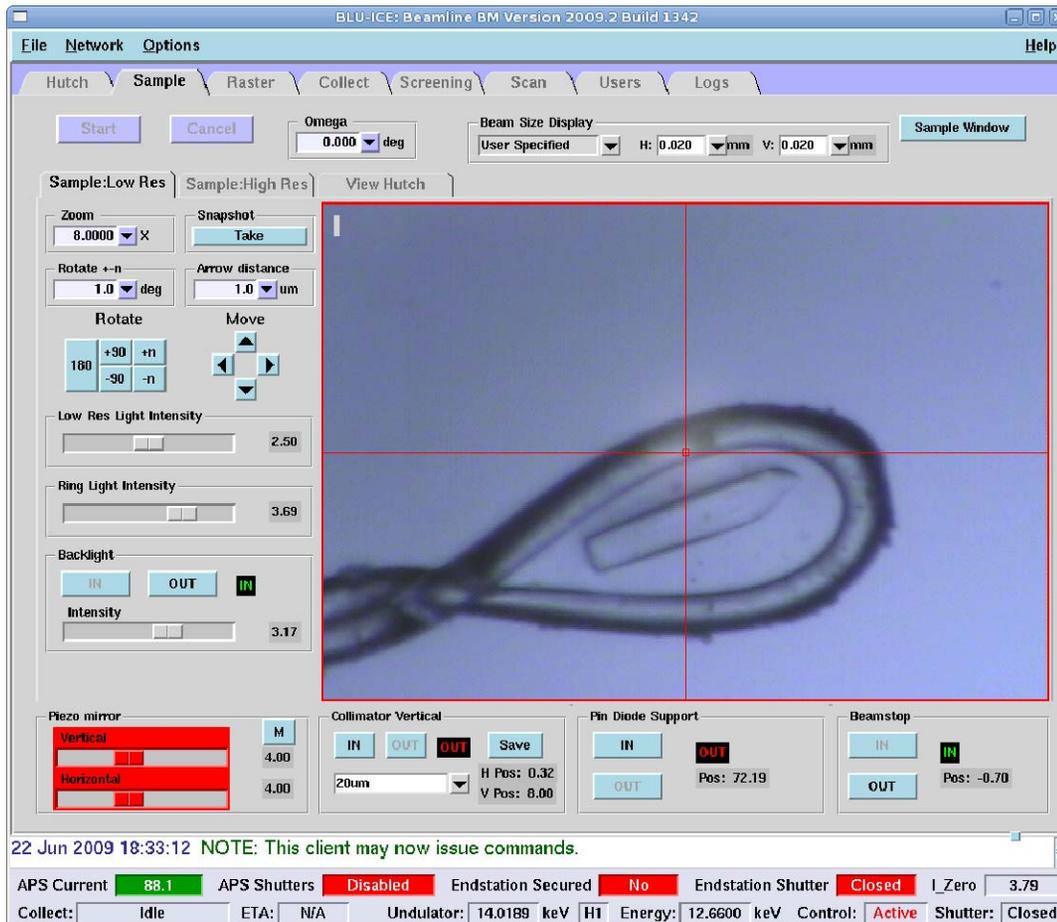


## BluIce-EPICS Tabs Overview

- ❑ **Sample & Rastering:** Mark Hilgart
- ❑ **Collect:** Oleg Makarov
- ❑ **Screening & Weblce:** Sudhir Pothineni
- ❑ **Scan:** Sergey Stepanov

*GM/CA CAT at the Advanced Photon Source,  
Biosciences Division of  
Argonne National Laboratory, USA*

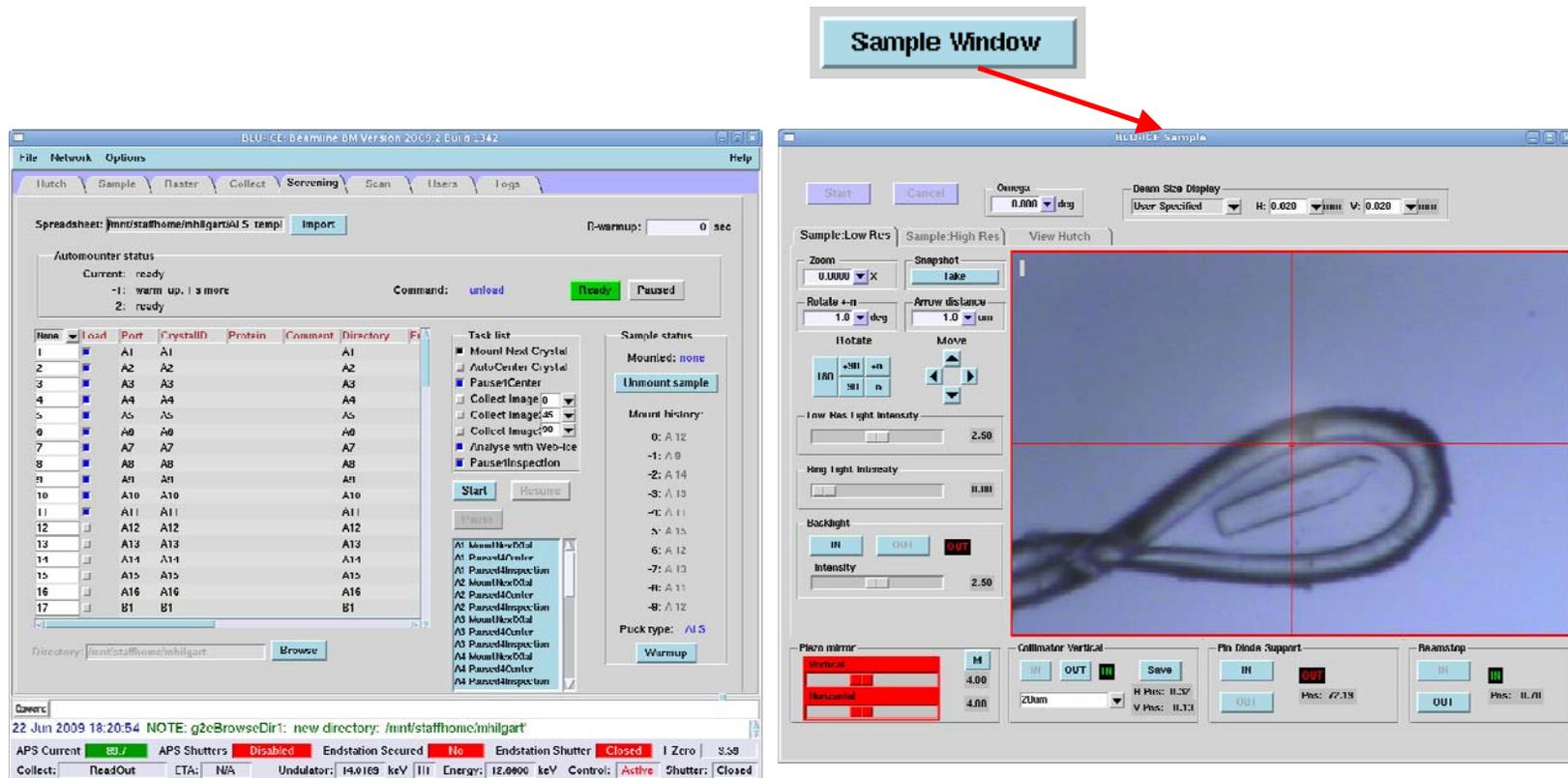
# Sample Tab



- What is it?
  - All controls related to visualization in one place
  - Pop-out window gives constant access to sample visualization
- Uses
  - Sample centering
  - Manual beam alignment
  - Rotation axis alignment
- Controls:
  - Pop-out button
  - Lighting
  - Move, zoom, snapshots
  - Beam size display
  - Related motors

Sample Tab

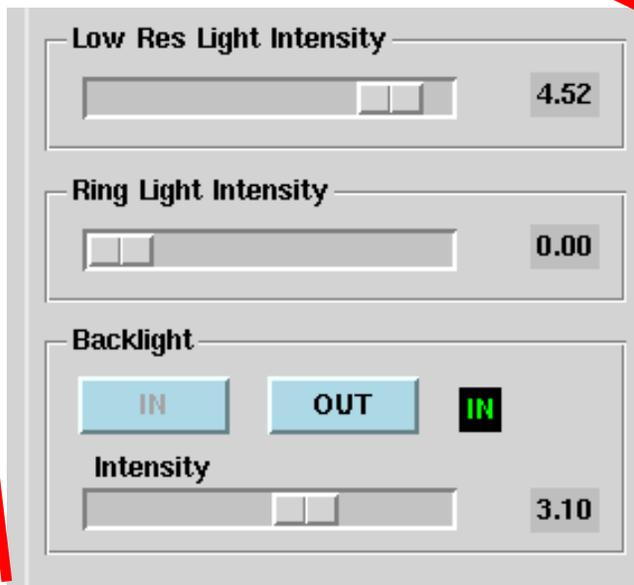
# Sample Tab: Pop-out feature



Blulce-EPICS with the sample tab popped out

- Button in the upper right of the sample tab pops up a second copy
- Uses large desktops or dual monitors more effectively
- Provides constant access to sample view and controls

# Sample Tab: Lighting



Lighting controls on the left side of the sample tab

- Fiber-optic lights
  - Low and high res
  - Along the camera axes
- Ring Light
  - High intensity LEDs
- Backlight
  - In while using the sample tab
  - Out for collection, since it blocks the beam
  - Move out is automatic before collection, scans
- Effective ranges
  - Only a portion of the slider is used
  - Hosts will show you how best to set each light

# Sample Tab: Move, Zoom, Snapshots

Zoom and movement controls on the left side of the sample tab

Sample tab video which allows point and click

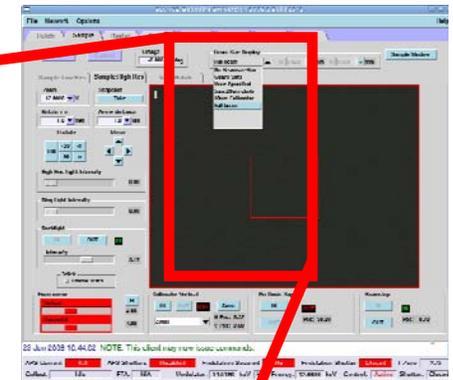
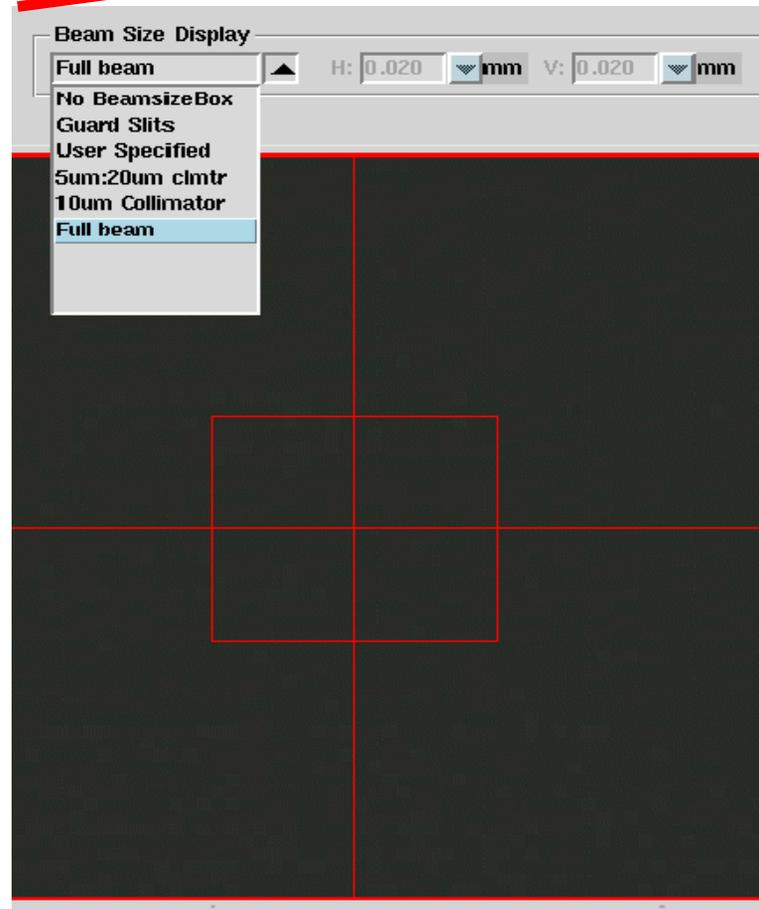
3click  
 Enable 3click

3-click selector

- Continuous Zoom
  - Separate for low, high res
  - Enter a value, click start
- Border
  - Red border indicates ready
- Rotate
  - 180, 90, n buttons
  - +-n field
- Translate
  - Point and click
  - Arrow buttons
  - Distance field
- Snapshot
  - Saves low-res and high-res camera views to a subdirectory in your home directory
- 3-click
  - Click to start, then click to center 3x
  - Sample will rotate between clicks

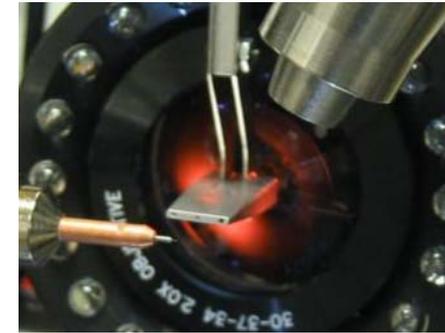
# Sample Tab: Beam Size Display

- Changes with zoom and camera
- Settings
  - Off
  - Guard slits
    - Defined on hutch tab
  - Collimators
    - 5um/20um
    - 10um
    - Full beam
  - User Specified
    - Can be used as a measuring tool

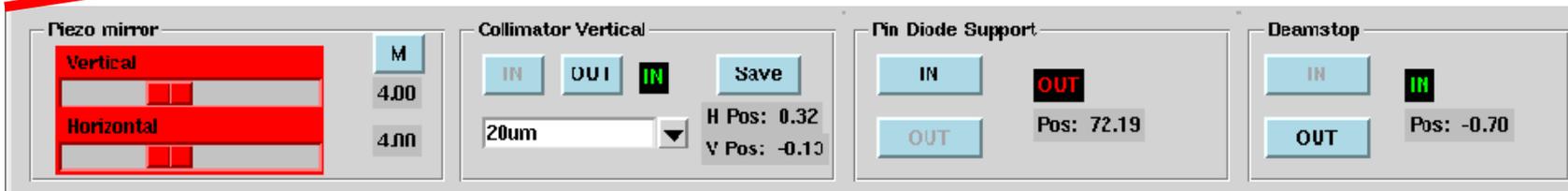
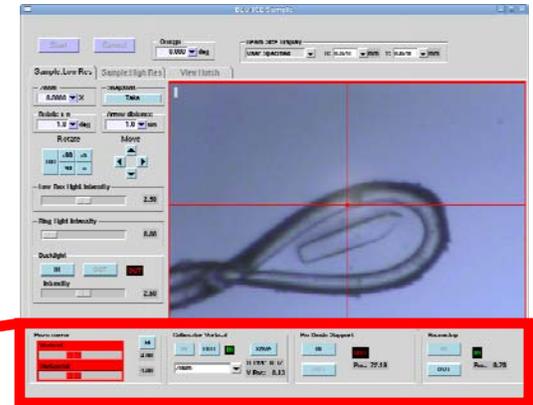


# Sample Tab: Related Motors

- Collimator
  - 5um, 10um, 20um, 300um (scatterguard)
  - Out when using sample tab, in for collection
  - Move in is automatic before collection, scans
- Piezo Mirror
  - Adjusts the beam position
  - Click 'M' to use the sliders
  - Not normally needed
- Beamstop
  - Either this or the pin diode must be in to protect the detector
  - Enforced in Blulce
- Pin Diode
  - Indicates beam strength at the sample
  - Not normally needed



Triple collimator



Motor controls at the bottom of the sample tab

# Raster Tab

- What is it?
  - A tool for finding crystals
- Uses
  - Find small, invisible crystals
  - Find the best diffracting areas of large crystals
- Diffraction vs Fluorescence
  - Complement each other
  - Diffraction measures directly what you want
  - Fluorescence is ~4x faster
    - 400-cell diffraction raster  
1/2 second exposure  
= 27 minutes
    - 400-cell fluorescence raster  
1/2 second exposure  
= 6.5 minutes
- Controls
  - Grid parameters
  - Collect parameters
  - Results table

BLU-ICE: Beamline ID-B Version 2009.1 Build 1182

File Network Options Help

Hutch Sample **Raster** Collect Screening Scan Users Logs

UNDER DEVELOPMENT

**Done**

Control: Start Stop Reset

Position: Omega 91.26, Sample X 0.17, Sample Y -0.029, Sample Z 15.368

Raster mode:  Diffraction  Fluorescence

Grid (um): Width: 220 Height: 100

Cell Size (um): Width: 40 Height: 35

Settings: Expose(sec): 1.0 Delta(deg): 0.5

Diffraction image options: Prefix: raster Dir: /mnt/evagfs1/user3/ra

Options:  Enable Processing

Status	X	Y	Frame	Row	Col	Spot Total	In-Resolution Total	Good Bragg C
DONE	60.0	-35.0	13	1	5	150	122	29
DONE	60.0	0.0	14	2	5	165	158	39
DONE	60.0	35.0	15	3	5	79	77	25
DONE	100.0	-35.0	16	1	6	108	73	29
DONE	100.0	0.0	17	2	6	141	132	39
DONE	100.0	35.0	18	3	6	38	31	9

10 Apr 2009 17:55:10 NOTE: collIn: move OK!

APS Current: 102.2 APS Shutters: Enabled Endstation Secured: Yes Endstation Shutter: Open I\_Zero: -0.02

Collect: Writing ETA: N/A Undulator: 8.4901 keV H1 Energy: 8.4001 keV Control: Active Shutter: Closed

Raster tab

# Raster Tab: Diffraction

BLU-ICE: Beamline ID-B Version 2009.1 Build 1182

File Network Options Help

Hutch Sample **Raster** Collect Screening Scan Users Logs

UNDER DEVELOPMENT

**Ready**

Control: Start Stop Reset

Position: Omega 90.86, Sample X 0.17, Sample Y -0.029, Sample Z 15.368

Raster mode:  Diffraction  Fluorescence

Grid (um): Width: 220 Height: 100

Cell Size (um): Width: 40 Height: 35

Settings: Expose(sec): 1.0 Delta(deg): 0.5

Diffraction image options: Prefix: raster Dir: /mnt/evagfs1/user0/ra Select

Options:  Enable Processing

Status	X	Y	Frame	Row	Col	Spot Total	In-Resolution Total	Good Bragg C
--	-100.0	-35.0	1	1	1			
--	-100.0	0.0	2	2	1			
--	-100.0	35.0	3	3	1			
--	-60.0	-35.0	4	1	2			
--	-60.0	0.0	5	2	2			
--	-60.0	35.0	6	3	2			

10 Apr 2009 17:52:46 NOTE: colln: move OK!

APS Current: 102.1 APS Shutters: Enabled Endstation Secured: Yes Endstation Shutter: Open I\_Zero: -0.02

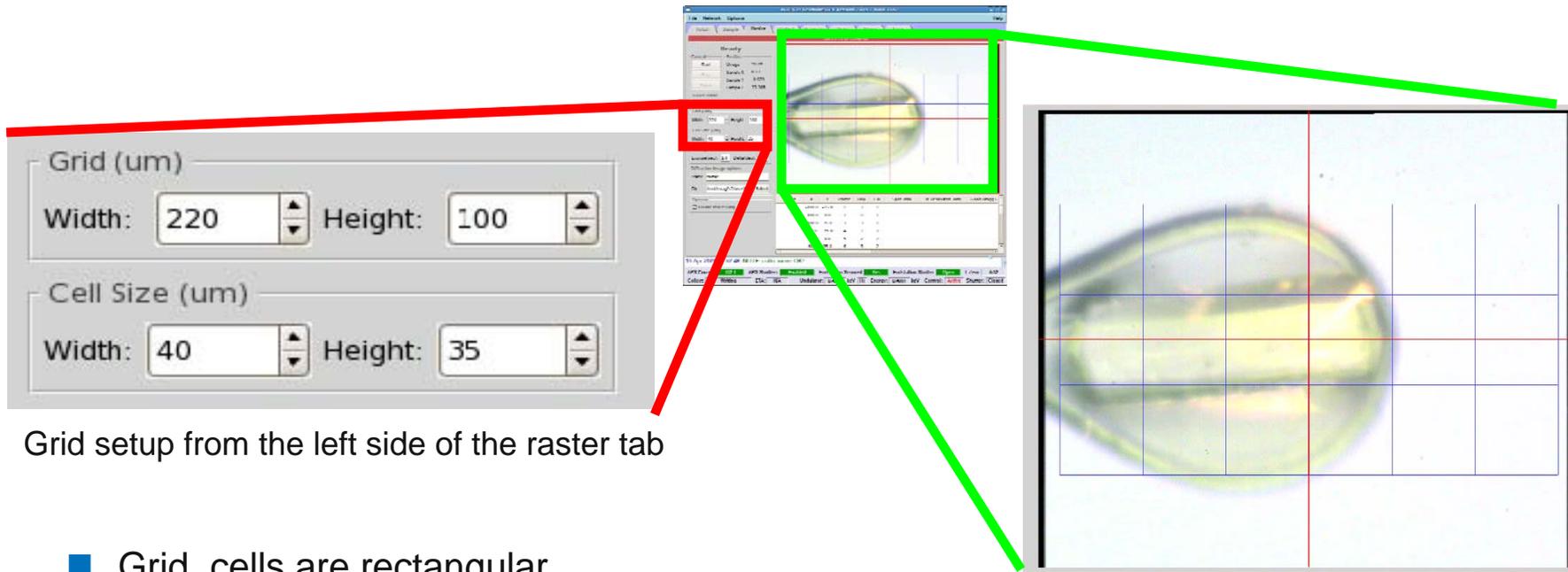
Collect: Writing ETA: N/A Undulator: 8.4901 keV HI Energy: 8.4001 keV Control: Active Shutter: Closed

## ■ Steps

- Grid setup
- Collection parameters
- Raster
- Results

Raster tab in diffraction mode

# Diffraction Rastering: Grid Setup

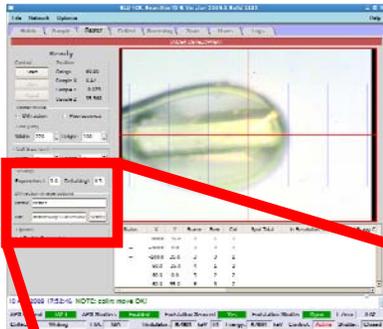


Grid setup from the left side of the raster tab

Grid display on the raster tab video

- Grid, cells are rectangular
- Typing immediately updates grid display
- Grid size is a minimum, will be rounded up
  - 35um cell height
  - 100um grid height
  - = 3 rows

# Diffraction Rastering: Collection Parameters



Settings

Expose(sec):  Delta(deg):

Diffraction image options

Prefix:

Dir:

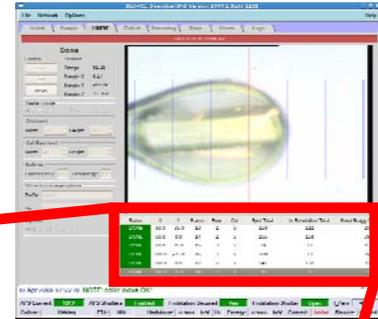
Options

Enable Processing

Diffraction collect parameters from the left side of the raster tab

- Same as collect tab
  - Exposure time
  - Delta
- Must be set beforehand on the hutch tab
  - Detector distance
  - Energy
  - Attenuation
- Output prefix and directory
  - “raster” prefix gives filenames like raster\_0.0001
- Enable processing
  - Does not affect speed

# Diffraction Rastering: Results

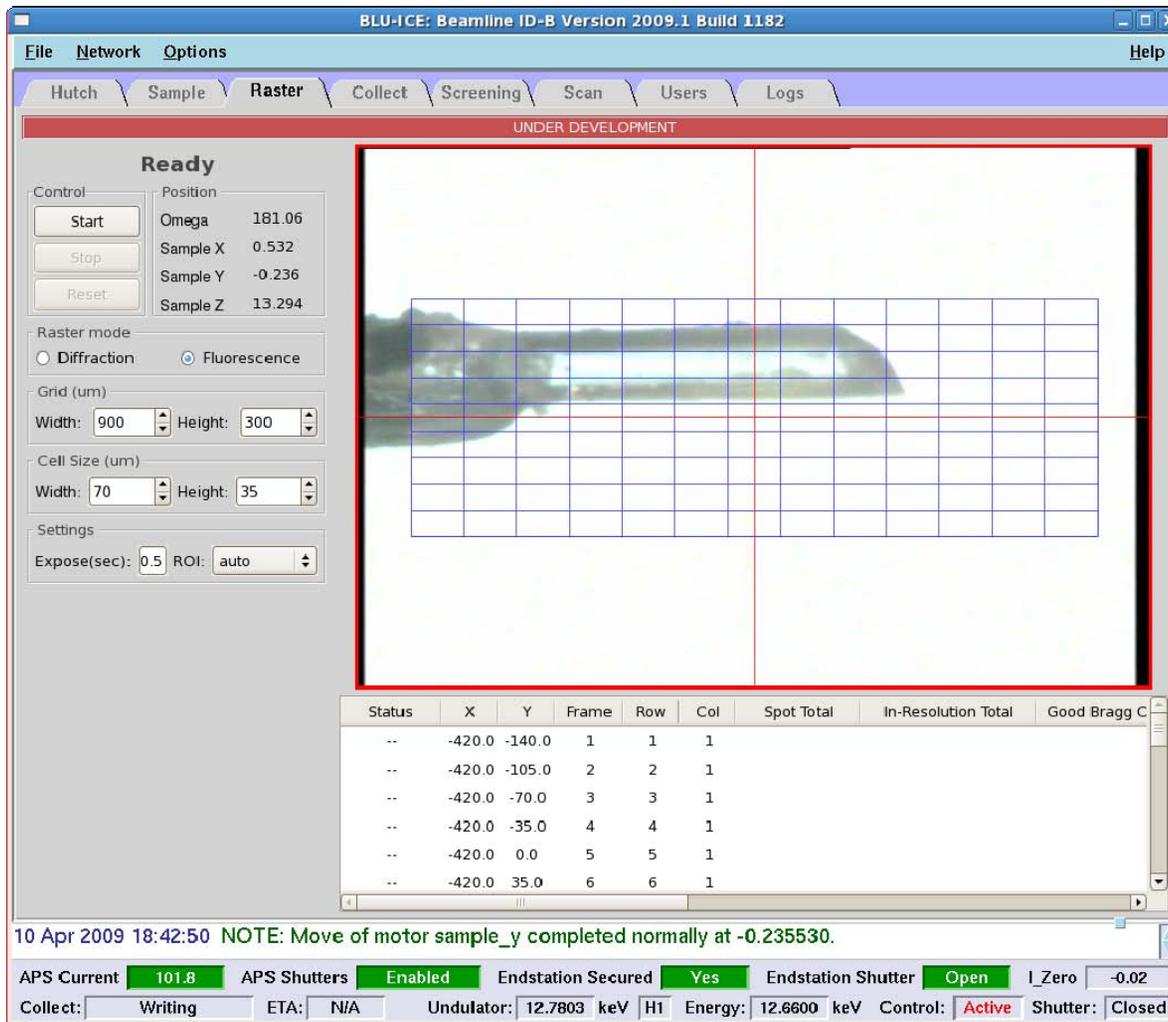


Status	X	Y	Frame	Row	Col	Spot Total	In-Resolution Total	Good Bragg C
DONE	60.0	-35.0	13	1	5	150	122	29
DONE	60.0	0.0	14	2	5	165	158	39
DONE	60.0	35.0	15	3	5	79	77	25
DONE	100.0	-35.0	16	1	6	108	73	29
DONE	100.0	0.0	17	2	6	141	132	39
DONE	100.0	35.0	18	3	6	38	31	9

Results table from diffraction rastering

- Click column headers to sort
- Double-click row to center
- Browse images on MAR computer (covered later)
  - Image name: raster\_0.0018
  - Frame column: 18

# Raster Tab: Fluorescence



BLU-ICE: Beamline ID-8 Version 2009.1 Build 1182

File Network Options Help

Hutch Sample **Raster** Collect Screening Scan Users Logs

UNDER DEVELOPMENT

**Ready**

Control: Start Stop Reset

Position: Omega 181.06, Sample X 0.532, Sample Y -0.236, Sample Z 13.294

Raster mode:  Diffraction  Fluorescence

Grid (um): Width: 900 Height: 300

Cell Size (um): Width: 70 Height: 35

Settings: Expose(sec): 0.5 ROI: auto

Status	X	Y	Frame	Row	Col	Spot Total	In-Resolution Total	Good Bragg C
--	-420.0	-140.0	1	1	1			
--	-420.0	-105.0	2	2	1			
--	-420.0	-70.0	3	3	1			
--	-420.0	-35.0	4	4	1			
--	-420.0	0.0	5	5	1			
--	-420.0	35.0	6	6	1			

10 Apr 2009 18:42:50 NOTE: Move of motor sample\_y completed normally at -0.235530.

APS Current: 101.8 APS Shutters: Enabled Endstation Secured: Yes Endstation Shutter: Open I\_Zero: -0.02

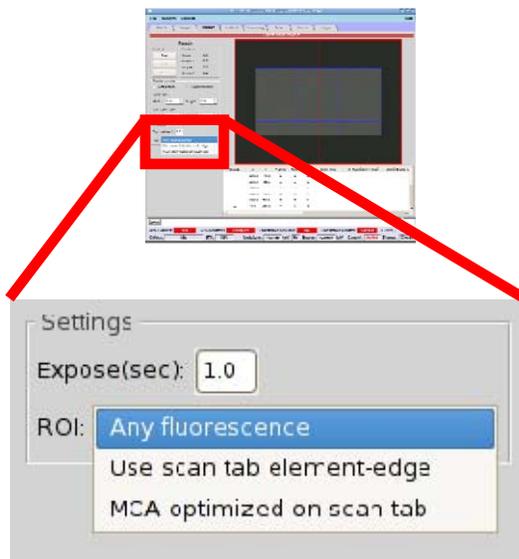
Collect: Writing ETA: N/A Undulator: 12.7803 keV HI Energy: 12.6600 keV Control: Active Shutter: Closed

## Steps

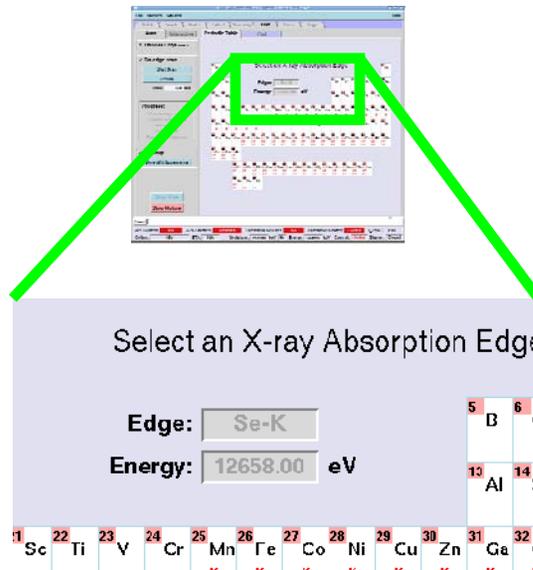
- Grid setup
- Exposure, ROI
- Raster
- Results

Raster tab in fluorescence mode

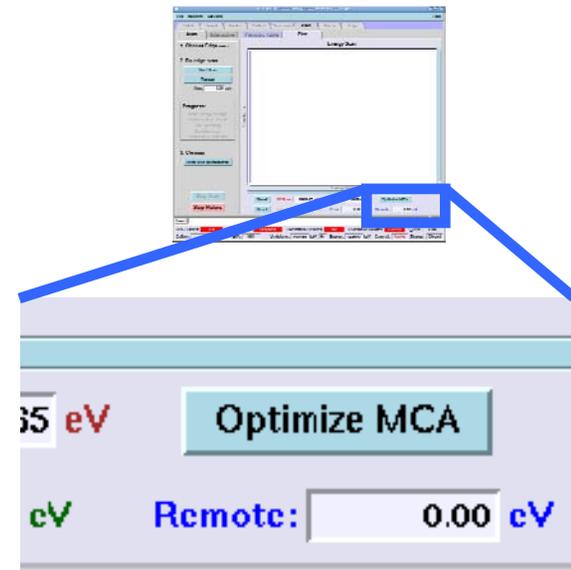
# Fluorescence Rastering: ROI



ROI selector in raster tab



Element-edge selector  
in scan tab

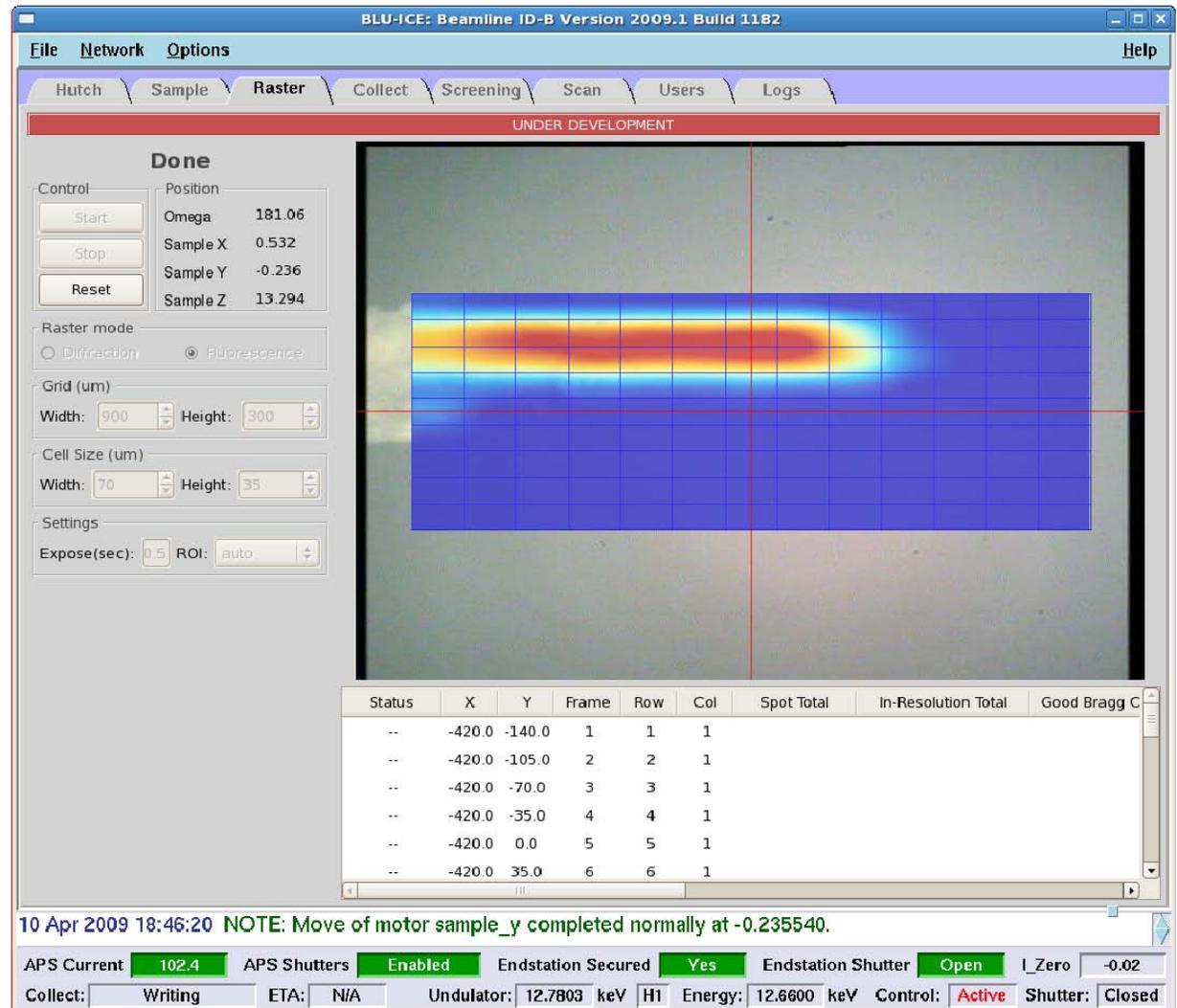


Optimize MCA button in scan tab

- Range determines which fluorescence is measured
- Any fluorescence
  - Range is set from 50eV to 100eV less than the beam energy
- Scan tab element-edge
  - A preset range is set based on the edge selected
- Multi-channel analyzer (MCA) optimized on scan tab
  - In interactive mode, the range can be manually set

# Fluorescence Rastering: Results

- Results are output as a color map
- Single-click on the map to center
- Collect on the collect tab



Results colormap from fluorescence rastering

# Rastering: Video Guide

Video tutorial on remote access & rastering:

<http://www.gmca.anl.gov/remote/demo>

# Blulce-EPICS: Collect tab

BLU-ICE: Beamline ID-B Version 2009.2 Build 1341

File Network Options Help

Hutch Sample Raster **Collect** Screening Scan Users Logs

/mnt/evagfs5/hnoller/06212009/JD5data/JD5\_2.0714

Collect  
Pause  
Abort

Current Position  
Phi: 0.00  
Omega: 0.00  
Distance: 900.00

Run Sequence

JD5_3.0001	180.00	11
JD5_3.0002	180.20	11
JD5_3.0003	180.40	11
JD5_3.0004	180.60	11
JD5_3.0005	180.80	11
JD5_3.0006	181.00	11
JD5_3.0007	181.20	11
JD5_3.0008	181.40	11
JD5_3.0009	181.60	11
JD5_3.0010	181.80	11
JD5_3.0011	182.00	11
JD5_3.0012	182.20	11
JD5_3.0013	182.40	11
JD5_3.0014	182.60	11
JD5_3.0015	182.80	11
JD5_3.0016	183.00	11
JD5_3.0017	183.20	11
JD5_3.0018	183.40	11
JD5_3.0019	183.60	11
JD5_3.0020	183.80	11
JD5_3.0021	184.00	11
JD5_3.0022	184.20	11
JD5_3.0023	184.40	11
JD5_3.0024	184.60	11

Run 3 ( inactive )

Default Update Delete Reset

Prefix: JD5  
Directory: /mnt/evagfs5/hnoller/0  
Browse

Distance: 617.950 mm  
Axis: gonio\_phi  
Delta: 0.20 deg  
Time: 1.00 s \* 0 = 0.00s

Frame gonio\_phi  
Start: 001 180.00 deg  
End: 900 360.00 deg  
Inverse Beam:  (phi axis only)  
Wedge: 180.0 deg  
Energy: 11.9996 keV

Open Contrast 200 Zoom 0.98

22 Jun 2009 14:56:00 NOTE: This client may now issue commands.

APS Current 5.3 APS Shutters Disabled Endstation Secured No Endstation Shutter Closed I\_Zero 0.02  
Collect: ReadOut ETA: N/A Undulator: 14.0189 keV H1 Energy: 11.9996 keV Control: Active Shutter: Closed



## Collect tab: outline

- Blulce Collect Tab
- Frame processing engine
- Hardware involved in data collection
- Frame Audit

## Collect tab: functionality

BLU-ICE: Beamline ID-B Version 2009.2 Build 1341

File Network Options Help

Hutch Sample Raster **Collect** Screening Scan Users Logs

/mnt/evagfs5/hnoller/06212009/JD5data/JD5\_2.0714

Collect  
Pause  
Abort

Current Position  
Phi: 0.00  
Omega: 0.00  
Distance: 900.00

Run Sequence

Frame	Phi	Omega	Time
JD5_3.0001	180.00	11	
JD5_3.0002	180.20	11	
JD5_3.0003	180.40	11	
JD5_3.0004	180.60	11	
JD5_3.0005	180.80	11	
JD5_3.0006	181.00	11	
JD5_3.0007	181.20	11	
JD5_3.0008	181.40	11	
JD5_3.0009	181.60	11	
JD5_3.0010	181.80	11	
JD5_3.0011	182.00	11	
JD5_3.0012	182.20	11	
JD5_3.0013	182.40	11	
JD5_3.0014	182.60	11	
JD5_3.0015	182.80	11	
JD5_3.0016	183.00	11	
JD5_3.0017	183.20	11	
JD5_3.0018	183.40	11	
JD5_3.0019	183.60	11	
JD5_3.0020	183.80	11	
JD5_3.0021	184.00	11	
JD5_3.0022	184.20	11	
JD5_3.0023	184.40	11	
JD5_3.0024	184.60	11	

Run 3 ( inactive )

Default Update Delete Reset

Prefix: JD5  
Directory: /mnt/evagfs5/hnoller/0  
Browse

Distance: 617.950 mm  
Axis: gonio\_phi  
Delta: 0.20 deg  
Time: 1.00 s \* 0 = 0.00s

Frame gonio\_phi  
Start: 001 180.00 deg  
End: 900 360.00 deg  
Inverse Beam:  (phi axis only)  
Wedge: 180.0 deg  
Energy: 11.9996 keV

Open Contrast 200 Zoom 0.98

22 Jun 2009 14:56:00 NOTE: This client may now issue commands.

APS Current 5.3 APS Shutters Disabled Endstation Secured No Endstation Shutter Closed I Zero 0.02  
Collect: ReadOut ETA: N/A Undulator: 14.0189 keV HI Energy: 11.9996 keV Control: Active Shutter: Closed

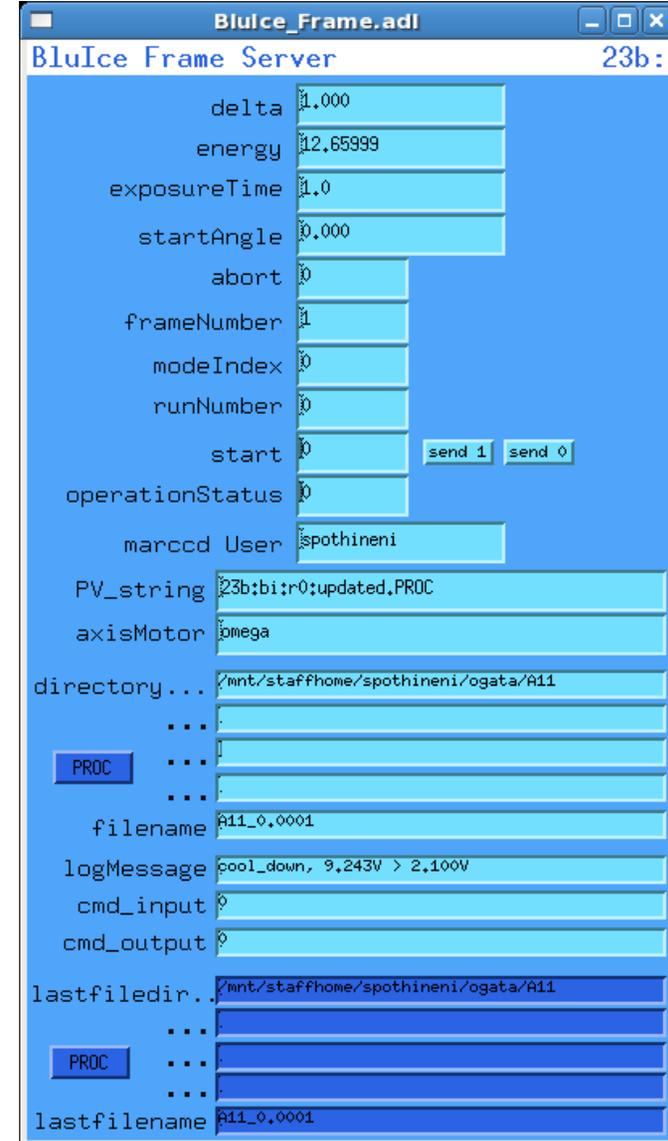
- Allows to acquire a dataset of X-ray diffraction images from the sample

### ■ Dataset parameters:

- **Prefix** – common filename part
- **Directory** – where to store files
- **Distance** – detector to sample distance
- **Axis** – gonio\_phi or gonio\_omega
- **Delta** – crystal oscillation angle
- **Time** – exposure time per image
- **Start** – the first frame # / angle
- **End** – the last frame # / angle
- **Inverse Beam**: Rotates the crystal by 180 deg to collect the friedel pairs for the input phi range. If wedges are used, the inverse beam is collected before changing the energy.
- **Wedge** - The phi rotation range that is collected successively at each energy
- **Energy** - As you enter an additional energy, an empty box appears for further energy entries.

## Collect tab: Frame Server

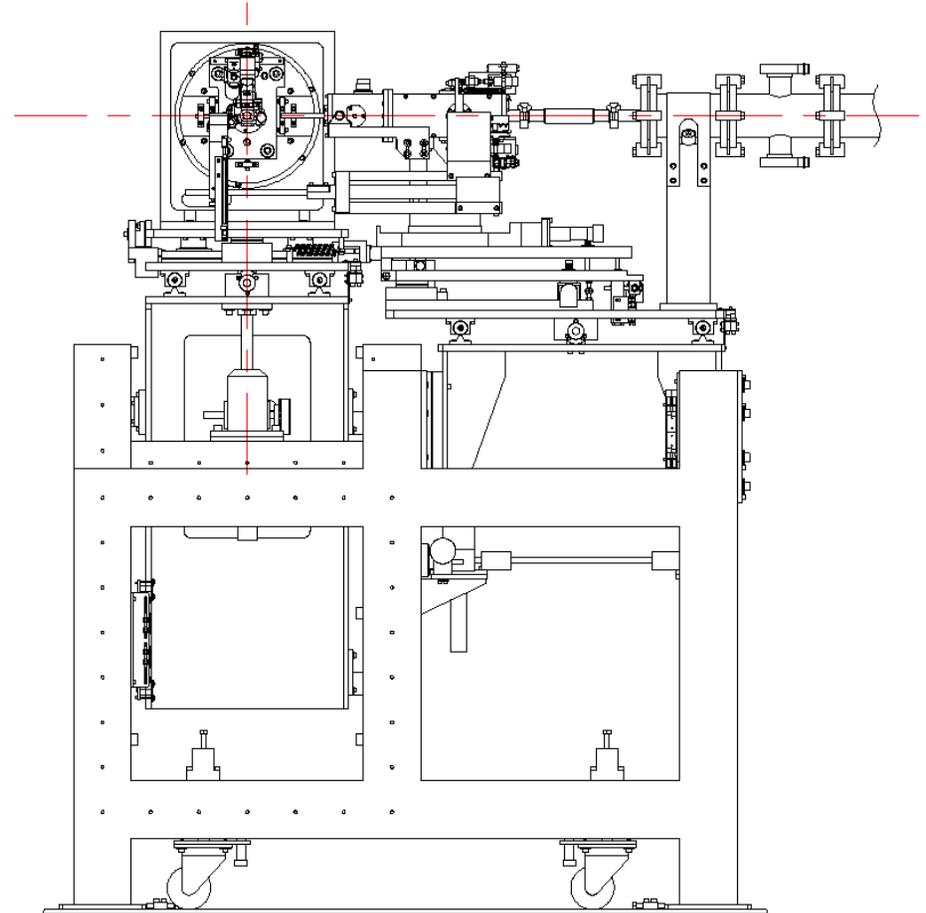
- BLU-ICE Frame Server is running on the MAR computer
- Frame Server receives requests from BLU-ICE with parameters for data acquisition
- Each request initiates acquisition of one diffraction image
- Coordinates crystal rotation, the fast shutter opening / closing, and operation of a CCD detector.
- Log file:
  - Epics-CCD-<DATE&TIME>.log



## Collect tab: Hardware involved in data collection



- MAR CCD area detector with computer
- EVA3000 storage
- Goniometer with Aerotech ABR1000 rotary table
- Fast Shutter
- PMAC motion controller



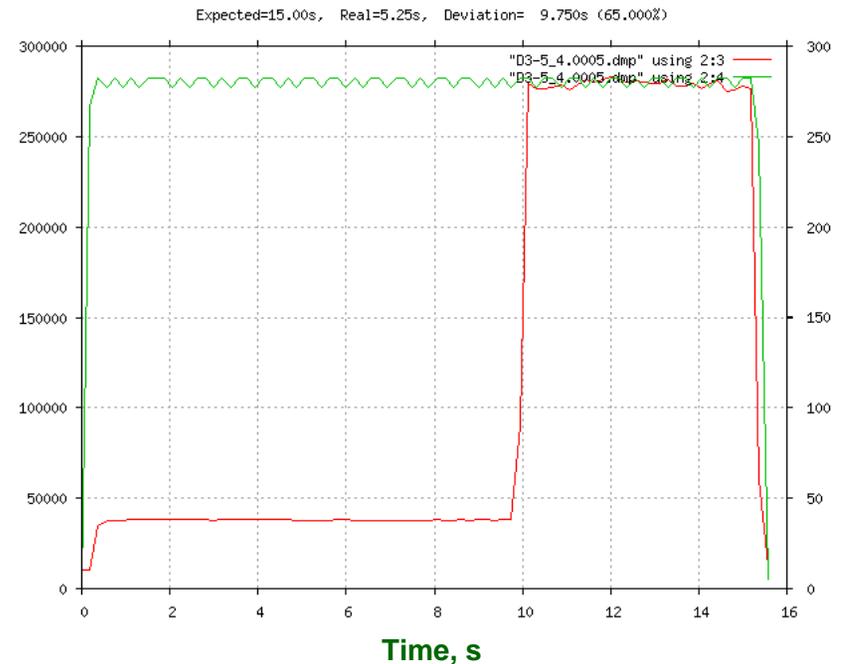
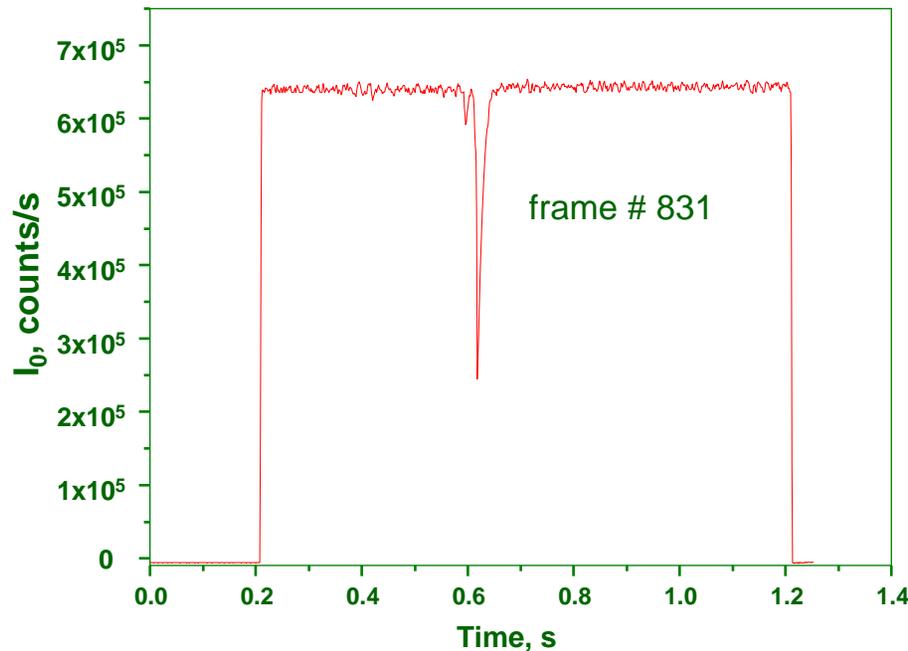
# Collect tab: Frame Audit

## ■ Log files:

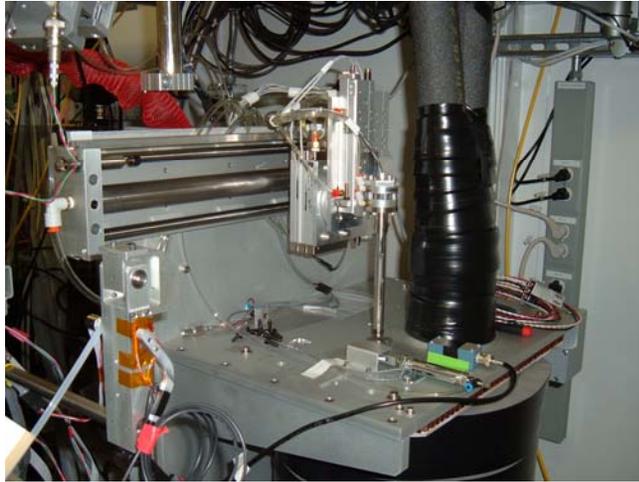
- frameAudit\_<DATE>\_<TIME>.log
- frameAudit\_<DATE>\_<TIME>.log\_camon

## ■ Data files:

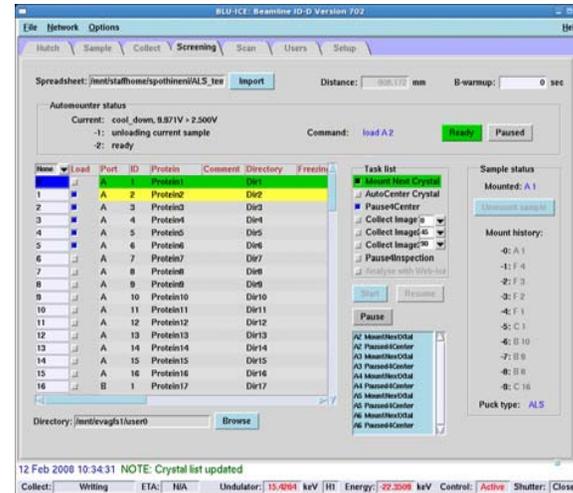
- <F\_NAME>.dmp
- <F\_NAME>.dmp.png



# Blulce-EPICS: Automated Screening



ALS Style Automounter

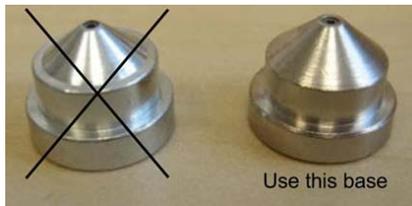


Blulce-Epics Screening Tab

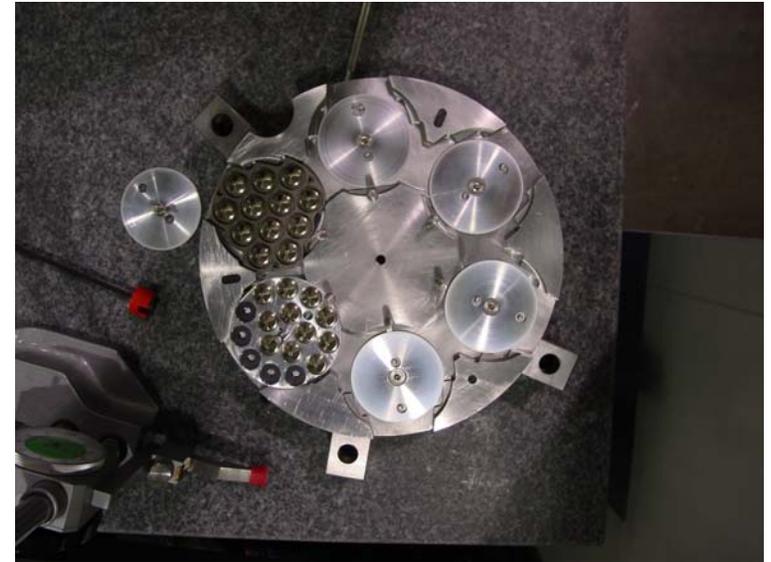
- Users can bring their samples in pucks and load into the sample changer dewar.
- Users can also bring the spreadsheet containing the samples information, which will be loaded to Blulce-Epics Screening Tab.
- User can select which samples to screen, and tasks to perform on them. Available tasks include auto-centering, taking diffraction test images and analyzing with Weblce.
- Blulce-Epics screening tab talks to Robot server for mounting and dismounting samples.
- The Spreadsheet contain the filenames prefix and the directory information for saving diffraction images.
- If selected the collected images automatically be posted for Weblce that provides crystal scoring and data collection strategy.
- For automated centering we have implemented interfaces to the XREC and C3D software packages developed at EMBL.
- We are developing new features for automated screening which are much more user friendly.

# Screening: Automounter Requirements

- The automounter requires a complete puck tool set and **specifically sized bases and pins**.
- We advise users to use **ONLY "ALS style" magnetic bases (Hampton part HR4-779, CrystalCap Magnetic (ALS))**.
- The only pins which can be used with the automounter are the "Hampton 18 mm" pins. This corresponds to breaking off the two end segments of a Hampton pin.



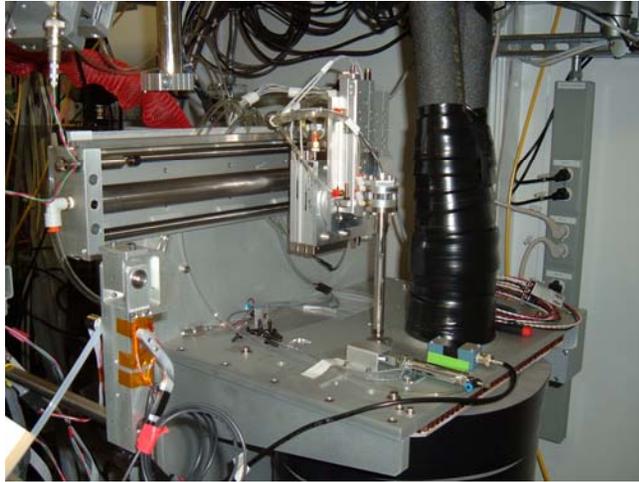
base



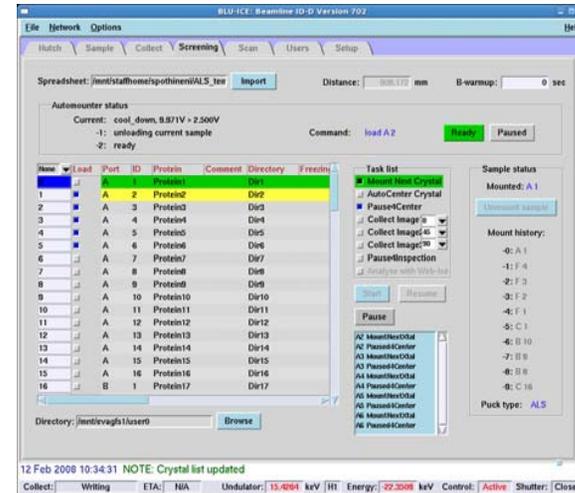
Baseplate in dewar



# Automated Screening



ALS Style Automounter



Blulce-Epics Screening Tab

- Users can bring their samples in pucks and load into the sample changer dewar.
- **Users can also bring the spreadsheet containing the samples information, which will be loaded to Blulce-Epics Screening Tab.**
- User can select which samples to screen, and tasks to perform on them. Available tasks include auto-centering, taking diffraction test images and analyzing with Weblce.
- Blulce-Epics screening tab talks to Robot server for mounting and dismounting samples.
- The Spreadsheet contain the filenames prefix and the directory information for saving diffraction images.
- If selected the collected images automatically be posted for Weblce that provides crystal scoring and data collection strategy.
- For automated centering we have implemented interfaces to the XREC and C3D software packages developed at EMBL.
- We are developing new features for automated screening which are much more user friendly.

# Screening: Sample information

	A	B	C	D	E	F	G	H	I	J
1	Port	CrystallID	Protein	Comment	Directory	FreezingCondition	CrystalCondition	Metal	Priority	Person
2	A1	A1			A1					
3	A2	A2			A2					
4	A3	A3			A3					
5	A4	A4			A4					
6	A5	A5			A5					
7	A6	A6			A6					
8	A7	A7			A7					
9	A8	A8			A8					
10	A9	A9			A9					
11	A10	A10			A10					
12	A11	A11			A11					
13	A12	A12			A12					
14	A13	A13			A13					
15	A14	A14			A14					
16	A15	A15			A15					
17	A16	A16			A16					
18	B1	B1			B1					
19	B2	B2			B2					
20	B3	B3			B3					
21	B4	B4			B4					
22	B5	B5			B5					
23	B6	B6			B6					
24	B7	B7			B7					
25	B8	B8			B8					
26	B9	B9			B9					
27	B10	B10			B10					
28	B11	B11			B11					

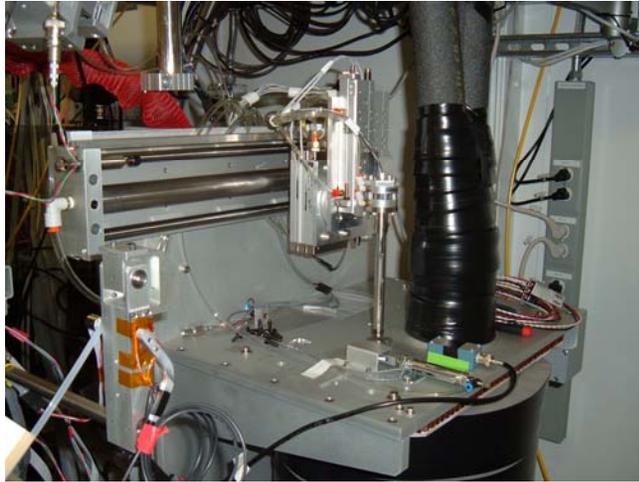
**Spreadsheet Instructions** Only three of the columns present in the spreadsheet are used by the screening system as described here:

**Port:**refers to a port in the puck. The robot will use this port to retrieve the sample. Don't change this column.

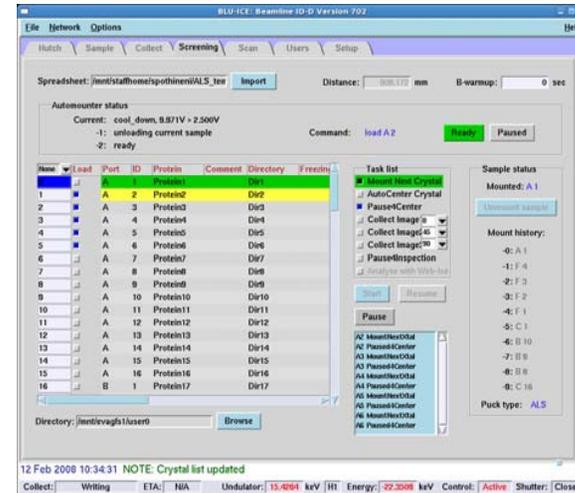
**CrystallID:**this label is used by the screening system to generate filenames. It is recommended that a unique ID be used for each sample.

**Directory:**If provided, this field will be used to generate subdirectories for each sample under the root screening directory. The default template Excel spreadsheet uses the **Port** as the subdirectory name.

# Automated Screening



ALS Style Automounter



Blulce-Epics Screening Tab

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BLU-ICE: Beamline BM Version 2009.2 Build 1341

File Network Options Help

Hutch Sample Raster Collect **Screening** Scan Users Logs

Spreadsheet: /mnt/staffhome/spothineni/ALS\_terr Import B-warmup: 0 sec

Automounter status  
 Current: cool\_down, 3.112V > 2.100V  
 -1: pin\_base warm-up, 1 s  
 -2: unloading current sample  
 Command: load A9 Ready Paused

None	Load	Port	CrystalID	Protein	Comment	Directory	Fi
1	<input type="checkbox"/>	A1	A1			A1	
2	<input type="checkbox"/>	A2	A2			A2	
3	<input type="checkbox"/>	A3	A3			A3	
4	<input checked="" type="checkbox"/>	A4	A4			A4	
5	<input checked="" type="checkbox"/>	A5	A5			A5	
6	<input checked="" type="checkbox"/>	A6	A6			A6	
7	<input checked="" type="checkbox"/>	A7	A7			A7	
8	<input checked="" type="checkbox"/>	A8	A8			A8	
9	<input checked="" type="checkbox"/>	A9	A9			A9	
10	<input checked="" type="checkbox"/>	A10	A10			A10	
11	<input checked="" type="checkbox"/>	A11	A11			A11	
12	<input type="checkbox"/>	A12	A12			A12	
13	<input type="checkbox"/>	A13	A13			A13	
14	<input type="checkbox"/>	A14	A14			A14	
15	<input type="checkbox"/>	A15	A15			A15	
16	<input type="checkbox"/>	A16	A16			A16	
17	<input type="checkbox"/>	B1	B1			B1	

Task list  
 Mount Next Crystal  
 AutoCenter Crystal  
 Pause4Center  
 Collect Image:0  
 Collect Image:45  
 Collect Image:90  
 Analyse with Web-Ice  
 Pause4Inspection  
 Start Resume  
 Pause

Sample status  
 Mounted: A8  
 Unmount sample  
 Mount history:  
 -0: A8  
 -1: A6  
 -2: A5  
 -3: A6  
 -4: A5  
 -5: A12  
 -6: A9  
 -7: A14  
 -8: A13  
 -9: A11  
 Puck type: ALS  
 Warmup

Directory: /mnt/staffhome/spothineni Browse

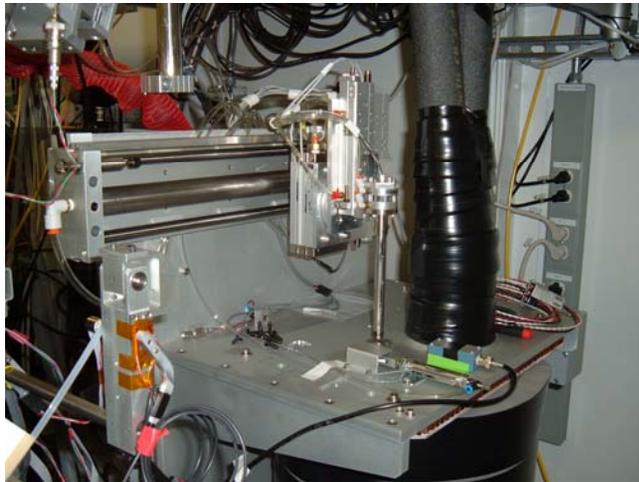
23 Jun 2009 16:03:13 NOTE: cool\_down, 3.263V > 2.100V

APS Current 102.0 APS Shutters Disabled Endstation Secured No Endstation Shutter Closed I Zero 2.82  
 Collect: ReadOut ETA: N/A Undulator: 14.0189 keV H1 Energy: 12.6600 keV Control: Active Shutter: Closed

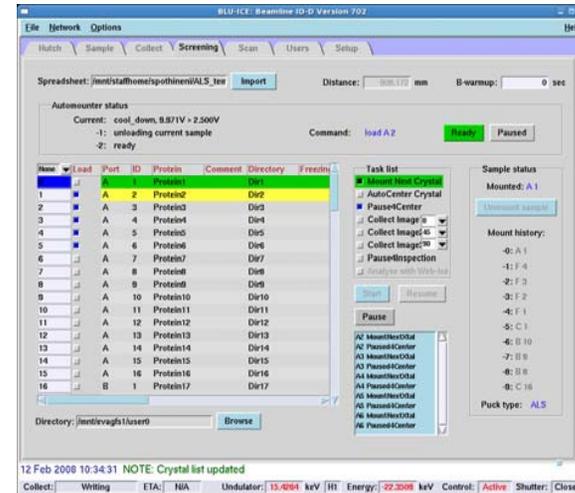
## Blulce-Epics ScreeningTab



# Automated Screening



ALS Style Automounter



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# Screening: Weblce

A. González, P. Moorhead, S. E. McPhillips, J. Song, K. Sharp, J. R. Taylor, P. D. Adams, N. K. Sauter and S. M. Soltis "Weblce: integrated data collection and analysis for macromolecular crystallography." *J. Appl. Cryst.* **41**, 176-184 (2008).

- Weblce is a web-browser application used for crystal scoring and data collection strategy calculations. It can be seen as a pipeline of programs for processing test images
- User is authenticated when loading the spreadsheet into Blulce-Epics. The spreadsheet information is stored in the crystal information server as a Sample Information List (SIL).
- During screening, the diffraction images and crystal images are posted to Weblce, and the crystal-analysis server automatically indexes these images and generates a strategy. The SIL is updated with the crystal scoring parameters.

## External software used by Web-Ice include:

- SPOTFINDER/DISTIL (diffraction spot location and image analysis): Z. Zhang, H. van den Bedem, N. K. Sauter, G. P. Snell and A. Deacon *J. Appl. Cryst.* **39**, 112-119. (2006).
- LABELIT (autoindexing): N. K. Sauter, R. W. Grosse-Kunstleve, and P. D. Adams. *J. Appl. Cryst.* **37**, 399-409. (2004)
- MOSFLM (data integration and overlap analysis): A. G. W. Leslie; in *Crystallographic Computing*, Oxford University Press. (1990)
- BEST (exposure time calculation and oscillation range): A. N. Popov and G. P. Bourenkov. *Acta Cryst.* **D59**, 1145-1153. (2003)
- RADDOSE (absorbed dose calculation): J. W. Murray, E. F. Garman and R. B. G. Ravelli. *J. Appl. Cryst.* **37**, 513-522. (2004)

# WebIce: Screening Results

User Cassettes   BL1-5 Cassettes   <b>Cassette Summary</b>   Cassette Details											
Spreadsheet ID: 5345   Update   Edit Crystal   Analyze Crystal   <b>A1</b>   View Strategy											
Port	CrystalID	Protein	Images	IceRings	Comment	Score	UnitCell	Mosaicity	Rmsd	BravaisLattice	Resolution
A8	A8	myo	A8_003.img A8_004.img	0 0	myoglobin, 9.5% xylytol, 9.5% glucose	0.669	90.25 90.25 45.35 90.00 90.00 120.00	0.75°	0.095 mm	P3,P312,P321,P6,P622	1.38 Å
A7	A7	myo	A7_003.img A7_004.img	3 3	myoglobin, 9.5% xylytol, 9.5% glucose	0.739	90.34 90.34 45.33 90.00 90.00 120.00	0.70°	0.057 mm	P3,P312,P321,P6,P622	1.34 Å
A2	A2	myo	A2_003.img A2_004.img	0 0	Collected several data sets on 7-1 - probably trashed. myoglobin, sucrose cryo	0.825	90.15 90.15 45.14 90.00 90.00 120.00	0.08°	0.086 mm	P3,P312,P321,P6,P622	1.28 Å

$$\text{Score} = 1.0 - (0.7 \times e^{-4/d}) - (1.5 \times rsmr) - (0.2 \times \mu)$$

**Score:** Calculated with above empirical formula where  $d$  is resolution limit in Å ,  $rsmr$  is in mm, and  $\mu$  is the mosaicity in degrees.

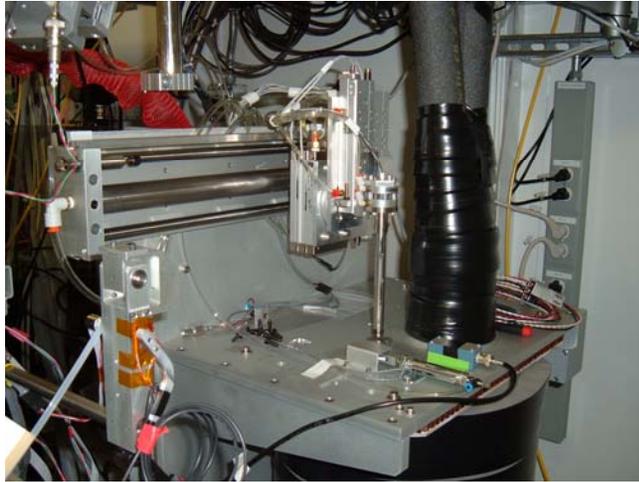
A score of 0.4-0.6 indicates borderline quality. Good crystals usually have a score of about 0.8 or higher.

This score is meant to be used as an initial indicator of the sample quality; although it has been found to agree reasonably well with human assessment in many cases, it is recommended to inspect the diffraction before choosing a sample for data collection.

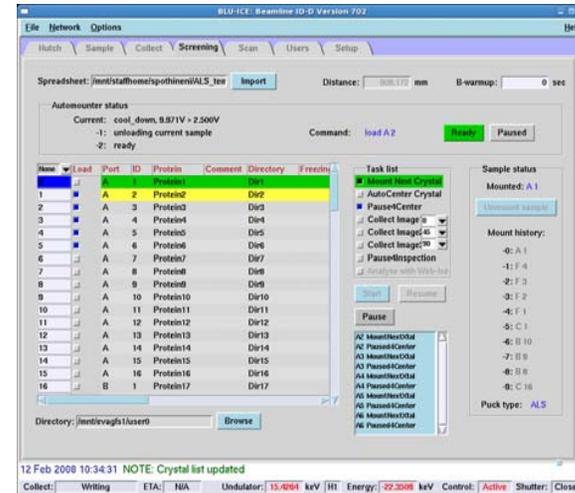
# WebIce: Diffraction Inspection

WebIce - Mozilla Firefox  
File Edit View History Bookmarks Tools Help  
https://bl1ws4.gmca.aps.anl.gov:8543/webice/setSilDisplayMode.do?silId=87&mode=silDetails&owner=user0  
WebIce Welcome ImageViewer Autoindex **Screening** Beamline Video Preferences Help Logout  
User Cassettes Browse Directories Beamline Cassettes Cassette Summary **Cassette Details** Beamline: Select beamline  
/mnt/share1/user0/webice\_test\_02012009/A1/A1\_0.0001  
Header | Spot Statistics | **Crystal Image** | Autoindex | Details  
File: /mnt/share1/user0/webice\_test\_02012009/A1/A1\_0.0001 Open  
Resolution: 1.34 Å  
Zoom: 1.0  
Brightness: 400  
Size: 400x400  
 Show spot overlay  
Analyze Image  
Prev Next  
Crystal ID: A1  
Spreadsheet ID: 87 Update Analyze Crystal **A1** View Strategy  
A1 A2 A3 A4 A5 A6 A7 A8 A9 A10 A11 A12 A13 A14 A15 A16 B1 B2 B3 B4 B5 B6 B7 B8 B9 B10 B11 B12 B13 B14 B15 B16  
C1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C12 C13 C14 C15 C16 D1 D2 D3 D4 D5 D6 D7 D8 D9 D10 D11 D12 D13 D14 D15 D16  
E1 E2 E3 E4 E5 E6 E7 E8 E9 E10 E11 E12 E13 E14 E15 E16 F1 F2 F3 F4 F5 F6 F7 F8 F9 F10 F11 F12 F13 F14 F15 F16  
Done bl1ws4.gmca.aps.anl.gov:8543

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ALS Style Automounter



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# Blulce-Epics: New Java Screening Tab

BLU-ICE: Beamline BM Version sudhir-piezo Build 1323

File Network Options Help

Hutch Sample Raster Collect Screening Scan Users Logs JScreening

/mnt/staffhome/spothineni/ALS\_template. Browse Update Spreadsheet Edit Export **A11 MountNextXtal**

Select	Next->	Port	CrystalID	Protein	Images	IceRings	Comment	Directory	Score
<input type="checkbox"/>		A8	A8					A8	
<input checked="" type="checkbox"/>		A9	A9					A9	
<input type="checkbox"/>		A10	A10					A10	
<input checked="" type="checkbox"/>	1	A11	A11					A11	
<input checked="" type="checkbox"/>	2	A12	A12					A12	
<input checked="" type="checkbox"/>	3	A13	A13					A13	
<input checked="" type="checkbox"/>	4	A14	A14					A14	
<input checked="" type="checkbox"/>	5	A15	A15					A15	
<input type="checkbox"/>		A16	A16					A16	
<input type="checkbox"/>		B1	B1					B1	
<input type="checkbox"/>		B2	B2					B2	

Settings

Detector Distance(mm): 900.0

Expose(sec): 1.0 Delta(deg): 1.0

Alignment

Mount

Yag F1 Alignment Pin F2

Puck Type

Puck : ALS

Actions

- Mount Next Crystal
- Auto Centering
- Pause
- Collect Image 0.0 1
- Collect Image 45.0 1
- Collect Image 90.0 1
- Pause

Robot

Ready Pause

None Mount

Unmount Warmup

Status

Current : gripper cold, 2.096V <=

-1 : cool\_down, 2.135V > 2.100V

-2 : unload

Mounted : A 9

23 Jun 2009 16:06:23 NOTE: gripper cold, 2.096V <= 2.100V

APS Current 101.9 APS Shutters Disabled Endstation Secured No Endstation Shutter Closed I\_Zero 2.3

Collect: ReadOut ETA: N/A Undulator: 14.0189 keV H1 Energy: 12.6600 keV Control: Active Shutter: Closed



# Scan Tab: interactive mode edge scans for determining inflection point

BLU-ICE: Beamline ID-B Version 2009.2 Build 1341

File Network Options Help

Hutch Sample Raster Collect Screening Scan Users Logs

Auto Interactive Periodic Table Plot

1. Choose Edge ---->

2. Prepare

Optimize fluor. signal

3. Analyze fluorescence spectrum

Take fluor. spectrum

Time: 4.00 sec

4. Do edge scan

Scan with fluor. peak selected on spectrum

Time: 1.00 sec

5. Cleanup

Done with fluorescence

Stop Scan

Stop Motors

Select an X-ray Absorption Edge

Edge: Se-K

Energy: 12658.00 eV

23 Jun 2009 10:03:57 NOTE: This client may now issue commands.

APS Current 0.0 APS Shutters Disabled Endstation Secured No Endstation Shutter Closed I\_Zero 0.02

Collect: Idle ETA: N/A Undulator: 14.0189 keV HI Energy: 11.9996 keV Control: Active Shutter: Closed

Fluor.signal tune

On-the-fly Edge Scans

Park Fluor.detector

# Scan Tab: auto mode edge scans

BLU-ICE: Beamline ID-B Version 2009.2 Build 1341

File Network Options Help

Hutch Sample Raster Collect Screening Scan Users Logs

Auto Interactive Periodic Table Plot

1. Choose Edge ---->

2. Do edge scan

Start Scan

Rescan

Time: 1.00 sec

Progress:

Move energy to edge  
Optimize fluor. signal  
Take spectrum  
Do edge scan  
Retract fluor. detector

3. Cleanup

Done with fluorescence

Stop Scan

Stop Motors

Select an X-ray Absorption Edge

Edge: Se-K  
Energy: 12658.00 eV

23 Jun 2009 10:03:57 NOTE: This client may now issue commands.

APS Current 0.0 APS Shutters Disabled Endstation Secured No Endstation Shutter Closed I\_Zero 0.02

Collect: Idle ETA: N/A Undulator: 14.0189 keV HI Energy: 11.9996 keV Control: Active Shutter: Closed

- Hardware-level sync between motor position and fluor.detector measurements
- 3-region (fine steps around the edge )
- Chooch for data analysis
- Auto mode: auto ROI selection from database (no need to make choice of ROI on the spectrum)