



Introduction to Remote at I24

Dr. Sam Horrell

Beamline Scientist at I24



@DrHorrell

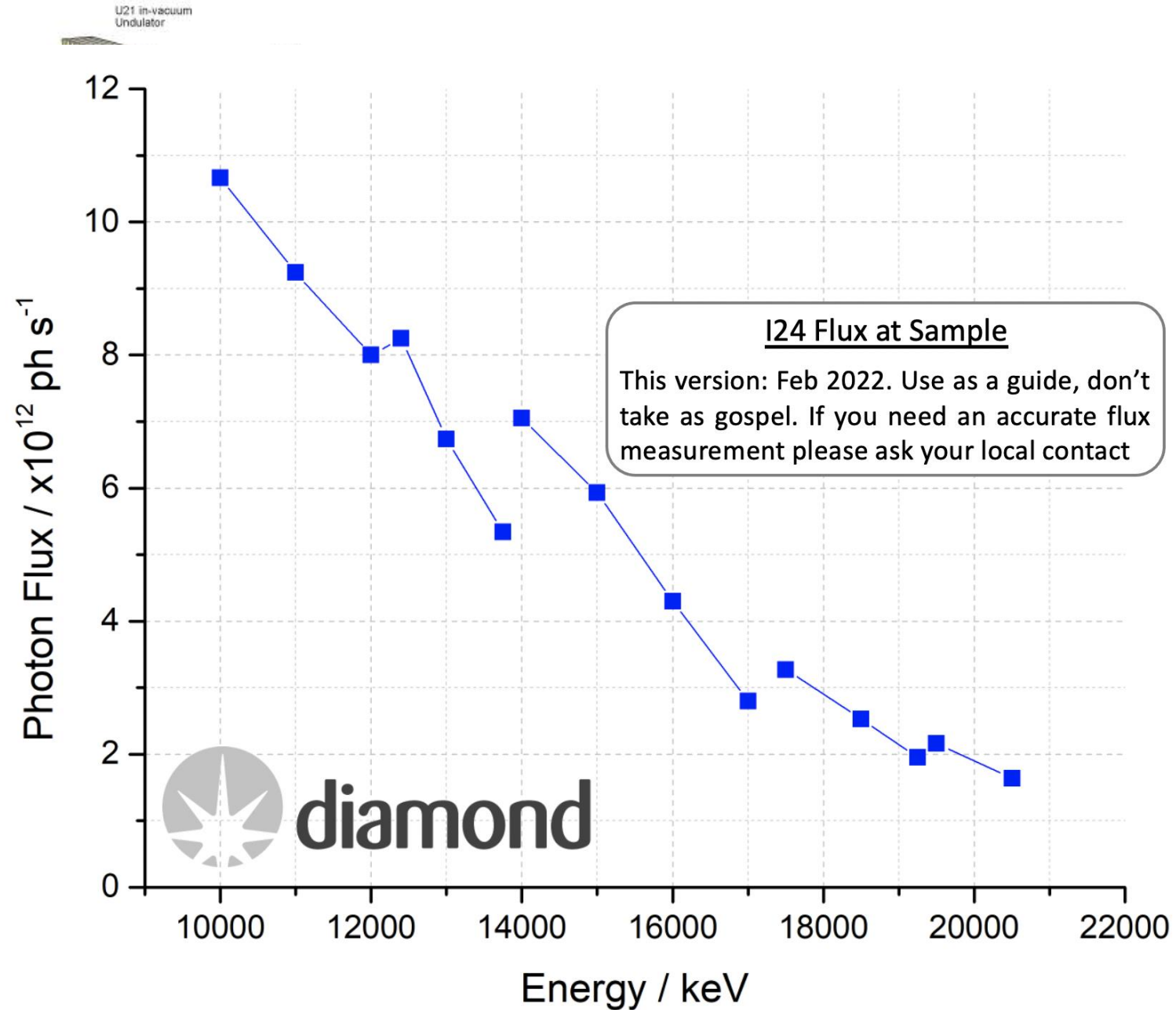


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Beamline Overview

- Tunable microfocus beamline
 - ~7.8-25 KeV
- High energy data collection
 - 7×10^{12} ph/s at 12.4 keV
 - 2×10^{12} ph/s at 20.0 keV
- Adaptable beam size
 - Minimum $7 \times 7 \mu\text{m}$
 - Maximum $50 \times 50 \mu\text{m}$
- Fluorescence Spectroscopy
 - K edges – Fe, Co, Ni, Cu, Zn, Se, N
 - L edges – Pt, Au, Hg

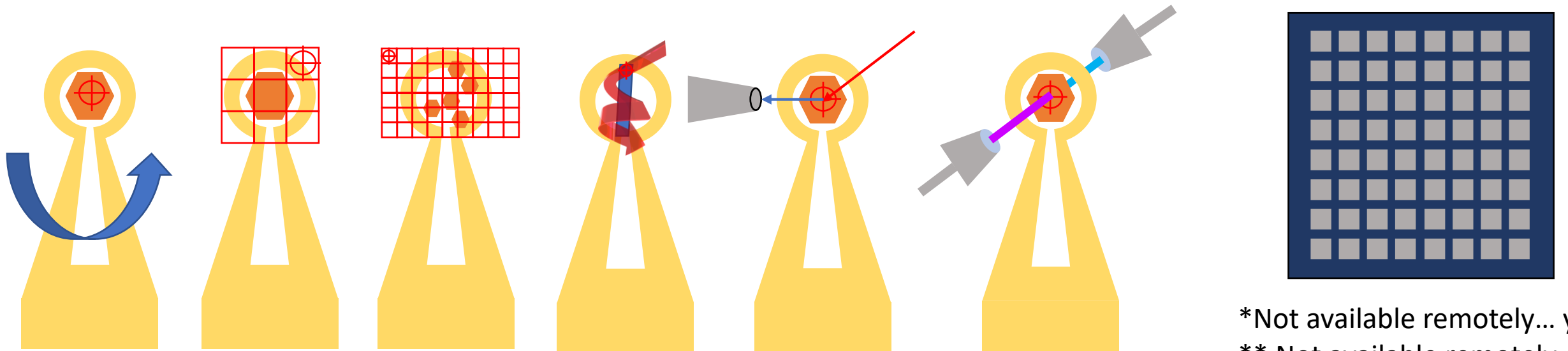


Modular End Station



What Can You Do At I24?

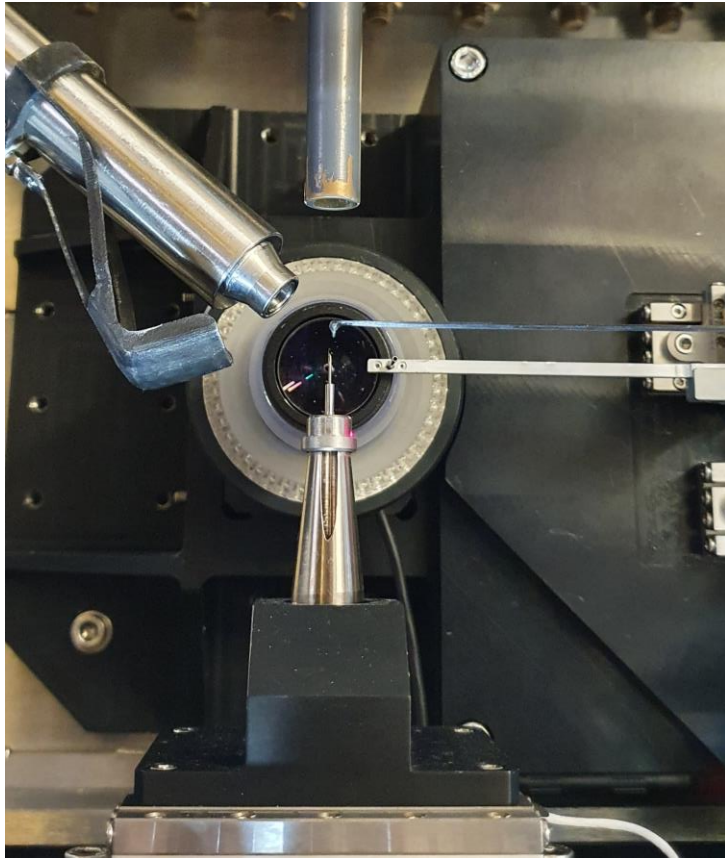
- Rotation data collection
- SAD and MAD phasing
- Fast grid scans
- Helical scans
- High energy data Collection
- Fluorescence Scans
- *UV-Vis Spectroscopy* *
- Serial crystallography **



*Not available remotely... yet

** Not available remotely

Pin Mode

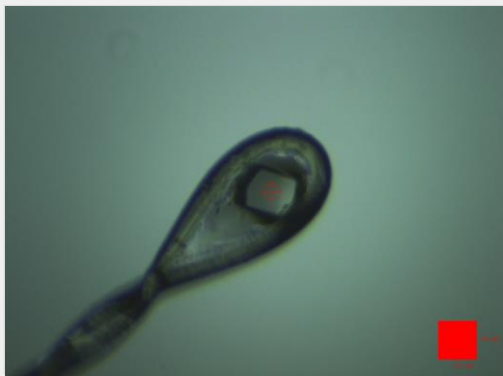


- Standard rotation data
- Multiplex data merging
- Helical scans
- Fast grid scans
- Fluorescence scans
- High-capacity robot

Auto-Processing Pipelines

03-02-2021 11:18:14 - hewl/Lys_006/Lys_006_1_#####.cbf

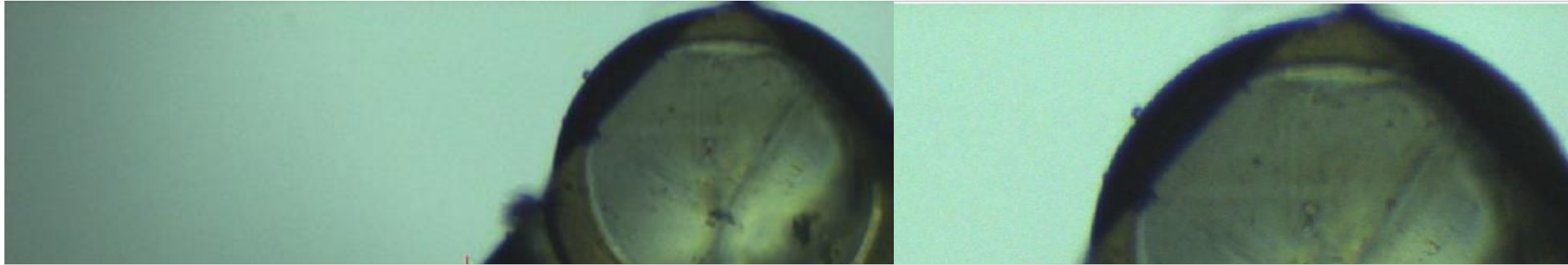
Sample: <u>Lys_006</u>	Flux: 2.77e+0
Ω Start: 0.0°	Ω Osc: 0.10°
Ω Overlap: 0°	No. Images: 1800
Resolution: 1.27Å	Wavelength: 0.9999Å
Exposure: 0.100s	Transmission: 10.04%
Beamsize: 7x7 μ m	Type: SAD
Comment: (-262,-57,472)	



Auto Processing Fast DP: ✓ Xia2/3dii: ✓ DIALS: ✓ Xia2/Multiplex: ? autoPROC: ✓

data	Resolution	Spacegroup	Mn</sig(i)>	Rmeas Inner	Rmeas Outer	Completeness	Cell	Status
fast_dp	27.68 - 1.28	P 4 2 2	21.0	0.032	0.730	99.2	78.29 78.29 37.00 90.00 90.00 90.00	processing successful
autoPROC	55.41 - 1.13	P 41 21 2	15.7	0.039	1.605	97.3	78.36 78.36 37.05 90.00 90.00 90.00	processing successful
autoPROC	19.00 - 1.13	P 43 21 2	15.9	0.038	1.495	97.2	78.34 78.34 37.04 90.00 90.00 90.00	processing successful
xia2 3dii	39.15 - 1.10	P 43 21 2	15.2	0.038	1.987	95.2	78.30 78.30 37.01 90.00 90.00 90.00	processing successful
xia2 3dii	39.15 - 1.10	P 41 21 2	15.2	0.038	1.987	95.2	78.30 78.30 37.01 90.00 90.00 90.00	processing successful
xia2 dials	55.44 - 1.12	P 41 21 2	14.0	0.023	3.127	96.4	78.40 78.40 37.02 90.00 90.00 90.00	processing successful
xia2 dials	39.20 - 1.13	P 43 21 2	13.8	0.023	2.977	97.0	78.40 78.40 37.02 90.00 90.00 90.00	processing successful
autoPROC+STARANISO	55.41 - 1.09	P 41 21 2	17.5	0.038	1.069	93.8	78.36 78.36 37.05 90.00 90.00 90.00	processing successful
autoPROC+STARANISO	19.59 - 1.09	P 43 21 2	17.9	0.037	1.033	93.0	78.34 78.34 37.04 90.00 90.00 90.00	processing successful

Grid Scan Wedge Collection



Box number	Motor positions
40	(224, -773, -842)
41	(230, -773, -834)
2	(158, -793, -917)
3	(165, -793, -910)
26	(165, -783, -910)
17	(224, -783, -842)
16	(230, -783, -834)
99	(237, -723, -827)
100	(230, -723, -834)
125	(230, -713, -834)
126	(237, -713, -827)

Default Folder

Default Prefix

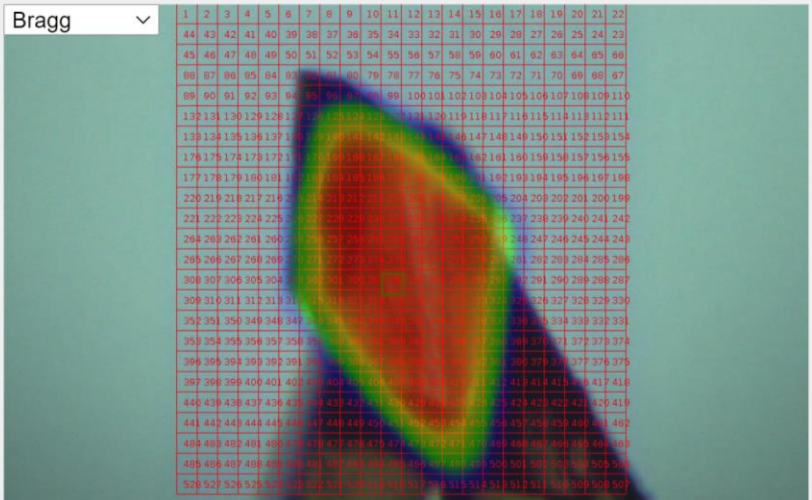
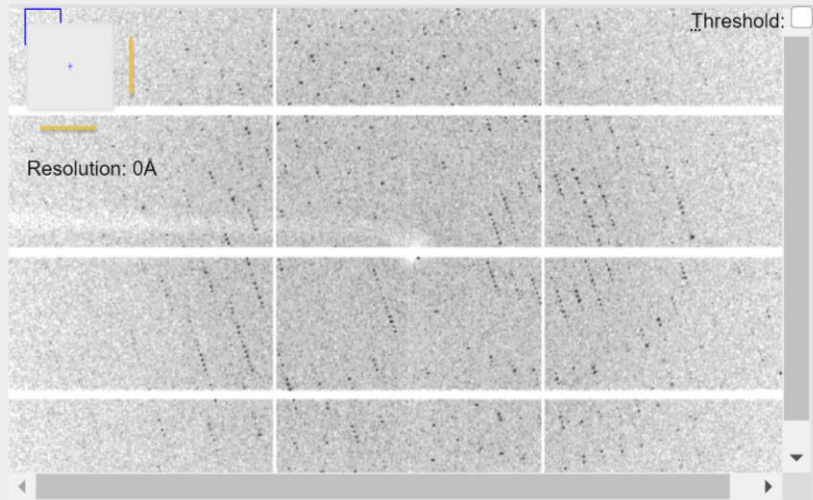
Run All

Run Selected

Position	Omega Start (°)	Omega Oscillation (°)	Omega Delta (°)	Kappa (°)	Phi (°)	X (μm)	Y (μm)	Z (μm)	Number of Images	Time per Image (s)	Maximum Resolution (Å)	Distance (mm)	Wavelength (Å)
	0.00	0.100	0.00	0.000	0.000	224.0	-773.0	-842.0	10	0.010	1.5000	269.2	0.9680
	-2.00	0.100	0.00	0.000	0.000	230.0	-773.0	-834.0	10	0.010	1.5000	269.2	0.9680
	2.00	0.100	0.00	0.000	0.000	158.0	-793.0	-917.0	10	0.010	1.5000	269.2	0.9680
	4.00	0.100	0.00	0.000	0.000	165.0	-793.0	-910.0	10	0.010	1.5000	269.2	0.9680
	-6.00	0.100	0.00	0.000	0.000	224.0	-783.0	-842.0	10	0.010	1.5000	269.2	0.9680
	8.00	0.100	0.00	0.000	0.000	230.0	-783.0	-834.0	10	0.010	1.5000	269.2	0.9680
	-3.00	0.100	0.00	0.000	0.000	237.0	-723.0	-827.0	10	0.010	1.5000	269.2	0.9680
	3.00	0.100	0.00	0.000	0.000	230.0	-723.0	-834.0	10	0.010	1.5000	269.2	0.9680
	3.00	0.100	0.00	0.000	0.000	230.0	-723.0	-834.0	10	0.010	1.5000	269.2	0.9680

09-02-2021 10:58:58 - 20210209/Eiger9p19/grid_Thau_Se_4/grid_2_master.h5

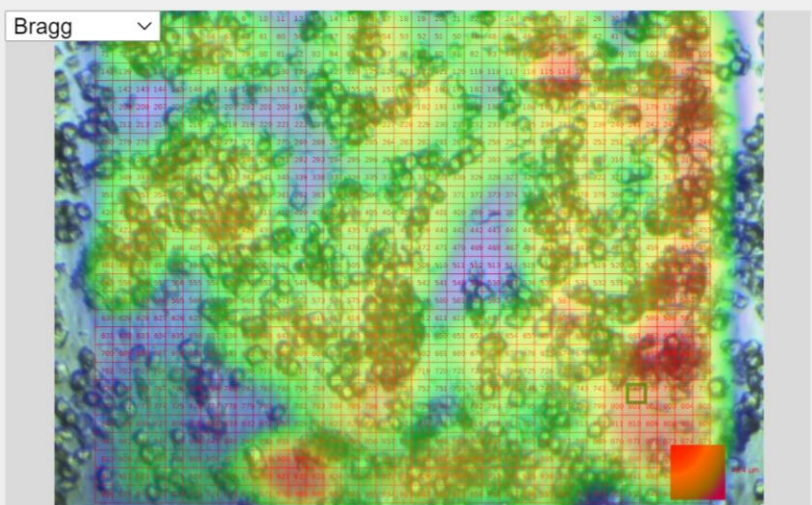
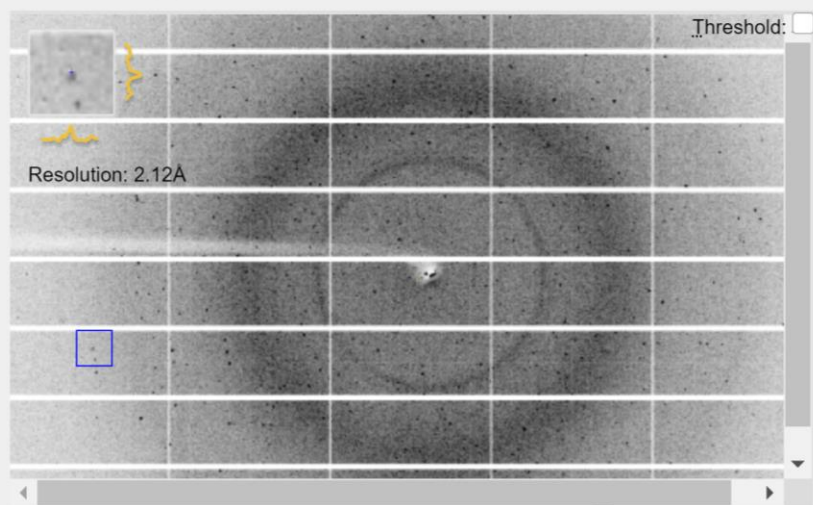
Sample: Thau_Se_4
 Ω Start: -0.0°
Resolution: 2.00Å
Wavelength: 0.9999Å
Exposure: 0.010s
Transmission: 4.95%
Beamsize: 7x7 μ m
Boxsize: 10x10 μ m
Comment: Diffraction grid scan of 22 by 24 images, Top left [352,106], Bottom right [833,630]
Image: 298 Value: 88
X: -281.50 Y: -519.58 Z: 243.00



Enlarge

05-02-2021 17:30:41 - agata/22Jan/NaBr/cryo2/grid10/grid10_1_#####.cbf

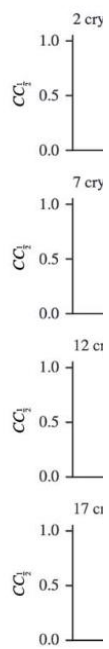
Ω Start: 164.0°
Resolution: 1.75Å
Wavelength: 0.9999Å
Exposure: 0.010s
Transmission: 100.00%
Beamsize: 7x7 μ m
Boxsize: 15x15 μ m
Comment: Diffraction grid scan of 35 by 28 images, Top left [59,19], Bottom right [961,741]
Image: 740 Value: 53
X: 1111.90 Y: 2115.17 Z: 374.58



Enlarge

Multiplex Pipeline

- Combining Small Wedges
- Combining Large Wedges
- Removing Outliers
- Provides Final Mtz
- Anomalous Signal
- Radiation Sensitive Samples



research papers



STRUCTURAL
BIOLOGY

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xia2.multiplex: a multi-crystal data-analysis pipeline

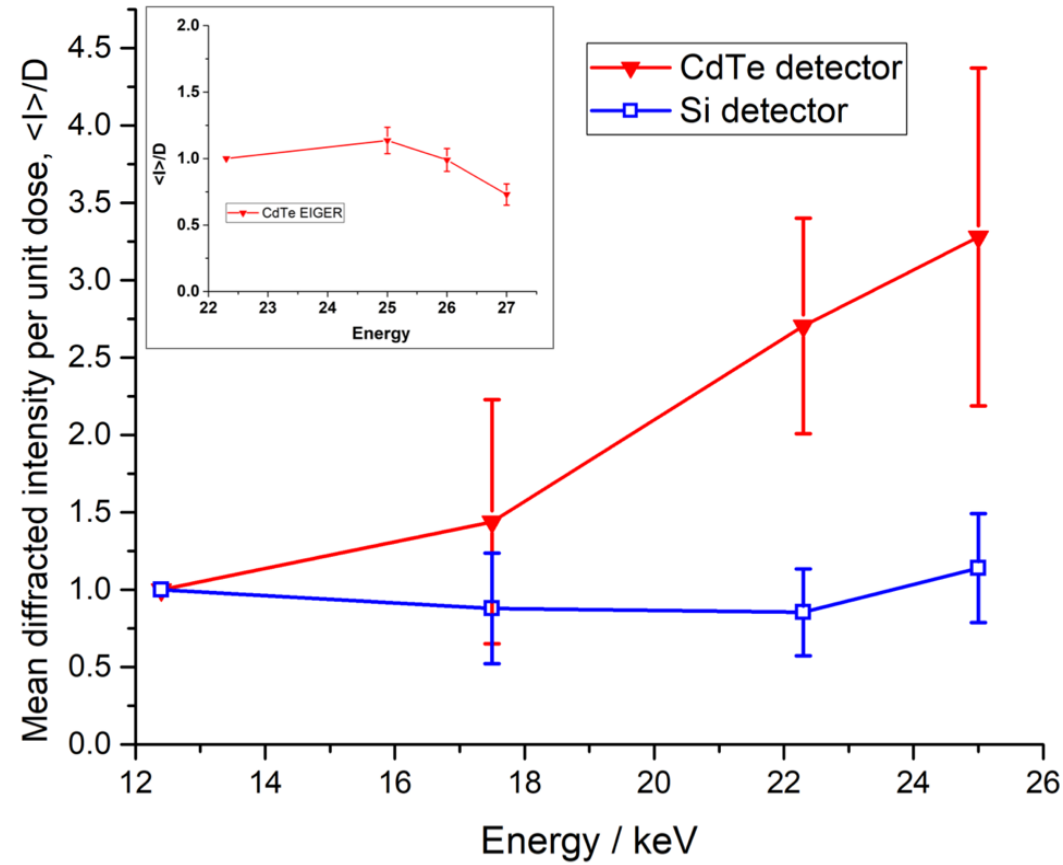
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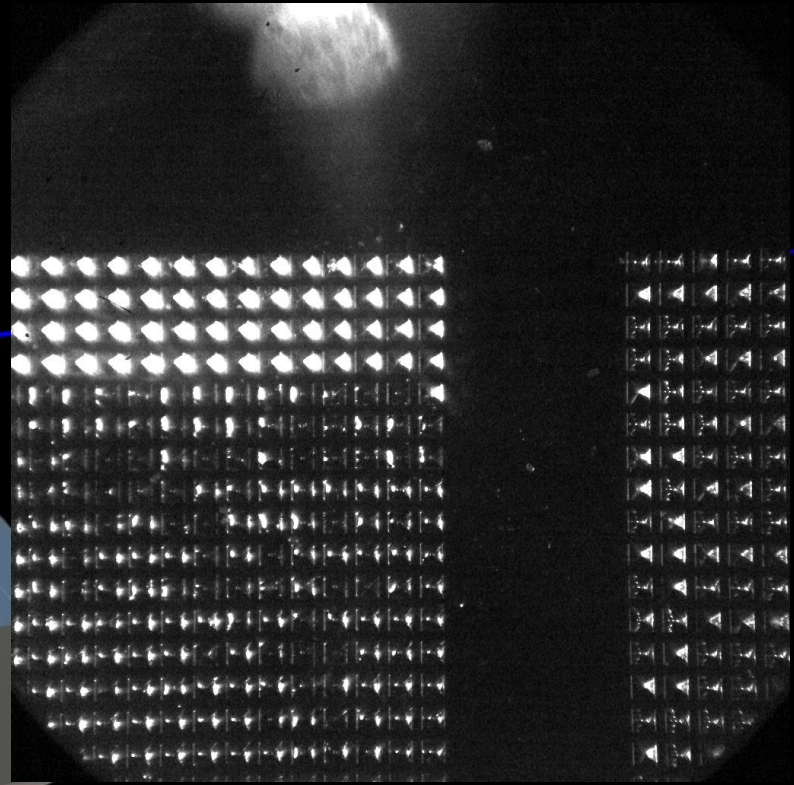
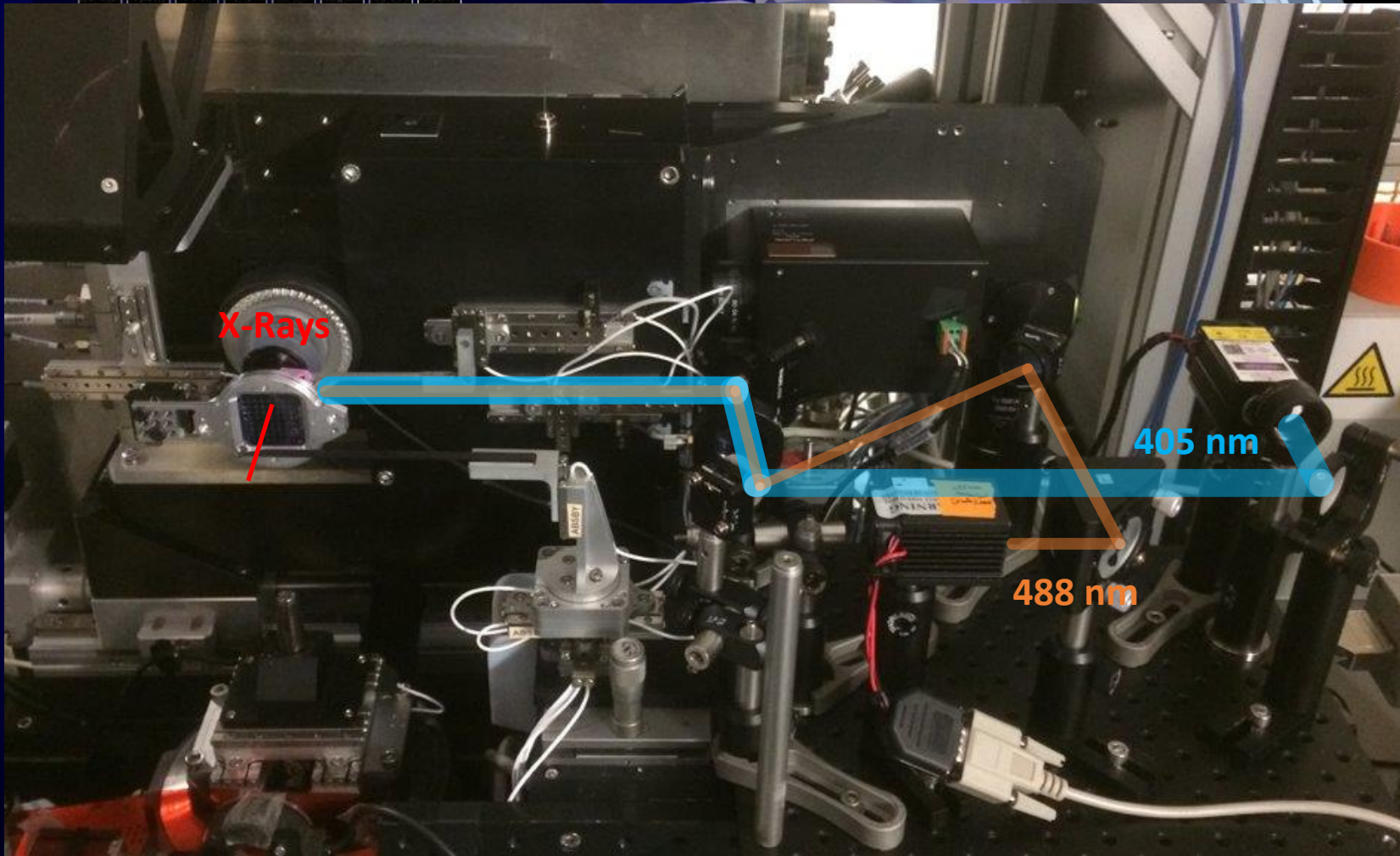
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High Energy Data Collection

- More data per unit dose
- Decreased absorption
- Increased elastic scattering
- Photoelectron escape





Serial Mode:
Fixed Target

Acknowledgements

I24 Team

- Robin Owen
- Danny Axford
- Sam Horrell
- Sofia Jaho
- Do-Heon Gu

XFEL Hub

- Pierre Aller
- Anastasiia Shilova

DIALS Team

- Richard Gildea

