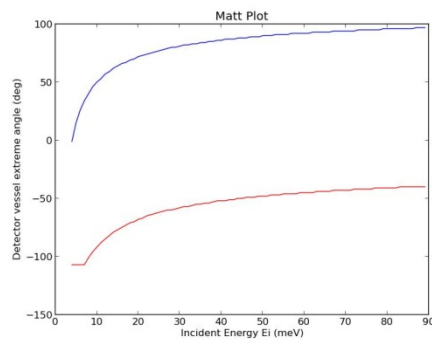
- i. Typically users know the desired momentum transfer Q and desired energy transfer E.
- ii. Planning tool functions

Plot\_PowderRange(Ei, S2)





PlotExtremeQ()



PlotExtremeQ(S2instead=True)

c. Single crystal planning tools

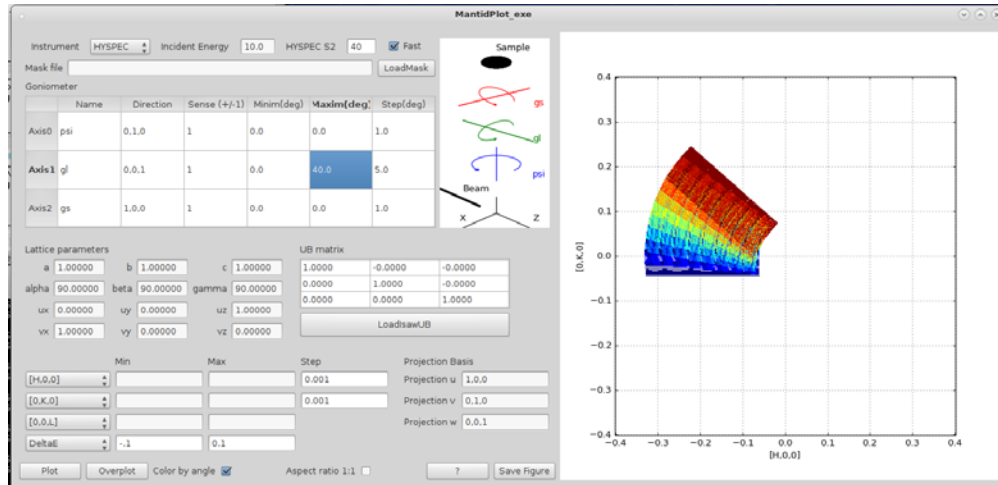
```
CubicCrystal=Crystal((4,4,4),(1,0,0),(0,1,0))
```

```
hexCrystal =
Crystal((4,4,4),(1,0,0),(0,1,0),alphabetagamma=(90.0,90.0,1
20.0))
```

```
CubicCrystal.WhereIsBragg((1,0,0),25)
CubicCrystal.WhereIsBragg((1,0,0),25,left=True)
```

```
Crystal.WhereIsBragg(hkl,Ei_meV,E_meV=0.0,left=False,
S1offset=0.0)
```

e. MANTID experiment planning GUI



f. HORACE planning GUI

i. Generating the PAR file

g. The final quick easy check

i. Simulate via very short runs with a larger rotation step size in the desired experiment configuration

ii. View using DAVE MSLICE. Is this what you really want?

h. Other strange considerations

i. When using a copper mount, common for DF inserts because copper doesn't go superconducting like Aluminum does at about 1 K, you can expect major multiple scattering background and major powder rings from the copper. However, if you use an  $E_i$  of 6 meV or less, all that disappears. It's because Cu is cubic with lattice spacing  $a=b=c=3.615$  Angstrom, so above 6.26 meV the scatter can be painful. An easy check of this is to look for powder rings on ICSD for copper at the appropriate energy or wavelength.

## 8. Moving to desired instrument configuration

### a. CSS Ei page

Incident Energy

Desired Incident Energy: 0.000 meV <-- "Enter" on desired energy starts update of motors & choppers!

Last successfully set: 13.000 meV

Fermi Chopper Speed: 300 Flat Focusing Test Mode

Fermi speed, flat focusing become active the next time a desired energy is entered. Consider using Test Mode before actual energy update.

Speed Req.	Energy Req.	Lock	OK
T0: 0 Hz	13.0 meV	<span style="color: orange;">●</span>	<span style="color: green;">●</span>
T1A:	13.0 meV	<span style="color: orange;">●</span>	<span style="color: green;">●</span>
T1B:	13.0 meV	<span style="color: orange;">●</span>	<span style="color: green;">●</span>
Fermi: 300 Hz 0 Hz	13.0 meV	<span style="color: orange;">●</span>	<span style="color: orange;">●</span>

Monochromator: PG

Heusler Rotation: 19.84750 deg ●

Heusler Focus: 0.857000 mm ●

P.G. Rotation: 21.95250 deg ●

P.G. Focus: 0.85200 mm ●

Detector Vessel: -50.0187 deg

Drum Shield: 1785.50086 mm

Drum Shield: 44.0001 deg ●

### b. CSS User Detector Vessel Page

Detector Vessel Motion

Motor BL14B:Mot:vs2

Det Vessel (s2) vMot

● -50.019 STOP

-50.000 More

**Sequence Program For Moving Detector Vessel**

Program Running ●

State Idle

Message Idle

Error Message

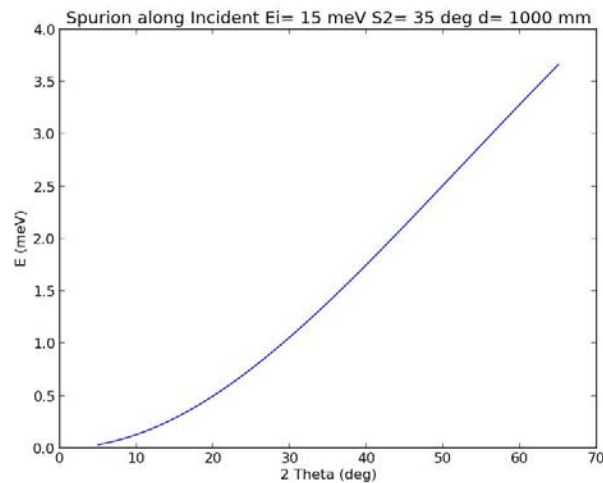
Error ●

- i. Why is my detector vessel not moving?
  - ii. When you know you're close to the wall...
- c. If you must avoid vertical focusing...
- i. CSS Heusler and PG Pages

## 9. Locate and minimize spurious scattering

- a. If you have a single crystal and have not done step 7.j., go back and get it done.
- b. Sit in one position, away from a Bragg peak, and do a 5-10 minute run in a fixed position.
- c. Observe the result in a E vs. Q geometry, either from the web interface or using one of the analysis tools.
- d. The following spurious planning tools can assist you in diagnosing any unexpected features:
  - i. A parabolic energy spurion that may have some aluminum Powder points, arising from scatter upstream or downstream of the sample, somewhere along the monochromatic incident beam. D\_along\_mm can be positive or negative, causing an energy loss or energy gain feature, respectively

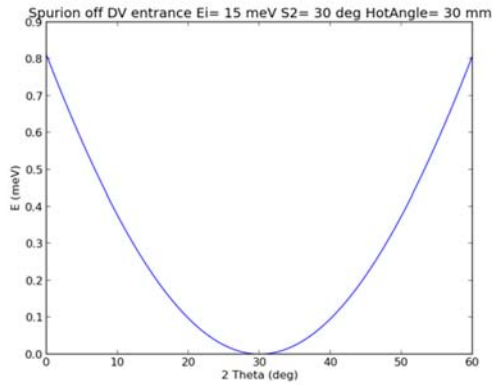
`Plot_Spurion_along_incident(Ei,S2,d_along_mm)`



`Plot_Spurion_along_incident(15,35,1000)`

- ii. Similarly, an incident beam or strong Bragg peak that hits the entrance window of the detector vessel (at angle 'TwoThetaHot') can also introduce an energy loss dependent background feature.

`Plot_Spurion_off_DV_Entrance(Ei,S2,TwoThetaHot)`



`Plot_Spurion_off_DV_Entrance (15,30,30)`

- iii. Spurion from isotropic scatter from sample position, scattering off of something cylindrically symmetric like our OVC, then back to detectors. Output is flat energy feature in meV.

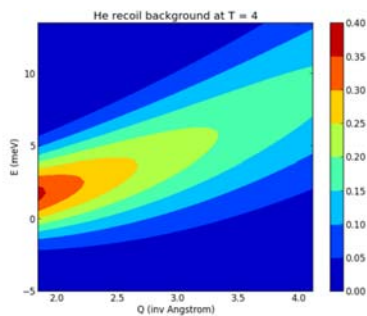
```
Spurion_fromSampleNBackscatter(Ei,r_mm)
Spurion_fromSampleNBackscatter(15,500)
output: flat energy spurion at 4.95 meV
```

- iv. Spurion from isotropic scatter from sample position, scattering directly above or below, then back to detectors. Output is flat energy feature in meV.

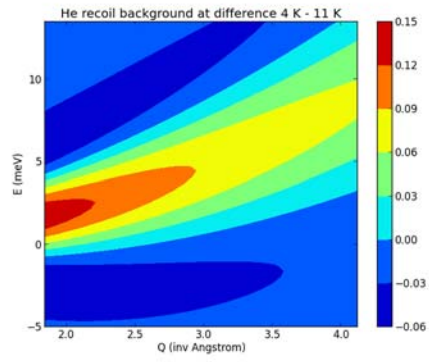
```
Spurion_fromVerticalOffscatter(Ei,r_mm)
Spurion_fromVerticalOffscatter(15,60)
output: flat energy spurion at 0.39 meV
```

- v. Spurion from Helium Recoil

```
RecoilRawContour(Ei,S2,T (temperature in Kelvin))
RecoilRawContour(15,70,4)
```



```
RecoilDiffContour(Ei,S2,T_low,T_high)
RecoilDiffContour(15,70,4,11)
```



## 10. Polarization mode

### a. Setup

psda

psr

### b. Acquisition

#### i. CSS Mezei Flipper Page

	Sum	Status	Voltage	Prot. V	Current	Over Voltage	Over Current	Over Temp.	Details
Comp		ON	3.84 V	22.00 V	9.530 A	OK	OK	OK	...
Flip		ON	1.94 V	22.00 V	5.008 A	OK	OK	OK	...
Guide		OFF	- 0.00 V	22.00 V	-0.001 A	OK	OK	OK	...
Z		OFF	0.01 V	55.00 V	0.013 A	OK	OK	OK	...

Summary Alarm

Control BL14B:Pol:Mez1:Comp

State ON Mode Voltage Range 8V

Calculated Power 36.6 W

Voltage		Current	
DC VOLTS (Volts)		DC Current (Amps)	
<input type="text" value="8.00"/>	3.8362	<input type="text" value="9.50"/>	9.5302
Protection Volt	22.00	Protect Level	22.00
Trip Status	ON	Trip Status	ON
<input type="button" value="ON"/> <input type="button" value="OFF"/> <input type="button" value="CLEAR"/>		<input type="button" value="ON"/> <input type="button" value="OFF"/> <input type="button" value="CLEAR"/>	


Status

Latched

Questionable Condition	<input type="button" value="CC operation"/>	Over Voltage	OK	
System Error	<input type="button" value="CC operation"/>	Over Current	OK	
		Overtemperature	OK	




ii. CSS Sample Coils Page

**3D Coils**      Coil Temp Alarm  Alarm Enable  Off  On


---

**Control Coil F**

Mode	Current	Curr	Volt	Voltage	Current
Output	OFF	ON	OFF	-0.0027 V	-0.0019 A
Rem/Loc	Rem	Rem	Loc	10.0	0.0
Coil Temp					

---

**Control Coil E**

Mode	Current	Curr	Volt	Voltage	Current
Output	OFF	ON	OFF	-0.0054 V	-0.0038 A
Rem/Loc	Rem	Rem	Loc	10.0	0.1
Coil Temp					


---

**Control Coil C**

Mode	Current	Curr	Volt	Voltage	Current
Output	OFF	ON	OFF	-0.0040 V	-0.0047 A
Rem/Loc	Rem	Rem	Loc	10.0	8.3
Coil Temp					


---

**Control Bottom**

Mode	Current	Curr	Volt	Voltage	Current
Output	OFF	ON	OFF	-0.0082 V	-0.0115 A
Rem/Loc	Rem	Rem	Loc	6.0	8.0
Coil Temp					

---

**Control Top**

Mode	Current	Curr	Volt	Voltage	Current
Output	OFF	ON	OFF	-0.0054 V	-0.0066 A
Rem/Loc	Rem	Rem	Loc	6.0	8.0
Coil Temp					

- iii. From direction and magnitude to currents on coils

Polarization Calculator			
p-angle	-125.000	out1 (c[0])	0.0000000000
s2	-40.000	out2 (c[1])	2.2648663818
field	20.000	out3 (c[2])	8.6766102630
ignoreCoils	0		

- iv. From HKL-w to currents on coils:

```
CurrentFromBasics(CrystalClass,Ei,hkl,w_meV,s2,left1=False,Fld=20.0, ignorecurrent=0)
```

```
run -i ForCoilOPI.py
```

```
CurrentFromBasics(NaCl,15.0,(1,0,0),5.0,-40.0,left1=False,Fld=20.0, ignorecurrent=0)
```

- v. Generate a table scan to track field along desired hkl-E space:  
-Edit MyTableGenerator.py, both routines.  
(this uses templates that have a static copy in the ForCoilOPI.py file)

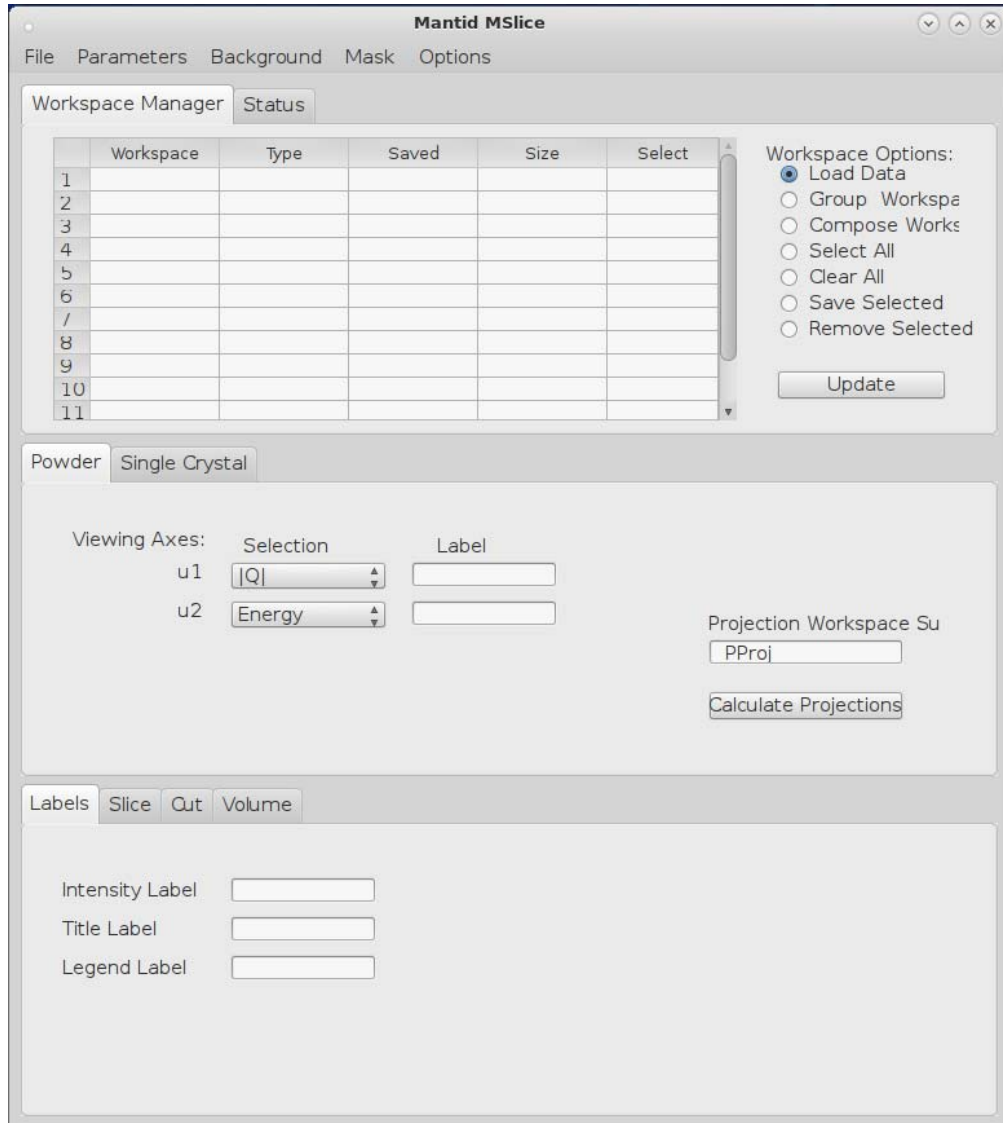
```
run -i MyTableGenerator.py  
MakeCSV_file_mine()
```

c. Analysis

- i. Done in autoreduction:
  1. TiZr normalization per-tube/pixel intensity normalization
  2. Angle correction
- ii. TiZr flip normalization (not done)
- iii. Done in script after autoreduction:
  1. Ef transmission normalization
  2. Flip ratio normalization
- iv. Sharpf equations: from 3-orthogonal-field with pre-sample flips to magnetic, nuclear coherent, isotope incoherent and spin-incoherent scattering. ONLY GOOD for POWDERS!
- v. Beyond Sharpf: multi-direction corrections (Ehlers et al), possibly useful for out of plane and low Q scattering

## 11. Visualize your results

- a. The HYSPEC Analysis computer
- b. Mantid MSLICE



- c. Mantid HORACE
- d. DAVE M-SLICE
  - i. Set up
    1. On analysis cluster, create a terminal window and enter  

```
dave
```
    2. On main screen, from the tab row at top, click on:
      - a. Data Reduction
        - i. NCNR
          1. DGS Reduction (Mslice)

2. Choose \*.nxspe format
3. On Mslice screen
  - a. Sample type:
    - i. Single Crystal
      1. Diffuse Scattering Multiple E
  - b. Energy Range
    - i. All
  - c. Option
    - i. View Axis
      1. Allow Extra Viewing Axis
  - d. Option
    - i. Binning Method
      1. Constant Intervals
        - a. Yes
- ii. Use: The MSLICE screen is divided into three sections vertically
  1. Top: Loading
    - a. Use files from the following directory:

`/SNS/HYS/IPTS-<your IPTS #>/shared/autoreduce/`

You have the option of either using '4pixel' data or 'msk\_tube' autoreduced data. The former bins pixels from each detector tube from 128 pixels into 32 groups, and masks the top and bottom 8 pixels. The latter bins the middle third of the (vertical) detector tube, roughly matching the vertical spread of the vertically focused Bragg peaks at 1.8 m focus element to sample distance. All these files ought to have the suffix \*.nxspe. If you prefer another format we can rereduce or modify our reduction script for autoreduction.

2. Middle: Calculating trajectories
  - a. Lattice parameters a,b,c in Angstroms; alpha,beta,gamma in degrees
  - b. U and V vectors are vectors in the scatter plane in r.l.u.  
They are most likely the vectors you used to initialize the Crystal class, unless you were not able to align in the plane. Then, you may need to use Mantid to determine these vectors. Their length is arbitrary (you don't have to normalize); only their direction matters.
  - c. Starting angle: the nominal starting angle for the first file of the set read in. If an offset angle was established during alignment, then you have to either add or subtract that offset angle (?).

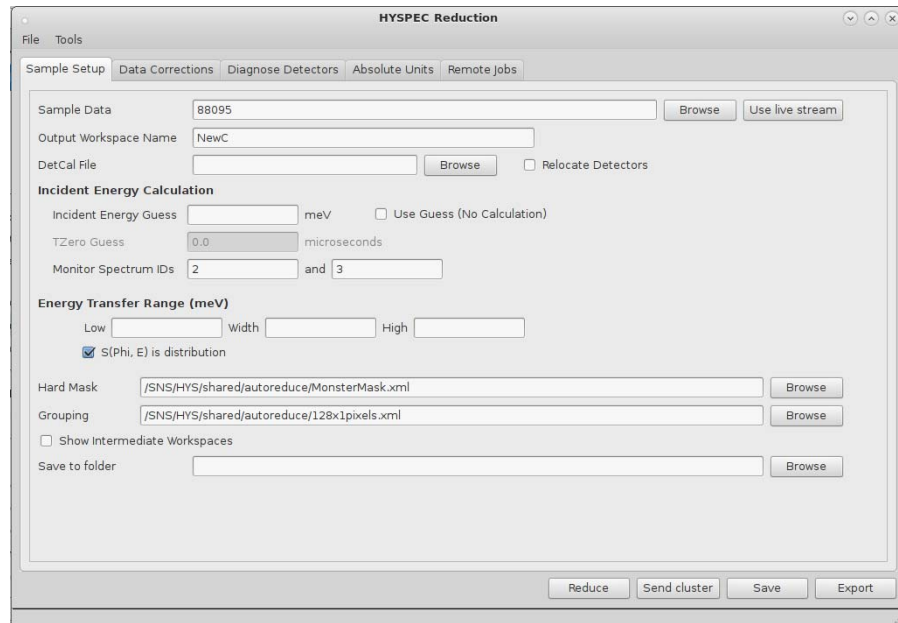
3. Bottom: viewing
  - a. Volume view is most flexible, allowing for slices and 1D's
- iii. Using MSLICE to plan and get trajectories
  1. Top section
    - a. Load at least one file for those you want to explore
    - b. Clear Data
  2. Middle section: Calculate projections
    - a. It asks if Ei is correct: hit OK
    - b. It then asks for the desired S1 angle range
  3. Bottom section: Detector trajectory tab
- e. Using Horace in MatLab
  - i. Open a terminal (either via menu or alt-f2 and type "gnome-terminal")
  - ii. Execute `/SNS/software/bin/setup_isis_matlab`
  - iii. Use Matlab-Horace link from the Analysis menu
  - iv. This will cause a file `~/startup.m` to be created in the user home directory, which means that all versions of Matlab should then try and use Horace. I don't know why the Matlab-Horace link points to r2011b, but I confirmed earlier that 2014a will run and says that it is using Horace.
  - v. You will need a \*.par file for each detector vessel geometry you use. For this, start MantidPlot, open up any raw data file that has the desired detector vessel geometry, and execute the algorithm SavePAR.
- f. Using TobyFit (????)

## 12. Autoreduction and Re-Reduction

- Autoreduction: what you're getting
- Also look for the following csv file that can be read by most spreadsheet programs:

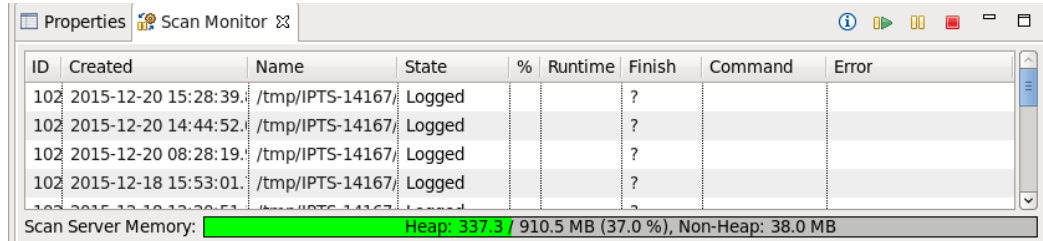
/SNS/HYS/IPTS-<your IPTS #>/shared/autoreduce/experiment\_log.csv

- Re-Reduction: in case you want to get something different
- Brute force GUI (almost never used but if you're curious...)



### 13. Automating your experiment acquisition

- a. General comments
  - i. Typically users set up scans to last ~20 to 24 hours, so they can come in the next day, look at analyzed data, and determine what the next step in the experiment needs to be
- b. CSS Scan Server Interface



ID	Created	Name	State	%	Runtime	Finish	Command	Error
102	2015-12-20 15:28:39.	/tmp/IPTS-14167/	Logged			?		
102	2015-12-20 14:44:52.	/tmp/IPTS-14167/	Logged			?		
102	2015-12-20 08:28:19.	/tmp/IPTS-14167/	Logged			?		
102	2015-12-18 15:53:01.	/tmp/IPTS-14167/	Logged			?		

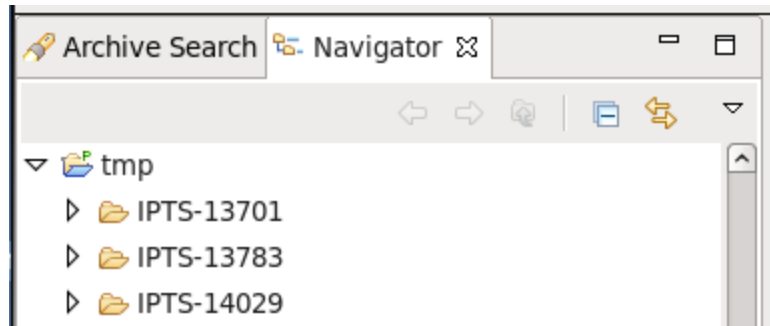
Scan Server Memory: **Heap: 337.3** 910.5 MB (37.0 %), Non-Heap: 38.0 MB

- i. If you have used the CSS Alignment Scan window, you have already used this software.
- ii. Note that when the scan server is active, some functions (buttons and blue fields) are frozen out for general users.
- iii. Bringing up Scan Server window from CSS
- iv. Stop Scan Server from CSS HYSPEC User page
- v. Stop / Pause / Resume Scan Server from CSS Server Window

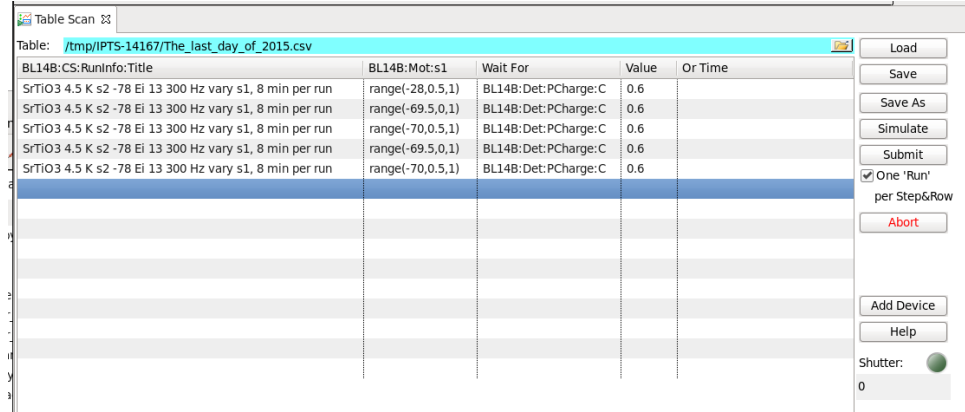


- vi. Show Scan status table. Right click on active scan.

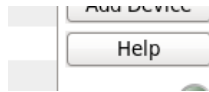
- c. CSS Table Scans
  - i. Generate your IPTS subdirectory



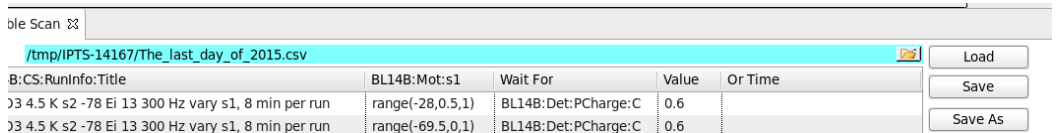
ii. CSS Table page



iii. Useful how-to radio button



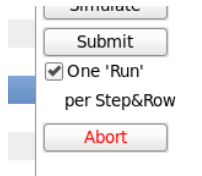
iv. Please be sure to save your scan so the Local Contact can view the same information via remote access



v. Reality check before submitting the scan



vi. Starting the scan

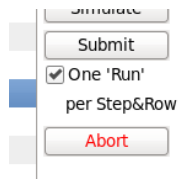


vii. Estimate when a scan will be completed

Name	State	%	Runtime	Finish
/tmp/IPTS-14167/	Logged			?
/tmp/IPTS-14167/	Logged			?

viii. Defaults

1. One NeXus run for the whole scan



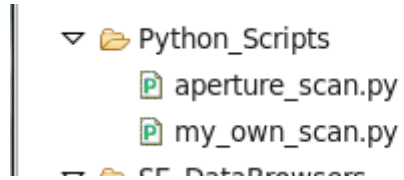
ix. List / table of typical PV's scanned for motors and sample environments <really need this table!>



x. Template subdirectory



d. CSS Script Scans



e. Monitoring your experiment

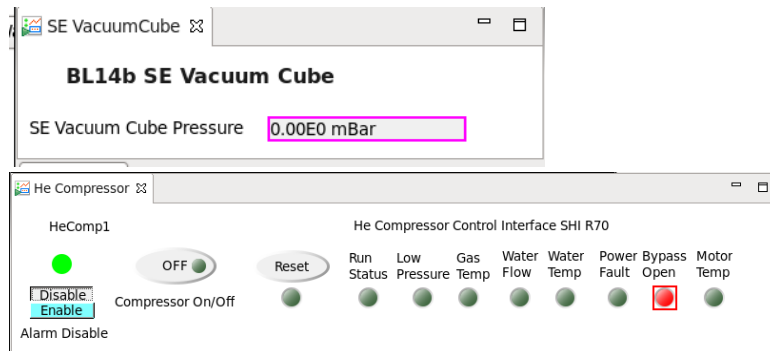
- i. At CSS
  1. CSS Monitor page
  2. CSS Scan Monitor functions
    - a. Scan status
- ii. On the Web

**14. What to do when you get home after your experiment is done**

- a. Accessing the Analysis Cluster
- b. Obtaining your data
- c. Preparing figures or movies
- d. Giving fantastic talks
- e. Presenting provocative posters
- f. Publishing results
- g. Letting us know

## 15. Software for data acquisition, under the hood

- a. EPICS
  - i. EPICS communication protocol
  - ii. EPICS database
  - iii. EPICS records
  - iv. EPICS alarming
  - v. EPICS equipment control (IOC software drivers)
- b. CSS
  - i. CSS Main Page
  - ii. CSS important mouse tricks
    - 1. For tablet and touchpad users: A mouse is moved over a surface (table or foam pad) to move a cursor around a screen. It also has one or more buttons and possibly a wheel at the finger positions, used to select various functions on various windows and regions of applications.
    - 2. For Mac users: Mice we use have two buttons. The left button usually makes a field active or enables the start of an application. The right button usually opens a pull-down menu from which to choose options with the left button.
  - iii. CSS plotting archived data
  - iv. CSS Chopper Pages
  - v. CSS Sample Environment Pages
    - 1. CCR-19 & CCR-10



BL14B Lakeshore Main 11

### Lakeshore

Input	Temperature	Alarm	Polling	Desc
A	0.000 K	Alarm	Enabled	
B	0.000 K	No Alarm	Disabled	
C	0.000 K	Alarm	Enabled	
D	0.000 K	Alarm	Enabled	
D2	0.000 K	No Alarm	Disabled	
D3	0.000 K	No Alarm	Disabled	
D4	0.000 K	No Alarm	Disabled	
D5	0.000 K	Alarm	Enabled	
Summary Alarm		No Alarm		
Alarm Disabled		Alarm Disabled		

Sample Temp: 0.000 K

Model:   
 Serial:   
 Firmware:

Output:	1	2	3	4	1	2
Control Input	None	None	None	None	M/S Done	
Setpoint	0.000 K	0.000 K	0.000 K	0.000 K	0.000 K	0.000 K
	0.000 K	0.000 K	0.000 K	0.000 K	Offset	0.0
Range	Off	Off	Off	Off	Offset Table	
Ramp Rate	0.000 K/min	0.000 K/min	0.000 K/min	0.000 K/min		
Ramp Status	Off	Off	Off	Off		
Manual Output	0	0	0	0		
P	0	0	0	0		
I	0	0	0	0		
D	0	0	0	0		
Output mode	Off	Off	Off	Off		
Power Up Enable	Off	Off	Off	Off		
Heater Output	0.0 %	0.0 %	N/A	N/A		
Analog Output	N/A	N/A	0.0 %	0.0 %		
Heater Status	No Error	No Error	N/A	N/A		

Set all Setpoints **Disconnected** (blocks until all temperatures are within tolerance windows)

BL14B Lakeshore Output 1

### Lakeshore Power Output Control

Output: 1

Setpoint (SETP)	0.000 K	0.000 K
Range (RANGE)	Off	Off
Ramp Rate (RAMP)	0.000 K/min	0.000 K/min
Ramp Status (RAMP on/off)	Off	Off
Manual Output (MOUT)	0	0
P	0	0
I	0	0
D	0	0
Output mode	Off	Off
Control Input	None	None
Power Up Enable	Off	Off
Tuning Mode	P Only	<input type="button" value="Start Tune"/>
Heater Output	0.0 %	
Heater Status	No Error	<input type="button" value="Reset"/>

2. CRYO-09

The screenshot displays the control interface for the BL14B Cryostat. The window title is "BL14B Cryostat". The main section is titled "Cryostat" and contains several parameters:

- Setpoint Temperature: 0.00 K (highlighted in cyan)
- Actual Temperature: 0.00 K (highlighted in magenta)
- VTI Pressure: 0.000 mBar (highlighted in magenta)
- Sample Space Pressure: 0.000 mBar (highlighted in magenta)
- Operating Mode: Manual
- Heating or Cooling: (empty field)
- Details: (button)

The "Cryostat Lakeshore Alarm" section shows:

- Alarm: No Alarm (radio button selected)
- Alarm Disabled: (button, highlighted in orange)

BL14B Orange Cryostat

### Operation Modes & Setpoint

Mode: Manual Manual  
 Lakeshore Setpoint: Channel 1 0.00 K 0.00 K  
 Lakeshore Input: Input A 0.00 K

### Needle Valve Control & Calibration

KP 8.00 8.00 Close Valve Open Valve  
 KI 1.00 1.00  
 KD 10.00 10.00  
 Control Disabled Off  
 Setpoint 8.50 8.50  
 Deadband 0.20 0.20  
 Settle Time 60 s 60 s  
 In Deadband & Time  
 Controlled Pressure (VTI) 0.00  
 PID Details  
 Set Close Position 40000  
 Set Open Position 130000  
 130000

### Controllers (Pfeiffer Gauge and lakeshore)

Pressure Temperature  
 VTI 0.000 mBar A 0.000 K  
 Sample Space 0.000 mBar B 0.000 K  
 C 0.000 K  
 D 0.000 K  
 Lakeshore

### Heating Table

	Low Temp	High Temp	Setpoint	Disabled	
1	0.00	10.00	8.50	Disabled	Detail
2	10.00	50.00	7.00	Disabled	Detail
3	50.00	100.00	1.00	Disabled	Detail
4	100.00	1000.00	1.00	Disabled	Detail
Lakeshore Input	Input A	0.00			All Rows

### Cooling Table

	Low Temp	High Temp	Setpoint	Disabled	
1	0.00	3.00	10.00	Disabled	Detail
2	3.00	10.00	12.00	Disabled	Detail
3	10.00	1000.00	20.00	Disabled	Detail
4	0.00	0.00	0.00	Disabled	Detail
Lakeshore Input	Input A	0.00			All Rows

BL14B Lakeshore Main

### Lakeshore

Input	Temperature	Alarm	Polling	Desc
A	0.000 K	Alarm	Enabled	
B	0.000 K	Alarm	Enabled	
C	0.000 K	No Alarm	Disabled	
D	0.000 K	No Alarm	Disabled	
D2	0.000 K	No Alarm	Disabled	
D3	0.000 K	No Alarm	Disabled	
D4	0.000 K	No Alarm	Disabled	
D5	0.000 K	No Alarm	Disabled	
Summary Alarm				No Alarm
Alarm Disabled				Alarm Disabled

Sample Temp 0.000 K Setup

Alarms / Input Status  
 Software Limits  
 Tolerance Windows  
 Descriptions  
 Raw Voltages

Model  
 Serial  
 Firmware  
 Epics Software Control

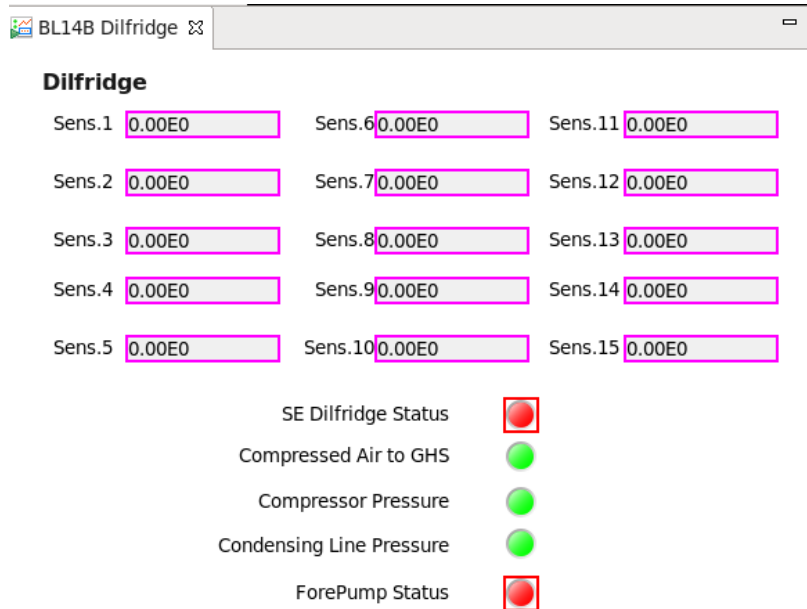
### Output: 1 2 3 4

Control Input: None None None None  
 Setpoint: 0.000 K 0.000 K 0.000 K 0.000 K  
 Range: Off Off Off Off  
 Ramp Rate: 0.000 K/min 0.000 K/min 0.000 K/min 0.000 K/min  
 Ramp Status: Off Off Off Off  
 Manual Output: 0 0 0 0  
 P: 0 0 0 0  
 I: 0 0 0 0  
 D: 0 0 0 0  
 Output mode: Off Off Off Off  
 Power Up Enable: Off Off Off Off  
 Heater Output: 0.0 % 0.0 % N/A N/A  
 Analog Output: N/A N/A 0.0 % 0.0 %  
 Heater Status: No Error No Error N/A N/A  
 Output 1 Output 2 Analog Out 3 Analog Out 4

Master/Slave: Discon Discon M/S Done Discon Discon Offset Discon Offset Table

Set all Setpoints Disconnected Dis (blocks until all temperatures are within tolerance windows)

### 3. CRYO-09 with DF



BL14B Dilfridge

**Dilfridge**


Sens.1 0.00E0    Sens.6 0.00E0    Sens.11 0.00E0


Sens.2 0.00E0    Sens.7 0.00E0    Sens.12 0.00E0


Sens.3 0.00E0    Sens.8 0.00E0    Sens.13 0.00E0


Sens.4 0.00E0    Sens.9 0.00E0    Sens.14 0.00E0


Sens.5 0.00E0    Sens.10 0.00E0    Sens.15 0.00E0

SE Dilfridge Status 

Compressed Air to GHS 

Compressor Pressure 

Condensing Line Pressure 

ForePump Status 

4. CRYO-09 with 3He: Using the Lakeshore shown in section 1 but with a different Lakeshore (350 instead of 336).

5. SLIM-SAM

vi. Least User Privileges

1. Your local contact can become a 'super user' that can do things you cannot, including
  - a. Modifying things while a scan is running
  - b. Change sample environments
  - c. Stop and restart software drivers associated with different instrument functions.

c. ADARA

i. Adding PV's to the NeXus file and for the HYS.MONITOR.GOV webpage remote monitoring:

1. On the OPI machine, even under the user account, edit the `/home/controls/bl14b/beamline.xml` file (not for the squeamish)

d. NEXUS

e. MANTID

- i. Mantid algorithms verified (?)
- ii. Live Viewing with Mantid
- iii. DGS Reduction Interface

f. Planning tools in Python

- i. Starting on Analysis Cluster or HYSPEC Analysis PC

```
cd /SNS/users/inelastic/HYSPEC
```

```
ipython
run -i rotations.py
run -i ubmatrix_out.py
run -i userlib_hys_out.py
```

ii. Starting on OPI

```
./mountHYS...
cd /SNS/PLAN
ipython
run -i rotations.py
run -i ubmatrix_out.py
run -i userlib_hys_out.py
```

iii. List of commands in alphabetical order, and section to go to for learning about them.



## 16. How HYSPEC is calibrated

- a. Assumptions at the start of calibration
  - i. Engineered drawings locate choppers, sample and detector 8-packs
  - ii. Position and time-delay profile of moderated pulse
    - i. From neutronics group (?)
    - ii. Same functional form used for chopper phase setting and Mantid autoreduction
- b. Functional form for Fermi chopper phase as a function of energy
  - i. Speed as a function of neutron kinetic energy
  - ii. Incorporate time delay profile of moderated pulse
  - iii. Chopper speed related phase offset when Top Dead Center (TDC) sensor is not exactly at chopper opening
  - iv. Confirm chopper direction and TDC sensing mode prior to calibration
  - v. Very slight empirical adjustment to fit to vanadium elastic line
    - i. First round, middle of each of 4 panels
    - ii. Plot, TOF vs detector tube
    - iii. Plot, converted to E vs detector tube
    - iv. Energy resolution FWHM for V is same as for predicted energy resolution
- c. Verifying that low-resolution choppers are centered

We can and should measure against neutron monitor 2 for this, to avoid any complications concerning possible misalignment downstream. All three choppers when scanning against phase have very broad plateaus due to the wide acceptance angles of these choppers.

  - i. T0
  - ii. T1A
  - iii. T1B
    - i. Temporary offset due to leak in Fermi chopper
- d. Focus array and drum shield calibration
  - i. Note the MTHU and MGHU motors are constrained as described in (), so we have set their positions, turned off their drives, and don't intend to run them again unless we observe some real problems.
  - ii. Ensure that sample is centered by confirming same count-rate at a variety of angles. Adjust STL and STU as needed to center.
- e. Scatter angles from powder samples: detector vessel calibration
  - i. Preferred material: alumina powder
  - ii. Either multiple S2 angles or verifying that ring is mostly on a single 8-pack ensures good coverage of a Powder ring
  - iii. Location in 2theta of powder ring on both sides determines nominal S2 offset
  - iv. Indirect measure of energy via 2theta angle
- f. Maintaining calibration
  - i. Periodic visual checks of calibration

- ii. Motorized stage position verification
  - i. S2 absolute encoder
  - ii. Msd stop
  - iii. M2 multiple encoders
  - iv. Focus array encoders
- g. Next round: possible multi-energy calibration using flat energy loss modes
  - i. Gamma picoline? Can be purchased easily.
  - ii. Para-hydrogen? Need gas handling sample environment with  $T < 14$  K. See flat excitation at 14.7 meV.
  - iii. Acetomenaphrin?
  - iv. Other?

## 17. Modeling excitations to compare against measurements

- a. Back of Envelope
- b. Density Functional Theory
  - i. CASTEP
  - ii. VASP
- c. Spin Waves
  - i. Spin Genie
  - ii. Spin W
- d. Crystal Field Excitations
  - i. McPhase
- e. Scattering kernel, monte carlo
  - i. McVine
- f. Phonons brute force
  - i.
- g. Accelerys Materials Studio

## 18. Accounting for corrections

- a. From model to measurement: sample & instrument simulation
  - a. Instrument simulation using McStas
  - b. Sample simulation using McVine
- b. From measurement backwards
  - a. Resolution function
    - i. Estimating using python functions
    - ii. Estimating using McStas
    - iii. Estimating using TobyPlot
    - iv. Deconvolution using TobyPlot
    - v. Mantid not there yet...
  - b. Multiple scattering correction
  - c. MultiPhonon scattering correction

## 19. Remote access

- a. When you're on the HYS-OPI or any analysis PC and need access to the FireFox browser for cameras or other useful things: from a command line in a terminal, type **fix-firefox-settings**, hit enter, and the browser on your other account on another machine will end so you can start afresh!

## 20. Camera views

[Hyspeccam.ornl.gov](http://Hyspeccam.ornl.gov)

[hyspecwcam.ornl.gov](http://hyspecwcam.ornl.gov)

[hyspecmezcaml.ornl.gov](http://hyspecmezcaml.ornl.gov)