## CLS Run Summer 2019 Logbook

June 12-14, 2019

Participants: Nazanin Samadi, Zisis Papandreou, Mehran Talebitaher, Benjamin Willis, and Richard Jones

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#### **Contact Information**

- Phone numbers
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  - b. Richard Jones, email: richard.t.jones@uconn.edu, cell: 860-377-5224
  - c. Mehran Talebitaher, email: <u>Alireza.Talebitaher@uregina.ca</u>, cell: 306-541-3848
  - d. Benjamin Willis, email: benjamin.willis@uconn.edu
  - e. Nazanin Samadi, email: Team Member, cell: 306-717-5469
  - f. Sergey Gasilov, email: <u>Sergey.Gasilov@lightsource.ca</u>, BMIT Staff Scientist, office: 306-657-3643
  - g. Adam Webb, BMIT Science Associate, office: 306-657-3846, cell: 306-372-8304
  - h. Denise Miller, email: Denise.Miller@lightsource.ca, office: 306-657-3815
  - i. BMIT and other CLS phone numbers are listed in the two images below.



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Canadian Centre canadien Light de rayennement Source synchrobron

#### BMIT BM Beamline 05B1-1 CONTACT LIST

\*\*Note: From any CLS phone you must dial '9' to access an external line. For CLSI internal numbers (prefix 657) you only need to dial the 4 digit extension

			306-227-3113 306-227-0759	
			306-227-0759	
			206 220 2002	
			300-230-2803	
	Roon	n P	hone	
	1128	30	306-657-3628	
	1129	30	06-657-3629	
tory	1112			
itory	1123	3	06-657-3843	
306-65	7-3815	Adam Webb	306-657-3846	
306-65	57-3589	BL Wireless	306-657-3630	
ce:			306-657-3639 306-657-3663 <sup>306-657-3700</sup>	
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Ught de rayonnement Source synchrotron	
Contact	
1-306-657-XX	XX
Floor Coordinator	3639
Sergey Gasilov	3653
Denise Miller	3815
Adam Webb	3846
Ning Zhu	3589
BMIT Mobile	3630
R. 1128 05ID-2	3628
R. 1113 Large Animal Lab	3843
R. 1129 05B1-1	3629
R. 1112 Small Animal Lab	3809
R. 1117 BMIT Computer Lab	3807
R. 1125 BMIT User Lounge	3831
R. 1123 BMIT Guest	3641
BMIT Hutch POE2	3631

## Goals for this run

- 1. Unpack the diamonds
- 2. Mount JD70-101 on holder and install in beamline
- 3. Check out beamline optics and verify camera focus
- 4. Take rocking curves of JD70-101 in 4 orientations
- 5. Transfer data from JD70-101 to UConn, verify data quality
- 6. Dismount JD70-101 and return to packaging
- 7. Mount JD70-103 on holder and install in beamline
- 8. Take rocking curves of JD70-103 in 4 orientations
- 9. Transfer data from JD70-103 to UConn, verify data quality
- 10. Dismount JD70-103 and return to packaging
- 11. Mount JD70-106 on holder and install in beamline
- 12. Take rocking curves of JD70-106 in 4 orientations
- 13. Transfer data from JD70-106 to UConn, verify data quality
- 14. Dismount JD70-106 and return to packaging
- 15. Mount JD70-107 on holder and install in beamline
- 16. Take rocking curves of JD70-107 in 4 orientations
- 17. Transfer data from JD70-107 to UConn, verify data quality
- 18. Dismount JD70-107 and return to packaging
- 19. Mount JD70-109 on holder and install in beamline
- 20. Take rocking curves of JD70-109 in 4 orientations
- 21. Transfer data from JD70-109 to UConn, verify data quality
- 22. Dismount JD70-109 and return to packaging
- 23. Mount JD70-100 on holder and install in beamline
- 24. Take rocking curves of JD70-100 in 4 orientations
- 25. Transfer data from JD70-100 to UConn, verify data quality
- 26. Dismount J70-100 and return to packaging
- 27. Mount JD70-104 on holder and install in beamline
- 28. Take rocking curves of JD70-104 in 4 orientations
- 29. Transfer data from JD70-104 to UConn, verify data quality
- 30. Dismount J70-104 and return to packaging
- 31. Mount JD70-105 on holder and install in beamline
- 32. Take rocking curves of JD70-105 in 4 orientations
- 33. Transfer data from JD70-105 to UConn, verify data quality
- 34. Dismount J70-105 and return to packaging
- 35. Transfer all remaining data, photos, and software tools to UConn
- 36. Clean up and check out

# **CLS Beam Permit document**

The Permit below is posted online (in previous years it was posted outside the BMIT door.

Session Peri Dashboard / My Projects /	nit — BMIT-BM_ 28G09539~Papandreou / BMIT-BM	2019-06-12 08:56	
28G09539 — Ro BMIT-BM On-Site Permi	ocking Curves of Artificia	al Diamond Radiators	
Active	Beamline: BMIT-BM	Staff: Adam Webb	Representative: Zisis Papandreou
Required Permissions: FACILITY-ACCESS (all) BMIT	-BM-USER (all)		

## **Experimental Sign-in**

Once the crew received its BSO (Beam Safety Operations) training, Adam Webb credited each member with the completion of the course. Then, each member had to log into their CLS account and accept the completion before the PI (ZP) could Sign in and take control of the experiment. At the end of the beam time, ZP will sign off. Also, if the experiment is to be left unattended, this can be indicated. All actions can be carried out by clicking on the respective button at the top right of the PI's account. See screenshot below.

Session Permit — BMIT-BM_2019-06-12 08:56 Dashboard / My Projects / 28609539-Papandreou / BMIT-BM_2019-06-12 08:56						Û		۲
28G09539 — Rocking Curves of Artificial Diamond Radiators				View Log	Unattend	Update	Project	() Sign-Off
Active	Beamline: BMIT-BM	Staff: Adam Webb	Representative: Zisis Papandreou			Jur June 14t	ne 12th/20 th/2019 0	019 08:56 - )8:00 (now)

## Info from previous runs

The logbooks from the August, 2016 run is a valuable store of useful information for how to carry out these rocking curve measurements at CLS. Use the link below to obtain read-only access.

- Logbook from GlueX CLS summer run 2016
- Link to photos taken during summer run 2016

- Logbook from CLS run in September, 2016
- Link to photo directory from September, 2016
- Logbook from GlueX CLS fall run 2017
- Link to photo directory from November, 2017

## Shift schedule

#### June 12, 8:00am [rtj, ns, zp, mt, bw, dw]

We have initiated the run, and are now setting the optics. To complete our plan, we need to run continuously 24/7 through 8:00 on Friday morning (48 hours). At the beginning all of us were on shift, but once we are underway and procedures are communicated, we made a plan for manning the counting room around the clock.

- June 12:
  - 08:00-22:00, all of us.
  - o 22:00-24:00, Nazanin, Richard and Zisis
- June 13:
  - o 00:00-08:00, Richard and Zisis
  - 08:00-16:00, Mehran, Nazanin and Ben
  - 16:00-24:00, all of us.
- June 14:
  - 00:00-08:00, Richard and Ben

# **Unpacking the diamonds**

The diamond were hand-carried to CLS by Richard in a locked carrying case. It did not need to be opened during airline security checks or customs. Here is a picture showing the inside of the case when it was opened, and the contents of the samples container.







# Setting up the goniometer, camera

None of the mountings for the target rotation stages or the camera were left over from last time we ran, so we had to reconstruct it from memory. The first thing we had to solve is how to mount the camera for down-bounce geometry. We tried various ways to align the holes in the aluminum mounting bracket and the vertical rail, but ran into the same problem as last time, that none of the holes in the hole pattern would allow us to (1) keep the camera aperture low enough to contain the down-bounce image, and (2) achieve close to the 28° angle for  $2\Theta$ =28.42° Bragg. The following images replicate the solution we had from last time.



## **Beamline optics**

For leveling purposes ensure that both horizontal lasers are set to the "MONO" setting.

The motor assignments are as follows:

- 1. cable 1 vertical motion stage on the target
- 2. cable 2 vertical motion stage on the camera
- 3. cable 3 target chi angle
- 4. cable 4 target theta (Bragg) angle
- 5. cable 7 target phi angle

The camera scintillator was YAG-500um. With that scintillator we were getting relatively low intensity images in the camera, even with the maximum shutter time set to 999 ms. To get a brighter image, we replaced the scintillator with a GADOX-20um. This should give us a factor of 2 increase in intensity. This is close to what we see. The Xray image below shows the top edge of the diamond of the diamond illuminated by the beam at close to the Bragg maximum. We adjusted the vertical height of the target until the intensities of the images at both the upper and lower edges were approximately equal. The **chi angle** was set to zero, and the position of the camera adjusted to center the diffracted image in the camera viewport.



We used a tungsten pin attached to the front of the camera scintillator to optimize the focus of the camera. We then selected a region of interest within the camera frame  $1120 \times 1156$  (height x width). The beam has a (2,2,0) Si double-bounce (downward) mono set to what we think is 20 keV, followed by 0.8mm aluminum filter. The aluminum takes out the soft X-rays, and it lowers the heat load on the white beam mono. We are now ready to run our first scan.

## **Beamline controls**



X BMIT_B1_Filters/bmitB1Filters.edl		_ = ×
	BMIT BM Beamline Filters Control	
Filter 1	Filter 2	Filter 3
Current Filters Aluminu	m none	none
0.883 (0.	800 ) mm 0.000 (0.000 ) mm	0.000 (0.000 ) mm
position: -890000 Ream Direction	-1109000	
Filters Enabled: O Photo	on Shutter Status OPEN	Filters Calibration:
Status: In position		Calibrate Filters Ston Calibration
Status. In position		Camprate Finters
Filter Position 1 (Upstream)	Filter Position 3 (Downstream)	
open (switch 5) 0.000 ( 0.000) mm in position: O	open (switch 5) 0.000 ( 0.000) mm in position:	open (switch 5) 0.000 ( 0.000) mm in position:
Filter 1 u Aluminum (switch 4) 0.883 ( 0.800) mm in position:	Filter 1 m Copper (switch 4) 0.276 ( 0.250) mm in position:	Filter 1d Silver (switch 4) 0.221 ( 0.200) mm in position:
Filter 2u Aluminum (switch 3) 0.441 ( 0.400) mm in position:	Filter 2m Aluminum (switch 3) 1.103 ( 1.000) mm in position:	Filter 2d Copper <sup>(switch 3)</sup> 0.055 ( 0.050) mm in position:
Filter 3u Aluminum (switch 2) 2.207 ( 2.000) mm in position:	Filter 3m Molybdenum (switch 2) 0.084 ( 0.076) mm in position:	Filter 3d Al 2mm+Sn 0.5 (switch 2) 2.758 ( 2.500) mm in position:
Filter 4u Aluminum (switch 1) 0.221 ( 0.200) mm in position:	Filter 4m Copper (switch 1) 0.552 ( 0.500) mm in position: O	Filter 4d Molybdenum (switch 1) 0.221 ( 0.200) mm in position:
Lock Filter STOP	Lock Filter STOP	Lock Filter STOP
Date of last visual inspection: 2018/04/19		

# **Data Acquisition System**

The data for the June 12-14, 2019 experiment were written on the DAQ pc WKS-W00258 on D:\DATA\Zisis-06-12-2019. The scans listed in the above table were saved to JD70-101\A, from where they were moved to network-mounted drive BMIT-USERS-DATA (drive unit Z) Z:\C29-BM\28-09539 for transfer to UConn.

In the process of taking these scans, we had to relearn what we knew before about running rocking curve scans because the GUI's had changed. Updated images of the DAQ gui's are found in <u>this google drive folder</u>. There is also a set of manuals for the stepping motors that Mehran highlighted to show the important sections, found in <u>another google drive folder</u>. Finally <u>another folder</u> is attached to this google drive area containing a long string of snapshots taken of the beamline and target + camera setup.

**DAQ Details** (courtesy of Adam Webb): The executables that are run but the various DAQ GUIs are in:

This PC> Local Disk (C:) > BMIT > LabVIEW

This folder contains a log of backups (not of interest to users) as well as all the executables, such as CT-Multiview, CT-HIPIC, etc. Enter the appropriate subfolder and launch its executable to get the GUI up. The folders contain additional support files, such as configuration settings (e.g. those can end in .ini filetype).

**CT-Multiview** screenshots. This shows the screens and numbers. On the first screen, under the Motion Setup tab, all the relevant Rotary Motion numbers for the GlueX diamond scans are listed. The bottom right corner has two buttons:

- <u>SimMode</u> refers to simulation mode. This should not be used by users. It is a program that Adam uses to test things.
- <u>Save Configuration</u> saves things into CT-Multiview folder, as a .ini file.

TION SETUP	Detector	CT SCAN DAT	A COLLECTION HELP	Mattiview er	]		
Best choice for ncr. (deg) # of 2 1 0.5	180 degrees Projections 90 180 360	Motor Steps 500 250 125	Vertical # of Vertical Views 1 Vertical Increment (mm) 0	Rotation # of projections 	Start (time/date) 4:09:42.762 PM 2019-06-12 Dock and Flat I	ed Elapsed Time Remaining n (s) (min) Time (min) 19 -1	Expected End (time/date) 4:27:14 PM 2019-06-12 Actual Duration (s) 1135.2
0.4 0.3 0.24 0.2 0.18 0.16 0.144 0.12 0.1	450 600 750 900 1000 1125 1250 1500 1800	100 75 60 50 45 40 36 30 25	Exposure time (ms) Fre $\frac{1}{\sqrt{990}}$ $\frac{1}{\sqrt{100}}$ Write file delay (ms) Dr $\frac{1}{\sqrt{150}}$ $\frac{1}{\sqrt{100}}$		Collect Images at Start and End Travel to take sample out-of-beam (mm)	# of Darks # of Fla 0 0 0 vertical direction ? Two	ts Enable o sets between views?
0.096 0.08 0.072 0.06 0.048 0.040 0.036	1875 2250 2500 3000 3750 4500 5000	24 20 18 15 12 10 9	SCANNING X-rays On SR current 208	View # 0 Vertical scan prog 0 10 20 30 40 Rotation scan pro 0 10 20 30 40 total images captured 878	ress 50 60 70 80 90 100 gress 50 60 70 80 90 100	Collecting projections Collecting "Flat" images Collecting "Dark" images Positioning sample Shutter closed Argus OK	Start Next View Control Shutter?

The screenshot below shows the CT Scan Data Collection tab of CT-Multiview. Typically the user only changes the # of projections and uses that same number also in the Collect Images at Start end End box.

#### When Start CT Scan is clicked, all configuration changes are saved!

The next screenshot shows the Bragg angle GUI. The Velocity and Travel Distance are modified accordingly by the user. Typically 1 deg is used as the travel distance when scanning to find the image, and then smaller steps, positive or negative, are used to fine tune and locate specific features on the HCImageLive screen, such as edges of the diamonds (marked on the screen with sticky flags) as well as the start and end points for the full scan. The numbers from the "Setting" Tab of the Bragg GUI are reflected in the "Motion Setup" tab, Rotary motor setup table of the CT-Multiview GUI. Examples of those are attached below.

Р	Pitch Stage (Bragg angle)	- 🗆 📉	Pitch Stage (Bragg angle) -	×
File E	dit Operate Tools Window Help		File Edit Operate Tools Window Help	
-	······································		♣ ֎	1
	Pitch Stage (Bragg angle)     Moving     Relative     Position       Setting     Run	1	Pitch Stage (Bragg angle) Moving Relative Position	Ŷ
	Velocity (Deg/s) ⊕ 0.005 Travel Distance (Deg) ⊕ -0.1229		Stage (axis)     Driver Microstep Value       Axis 4     250       Acceleration Time (s)     Motor steps per rev       0.5     500       Lead screw pitch^-1       Board ID     (rev/deg)       1.6667     SA16A-RM = 1.6667	
	Progress (%)		Motor Velocity (RPM) Travel Distance (steps)	
	RUN STOP EXIT		name Save Configuration Pitch_Stage Save	
<		×	v 	> .::

<b>1</b>		CT-multiview		-	
File Edit Operate Tools Window Help					
🖷 🕸 🔘					- 2
MOTION SETUP Detector CT SCAN D	ATA COLLECTION HELP	MultiView CT			
Vertical motion setup	Flat motion setup	Rotary motion setup	Detector trigger setup	Fast Shutter setup	
Board ID Vertical         2         Stage (Axis) Vertical         Axis 1         Lead screw pitch^-1 (rev/mm) Vertical         1         Motor steps per rev Vertical         500         Driver Microstep Value Vertical         2         Velocity Vertical (mn/s)         1         Acceleration Time (s) Vertical         0.1         Rewind Factor Vertical         1         Backbach vertical (steps)         0	Board ID flat	Board ID rotation 2 Stage (Axis) rotation Axis 4 Lead screw pitch~1 (rev/mm) Rotation 10007 Motor steps per rev rotation 500 Driver Microstep Value Rotation 250 Velocity rotation (deg/s) 0.1 Acceleration (deg/s) 0.1 Rewind Factor Rotation 1 Baddash rotation (steps) 0 0	Counter(5) B Dev2/ctr1  Counter(5) Count	Shutter input Shutter output open Shutter output open Shutter output dose Dev3/port0/line1 * Shutter output dose Dev3/port0/line1 * Shutter Shutter output dose Dev3/port0/line1 * Shutter Shu	

All these were taken using the *Snipping Tool* in Windows, and moved off the DAQ machine using *sftp* (terminal operated).

# **Diamond Scans**

## Mount JD70-101, install in beamline

We found the single-axis rotary sample mount (pictured below) that we used to hold the diamond during our previous runs.







I used a piece of printer paper cut at a 45 degree angle to camp the diamond mounting bar to the sample holder at a 45° angle. A second mounting bar was stuck into the same clamps to prevent the clamps from twisting off the diagonal bar, as it is barely long enough to span the height between the two clamps at 45 degrees.

To represent the orientation of the diamond during a scan, I use the notation "/X" etc., to represent which side of the diamond the beam enters from and whether the mounting bar leans left or right from the beam particles' perspective. The configuration shown at the right is  $X \setminus$ because the crystal is on the upstream side of the bar, and the bar is leaning beam-left like the backslash character. The 4 independent orientations for the scans to be taken of each diamond are X\, /X, X/, and \X. The first pair and the second pair can be reached by a 180 flip around the horizontal rotation axis of the mounting frame shown in the above photo. Switching between the first and second pair requires rotating the mounting bar around the beam axis by 90° inside its slot on the frame.



(Right) Photograph of the target holder frame on the crystal goniometer, from the viewpoint of a beam photon. Through the target frame one can see the controls of the X-ray camera.

#### Take rocking curves (4) of JD70-101

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10	X١	(0.3979, 0.4958)	700	2.44	JD70-101-10
20 <sup>1</sup>	/X	(1.0477, 1.1526)	750	"	JD70-101-20
30	/X	(0.9257,1.0486) <sup>2</sup>	878	"	JD70-101-30
40	X/	(1.6229,1.7330)	786	"	JD70-101-40
50	١X	(3.3430,3.4530)	786	"	JD70-101-50

<sup>1</sup>The storage ring tripped during this run at around step 639, had to repeat.

<sup>2</sup>The previous run failed to complete, had to reset the DAQ, lost the reference position in theta.

#### Transfer data from JD70-101 to UConn

#### June 13, 2019 [rtj]

To do this, we set up a globus personal endpoint on WKS-W00258 and created an alias in the globus web interface named CLS-BMIT-1. I then enabled the globus endpoint at uconn named by the alias jonesrt#grinch. I then issued a copy from D:\DATA\Zisis-06-12-2019\JD70-101 on WKS-W00258 to grinch. For this to work, I had to disable the firewall on grinch. In the future, I need to work out a way to whitelist connections from CLS so I do not have to disable iptables to get these transfers to complete.

```
[root@grinch ~]# ls /export/data0/Zisis-06-12-2019/JD70-101/A
JD70-101-10_00001.tif ... JD70-101-10_00700.tif
JD70-101-20_00001.tif ... JD70-101-20_00750.tif
JD70-101-30_00001.tif ... JD70-101-30_00878.tif
[root@grinch ~]# ls /export/data0/Zisis-06-12-2019/JD70-101/B
JD70-101-40_00001.tif ... JD70-101-40_00786.tif
JD70-101-50_00001.tif ... JD70-101-50_00786.tif
```

Note added later: What I had to do is to add ip subnet 128.233.249.248/24 to the list of trusted subnets in iptables on grinch. That name is not registered with the public DNS, but I think it must correspond to the workstation at CLS where these data are being sent from. After I added this rule, I still find that I get occasional connection resets and failed transfers when the firewall is enabled. Watching netstat during a globus transfer, I see a couple of extra listeners starting up from the globus-gridftp-server process on grinch. These were on odd port numbers that did not look like regular globus daemon ports to me, so I am not sure what they are for. They only last

for the duration of a transfer and then they disappear, unlike the listener on 2811 that remains active all the time the server is running. I will need to figure out how to control the port numbers on these ephemeral listening ports, otherwise I will never be fully able to run globus transfers while the firewall is enabled.

## Verify data quality

I copied the following data analysis procedures from the logbook for the November 2017 CLS run, and adapted them for this run period.

#### Rocking curve analysis procedure

- 1. Use globus online to transfer the folder containing all of the images taken in the previous scan to jonesrt#grinch. These data should land in grinch.phys.uconn.edu:/export/data0.
- 2. Create a data analysis area on /nfs/direct/jonesrt, e.g. /nfs/direct/jonesrt/cls-6-2019 and create a work directory for this sample, eg. /nfs/direct/jonesrt/cls-6-2019/JD70-101, then use rsync to copy image files from grinch to this work area. This separation between directories used for transfer and analysis is useful so that one can rename files in the analysis area without having them overwritten by the next globus transfer. This renaming happens whenever someone mistypes the image prefix or sequence numbering options during image acquisition, and lets the names be rewritten into canonical form before attempting to run the analysis. Canonical form for images is <sample>-<scan>\_<N>.tif where step number N ranges from 1 to the number of steps and has leading zeros to make the total number of digits equal to 5.
- 3. Go to /home/www/docs/halld/diamonds on gluey.phys.uconn.edu and make a new directory for this run, e.g. cls-6-2019. Inside this directory, create a symlink called "data" to the work area on /nfs/direct/jonesrt/<run> created in step 2 above. Make another folder next to "data" called "photos" where photographs from the run will be stored. Then cd into data and add a symlink back to /home/www/docs/halld/diamonds/Analysis called Analysis. Finally, from within Analysis, create a symlink to the same destination as /home/www/docs/halld/diamonds/<run>/data, and name it <run>. This completes the directory linkage structure assumed in the code and in these instructions.
- 4. Make a local copy of rcmaker.C (one can be found in the Analysis directory) in the sample directory under /home/www/docs/halld/diamonds/<run>/data/<sample>. Open a new terminal window and cd into this directory where the copy of rcmaker.C is found.
- 5. Start root in this window, and initialize the root session as follows:
  - a. .L /usr/lib64/libtiff.so
  - b. .L rcmaker.C+O
- Each time a new scan is made and the data are pushed into the analysis area through globus + rsync steps, a new root command illustrated below must be issued to convert the raw image files into root histograms.
  - a. rcmaker("<sample>",<scan>,<steps>,1)

- 7. When this completes, use uberftp to push the output root file that contains all of the raw data from this scan to pnfs. The file is named <sample>-<scan>\_rocking\_curves.root and should be found in the same directory as the tiff files that were used to create it. Ignore the warnings from the tiff conversion library about unexpected tags in the tiff header, as these do not cause any real problems. The destination directory on pnfs should be /pnfs/phys.uconn.edu/data/Gluex/beamline/diamonds/<run>/results. If this directory does not exist yet, it should be created and owned by the gluexuser user. Copying into this directory requires that the person doing the transfer have a valid voms proxy issued by the Gluex vo.
- 8. As soon as the X\_rocking\_curves.root file is uploaded to pnfs, the root process that fits the rocking curves to a gaussian peak over a constant background can be started. I use proof for this step, although if you are patient you can just run it in a regular root client session. The configuration of the proof service at UConn makes using this pretty straight-forward. Use the UConn-proof web interface to start your own private proof service, and then connect to that service to do your analysis. All of this is automated by the dofits.C script found in Analysis. The following session illustrates how to use it, from a root session started in the Analysis directory. Before you start this, edit the dofits.C file to make sure it points to your private proof service, and that the appropriate set of lines have been commented out so that only the scans that you want to fit are processed. All you need to do as the run progresses is just add a single line in the appropriate function within dofits.C for each scan you want to process, and comment them out as you finish each one.
  - a. .L Map2D.cc+O
  - b. .L rcfitter.C+O
  - c. .L rcpicker.C+O
  - d. .L run\_rcfitter.C+O
  - e. .x dofits.C
- The above step creates a new root output file <sample>-<scan>\_results.root in the Analysis directory. Use uberftp to copy it to the same area on pnfs where you stored the X\_rocking\_curves.root file in one of the previous steps.
- 10. Edit the python script plotgen.py and follow the examples in the code to add a line to generate rocking curve topograph images for each scan with a X\_results.root file that has been uploaded to pnfs, as described in the previous step. Run this file within a python session as follows.
  - a. import plotgen
- 11. Move the \*.png files created in the last step into <run>/<sample>. Eventually at the end of the run, you will back up these <sample> directories containing all of the raw image files into a compressed archive and then remove the tiff files, leaving behind only these png images. These are the final results from this analysis.
- 12. Delete the .root files created in the above steps after they have been copied into pnfs. This leaves behind a very small data footprint in the /home/www and /nfs/direct/jonesrt

nfs areas, containing only a few png images and text files from each scan. The raw data and fitting results are stored in the root files that are archived on pnfs.

#### Dismount JD70-101, repackage

JD70-101 was returned to its position in sleeve 4 without incident.

#### Mount JD70-103, install in beamline

JD70-103 was successfully mounted in the target frame and aligned using the vertical and horizontal alignment lasers on the beamline. At first there was confusion about the horiztonal alignment, which eventually was tracked down to the two horizontal lasers being set at different heights: one of them at the height of white beam, and the other at the height of diffracted beam from the mono. We set both of them to the level of the diffracted beam from the mono.

#### Take rocking curves (4) of JD70-103

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10	Х/	(-0.4150,-0.3750)	286	2.44	JD70-103-10
20 <sup>1</sup>	١X	(-0.1800,-0.1300)	358	"	JD70-103-20
30	X/	(0.9091,0.9420)	235	"	JD70-103-30
40	/X	(2.0490,2.0910)	300	"	JD70-103-40

<sup>1</sup>Somewhere during this run there were 3 frames that were lost, image sync is off by 3, ignoring.

In former run periods, we always used the NTSB 30 Hz camera and a TV monitor to find the Bragg peak each time we changed the target orientation. But this time we decided to use the <u>camera in internal trigger mode</u>. The camera integrates over a 1s period, so if one moves the Bragg angle continuously over a broad range at a steady speed, not too fast, you can see the image of the crystal show up in a live updating view of the camera output. This is much more efficient because we don't have to keep going in to install the fluorescent paper and then remove it to switch to camera viewing.

#### Transfer data, verify data quality

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-103/A
JD70-103-10_00001.tif ... JD70-103-10_00286.tif
JD70-103-20 00001.tif ... JD70-103-20 00358.tif
```

JD70-103-30\_00001.tif ... JD70-103-30\_00235.tif JD70-103-40\_00001.tif ... JD70-103-40\_00300.tif

When I transferred the files, I noticed that the size of the image files in this set are a factor 2 smaller than what was seen in the JD70-101 images. Later on when I went to analyze them, I discovered that these files were saved in a different format from the standard one I had been using in the past: 8-bit instead of 16-bit encoding. Here is the output from imagemagick identify comparing the 8-bit and 16-bit image encodings.

grinch.phys.uconn.edu> identify JD70-103-10\_00040.tif JD70-103-10\_00040.tif TIFF 888x872 888x872+0+0 8-bit PseudoClass 256c 777KB grinch.phys.uconn.edu> identify ../JD70-101/JD70-101-10\_00040.tif ../JD70-101/JD70-101-10\_00040.tif TIFF 1156x1120 1156x1120+0+0 16-bit Grayscale DirectClass 2.59MB

Apart from the different overall dimensions of the image, the two encodings are quite different. The 16-bit encoding is called 16-bit Grayscale DirectClass which means the 3 color values recorded for each pixel are the actual intensities of the three primary colors at that spot. By contrast, the 8-bit encoding is called 8-bit PseudoClass 256c, which I take to mean that the intensities of the three primary colors at each pixel are recorded as a value 0..255 that represents an index into a lookup table of actual intensities.

The command "convert JD70-103-10\_00040.tif -verbose info:" generates the same output display Miscellany -> Image Info, printing it to the screen in plain text. This shows that the PseudoClass color lookup table for 8-bit grayscale that the camera is using simply maps the 256 values 0..255 onto themselves for each of the 3 primary colors. The histogram of these 8-bit images shows the background (pedestal) value peaks around 10, with most of the remaining pixels being at the level 25 or less, indicating 4-bit accuracy in the image brightness. This can be compared with the 16-bit grayscale images for which the pedestal sits around value 170 and the high-intensity tail cuts off around 250, indicating more like 6 bits of accuracy in the brightness. So there is roughly a factor 10 in resolution between the 8-bit intensity maps and the 16-bit variants., Still it should be possible to determine the rocking curve width with just 4 bits of accuracy.

#### Dismount JD70-103, repackage

JD70-103 was returned to its cell in sleeve 4 without incident.

#### Mount JD70-106, install in beamline

Diamond JD70-106 was removed from its slot in sleeve 4 and aligned on the beamline.

#### Take rocking curves (4) of JD70-106

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10	X/	(2.5060,2.6511)	1036	2.44	JD70-106-10
20	/X	(4.8572,4.9761)	850	"	JD70-106-20
30	X/	(-3.2240,-3.0780)	1043	"	JD70-106-30
40	١X	(-2.8600,-2.7000)	1143	"	JD70-106-40

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-106/A
JD70-106-10_00001.tif ... JD70-106-10_01036.tif
JD70-106-20_00001.tif ... JD70-106-20_00850.tif
[root@grinch data0]# ls Zisis-06-12-2019/JD70-106/B
JD70-106-30_00001.tif ... JD70-106-30_01043.tif
JD70-106-40_00001.tif ... JD70-106-40_01143.tif
```

Once again, the image files in this dataset are encoded as 8 bits, not 16 as is usually used. This was apparently due to a wrong mouse click that changed the camera image encoder to write 8-bit tiffs instead of 16-bit. Visually, the images look ok to me so I am hoping that I can find tweaks to my analysis code that will allow these data to be analyzed on the same basis as the standard 16-bit images.

#### Dismount JD70-106, repackage

JD70-106 was returned to its pocket in sleeve 4 without incident.

## Mount JD70-107, install in beamline

JD70-107 was mounted on the target frame and aligned on the beamline.

## Take rocking curves (4) of JD70-107

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10 <sup>1</sup>	Х/	(-0.2710,-0.2200)	364	2.44	JD70-107-10
20 <sup>2</sup>	١X	(-0.3400,-0.2850)	393	"	JD70-107-20

30	X١	(0.8100,0.8600)	357	u	JD70-107-30
40	/X	(0.5800,0.6200)	286	ű	JD70-107-40

<sup>1</sup>This run was originally saved in directory HD70-107 but with filenames JD70-106-40\_nnnnn.tif which was confusing. After the files were transferred to UConn, I renamed them using the correct suffix JD70-107-10.

<sup>2</sup>The DAQ stopped working at the start of this scan, so we had to restart the camera vi, which is named HCImageLive. Then, after we restarted that vi, the scan controller vi stopped working so we had to restart that one. This was more problematic because when we restarted it, all of the configuration settings returned to their default values and we had to restore them with guesses. Our guesses can be seen in the GUI snapshots below. We will ask Nazanin to review these in the morning.



N SETUP CT SCAN DATA COLLECTION	Vertical # of Vertical Views	Rotation # of projections	Start (time/date)	Estimated	Elapsed Time	Remaining	Expected End (time/date)
est choice for 180 degrees rotation	Vertical Increment (mm)	Rotation Increment (deg)	5:11:01.981 AM 2019-06-13	Duration (s)	(min) 0	0	5:11:11 AM 2019-06-13
2 90 500	90	0.00014		(IIIII)	alles see		Actual Duration (s)
1 180 250 0.5 360 125	Detector	setup	Dark a	nd Flat Image	Collection set	up	3.555
0.3 600 75 0.2 900 50 0.18 1000 45 0.16 1125 40 0.144 1250 36 0.12 1500 30	Exposure time (ms) 990 Write file delay (ms) 1000 1000	# of mages tegration 0 1 elay (ms) Image Delay (ms) 50	Collect Flat and Dar images every Travel to take sampl out-of-beam (mm)	k () 250 e () 0	# of Darks	# of Flats	Enable
0.1 1800 23 0.096 1875 24 0.08 2250 20 0.072 2500 18 0.06 3000 15	SCANNING Vie	Vertical scan prog ew # 0 0 10 20 30 40 Rotation scan pro ion # 0 4	ress 50 60 70 80 90 10 igress		Collecting projecti Collecting "Flat" in Ollecting "Dark" in	ons nages mages	Start Next View Control Shutter?

Note added later by RTJ: I learned afterward from Adam Webb that the factor 1667 / 500 that we ended up with is correct, but the configuration parameters should be written differently. We had the primary screw pitch left at its default value of 0.5 mm/rev and set the steps per revolution to 1667, whereas it would be more correct to set the primary screw pitch to 1.6667 mm/rev and leave the steps per revolution at the default value 500. Either way, the resulting scans are the same.

#### Transfer data, verify data quality

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-107/A
JD70-107-10_00001.tif ... JD70-107-10_00364.tif [after renaming from original 106-40]
JD70-107-20_00001.tif ... JD70-107-20_00393.tif
JD70-107-30_00001.tif ... JD70-107-30_00357.tif
JD70-107-40_00001.tif ... JD70-107-40_00286.tif
```

#### Dismount JD70-107, repackage

Diamond JD70-107 was dismounted and returned to its pocket in sleeve 4 without incident.

#### Mount JD70-109, install in beamline

Diamond JD70-109 was mounted on the target frame and aligned on the beamline.

#### Take rocking curves (4) of JD70-109

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10 <sup>1</sup>	X/	(-4.8590,-4.7730)	614	2.44	JD70-109-10
11	X/	(-4.8590,-4.7730)	615	"	JD70-109-11
20 <sup>2</sup>	/X	(-4.62705,-4.557)	500	"	JD70-109-20
30	X/	(1.36202,1.39896)	264	"	JD70-109-30
40	١X	(2.71298,2.74995)	264	"	JD70-109-40

<sup>1</sup>This scan was repeated because a refill happened during the first one.

<sup>2</sup>Detector was moved 20mm downstream and 10mm down. (reason: crystal stage and detector stage were colliding!)

#### Transfer data, verify data quality

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-109/A
JD70-109-10_00001.tif ... JD70-109-10_00614.tif
JD70-109-11_00001.tif ... JD70-109-20_00500.tif
JD70-109-30_00001.tif ... JD70-109-30_00264.tif
JD70-109-40_00001.tif ... JD70-109-40_00264.tif
```

#### Dismount JD70-109, repackage

Diamond JD70-109 was removed from the target frame and returned to its pocket in sleeve 4 without incident.

#### Mount JD70-100, install in beamline

Used diamond JD70-100 was removed from its pocket in sleeve 4 and mounted in the target frame, aligned on the beamline.

#### Take rocking curves (4) of JD70-100

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
------	-------------	-------------------	-----------	------------------	--------------

10	X/	(-1.03496,-0.959088)	542	2.44	JD70-100-10
20	١X	(-1.10203,-1.00298)	708	ű	JD70-100-20
30	X١	(0.479981,0.542029)	444	ű	JD70-100-30
40	/X	(532031,0.598082)	472	ű	JD70-100-40

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-100/A
JD70-100-10_00001.tif ... JD70-100-10_00542.tif
JD70-100-20_00001.tif ... JD70-100-20_00708.tif
JD70-100-30_00001.tif ... JD70-100-30_00444.tif
JD70-100-40 00001.tif ... JD70-100-40 00472.tif
```

#### Dismount J70-100, repackage

Diamond JD70-100 was removed from the target frame and returned to its pocket in sleeve 4 without incident.

#### Mount JD70-104, install in beamline

Used target JD70-104 was removed from its individual pillbox in the diamond case and installed in the mounting frame, aligned on the beamline.

#### Take rocking curves (4) of JD70-104

It was decided to use a larger step size for the radiation-damaged diamonds, JD70-104, as compared to the virgin diamonds measured to this point. This was done in order to make the data taking per orientation more manageable, yet offering a more detailed scan of the damaged diamonds, for the purpose of a more detailed scan-analysis.

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10	X١	(4.83554,5.5906)	1349	9.76	JD70-104-10
20	/X	(4.8990,5.6490)	1340	u	JD70-104-20

30	X/	(-2.2200,-1.4700)	1340	u	JD70-104-30
40	١X	(-2.26,-1.51)	1340	"	JD70-104-40

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-104/A
JD70-104-10_00001.tif ... JD70-104-10_01349.tif
JD70-104-20_00001.tif ... JD70-104-20_01340.tif
JD70-104-30_00001.tif ... JD70-104-30_01340.tif
JD70-104-40_00001.tif ... JD70-104-40_01340.tif
```

#### Dismount J70-104, repackage

Diamond JD70-104 was removed from the target frame and returned to its pillbox without incident.

#### Mount JD70-105, install in beamline

Used target JD70-105 was removed from its individual pillbox in the diamond case and installed in the mounting frame, aligned on the beamline.

## Take rocking curves (4) of JD70-105

scan	orientation	theta range (deg)	no. steps	step size (urad)	image prefix
10	Х/	(0.7430,0.796976)	386	2.44	JD70-105-10
20	١X	(0.598035,0.654035)	400	"	JD70-105- <mark>201</mark>
30	X١	(-0.764,-0.718)	329	"	JD70-105- <mark>30²</mark>
40	/X	(-0.890032,-0.8299850	429	"	JD70-105-40

<sup>1</sup>These files were originally labeled as JD70-105-30, later the labels were swapped back. <sup>2</sup>Originally labeled as JD70-105-20, later swapped back to the correct ones shown here.

Data from the above scans were transferred to UConn using globus. Here is a listing of what arrived when the transfer completed.

```
[root@grinch data0]# ls Zisis-06-12-2019/JD70-105/A
JD70-105-10_00001.tif ... JD70-105-10_00386.tif
JD70-105-20_00001.tif ... JD70-105-20_00400.tif [after the names were corrected]
JD70-105-30_00001.tif ... JD70-105-30_00329.tif [after the names were corrected]
JD70-105-40_00001.tif ... JD70-105-40_00429.tif
```

#### Dismount J70-105, repackage

The JD70-105 diamond was removed from the target frame and returned to its pillbox, placed back in the diamond case.

# Transfer all remaining data, photos, and software tools to UConn

June 14, 2019 [rtj]

I created a single directory to hold all of the photos that I took during this run.

• photo directory for June, 2019 run

There were no new software tools that we used at CLS this time, everything that was new was developed and run remotely from the UConn cluster. Here is a selection of our photos taken on the second day of the run.

















# **Clean up and Sign Out**

Richard and Zisis cleaned up the counting room and the experimental area and put away all tools.

Session Perm Dashboard / My Projects / 28	¢			
28G09539 — Rock BMIT-BM On-Site Permit	king Curves of Artifici	al Diamond Radiators		View Log Project
Complete	Beamline: BMIT-BM	<sub>Staff:</sub> Adam Webb	Representative: Zisis Papandreou	June 12th/2019 08:56 – June 14th/2019 07:25 (now)
Required Permissions: ACUTY-ACCESS (all) BMIT-BM ACTIVITY LOG • Hand over by Adam We • Sign-On updated by Zis 'Sergey Gasilov,' Adam We	-USER (all) ebb for BMIT-BM at Wed Jun 12 Z iss Papandreou on Wed Jun 12 20 ebb';	2019, 08:02. 119, 08:56; Added samples: 'Diamond o	rystals (6 * 1)';; Added team: 'Mehran Talebitaher,' Ben Wil	ilis', 'Zisis Papandreou', 'Nazanin Samadi', 'Richard Jones',



SLEEVE 103 104 101 108 105 106 101- 102 103 104 105 100 107-108 107 110 111 107-100 100 111 JD70-100 -> JD70-111 (12) +





Zisis, signing off on the successful completion of our beam time!

Thank you to Sergei, Adam, and everyone at CLS for your help!