# BluIce at SSRL

## Special features of GUI and framework

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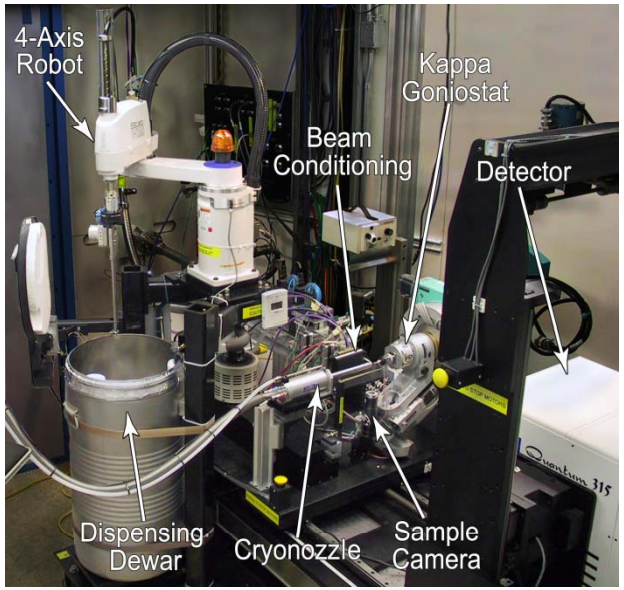
Stanford Synchrotron Radiation Laboratory

**Data Acquisition, User Interfaces and Scientific Computing Requirements Workshop on 19-21 April 2010 at NSLS2 BNL**

# The SSRL Protein Crystallography Resource

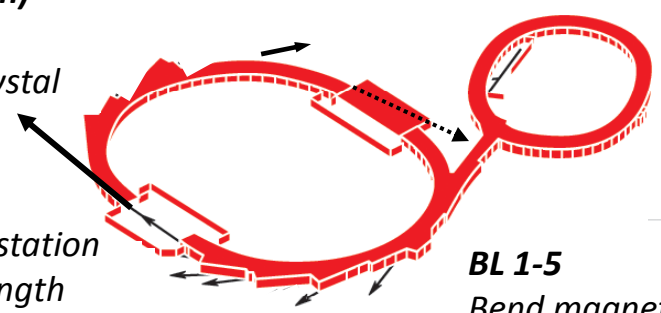



http://smb.slac.stanford.edu/

***BL 11-1 (Stanford-Scripps)***
*Wiggler side-station*
*Multi-wavelength*

***BL 14-1 (JCSG-Genentech)***
*Bend magnent*
*MAD*

***BL12-2 (Caltech)***
*Undulator*
*MAD, Microcrystal*



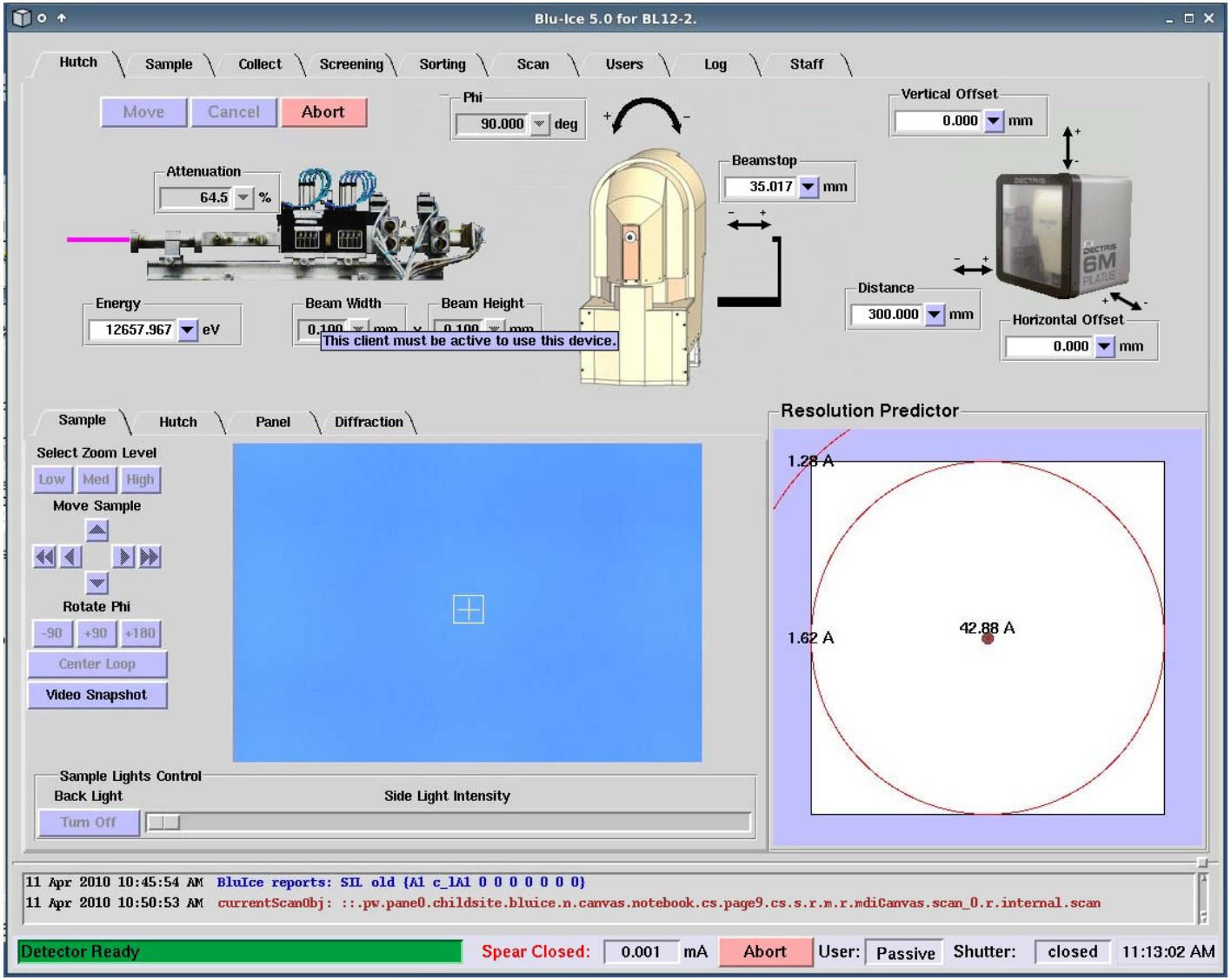
***BL 9-1***
*Wiggler side-station*
*Multi-wavelength*

***BL 1-5***
*Bend magnet*
*MAD*

***BL 7-1***
*Wiggler side-station*
*Multi-wavelength*

***BL 9-2***
*Wiggler*
*MAD*

# BluIce, the GUI



# BluIce History

- 2000 By Tim McPhillips
- Goal
  - Simplified control, universal across all beamlines
  - Less user editing
  - Automation for high throughput
  - Remote control
  - Secure

# BluIce History

- 1.0: Centralized Message Routing Architecture
- 2.0: Scripted Motors
- 3.0: Scripted Operations
- 4.0: Object-Oriented with incrTcl/TK.
- 5.0: SSL

# BluIce, the GUI

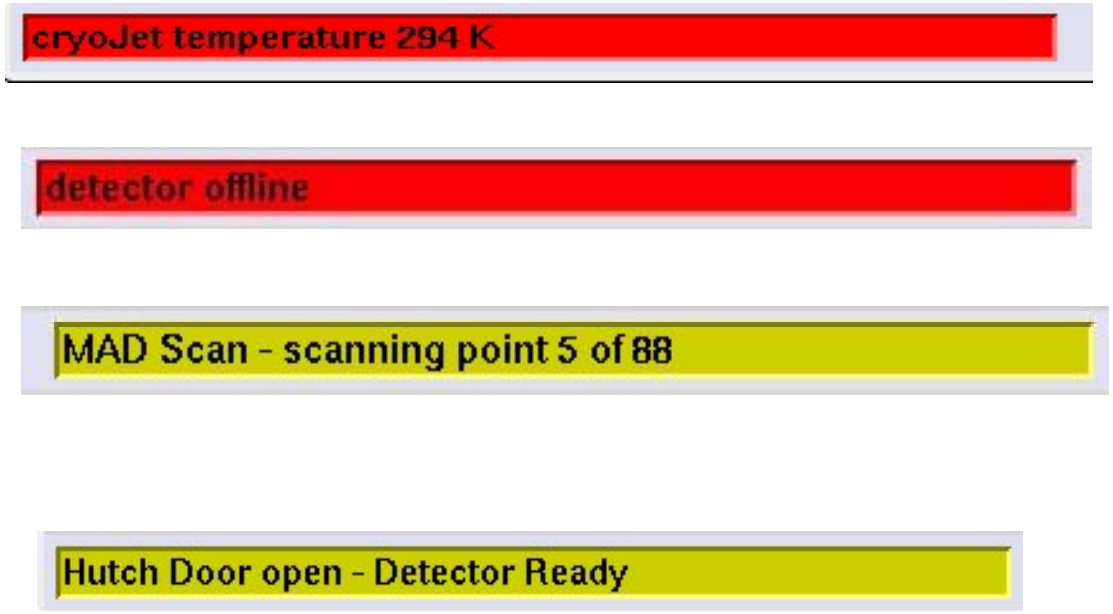
Point of view of user

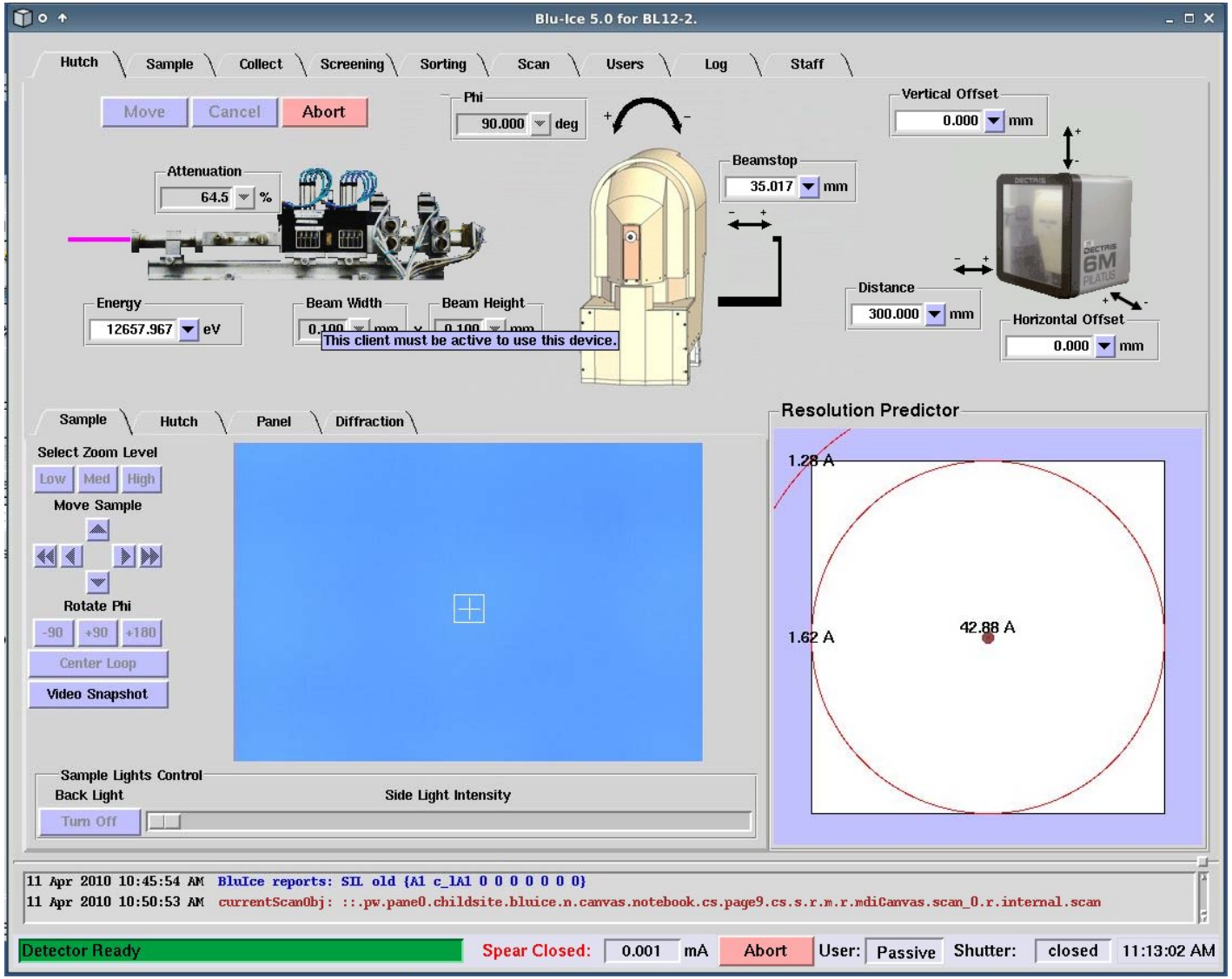
- Tab Style: Maximizes use of GUI real estate
- Less is Better: hide details from user.
- Comprehensive: diverse user base
- GUI, no scripting for normal user.
- Convenient (easy to say)

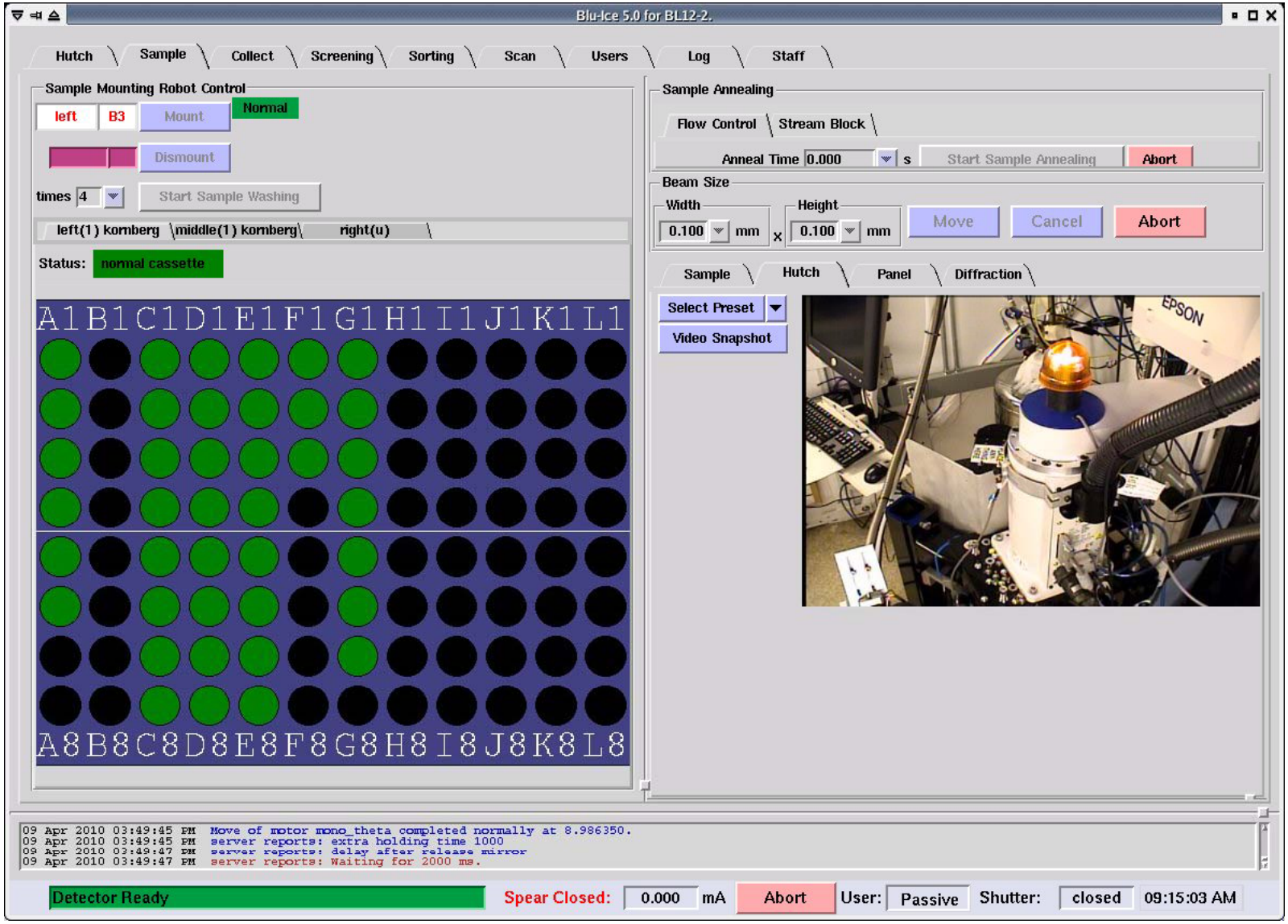
# Convenient

- Major System Status on status bar
- Balloon Hints for disabled inputs
- Resolution calculator
- Auto-Correction and Preview: spot mistakes
- Dropdown list for motor positions.
- Click and move sample
- Customize column display for spreadsheet

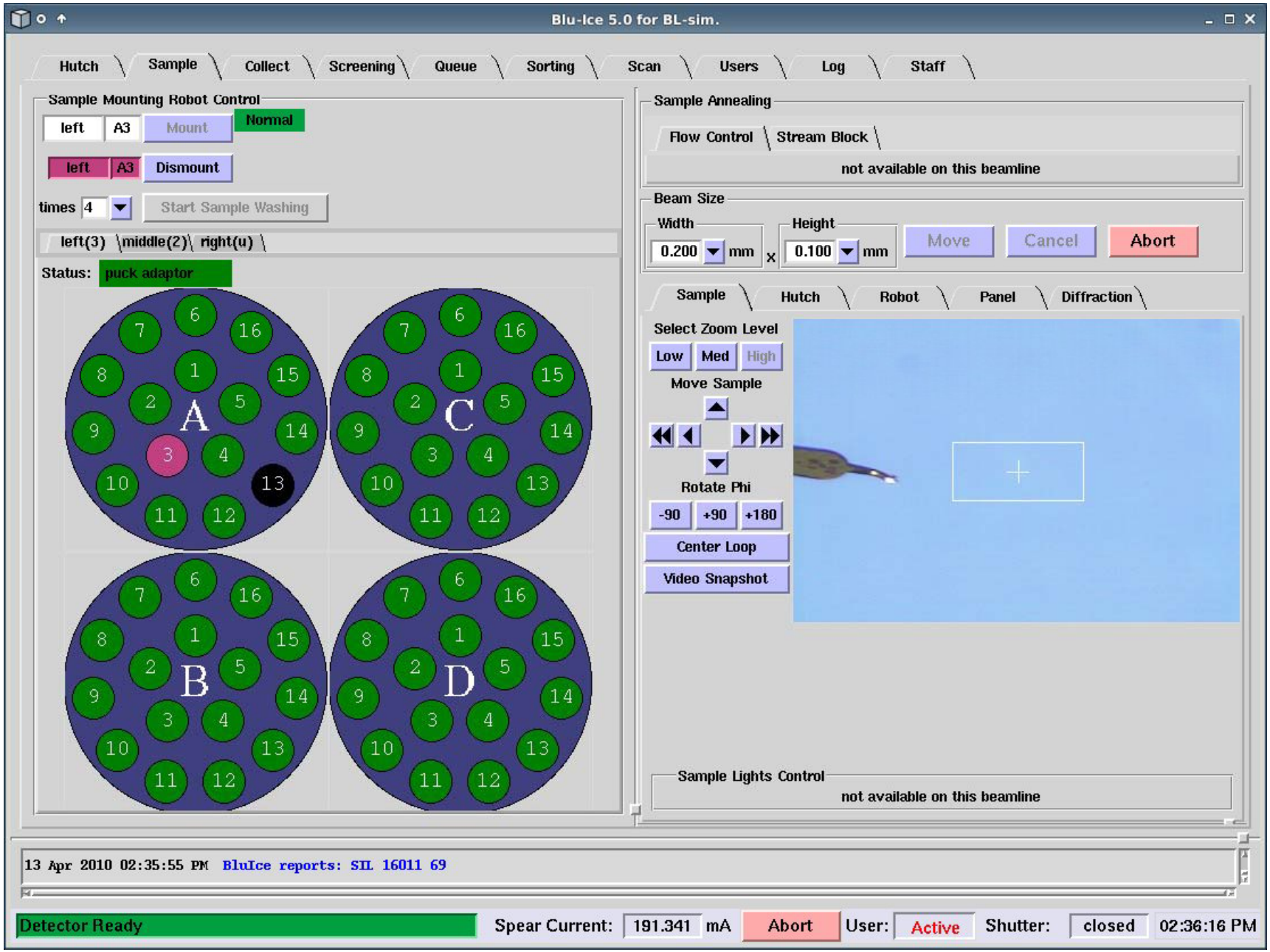
- Major Status:

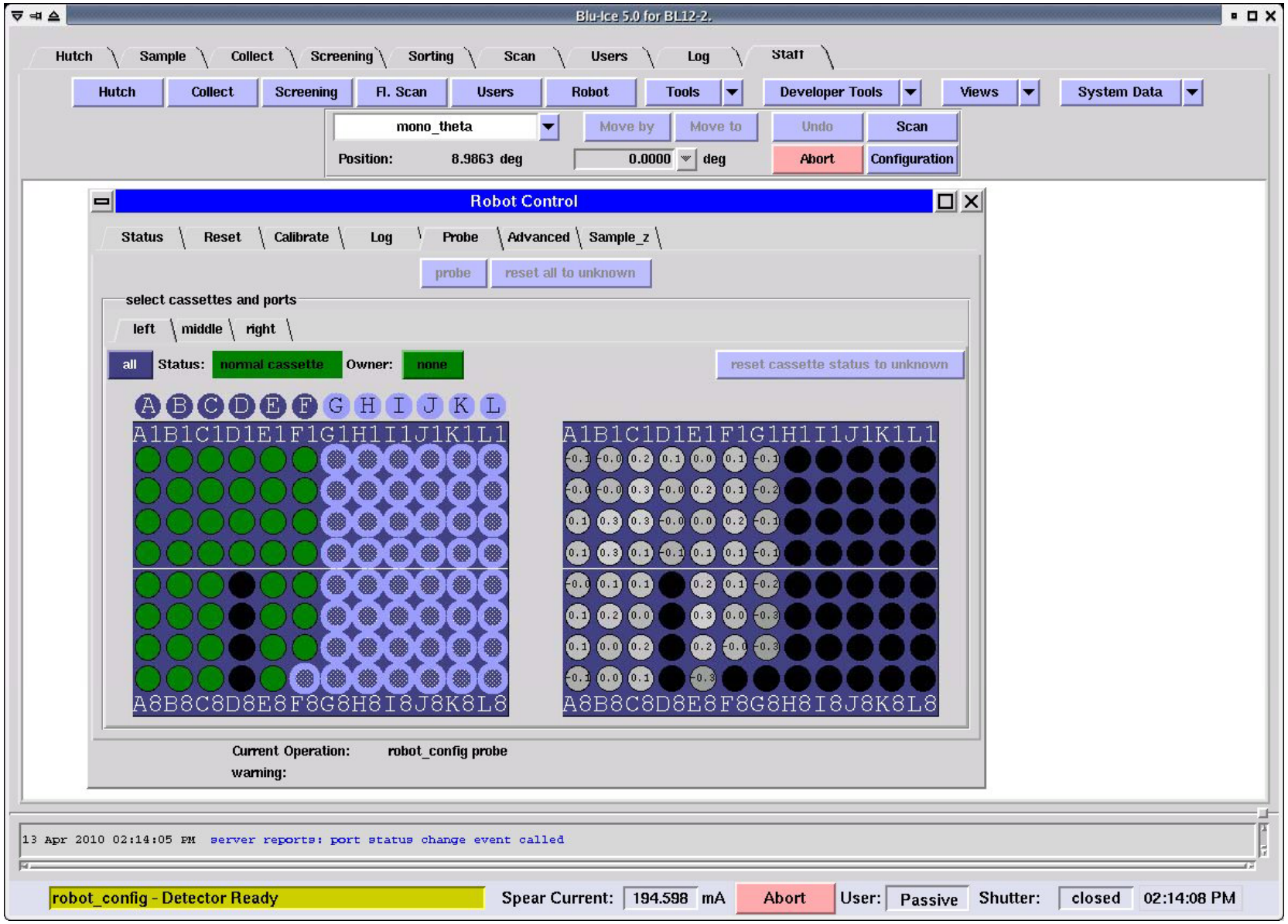



Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Move
Cancel
Abort
Phi
90.000
deg
Vertical Offset
0.000
mm
Attenuation
64.5
%
Beamstop
35.017
mm
Energy
12657.967
eV
Beam Width
Beam Height
This client must be active to use this device.
Distance
300.000
mm
Horizontal Offset
0.000
mm
Sample
Hutch
Panel
Diffraction
Select Zoom Level
Low
Med
High
Move Sample
Rotate Phi
-90
+90
+180
Center Loop
Video Snapshot
Resolution Predictor
1.28 A
1.62 A
42.88 A
Sample Lights Control
Back Light
Side Light Intensity
Turn Off
11 Apr 2010 10:45:54 AM BluIce reports: SIL old {A1 c_lA1 0 0 0 0 0 0 0}
11 Apr 2010 10:50:53 AM currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page9.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
Detector Ready
Spear Closed:
0.001
mA
Abort
User:
Passive
Shutter:
closed
11:13:02 AM

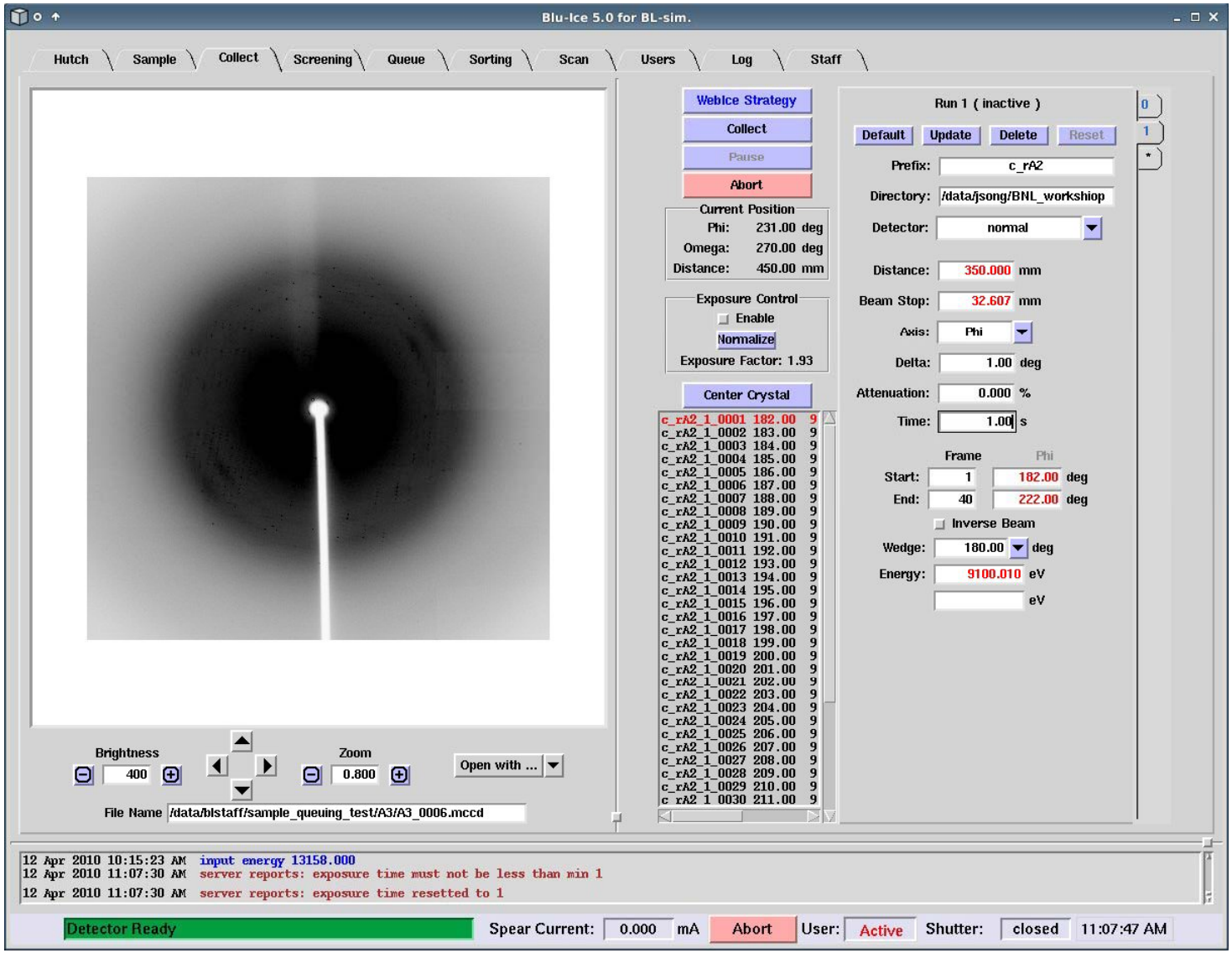

Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Sample Mounting Robot Control
left
B3
Mount
Normal
Dismount
times
4
Start Sample Washing
left(1) kornberg
middle(1) kornberg
right(u)
Status:
normal cassette
A1B1C1D1E1F1G1H1I1J1K1L1
A8B8C8D8E8F8G8H8I8J8K8L8
Sample Annealing
Flow Control
Stream Block
Anneal Time
0.000
s
Start Sample Annealing
Abort
Beam Size
Width
0.100
mm
x
Height
0.100
mm
Move
Cancel
Abort
Sample
Hutch
Panel
Diffraction
Select Preset
Video Snapshot
EPSON
09 Apr 2010 03:49:45 PM Move of motor mono_theta completed normally at 8.986350.
09 Apr 2010 03:49:45 PM server reports: extra holding time 1000
09 Apr 2010 03:49:47 PM server reports: delay after release mirror
09 Apr 2010 03:49:47 PM server reports: Waiting for 2000 ms.
Detector Ready
Spear Closed:
0.000
mA
Abort
User:
Passive
Shutter:
closed
09:15:03 AM

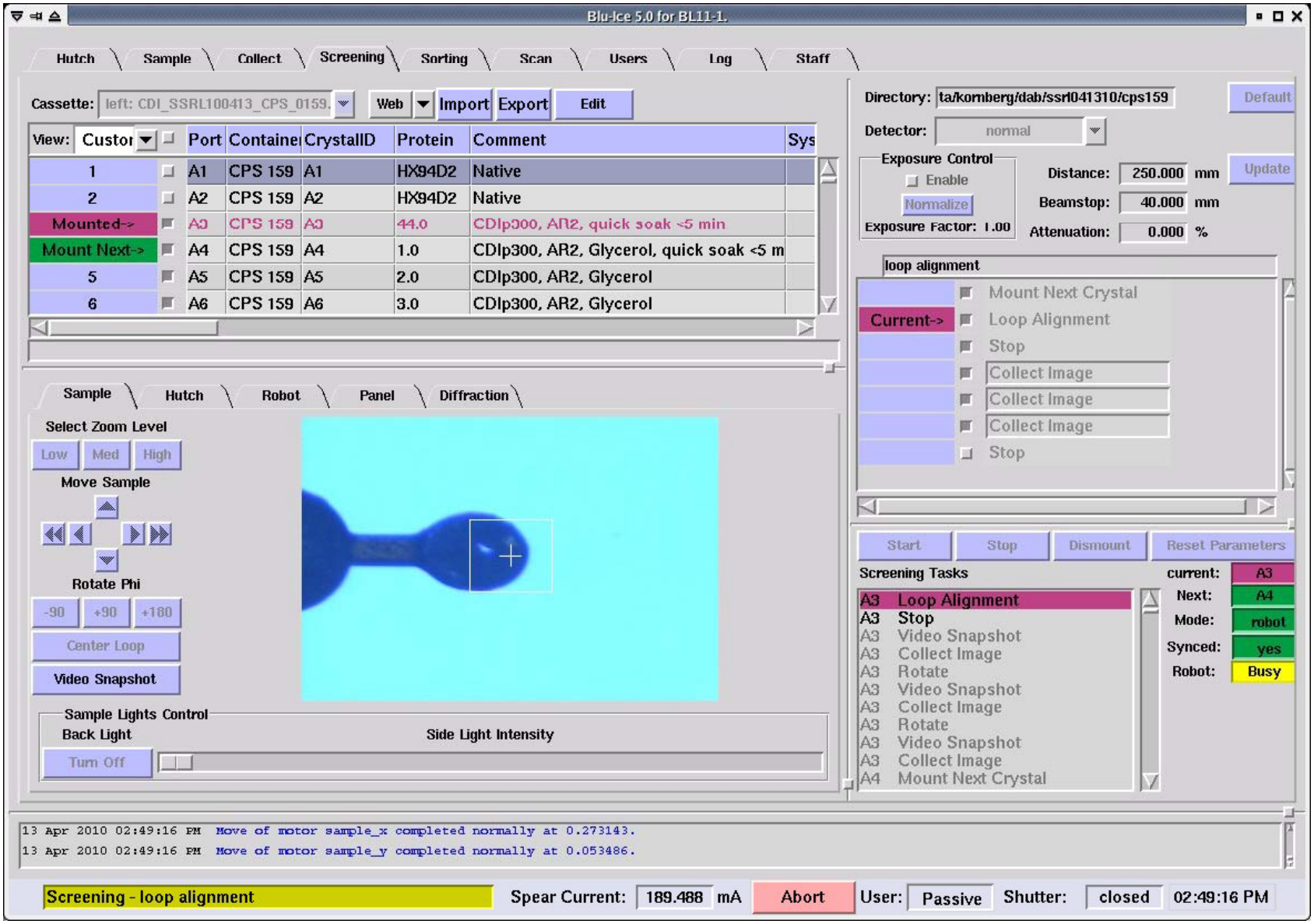
# Sample Storage Cassette/Puck

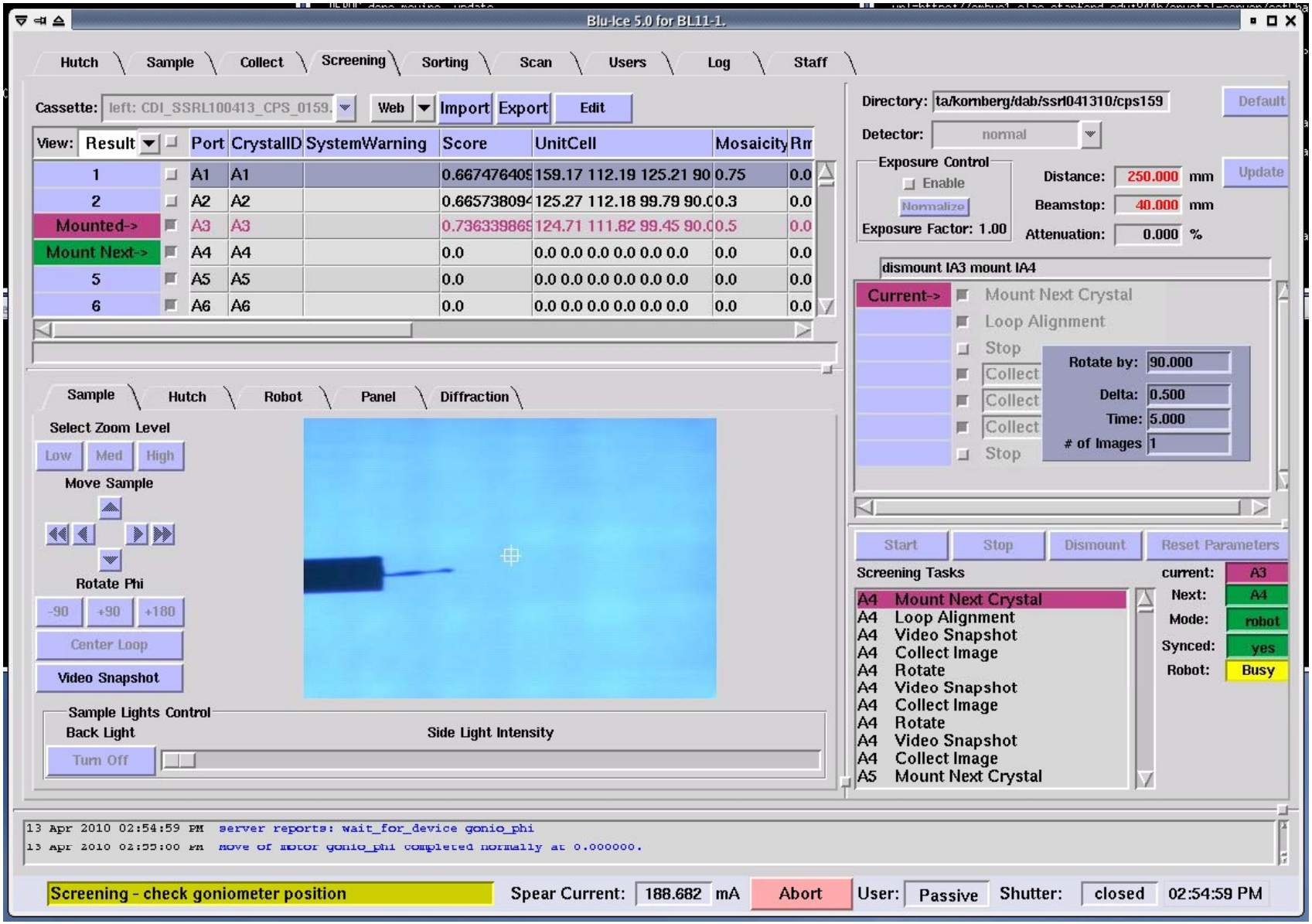

Blu-Ice 5.0 for BL-sim.
Hutch
Sample
Collect
Screening
Queue
Sorting
Scan
Users
Log
Staff
Sample Mounting Robot Control
left
A3
Mount
Normal
left
A3
Dismount
times
4
Start Sample Washing
left(3)
middle(2)
right(u)
Status:
puck adaptor
A
B
C
D
Sample Annealing
Flow Control
Stream Block
not available on this beamline
Beam Size
Width
0.200
mm
Height
0.100
mm
Move
Cancel
Abort
Sample
Hutch
Robot
Panel
Diffraction
Select Zoom Level
Low
Med
High
Move Sample
Rotate Phi
-90
+90
+180
Center Loop
Video Snapshot
Sample Lights Control
not available on this beamline
13 Apr 2010 02:35:55 PM BluIce reports: SIL 16011 69
Detector Ready
Spear Current:
191.341
mA
Abort
User:
Active
Shutter:
closed
02:36:16 PM

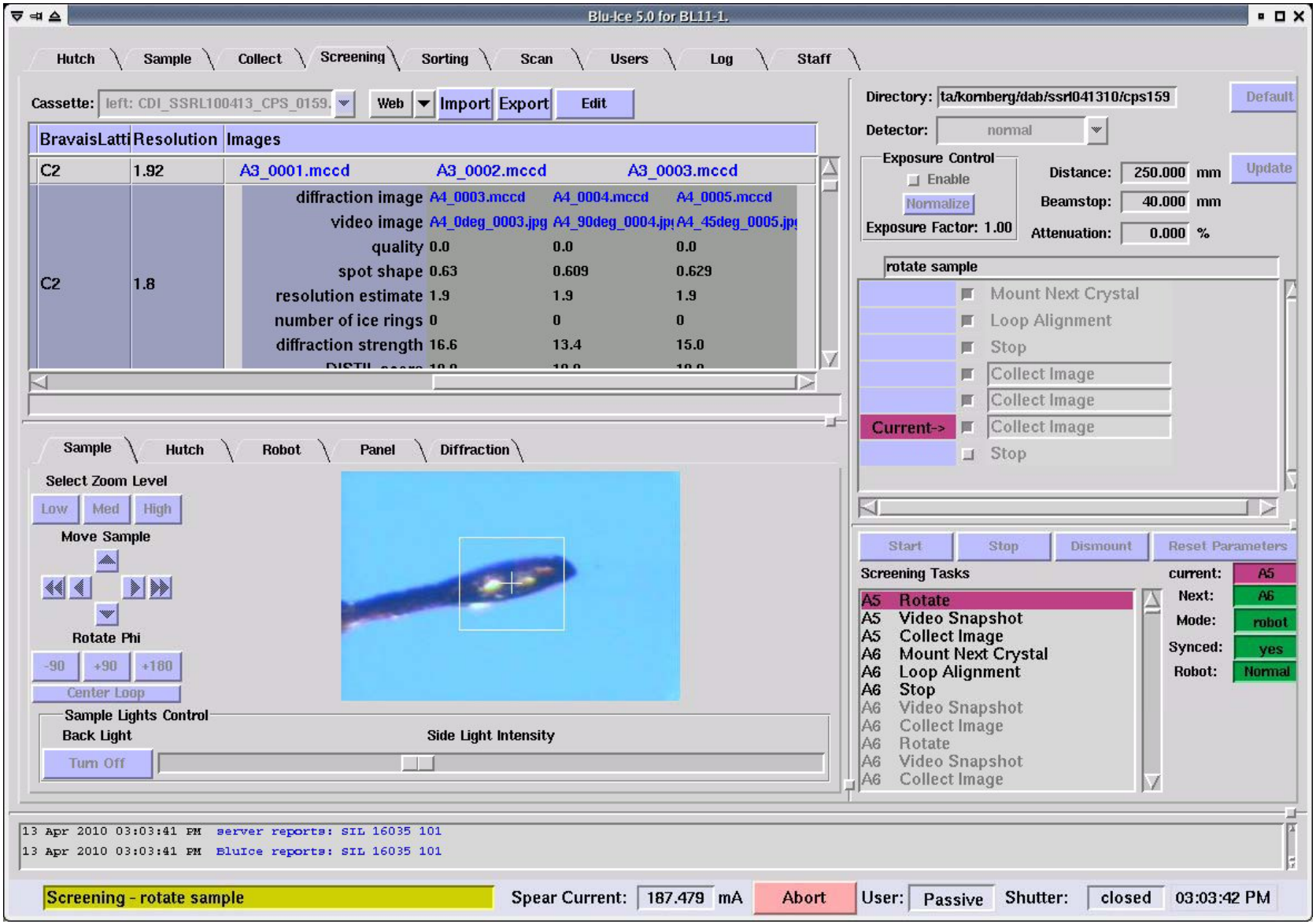

Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
mono_theta
Move by
Move to
Undo
Scan
Position:
8.9863 deg
0.0000
deg
Abort
Configuration
Robot Control
Status
Reset
Calibrate
Log
Probe
Advanced
Sample_z
probe
reset all to unknown
select cassettes and ports
left
middle
right
all
Status:
normal cassette
Owner:
none
reset cassette status to unknown
A B C D E F G H I J K L
A1B1C1D1E1F1G1H1I1J1K1L1
A8B8C8D8E8F8G8H8I8J8K8L8
A1B1C1D1E1F1G1H1I1J1K1L1
A8B8C8D8E8F8G8H8I8J8K8L8
Current Operation:
robot_config probe
warning:
13 Apr 2010 02:14:05 PM
server reports: port status change event called
robot_config - Detector Ready
Spear Current:
194.598
mA
Abort
User:
Passive
Shutter:
closed
02:14:08 PM

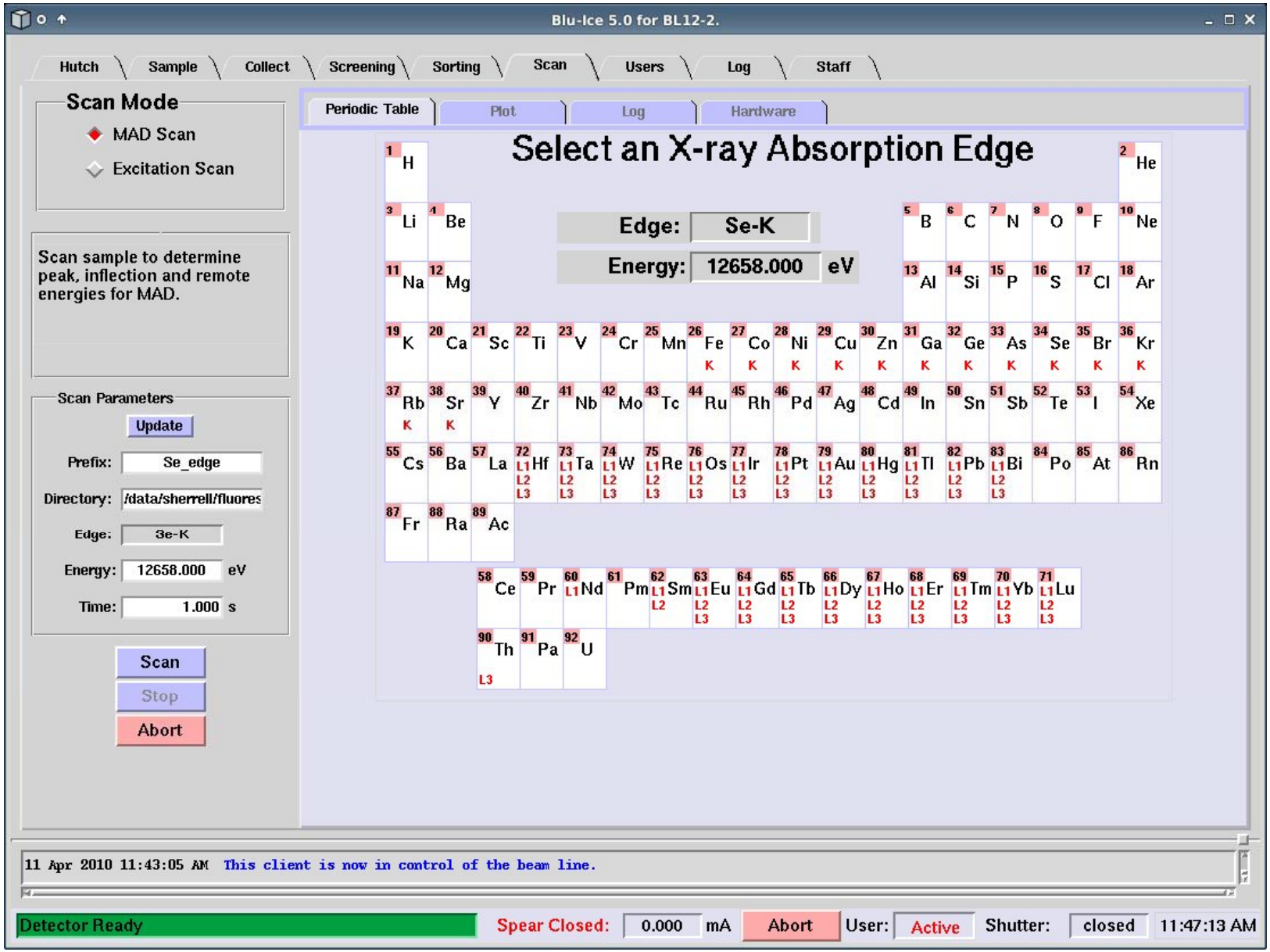
# Auto-Correction and Preview

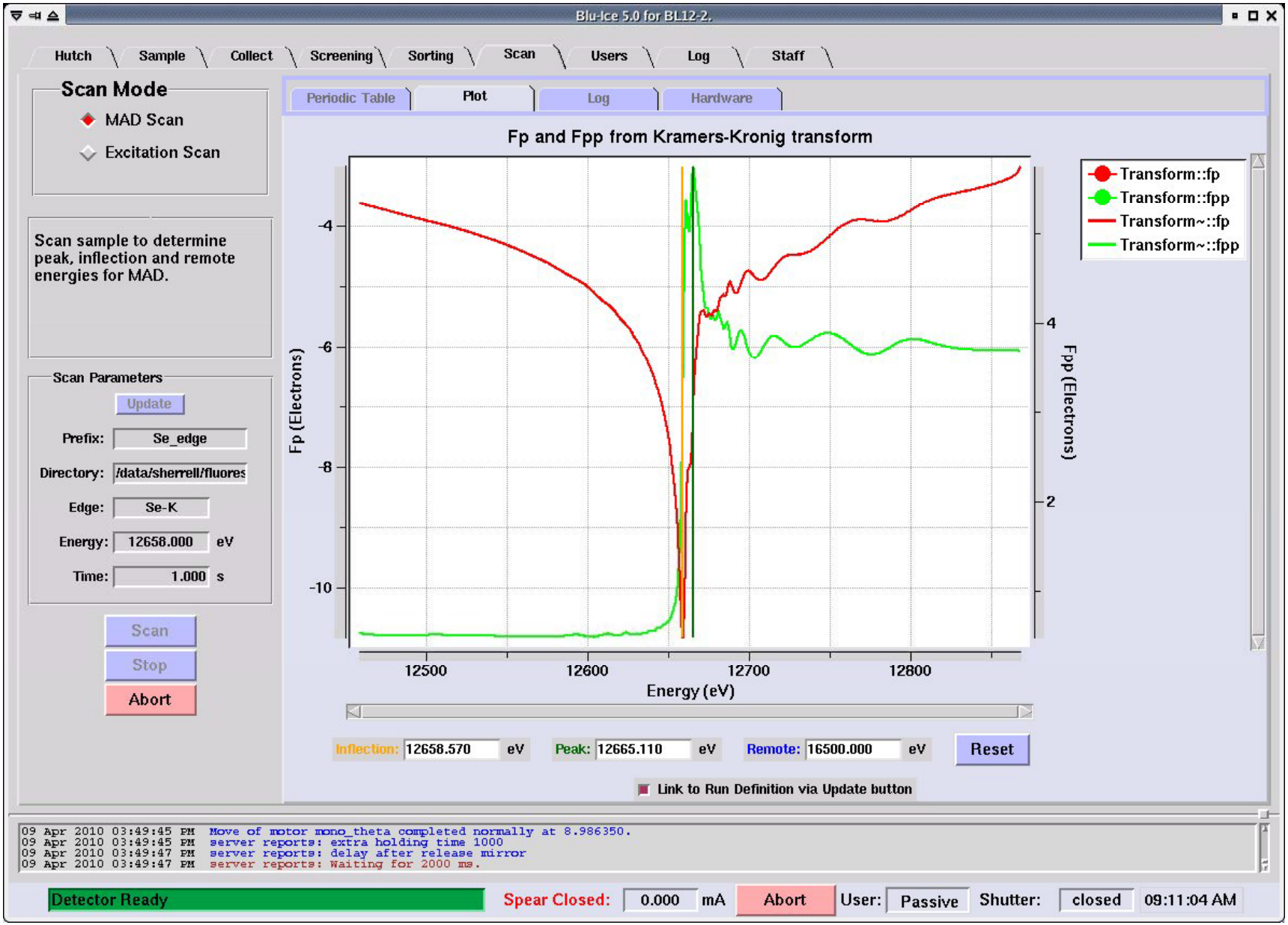


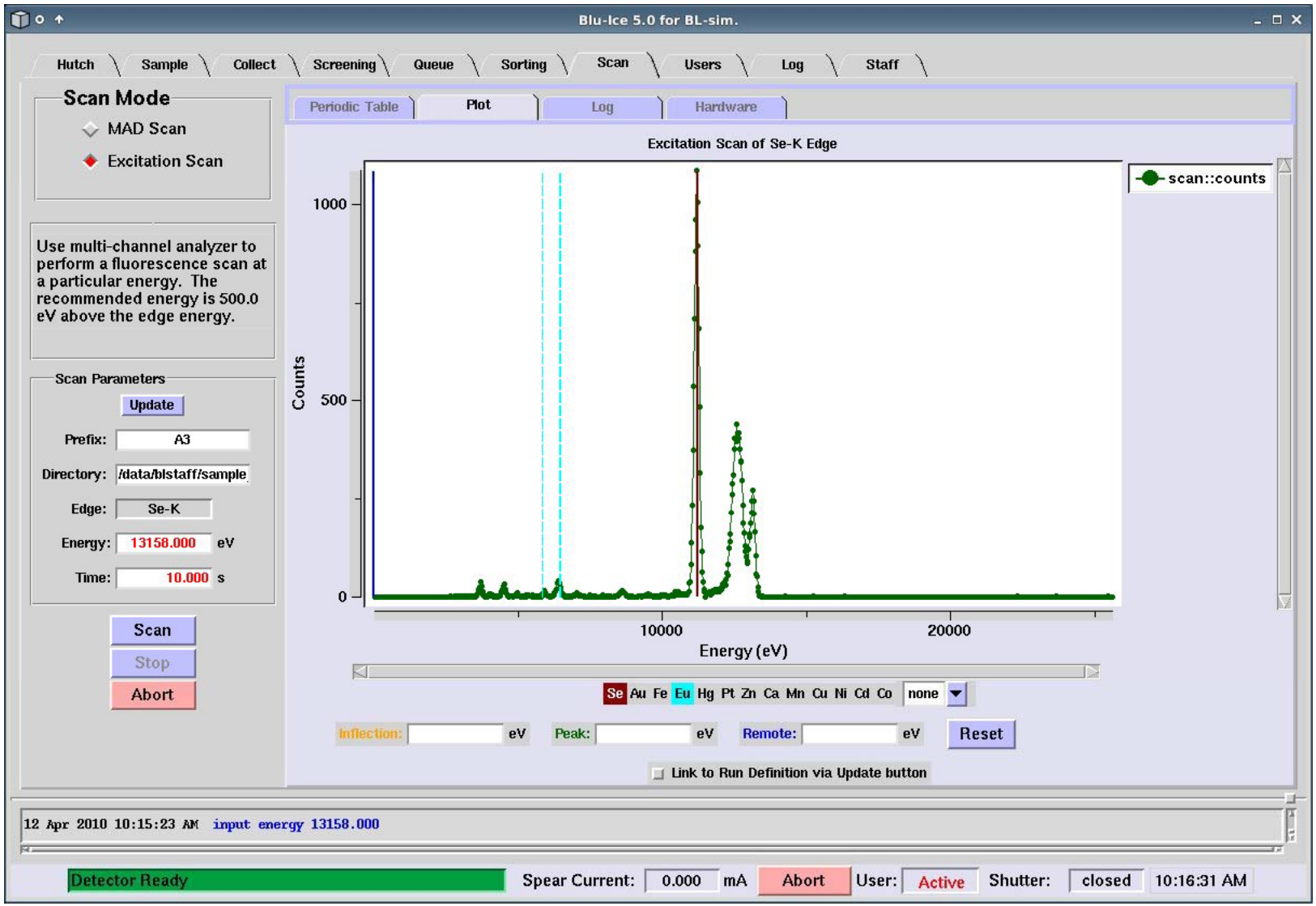

Blu-Ice 5.0 for BL11-1.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Cassette: left: CDI_SSRL100413_CPS_0159.
Web
Import
Export
Edit
View: Custor
Port Containe CrystalID Protein Comment Sys
1 A1 CPS 159 A1 HX94D2 Native
2 A2 CPS 159 A2 HX94D2 Native
Mounted-> A3 CPS 159 A3 44.0 CDIp300, AR2, quick soak <5 min
Mount Next-> A4 CPS 159 A4 1.0 CDIp300, AR2, Glycerol, quick soak <5 m
5 A5 CPS 159 A5 2.0 CDIp300, AR2, Glycerol
6 A6 CPS 159 A6 3.0 CDIp300, AR2, Glycerol
Directory: ta/kornberg/dab/ssrl041310/cps159
Default
Detector: normal
Exposure Control
Enable
Normalize
Exposure Factor: 1.00
Distance: 250.000 mm
Beamstop: 40.000 mm
Attenuation: 0.000 %
Update
loop alignment
Mount Next Crystal
Current-> Loop Alignment
Stop
Collect Image
Collect Image
Collect Image
Stop
Sample
Hutch
Robot
Panel
Diffraction
Select Zoom Level
Low
Med
High
Move Sample
Rotate Phi
-90
+90
+180
Center Loop
Video Snapshot
Sample Lights Control
Back Light
Side Light Intensity
Turn Off
Start
Stop
Dismount
Reset Parameters
Screening Tasks
current: A3
Next: A4
Mode: robot
Synced: yes
Robot: Busy
A3 Loop Alignment
A3 Stop
A3 Video Snapshot
A3 Collect Image
A3 Rotate
A3 Video Snapshot
A3 Collect Image
A3 Rotate
A3 Video Snapshot
A3 Collect Image
A4 Mount Next Crystal
13 Apr 2010 02:49:16 PM Move of motor sample_x completed normally at 0.273143.
13 Apr 2010 02:49:16 PM Move of motor sample_y completed normally at 0.053486.
Screening - loop alignment
Spear Current: 189.488 mA
Abort
User: Passive
Shutter: closed
02:49:16 PM


Blu-Ice 5.0 for BL11-1.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Cassette: left: CDI_SSRL100413_CPS_0159.
Web
Import
Export
Edit
View: Result
Port CrystalID SystemWarning Score UnitCell Mosaicity Rm
1 A1 A1 0.667476409 159.17 112.19 125.21 90 0.75 0.0
2 A2 A2 0.665738094 125.27 112.18 99.79 90.0 0.3 0.0
Mounted-> A3 A3 0.736339869 124.71 111.82 99.45 90.0 0.5 0.0
Mount Next-> A4 A4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
5 A5 A5 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
6 A6 A6 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
Directory: ta/kornberg/dab/ssrl041310/cps159
Default
Detector: normal
Exposure Control
Enable
Normalize
Exposure Factor: 1.00
Distance: 250.000 mm
Update
Beamstop: 40.000 mm
Attenuation: 0.000 %
dismount IA3 mount IA4
Current->
Mount Next Crystal
Loop Alignment
Stop
Collect
Collect
Collect
Stop
Rotate by: 90.000
Delta: 0.500
Time: 5.000
# of Images 1
Start
Stop
Dismount
Reset Parameters
Screening Tasks
A4 Mount Next Crystal
A4 Loop Alignment
A4 Video Snapshot
A4 Collect Image
A4 Rotate
A4 Video Snapshot
A4 Collect Image
A4 Rotate
A4 Video Snapshot
A4 Collect Image
A5 Mount Next Crystal
current: A3
Next: A4
Mode: robot
Synced: yes
Robot: Busy
Sample
Hutch
Robot
Panel
Diffraction
Select Zoom Level
Low
Med
High
Move Sample
Rotate Phi
-90
+90
+180
Center Loop
Video Snapshot
Sample Lights Control
Back Light
Side Light Intensity
Turn Off
13 Apr 2010 02:54:59 PM server reports: wait_for_device gonio_phi
13 Apr 2010 02:55:00 PM move of motor gonio_phi completed normally at 0.000000.
Screening - check goniometer position
Spear Current: 188.682 mA
Abort
User: Passive
Shutter: closed
02:54:59 PM


Blu-Ice 5.0 for BL11-1.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Cassette: left: CDI_SSRL100413_CPS_0159.
Web
Import
Export
Edit
BravaisLatti
Resolution
Images
C2
1.92
A3_0001.mccd
A3_0002.mccd
A3_0003.mccd
C2
1.8
diffraction image
A4_0003.mccd
A4_0004.mccd
A4_0005.mccd
video image
A4_0deg_0003.jpg
A4_90deg_0004.jp
A4_45deg_0005.jp
quality
0.0
0.0
0.0
spot shape
0.63
0.609
0.629
resolution estimate
1.9
1.9
1.9
number of ice rings
0
0
0
diffraction strength
16.6
13.4
15.0
Sample
Hutch
Robot
Panel
Diffraction
Select Zoom Level
Low
Med
High
Move Sample
Rotate Phi
-90
+90
+180
Center Loop
Sample Lights Control
Back Light
Turn Off
Side Light Intensity
Directory: ta/kornberg/dab/ssrl041310/cps159
Default
Detector: normal
Exposure Control
Enable
Normalize
Exposure Factor: 1.00
Distance: 250.000 mm
Beamstop: 40.000 mm
Attenuation: 0.000 %
Update
rotate sample
Mount Next Crystal
Loop Alignment
Stop
Collect Image
Collect Image
Current->
Collect Image
Stop
Start
Stop
Dismount
Reset Parameters
Screening Tasks
A5 Rotate
A5 Video Snapshot
A5 Collect Image
A6 Mount Next Crystal
A6 Loop Alignment
A6 Stop
A6 Video Snapshot
A6 Collect Image
A6 Rotate
A6 Video Snapshot
A6 Collect Image
current: A5
Next: A6
Mode: robot
Synced: yes
Robot: Normal
13 Apr 2010 03:03:41 PM server reports: SIL 16035 101
13 Apr 2010 03:03:41 PM BluIce reports: SIL 16035 101
Screening - rotate sample
Spear Current: 187.479 mA
Abort
User: Passive
Shutter: closed
03:03:42 PM


Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Scan Mode
MAD Scan
Excitation Scan
Scan sample to determine peak, inflection and remote energies for MAD.
Scan Parameters
Update
Prefix: Se_edge
Directory: /data/sherrell/fluores
Edge: Se-K
Energy: 12658.000 eV
Time: 1.000 s
Scan
Stop
Abort
Periodic Table
Plot
Log
Hardware
Select an X-ray Absorption Edge
Edge: Se-K
Energy: 12658.000 eV
11 Apr 2010 11:43:05 AM This client is now in control of the beam line.
Detector Ready
Spear Closed: 0.000 mA
Abort
User: Active
Shutter: closed
11:47:13 AM


Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Scan Mode
MAD Scan
Excitation Scan
Scan sample to determine peak, inflection and remote energies for MAD.
Scan Parameters
Update
Prefix: Se_edge
Directory: /data/sherrell/fluores
Edge: Se-K
Energy: 12658.000 eV
Time: 1.000 s
Scan
Stop
Abort
Periodic Table
Plot
Log
Hardware
Fp and Fpp from Kramers-Kronig transform
Transform::fp
Transform::fpp
Transform~::fp
Transform~::fpp
Fp (Electrons)
Fpp (Electrons)
Energy (eV)
Inflection: 12658.570 eV
Peak: 12665.110 eV
Remote: 16500.000 eV
Reset
Link to Run Definition via Update button
09 Apr 2010 03:49:45 PM Move of motor mono_theta completed normally at 8.986350.
09 Apr 2010 03:49:45 PM server reports: extra holding time 1000
09 Apr 2010 03:49:47 PM server reports: delay after release mirror
09 Apr 2010 03:49:47 PM server reports: Waiting for 2000 ms.
Detector Ready
Spear Closed: 0.000 mA
Abort
User: Passive
Shutter: closed
09:11:04 AM


Blu-Ice 5.0 for BL-sim.
Hutch
Sample
Collect
Screening
Queue
Sorting
Scan
Users
Log
Staff
Scan Mode
MAD Scan
Excitation Scan
Use multi-channel analyzer to perform a fluorescence scan at a particular energy. The recommended energy is 500.0 eV above the edge energy.
Scan Parameters
Update
Prefix: A3
Directory: /data/blstaff/sample
Edge: Se-K
Energy: 13158.000 eV
Time: 10.000 s
Scan
Stop
Abort
Periodic Table
Plot
Log
Hardware
Excitation Scan of Se-K Edge
scan::counts
Counts
1000
500
0
10000
20000
Energy (eV)
Se Au Fe Eu Hg Pt Zn Ca Mn Cu Ni Cd Co none
Inflection: eV
Peak: eV
Remote: eV
Reset
Link to Run Definition via Update button
12 Apr 2010 10:15:23 AM input energy 13158.000
Detector Ready
Spear Current: 0.000 mA
Abort
User: Active
Shutter: closed
10:16:31 AM

Blu-Ice 5.0 for BL12-2.

Hutch | Sample | Collect | Screening | Sorting | Scan | Users | Log | Staff

Users

| | User Name | Staff | Roaming | Location | |
|---|---|---|---|---|---|
| | Jinhu Song | Yes | Yes | REMOTE | |
| | Staff Account | Yes | Yes | HUTCH | Pete |
| | Staff Account | Yes | Yes | REMOTE | Mike |
| | Graeme Card | Yes | Yes | REMOTE | Graeme Card at lab x 5594 |
| Active--> | Jinhu Song | Yes | Yes | REMOTE | at home |

Notification Setup (email addresses separated by "," )

Submit | Cancel | Send Test Message | Clear All

jinhu@stanford.edu

- [x] Spear State
- [x] Screening
- [ ] Collect
- [ ] Sorting Crysta
- [ ] Motor Scans

Chat Room

load file | refresh | download | new chat | pause

11 Apr 2010 11:41:56 AM jsong: {Test message for BNL workshop}

Type message then hit Enter

Color: Blue | Brown | Red

11 Apr 2010 11:43:05 AM This client is now in control of the beam line.

Detector Ready | Spear Closed: 0.000 mA | Abort | User: Active | Shutter: closed | 11:43:51 AM

Blu-Ice 5.0 for BL14-1.

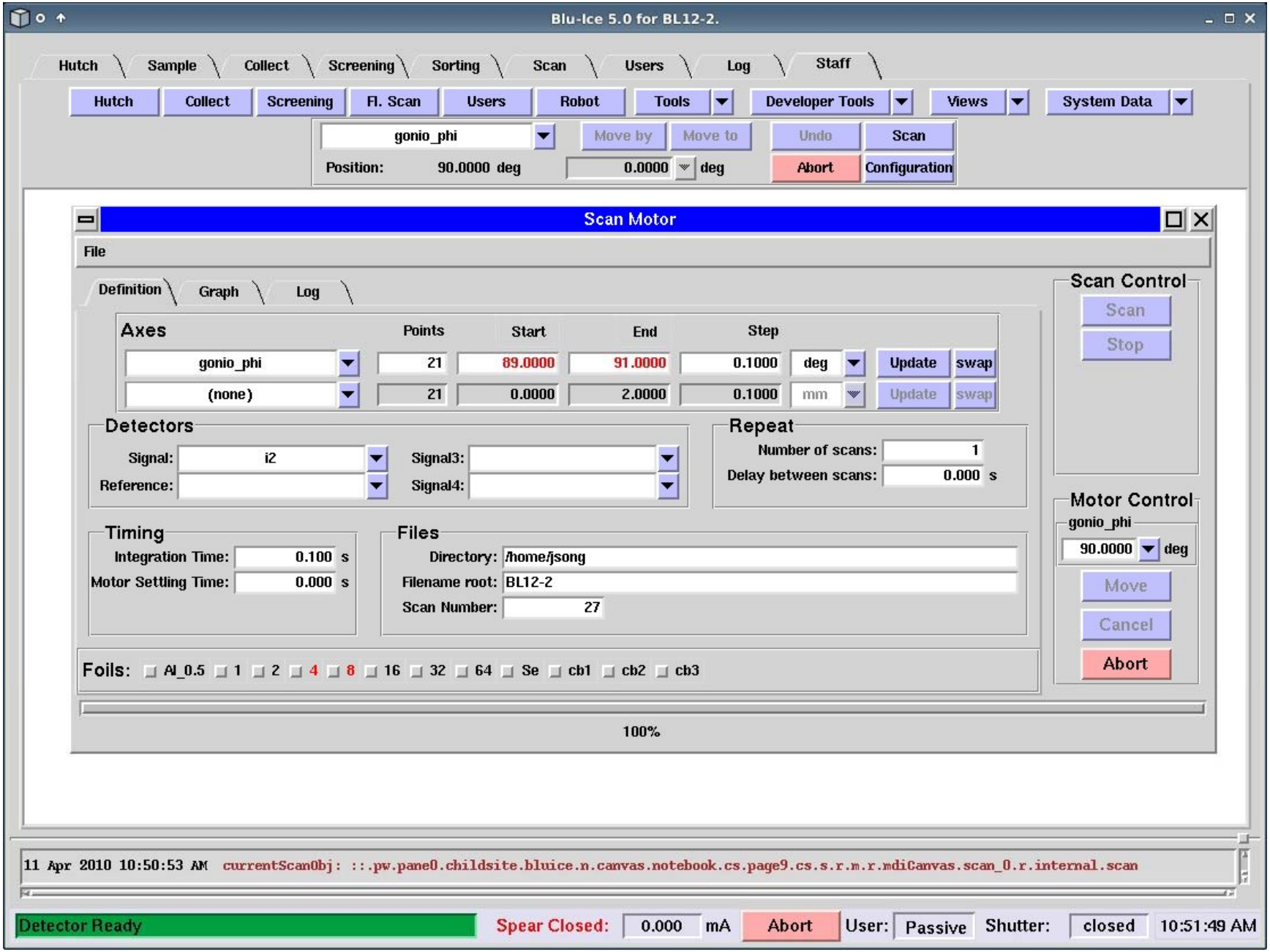
Hutch | Sample | Collect | Screening | Sorting | Scan | Users | Log | Staff

load file | refresh | download | new log | pause

```
24 Feb 2010 03:18:46 PM  madscan scan66 12680.0 748.989690722 0.518546 1444.40356443 3%
24 Feb 2010 03:18:49 PM  madscan scan67 12681.0 734.127835052 0.517591 1418.35510094 3%
24 Feb 2010 03:18:52 PM  madscan scan68 12682.0 753.929896907 0.516854 1458.69026245 3%
24 Feb 2010 03:18:55 PM  madscan scan69 12683.0 690.733333333 0.515547 1339.80671662 4%
24 Feb 2010 03:18:58 PM  madscan scan70 12684.0 756.593814433 0.514767 1469.77917083 3%
24 Feb 2010 03:19:00 PM  madscan scan71 12685.0 732.494845361 0.513788 1425.67526949 3%
24 Feb 2010 03:19:03 PM  madscan scan72 12686.0 735.85 0.512659 1435.3595665 4%
24 Feb 2010 03:19:05 PM  madscan scan73 12687.0 743.513402062 0.511916 1452.41289989 3%
24 Feb 2010 03:19:08 PM  madscan scan74 12688.0 691.859793814 0.510981 1353.98340411 3%
24 Feb 2010 03:19:11 PM  madscan scan75 12689.5 762.070103093 0.510182 1493.72205035 3%
24 Feb 2010 03:19:14 PM  madscan scan76 12693.0 666.991666667 0.506651 1316.47162774 4%
24 Feb 2010 03:19:16 PM  madscan scan77 12698.0 661.146391753 0.501931 1317.20573496 3%
24 Feb 2010 03:19:19 PM  madscan scan78 12704.5 672.981443299 0.496079 1356.60135442 3%
24 Feb 2010 03:19:22 PM  madscan scan79 12712.5 621.542268041 0.488524 1272.2860454 3%
24 Feb 2010 03:19:25 PM  madscan scan80 12722.0 648.668041237 0.48022 1350.77264845 3%
24 Feb 2010 03:19:27 PM  madscan scan81 12733.0 713.616494845 0.470748 1515.92039657 3%
24 Feb 2010 03:19:30 PM  madscan scan82 12745.5 667.826804124 0.45984 1452.30254898 3%
24 Feb 2010 03:19:33 PM  madscan scan83 12759.5 655.670103093 0.447471 1465.27954458 3%
24 Feb 2010 03:19:36 PM  madscan scan84 12775.0 646.391752577 0.434831 1486.53557952 3%
24 Feb 2010 03:19:38 PM  madscan scan85 12792.0 647.257142857 0.421153 1536.86936305 2%
24 Feb 2010 03:19:41 PM  madscan scan86 12810.5 603.016666667 0.40581 1485.9581249 4%
24 Feb 2010 03:19:44 PM  madscan scan87 12838.0 556.593814433 0.383806 1450.19570938 3%
24 Feb 2010 03:19:47 PM  madscan scan88 12868.0 585.183673469 0.360562 1622.97655734 2%
24 Feb 2010 03:19:47 PM  madscan averate dead time ration 2%
24 Feb 2010 03:19:57 PM  madscan autochooch 12657.950195 -9.705869 2.793999 12664.490234 -7.007955 5.457547 9000.000000 -1.000000 0.900000 NULL/Sescan Sesmooth_ex
24 Feb 2010 03:19:57 PM  madscan ==================end==========================
24 Feb 2010 04:13:48 PM  screening ========eigenbro start /data/eigenbro/2010_02_24_SSRL_141/p124/x02=========
24 Feb 2010 04:13:48 PM  screening cassette: puck_loading_2010_02_24_14_1_1.xls(eigenbro|UNKNOWN|15834)
24 Feb 2010 04:13:48 PM  screening energy                12657.982 ev
24 Feb 2010 04:13:48 PM  screening attenuation           0.000 %
24 Feb 2010 04:16:53 PM  screening ==================stopped================
24 Feb 2010 04:19:37 PM  collecting ======eigenbro start collectRun 0======
24 Feb 2010 04:20:27 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x01/test_p124x02__0_0001.mccd 0.000 deg
24 Feb 2010 04:20:27 PM  collecting =======end collectRun 0========
24 Feb 2010 04:22:49 PM  collecting ======eigenbro start collectRun 0======
24 Feb 2010 04:22:56 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x01/test_p124x02__0_0002.mccd 0.000 deg
24 Feb 2010 04:22:57 PM  collecting =======end collectRun 0========
24 Feb 2010 04:25:48 PM  collecting ======eigenbro start collectRuns 1=====
24 Feb 2010 04:25:49 PM  collecting =========run 1========
24 Feb 2010 04:25:56 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0001.mccd 0.000 deg
24 Feb 2010 04:26:05 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0002.mccd 1.000 deg
24 Feb 2010 04:26:13 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0003.mccd 2.000 deg
24 Feb 2010 04:26:21 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0004.mccd 3.000 deg
24 Feb 2010 04:26:30 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0005.mccd 4.000 deg
24 Feb 2010 04:26:38 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0006.mccd 5.000 deg
24 Feb 2010 04:26:46 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0007.mccd 6.000 deg
24 Feb 2010 04:26:54 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0008.mccd 7.000 deg
24 Feb 2010 04:27:03 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0009.mccd 8.000 deg
24 Feb 2010 04:27:11 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0010.mccd 9.000 deg
24 Feb 2010 04:27:19 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0011.mccd 10.000 deg
24 Feb 2010 04:27:28 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0012.mccd 11.000 deg
24 Feb 2010 04:27:36 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0013.mccd 12.000 deg
24 Feb 2010 04:27:45 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0014.mccd 13.000 deg
24 Feb 2010 04:27:53 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0015.mccd 14.000 deg
24 Feb 2010 04:28:01 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0016.mccd 15.000 deg
24 Feb 2010 04:28:10 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0017.mccd 16.000 deg
24 Feb 2010 04:28:18 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0018.mccd 17.000 deg
24 Feb 2010 04:28:26 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0019.mccd 18.000 deg
24 Feb 2010 04:28:34 PM  collecting 1A2 collect /data/eigenbro/2010_02_24_SSRL_141/p124/x02/p124x02__1_0020.mccd 19.000 deg
```

```
13 Apr 2010 03:17:05 PM  Move of motor sample_z completed normally at 0.000000.
```

Screening - mount IA3 | Spear Current: 185.656 mA | Abort | User: Passive | Shutter: closed | 03:17:06 PM


Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
gonio_phi
Move by
Move to
Undo
Scan
Position:
90.0000 deg
0.0000
deg
Abort
Configuration
Scan Motor
File
Definition
Graph
Log
Axes
Points
Start
End
Step
gonio_phi
21
89.0000
91.0000
0.1000
deg
Update
swap
(none)
21
0.0000
2.0000
0.1000
mm
Update
swap
Detectors
Signal:
i2
Signal3:
Reference:
Signal4:
Repeat
Number of scans:
1
Delay between scans:
0.000
s
Timing
Integration Time:
0.100
s
Motor Settling Time:
0.000
s
Files
Directory:
/home/jsong
Filename root:
BL12-2
Scan Number:
27
Foils:
Al_0.5
1
2
4
8
16
32
64
Se
cb1
cb2
cb3
Scan Control
Scan
Stop
Motor Control
gonio_phi
90.0000
deg
Move
Cancel
Abort
100%
11 Apr 2010 10:50:53 AM
currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page9.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
Detector Ready
Spear Closed:
0.000
mA
Abort
User:
Passive
Shutter:
closed
10:51:49 AM

Blu-Ice 5.0 for BL9-1.

Hutch | Sample | Collect | Screening | Sorting | Scan | Users | Log | Staff

Hutch | Collect | Screening | Fl. Scan | Users | Robot | Tools | Developer Tools | Views | System Data

beamstop_z | Move by | Move to | Undo | Scan

Position: 40.0051 mm | 0.00000 mm | Abort | Configuration

## Scan Motor

File

Definition | Graph | Log

**Axes**

| | Points | Start | End | Step | | | |
|---|---|---|---|---|---|---|---|
| beamstop_z | 21 | 39.01 | 41.01 | 0.10 | mm | Update | swap |
| (none) | 21 | 0.0000 | 2.0000 | 0.1000 | mm | Update | swap |

**Detectors**

Signal: i2 | Signal3:

Reference: | Signal4:

**Repeat**

Number of scans: 1

Delay between scans: 0.000 s

**Timing**

Integration Time: 0.100 s

Motor Settling Time: 0.000 s

**Files**

Directory: /home/jsong

Filename root: BL9-1

Scan Number: 6

Foils: 1 2 4 8 16 32 Se

**Scan Control**

Backlash

Scan

Stop

**Motor Control**

beamstop_z

40.01 mm

Move

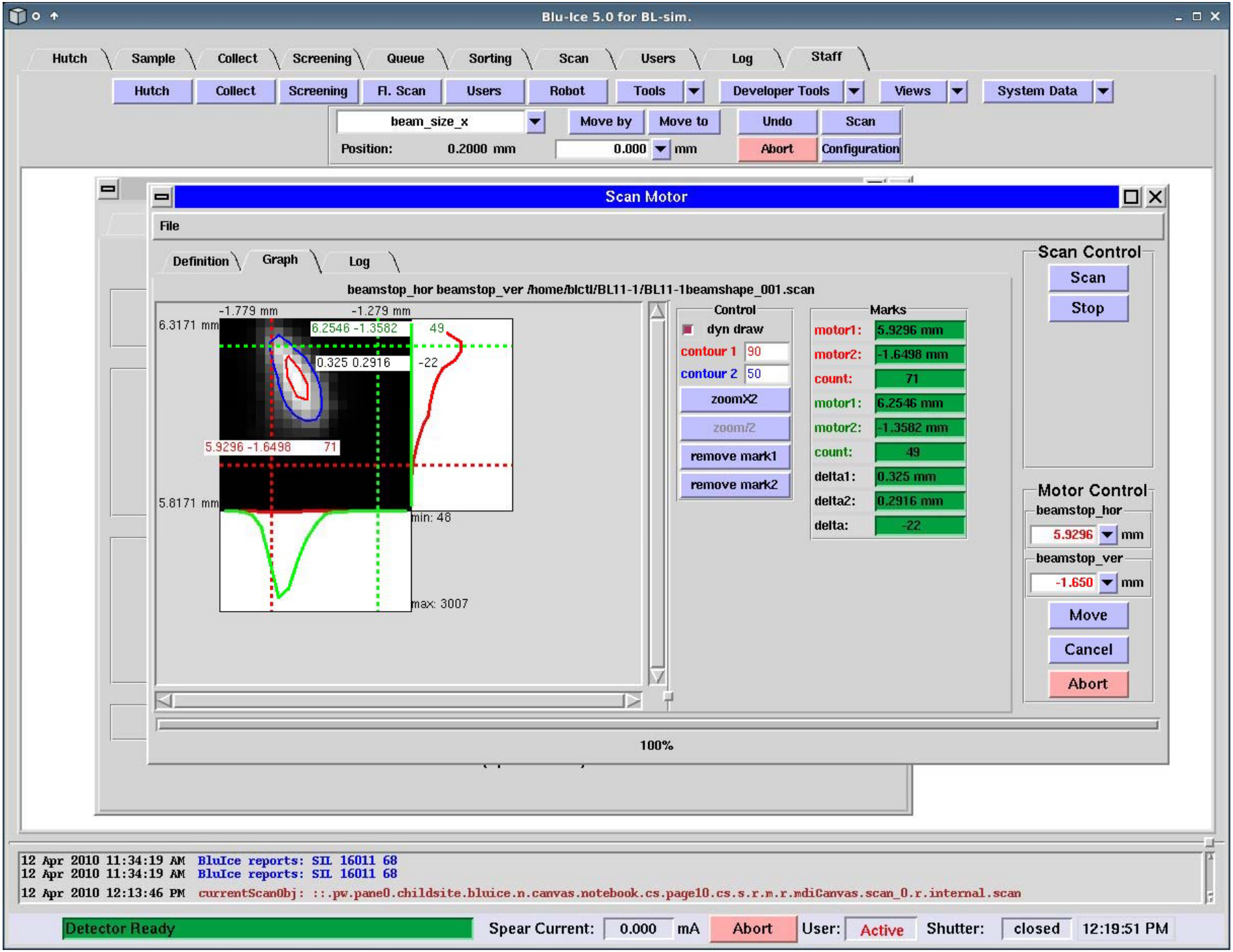
Cancel

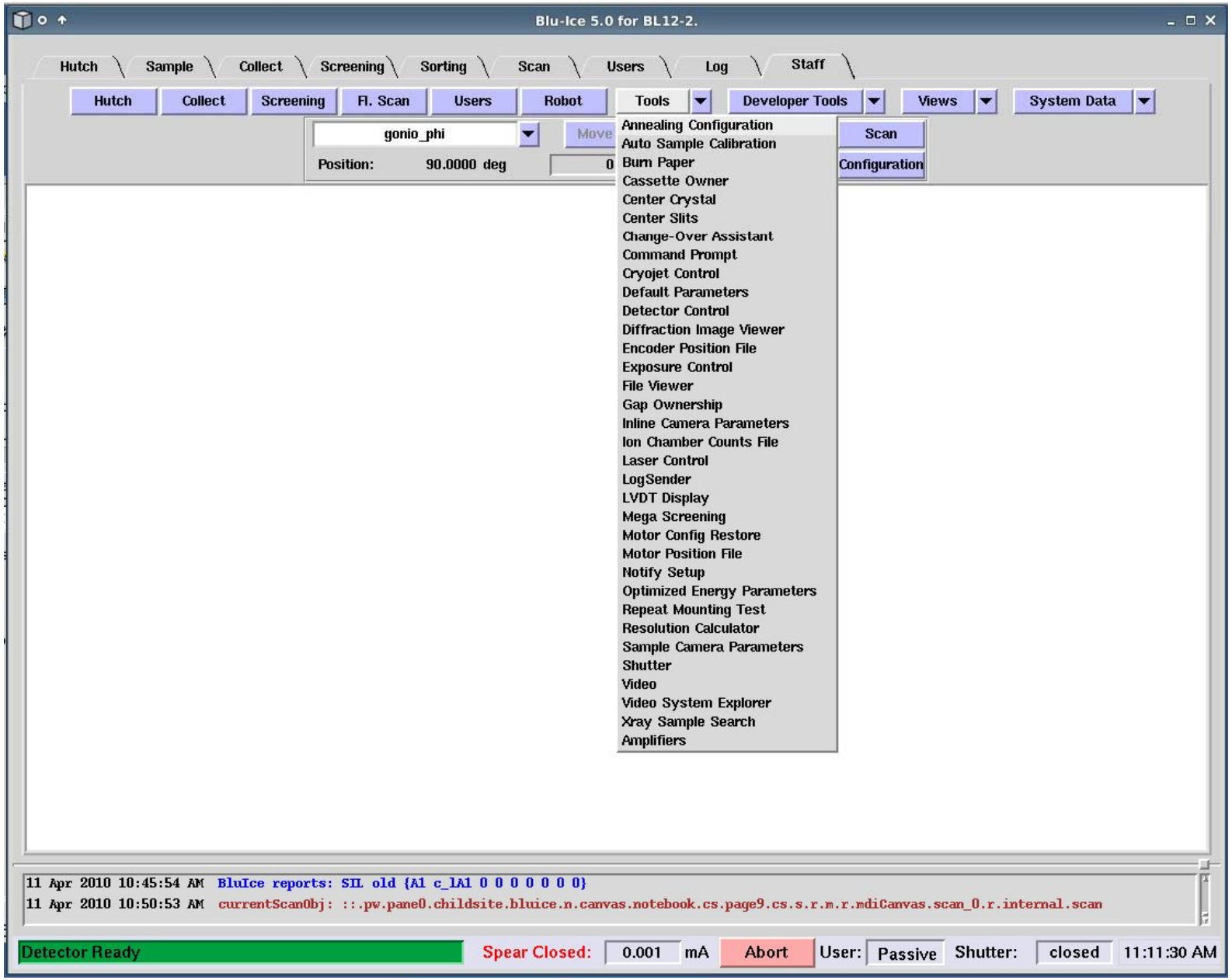
Abort

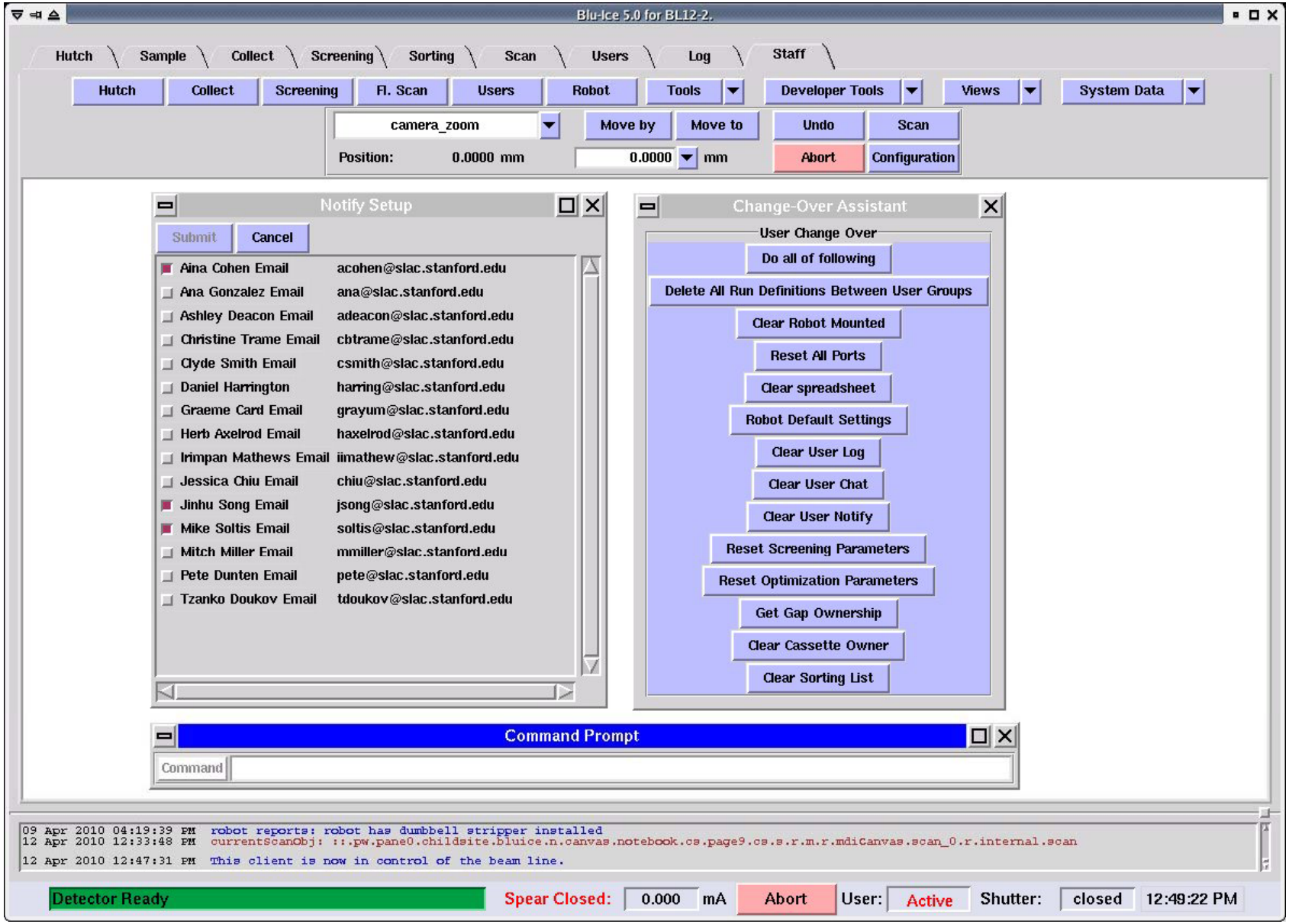
100%

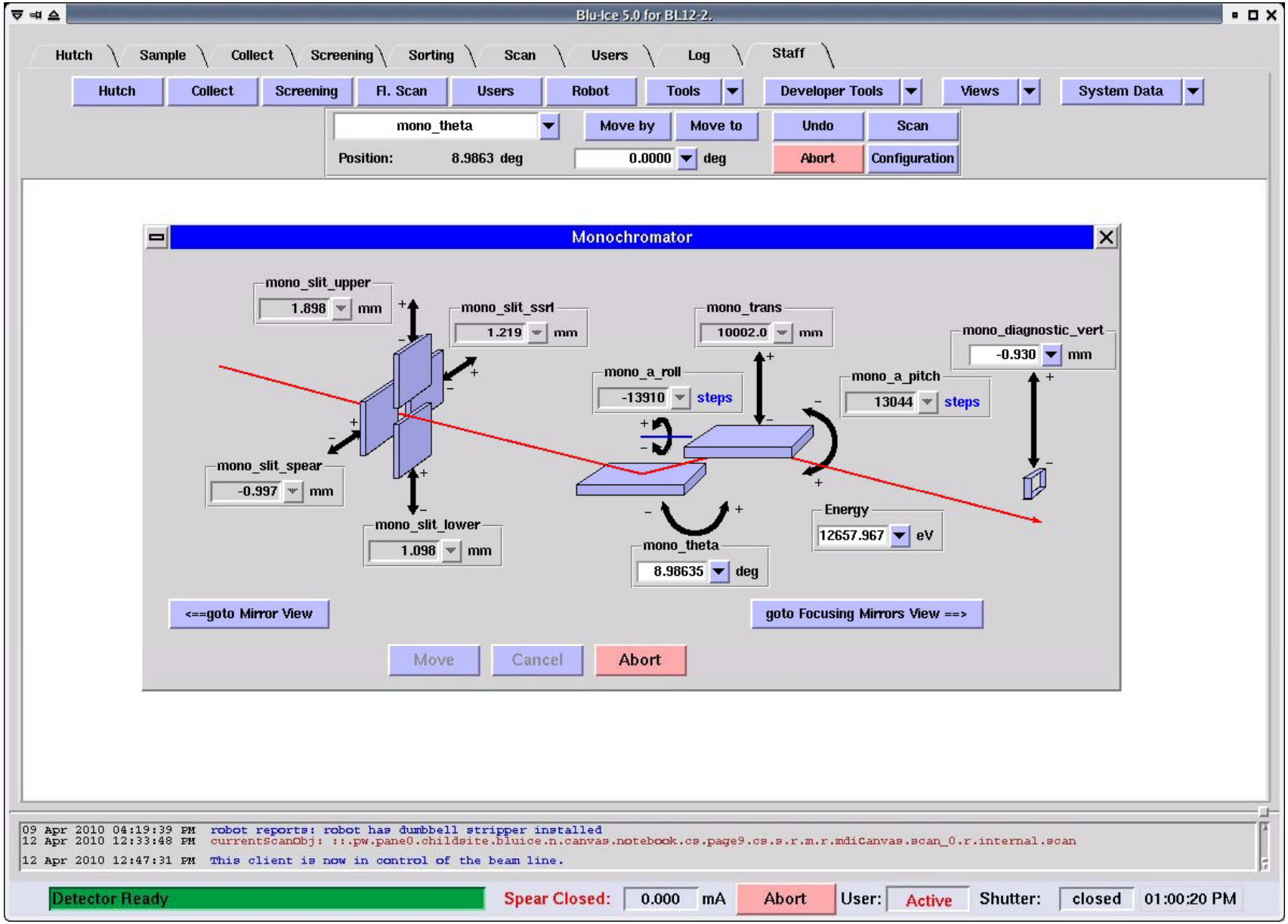
```
10 Apr 2010 12:03:43 AM  cryojet_mode open
12 Apr 2010 12:28:14 PM  currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page9.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
```

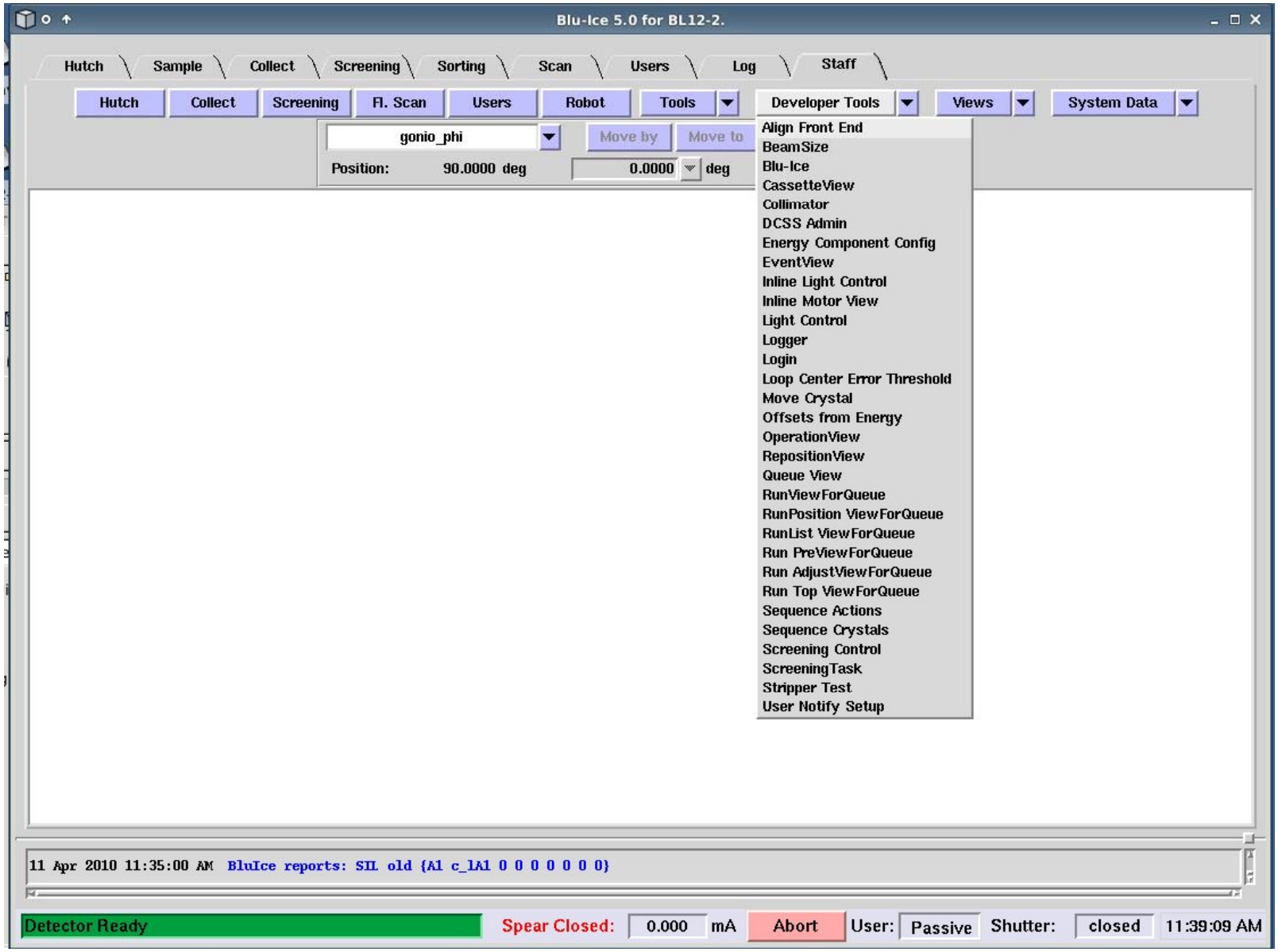
cryoJet temperature 297 K | Spear Closed: 0.000 mA | Abort | User: Passive | Shutter: closed | 12:30:55 PM


Blu-Ice 5.0 for BL-sim.
Hutch
Sample
Collect
Screening
Queue
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
beam_size_x
Move by
Move to
Undo
Scan
Position:
0.2000 mm
0.000
mm
Abort
Configuration
Scan Motor
File
Definition
Graph
Log
beamstop_hor beamstop_ver /home/blctl/BL11-1/BL11-1beamshape_001.scan
-1.779 mm
-1.279 mm
6.3171 mm
6.2546 -1.3582
49
0.325 0.2916
-22
5.9296 -1.6498
71
5.8171 mm
min: 48
max: 3007
Control
dyn draw
contour 1
90
contour 2
50
zoomX2
zoom/2
remove mark1
remove mark2
Marks
motor1:
5.9296 mm
motor2:
-1.6498 mm
count:
71
motor1:
6.2546 mm
motor2:
-1.3582 mm
count:
49
delta1:
0.325 mm
delta2:
0.2916 mm
delta:
-22
Scan Control
Scan
Stop
Motor Control
beamstop_hor
5.9296
mm
beamstop_ver
-1.650
mm
Move
Cancel
Abort
100%
12 Apr 2010 11:34:19 AM BluIce reports: SIL 16011 68
12 Apr 2010 11:34:19 AM BluIce reports: SIL 16011 68
12 Apr 2010 12:13:46 PM currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page10.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
Detector Ready
Spear Current:
0.000
mA
Abort
User:
Active
Shutter:
closed
12:19:51 PM


Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
gonio_phi
Move
Scan
Position:
90.0000 deg
0
Configuration
Annealing Configuration
Auto Sample Calibration
Burn Paper
Cassette Owner
Center Crystal
Center Slits
Change-Over Assistant
Command Prompt
Cryojet Control
Default Parameters
Detector Control
Diffraction Image Viewer
Encoder Position File
Exposure Control
File Viewer
Gap Ownership
Inline Camera Parameters
Ion Chamber Counts File
Laser Control
LogSender
LVDT Display
Mega Screening
Motor Config Restore
Motor Position File
Notify Setup
Optimized Energy Parameters
Repeat Mounting Test
Resolution Calculator
Sample Camera Parameters
Shutter
Video
Video System Explorer
Xray Sample Search
Amplifiers
11 Apr 2010 10:45:54 AM BluIce reports: SIL old {A1 c_lA1 0 0 0 0 0 0 0}
11 Apr 2010 10:50:53 AM currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page9.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
Detector Ready
Spear Closed:
0.001
mA
Abort
User:
Passive
Shutter:
closed
11:11:30 AM


Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
camera_zoom
Move by
Move to
Undo
Scan
Position: 0.0000 mm
0.0000
mm
Abort
Configuration
Notify Setup
Submit
Cancel
Aina Cohen Email acohen@slac.stanford.edu
Ana Gonzalez Email ana@slac.stanford.edu
Ashley Deacon Email adeacon@slac.stanford.edu
Christine Trame Email cbtrame@slac.stanford.edu
Clyde Smith Email csmith@slac.stanford.edu
Daniel Harrington harring@slac.stanford.edu
Graeme Card Email grayum@slac.stanford.edu
Herb Axelrod Email haxelrod@slac.stanford.edu
Irimpan Mathews Email iimathew@slac.stanford.edu
Jessica Chiu Email chiu@slac.stanford.edu
Jinhu Song Email jsong@slac.stanford.edu
Mike Soltis Email soltis@slac.stanford.edu
Mitch Miller Email mmiller@slac.stanford.edu
Pete Dunten Email pete@slac.stanford.edu
Tzanko Doukov Email tdoukov@slac.stanford.edu
Change-Over Assistant
User Change Over
Do all of following
Delete All Run Definitions Between User Groups
Clear Robot Mounted
Reset All Ports
Clear spreadsheet
Robot Default Settings
Clear User Log
Clear User Chat
Clear User Notify
Reset Screening Parameters
Reset Optimization Parameters
Get Gap Ownership
Clear Cassette Owner
Clear Sorting List
Command Prompt
Command
09 Apr 2010 04:19:39 PM robot reports: robot has dumbbell stripper installed
12 Apr 2010 12:33:48 PM currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page9.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
12 Apr 2010 12:47:31 PM This client is now in control of the beam line.
Detector Ready
Spear Closed:
0.000
mA
Abort
User:
Active
Shutter:
closed
12:49:22 PM


Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
mono_theta
Move by
Move to
Undo
Scan
Position:
8.9863 deg
0.0000
deg
Abort
Configuration
Monochromator
mono_slit_upper
1.898
mm
mono_slit_ssrl
1.219
mm
mono_trans
10002.0
mm
mono_diagnostic_vert
-0.930
mm
mono_a_roll
-13910
steps
mono_a_pitch
13044
steps
mono_slit_spear
-0.997
mm
mono_slit_lower
1.098
mm
mono_theta
8.98635
deg
Energy
12657.967
eV
<==goto Mirror View
goto Focusing Mirrors View ==>
Move
Cancel
Abort
09 Apr 2010 04:19:39 PM robot reports: robot has dumbbell stripper installed
12 Apr 2010 12:33:48 PM currentScanObj: ::.pw.pane0.childsite.bluice.n.canvas.notebook.cs.page9.cs.s.r.m.r.mdiCanvas.scan_0.r.internal.scan
12 Apr 2010 12:47:31 PM This client is now in control of the beam line.
Detector Ready
Spear Closed:
0.000
mA
Abort
User:
Active
Shutter:
closed
01:00:20 PM

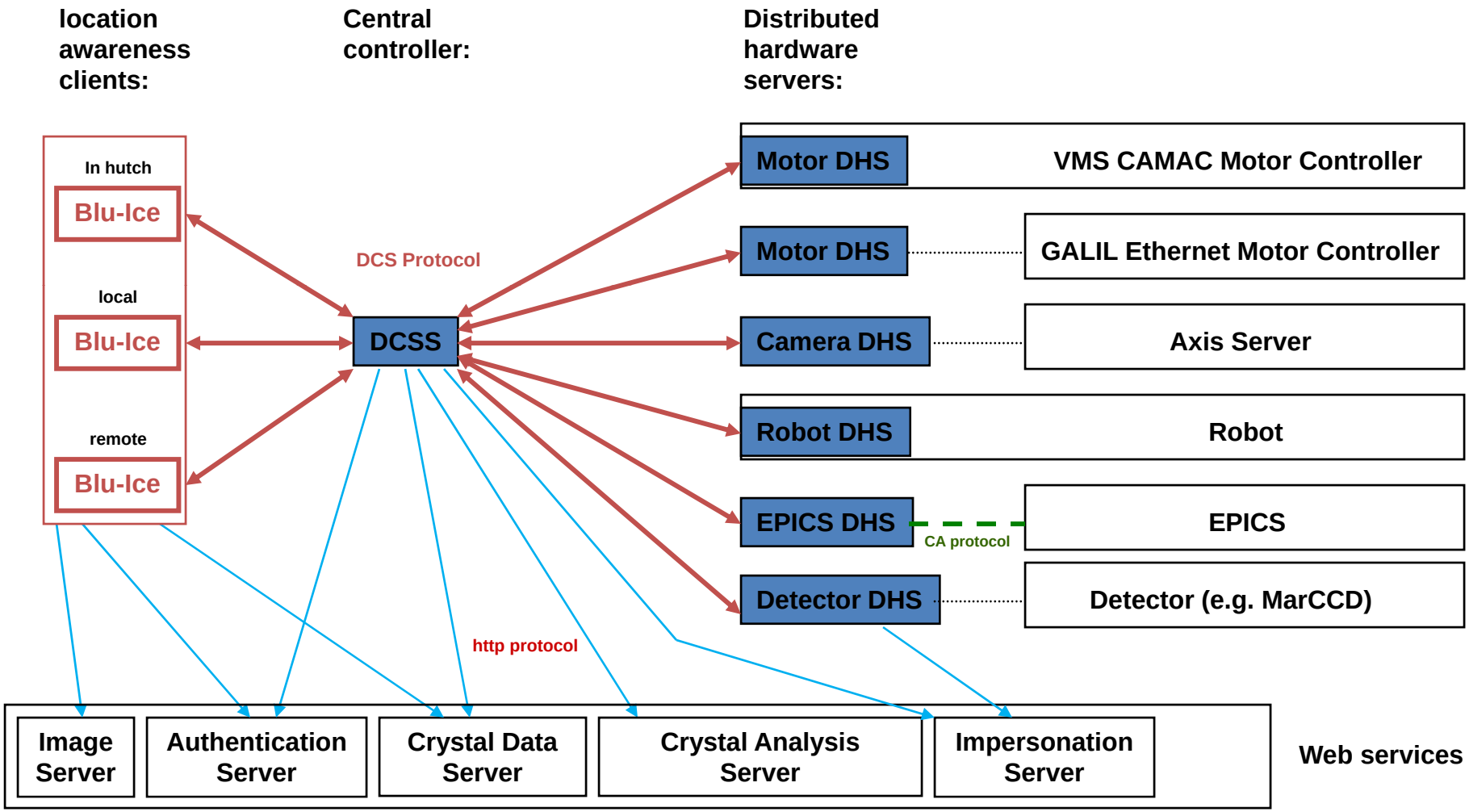

Blu-Ice 5.0 for BL12-2.
Hutch
Sample
Collect
Screening
Sorting
Scan
Users
Log
Staff
Hutch
Collect
Screening
Fl. Scan
Users
Robot
Tools
Developer Tools
Views
System Data
gonio_phi
Move by
Move to
Position:
90.0000 deg
0.0000
deg
Align Front End
BeamSize
Blu-Ice
CassetteView
Collimator
DCSS Admin
Energy Component Config
EventView
Inline Light Control
Inline Motor View
Light Control
Logger
Login
Loop Center Error Threshold
Move Crystal
Offsets from Energy
OperationView
RepositionView
Queue View
RunViewForQueue
RunPosition ViewForQueue
RunList ViewForQueue
Run PreViewForQueue
Run AdjustViewForQueue
Run Top ViewForQueue
Sequence Actions
Sequence Crystals
Screening Control
ScreeningTask
Stripper Test
User Notify Setup
11 Apr 2010 11:35:00 AM BluIce reports: SIL old {A1 c_lA1 0 0 0 0 0 0 0}
Detector Ready
Spear Closed:
0.000
mA
Abort
User:
Passive
Shutter:
closed
11:39:09 AM

# BluIce, the GUI

Point of view of programmer

- Object Oriented (incrTcl/TK): reusable widgets from small single button to the whole BluIce.
- Component Framework:  publish attributes for subscription
- GateExtension: Automatic message for balloon hints.
- Configure support,
- Log support.

# DCS framework



# Special features of framwork

- Central Control
- Ultra-light text wire protocol
- Security:
  - Authentication Server
  - Impersonation Server
- WebIce Services:
  - Crystal Information Server
  - Crystal Analysis Server

The Dcs Message Format:
Header: 26 bytes NULL ended text with 2 numbers in ASCII format.

Message sequence for a motor move command:
Active BluIce ➔DCSS: gtos_start_motor_move beam_stop_z 12.0
DCSS ➔ galil1: stog_start_motor_move beam_stop_z 12.0
Galil1 ➔ DCSS: htos_motor_move_started beam_stop_z 12.0
Galil1 ➔ DCSS: htos_update_motor_position beam_stop_z 30.0
Galil1 ➔ DCSS: htos_update_motor_position beam_stop_z 20.0
Galil1 ➔ DCSS: htos_update_motor_position beam_stop_z 12.0
Galil1 ➔ DCSS: htos_motor_move_completed beam_stop_z 12.0 normal

DCSS will broadcast all message from Galil1 to all BluIce clients.
The Galil1 sends the update message at around 10Hz.

# DCSS

Switching:

Relay message from BluIce to the devices's host DHS
Broadcast message from DHS to all BluIce

"self": a special build-in DCSS client: registered as both DHS and BluIce

It is the script engine, supports devices: operation, motor, string, ion chamber….

It is also an GUI client so that it can receive all messages from all DHS to keep track of all devices and send command to DCSS to access other DHS.

There is no special treatment for "self" in DCSS, except it does not need authentication.

# Script engine

- A place to integrate devices from different DHS into a super device (like energy)
- A place to write operations (scripts) to finish a task, especially if the task need to access more than one devices (like screening)

# An operation

- proc NAME_initialize {}
- proc NAME_start {argument list}
- proc NAME_cleanup {}

# A motor

- Proc NAME_initialize {}
- Proc NAME_move { new_position}
- Proc NAME_set { new_position }
- Proc NAME_update {}
- Proc NAME_calculate { child_motor_list_if_any }

# Device Mapping

- energy
  2
  self energy_bl92
  0 1 1 1 1
  0 0 1 1 1
  1
  12666.012477 15000 6000 0 0 0 0 ev
  mono_theta_corr

# Security

- Authentication Server (Tomcat jsessionID, CAS as reference)
  - single sign-on
  - Support one-time ticket with short time span
  - https
- Impersonation Server
  - Access file on behave of user
  - Run data processing scripts as user
- SSL

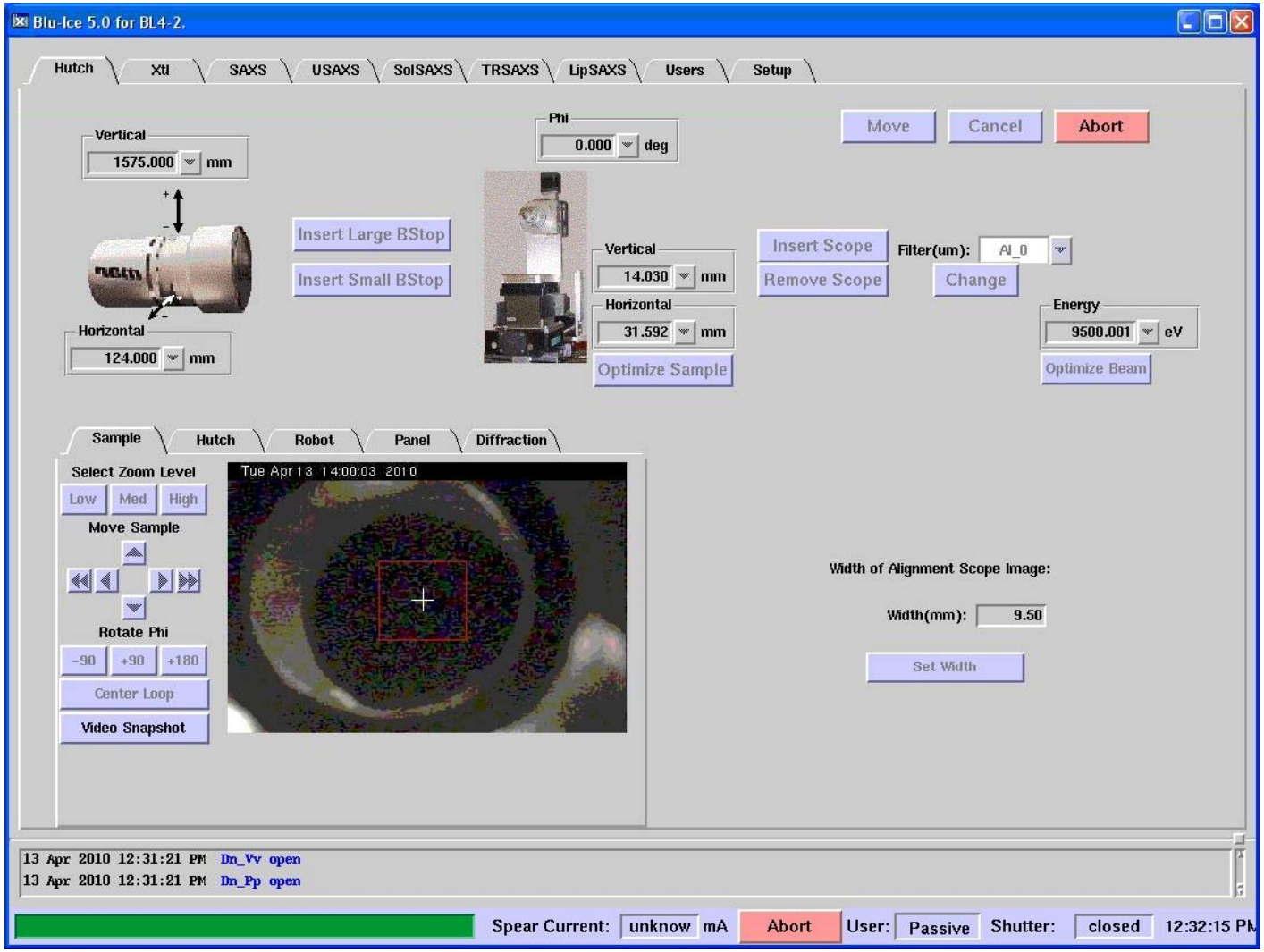
# Security

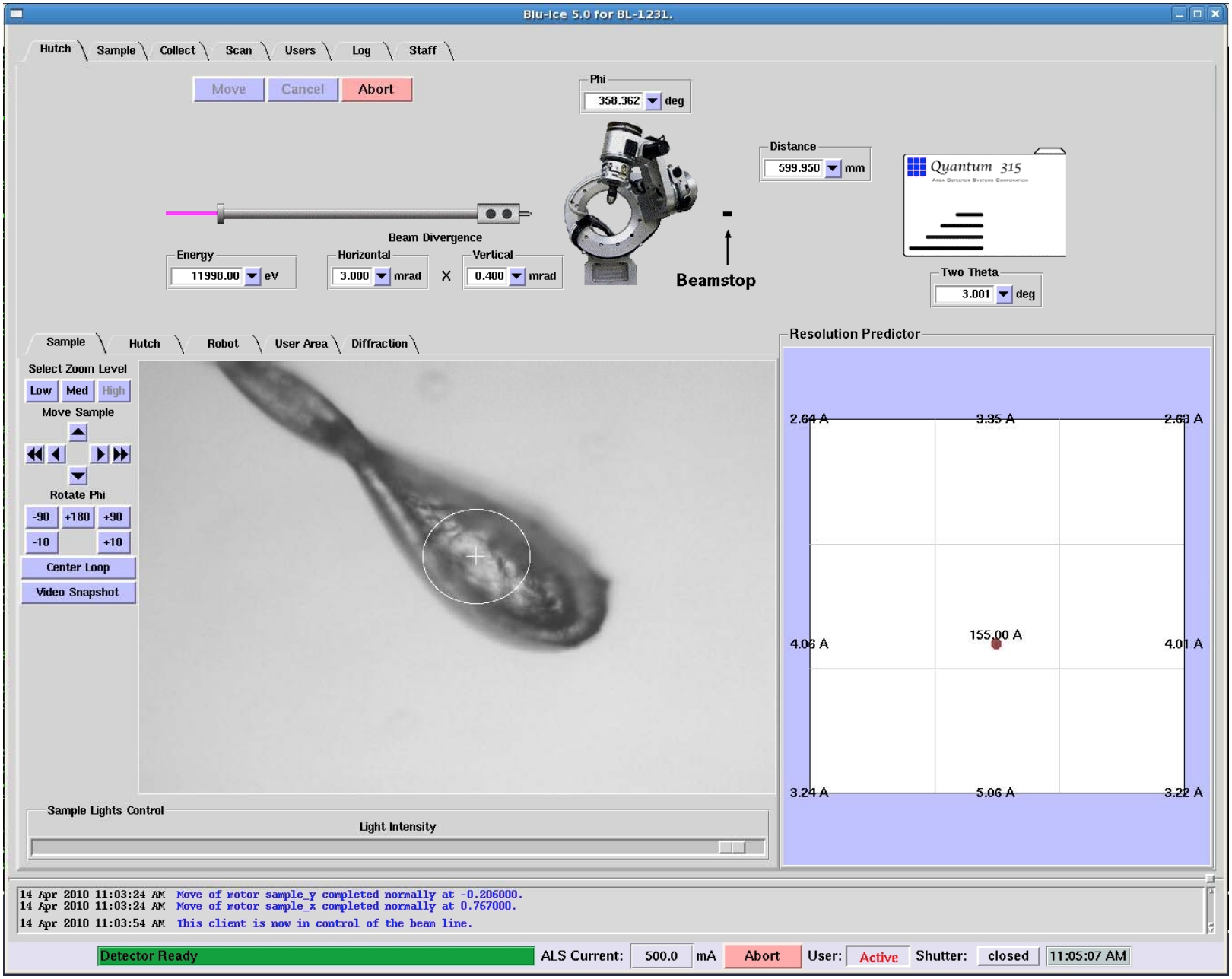
- SSL on most communications:
  - Authentication (very frequent)
  - BluIce to DCSS (not frequent)
  - BluIce to Crystal and Analysis Servers (frequent)
- One-time-ticket for others:
  - BluIce to Image server (frequent)
  - Detector DHS to Impersonal Server (frequent)
- Users only login to terminal machines.

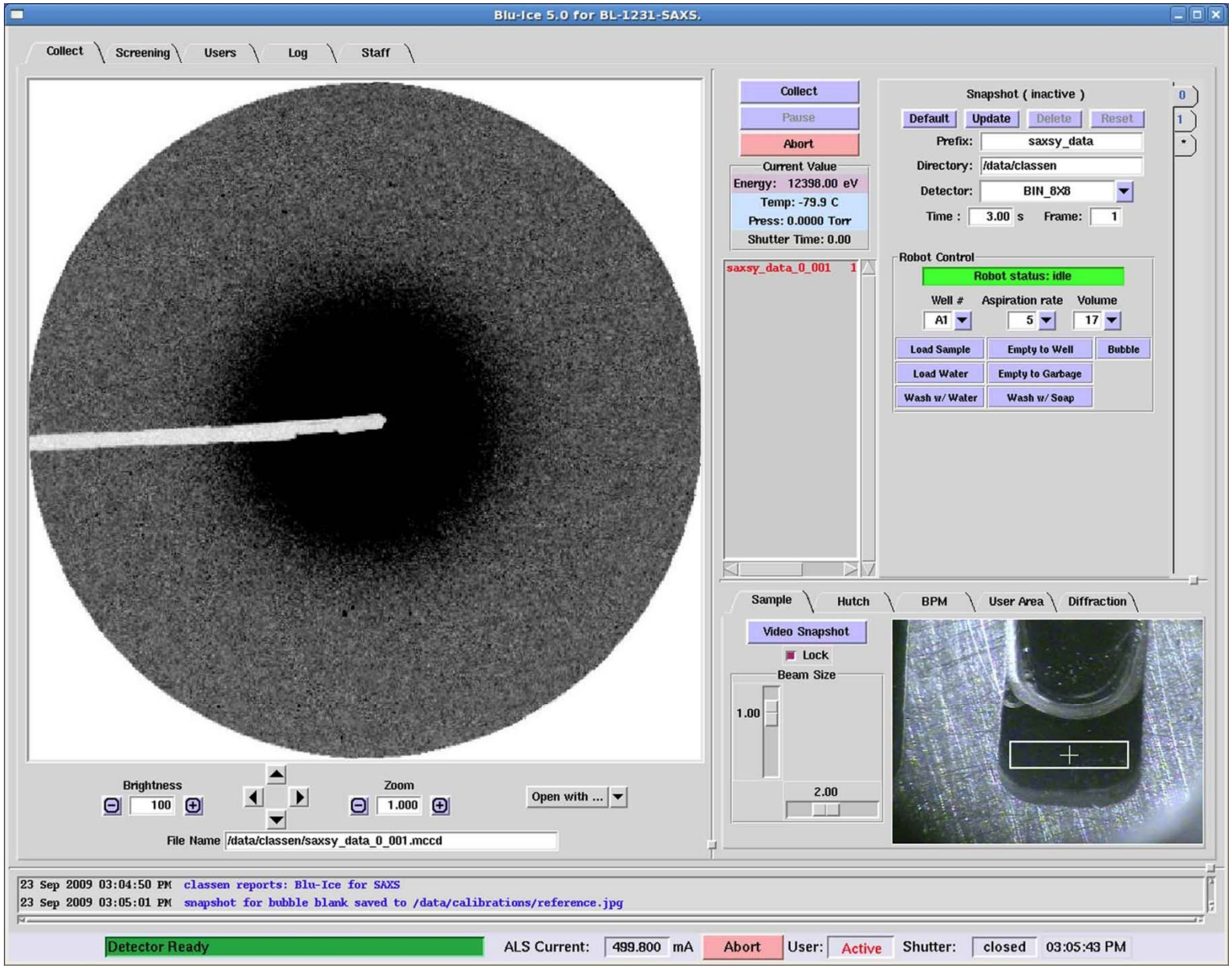
# imgsrv

- Staff can see any user’s image file.
- Cached image list
- Zoom, pan, brightness

# Collaboration




Blu-Ice 5.0 for BL-1231.
Hutch
Sample
Collect
Scan
Users
Log
Staff
Move
Cancel
Abort
Phi
358.362
deg
Distance
599.950
mm
Quantum 315
Beam Divergence
Energy
11998.00
eV
Horizontal
3.000
mrad
X
Vertical
0.400
mrad
Beamstop
Two Theta
3.001
deg
Sample
Hutch
Robot
User Area
Diffraction
Select Zoom Level
Low
Med
High
Move Sample
Rotate Phi
-90
+180
+90
-10
+10
Center Loop
Video Snapshot
Resolution Predictor
2.64 A
3.35 A
2.63 A
4.06 A
155.00 A
4.01 A
3.24 A
5.06 A
3.22 A
Sample Lights Control
Light Intensity
14 Apr 2010 11:03:24 AM Move of motor sample_y completed normally at -0.206000.
14 Apr 2010 11:03:24 AM Move of motor sample_x completed normally at 0.767000.
14 Apr 2010 11:03:54 AM This client is now in control of the beam line.
Detector Ready
ALS Current:
500.0
mA
Abort
User:
Active
Shutter:
closed
11:05:07 AM


Blu-Ice 5.0 for BL-1231-SAXS.
Collect
Screening
Users
Log
Staff
Collect
Pause
Abort
Current Value
Energy: 12398.00 eV
Temp: -79.9 C
Press: 0.0000 Torr
Shutter Time: 0.00
saxsy_data_0_001 1
Snapshot ( inactive )
Default
Update
Delete
Reset
Prefix: saxsy_data
Directory: /data/classen
Detector: BIN_8X8
Time : 3.00 s
Frame: 1
Robot Control
Robot status: idle
Well #
Aspiration rate
Volume
A1
5
17
Load Sample
Empty to Well
Bubble
Load Water
Empty to Garbage
Wash w/ Water
Wash w/ Soap
Sample
Hutch
BPM
User Area
Diffraction
Video Snapshot
Lock
Beam Size
1.00
2.00
Brightness
100
Zoom
1.000
Open with ...
File Name /data/classen/saxsy_data_0_001.mccd
23 Sep 2009 03:04:50 PM classen reports: Blu-Ice for SAXS
23 Sep 2009 03:05:01 PM snapshot for bubble blank saved to /data/calibrations/reference.jpg
Detector Ready
ALS Current: 499.800 mA
Abort
User: Active
Shutter: closed
03:05:43 PM

Blu-Ice 5.0 for BL-1231-SAXS.

Collect | Screening | Users | Log | Staff

96-well Tray: Position_1 | Web | Import | Export | Edit

View: Full

| Well | W | B | Well | SampleID | Protein | Buffer | Salt | pH | Additives | Comment | Directory |
|---|---|---|---|---|---|---|---|---|---|---|---|
| A1 | | | A1 | salt_v_ph1 | Nbs1 | 20mM Tris | 10mM NaCl | 5.5 | 1mM TCEP | 20deg C | /data/class |
| A2 | | | A2 | salt_v_ph2 | Nbs1 | 20mM Tris | 50mM NaCl | 5.5 | 1mM TCEP | 20deg C | /data/class |
| A3 | | | A3 | salt_v_ph3 | Nbs1 | 20mM Tris | 100mM NaCl | 5.5 | 1mM TCEP | 20deg C | /data/class |
| A4 | | | A4 | salt_v_ph4 | Nbs1 | 20mM Tris | 200mM NaCl | 5.5 | 1mM TCEP | 20deg C | /data/class |
| A5 | | | A5 | salt_v_ph5 | Nbs1 | 20mM Tris | 10mM NaCl | 6.5 | 1mM TCEP | 20deg C | /data/class |
| A6 | | | A6 | salt_v_ph6 | Nbs1 | 20mM Tris | 50mM NaCl | 6.5 | 1mM TCEP | 20deg C | /data/class |
| A7 | | | A7 | salt_v_ph7 | Nbs1 | 20mM Tris | 100mM NaCl | 6.5 | 1mM TCEP | 20deg C | /data/class |
| A8 | | | A8 | salt_v_ph8 | Nbs1 | 20mM Tris | 200mM NaCl | 6.5 | 1mM TCEP | 20deg C | /data/class |
| A9 | | | A9 | salt_v_ph9 | Nbs1 | 20mM Tris | 10mM NaCl | 7.5 | 1mM TCEP | 20deg C | /data/class |
| A10 | | | A10 | salt_v_ph10 | Nbs1 | 20mM Tris | 50mM NaCl | 7.5 | 1mM TCEP | 20deg C | /data/class |
| A11 | | | A11 | salt_v_ph11 | Nbs1 | 20mM Tris | 100mM NaCl | 7.5 | 1mM TCEP | 20deg C | /data/class |
| A12 | | | A12 | salt_v_ph12 | Nbs1 | 20mM Tris | 200mM NaCl | 7.5 | 1mM TCEP | 20deg C | /data/class |
| B1 | | | B1 | salt_v_ph13 | Nbs1 | 20mM Tris | 10mM NaCl | 8.5 | 1mM TCEP | 20deg C | /data/class |
| B2 | | | B2 | salt_v_ph14 | Nbs1 | 20mM Tris | 50mM NaCl | 8.5 | 1mM TCEP | 20deg C | /data/class |
| B3 | | | B3 | salt_v_ph15 | Nbs1 | 20mM Tris | 100mM NaCl | 8.5 | 1mM TCEP | 20deg C | /data/class |
| B4 | | | B4 | salt_v_ph16 | Nbs1 | 20mM Tris | 200mM NaCl | 8.5 | 1mM TCEP | 20deg C | /data/class |
| B5 | | | B5 | salt_v_ph17 | Nbs1 | 20mM Tris | 10mM NaCl | 9.5 | 1mM TCEP | 20deg C | /data/class |

Sample | Hutch | BPM | User Area | Diffraction

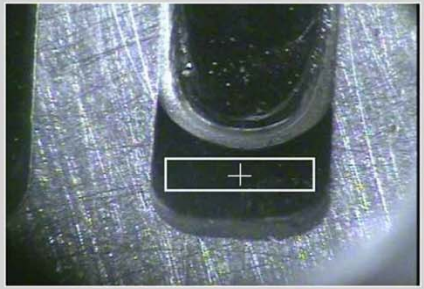
Video Snapshot

Lock

Beam Size

1.00

2.00



Directory: /data/classen/saxsy_data | Default

Detector: BIN_8X8

Prefix: sample

Sequence 1

| | | | |
|---|---|---|---|
| Step 1: | Load Sample | Time1: | 1.00 |
| Step 2: | Bubble | Time2: | 2.00 |
| Step 3: | Expose | Time3: | 5.00 |
| Step 4: | Empty to Well | Time4: | 4.00 |
| Step 5: | none | Time5: | 5.00 |
| Step 6: | none | | |
| Step 7: | none | | |
| Step 8: | none | | |

Volume 15 | Aspiration 5

Start | Abort

Current Well: NONE

Current Step: NONE

Screening Tasks

A1 Load Sample
A1 Bubble
A1 Expose
A1 Empty to Well
A2 Load Sample
A2 Bubble
A2 Expose
A2 Empty to Well
A3 Load Sample
A3 Bubble
A3 Expose
A3 Empty to Well
A4 Load Sample
A4 Bubble
A4 Expose
A4 Empty to Well
A4 Water Wash
A5 Load Sample
A5 Bubble
A5 Expose
A5 Empty to Well
A6 Load Sample

```
23 Sep 2009 05:06:29 PM  classen reports: Blu-Ice for SAXS
23 Sep 2009 05:06:30 PM  classen reports: Blu-Ice for SAXS
23 Sep 2009 05:07:10 PM  snapshot for bubble blank saved to /data/calibrations/reference.jpg
```

Detector Ready | ALS Current: 499.800 mA | Abort | User: Active | Shutter: closed | 05:07:32 PM

# EPICS Gateway DHS

| DCS | EPICS |
|---|---|
| Real Motor | Motor: scale factor, speed, … |
| Pseudo Motor | Motor |
| Shutter | Shutter |
| String | All others (ai, ao, Li, Lo, si, so,…) |

Standard EPICS motor record (old and new)
Australia Light Source motor template
Lyncean Tech motor template
Canadian Light Source motor template
SSRL Undulator Gap motor template

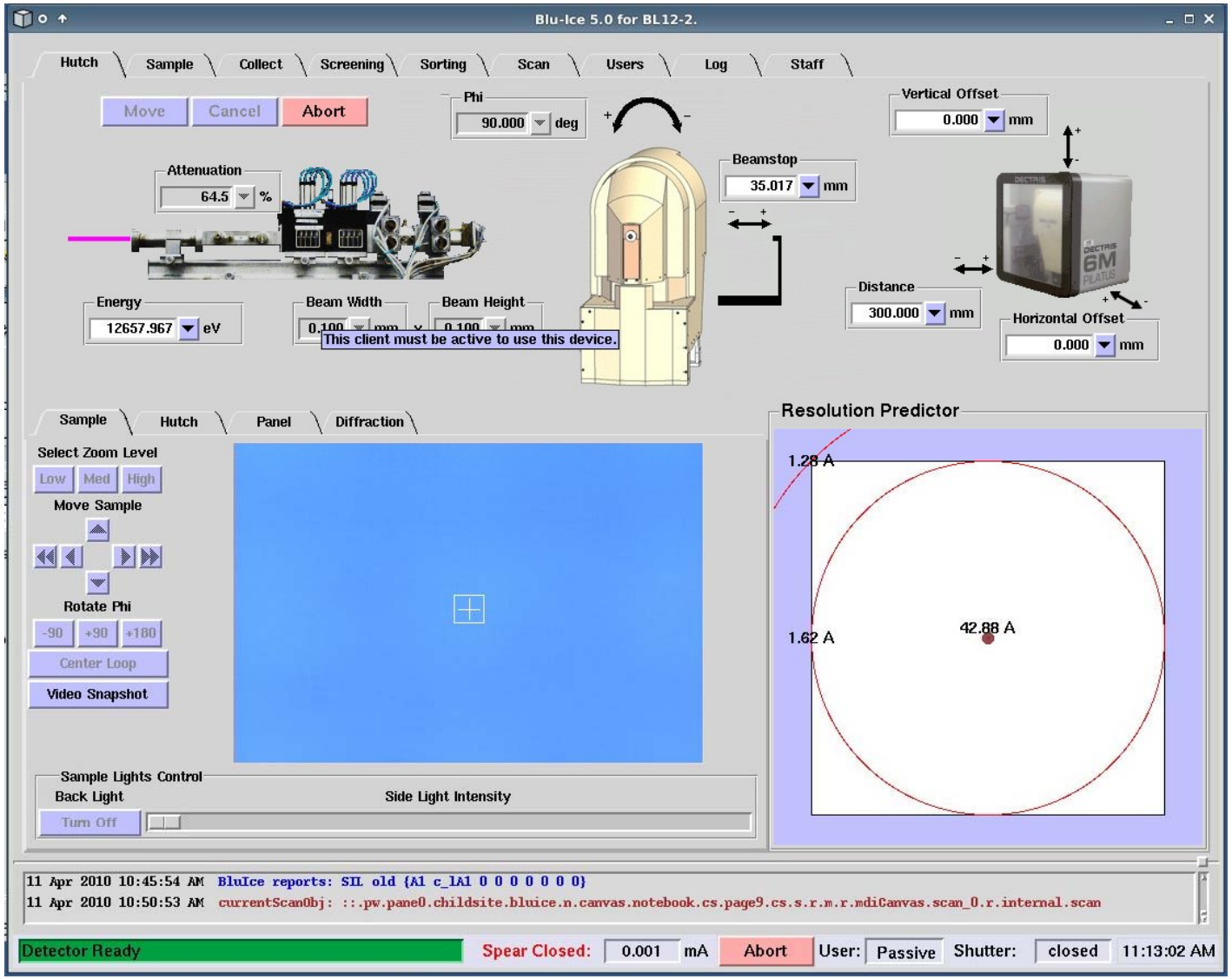
# EPICS gateway DHS

spear_current
13
epics_gateway SPEAR:BeamCurrAvg1S
0 0 0 0 0
0 0 0 0 0

sample_x
1
epics_gateway SMTR99993I1012:mm
0 1 1 1 1
0 1 1 1 1
0
0.0 500 -500 6768.189 1000 500 10 1 1 0 1 0 0 mm

# EPICS Gateway DHS

- 7 Motors: energy, beam size (2), attenuation, beam stop, detector distance, phi
- Detector DHS or 3 operations and 1 string: collect_image, oscillation_ready, transfer_image, lastImageCollected




Users love Blu-Ice because…

# Reasons for Blu-Ice's ease-of-use & popularity

- The programmers belong to the beamline support group.
- The programmers' boss and colleagues are the main users
- The boss uses and messes with the GUI
- Support staff complain after a call from a confused user
- Staff are tired/confused during startup

# The SSRL Macromolecular Crystallography Group

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Office of Science
Department of Energy

Office of Biological and Environmental Research

National Center For Research Resources

National Institute of General Medical Sciences
NATIONAL INSTITUTES OF HEALTH

ARRAY BIOPHARMA

THE SCRIPPS RESEARCH INSTITUTE

NOVARTIS

GENENCOR
A Danisco Division

CALTECH

Roche

Genentech
IN BUSINESS FOR LIFE

EXELIXIS

Plexxikon