STATES OF BL13-XALOC

Macromolegular Skystallography

beamline

ALBA

F

Jordi Suanhuix

XALOC: Layout reminder

Beamline concept : In-vacuum Undulator IVU21.6 + Channel-cut Si(111) monochromator + KB focusing mirrors





Experimental Hutch

MD2M CATS PILATUS 6M

XALOC: Beam Shaping - larger sizes

Beam size be expanded by unbending the mirrors and defocusing the beam

- \odot From 50×5.7 to 250×250 μm
- \circ Increasingly popular for beamtimes with a variety of projects











Beam Shaping - smaller sizes

The MD2 penta-aperture consisting in 5 round pinholes is used to reduce the beam size

- Variety of smaller beam sizes for small crystals
- More accurate raster scans possible

BUT:

- Flux is reduced linearly with size
- Data have slightly but consistently better quality (ISas) when defocusing the beam
- Seeking for beam vibrations...







MXCuBE meeting, Nov 30-Dec 1, 2015

Beam vibrations

- Beam center found by Gaussian fitting of images at focal point recorded at 480 Hz
- High speed camera coupled with a 20 um-thick YAG:Ce screen
- Vibrations with the beamline at rest (no excitations)



BL13-XALOC Beamline status

MXCuBE meeting, Nov 30-Dec 1, 2015

Beam vibrations

- The origin of the resonances can be found by hitting the vacuum vessels of the critical elements
- All resonances have frequencies higher that the maximum detector frame rate (12 Hz)



Mono eigenfrequencies



VFM eigenfrequencies



HFM eigenfrequencies



- Horizontal beam vibrations are dominated by a 48 Hz coming from HFM
- Vertical beam vibrations are dominated by a series frequencies at ~75 Hz and one at 100 H from Mono and VFM
- Still no conclusions on the effect on the quality of data.

Spectrum of the beam motion at detector position (no-excitation): Amplitudes

				ratio to		ratio to		
			х-	total	У -	total		
	frequency	frequency	amplitude	amplitude	amplitude	amplitude		
ID	interval (Hz)	(Hz)	(um rms)	(%)	(um rms)	(%)		Resonance
1	0.00-15.00	6.53	0.034	2.08	0.06	3.05		
2	15.00-22.00	19.16	0.01	0.17	0.029	0.71		
3	22.00-35.00	26.13	0.011	0.22	0.026	0.55		
4	35.00-41.00	39.42	0.011	0.21	0.014	0.15		
5	41.00-45.00	43.2	0.014	0.35	0.019	0.31		VFM
6	45.00-49.60	48.71	0.164	47.66	0.017	0.23	Н	HFM
7	49.60-52.00	50.04	0.038	2.55	0.021	0.38		
8	52.00-67.00	58.53	0.042	3.14	0.113	10.73		
9	67.00-72.00	69.6	0.048	4.05	0.092	7.15		
								HFM, VFM,
10	72.00-78.00	73.47	0.121	25.83	0.131	14.37	Both	MONO
11	78.00-88.00	78.8	0.036	2.25	0.102	8.78		
12	88.00-98.00	95.82	0.016	0.43	0.058	2.82		Mono
13	98.00-106.00	100.36	0.036	2.25	0.165	22.9	V	
14	106.00-110.00	108.93	0.009	0.15	0.043	1.57		VFM
15	110.00-116.00	112.93	0.01	0.18	0.054	2.4		
16	116.00-124.00	116.98	0.013	0.31	0.09	6.82		
17	124.00-129.00	126.27	0.009	0.13	0.038	1.18		
18	129.00-142.00	137.42	0.017	0.48	0.035	1.04		
19	142.00-145.00	143.2	0.008	0.11	0.02	0.32		
20	145.00-149.00	148.27	0.009	0.15	0.053	2.33		
21	149.00-150.50	150.04	0.037	2.4	0.029	0.71		
22	150.50-154.00	151.24	0.011	0.21	0.049	2.05		
23	154.00-160.00	156.13	0.012	0.26	0.038	1.24		Mono
24	160.00-168.00	164.18	0.021	0.75	0.056	2.66		
25	168.00-200.00	169.6	0.046	3.74	0.082	5.7		

XALOC: Crystallization plates

- Plates are mounted on the robot, using the plates tool
- The new XYZ moveable beam stop required for plates is already installed
- The cryostream is swung out remotely
- A special widget is used for collection. Integration in the standard collection widget is foreseen before Summer 2016
- A TRIS crystal was positioned in the beam using manual operation of the robot
- An still image was recorded using an exposure of 0.5 s
- Now able to scan plates, but not ready for users

Plate data collection (collect, bl13_collect_widget_plate_RB.py) (on pcbl1301)	
File View Taurus Tools Help	
Ealign 12.6610 12.6610 Abs • keV mbattrans • 12.990 30.00 Abs • % detsamdis • 502.422 502.422 Abs • mm rescomp • 2.49 Abs • A	Data Dir [beamlines/b113/inhouse/rboer/scripts/plate_widget.] Prefix test Run 1 Template test_1####.cbf 10 + Shoot Plate open EH - ->> Shoot Plate ->>





XALOC: Controls upgrades

- EDNA implemented and integrated in the experiment pipeline
- Automatic data processing
 - Using the cluster
 - AutoPROC (Global Phasing Ltd) implemented
 - Implementing Phaser in the pipeline
- Diffraction data queues ready.
 - Inverse beam (wedged) anomalous data collection
 - Many others to be implemented
- Multiple crystal position data collection: crystal cartography
- Reorientation of the crystal after indexing with EDNA
- Beamline diagnostic tool
- sftp service for users



Rai and filename info No sample detected Status: waiting for user input					
Data Dr Anomelocal/upb/13	n Dr Anmeiocallyph13				
prefix no_sample				nun 1	
Auto template no_sample_1_####.cbf				Auto Filename	
Dailection mode	Parameters for Te	sting	Parameters for Collec	cáng	
Natve	Set transmissi	on to 50	_		
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MAD	Test exposure time	0.500		Realign star	Collect
	Test angles	•			
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bl13_kappacalc.py (on pcbl1301)				100	
Reload EDNA file	Get XDS/Mosfim matrix file				Exit
			Kappa	Phi	Closest Angle
to align a* with omega			26.62	27 149.2	83 0.000
to align b* with omega			75.00	00 -61.72	26 50.687
to align c* with omega			75.00	00 28.55	55 59.831
User HKL ✔ 1.000000 ♦ 0.000000 ♦	0.000	000	\$ 26.62	27 149.2	83 0.000

Remote data collection

WORKFLOW REMOTE ACCESS XALOC

- NX based (Server ready)
- User needs to install NX Enterprise client for Windows/Linux/Mac (exe file)
- Connect to:
 - Host: remotenx.cells.es Port: 443
- Currently in beta testing
- Still to be done: script giving user authentication



XALOC: Future upgrades

Mechanical

- Installation of a (de)humidifier device
 - Control system required
- Mechanized crystal annealing
- New viewing camera



Controls

- Installation of MXCuBE
- Implementation of (pending MxCUBE??):
 - Helical data collection
 - MAD data collection pipeline
 - Multiple kappa angle data collection
 - Automated crystal centering
- Automatic beam alignment to be started when the fluorescence screen can be automatically placed at sample position
- Automatic loop centering : waiting for MXCuBE?





The XALOC Team

Engineering

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Administration



BL13-XALOC Beamline status