

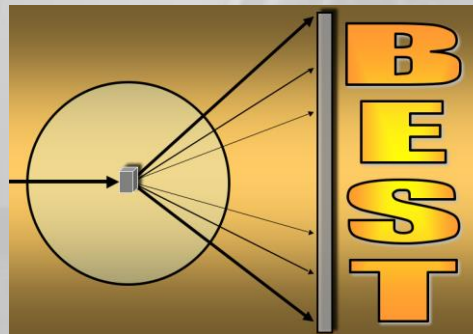
A Light for Science



European Synchrotron Radiation Facility

Looking forward to the fully automated and optimal data collection using synchrotron radiation

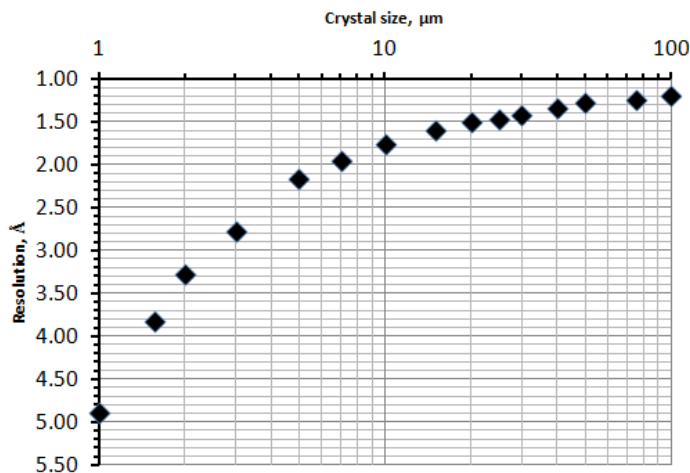
*Alexander Popov
ESRF, MX group*



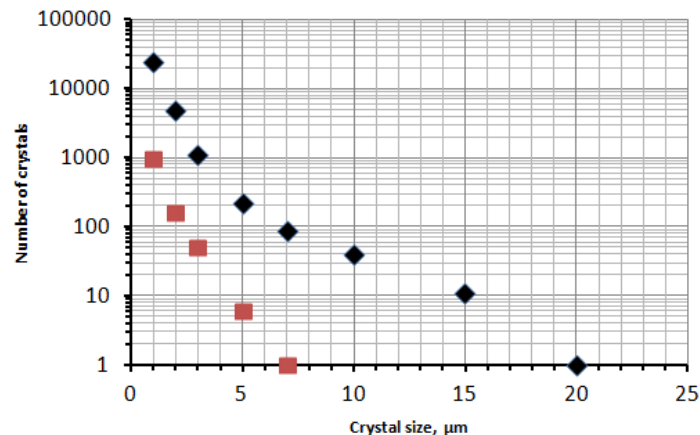
- *Data quality is better*
- *Measurements are too difficult*

Micro-crystallography

- Thermolysin, Space Group $P6_122$; B-factor = 11.5 \AA^2



Complete data set resolution vs. crystal size

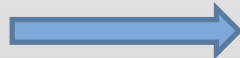


Number of cryocooled crystals of a given size required to achieve dataset resolutions of 1.5 \AA (black) and 2.0 \AA (blue).

- For a crystal $1 \times 1 \times 1 \text{ \mu m}^3$ in dimensions partial data sets *from about 1000 crystals* would be needed to achieve a final data set resolution of $d_{\min} = 2.0 \text{ \AA}$.

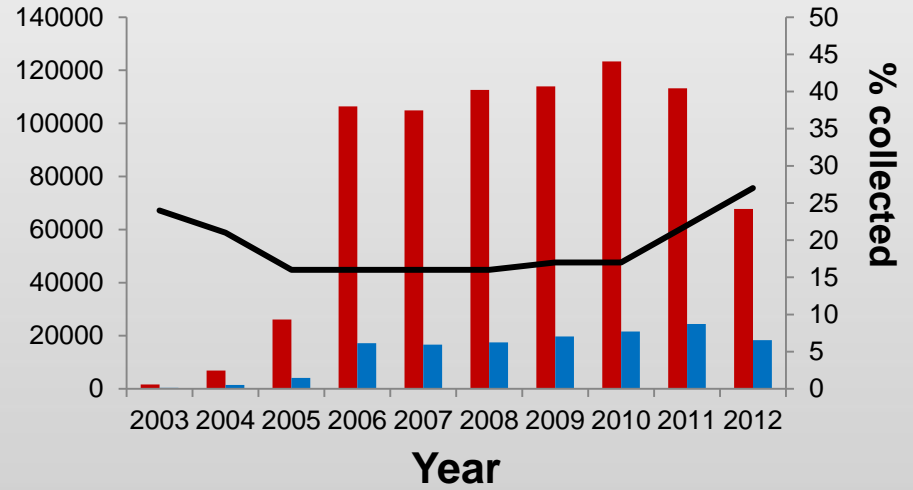
- We are lazy and we don't want to do boring work. We don't know and we don't want to know a crystallography.*

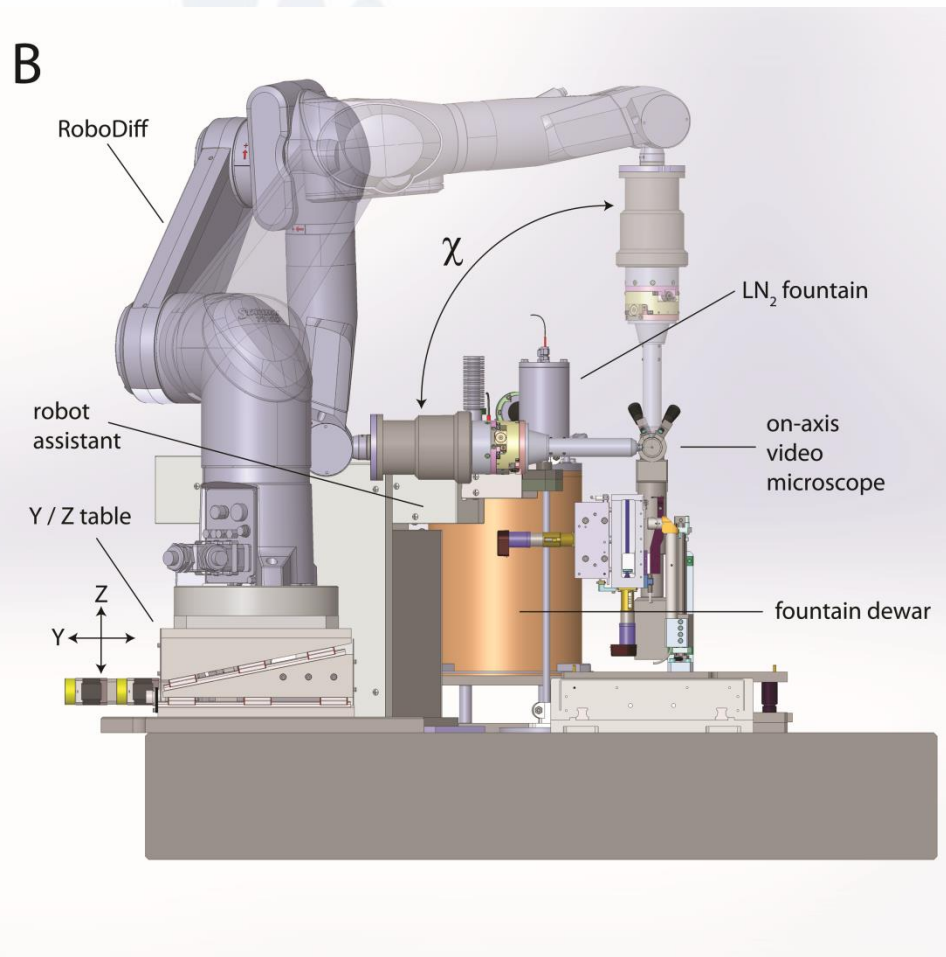
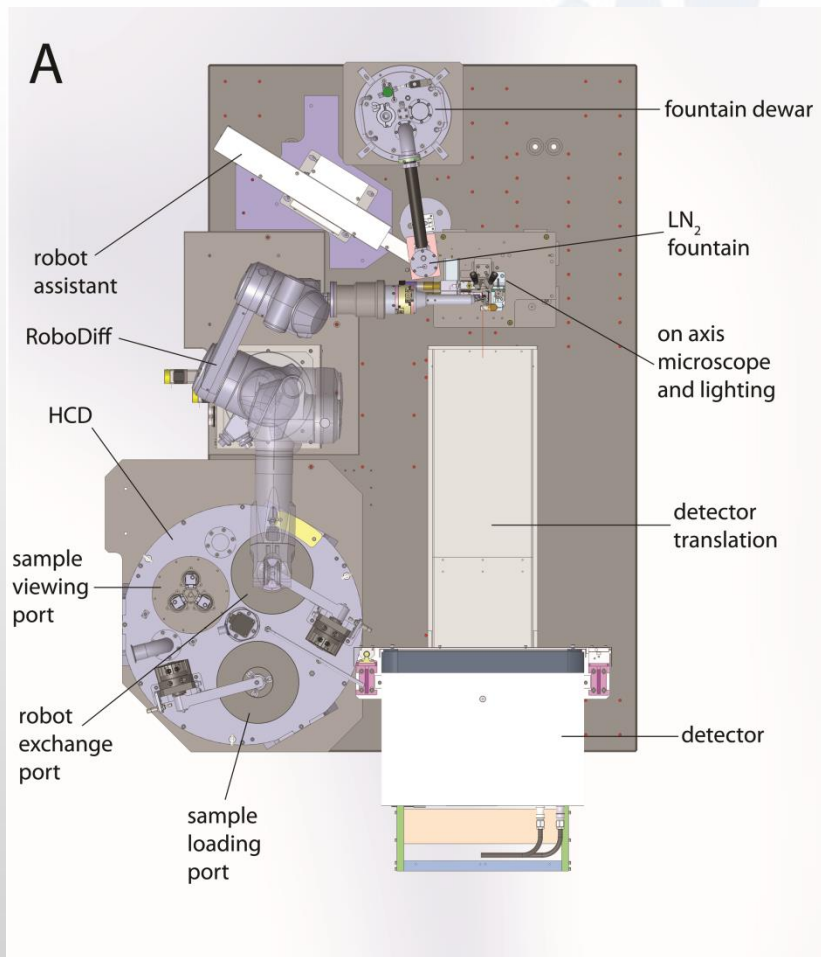
High-throughput crystallization



collections

ESRF beamlines



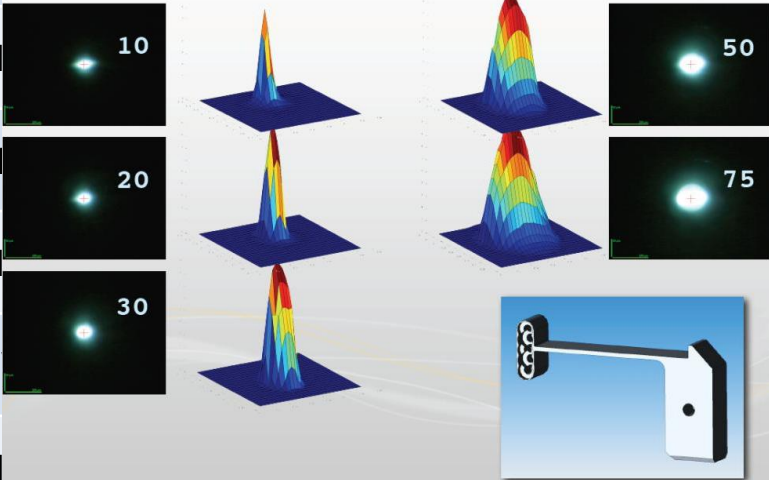


RoboDiff

Nurizzo D, Bowler MW, *et al.* (2016), *Acta Cryst D*. accepted

how we can realize automation?

Old available SB beam lines

	Energy [keV]	Beam size [mm ²]	Flux [ph/s]	detector	Frame rate [Hz]
ID23-1	6-20	10-40	3x10 ¹³		50
ID23-2	14.2	5x7	4x10 ¹³		20
ID29	6-20	10-50	5x10 ¹³		30
ID29S	optical spectroscopy (CRYOBENCH; U)				
BM29	7-15	500 (100)	2x10 ¹³		

New SB beam lines

MASSIF-1	12.8	20-150	10 ¹³	Pilatus3 2M	250
MASSIF-2	12.8	20-100	10 ¹³	tbd	Not finished
MASSIF-3	12.8	>10	5x10 ¹³	Eiger 4M	750
ID30B	6-20	20-200	10 ¹³	Pilatus3 6M	100



PILATUS3 S Series

ADVANTAGES S SERIES

- Maximum frame rate of 25 Hz
- Readout time of 2.03 ms
- Upgradeable to X series



PILATUS3 X Series

ADVANTAGES X SERIES

- Frame rates up to 500 Hz
- Readout time of 0.95 ms
- Region of interest readout

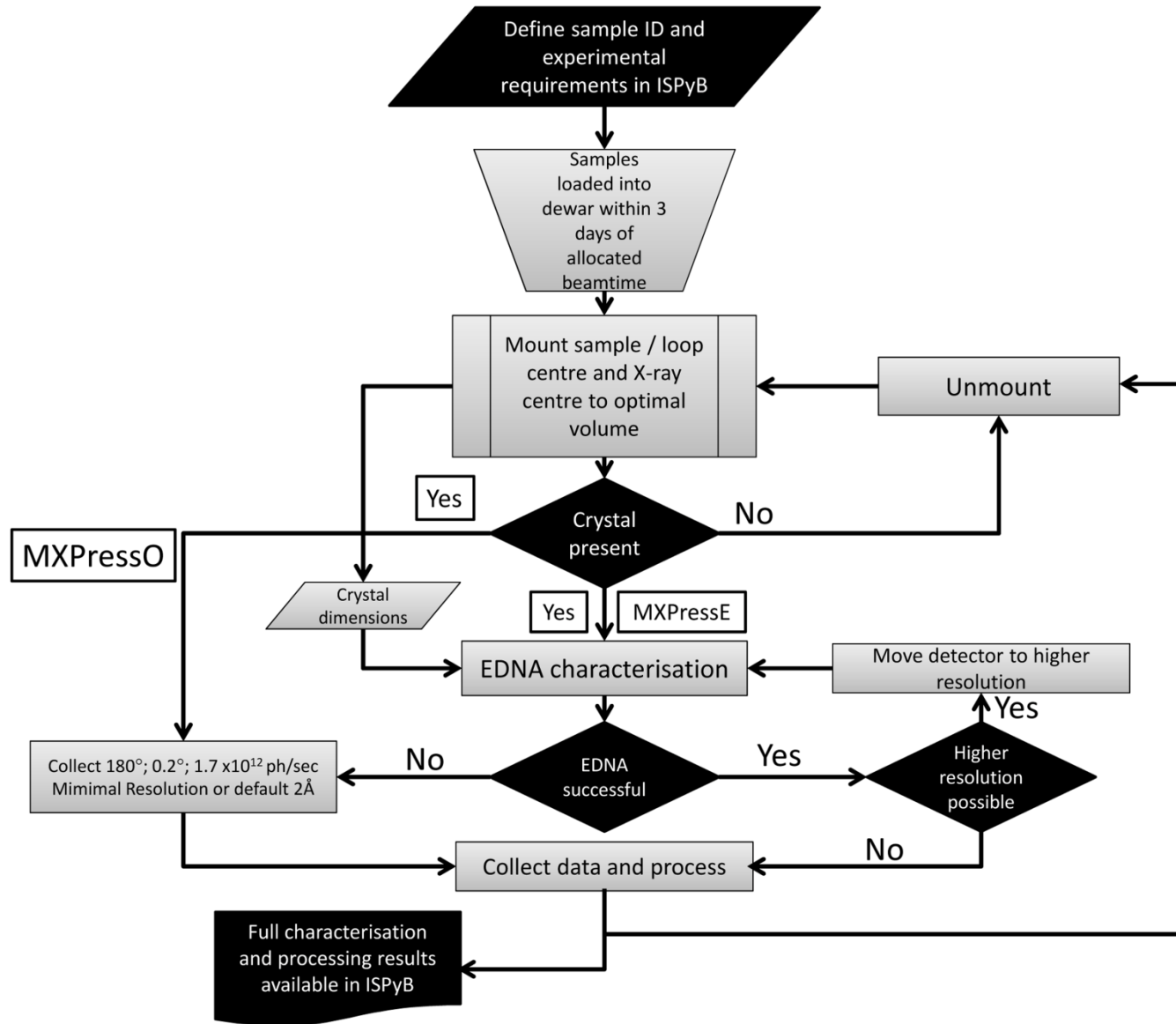
EIGER X SYNCHROTRON SERIES



The new EIGER X series provides ultimate performance for the most demanding synchrotron applications. Frame rates in the kilohertz range in combination with continuous readout open new horizons in time-resolved experiments and XPCS. Hitherto prohibitively slow scanning beam imaging techniques like ptychography become routinely possible. High resolution and coherent diffraction experiments benefit from the small pixel size and an outstanding point-spread function that is enabled by direct conversion of X-rays. Highest count rates per unit area ideally match the ever-increasing beamline brightness. Read more about the EIGER X series [here](#).

PILATUS3 X detector series technical specifications

PILATUS3 X	200K-A	300K	300K-W	1M	2M	6M
Number of detector modules	1 x 2	1 x 3	3 x 1	2 x 5	3 x 8	5 x 12
Sensitive area: width x height [mm²]	83.8 x 70.0	83.8 x 106.5	253.7 x 33.5	168.7 x 179.4	253.7 x 288.8	423.6 x 434.6
Pixel size [μm²]	172 x 172					
Number of pixels: hor. x ver.	487 x 407	487 x 619	1475 x 195	981 x 1043	1475 x 1679	2463 x 2527
Gap width: hor. / ver. [pixel]	- / 17	- / 17	7 / -	7 / 17	7 / 17	7 / 17
Dead area [%]	4.3	5.5	0.9	7.2	8.0	8.5
Defective pixels	< 0.03%					
Maximum frame rate, full frame [Hz]	500	500	500	500	250	100
Maximum frame rate, ROI [Hz]	-	-	-	500	500	500
Readout time [ms]	0.95					
Point-spread function	1 pixel (FWHM)					
Threshold energy [keV]	3.5 - 18	2.7 - 18	2.7 - 18	2.7 - 18	2.7 - 18	2.7 - 18
Counter depth	20 bits (1,048,576 counts)					
Power consumption [W]	30	30	30	165	250	580
Dimensions (WHD) [mm³]	156 x 155 x 284	158 x 193 x 262	280 x 62 x 296	265 x 286 x 455	384 x 424 x 456	590 x 603 x 455
Weight [kg]	5.4	7.5	7.0	25	46	92
Module cooling	Air-cooled	Water-cooled	Water-cooled	Water-cooled	Water-cooled	Water-cooled
Electronics cooling	Air-cooled	Water-cooled	Water-cooled	Air-cooled	Air-cooled	Air-cooled
Standard configuration	450 μm silicon sensor					
	detector, detector server	detector, detector server, water-cooling unit		detector, detector server, water-cooling unit, PPU mini		
	1000 μm silicon sensor					
Detector options	PPU mini, L or XL	PPU mini, L or XL	PPU mini, L or XL	PPU L or XL	PPU L or XL	PPU L or XL
	-	vacuum compatibility		-	-	-
	320 μm silicon sensor					



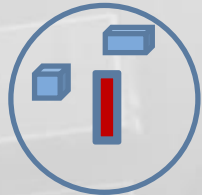
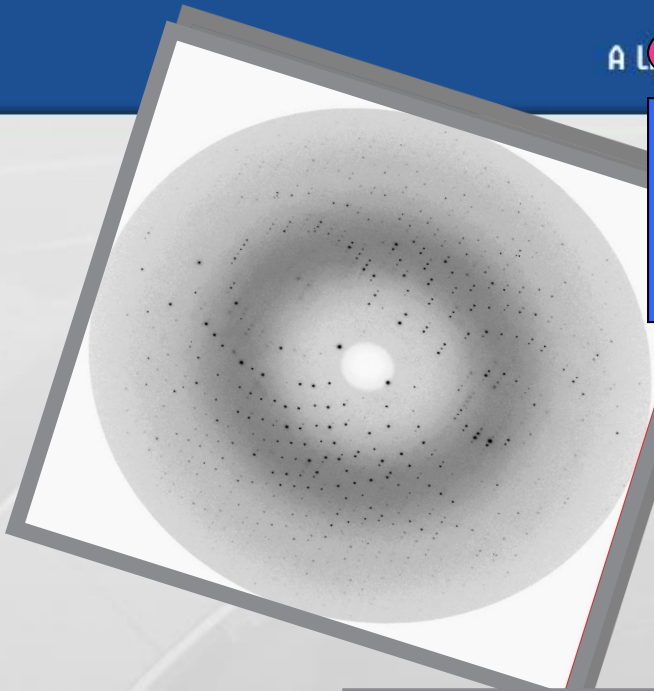
Svensson, O., Monaco, S., Popov, A., Nurizzo, D. and Bowler, M. W. (2015), The fully automatic characterization and data collection from crystals of biological macromolecules. *Acta Cryst.* **D71** 1757-1767

Detector

Data quality
Completeness, Resolution, Statistics

What the data is going to be used for?

Size
N. of pixels
T readout
Noise
Sensitivity
Dynamic range



Crystal(s?)

Space group
Cell parameters
Orientation
B-factor
Mosaicity
Anisotropy
Size
Number ?
Radiation damage

Crystal-to-detector distance
Resolution
 I_p/I_b
spot overlap

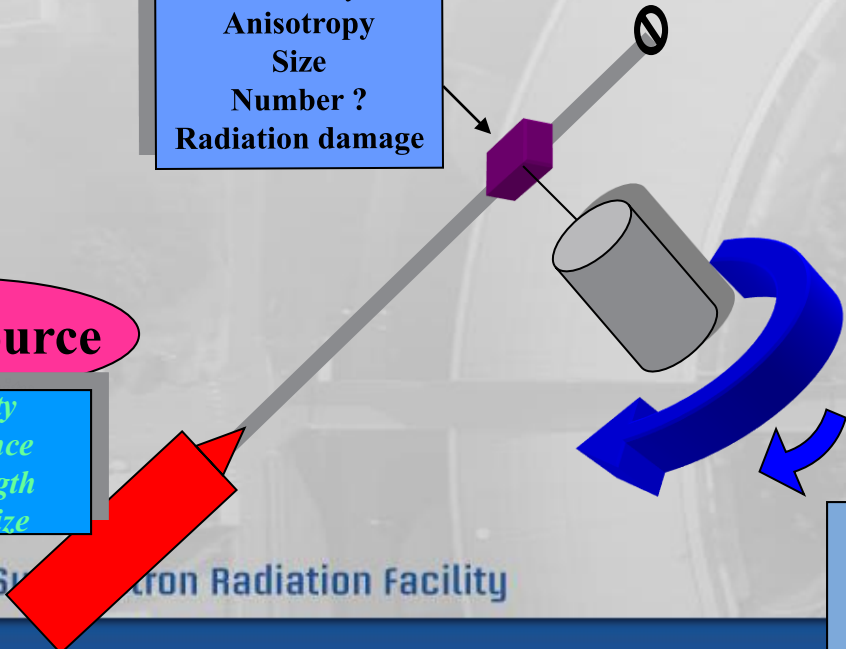
Starting angle and total rotation range
Completeness
Multiplicity
d.c. time

Rotation width
 I_p/I_b ,
spot overlap,
total d.c. time

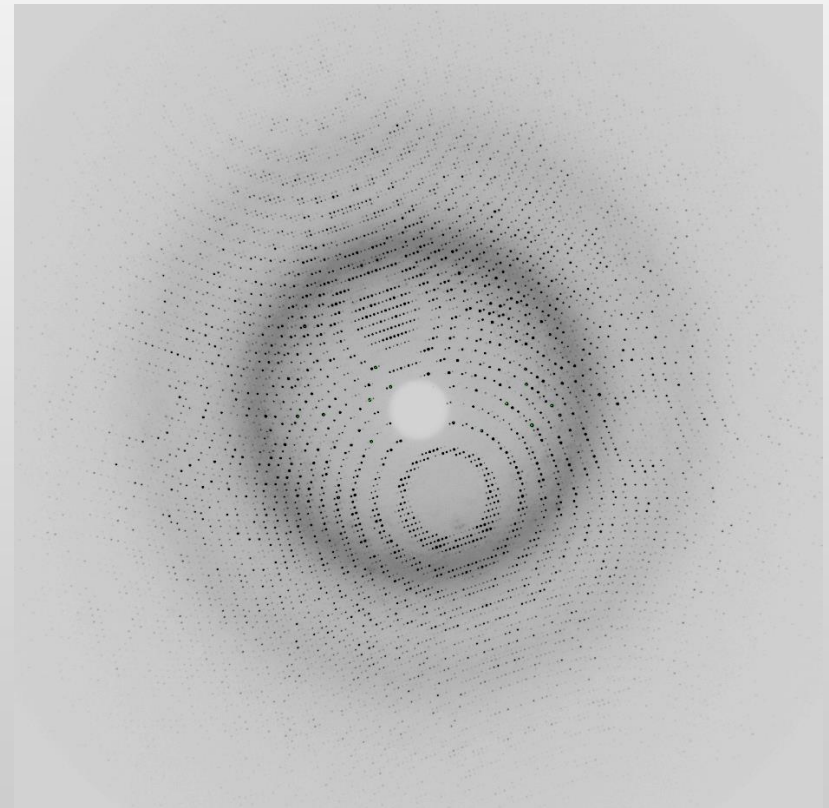
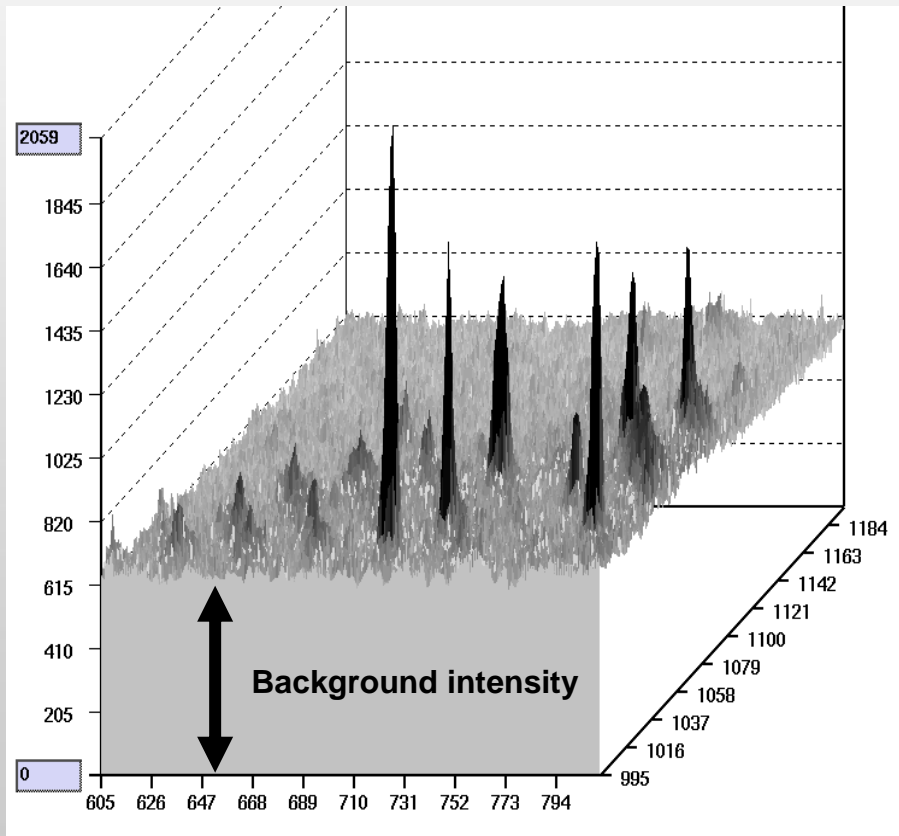
Exposure time
statistics
overloads
total d.c. time

X-ray source

Intensity
Divergence
Wavelength
Beam size

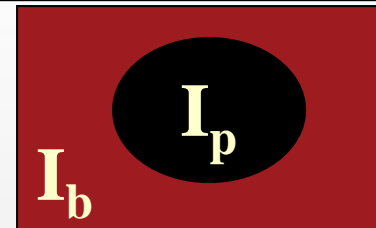


- Large cell parameters
- Weak diffraction intensity – light atoms
- Poor crystal quality – big B- factor
- Background intensity > diffraction intensity

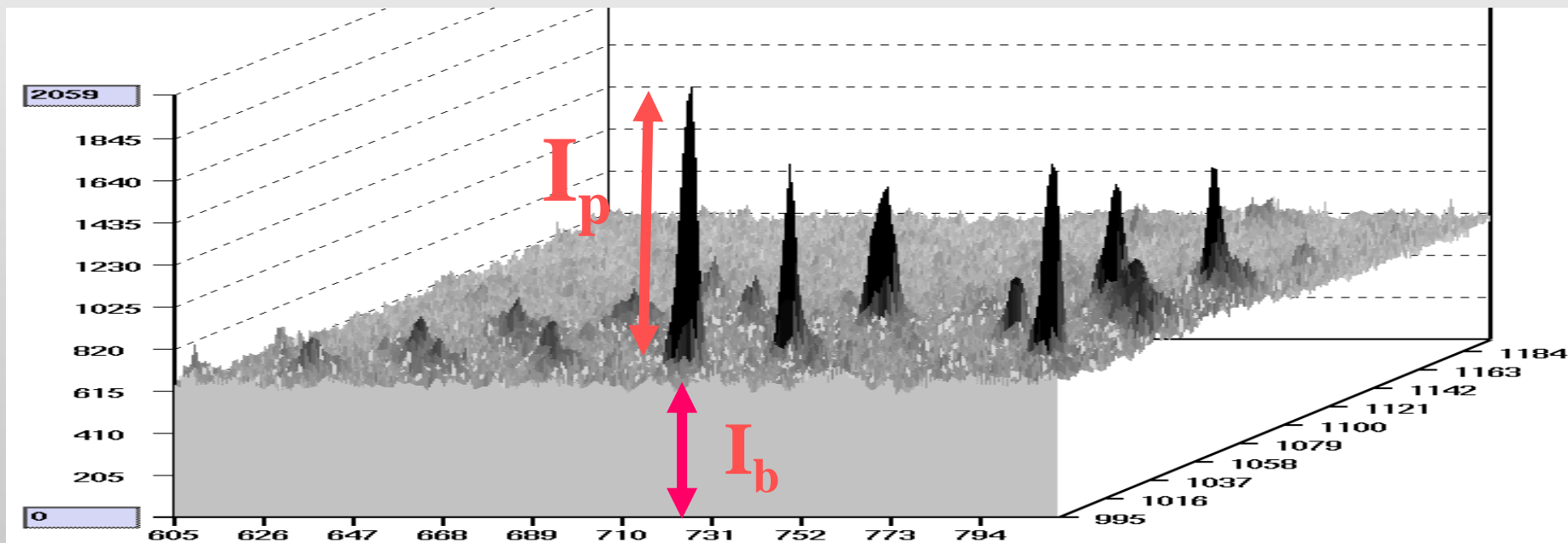


Main uncertainties of the observed intensities are determined by counting statistics

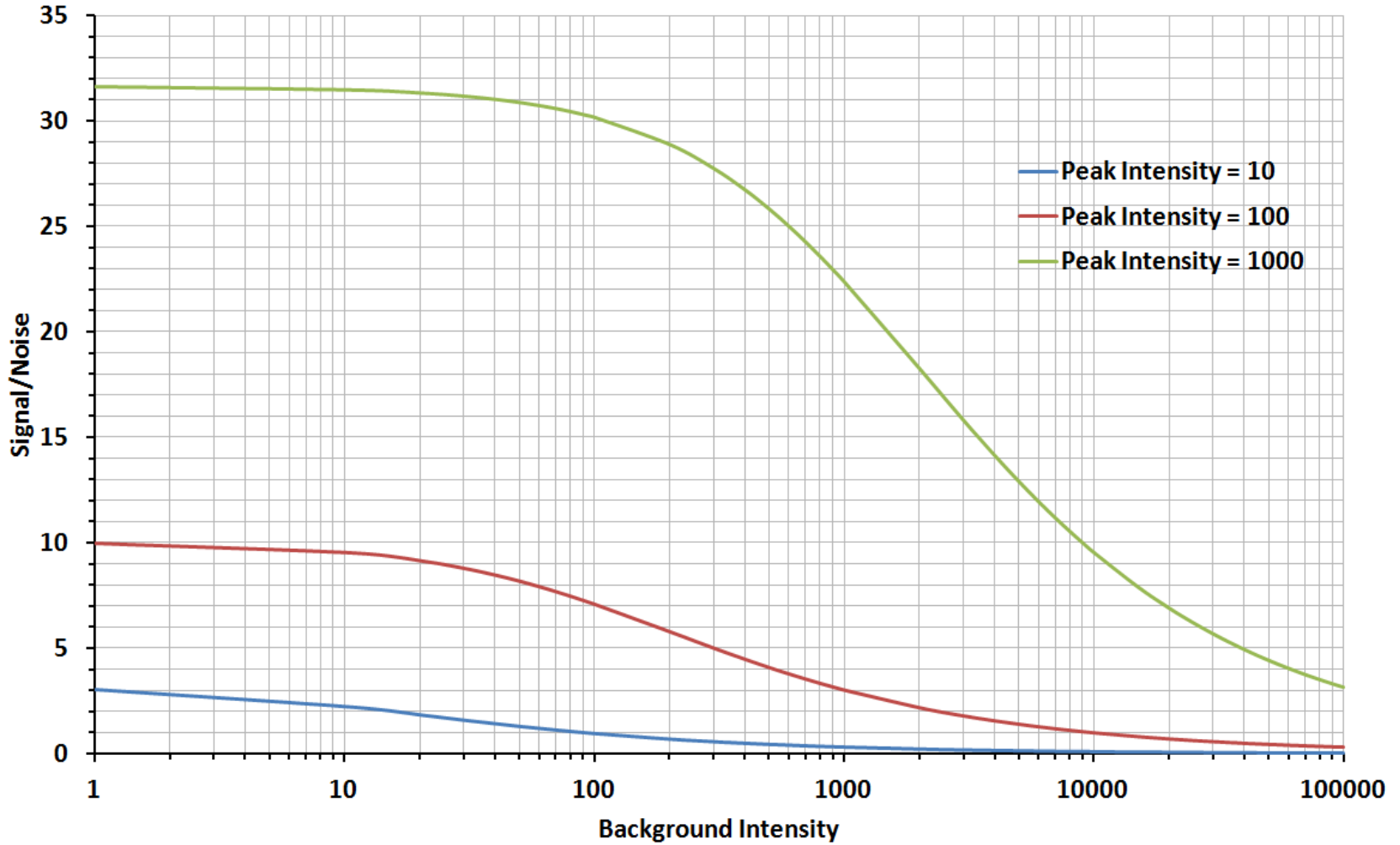
$$\sigma_{I_p}^2 = \left(I_p + I_b \cdot \frac{m \cdot (m + n)}{n} \right) \cdot G$$



where m and n are number of pixels in the peak and background region of the measurement box respectively. G is the detector gain, which converts pixel counts to equivalent X-ray photons. K_{ins} is a proportionality constant for the instrument-error term

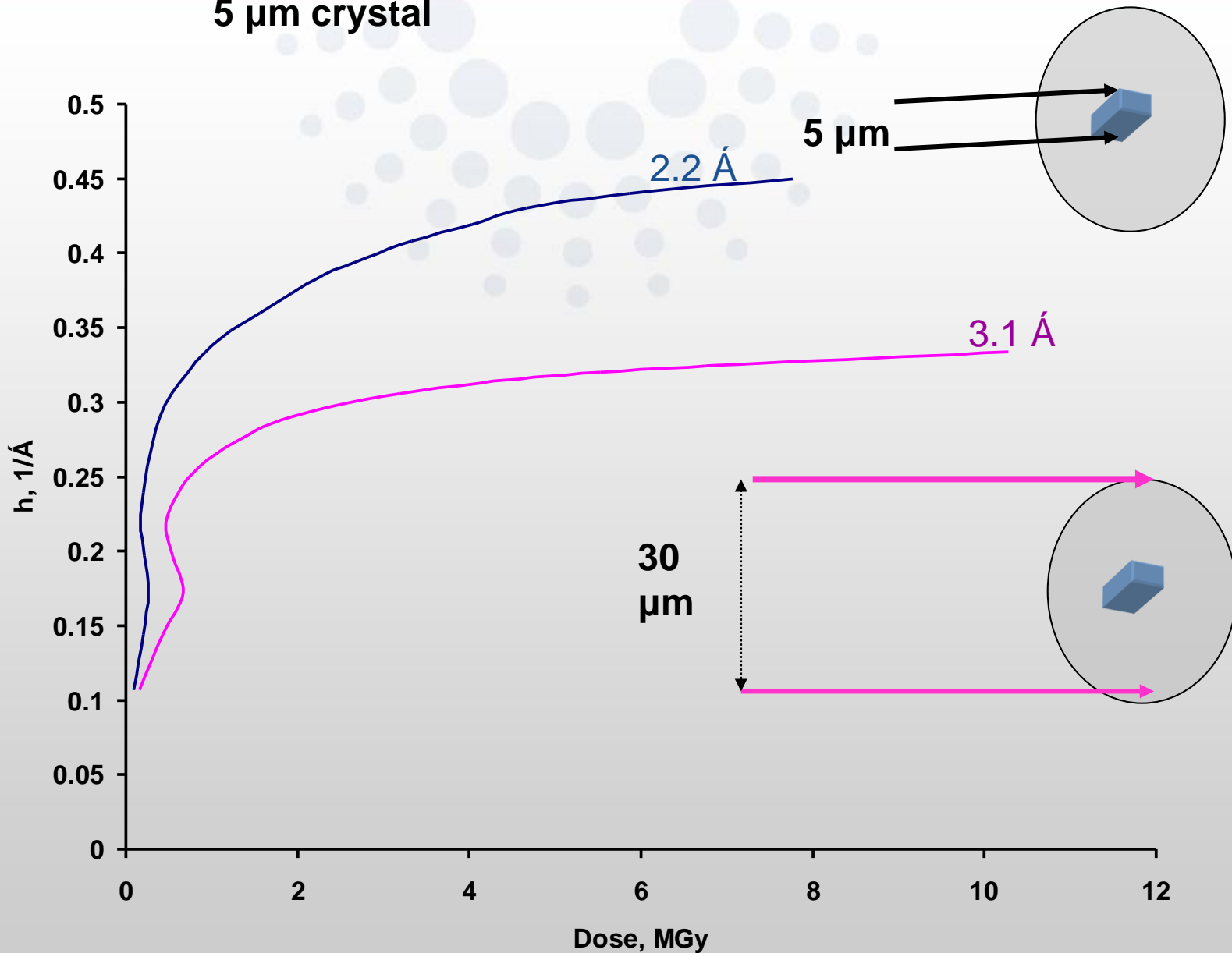


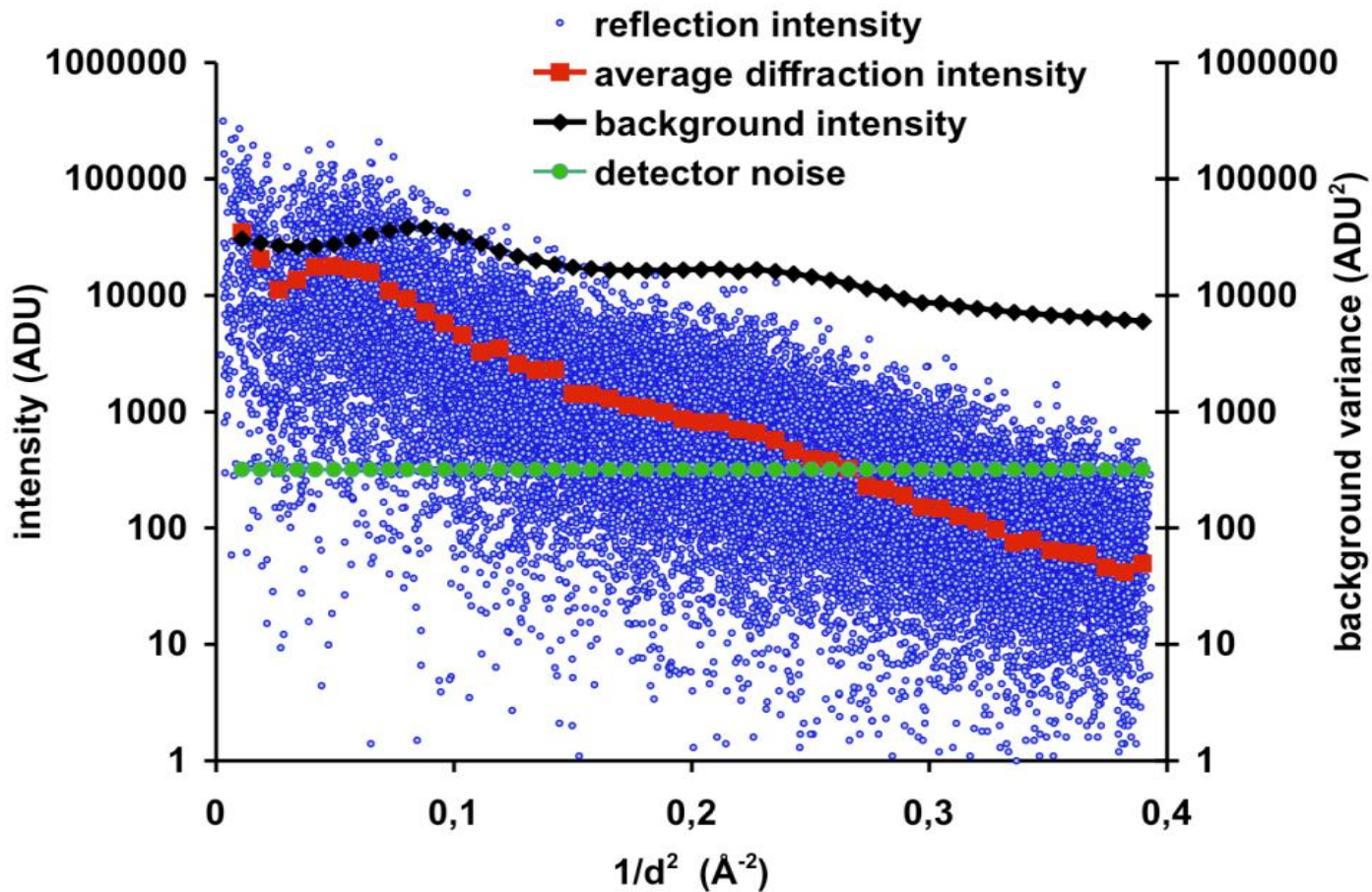
Signal/Noise vs. $I_{\text{background}}$



Diffraction resolution vs. absorbed dose

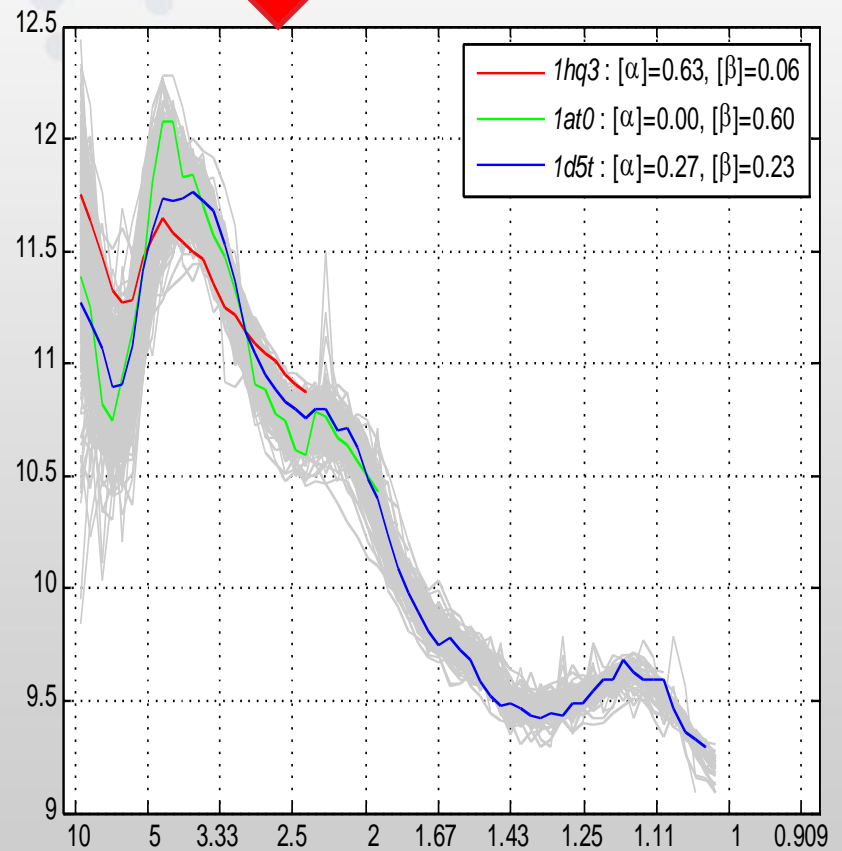
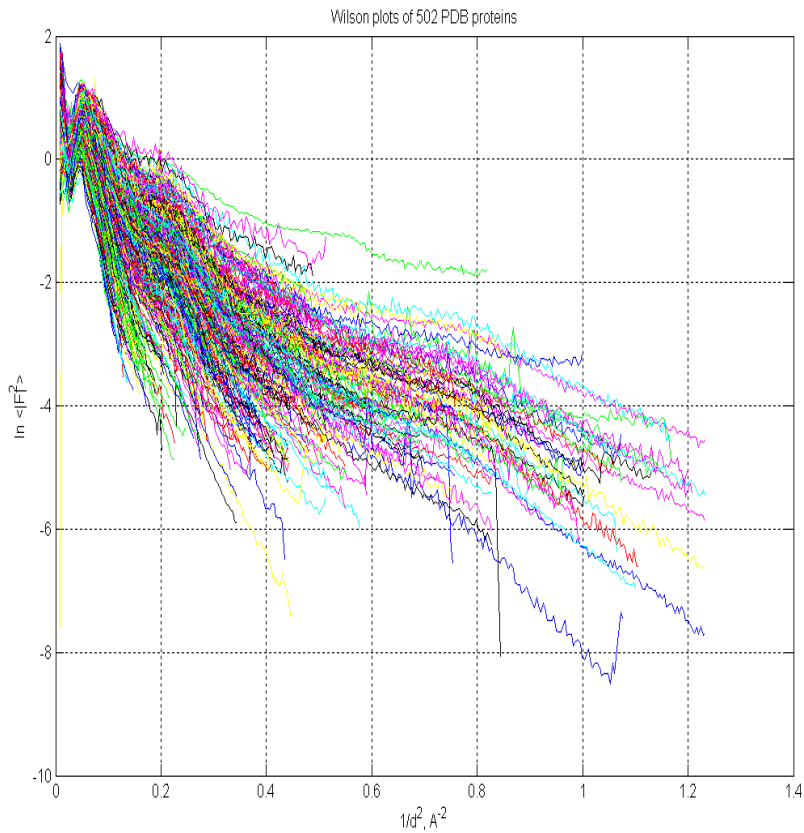
5 μm crystal

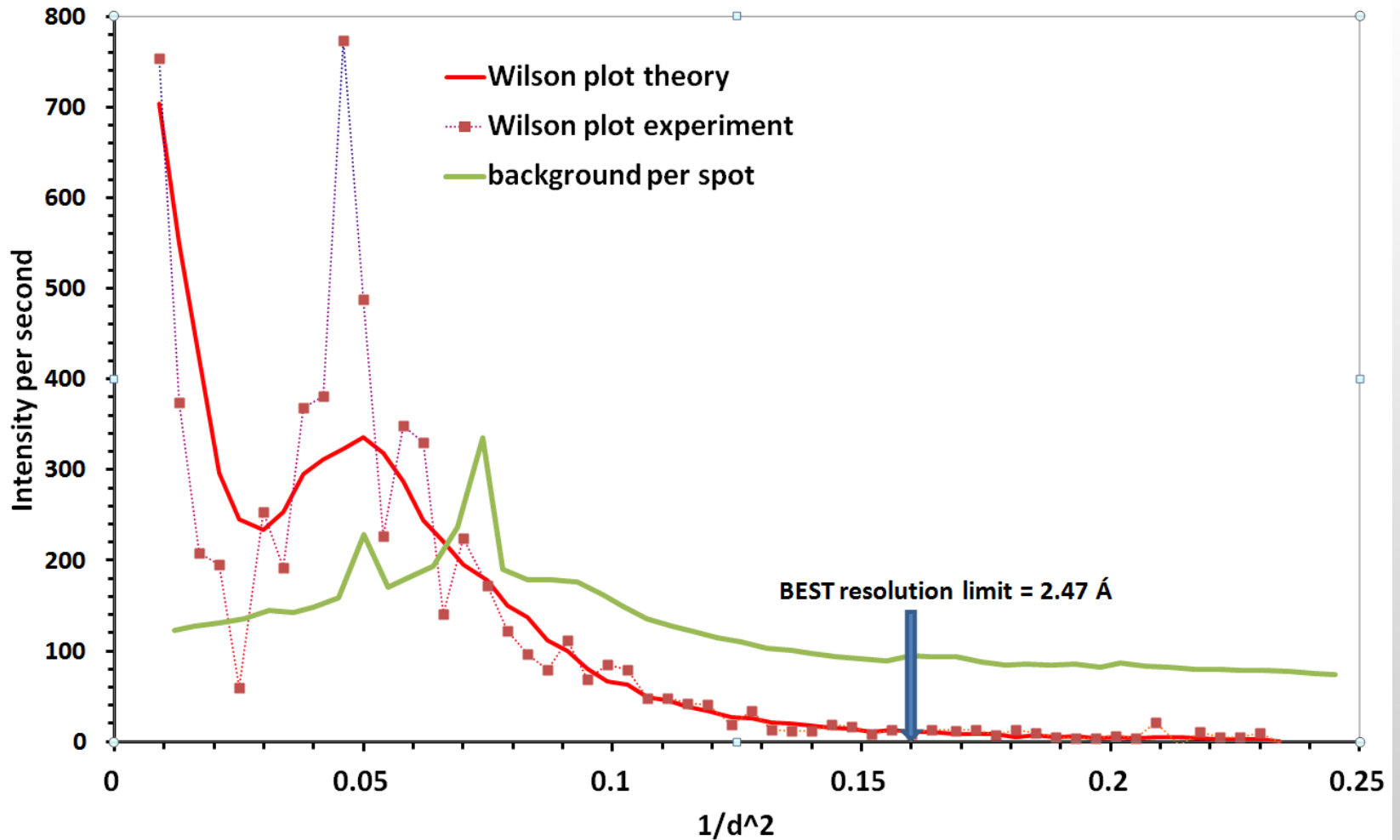


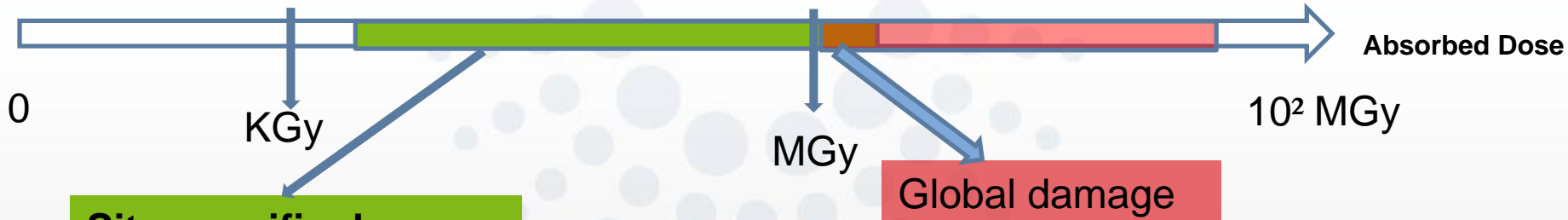
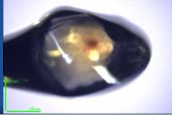


Wilson plot

$$\hat{J}(\mathbf{h}) \propto \hat{J}_u(h) \cdot \text{Exp}(-\mathbf{h} \cdot \mathbf{B} \cdot \mathbf{h}^T)$$





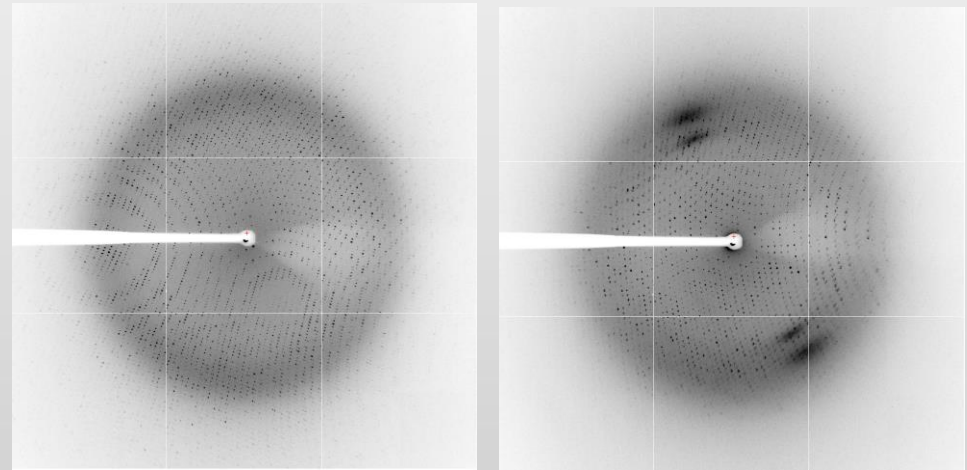
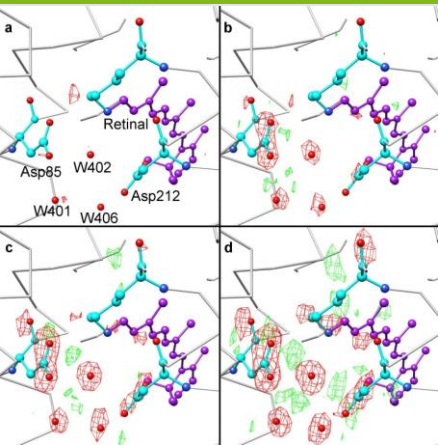


Site-specific damage

1. Dose of 0.3 MGy - X-ray radiation damage effects are not detectable even at atomic resolution.
2. Doses above 2 MGy lead to partial decarboxylation of the most sensitive residues
3. Doses above 6 MGy may lead to wrong interpretation of chemistry for some protein residues

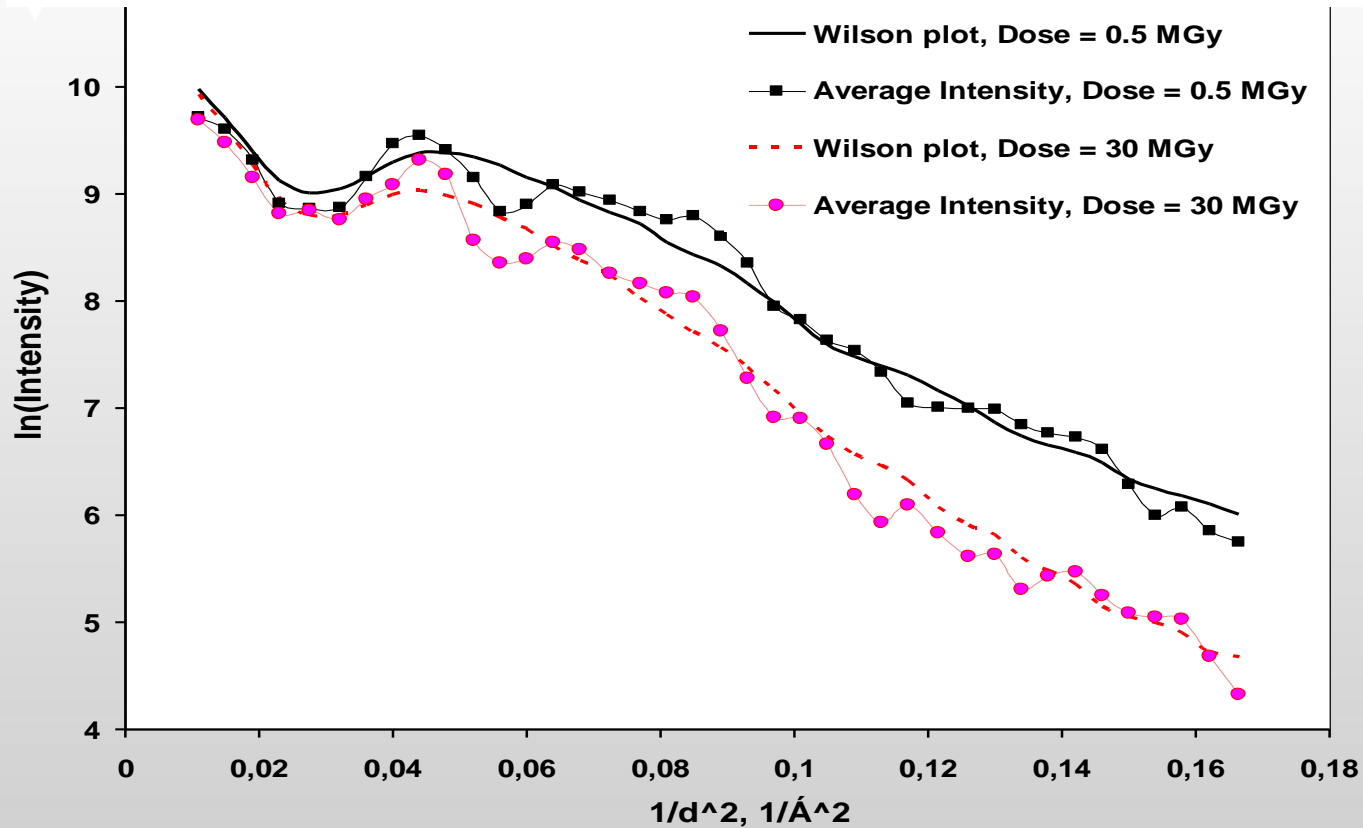
Global damage

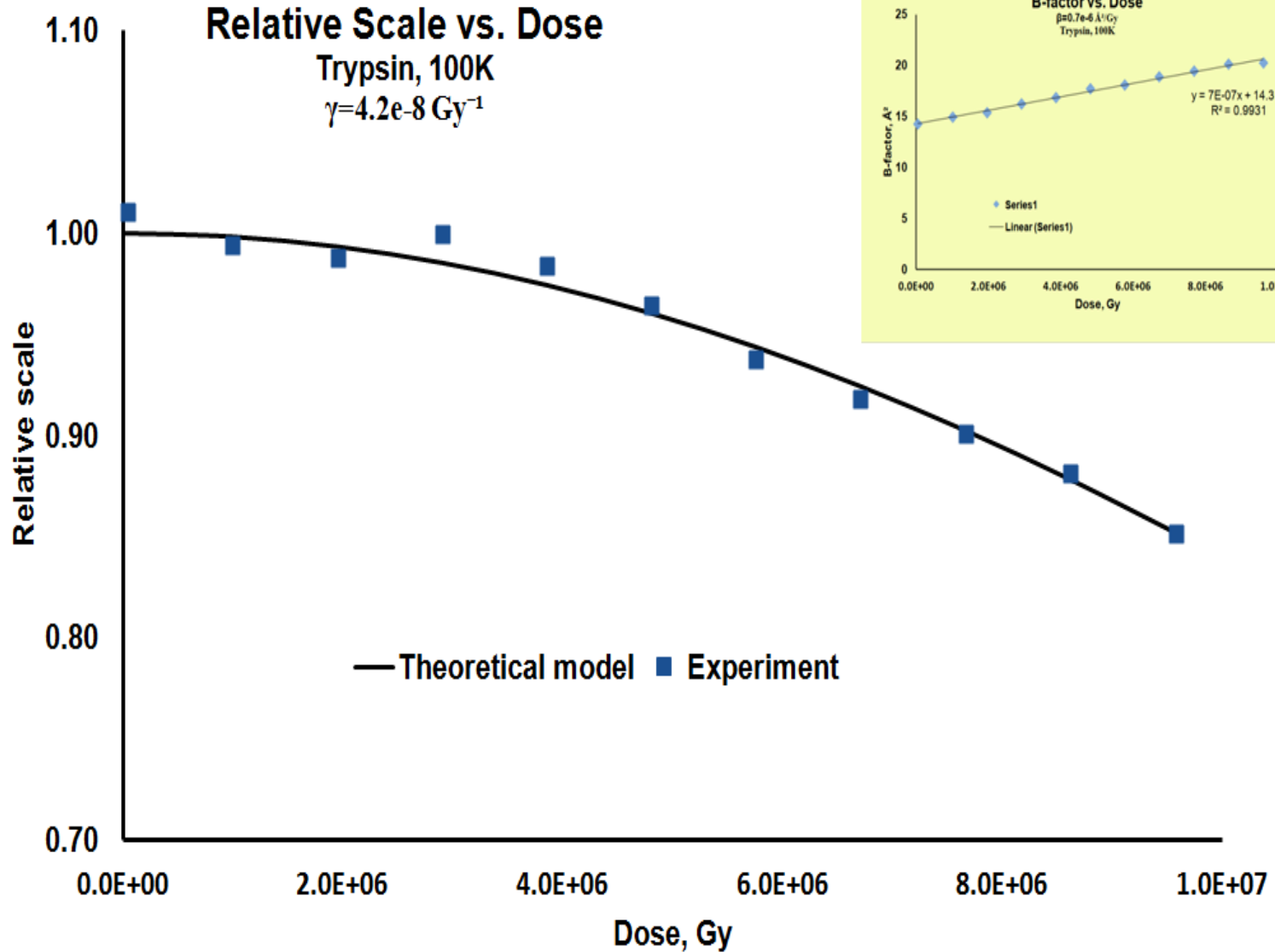
- Overall and q-dependent loss of diffraction peak intensity
- Non-specific non-isomorphism
- Changes in unit-cell parameters
- Increase in the mosaicity

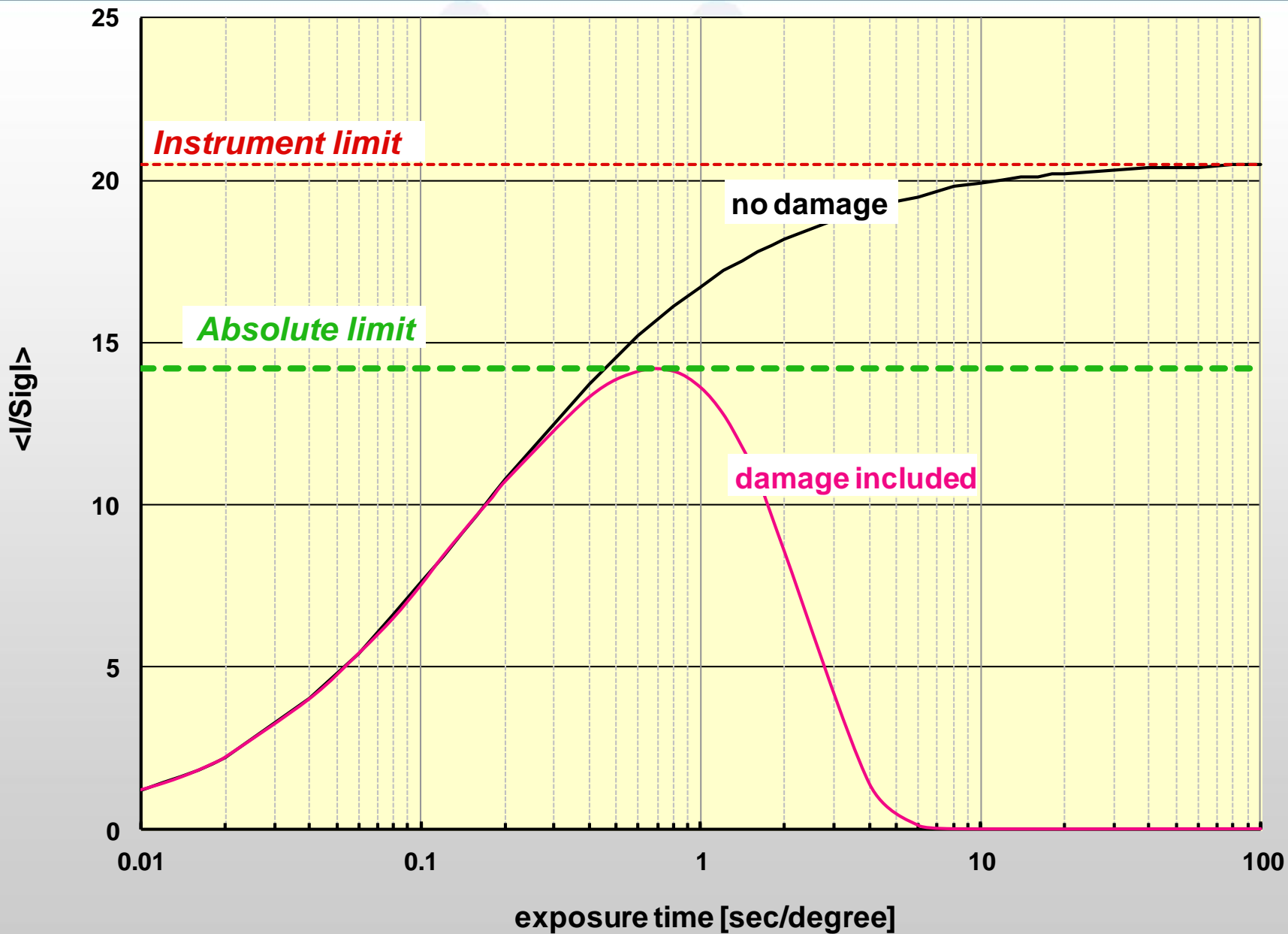


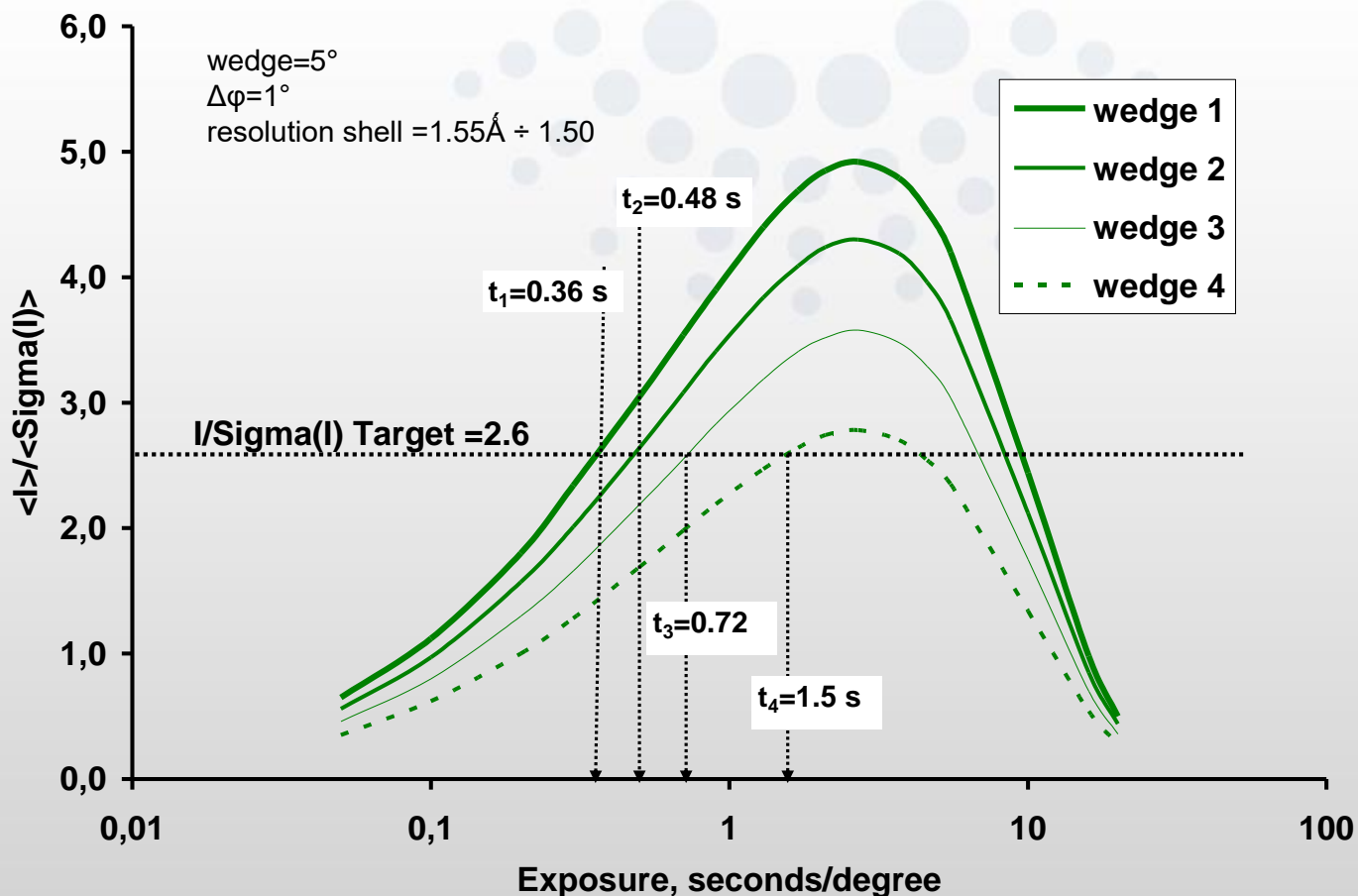
X-Ray-Radiation-Induced changes in Bacteriorhodopsin Structure
 Borshevskiy et al. 2011,
J.Mol.Biol. V.409,813-825

$$\hat{J}(h, D) \propto \text{scale}(D) \cdot \hat{J}_u(h) \cdot \text{Exp}(-B(D) \cdot h^2 / 2)$$









Graphical solution of the equation at resolution 1.5 Å and fixed rot. width for 5° sequential rotation wedges.

$$\frac{\hat{J}}{\hat{\sigma}_J}(t_{\text{exposure}}, D) = \frac{C}{\sqrt{M}} = \frac{4.0}{\sqrt{2.4}} = 2.58$$

Semi-empirical model for diffraction intensity vs reciprocal space coordinate

$$\hat{J}(\mathbf{h}) = \frac{1}{s} \cdot \hat{J}_u(h) \cdot \text{Exp}(-\mathbf{h} \cdot \mathbf{B} \cdot \mathbf{h}^T)$$

Semi-empirical model of variance vs integrated intensity

$$\sigma^2_i(\mathbf{J}) = k_0 + k_1 \mathbf{J} + k_2 \mathbf{J}^2$$

Integration over the scanned reciprocal space using Wilson distribution

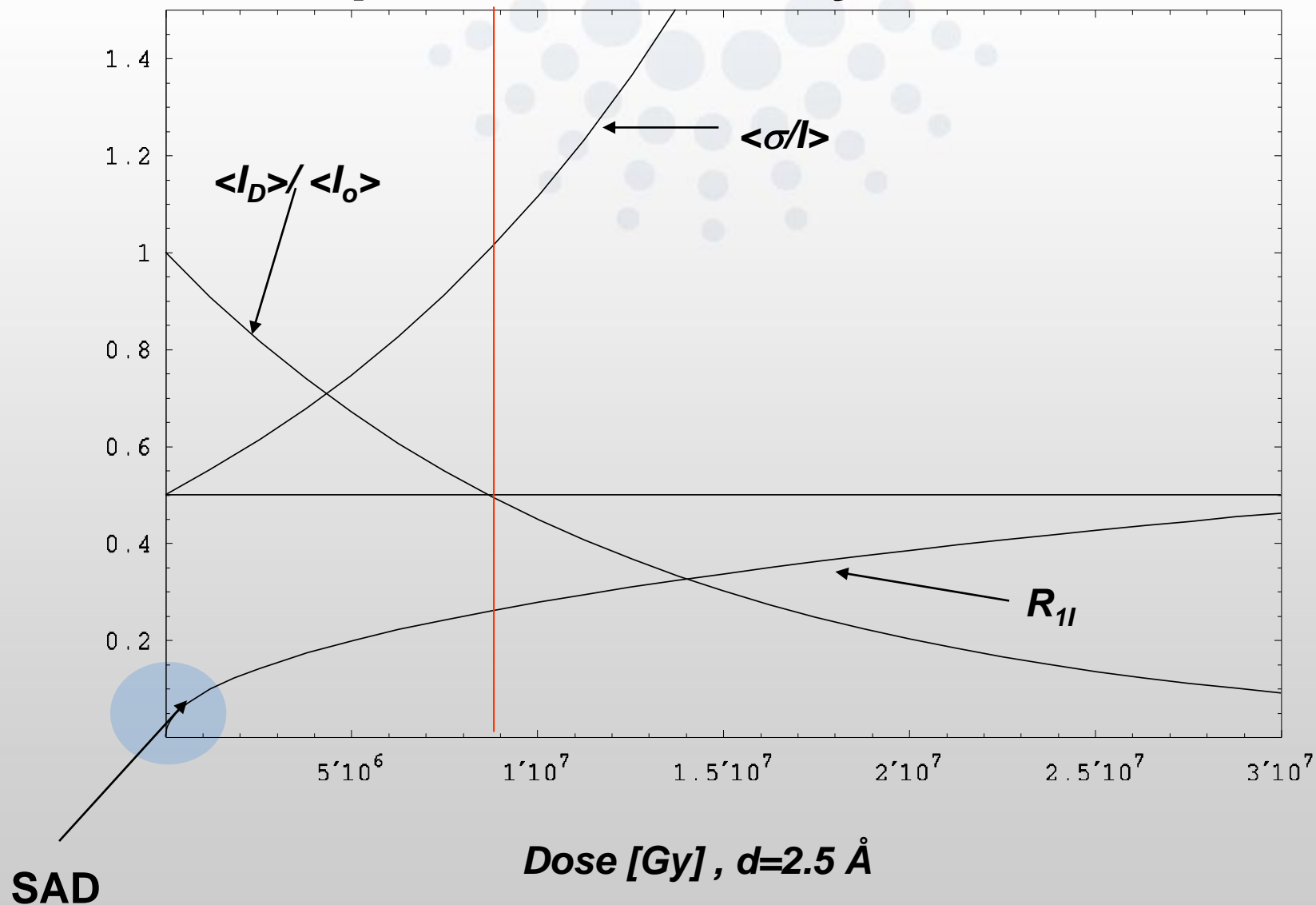
$$\hat{\sigma}_J(h, \varphi) = \frac{1}{2N} \sum_{i=1}^N \int_0^{\infty} \sqrt{k_{0i} + k_{1i} J + k_2 J^2} \left(p(J | \hat{J}(\mathbf{h}_{i1})) + p(J | \hat{J}(\mathbf{h}_{i2})) \right) dJ$$

Radiation-damage model

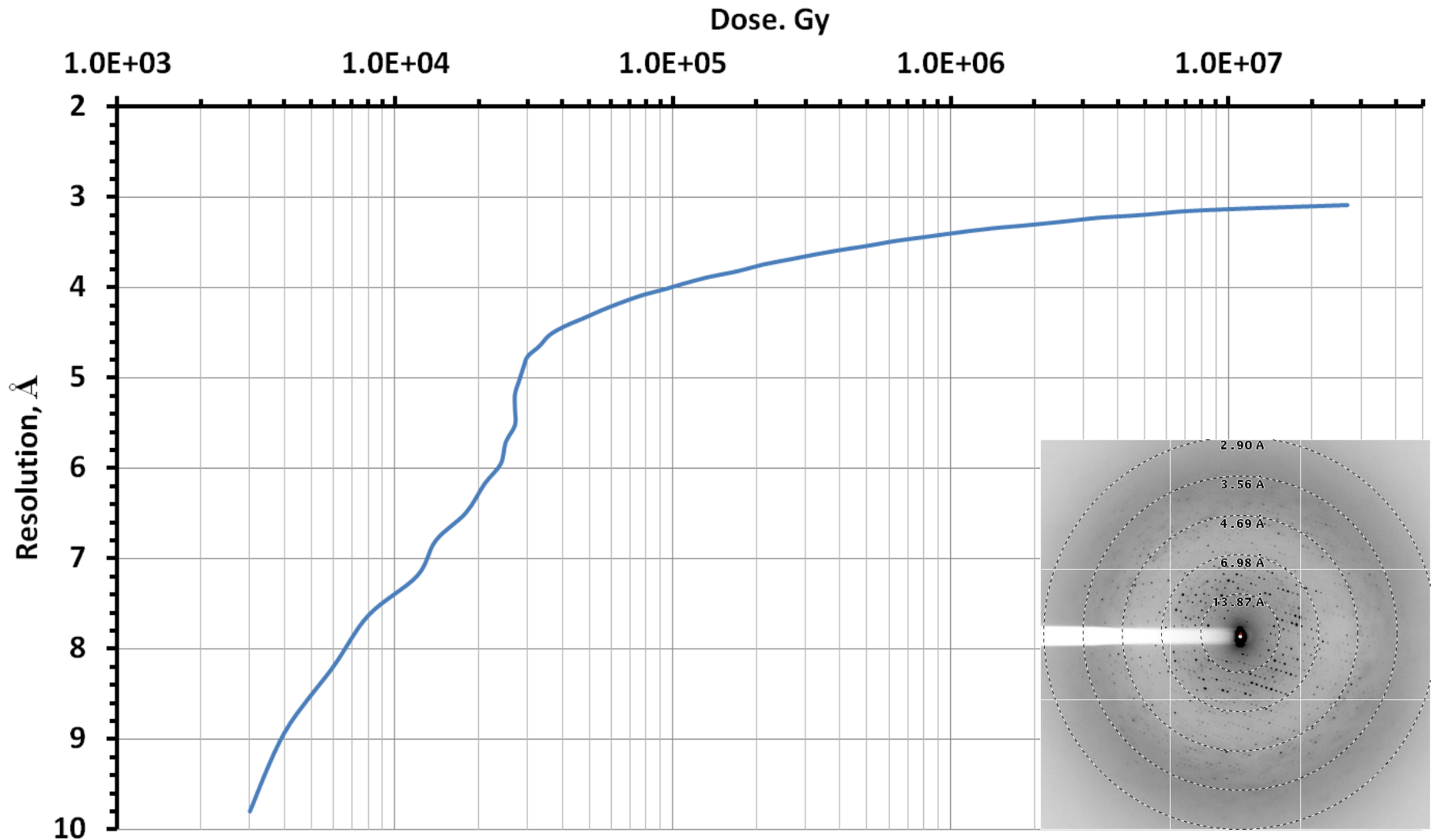
Resolution-dependent intensity decay:

$$\hat{J}(\mathbf{h}, D) = \hat{J}(\mathbf{h}, D = 0) \text{scale}(D) \exp(-B(D)h^2 / 2)$$

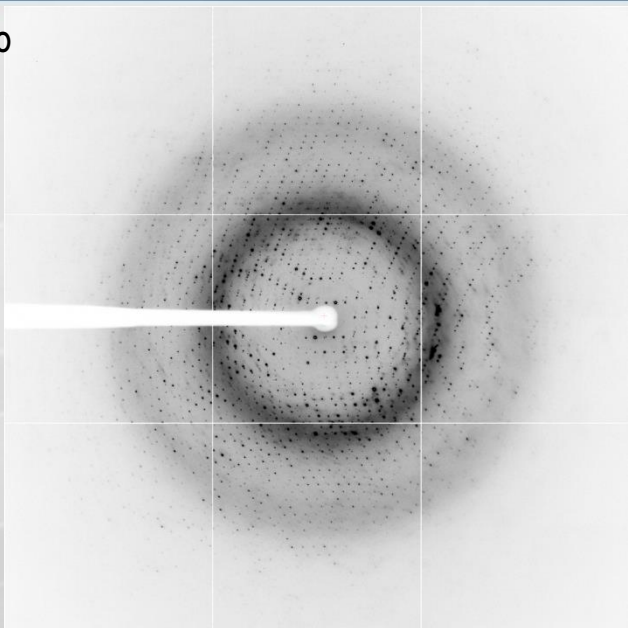
Expected Intensity Variation



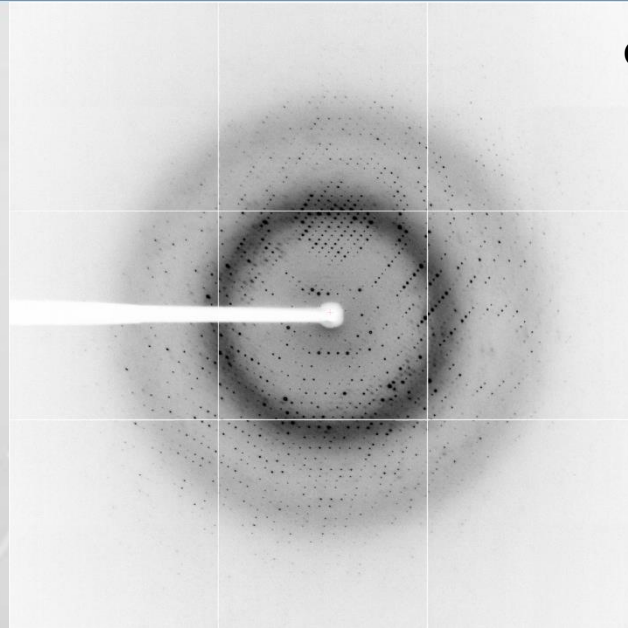
The 70 kDa membrane protein FtsH from
Aquifex aeolicus I222, $a = 137.9 \text{ \AA}$, $b = 162.1 \text{ \AA}$, $c = 170 \text{ \AA}$



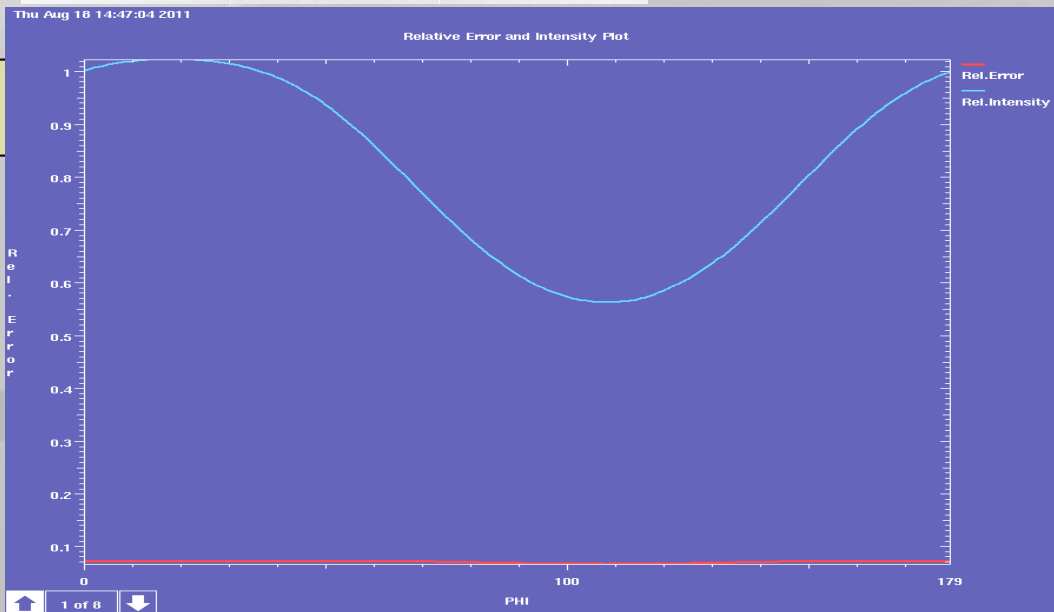
$\varphi=0^\circ$



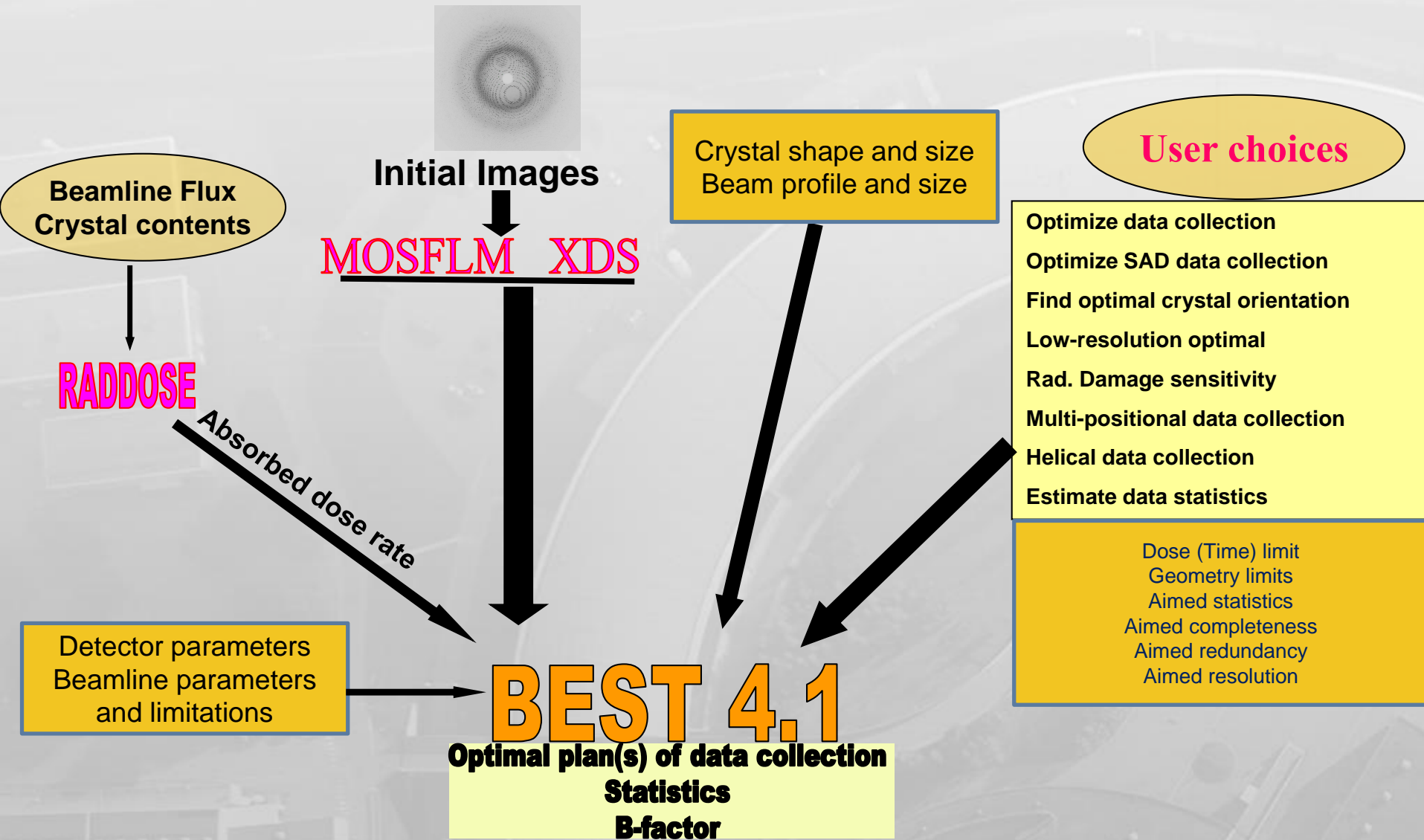
$\varphi=90^\circ$



Intensity vs. crystal position

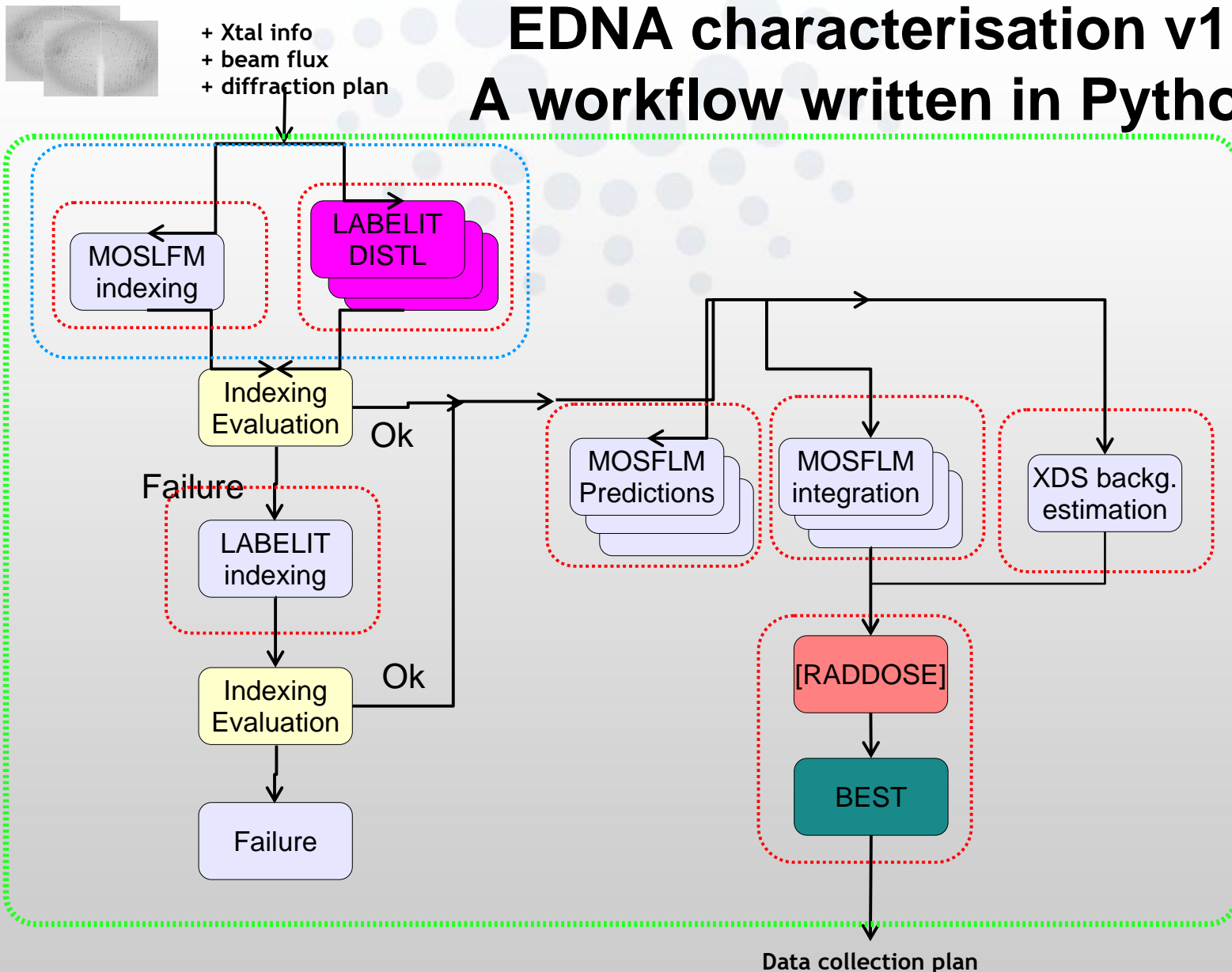


Data collection strategy accounting radiation damage



EDNA characterisation v1.3

A workflow written in Python



File Instrumentation Help

User: **opld-231 operator on ID23eh1** (operator on ID23eh1 ID23eh1 Dates: 2013-09-05 to 2013-09-06)

Hutch Collect Energy scan XRF spectrum EDNA Log

Time and date Prefix Run number

2013-03-07 00:	propdiol_7	1
2013-03-28 19:	x2	2
2013-03-07 00:	mi_4	2
2013-03-06 23:	black_x9	2
2013-04-01 17:	xtal16	3
2013-04-01 16:	xtal7	2
2013-03-28 21:	x1	1
2013-04-01 14:	xtal2	3
2013-03-07 00:	propdiol_9	1
2013-03-28 21:	x1	2
2013-03-28 18:	x5	1
2013-04-01 15:	xtal2	5
2013-03-06 23:	mi_2	1
2013-04-01 15:	xtal5	5
2013-03-07 00:	mi_5	1
2013-03-28 18:	x6	1
2013-04-01 17:	xtal13	1
2013-04-01 15:	xtal4	1
2013-04-01 18:	xtal2	1
2013-04-01 17:	xtal14	5
2013-04-01 17:	xtal14	1
2013-04-01 17:	xtal16	1
2013-03-28 21:	x5	1
2013-03-06 23:	black_x3	3
2013-04-01 17:	xtal14	6
2013-03-28 20:	x4	1
2013-04-01 17:	xtal15	1
2013-03-06 23:	cf042a_x2	2
2013-03-06 21:	black_x3	1
2013-04-01 16:	xtal8	2
2013-04-01 19:	xtal10	2
2013-03-28 18:	x4	1
2013-03-06 21:	black_x9	1
2013-04-01 17:	xtal13	2
2013-03-06 21:	blue_x4	1
2013-03-28 15:	ins	1
2013-03-06 22:	cd468a_x5	1
2013-03-06 22:	cd468a_x2	1
2013-04-01 14:	xtal2	2
2013-04-01 18:	xtal7	1
2013-03-06 21:	blue_x3	1

Clear history

Back Forward

Data collection info

Data collection date	2013/Mar/06 21:26:18.859
Image prefix	ref-black_x9_1
Directory	/data/id23eh1/inhouse/opld231/20130306/RAW_DATA/daniele/j/black/x9

Diffraction Plan

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)
None	False	Default (optimized)	Default (>= 0.99)	3.00	Default (highest possible)

Collection plan strategy ([RADDOSSE log file](#) , [BEST log file](#))

Resolution limit is set by the radiation damage								
Wedge	Subwedge	Start (°)	Width (°)	No Images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	90.00	0.15	480	0.32	2.68	100.00	564.25

Wilson plot (factor = 0.5, 3.0)

Measured vs theoretical multiplicity

Measured vs theoretical I/sigma

Relative decay rate vs time (2012 - 2013)

Indexing summary: Selected spacegroup: P3

Refined unit cell parameters (Å/degrees)					
a (Å)	b (Å)	c (Å)	alpha (°)	beta (°)	gamma (°)
133.844	133.844	38.022	90.000	90.000	120.000

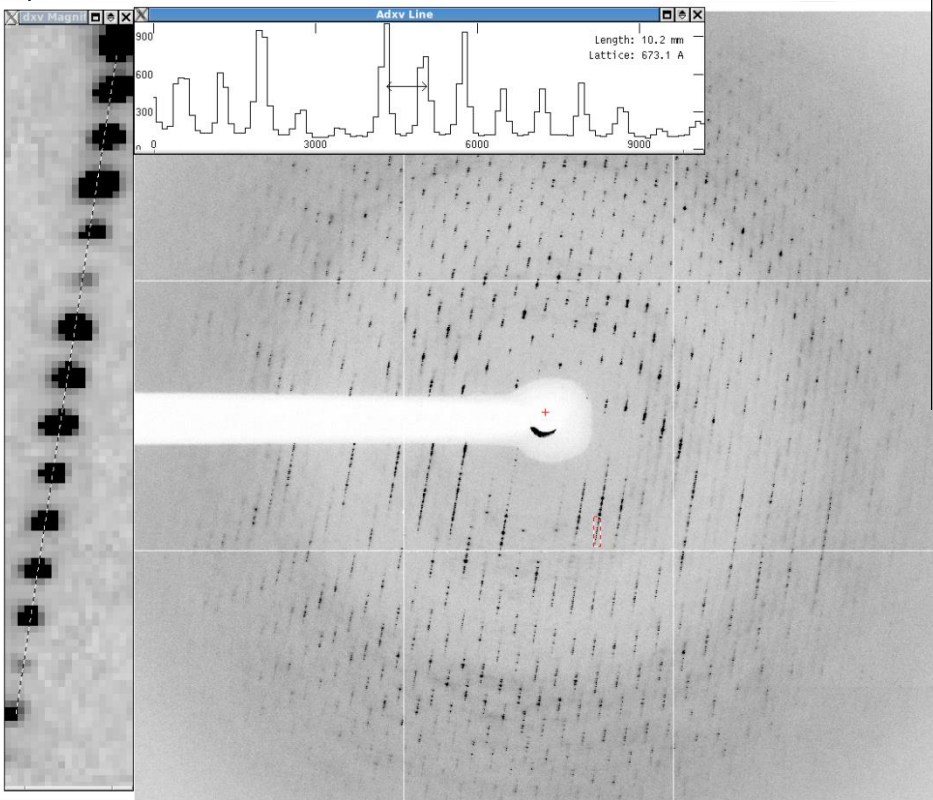
[Indexing log file](#)

ref-black_x9_1_0002.cbf

ref-black_x9_1_0001.cbf

[Integration log file 1](#)
[Integration log file 2](#)

Crystal
 Space Group : P 4
 Cell : 141.55 141.55 671.01 90.00 90.00 90.00
 Mosaicity : 0.17 degree

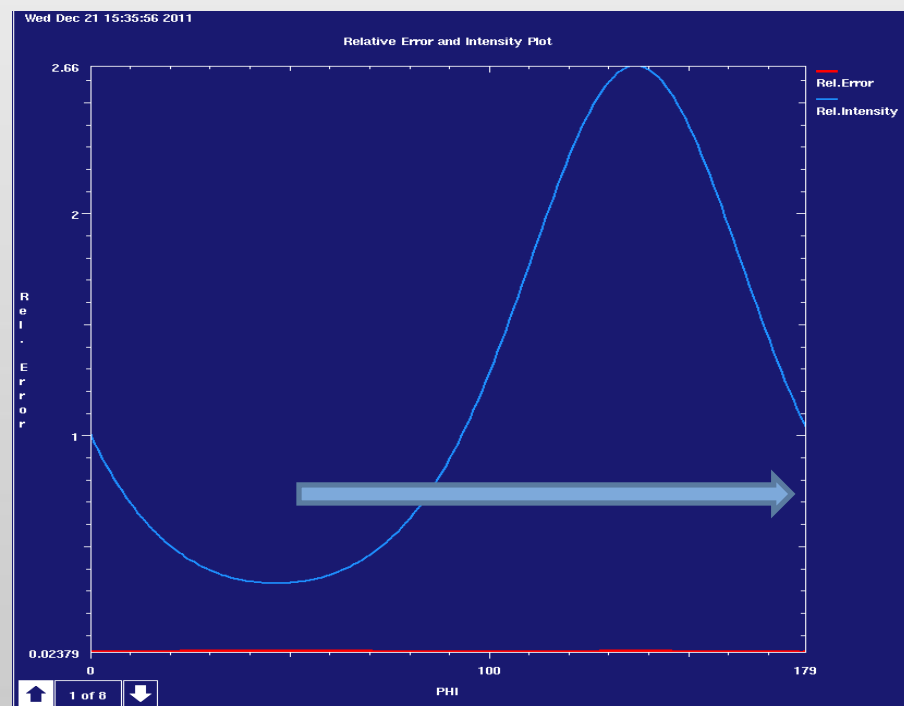


Main Wedge
 =====
 Resolution limit is set by the radiation damage
 Resolution limit = 3.59 Angstrom Transmission = 40.6% Distance = 562.2mm

WEDGE PARAMETERS						INFORMATION					
sub-We- dge	Phi- start degree	Rot. width degree	Exposure /image s	N.of ima- ges	Over- lap width degree	Exposure /sWedge s	Exposure total s	Dose /sWedge MGy	Dose total MGy	Comple- teness %	
1	53.00	0.10	0.169	100	No	10.00	16.9	16.9	8.711	8.711	32.9
2	63.00	0.10	0.156	300	Yes	30.00	46.9	63.8	24.156	32.867	76.0
3	93.00	0.10	0.100	150	No	15.00	15.0	78.8	7.729	40.596	90.2
4	108.00	0.50	0.437	140	No	70.00	61.2	140.0	31.530	72.126	100.0

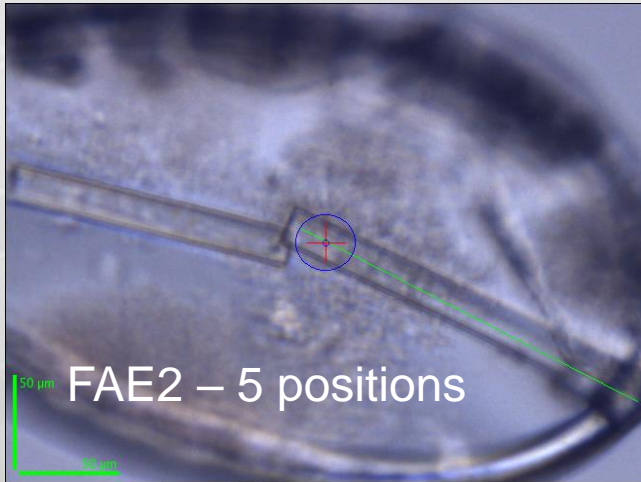
Phi_start - Phi_finish : 53.00 - 178.00
 Total rotation range : 125.00 degree
 Total N.of images : 690
 Overall Completeness : 100.0%
 Redundancy : 5.46
 R-factor (outer shell) : 13.3% (63.2%)
 I/Sigma (outer shell) : 17.3 (3.4)
 Total Exposure time : 140.0 sec (0.039 hour)
 Total Data Collection time : 1948.2 sec (0.541 hour)

Scaling
 Relative scale : 31.44
 Overall B-factor : 82.17 Angstrom^2
 B-factor eigenvalues : 51.11 118.04 118.04 Angstrom^2
 Scaling error : 3% at the resolution limit

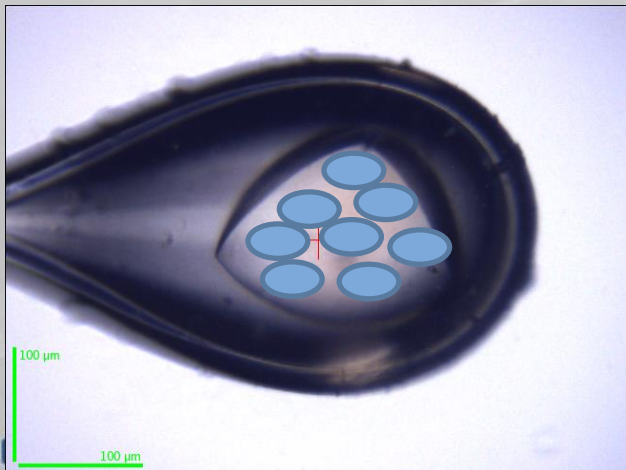


FAE crystals ID23-1

E=12.75Kev, I=35 mA, Aperture=0.03 mm
Flux=1.5x10¹¹ Photon/sec



The 70 kDa membrane protein FtsH from
Aquifex aeolicus I222, a = 137.9, b = 162.1, c = 170

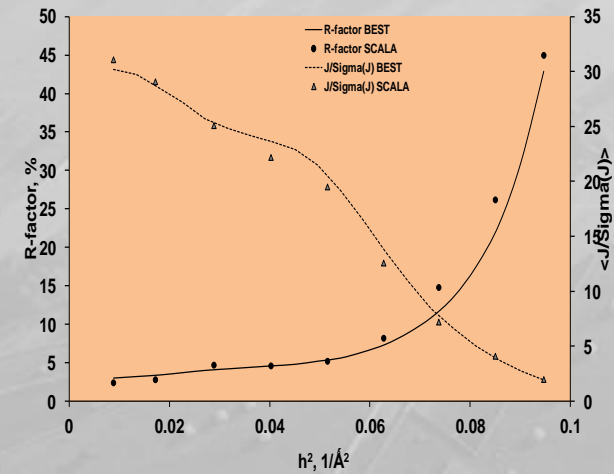
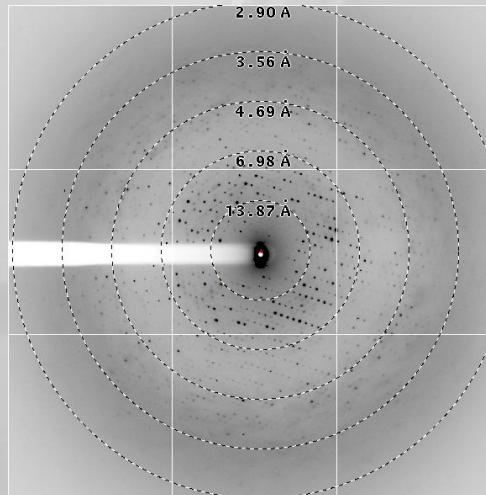


Multi-positions data collection

Resolution limit is set by the radiation damage
Resolution limit = 1.73 Angstrom Transmission = 100.0% Distance = 244.6mm

WEDGE PARAMETERS					INFORMATION						
sub-We- dge	Phi start degree	Rot. width degree	Exposure /image s	N.of ima- ges	Over- lap	sWedge width degree	Exposure /sWedge s	Exposure total s	Dose /sWedge MGy	Dose total MGy	Comple- teness %
1	0.00	0.25	1.338	80	No	20.00	107.0	107.0	4.067	4.067	51.9
1	20.00	0.25	1.338	80	No	20.00	107.0	107.0	4.067	4.067	85.6
1	40.00	0.25	1.338	80	No	20.00	107.0	107.0	4.067	4.067	75.2
1	60.00	0.25	1.338	80	No	20.00	107.0	107.0	4.067	4.067	88.1

Phi_start - Phi_finish	: 0.00 - 80.00
Total rotation range	: 80.00 degree
Total N.of images	: 320
Overall Completeness	: 98.6%
Redundancy	: 3.18
R-factor (outer shell)	: 5.6% (36.8%)
I/Sigma (outer shell)	: 22.9 (3.3)
Total Exposure time	: 428.1 sec (0.119 hour)
Total Data Collection time	: 1228.1 sec (0.341 hour)



..... SAD data collection.....

-asad, strategy for SAD data collection, resolution selected automatically, rot.interval=360 dg.

-SAD {no|yes|graph}, strategy for SAD data collection if "yes", "graph" - estimation of resolution for SAD

Minimum of RFriedel = $\langle |E_2+w| \rangle - \langle |E_2-w| \rangle$ is a target noise only, no anomalous scattering itself:
 decay, non-isomorphism
 exact pair-wise dose differences for Bijvoet mates

Resolution	RFriedel (%)	I/Sigma	Redundancy
10.12	0.8	74.1	23.7
6.90	0.8	43.6	23.7
5.34	1.1	48.4	23.0
4.51	1.2	47.5	23.5
3.98	1.6	34.5	20.6
3.60	2.5	22.4	13.9
3.31	4.0	14.0	11.9
3.08	6.6	8.3	7.0
2.89	10.5	5.2	6.1
2.73	15.6	3.7	2.5
2.60	23.0	2.4	3.8

http://skuld.bmsc.washington.edu/cgi-bin/MAD_power.pl

Estimate of signal from MAD experiment

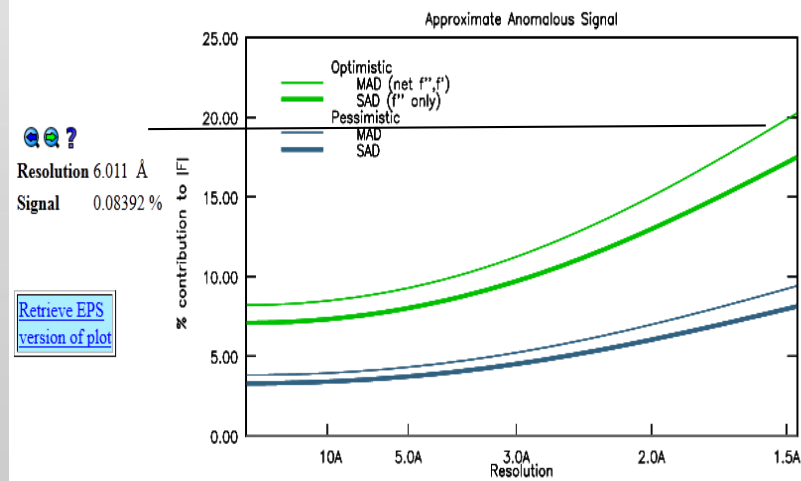
8 Se atoms per 300 protein residues and 0 nucleic acid residues

Se scattering factor estimates:

$$\min f' = -9 \quad \max f' = -2 \quad \max f'' = 6$$

Pessimistic scenario:

60% of anomalous scatterers ordered; 60% of optimal f' and f'' achieved



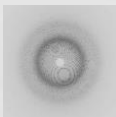
Induced Burn Strategy

Beamline Flux
Crystal contents
Crystal sizes

RADDOSE

Absorbed dose rate

Initial Images



MOSFLM XDS

BEST

Plan of data collection

11 cycles for testing
10 cycles for burning

User

Rad. Damage sensitivity

- Minimal RD inside the testing cycles
- Must induce significant changes in Intensity
- The intensity measurements remain statistically significant up to the last cycle of data collection

Measurements

XDS auto

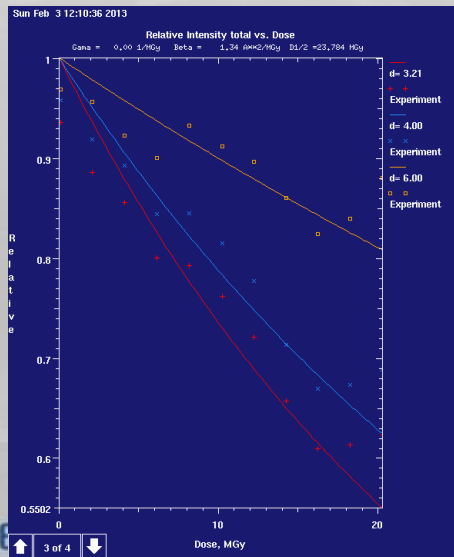
RDFIT

Program RDFIT /A.Popov & G.Bourenkov/
Version 1.1.0// 16.11.2012
Copyright 2012 by Alexander Popov and Gleb Bourenkov

PROJECT: BEST plan

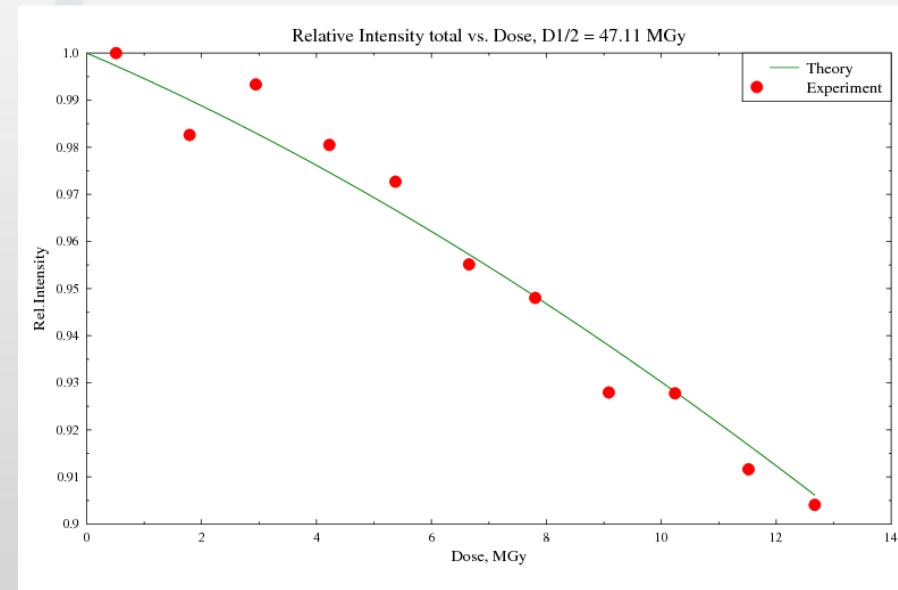
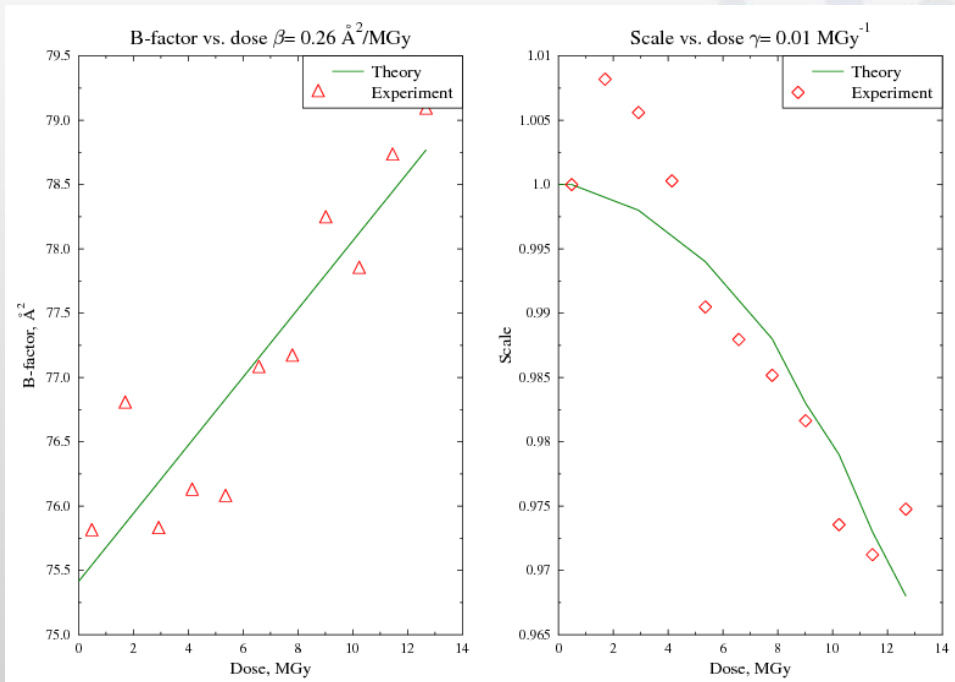
Wedge	dose MGy	max Resol. Angstr.	B-factor Angstr**2	Scale	del_Volum cell, %
0	0.0000	2.07	24.69	1669.62	
1	0.0081	2.07	24.24	1536.05	0.000
2	0.0246	2.07	25.48	1625.30	-0.061
3	0.0411	2.07	26.76	1669.59	0.008
4	0.0576	2.07	26.82	1879.64	-0.026
5	0.0741	2.07	27.49	2038.74	0.018
6	0.0906	2.11	27.36	2207.69	0.059
7	0.1071	2.11	27.90	2346.92	0.044
8	0.1236	2.07	28.22	2466.71	0.071
9	0.1401	2.11	28.18	2665.51	0.121
10	0.1566	2.58	30.37	2618.73	0.133
11	0.1731	2.58	30.33	2691.93	0.084

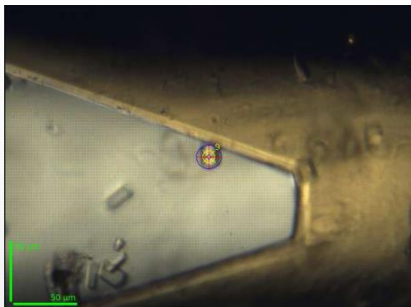
beta = 31.65 A**2/MGy gama = 4.29 1/MGy
Dose 1/2_th = 0.157 MGy Dose 1/2 = 0.163 MGy
Relative Radiation Sensitivity = 59.12



ation Facility

Example results from "burning strategy"

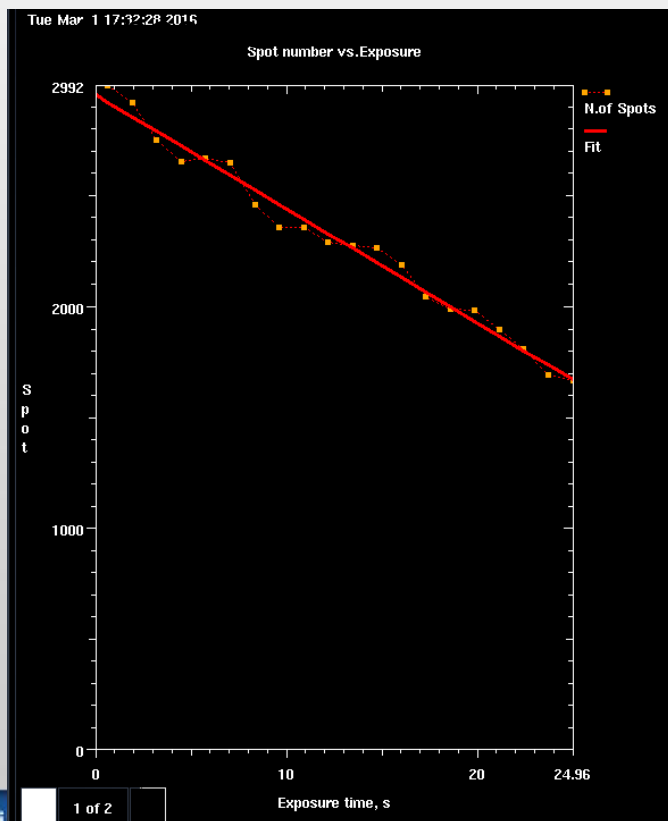




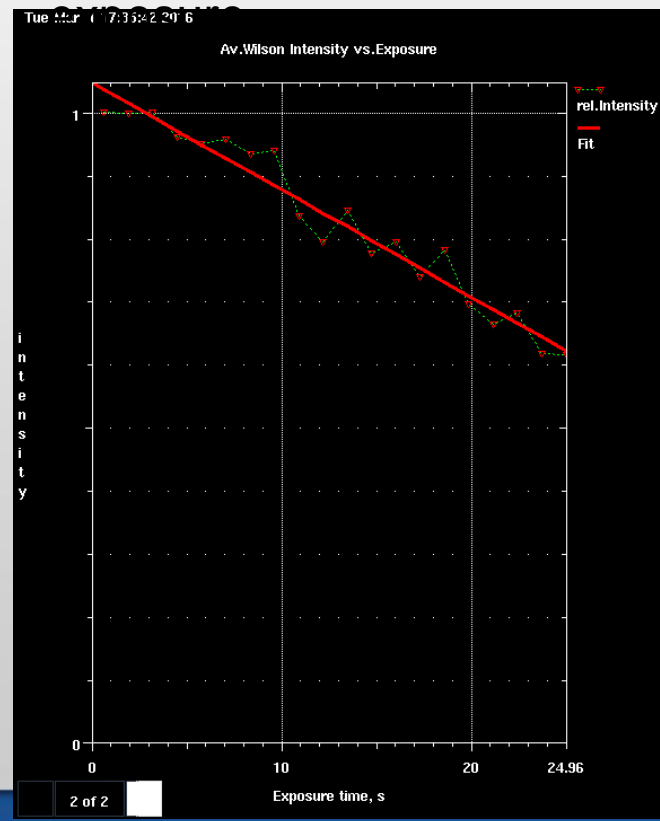
One cycle
10 images, total rotation 2°



Spot number vs.

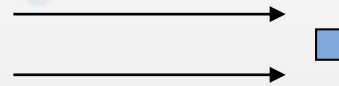


Average intensity vs.



$$\sigma (I_{\text{peak}}) = \text{SQRT} (I_{\text{peak}} + I_{\text{background}})$$

$$I_{\text{peak}} / \sigma(I_{\text{peak}}) = n$$

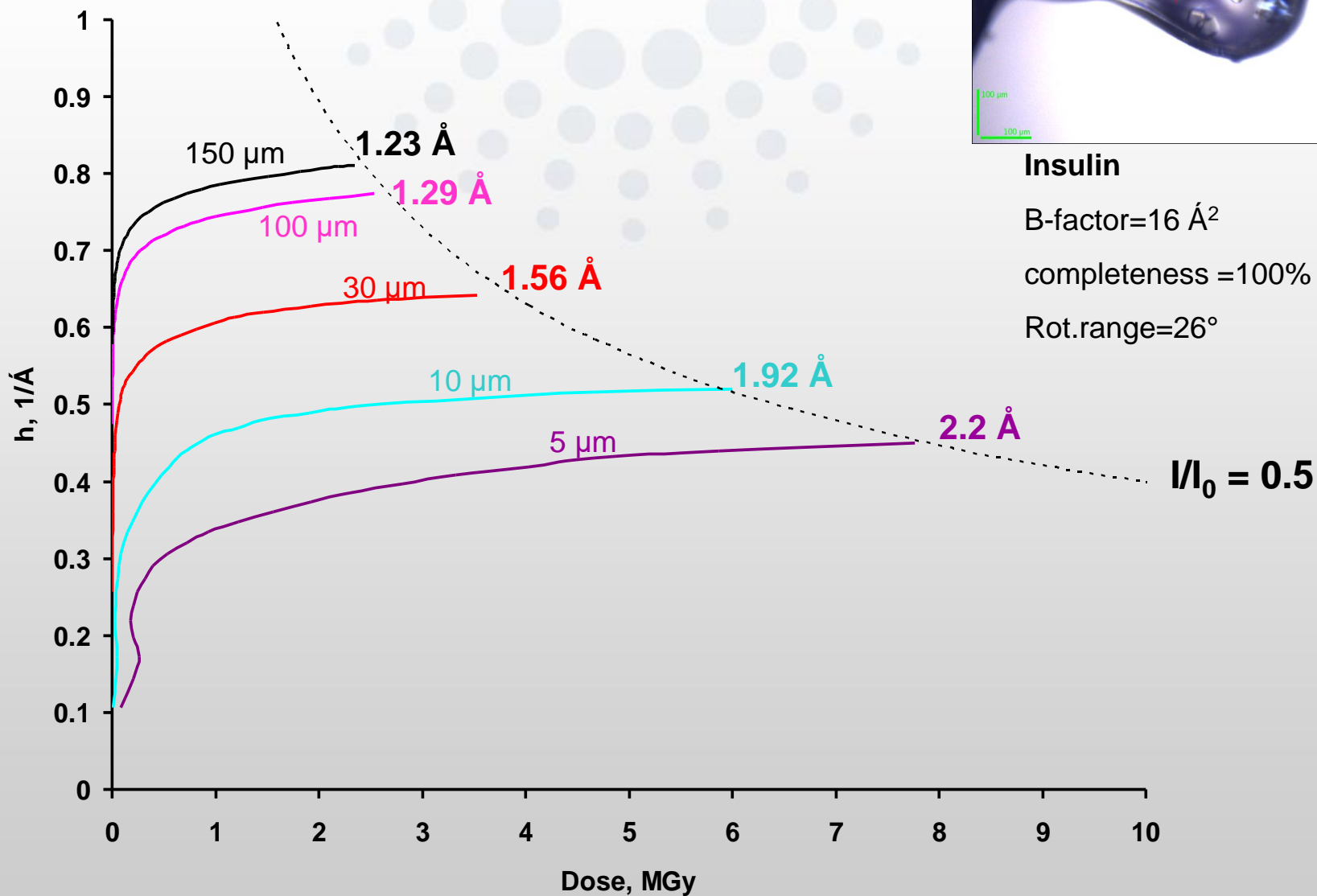


$$I_{\text{peak}} / \sigma(I_{\text{peak}}) = n * \text{Sqrt}(k)$$



Diffraction resolution vs. absorbed dose

for different crystal size



Insulin

B-factor = 16 Å^2

completeness = 100%

Rot. range = 26°

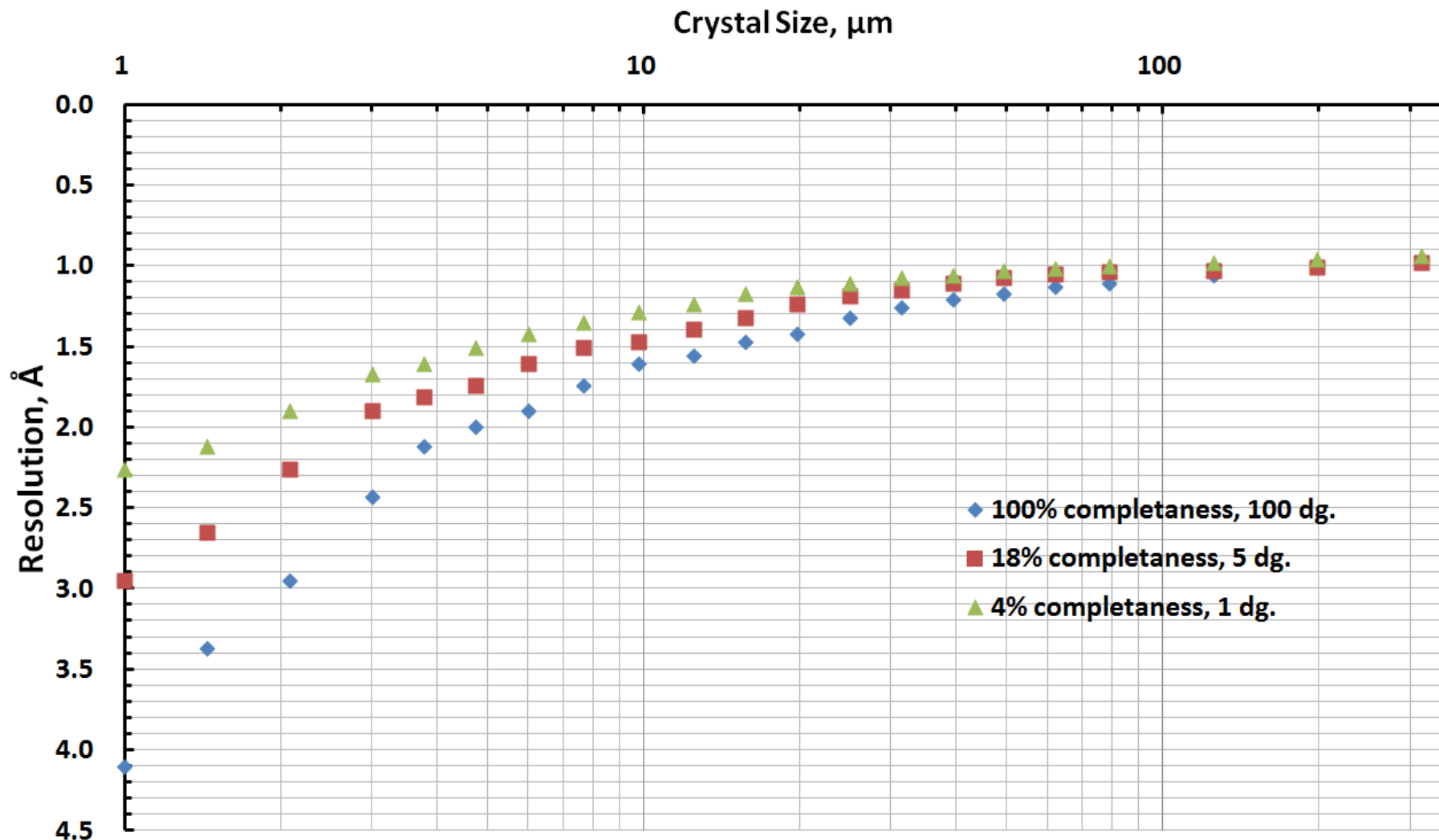
$I/I_0 = 0.5$

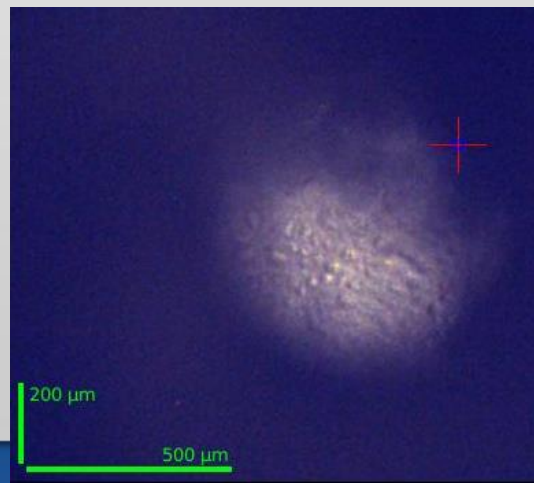
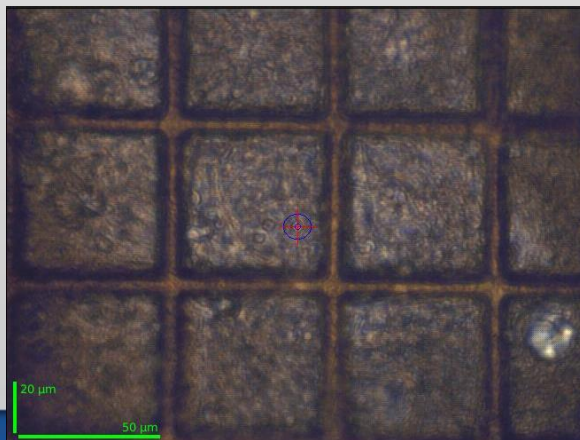
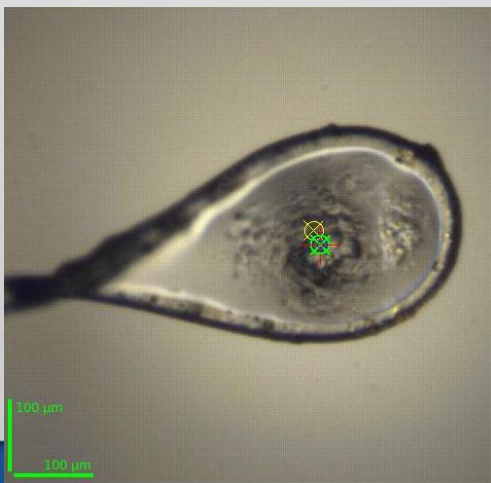
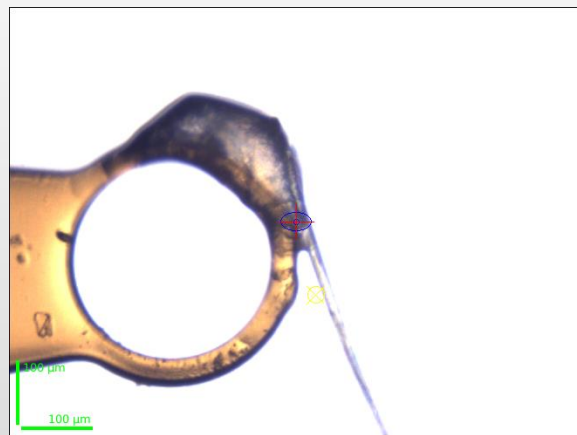
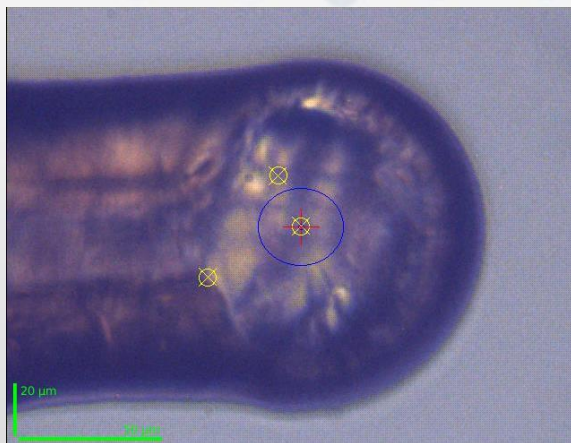
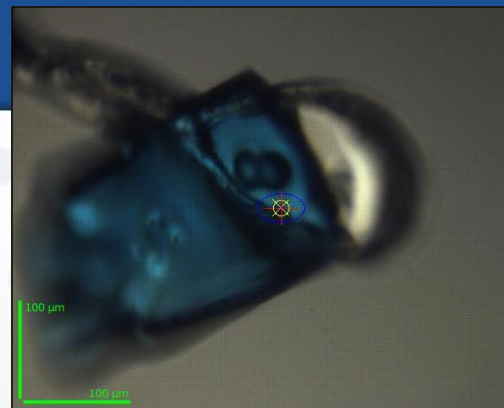
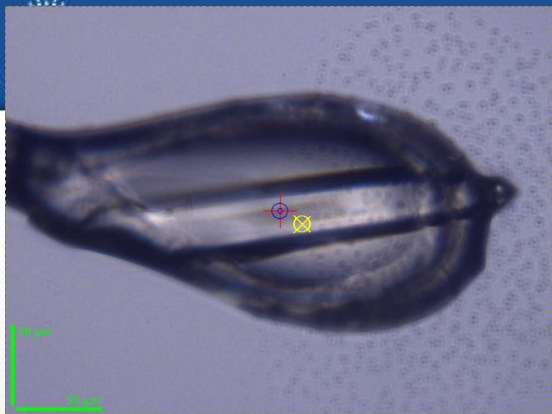


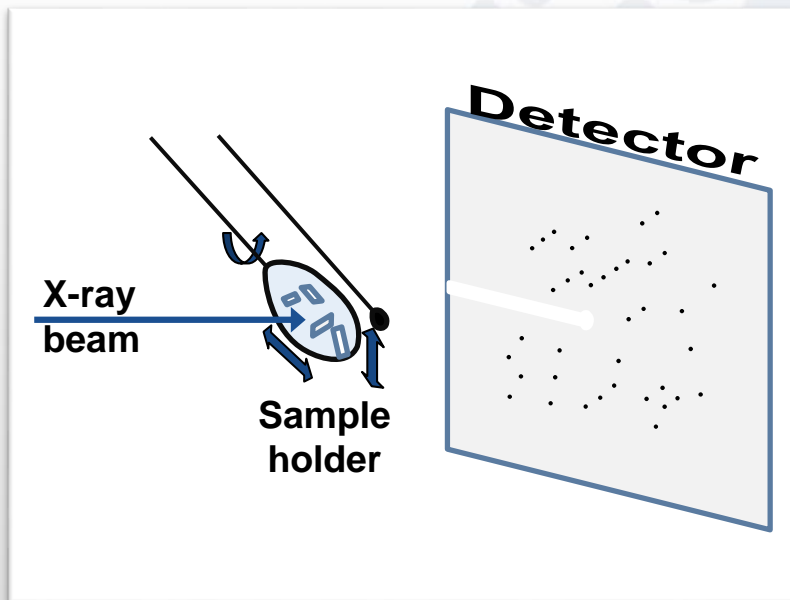
Achievable resolution vs. crystal size

Lactase, B-factor=9.6 Å²

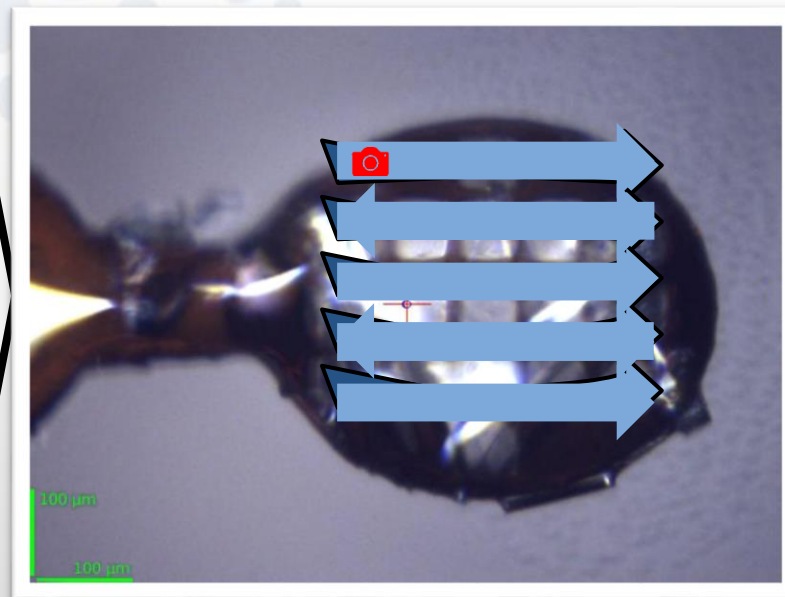
P222







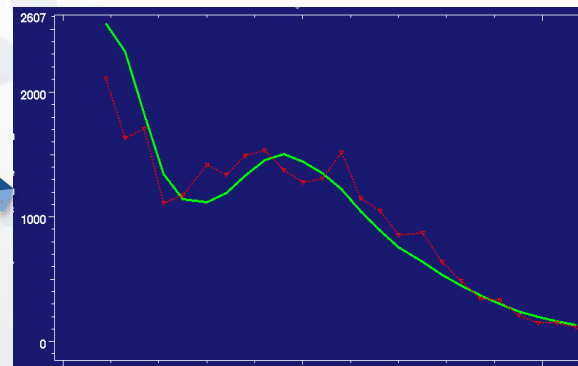
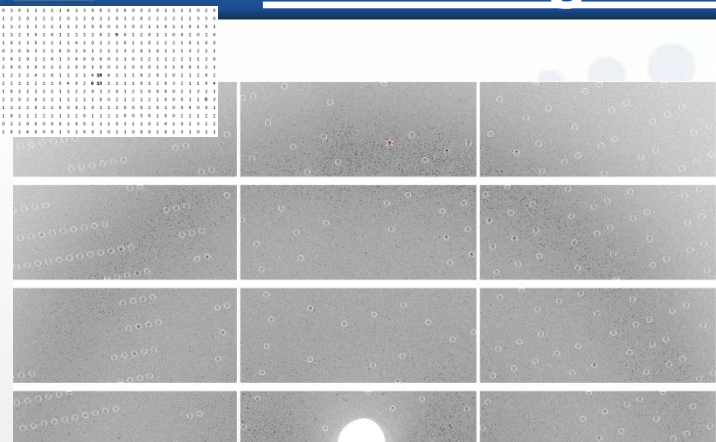
Experimental setup for X-ray crystallography



The data are accumulated during translational movement

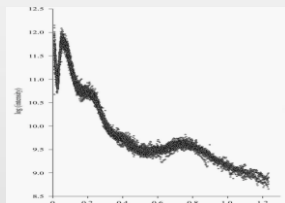
X-ray centering

- Use Wilson plot as a prior
- Use all pixels, not just the local maxima

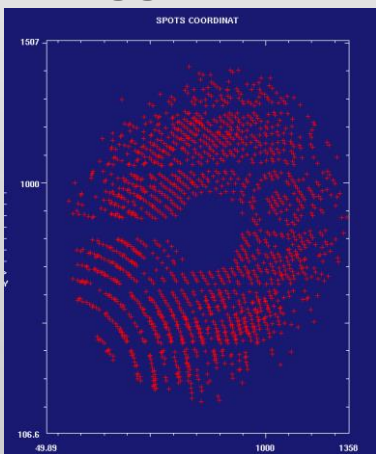


score =

total scattered intensity × radial shape similarity



Bragg spots search



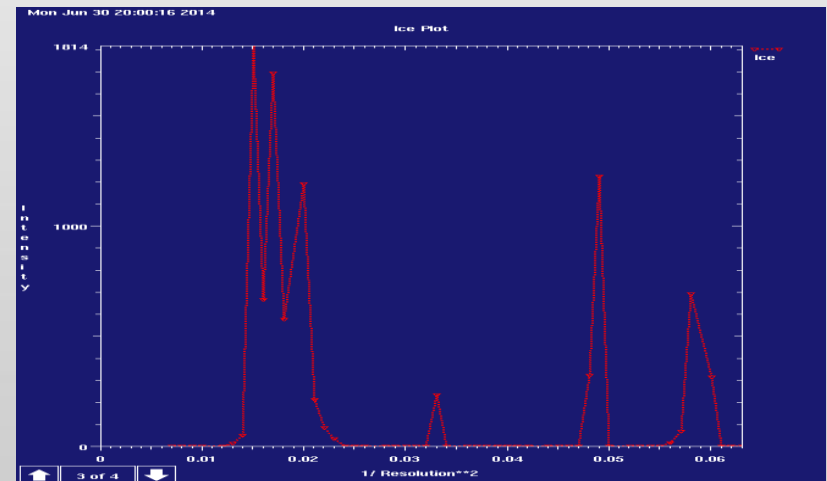
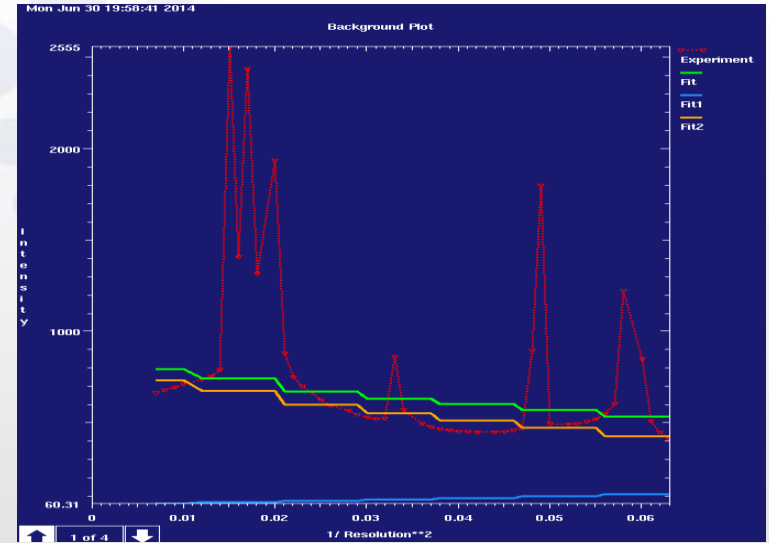
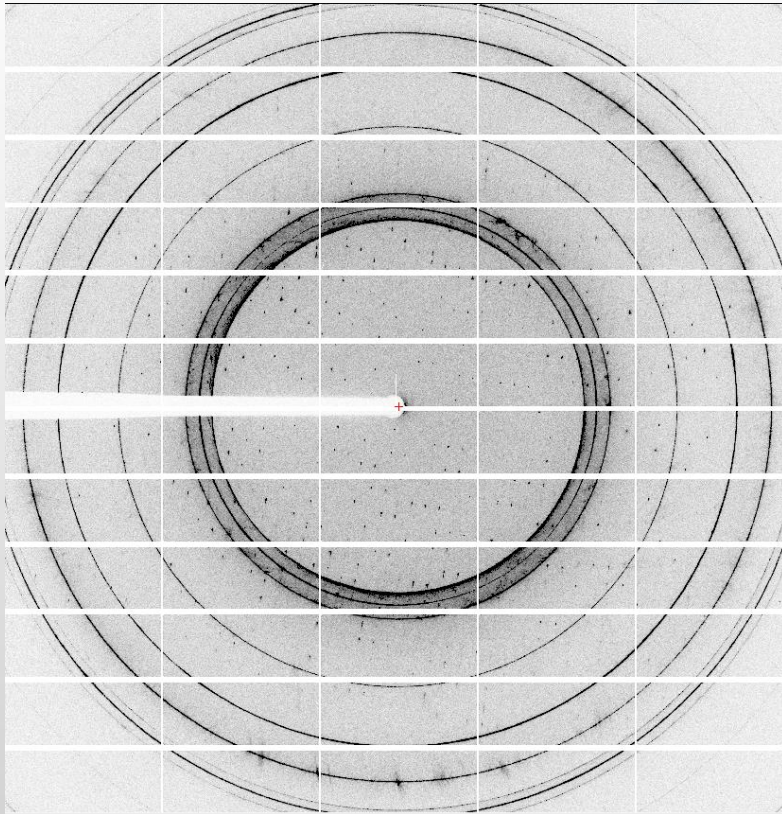
Spots list

```

Program dozor /A.Popov & G.Bourenkov/
Version 1.3.6 // 02.02.2016
Copyright 2014 by Alexander Popov and Gleb Bourenkov
  
```

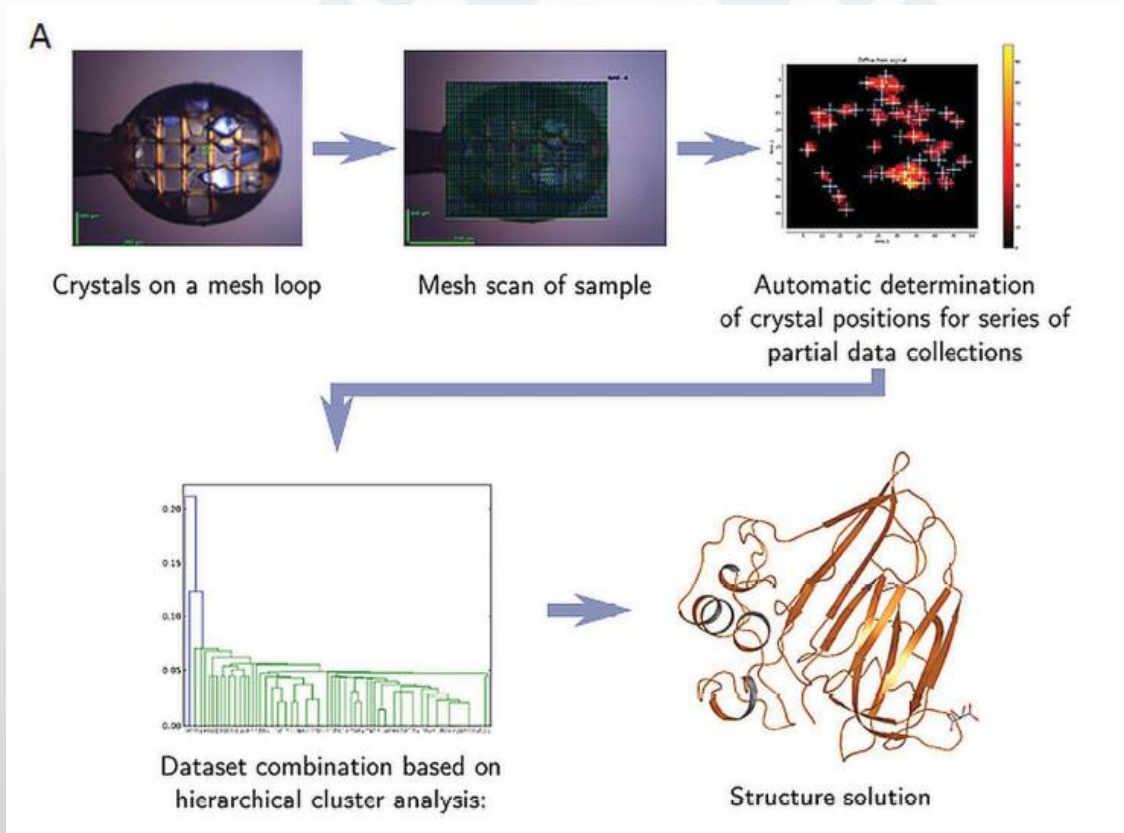
Image	N	SPOTS		Powder Wilson					Main Score	Spot Score	Visible Resolution
		num.of	INTaver	Res.	Scale	B-fac.	Res.	Corr.			
1	44	4.	3.4	154.25	26.5	2.9	72.0	26.7	1.426	1.74	2.73
2	46	39.	3.6	21.35	28.0	2.9	61.2	25.7	9.097	12.40	2.86
3	40	76.	3.4	5.88	44.6	2.8	69.1	28.2	22.485	29.69	2.73
4	51	44.	3.4	18.10	24.2	2.8	64.0	24.8	12.837	16.96	2.69
5	46	32.	3.3	22.98	30.4	2.9	71.6	24.9	9.561	13.63	2.62
6	11	5.	6.4	142.22	18.1	2.9	62.8	29.6	0.235	0.13	5.09
7	43	4.	3.4	232.69	16.7	2.8	62.9	31.0	1.258	1.97	2.69
8	30	78.	3.4	19.31	13.1	2.9	56.1	31.3	15.888	30.38	2.69
9	33	83.	3.2	9.34	28.5	2.9	52.3	25.0	20.799	40.67	2.59
10	31	66.	3.4	8.86	39.8	3.0	62.3	24.7	16.076	24.23	2.69

DOZOR - indication on the ice or salt diffraction contaminations



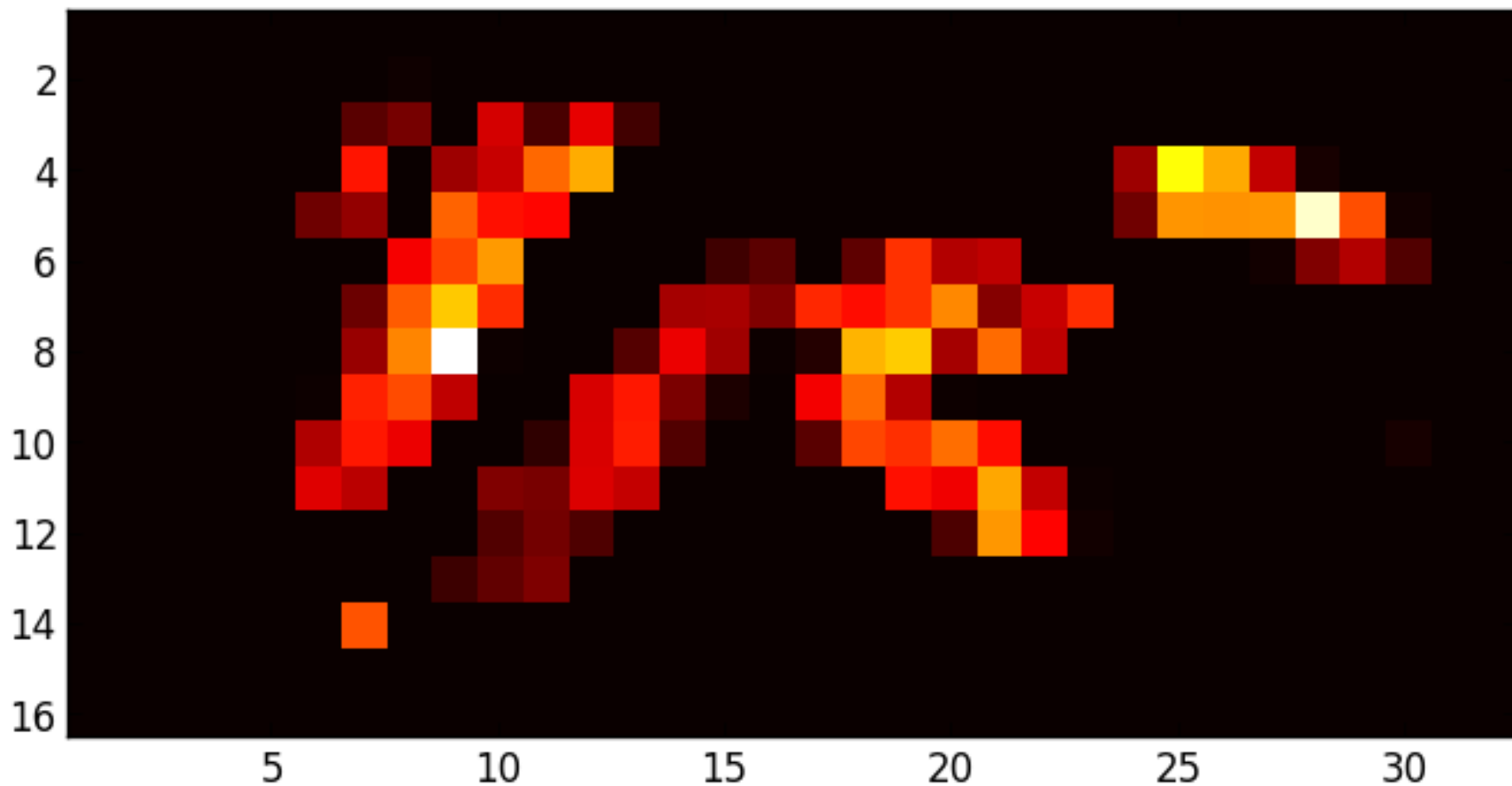
MeshAndCollect: an automated multi-crystal data collection workflow for synchrotron macromolecular crystallography beamlines

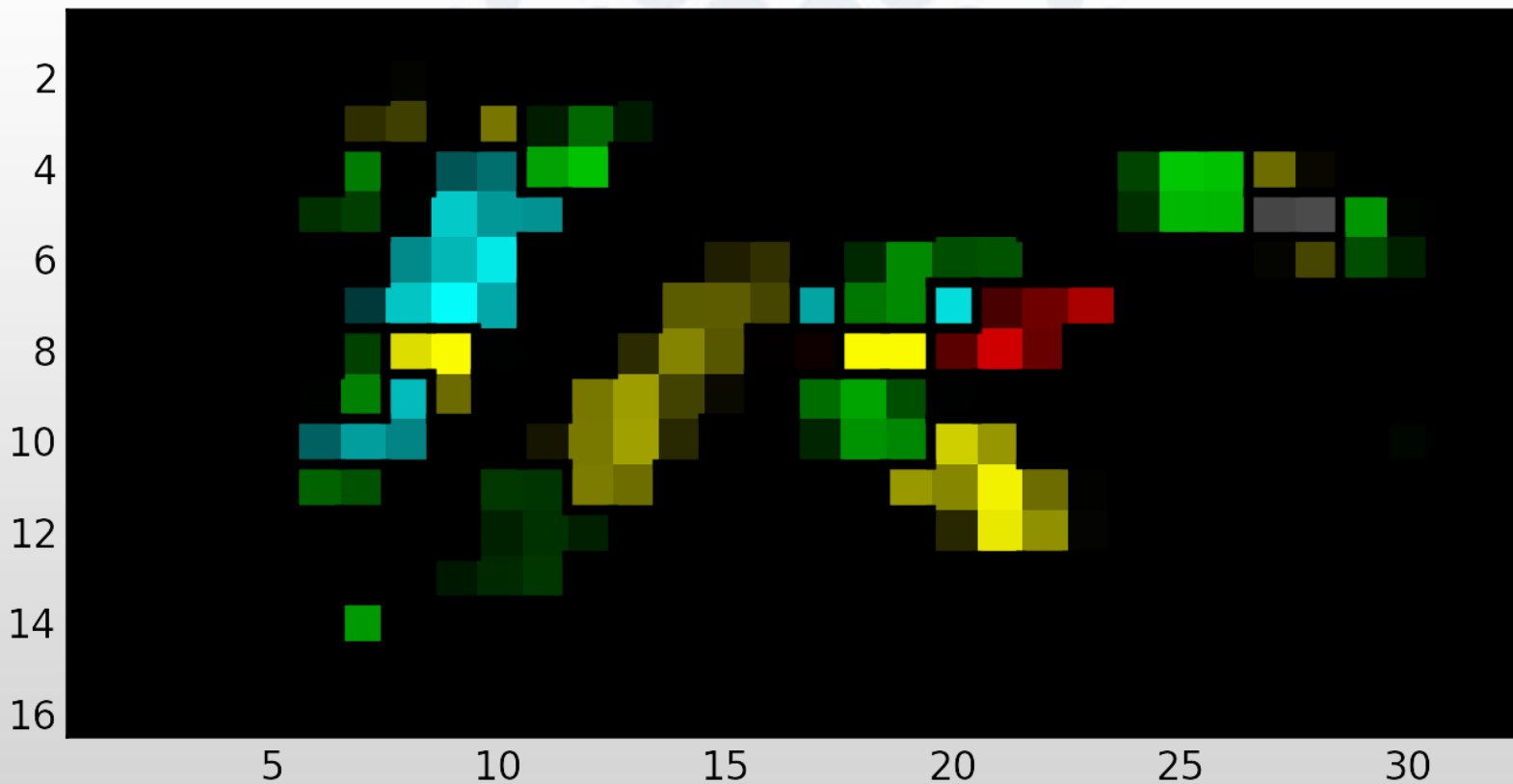
Ulrich Zander *et al.*, *Acta Crystallographica* (2015) D71, 2328-43

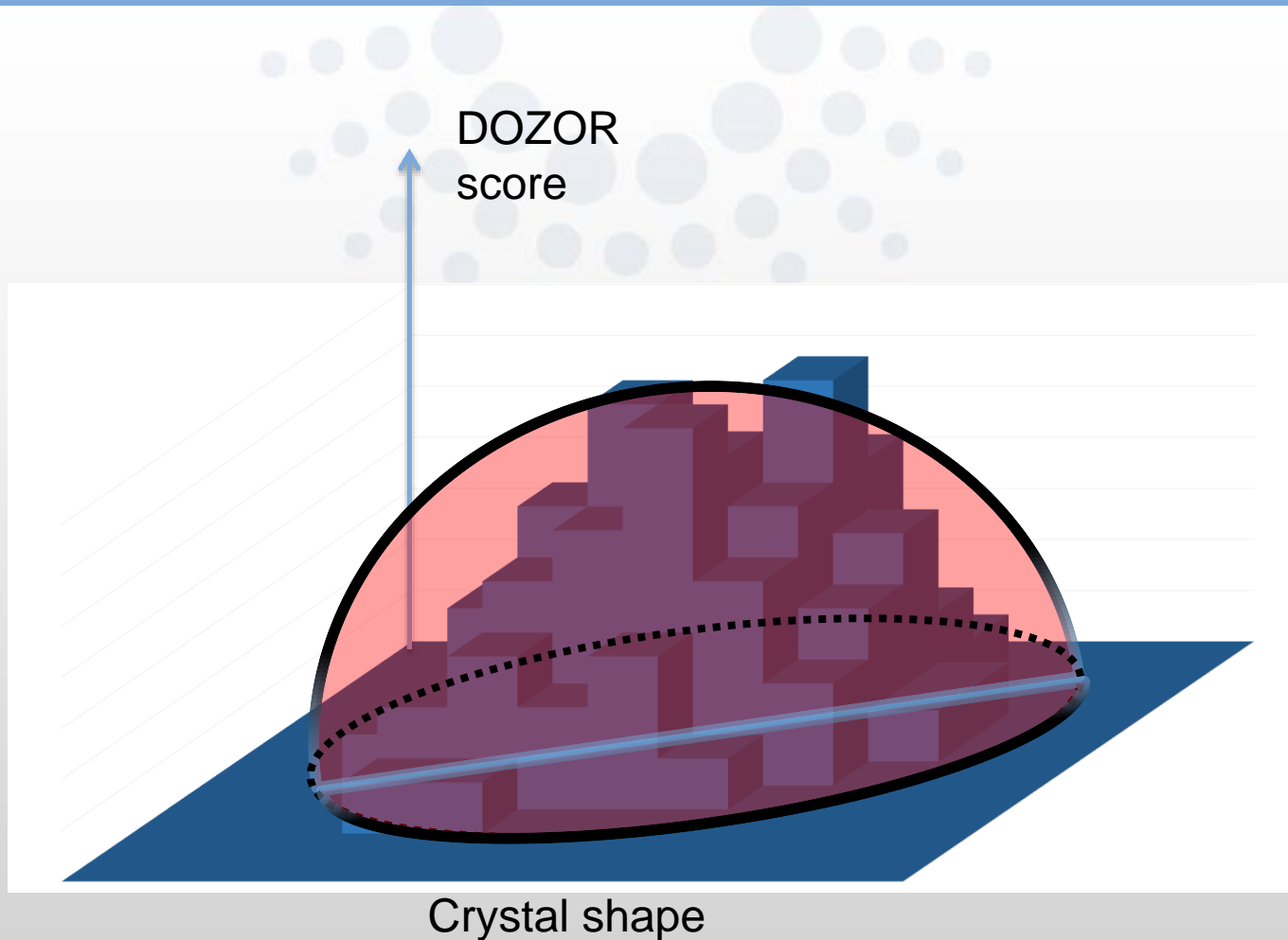


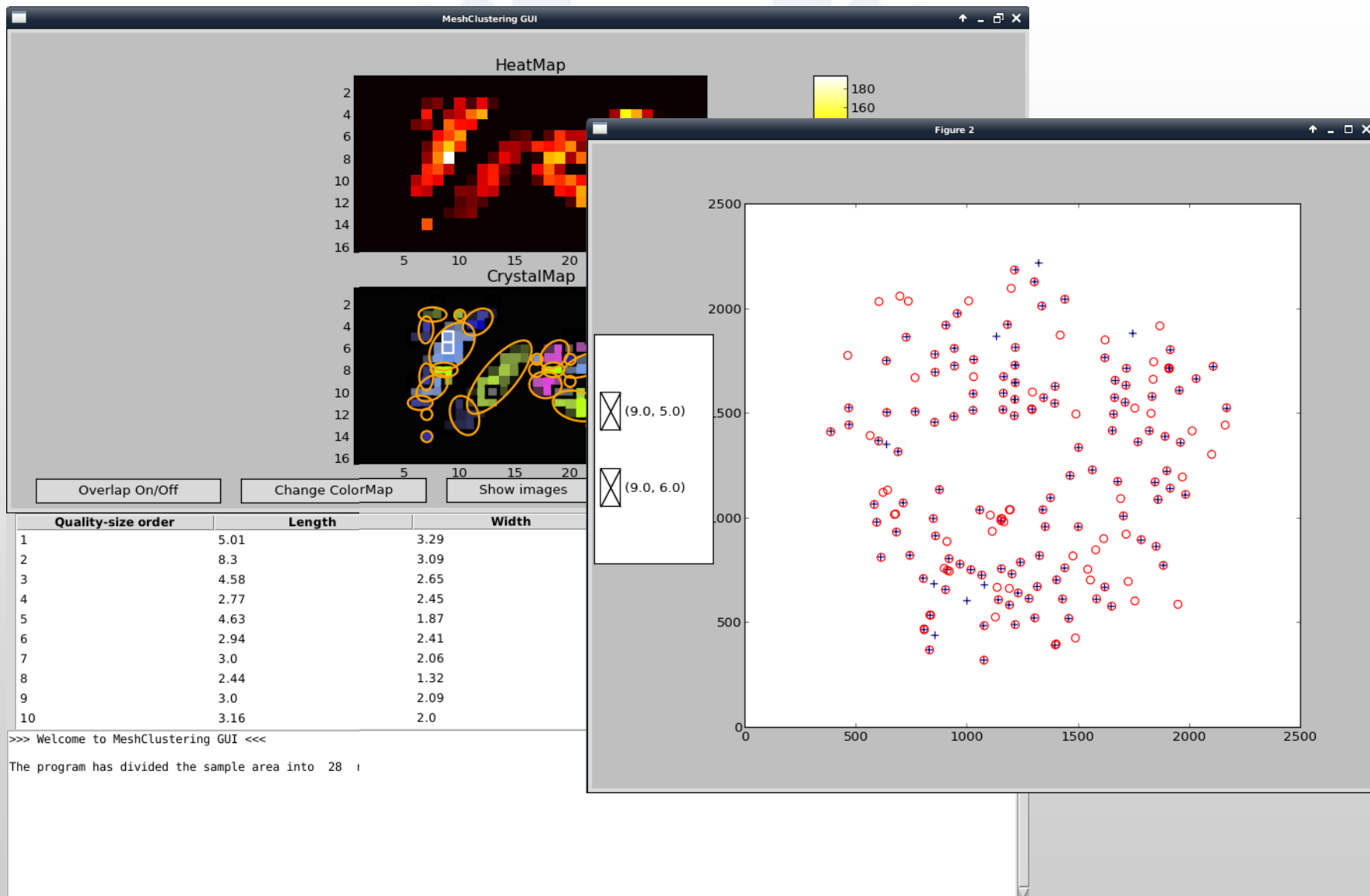
The 'MeshAndCollect' workflow for multi crystal data collection method.

mesh scan is performed on the sample. The resulting images are automatically inspected for protein diffraction and scored according to diffraction strength. A heat map is generated that represents the diffraction intensity where the positions for partial data collections are marked. After the user has selected the settings for the partial data collections, the MxCuBE2 data collection queue is automatically filled and all partial data sets collected. Once the partial datasets have been automatically processed, HCA can then be used to choose which data sets to merge to produce a final data set for structure solution.

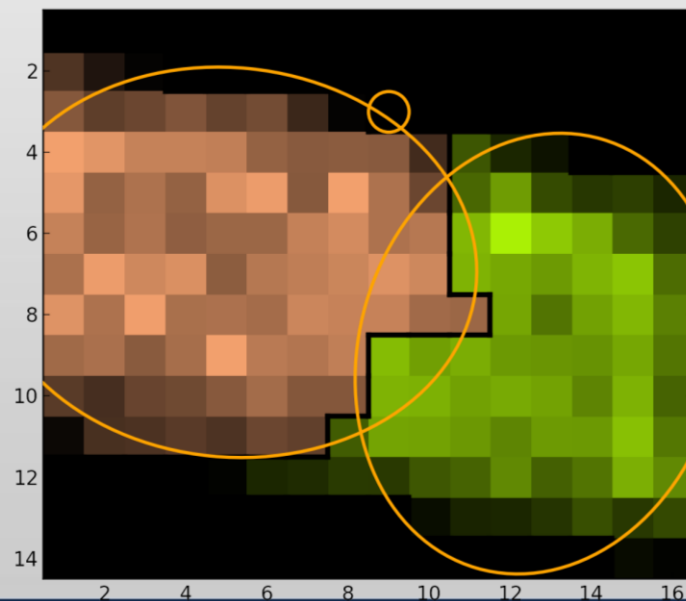
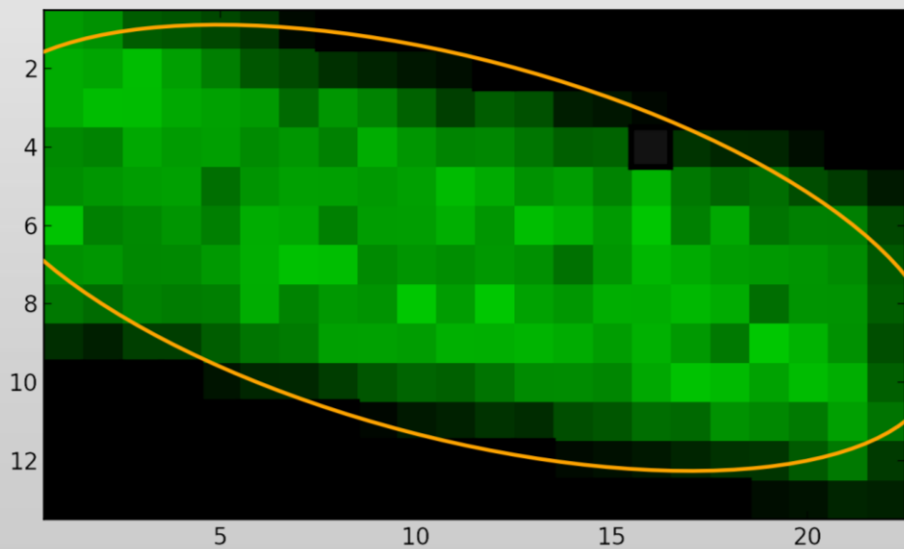
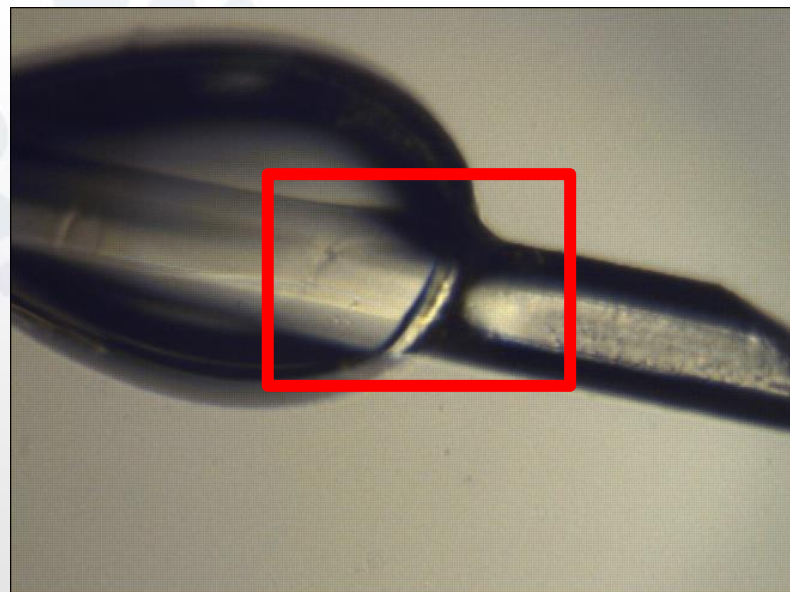
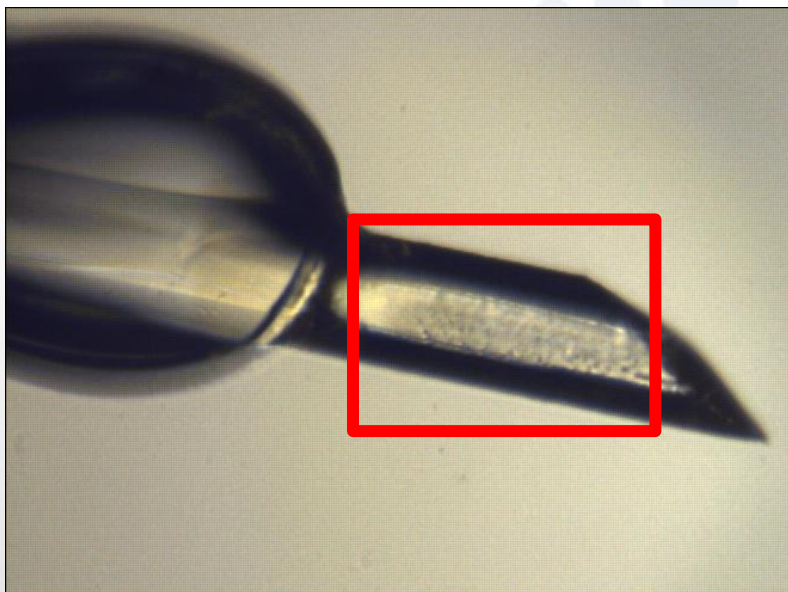


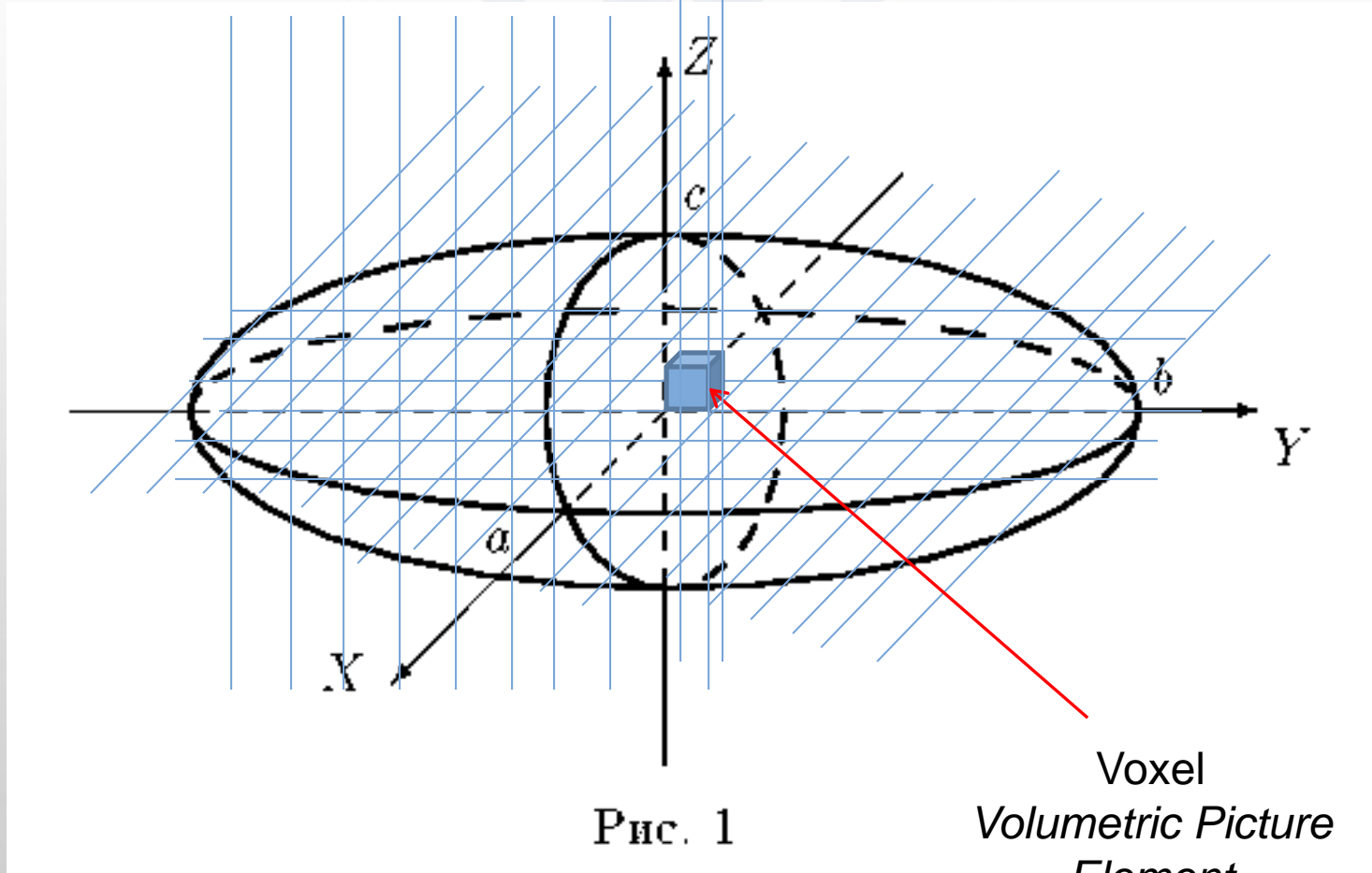






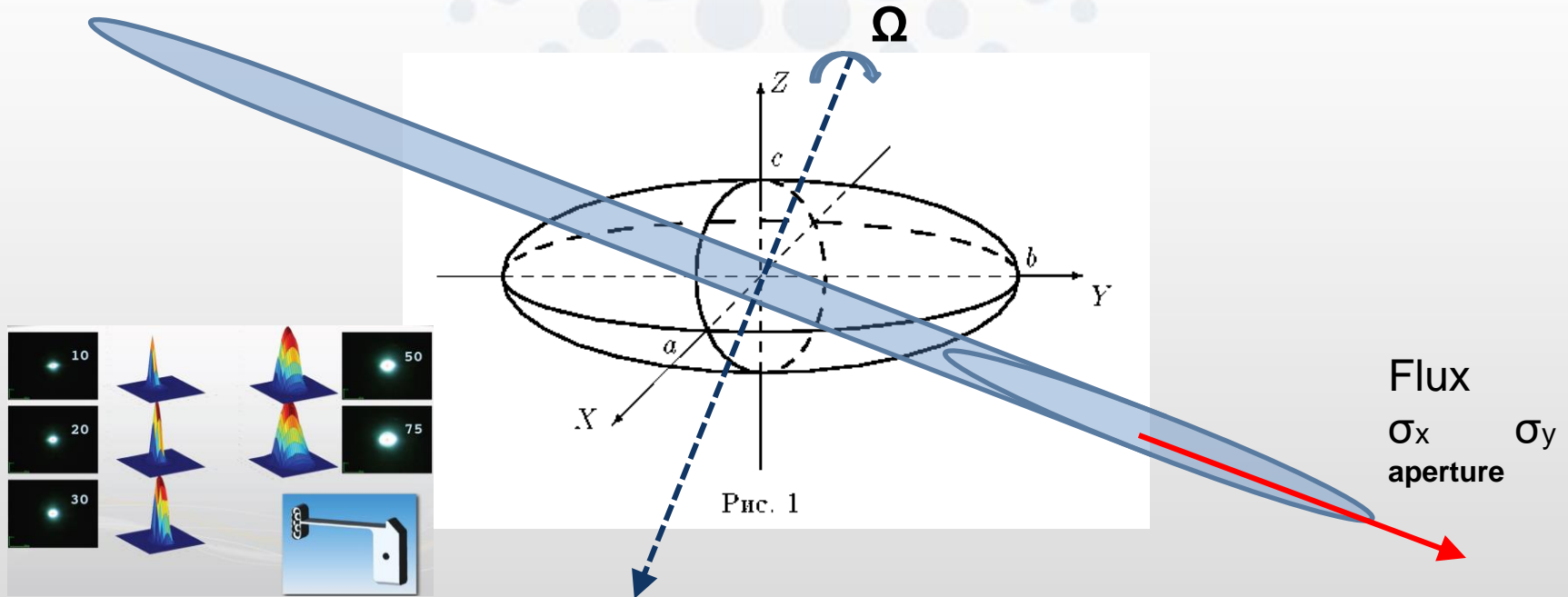
Some test examples





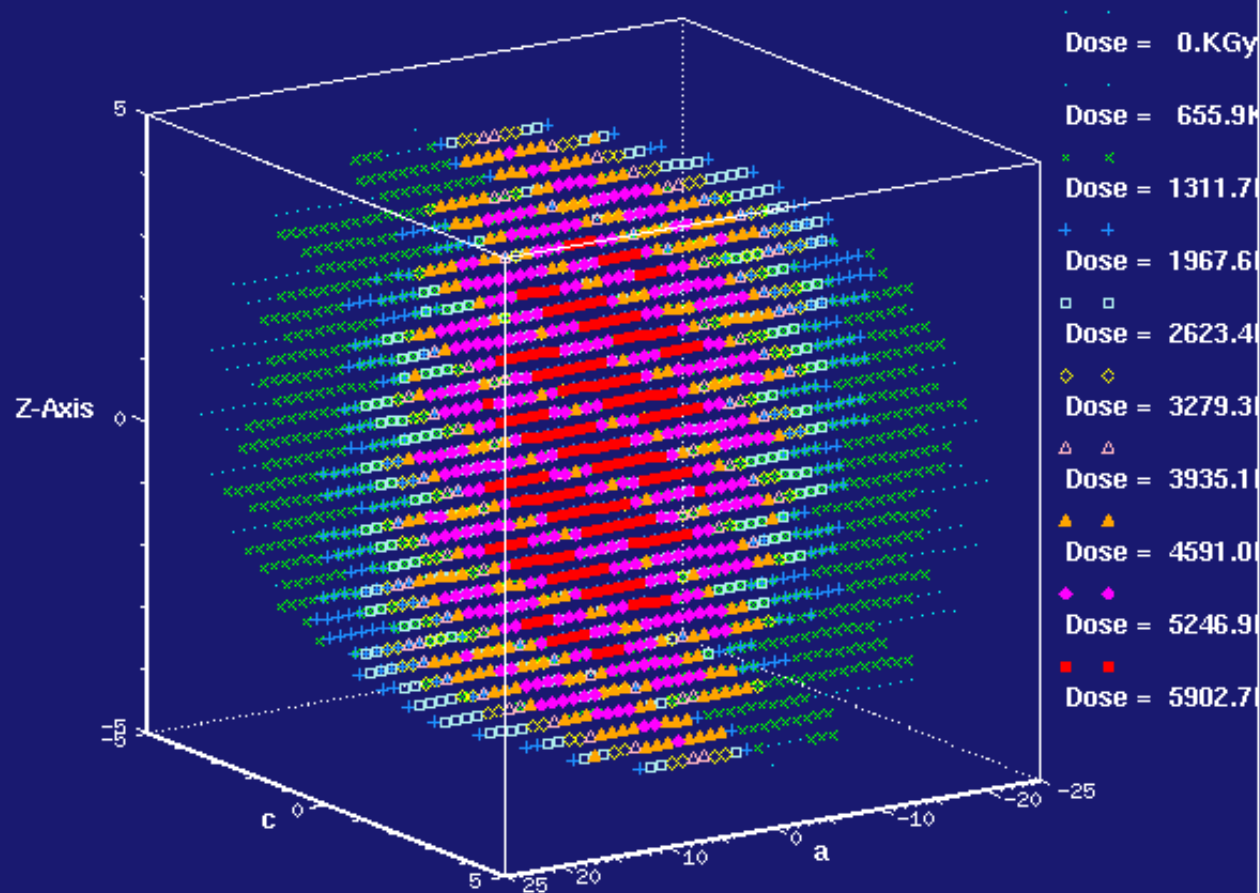
Voxel
Volumetric Picture
Element

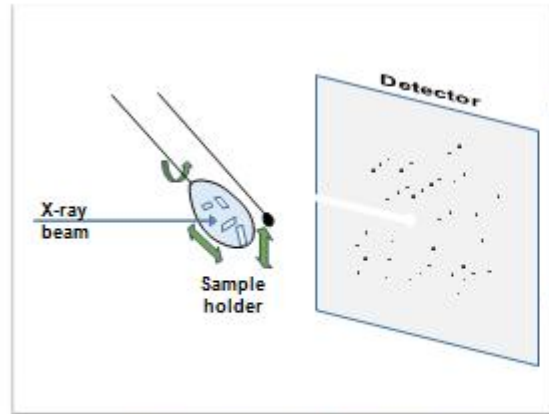
$$Scale(\Omega) = Scale(voxel) \times NumberVoxel(\Omega)$$



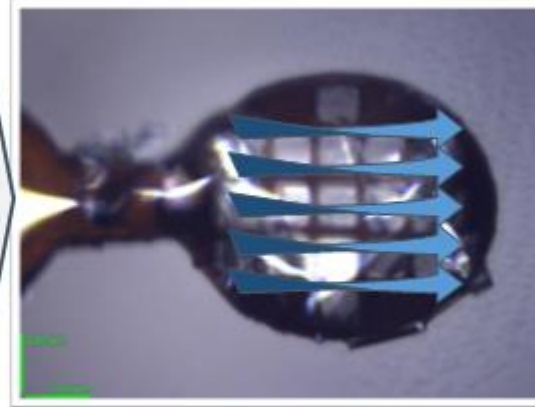
$$\hat{J}(\mathbf{h}, D) = \hat{J}_o(h) \sum_{voxel} \sum_{x,y} I_{x,y}(beam) \times scale(voxel, D_{voxel}) \exp(-\mathbf{h} \cdot \mathbf{B}(D_{voxel}) \cdot \mathbf{h}^T / 2)$$

Dose vs. sample





Experimental setup for X-ray crystallography



Translation with slight rotation is the principle of Mesh Scan data collection

The Complex Analysis of the X-ray Mesh Scan

DOZOR

Crystals Mapping – positions, size, diffraction quality

BEST – Data Collection Strategy accounting radiation damage

Data Collection and Processing

Acknowledgements

- Gleb Bourenkov
- Igor Melnikov
- ESRF MX Group
- Olof Svensson & EDNA developers team