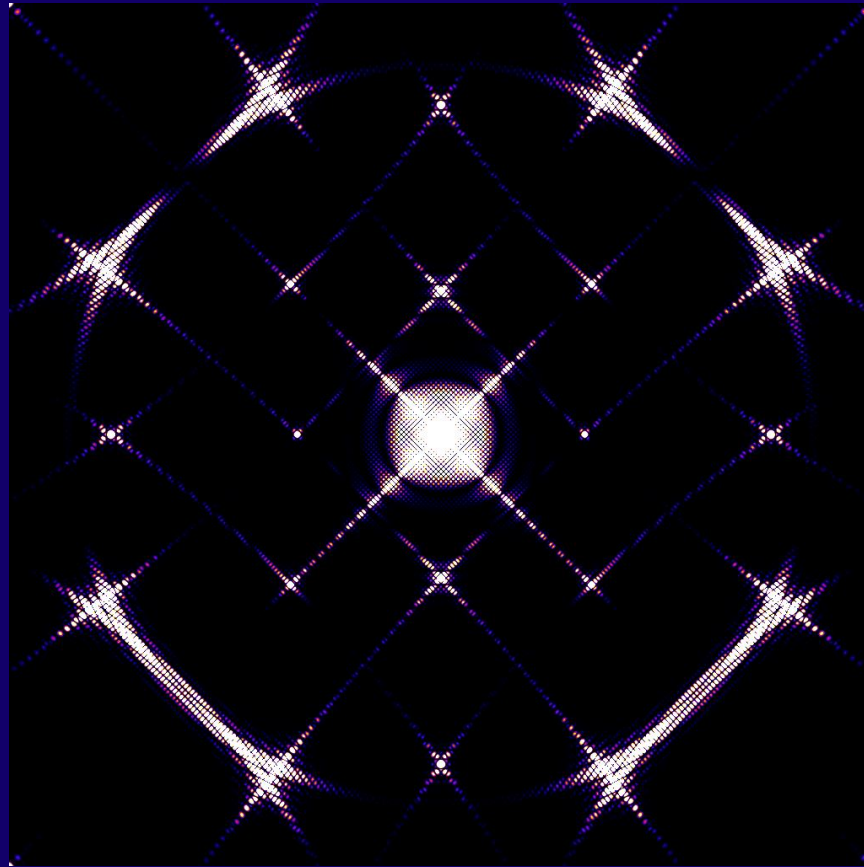


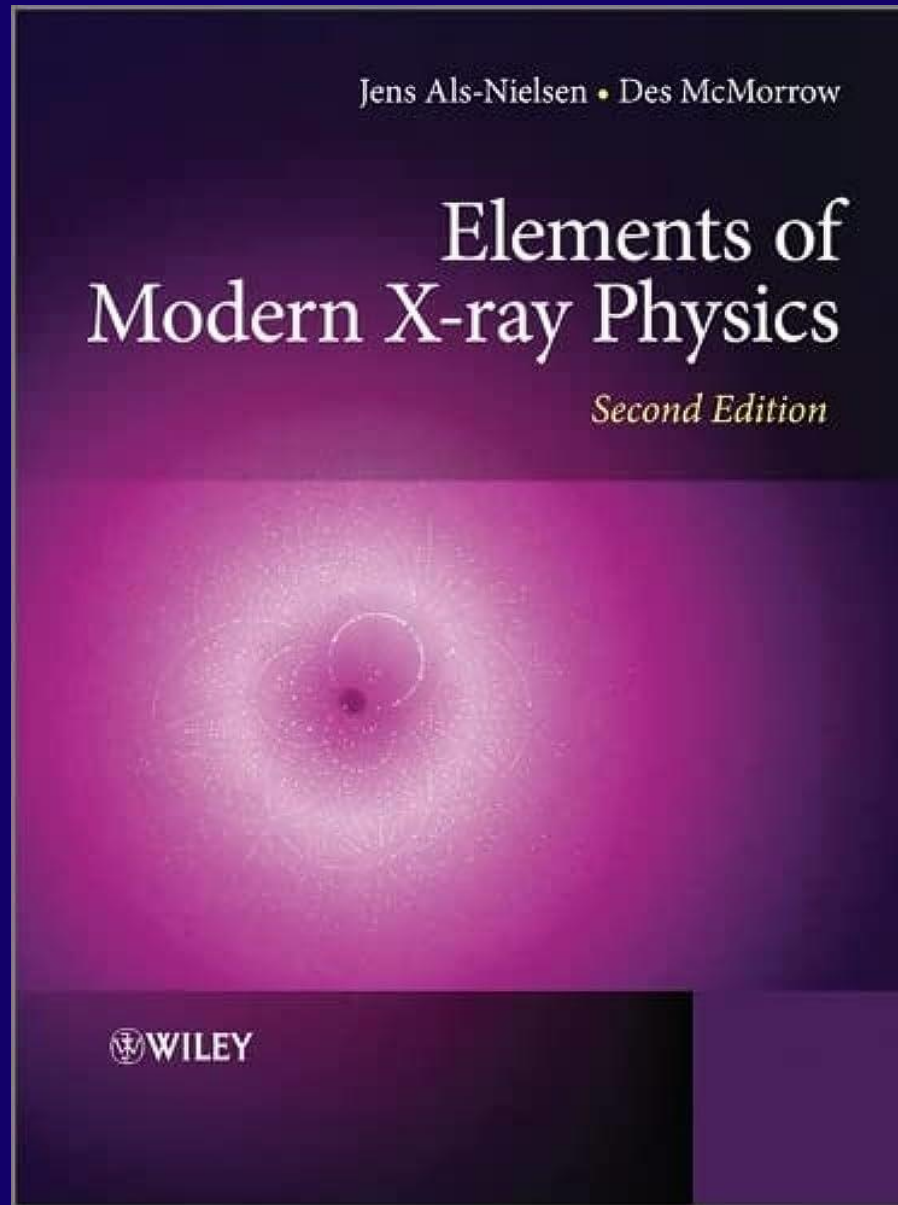
Reciprocal space. Part 2



O. M. Yefanov

CFEL at DESY, Hamburg, Germany

To read



What we'll be talking about:

- **Non-crystalline objects**
- **High resolution**
- **Ewald sphere (again ☹)**
- **Single particle imaging**
- **Why crystals?**
- **Protein crystallography**
- **Pink and convergent beams**
- **Dynamical theory (multiple scattering)**
- **Processing lots of data**

Again some basics

a, b, c - real lattice vectors

a*, b*, c* - reciprocal lattice

H – reciprocal lattice vector

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

h, k, l – Miller indexes

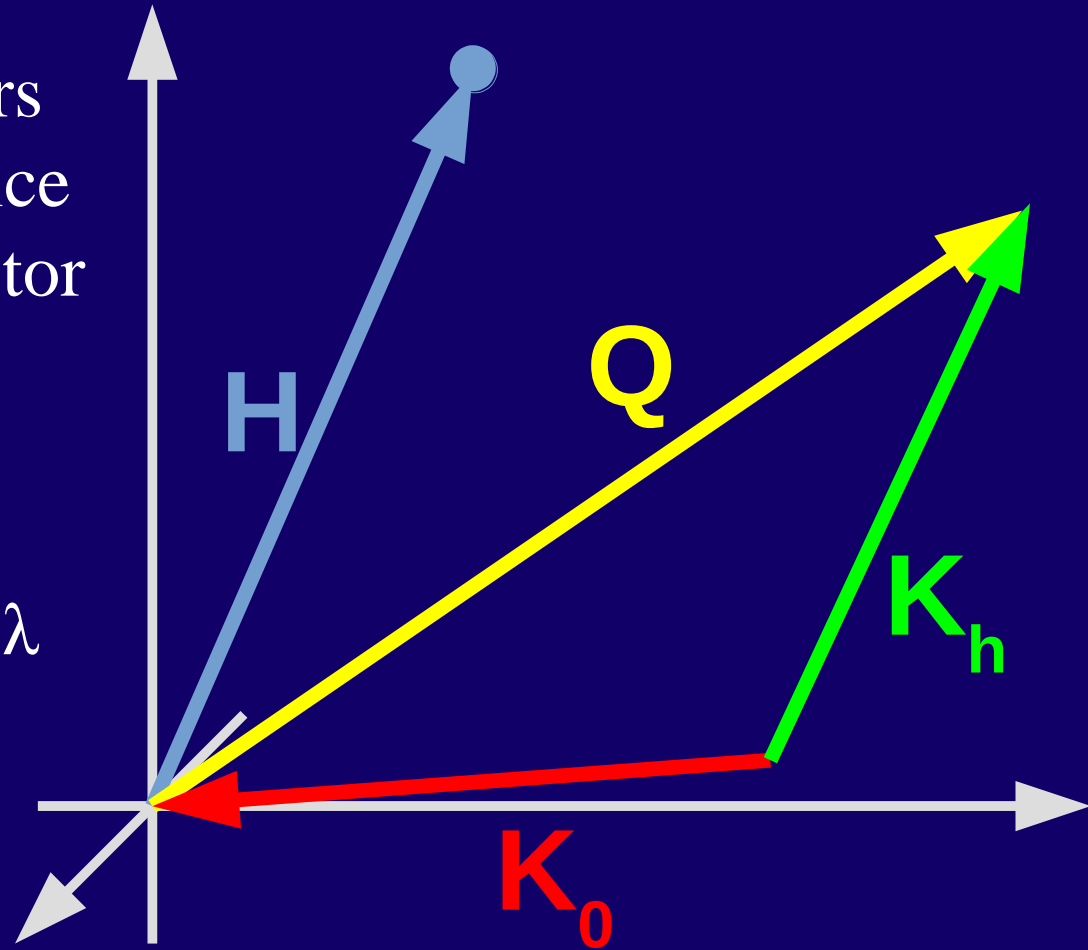
λ – wavelength ($\sim 1\text{\AA}$)

K – wavevector, $|\mathbf{K}| = 1/\lambda$

Q – scattering vector

$$\mathbf{Q} = \mathbf{K}_h - \mathbf{K}_0$$

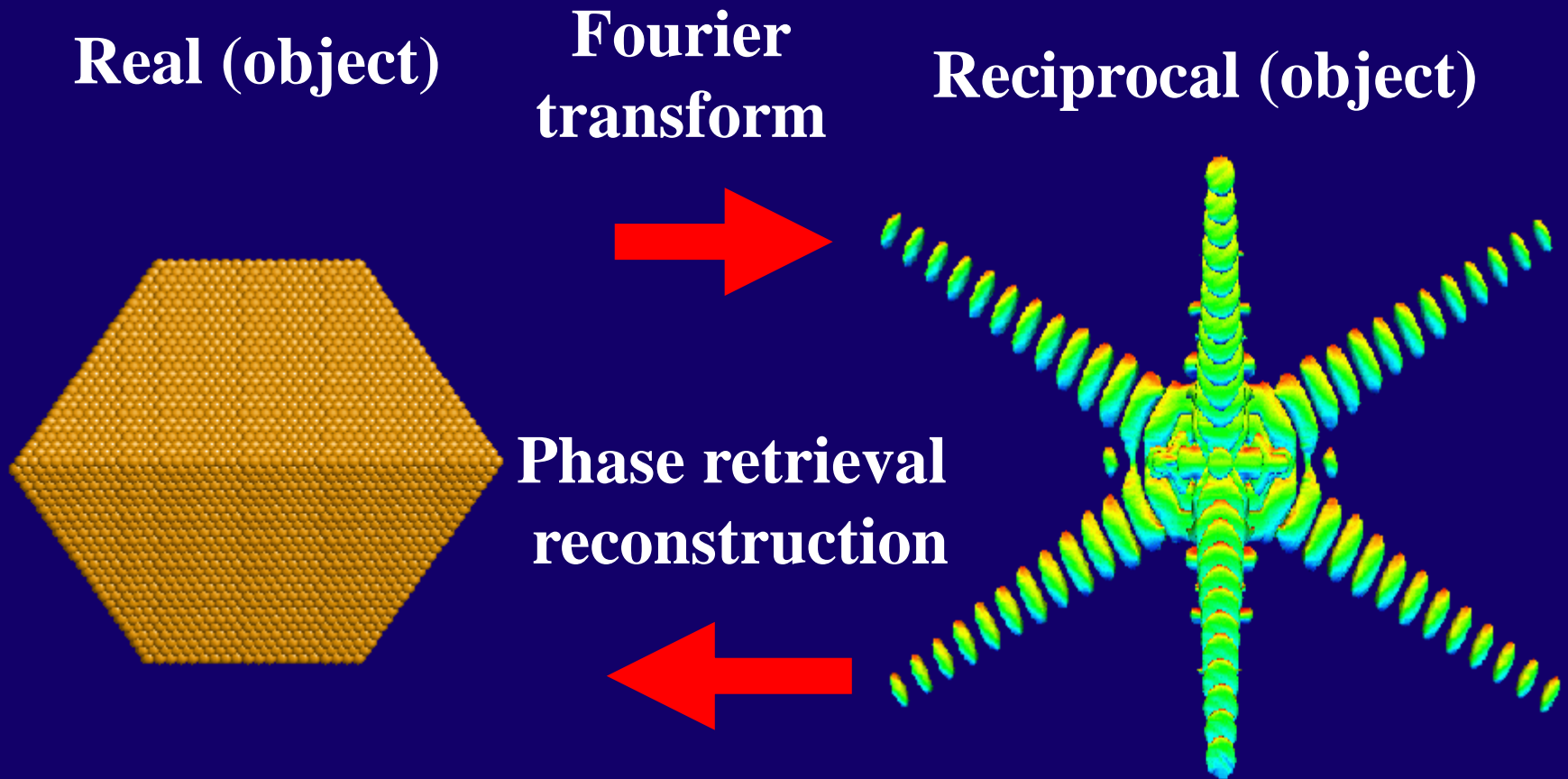
H = Q – Bragg's law



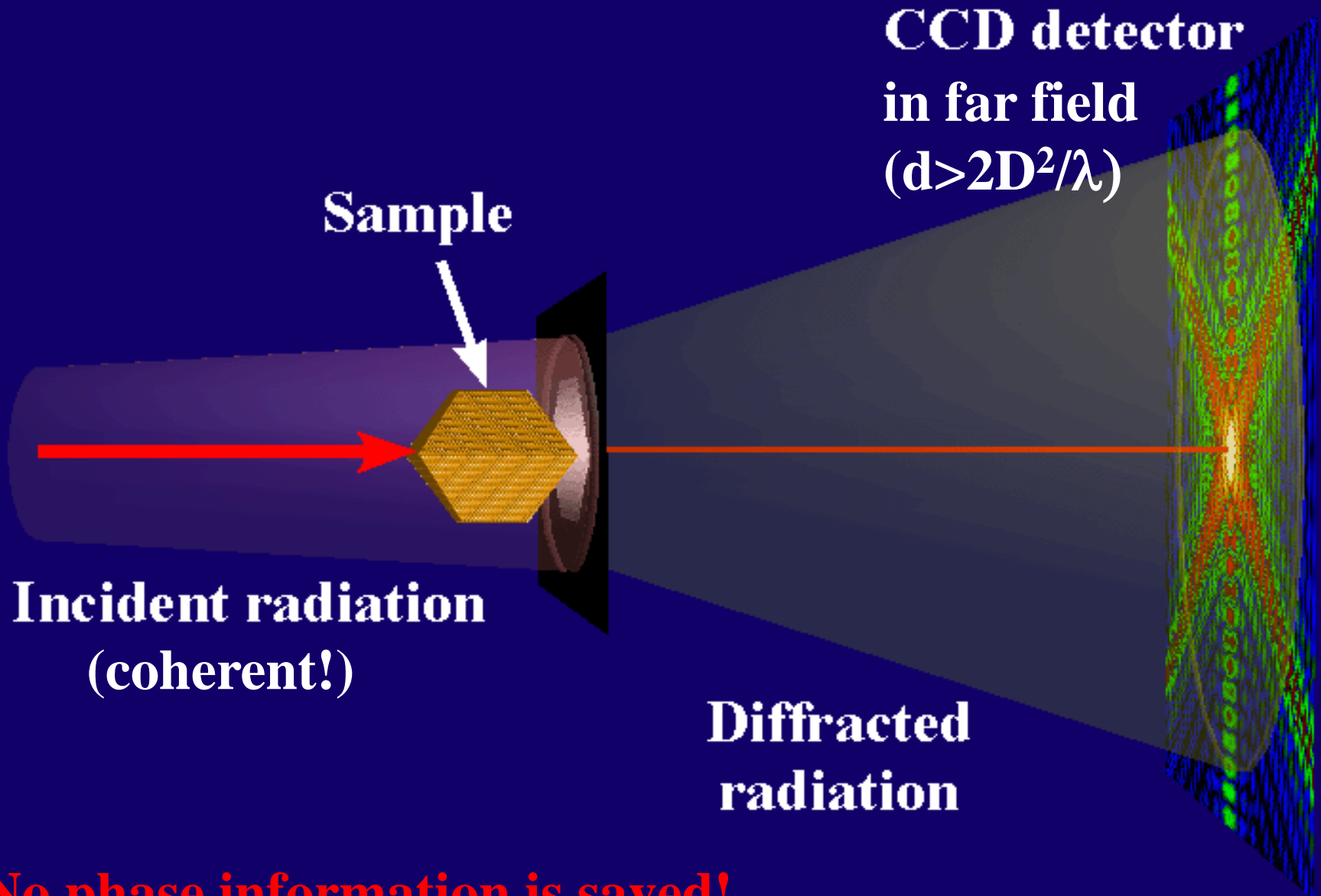


Non-crystalline objects

Reciprocal space in 3D



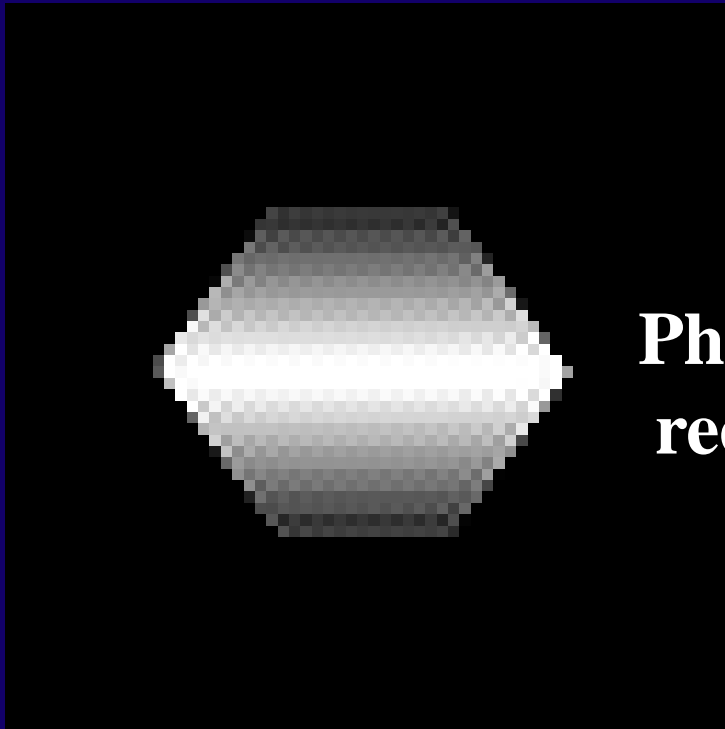
Coherent X-ray Diffraction Imaging



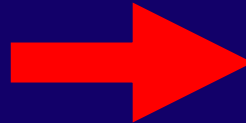
No phase information is saved!

Reciprocal space in 2D

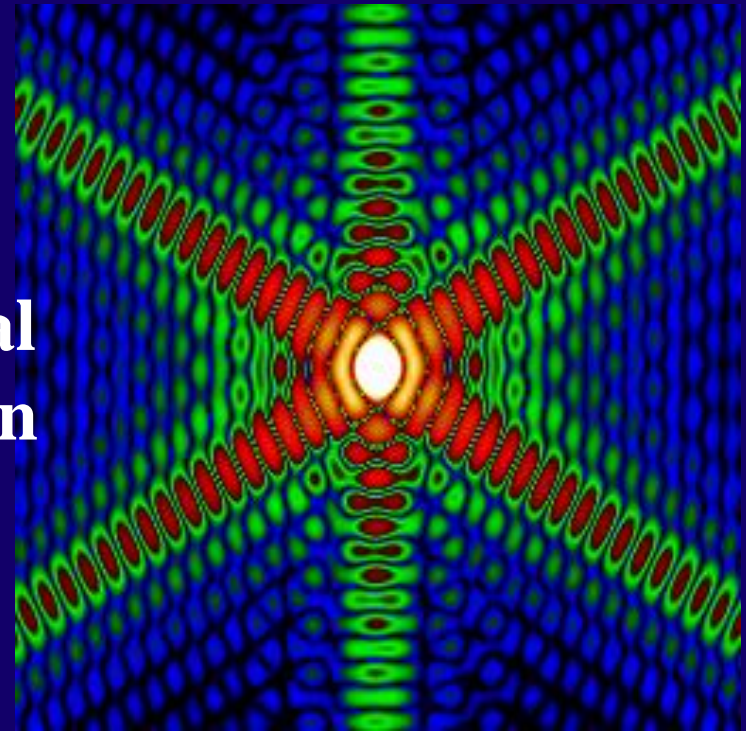
Projection
of the object



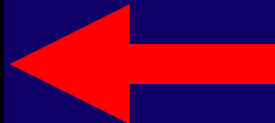
Fourier
transform



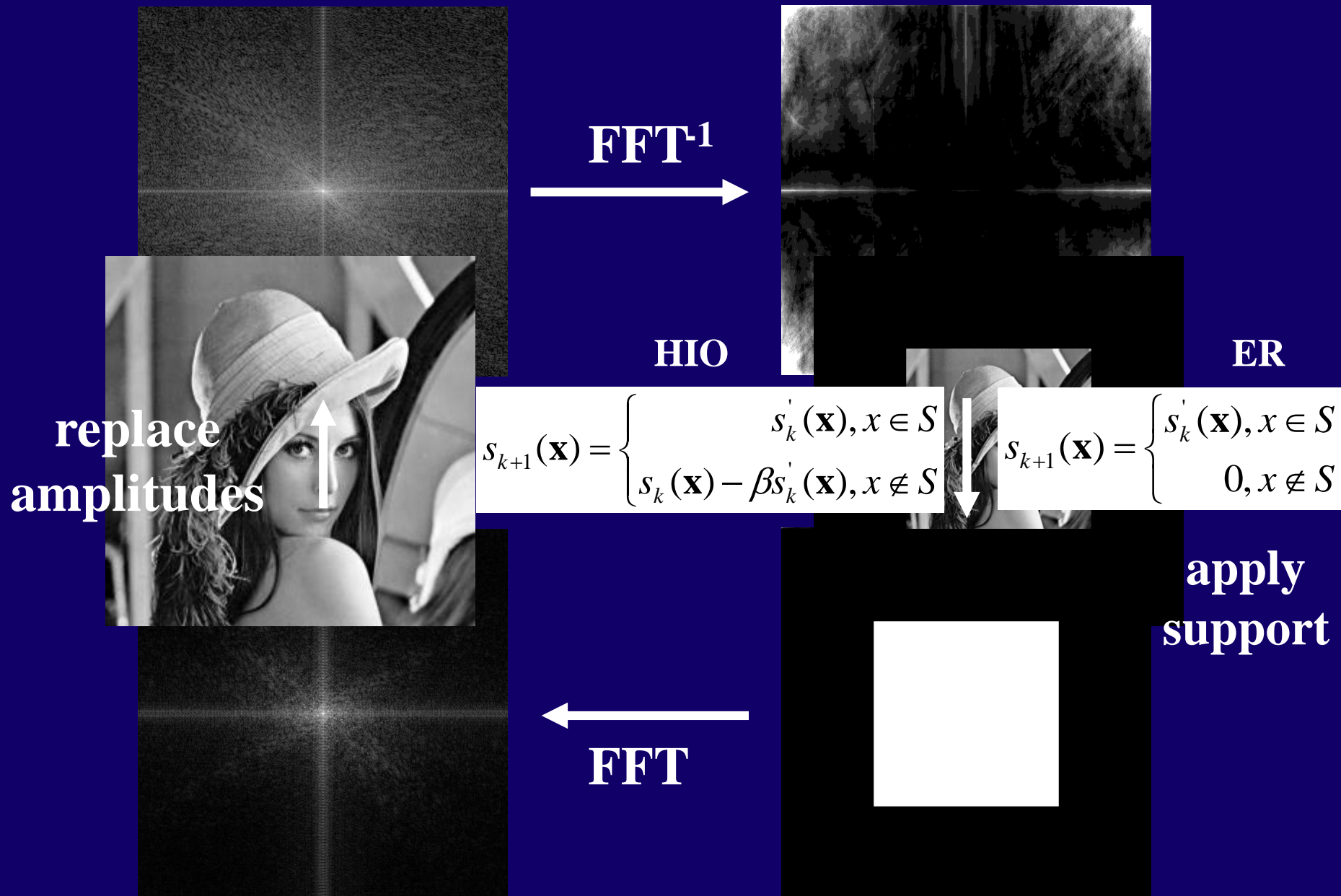
Section through
reciprocal space



Phase retrieval
reconstruction



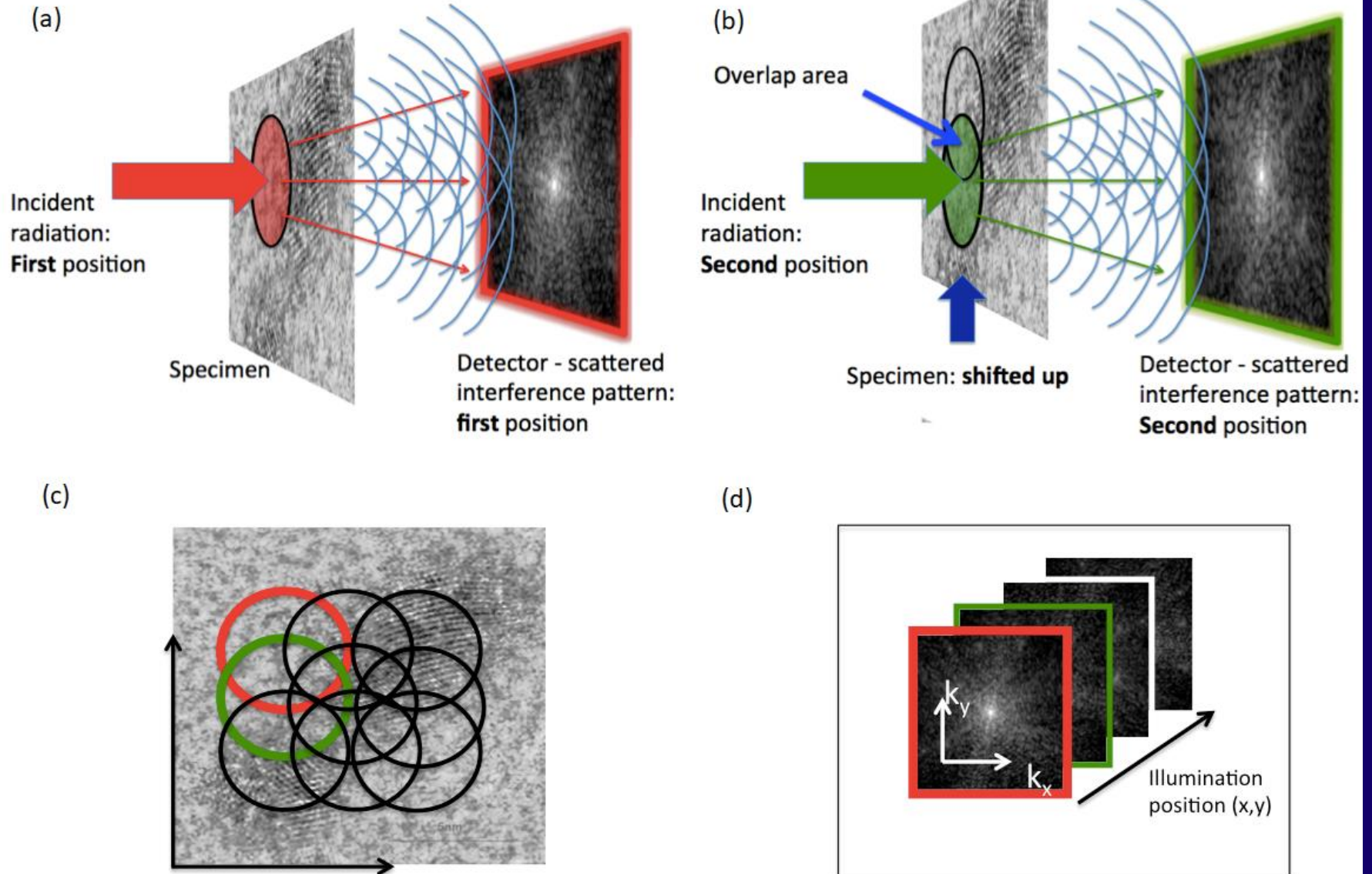
Phase retrieval algorithm:



Phase retrieval algorithm:



Ptychography

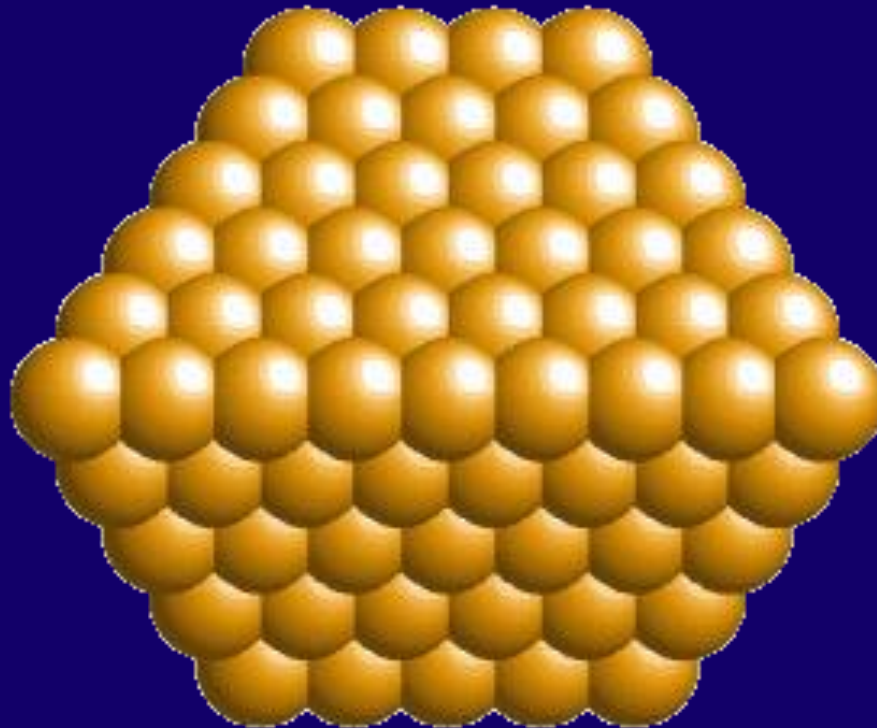


From Wiki

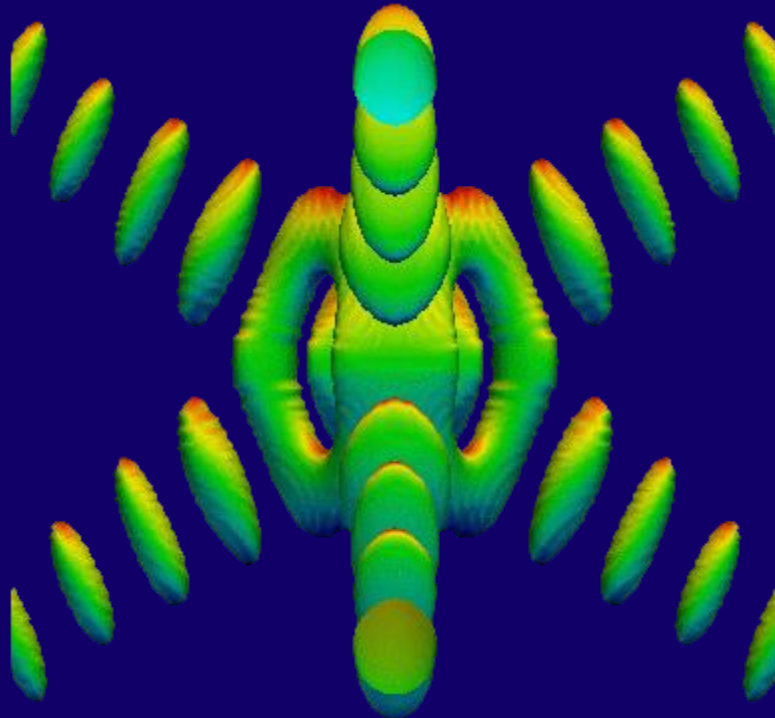


Why do we need high resolution?

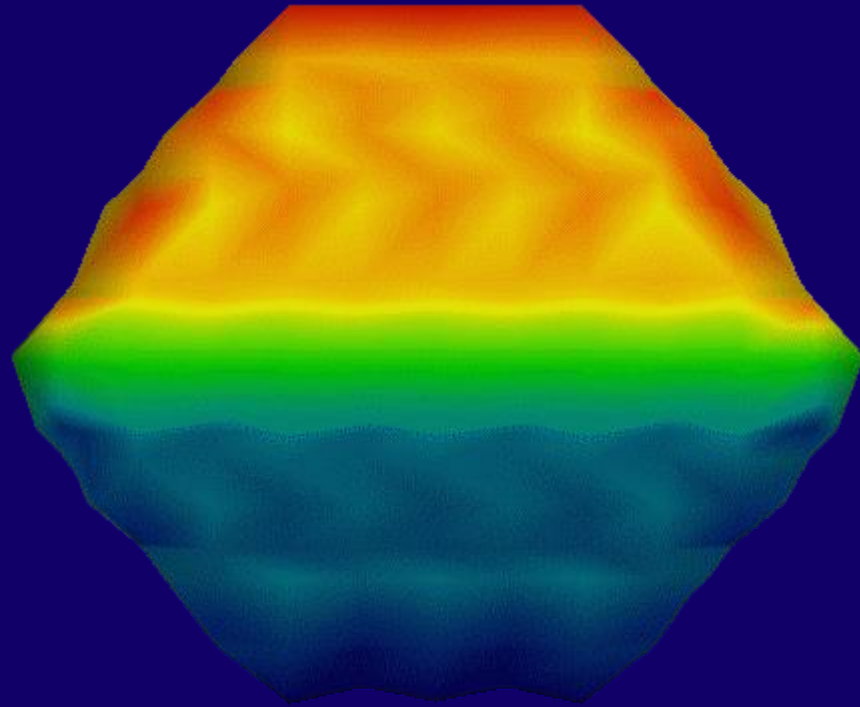
3D crystalline sample



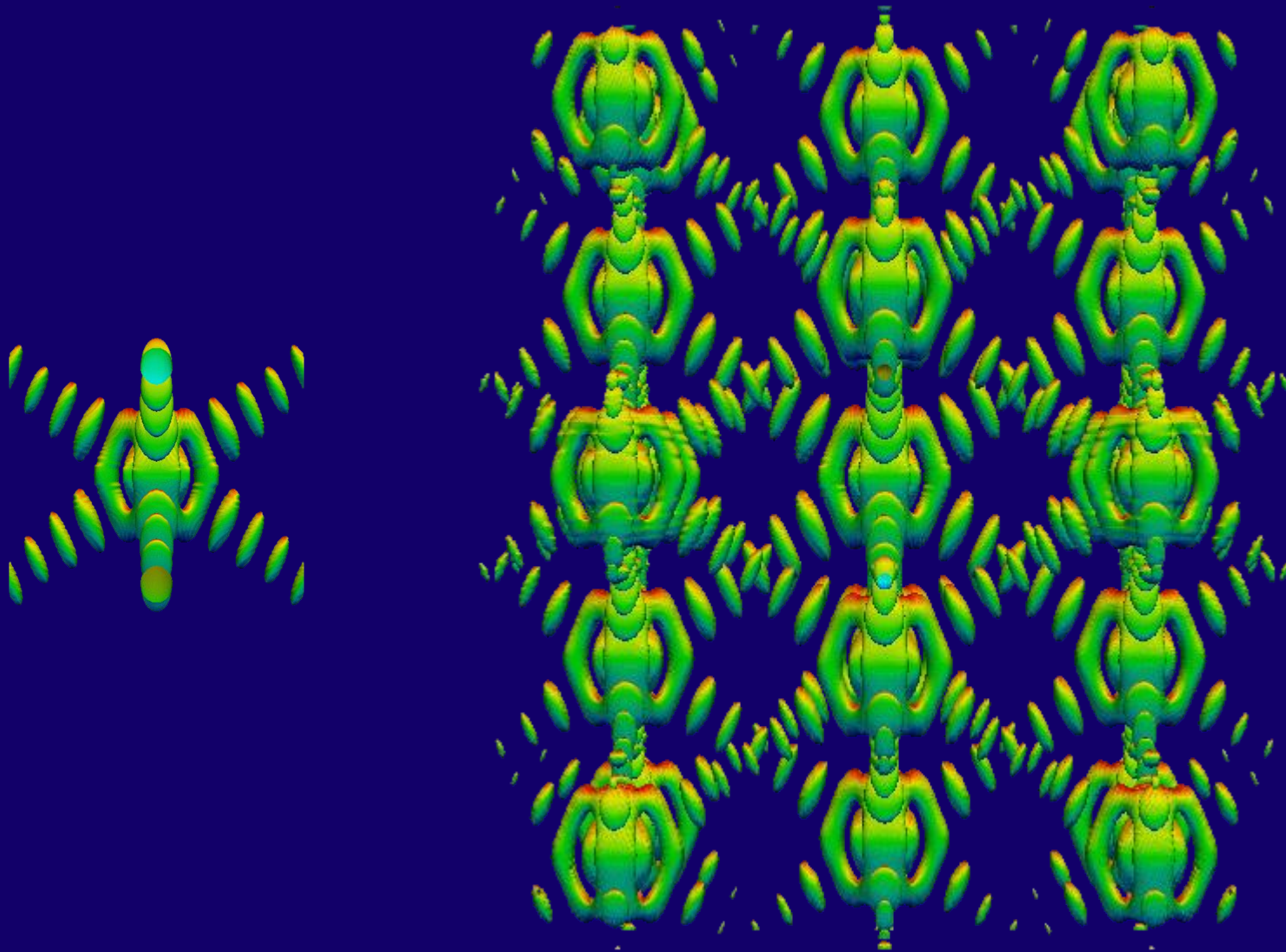
Reciprocal space for low Q



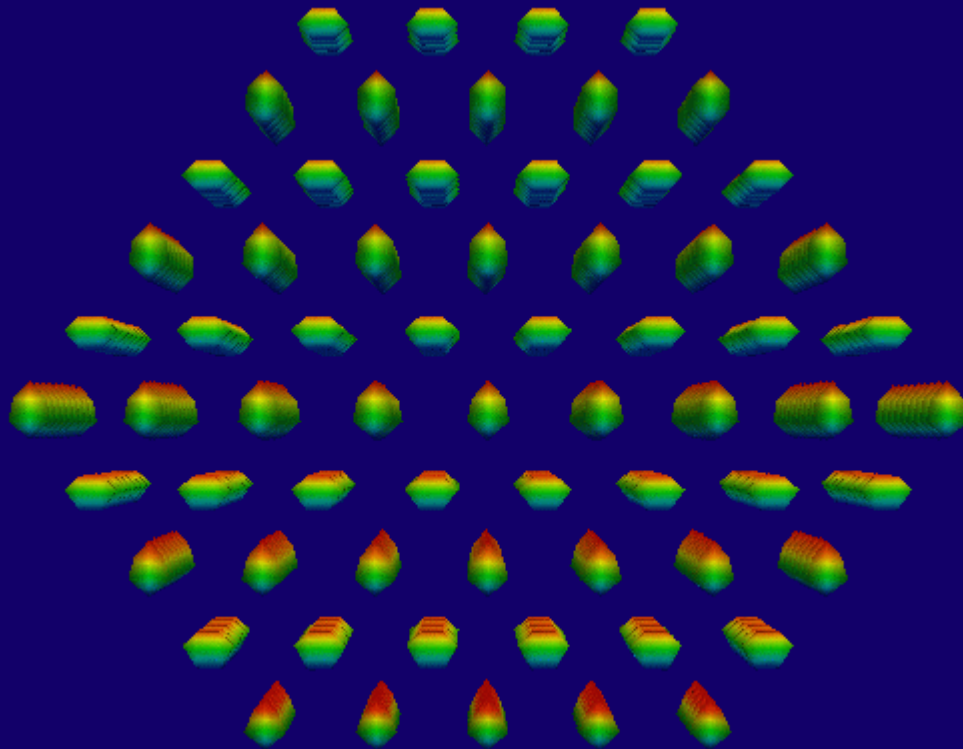
Reconstruction for low Q



Reciprocal space for high Q



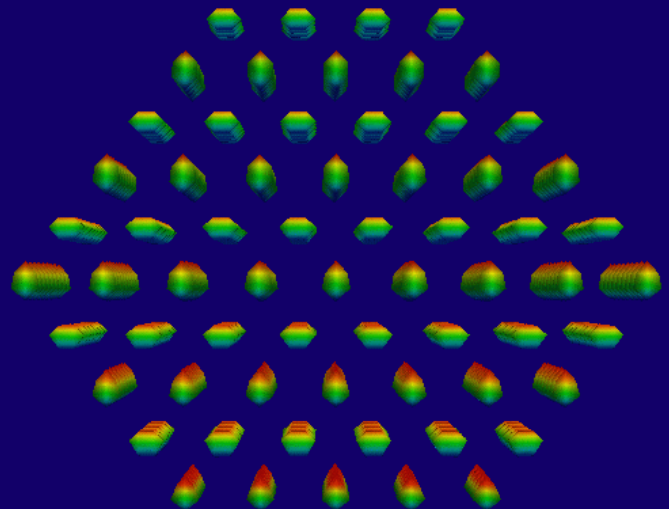
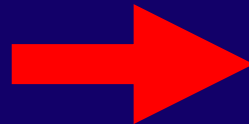
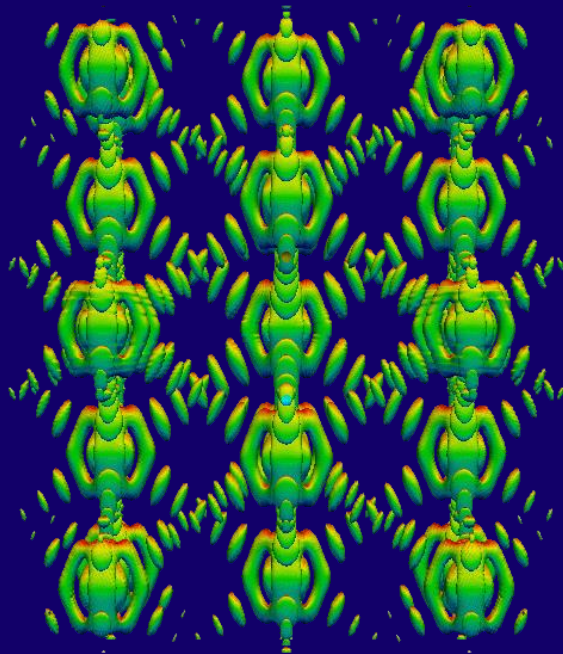
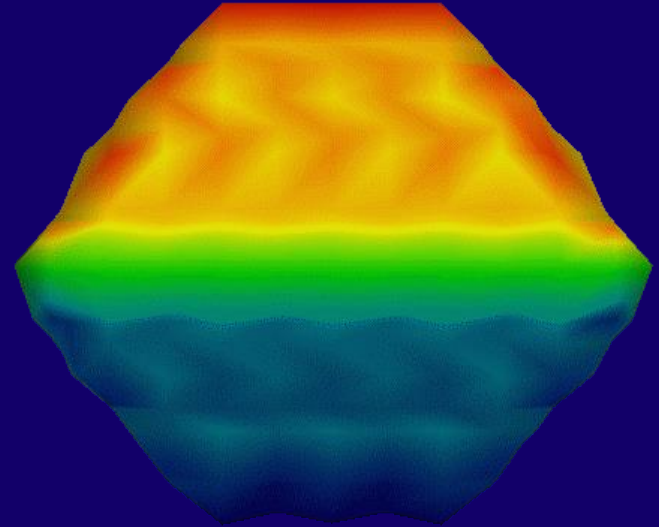
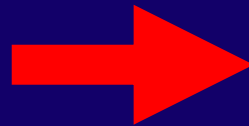
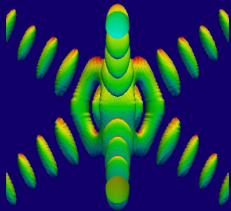
Reconstruction for high Q



High vs low Q:

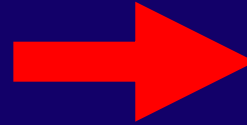
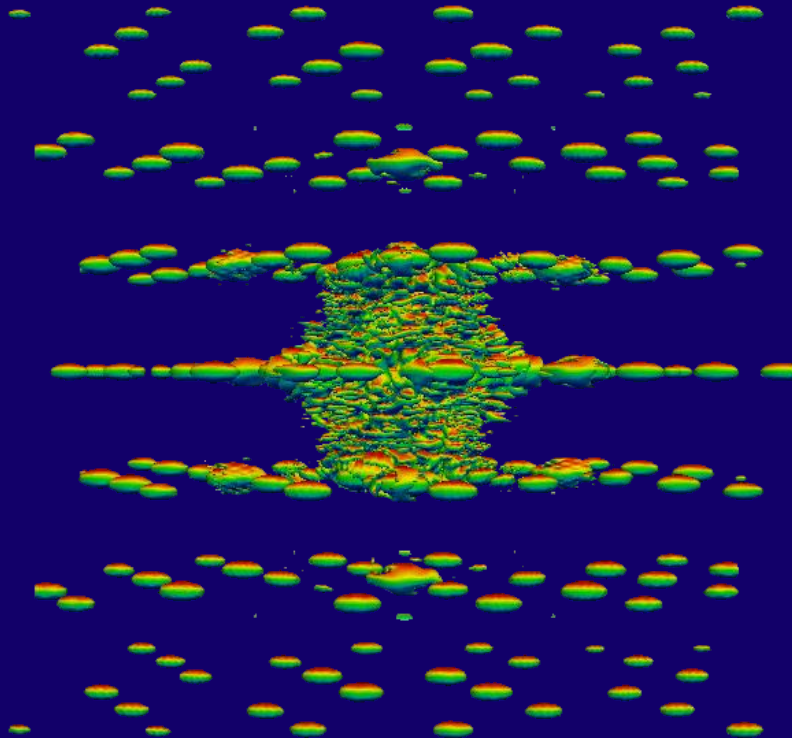
Reciprocal space

Real space

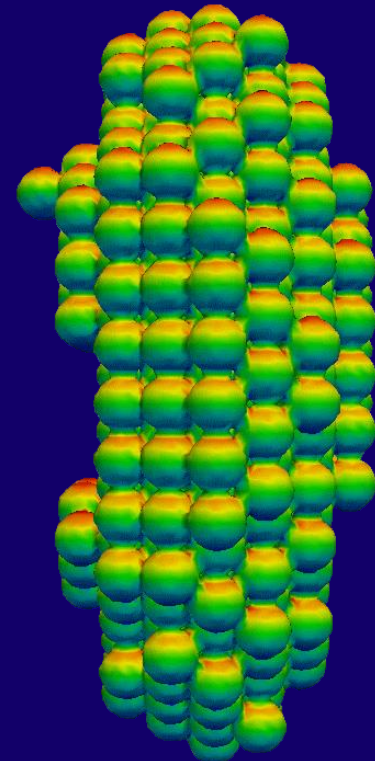


Another example

Reciprocal space



Real space

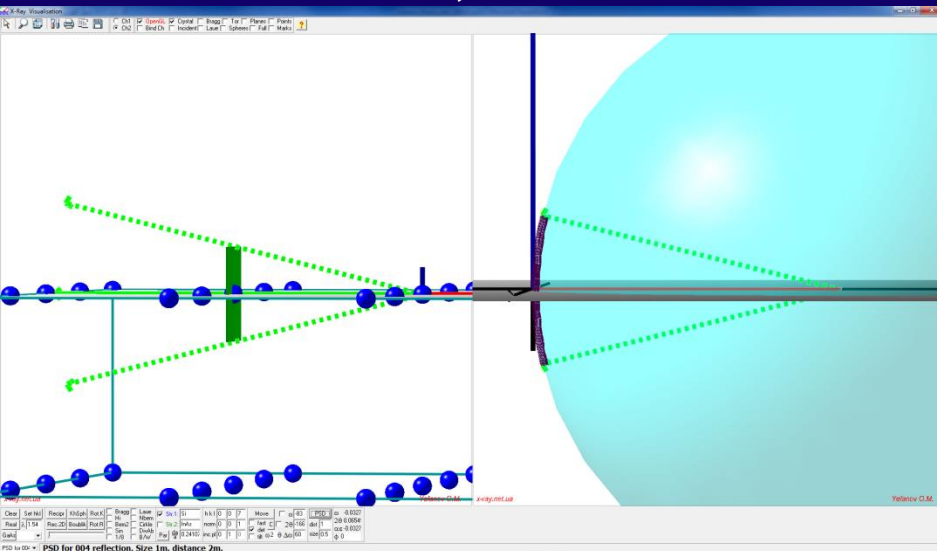




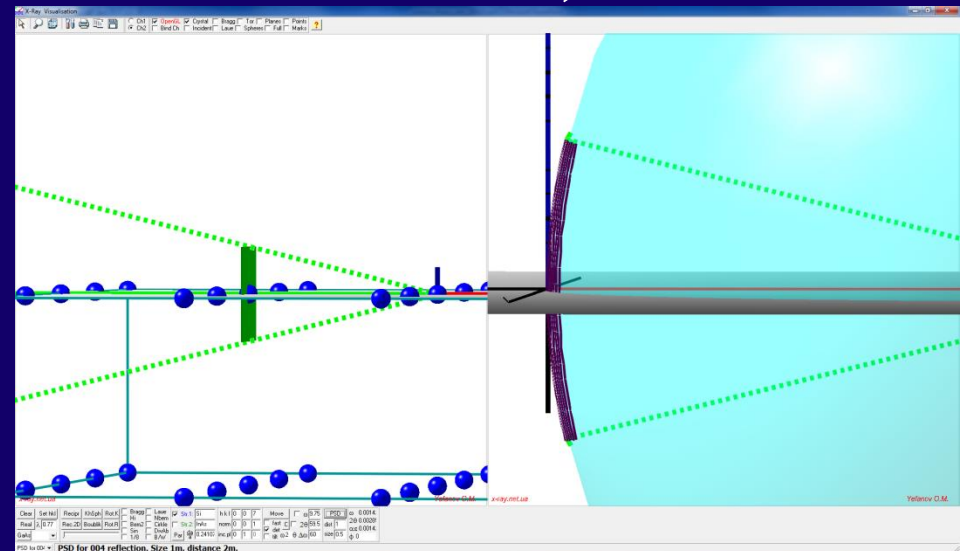
Ewald sphere

Ewald sphere

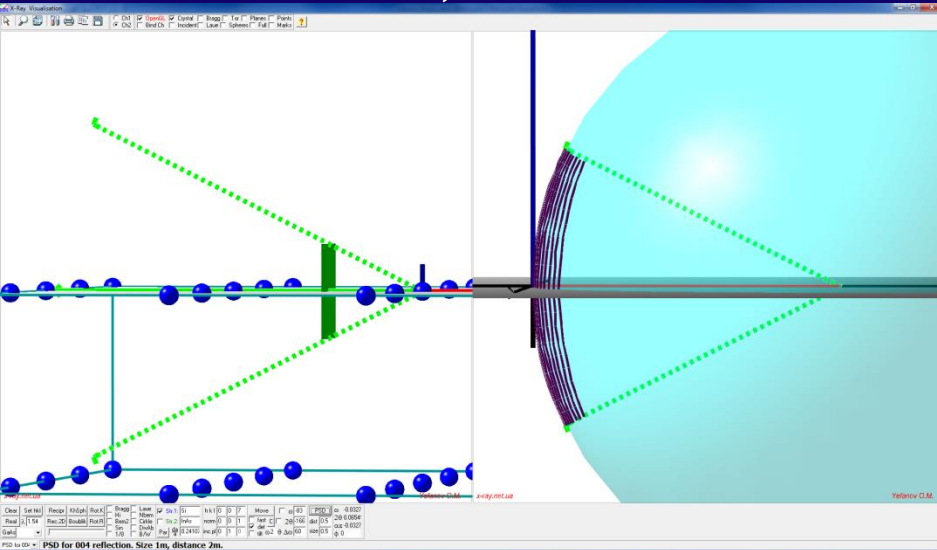
8keV, 1m



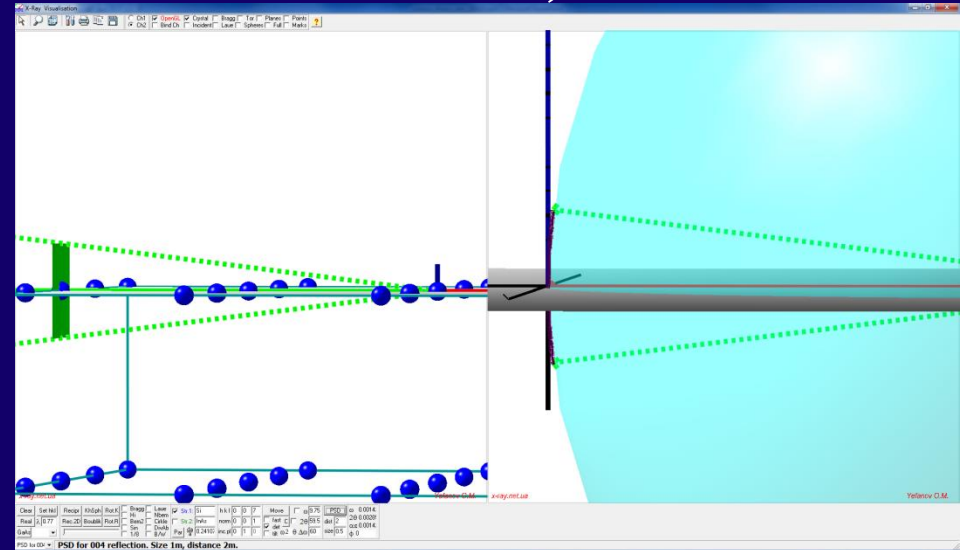
16keV, 1m



8keV, 0.5m

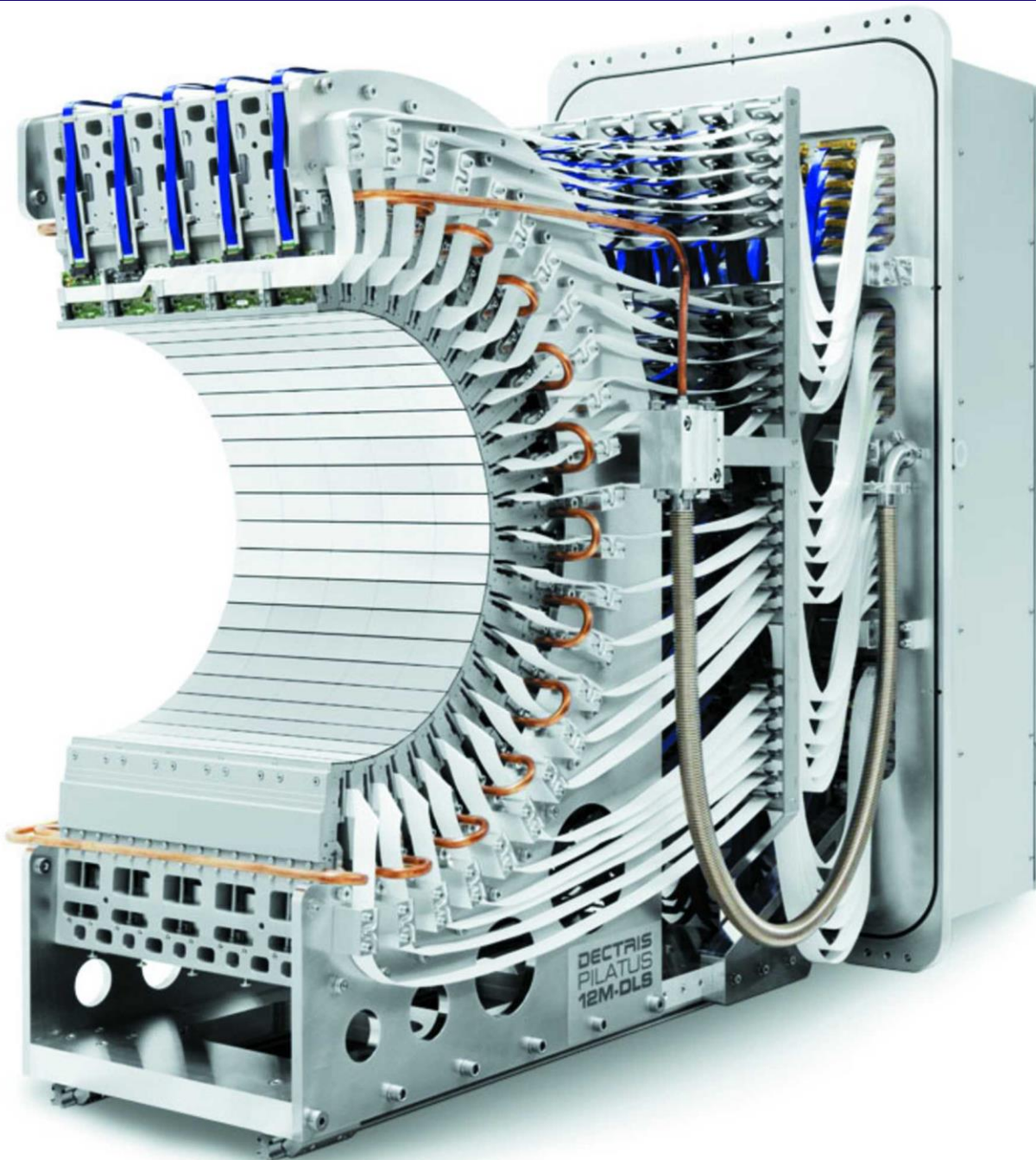


16keV, 2m



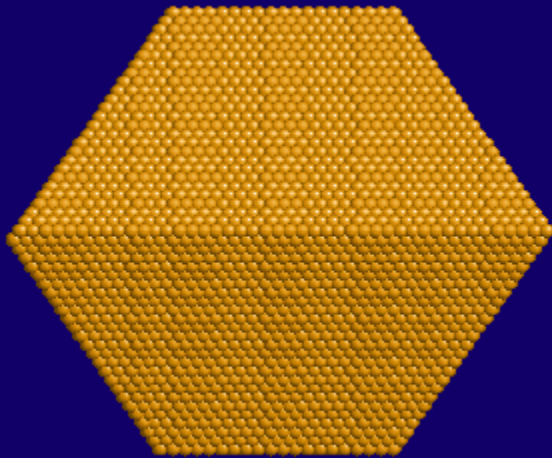
Soft x-rays are difficult for high resolution

**Ewald sphere,
low energy**

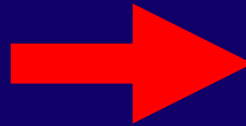


Reciprocal space in 3D

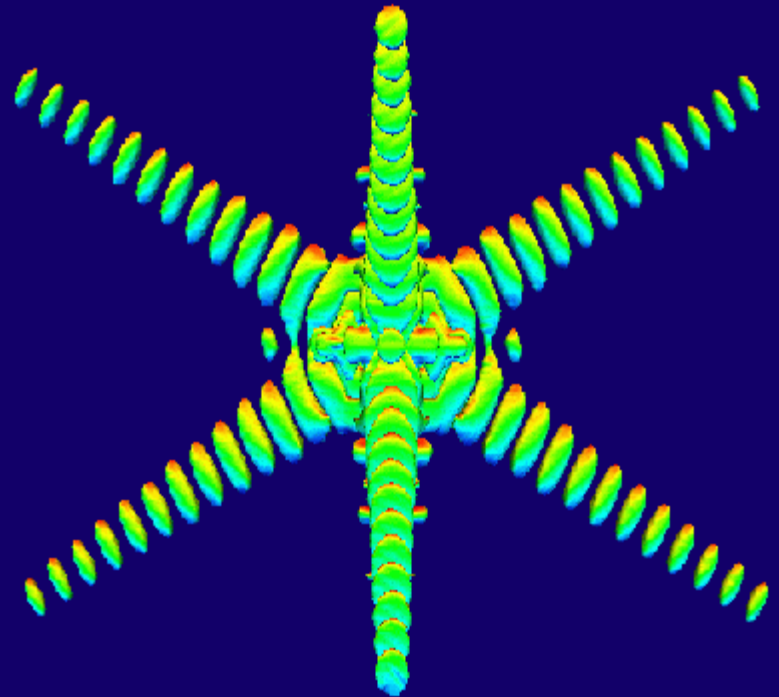
Real (object)



\approx Fourier
transform



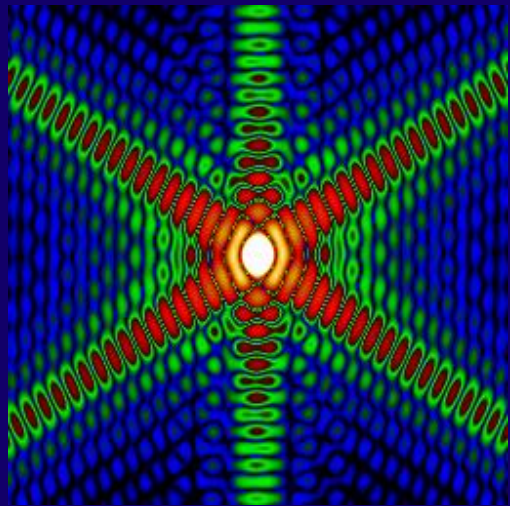
Reciprocal (object)



Truncation rods

Diffraction in real space

7

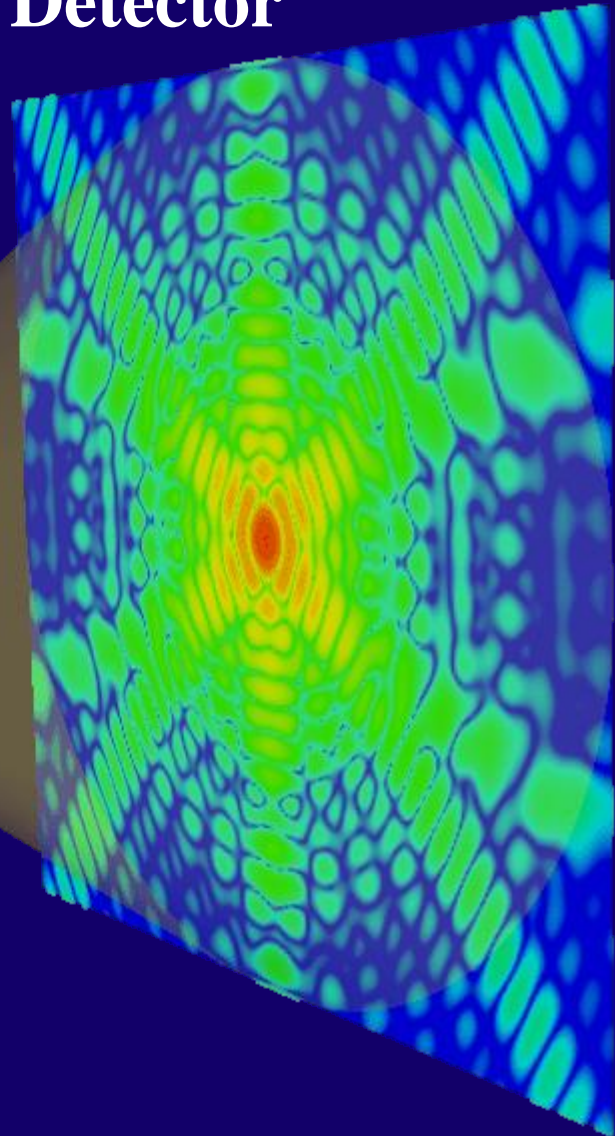


Incident beam



Sample

Detector



Diffraction in reciprocal space

Ewald
sphere

Reciprocal
space of
the object

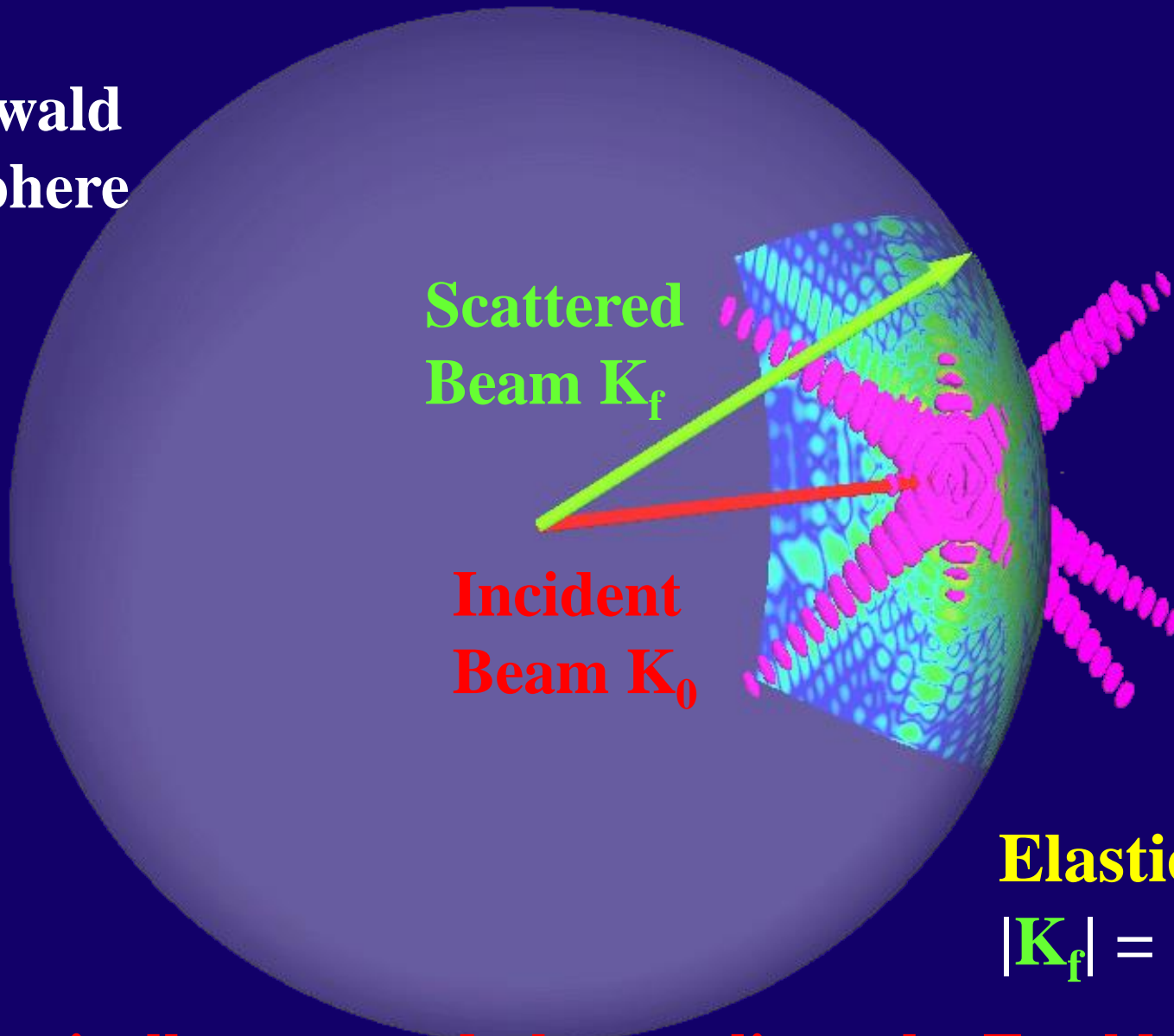
Scattered
Beam \mathbf{K}_f

Incident
Beam \mathbf{K}_0

Elastic scattering:

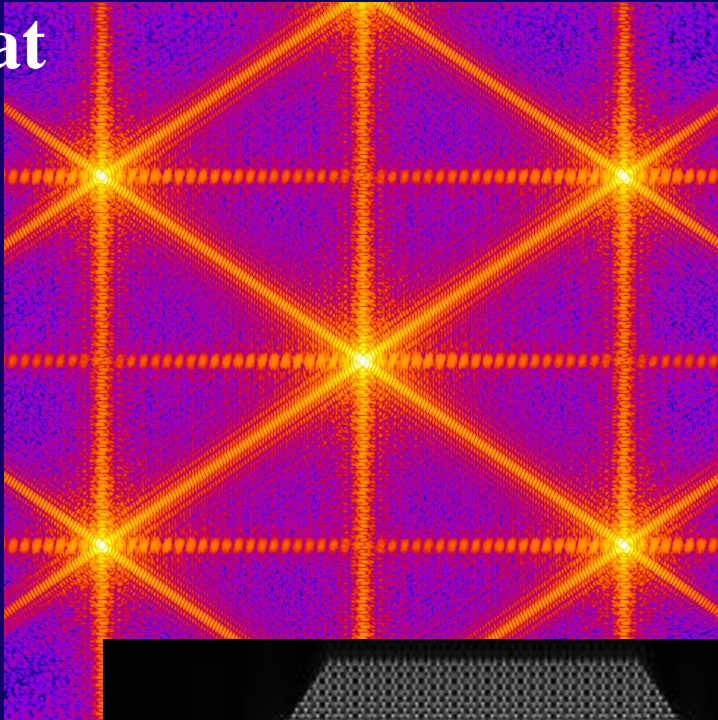
$$|\mathbf{K}_f| = |\mathbf{K}_0| = 2\pi/\lambda$$

Elastically scattered photons lie at the Ewald sphere

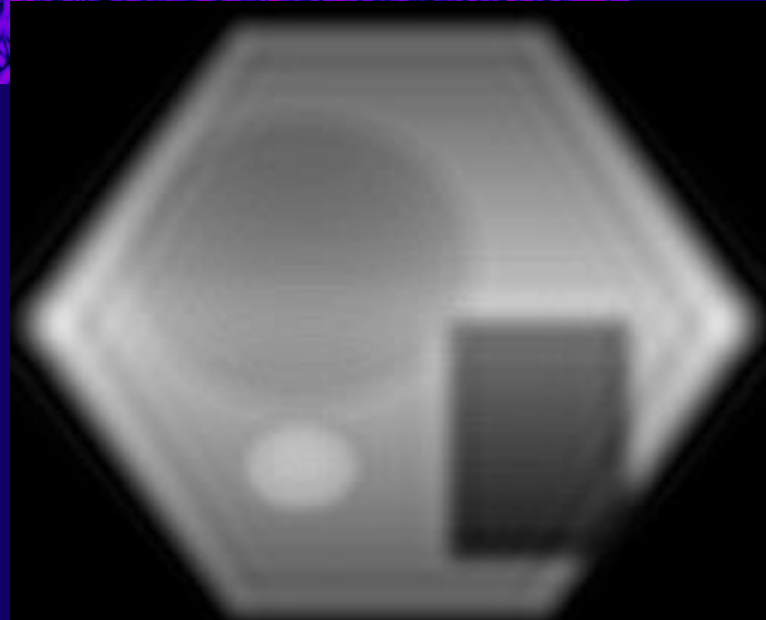
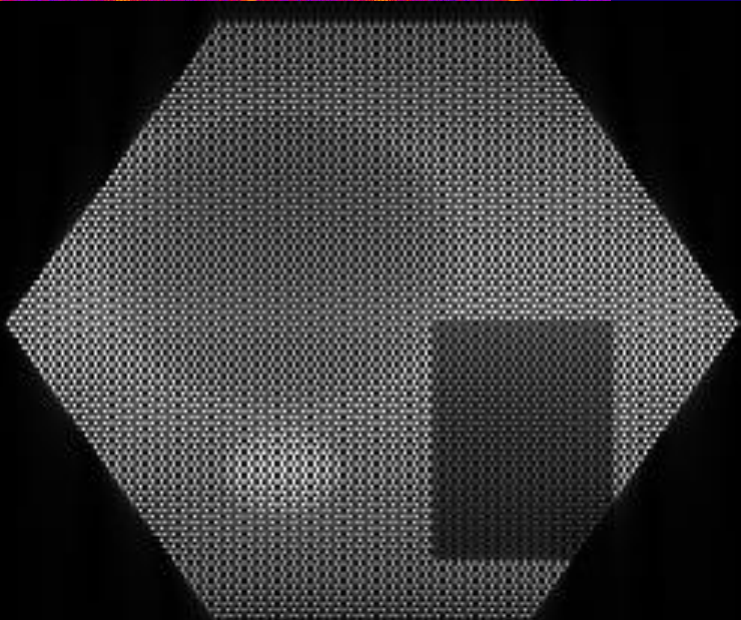
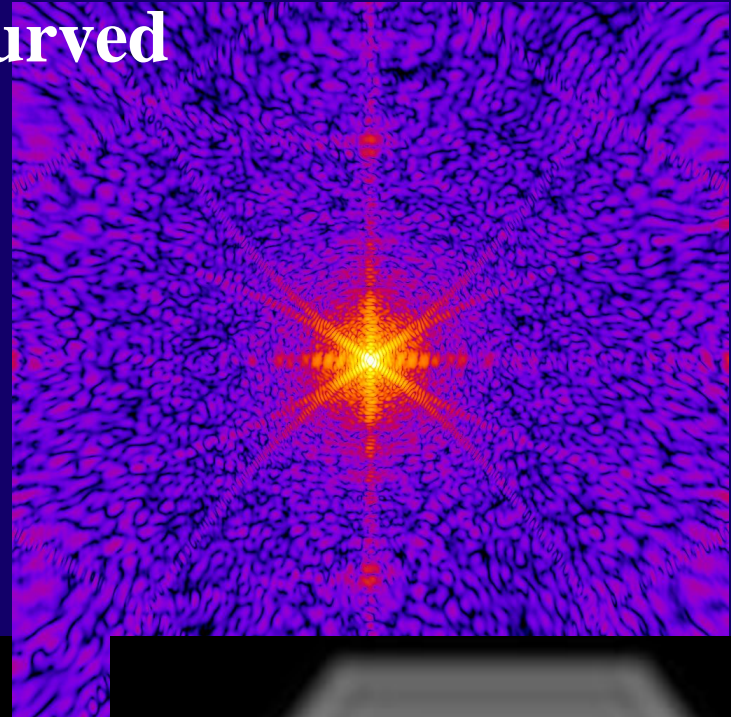


Ewald sphere “effects”

Flat

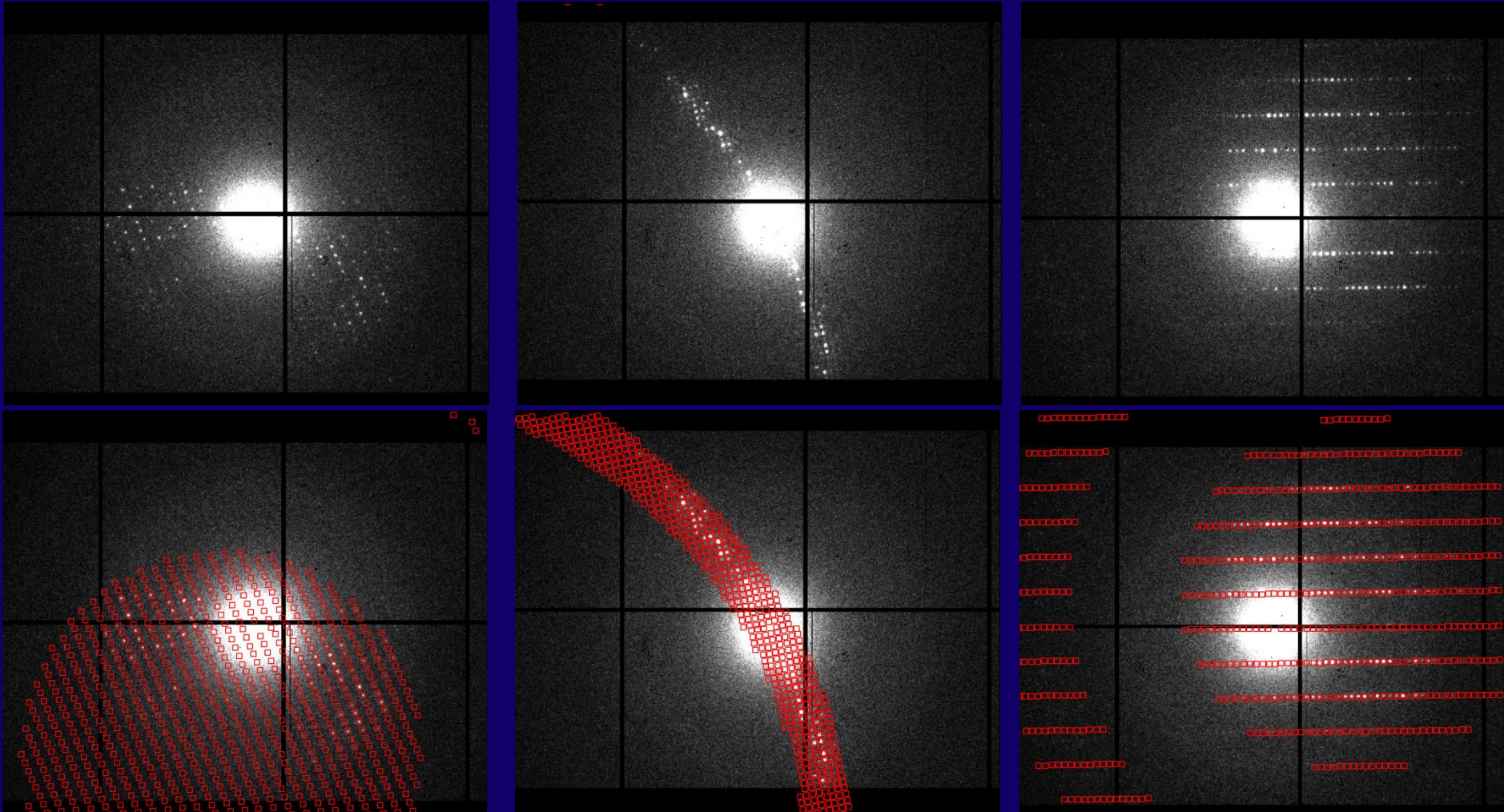


Curved



Electron Diffraction

500keV, $L = 1570\text{mm}$, $D \text{ (vert)} = 34\text{mm}$, so $L/D = 50!$

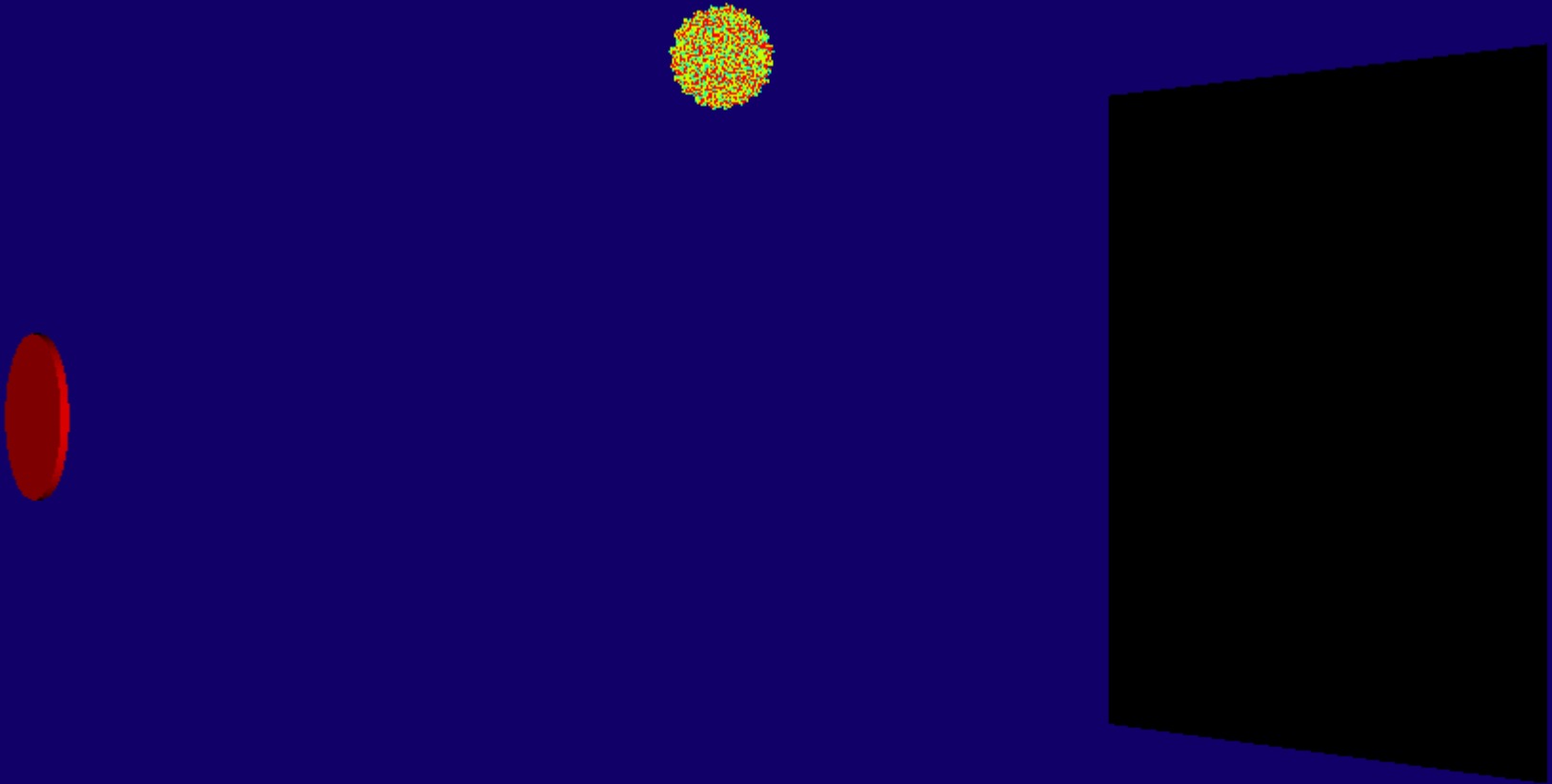


Even for electrons Ewald sphere is not “flat”!

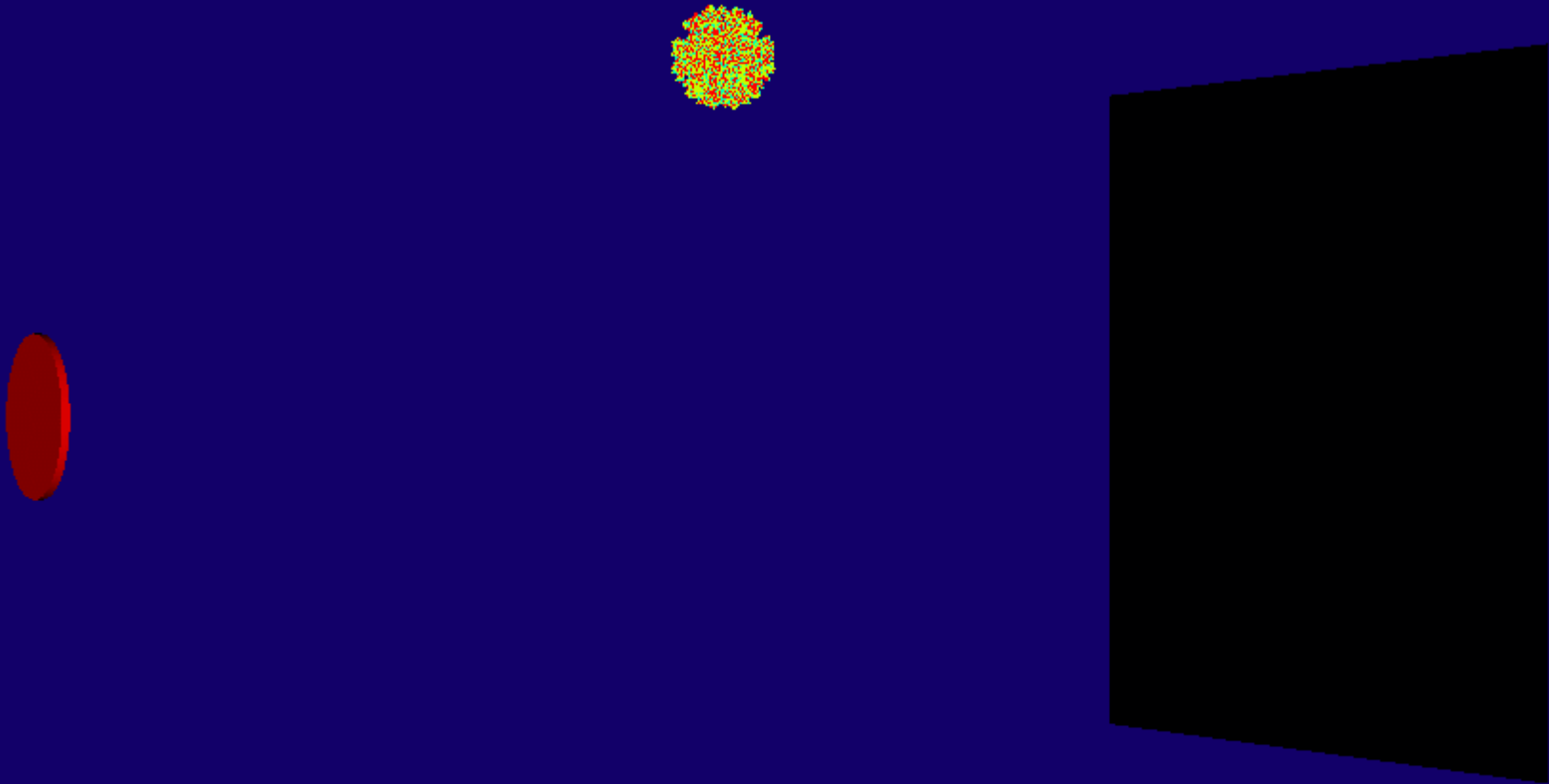


Single Particle Imaging (SPI)

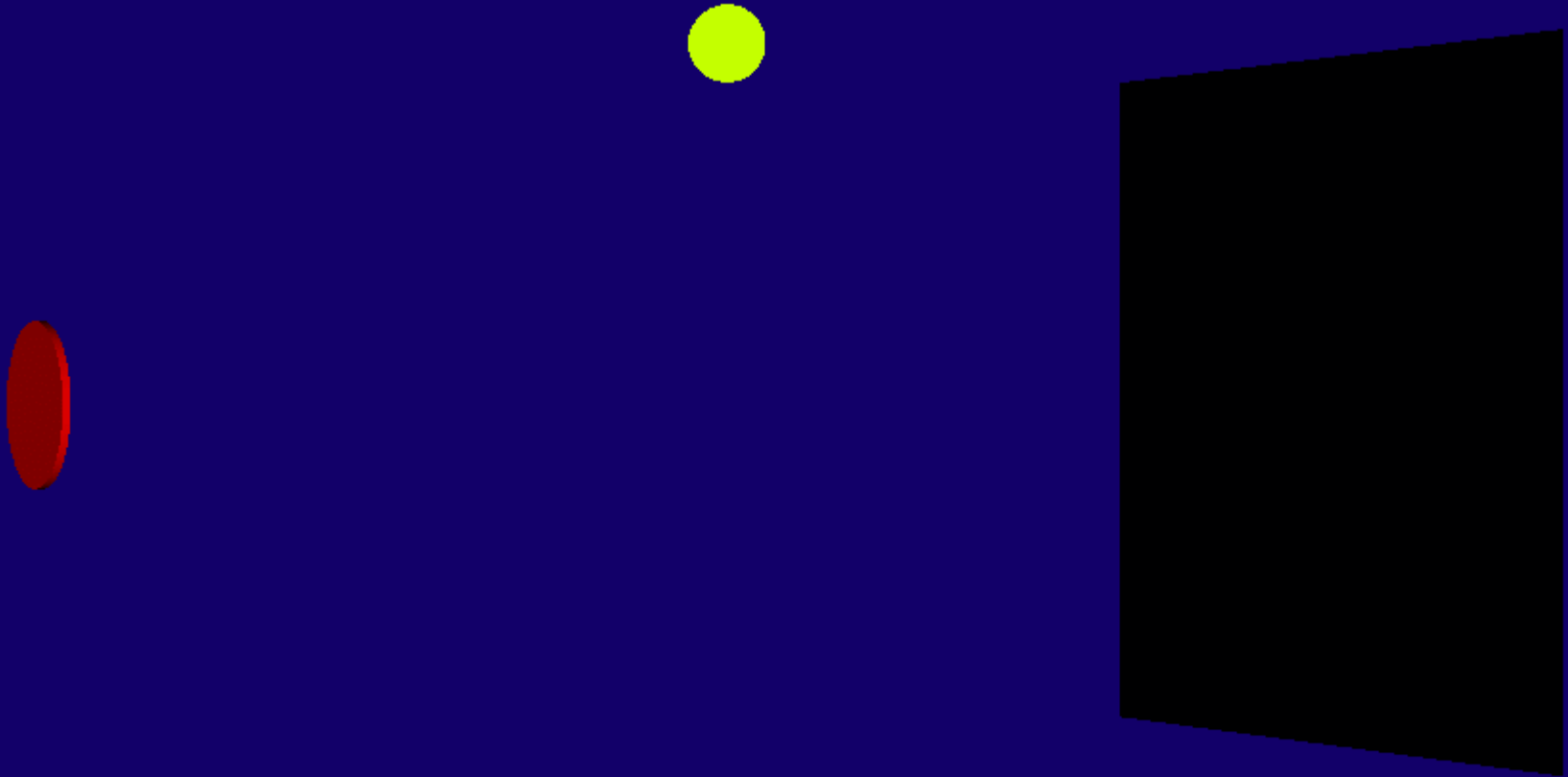
Diffraction on a single virus



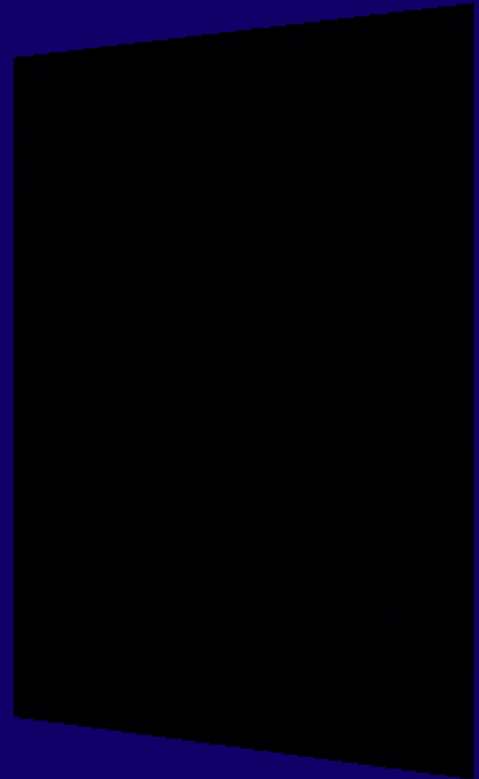
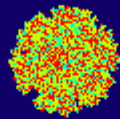
Diffraction on a single virus



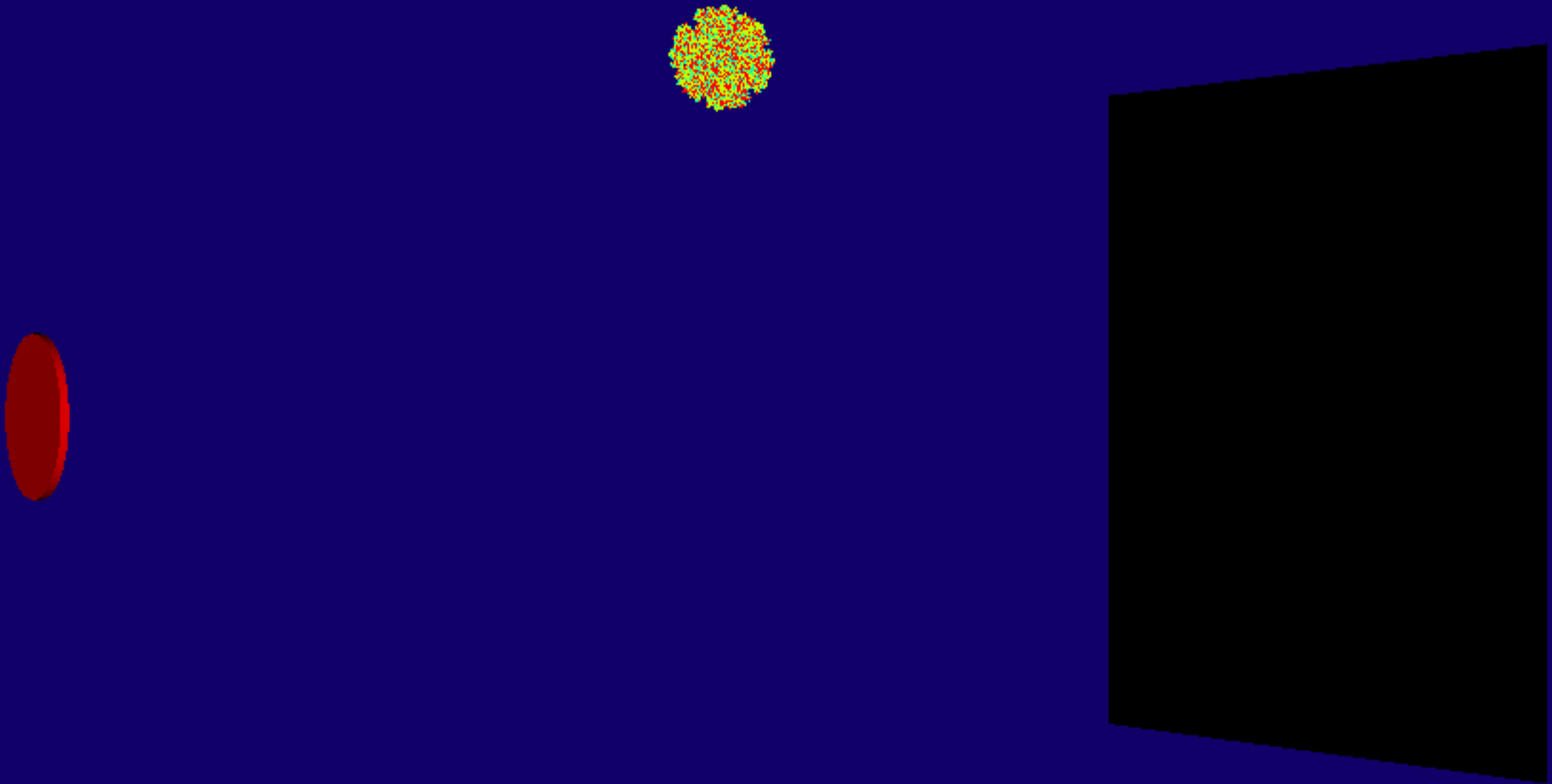
Diffraction on a a drop of water



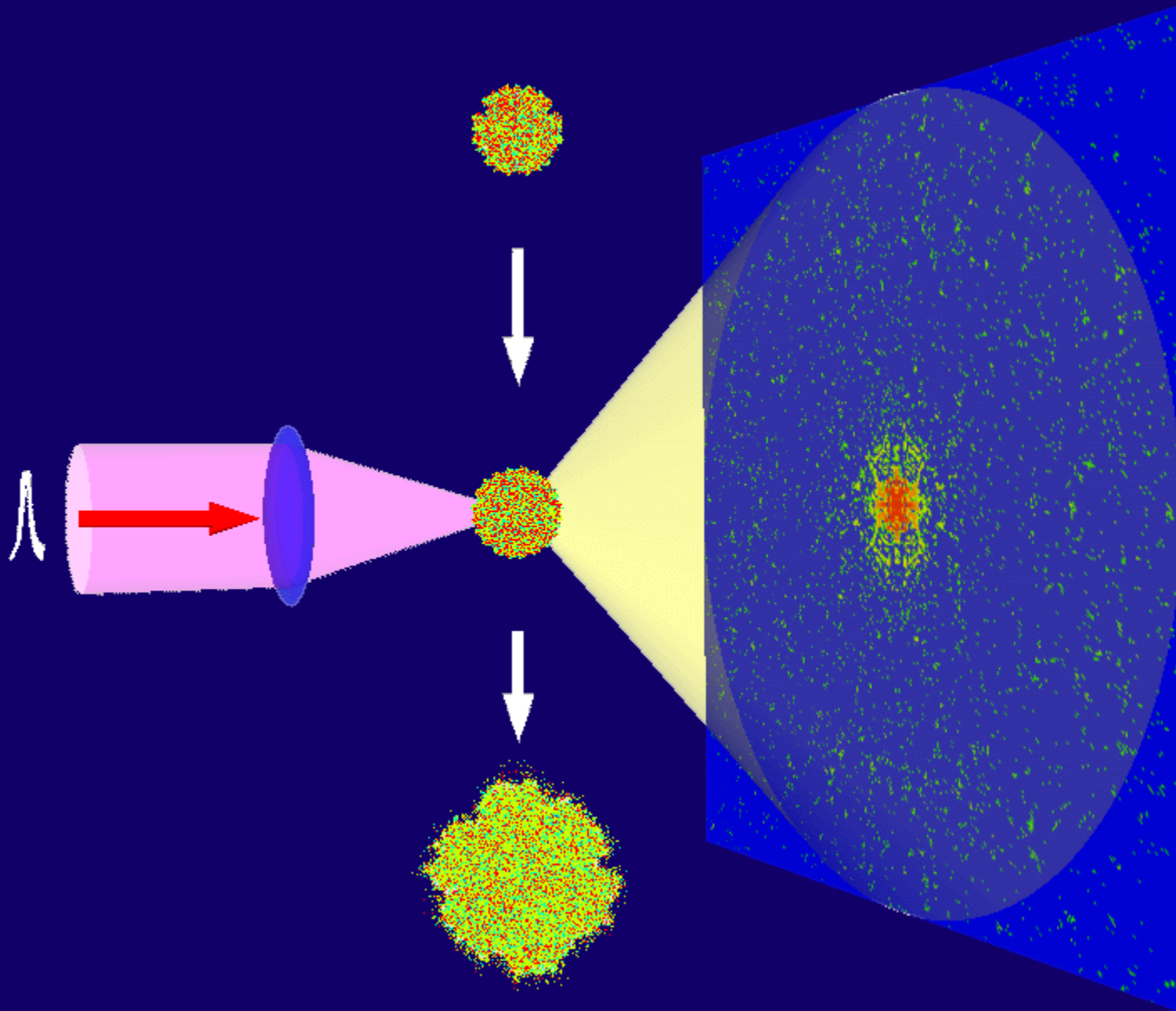
Miss the target



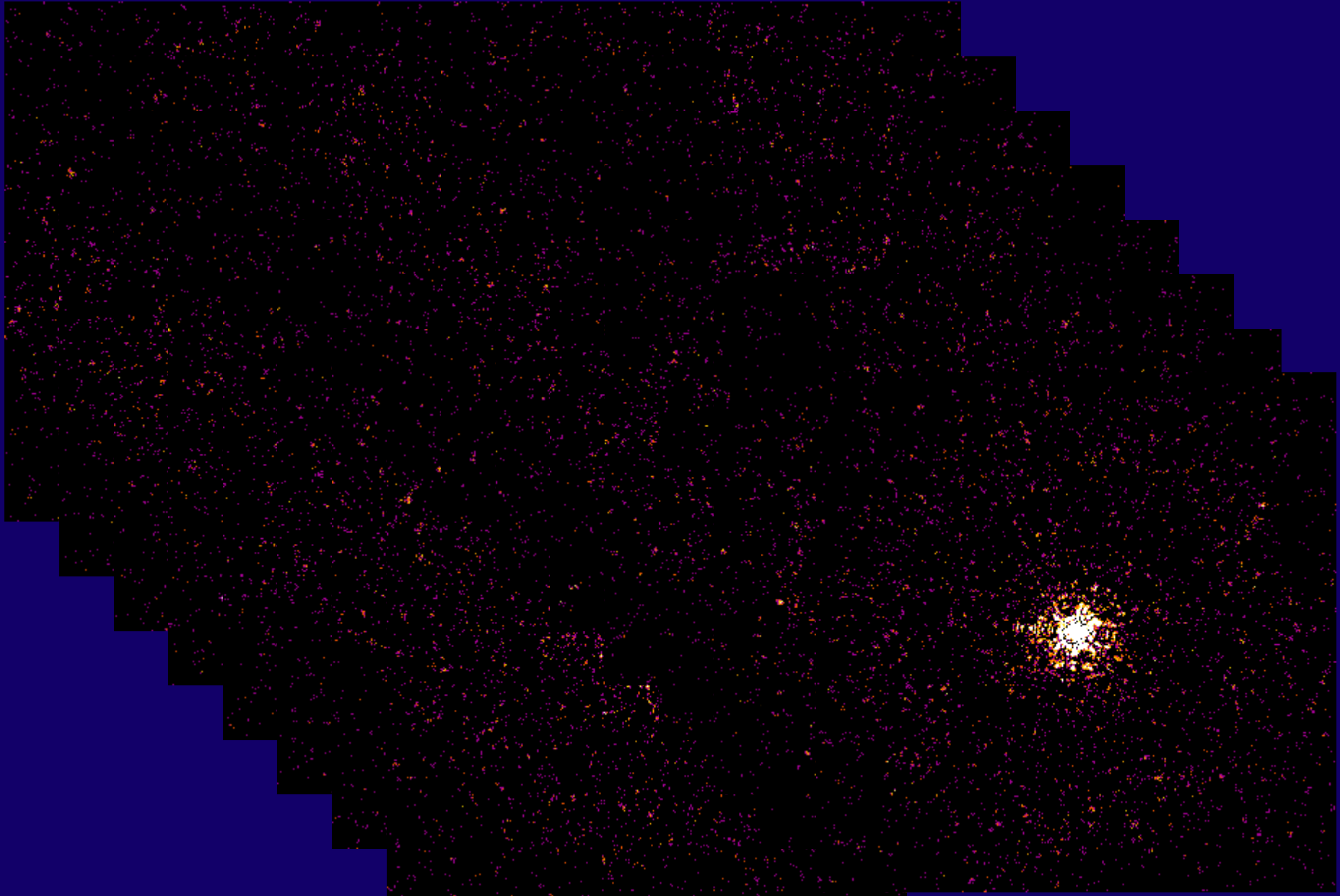
Diffraction on a single virus



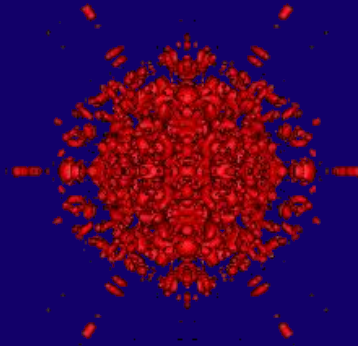
Real experiment schematic



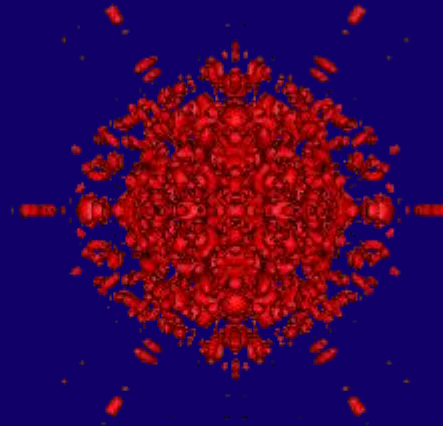
Single shot diffraction patterns



SPI, 3D merging



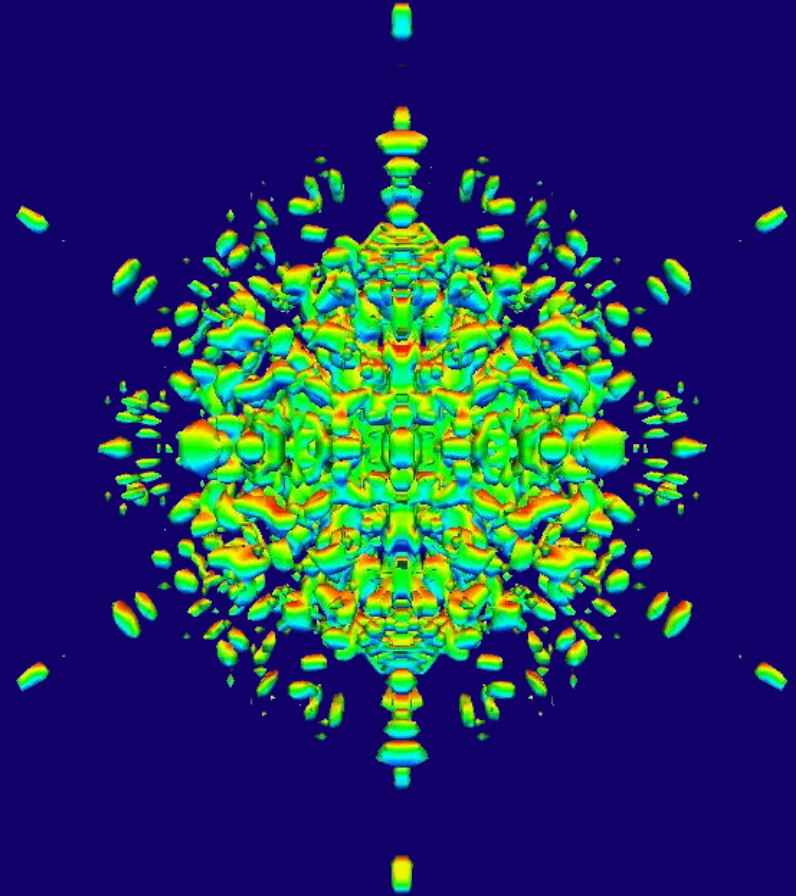
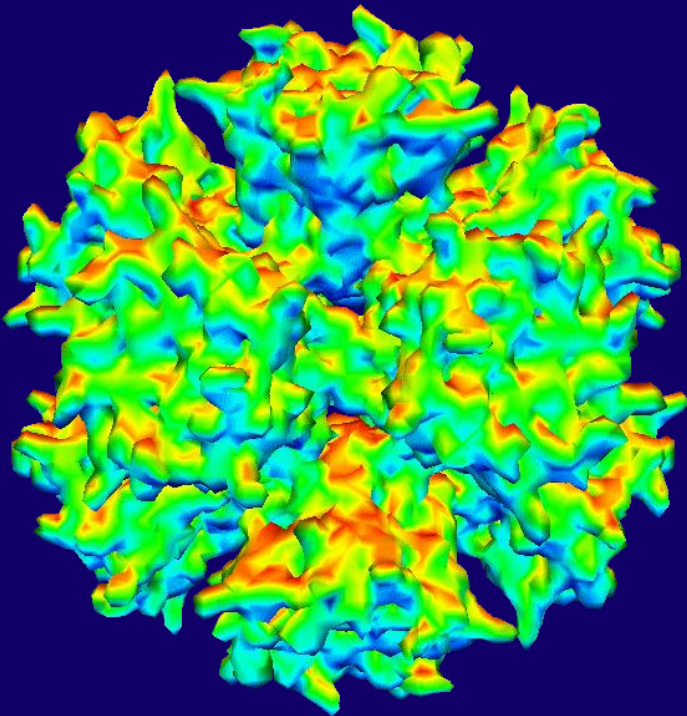
SPI, orientation refinement



Virus 2c6s (200k atoms), 27nm
12000 random oriented patterns

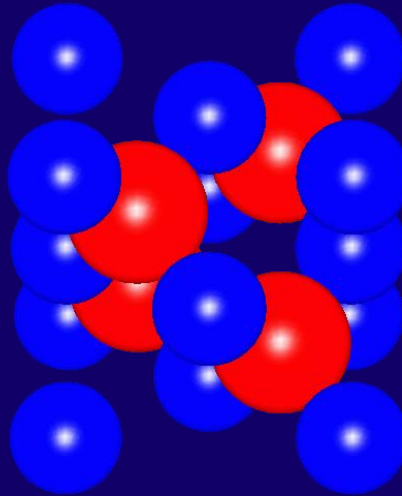
Real space

Reciprocal space



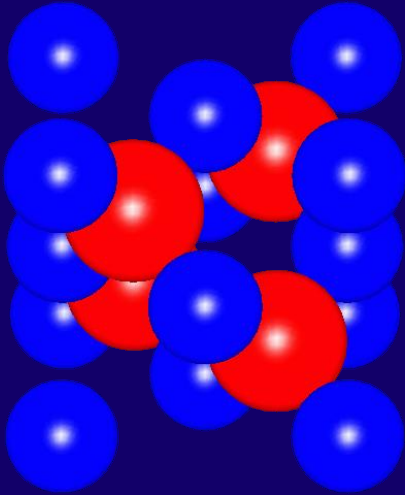


Why crystals?

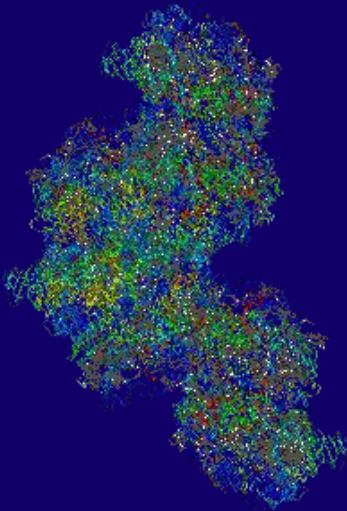


Unit cells

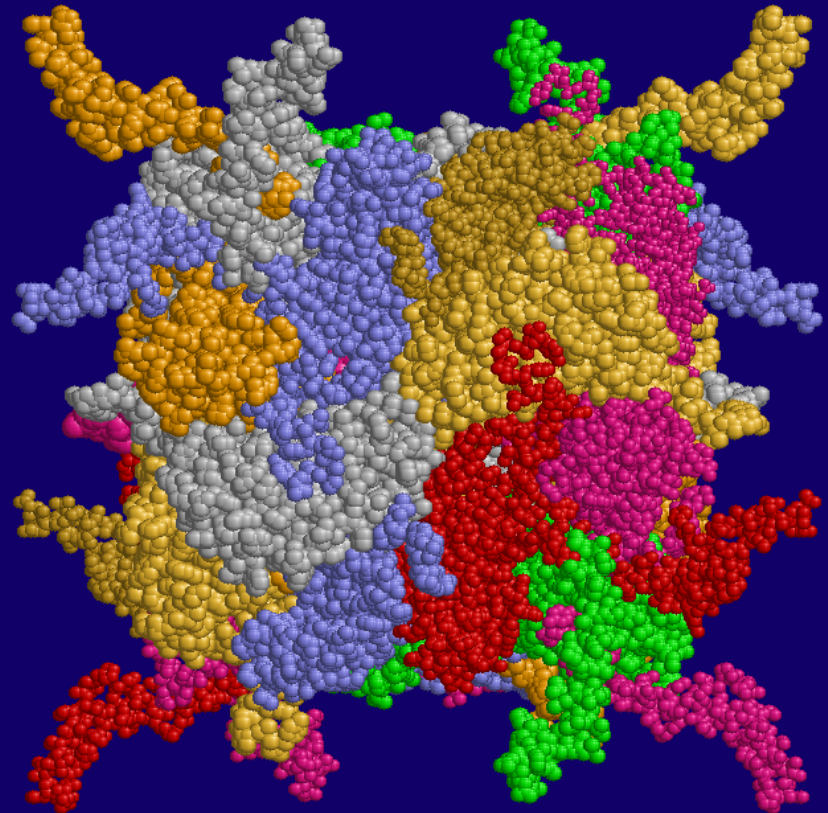
GaAs



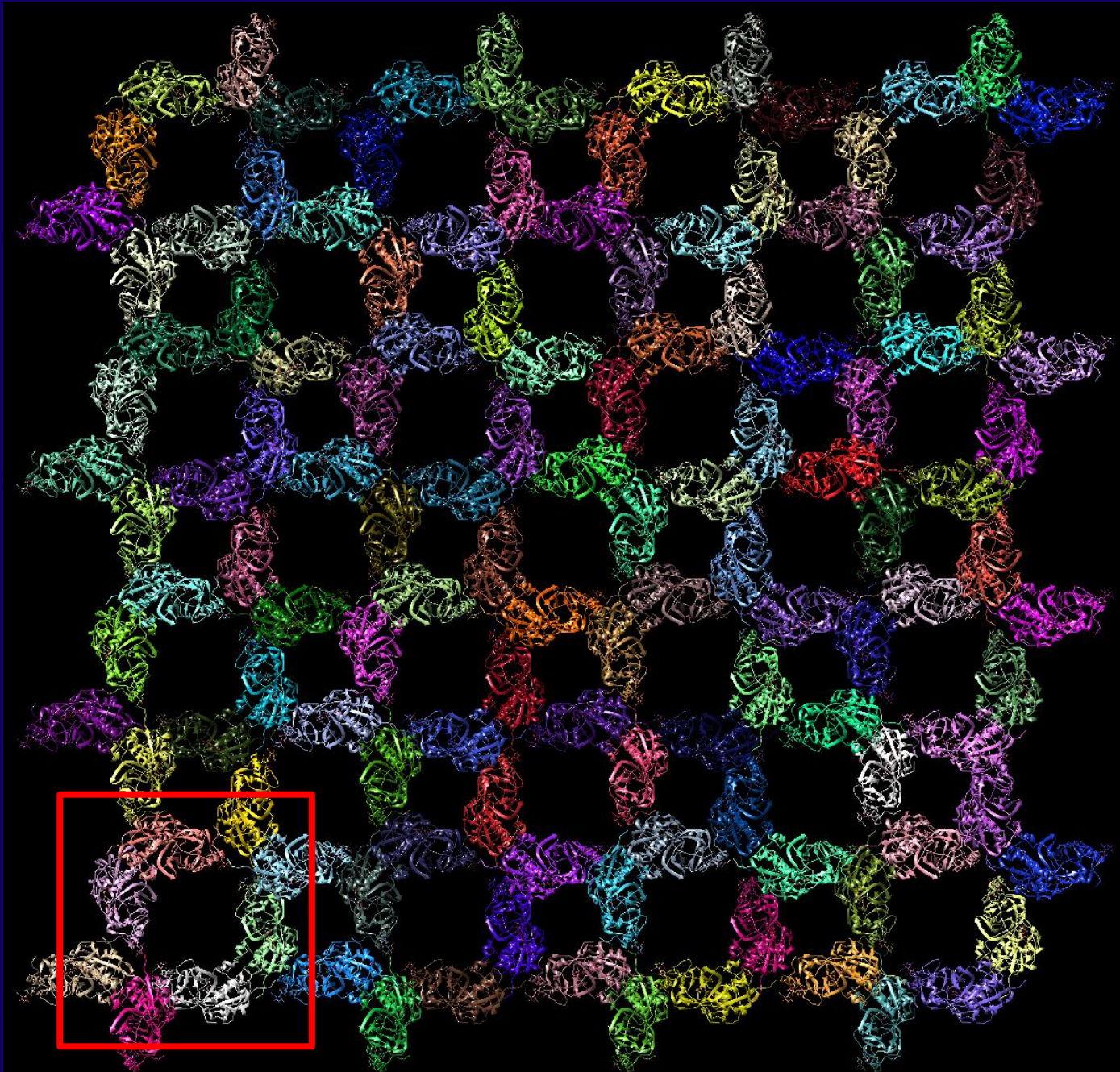
PS2



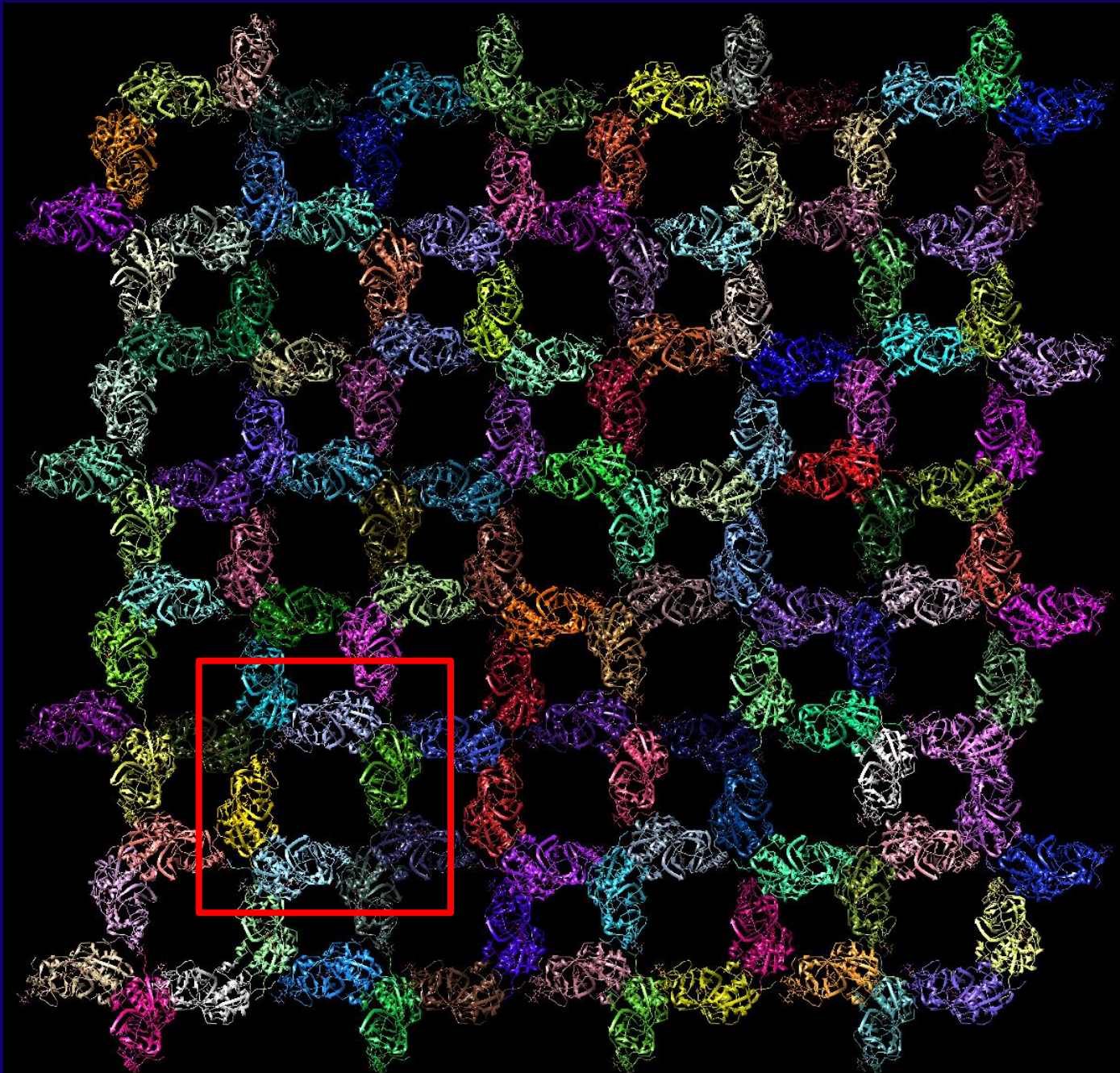
GV



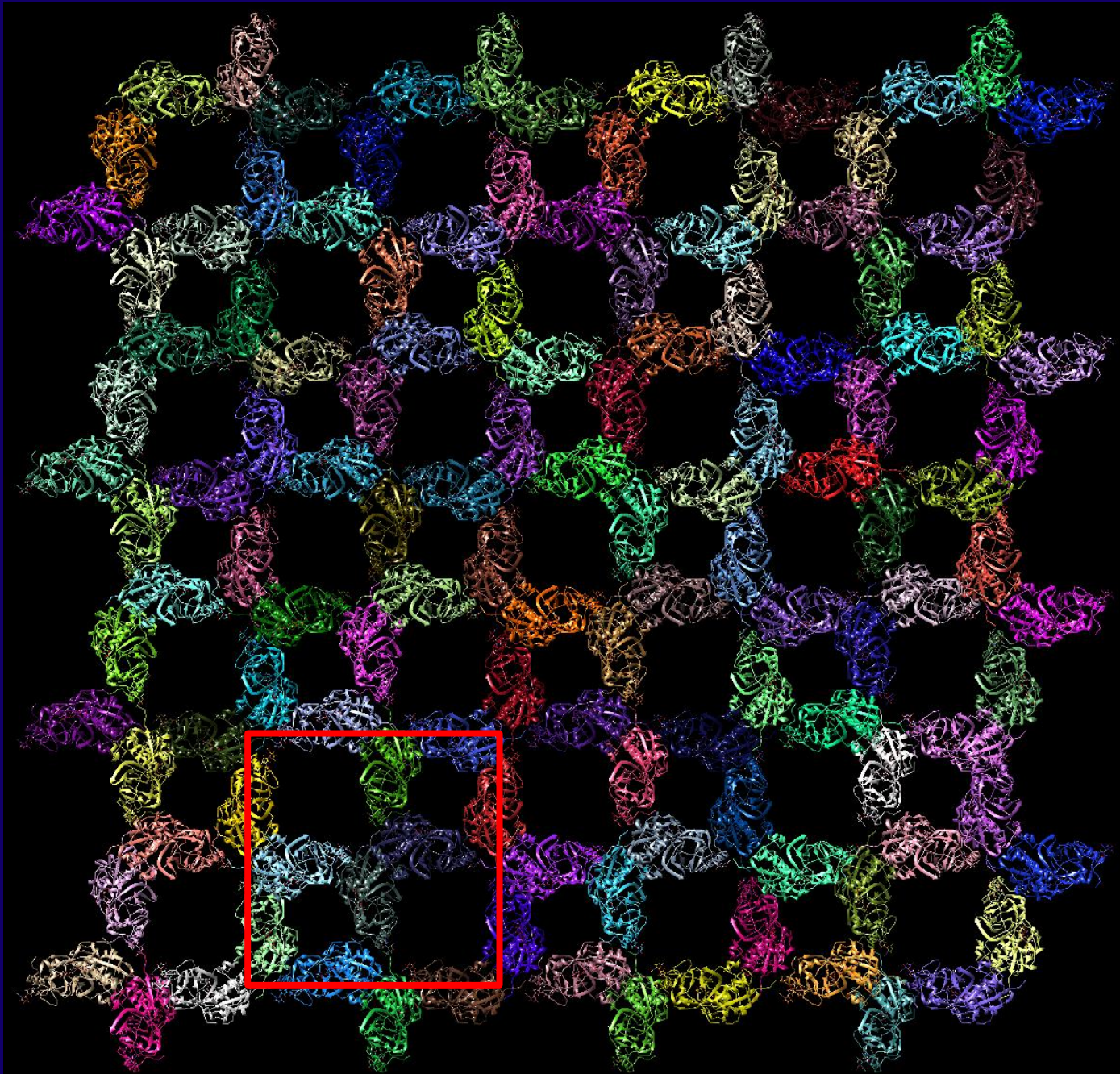
The choice of a unit cell



The choice of a unit cell

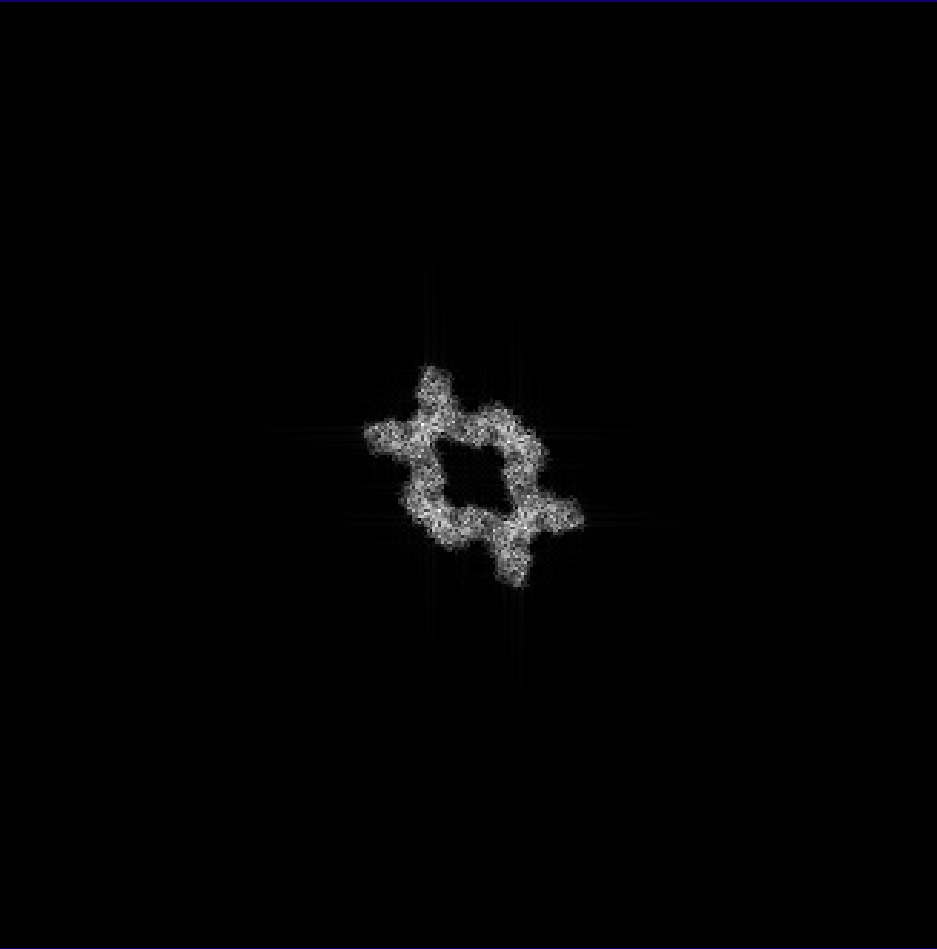


The choice of a unit cell

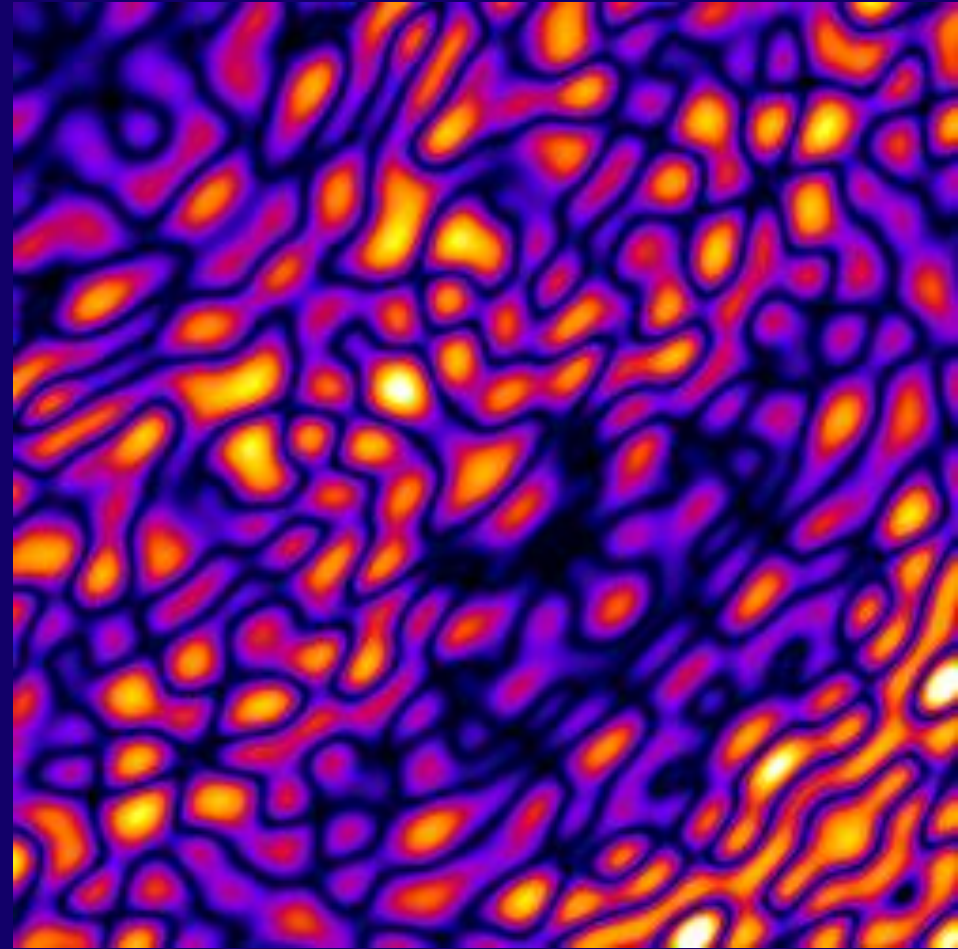


Introduction into crystallography

1 unit cell (CatB)



Ideal diffraction pattern

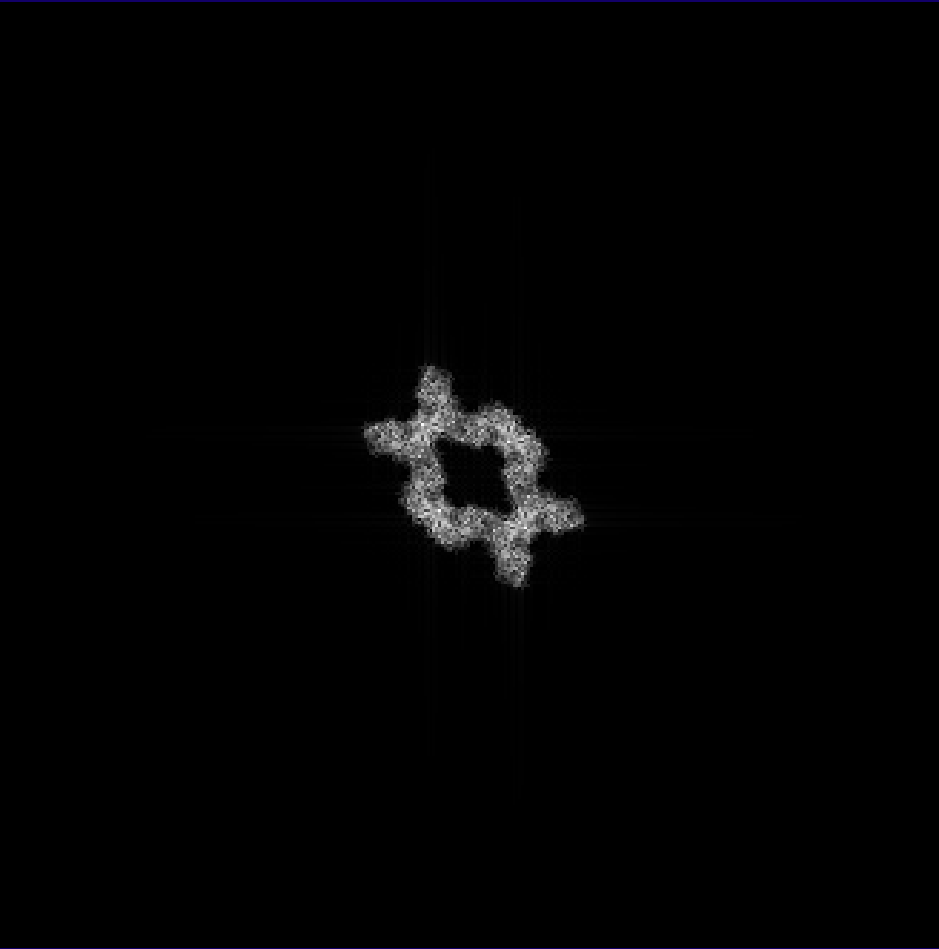




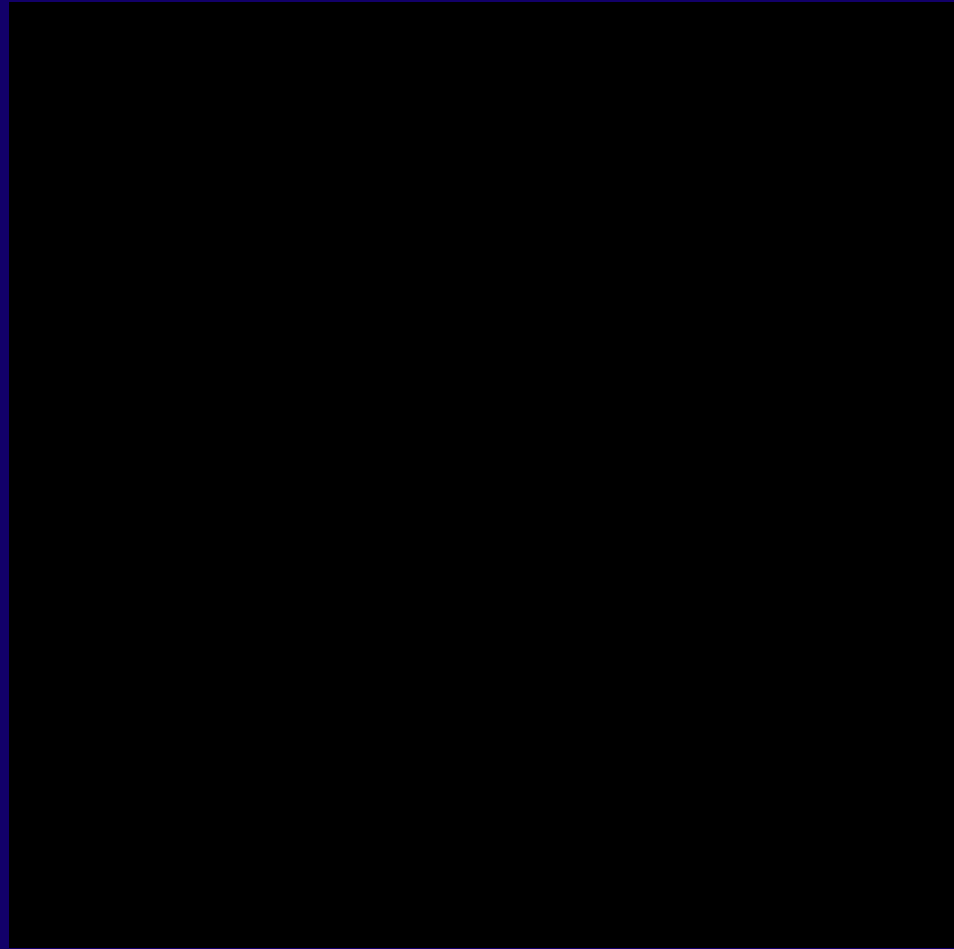
Again, why crystals?

Introduction into crystallography

1 unit cell (CatB)

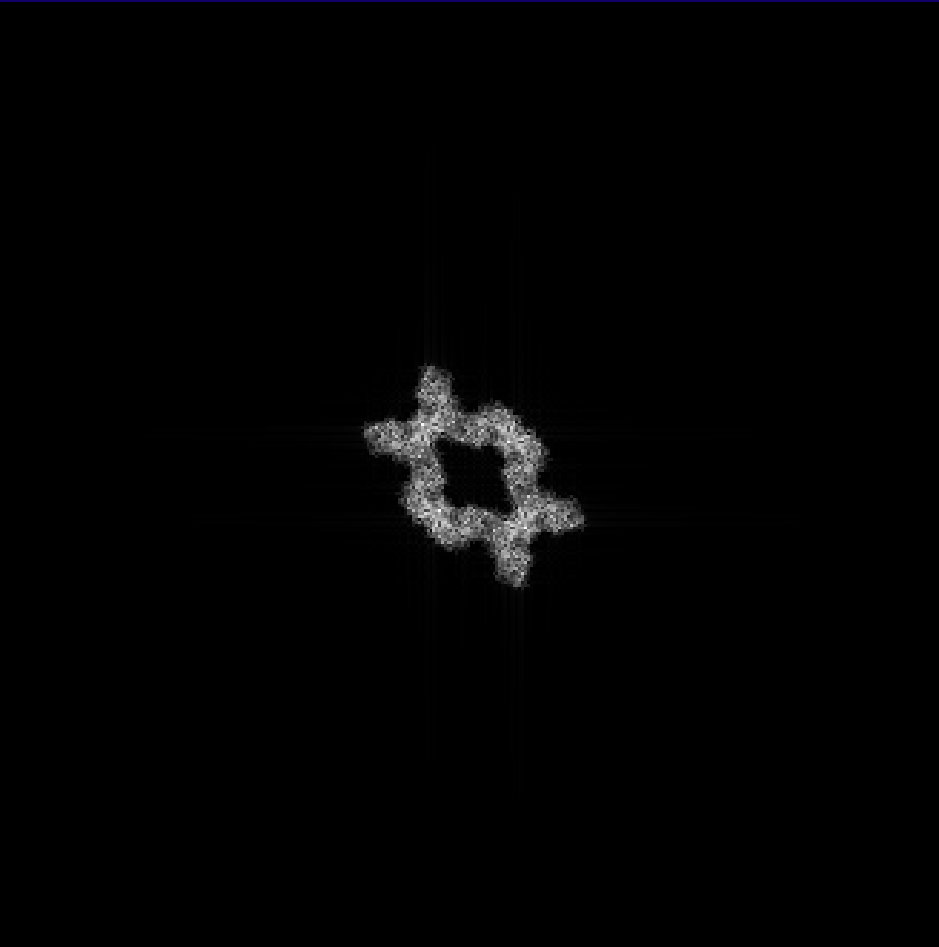


Realistic diffraction pattern

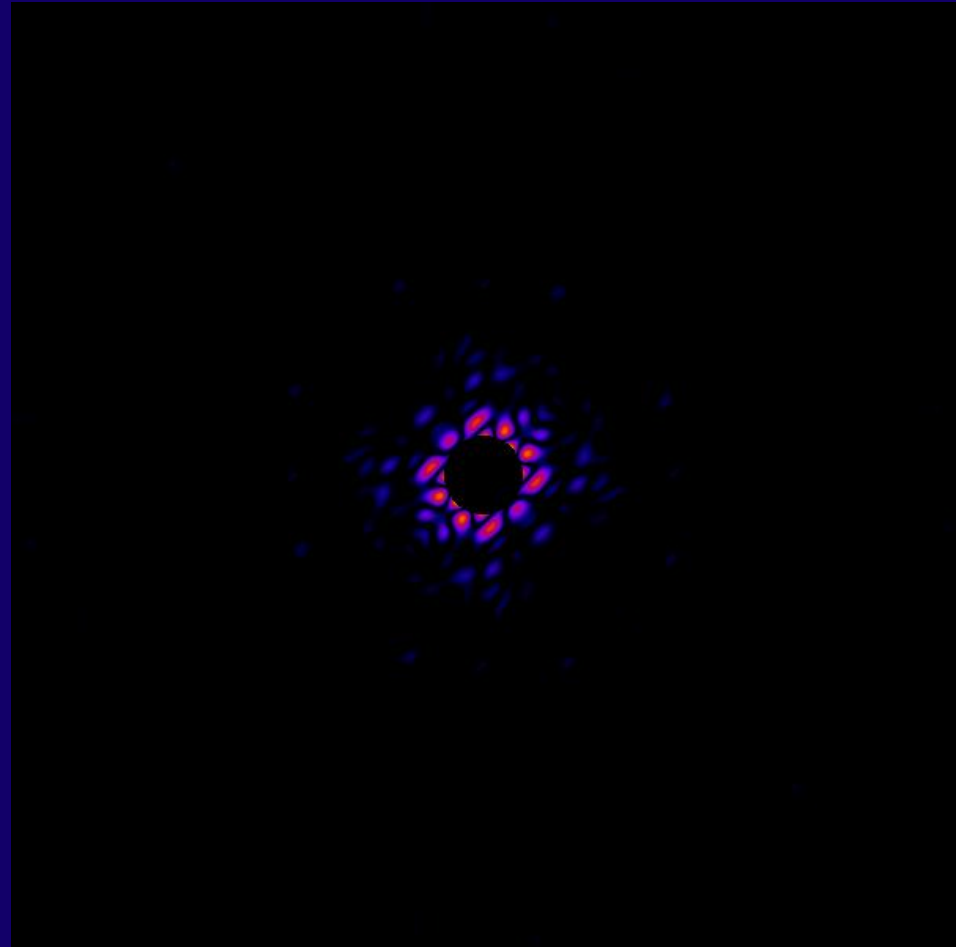


Introduction into crystallography

1 unit cell (CatB)



Diffraction pattern

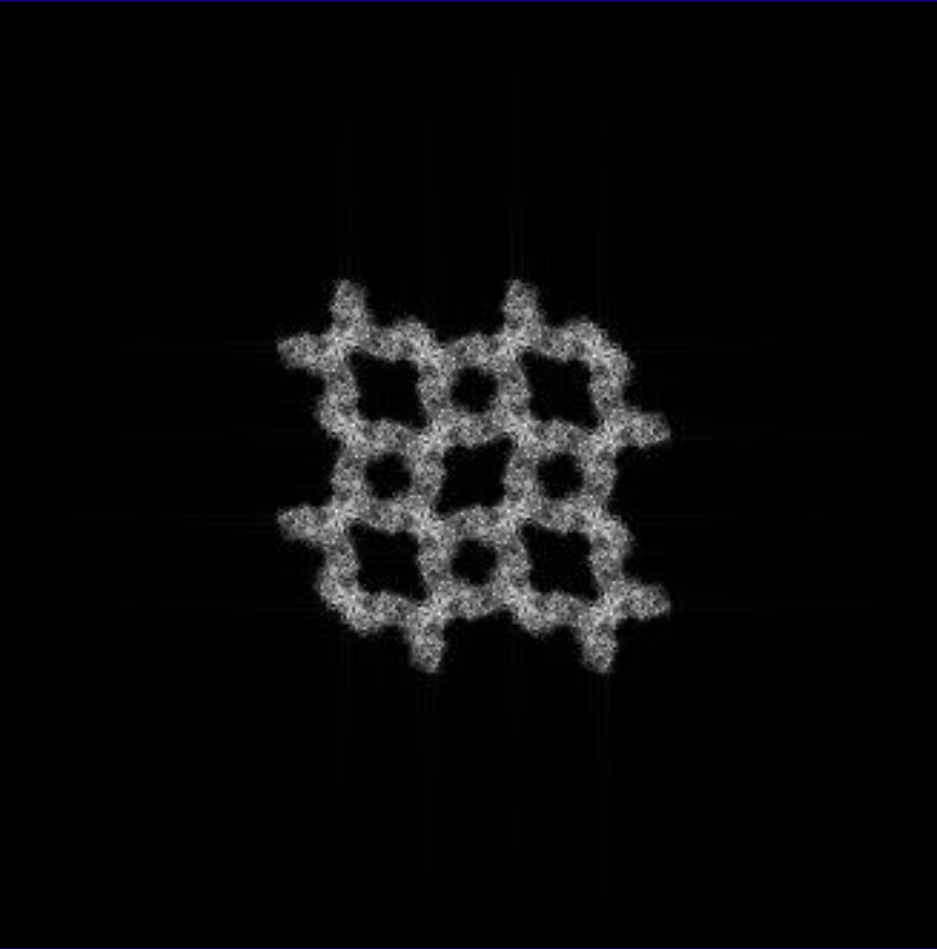


All simulations made with Moltrans

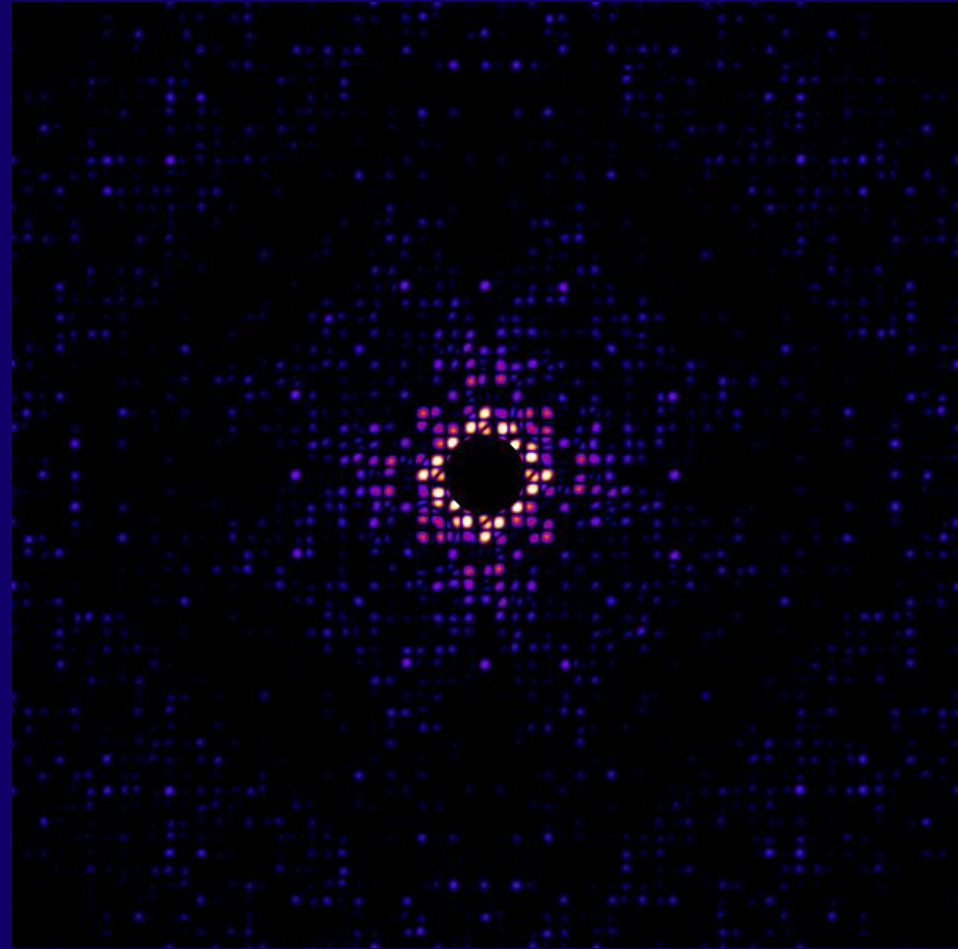
Unreal flux (1e20 photons)

Introduction into crystallography

2x2 unit cells (CatB)



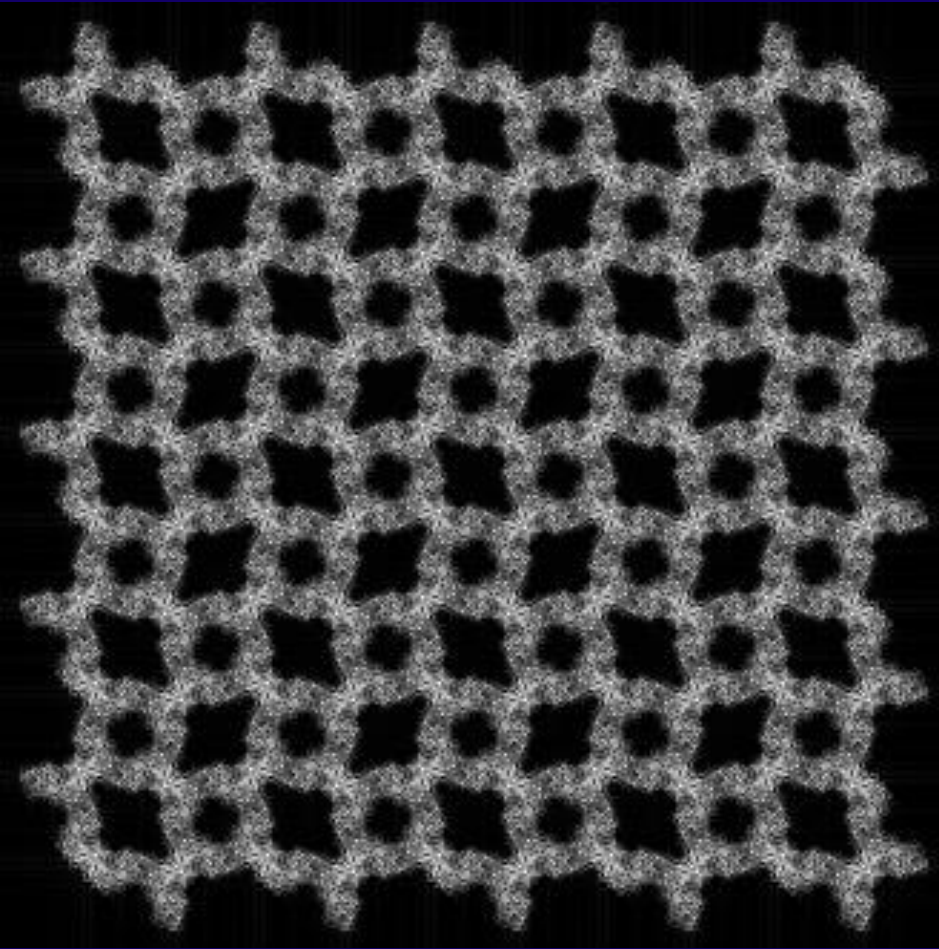
Diffraction pattern



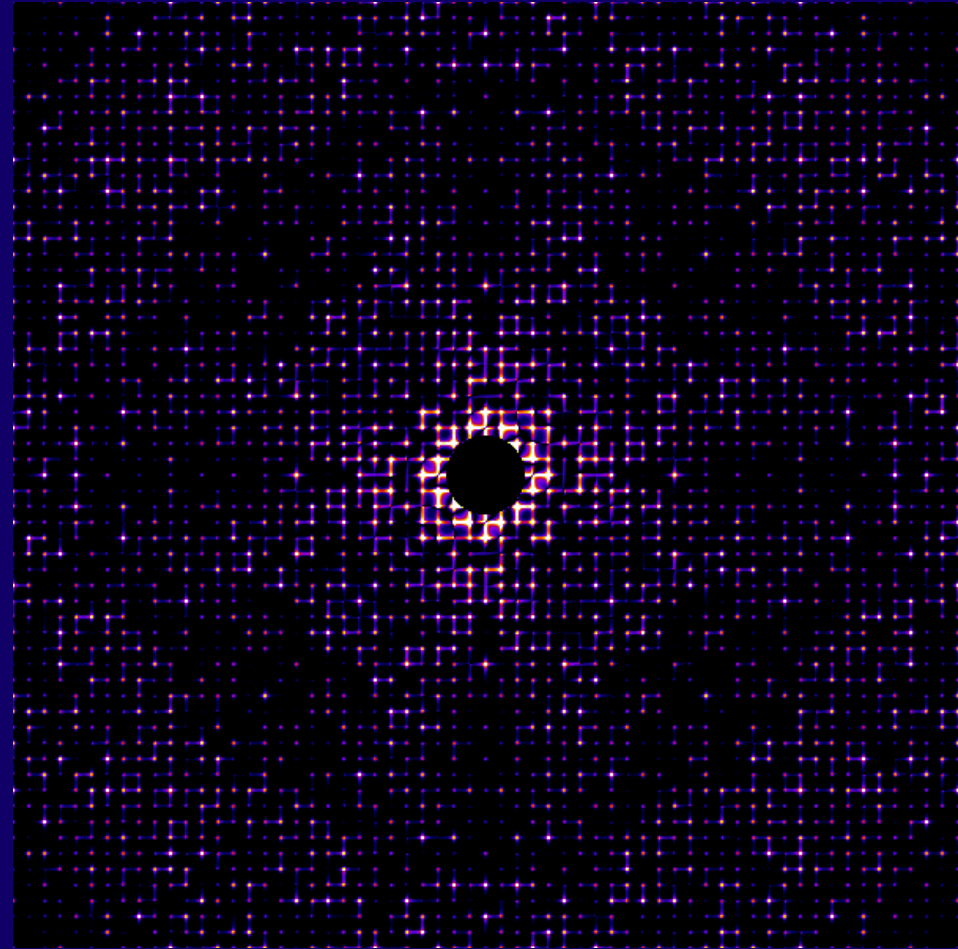
All simulations made with Moltrans

Introduction into crystallography

5x5 unit cells (CatB)



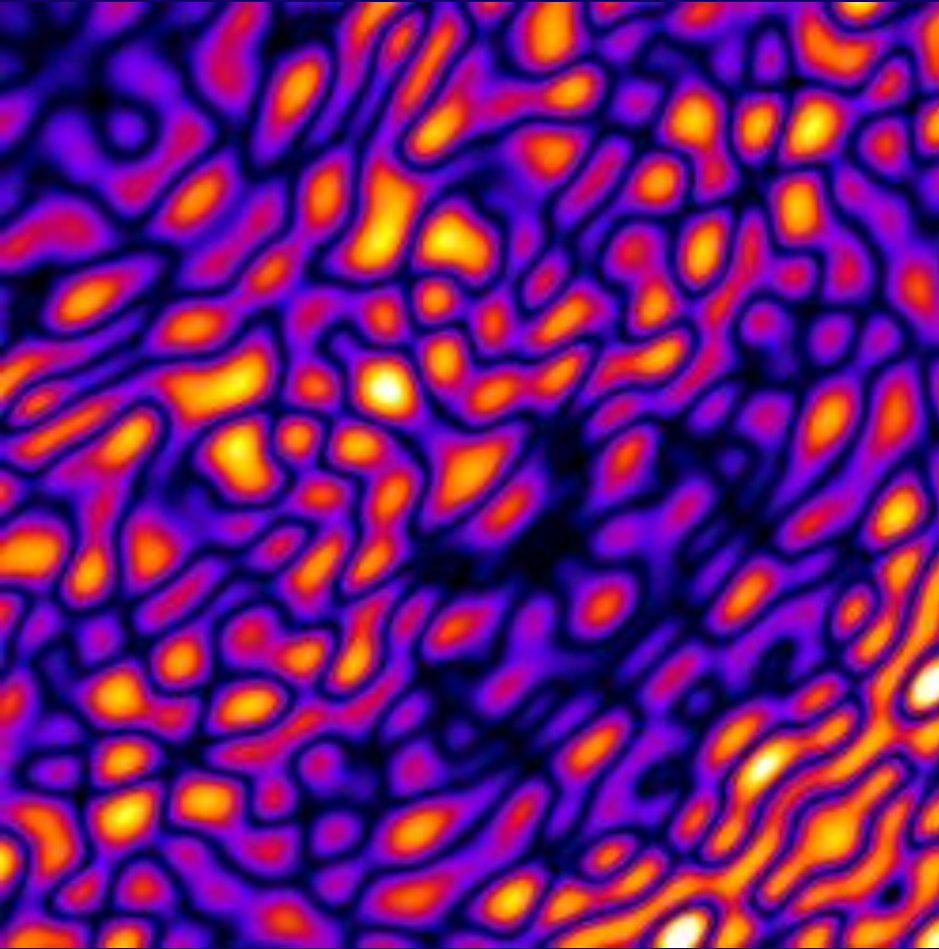
Diffraction pattern



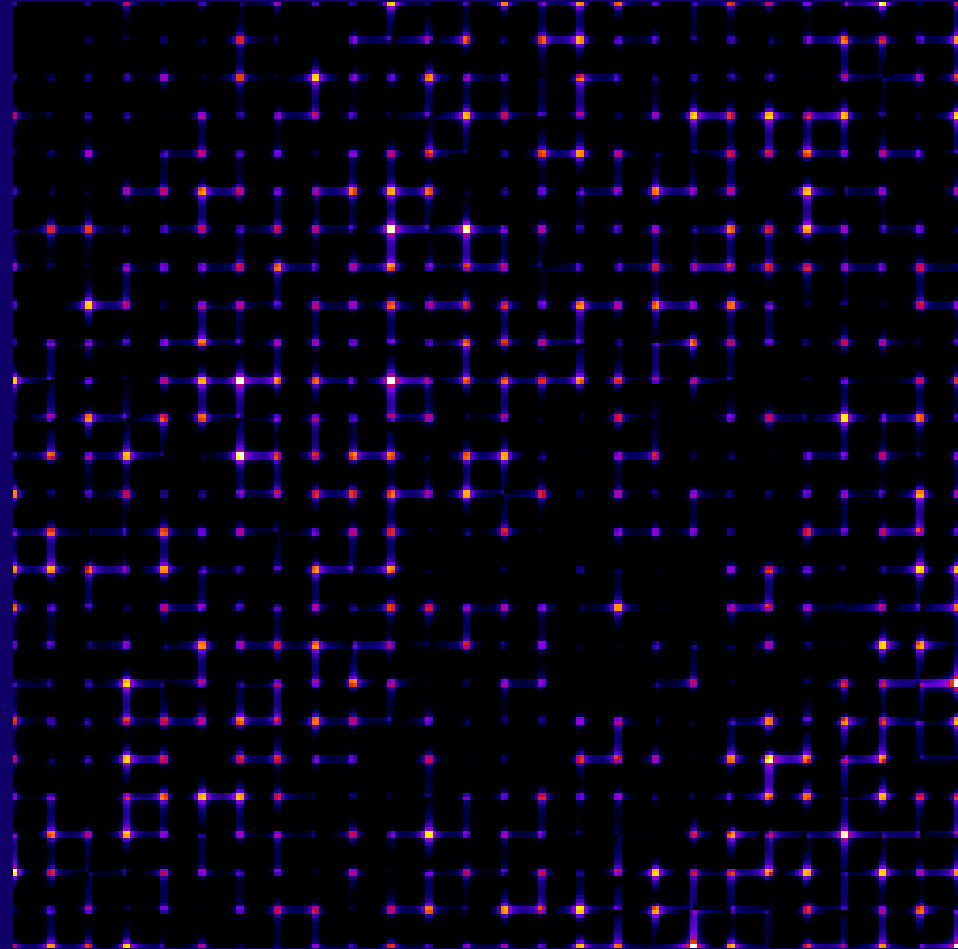
All simulations made with Moltrans

Introduction into crystallography

Pattern of 1 unit cell (CatB)



Pattern of 5x5 unit cells

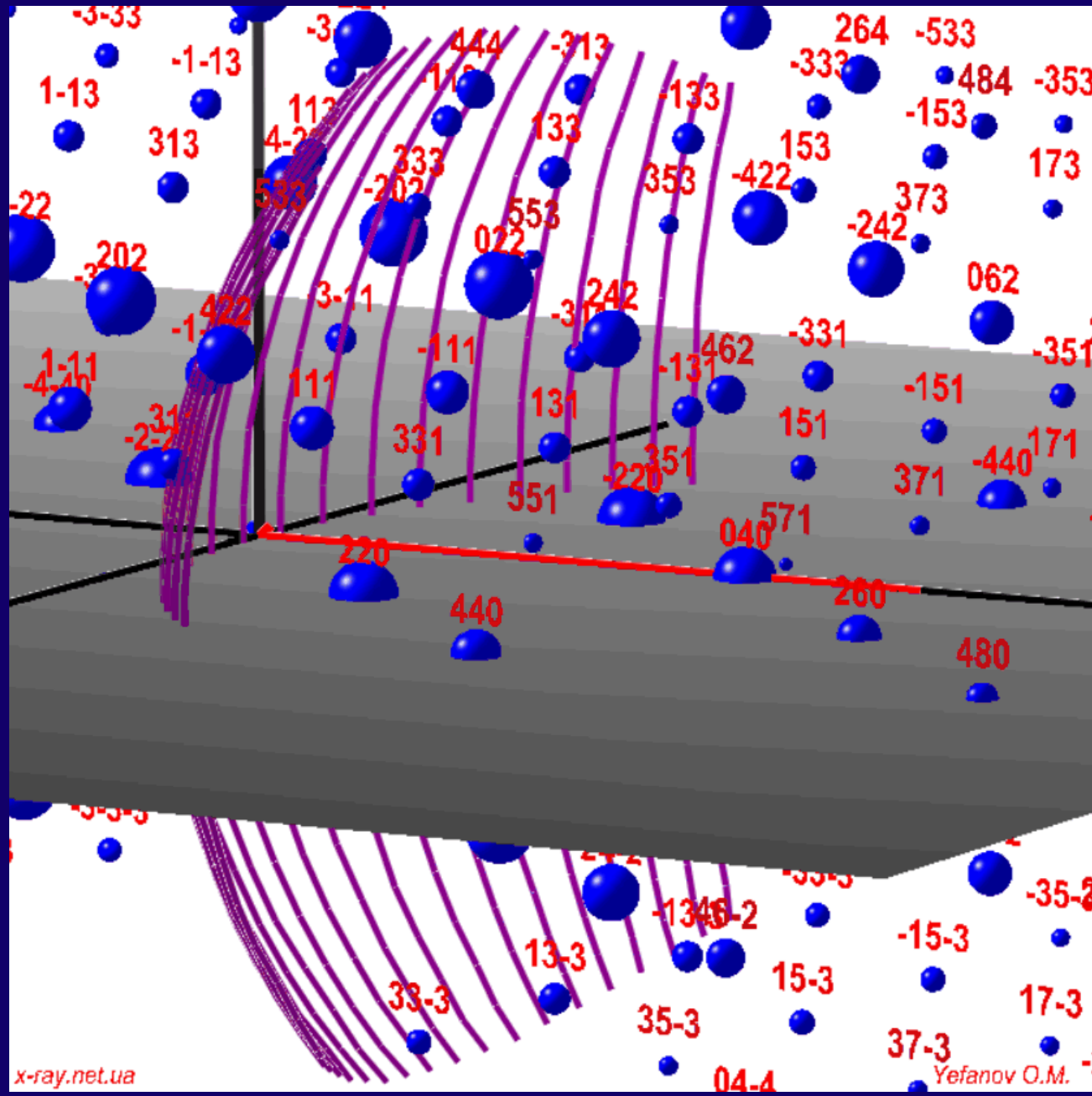


Bragg peaks intensities are modulated by the FFT of the UC



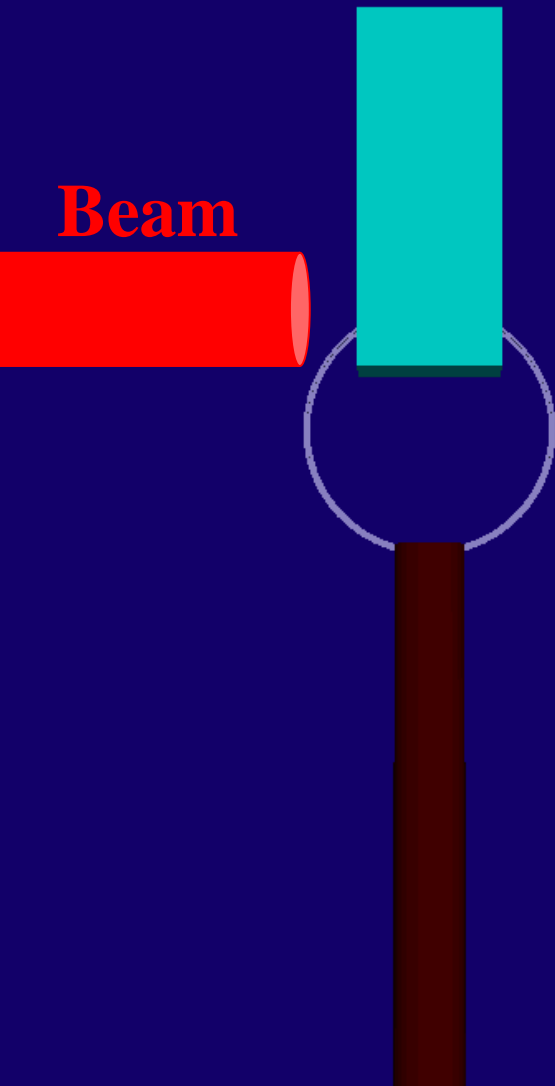
Measuring protein crystals

Typical “tomographic” measurement

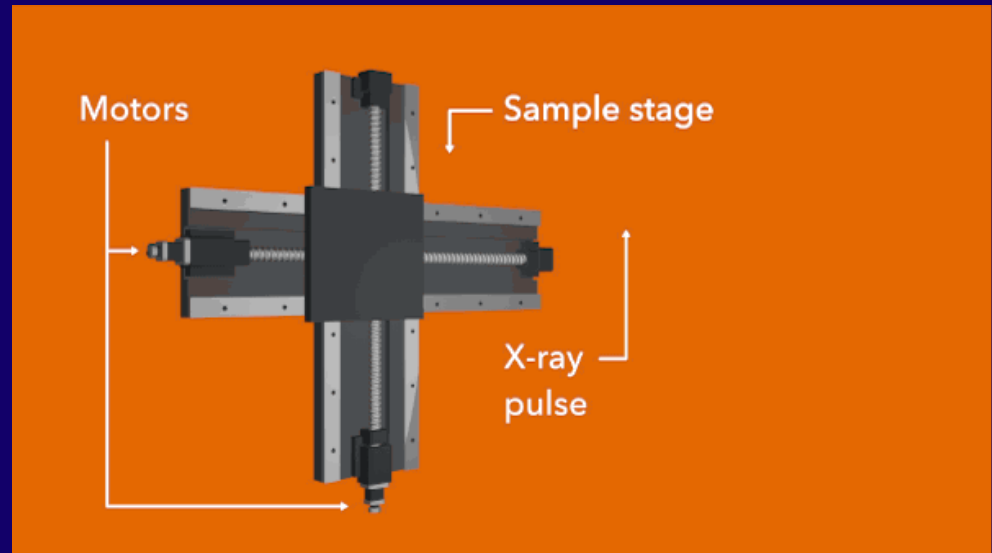
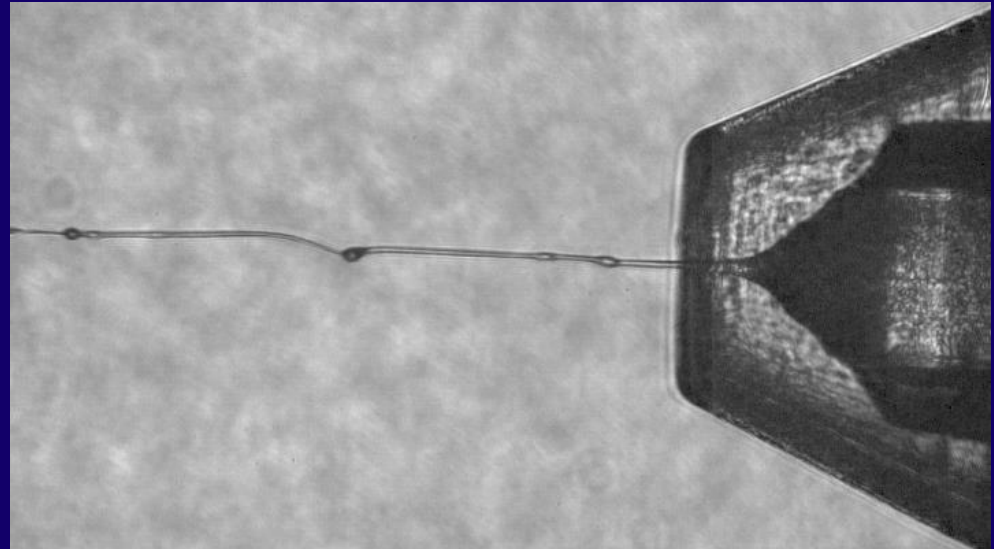


Single crystal and serial crystallography

Single crystal

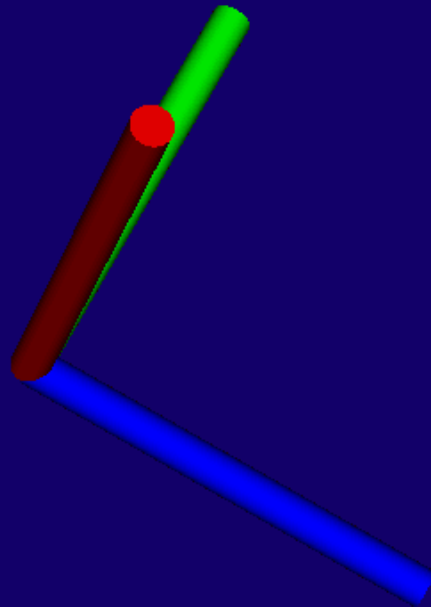


Serial

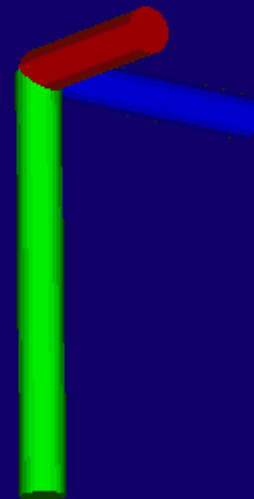


Unit cell vectors

Single crystal



Serial



Measured patterns

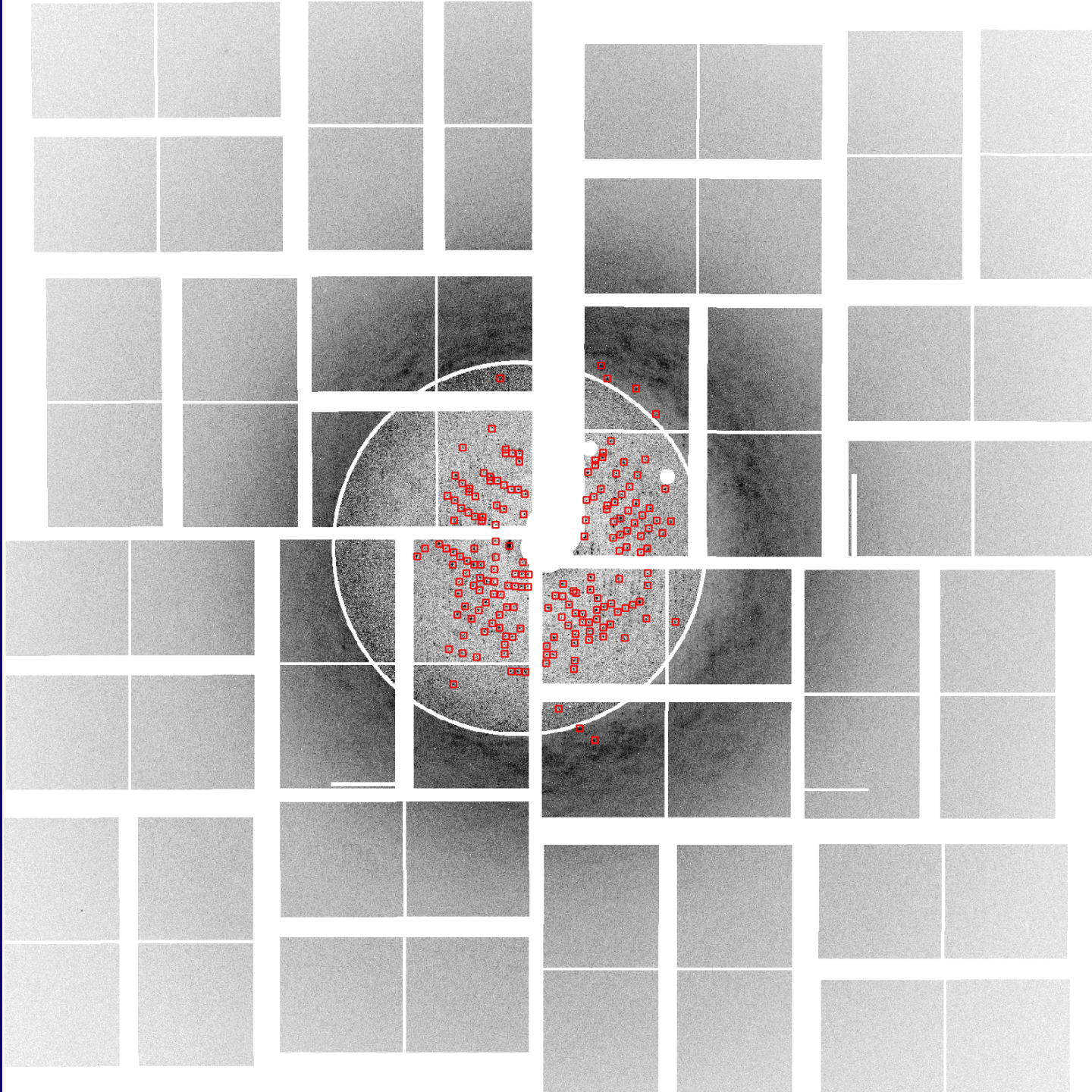
Single crystal

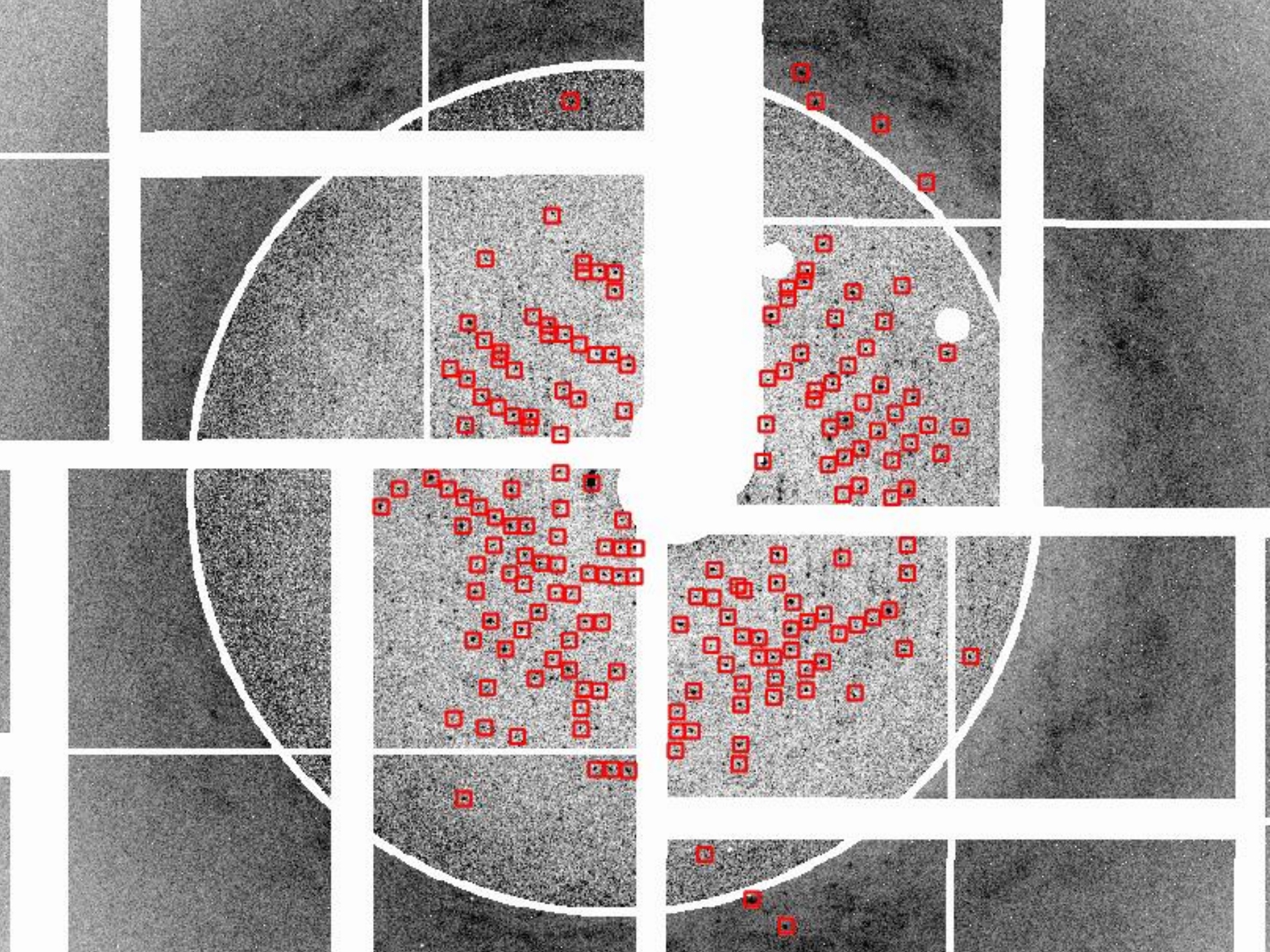


Serial

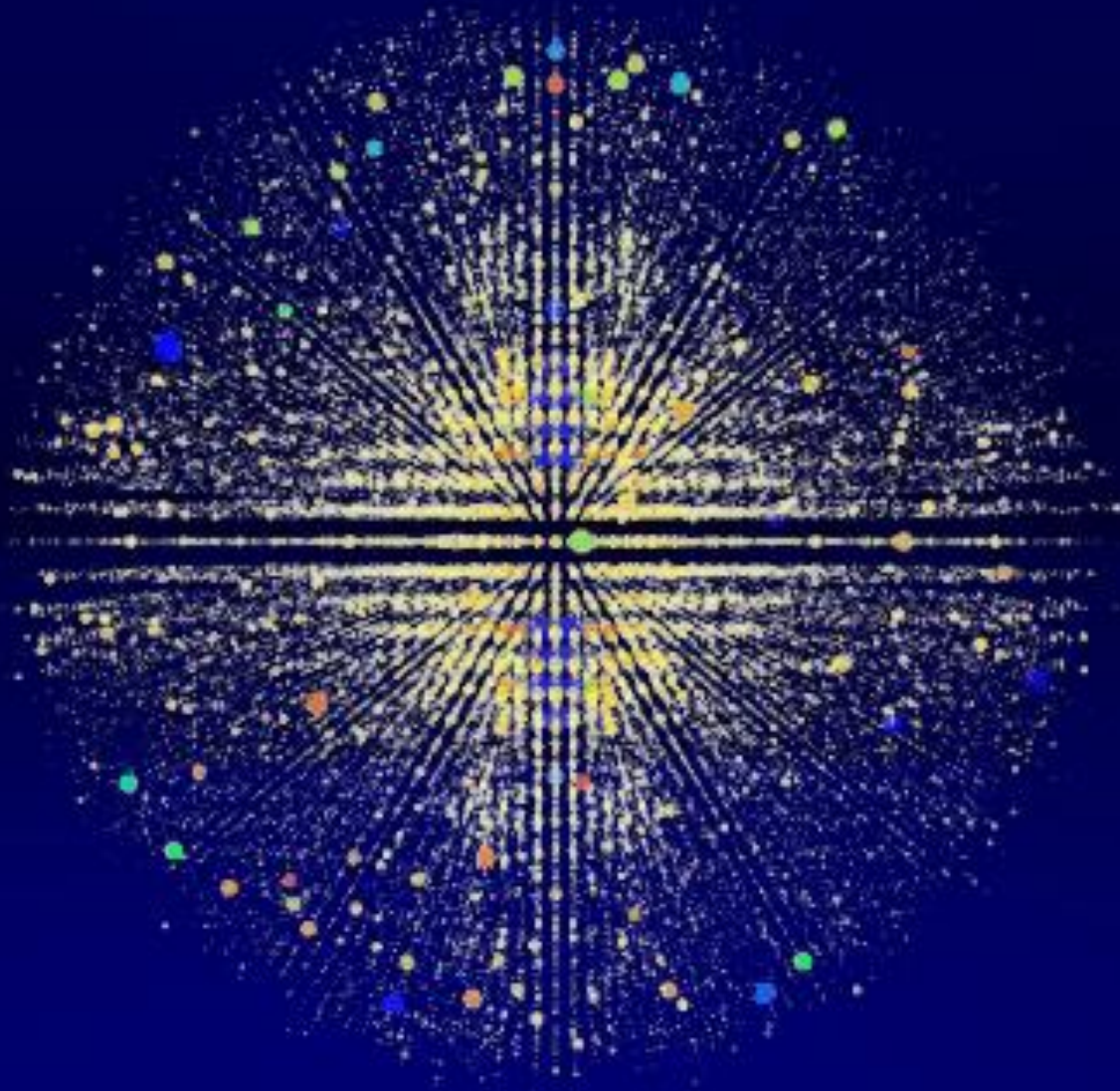


An indexed pattern (CS-PAD detector)





hkl reflections in 3D

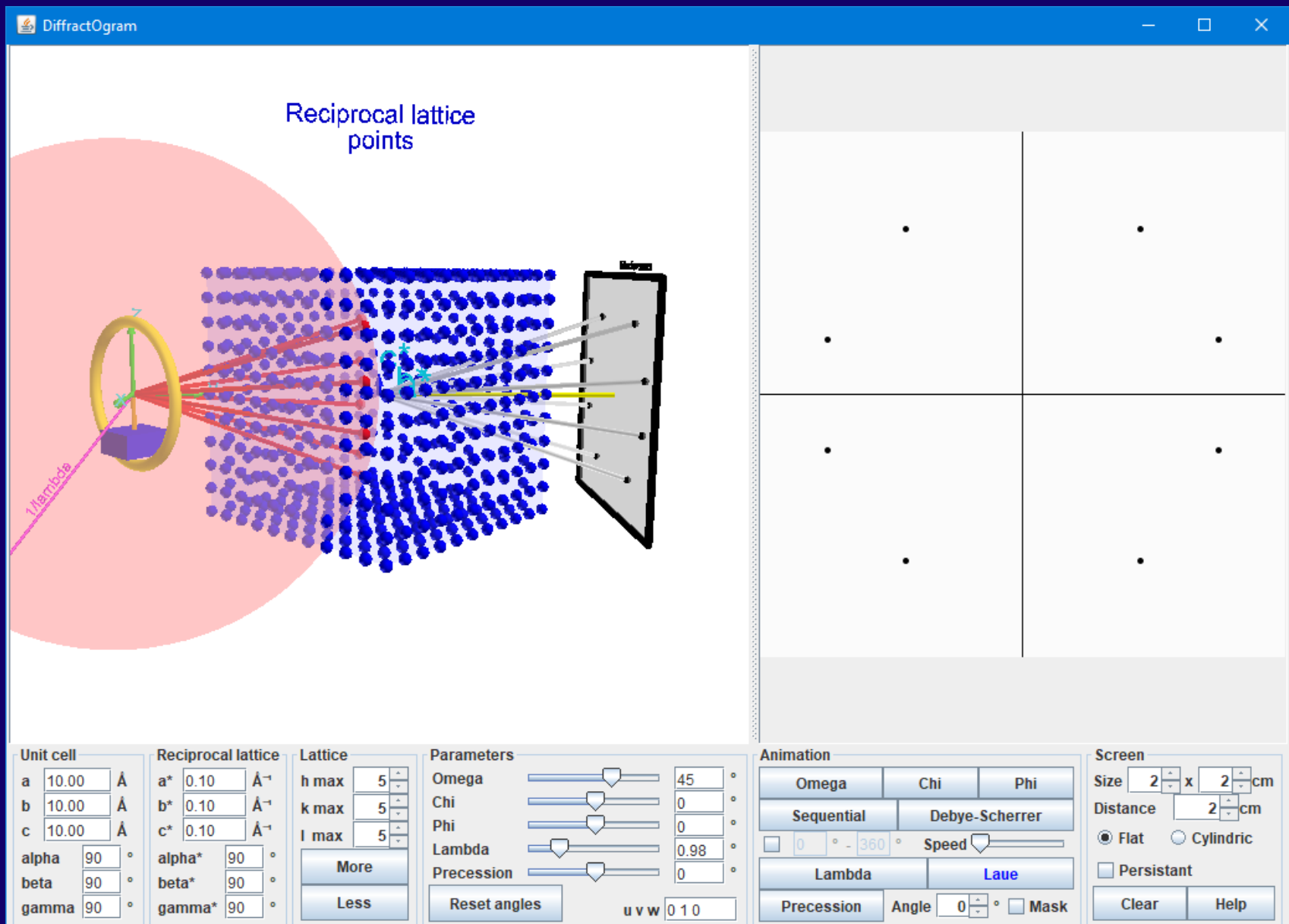




DiffractOrgam

Diffractogram

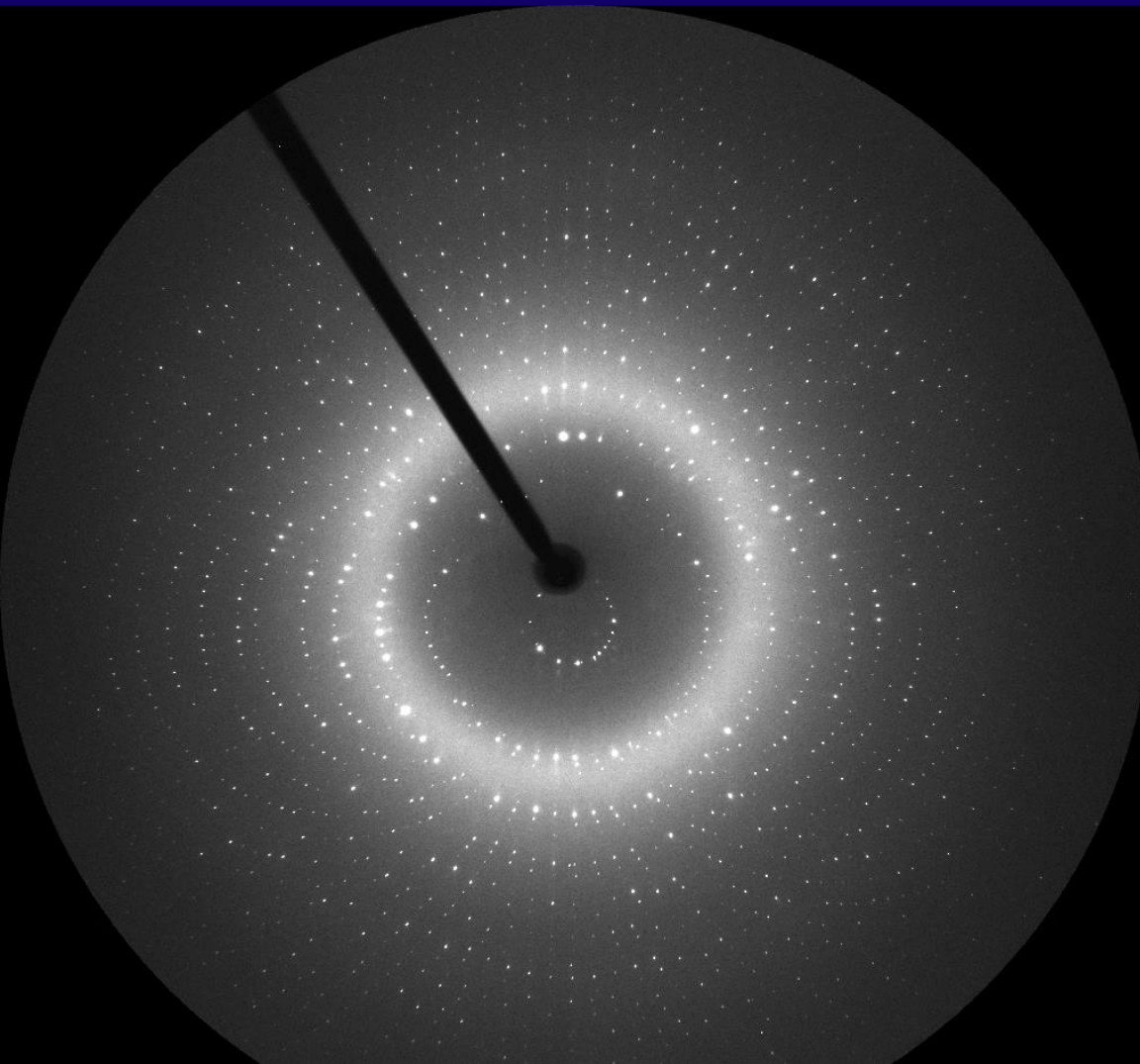
<https://www.epfl.ch/schools/sb/research/iphys/teaching/crystallography/diffractogram/>



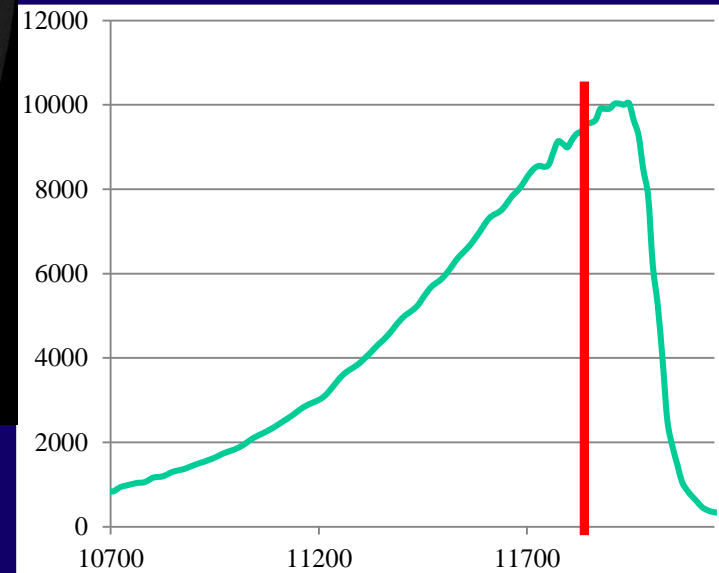


Pink and Convergent beams

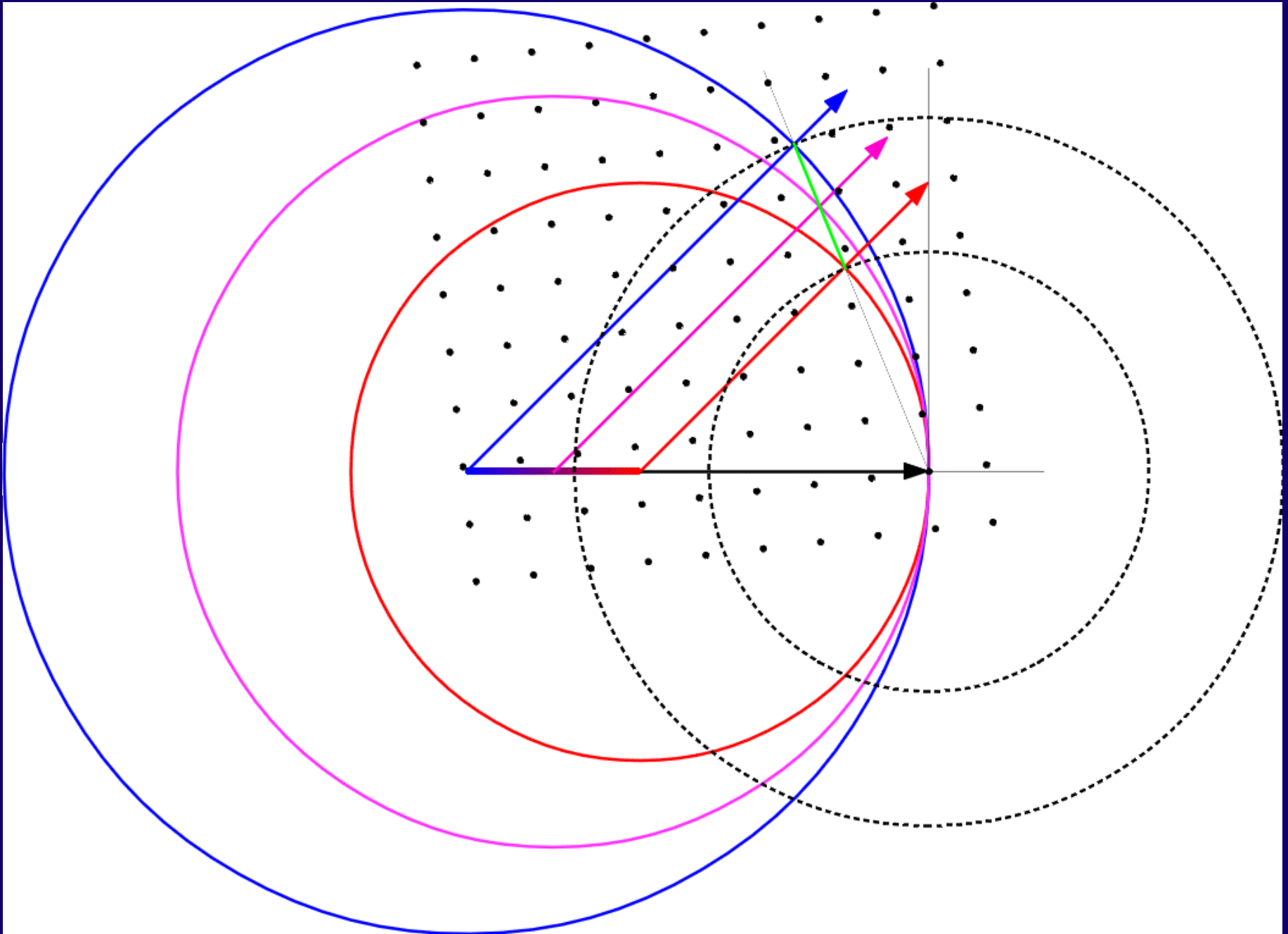
Pink beam (Laue diffraction)



- $1e15$ ph/sec
- Single 100ps bunch from sync. is enough
- 5% bandwidth
- New algorithms needed

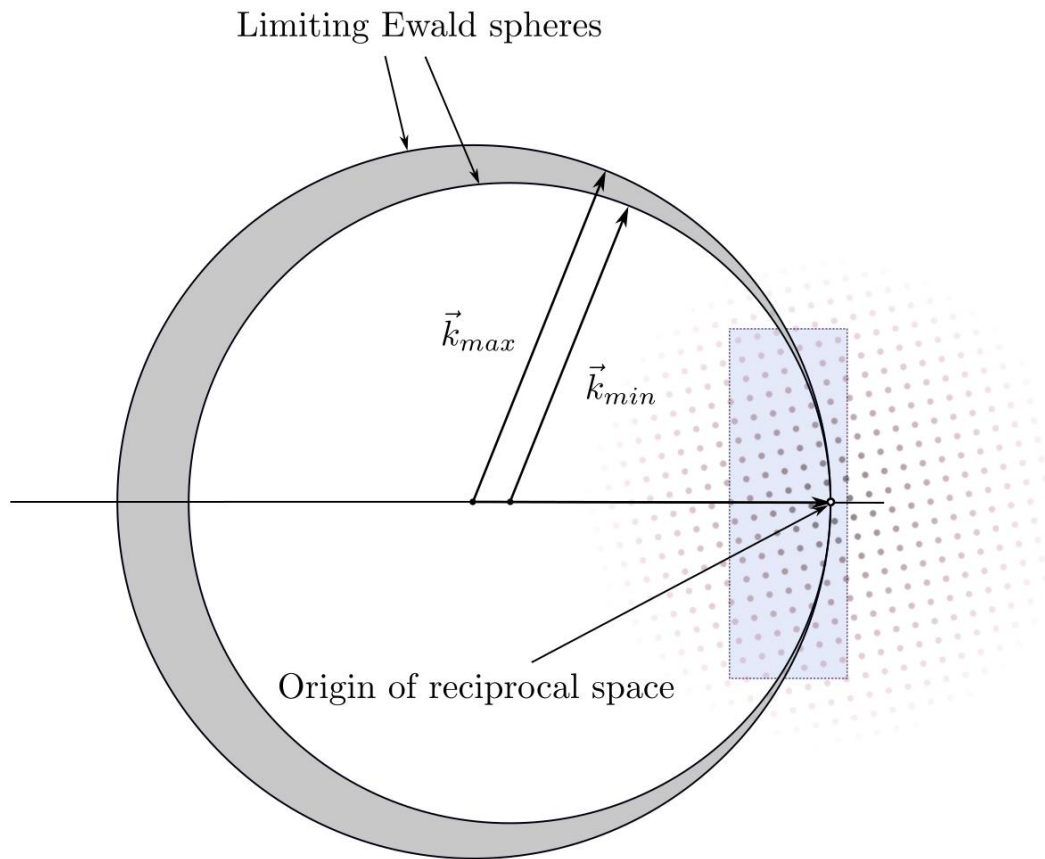


Pink beam in reciprocal space

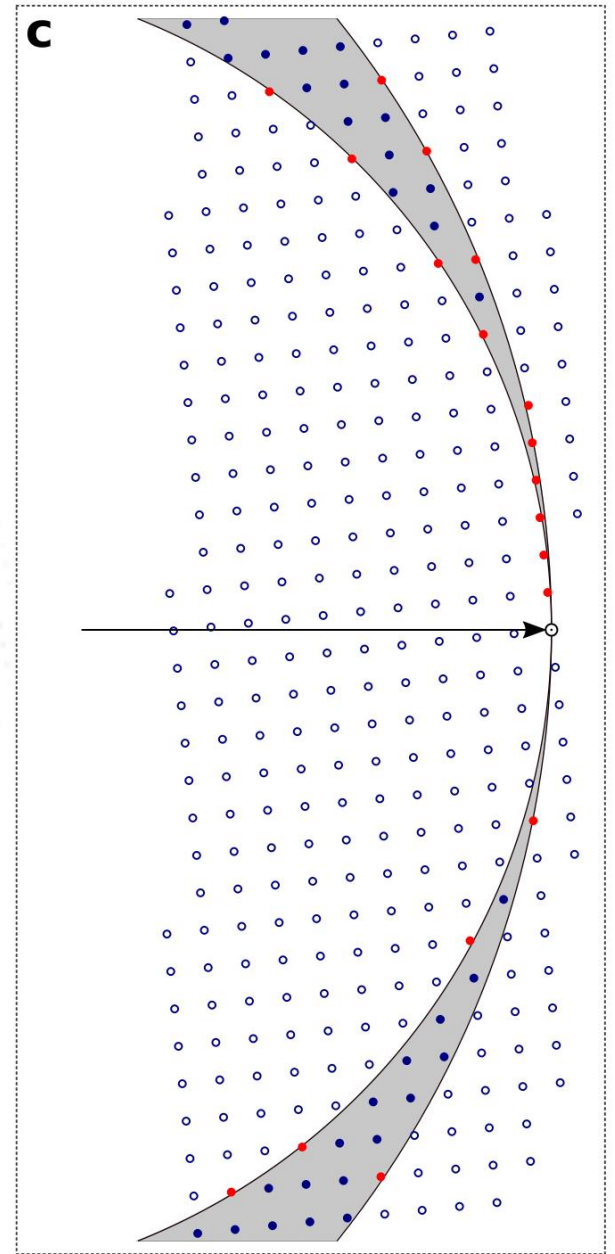


Partiality with pink beam

b

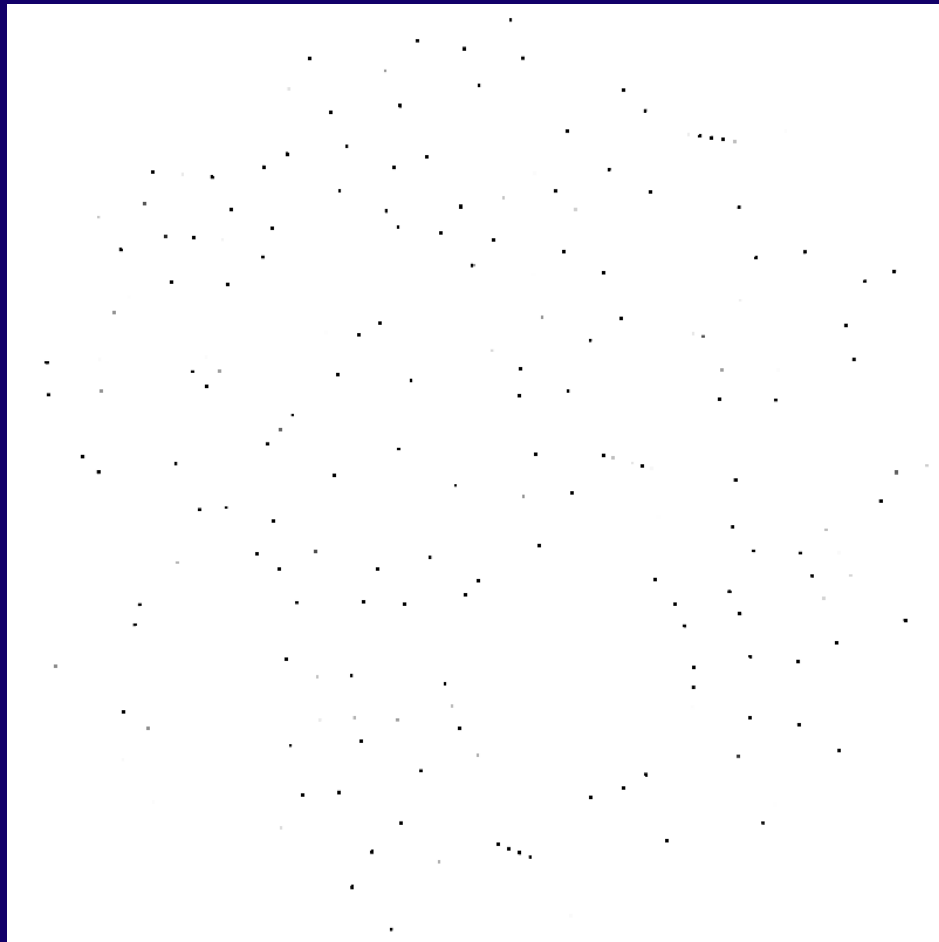


c

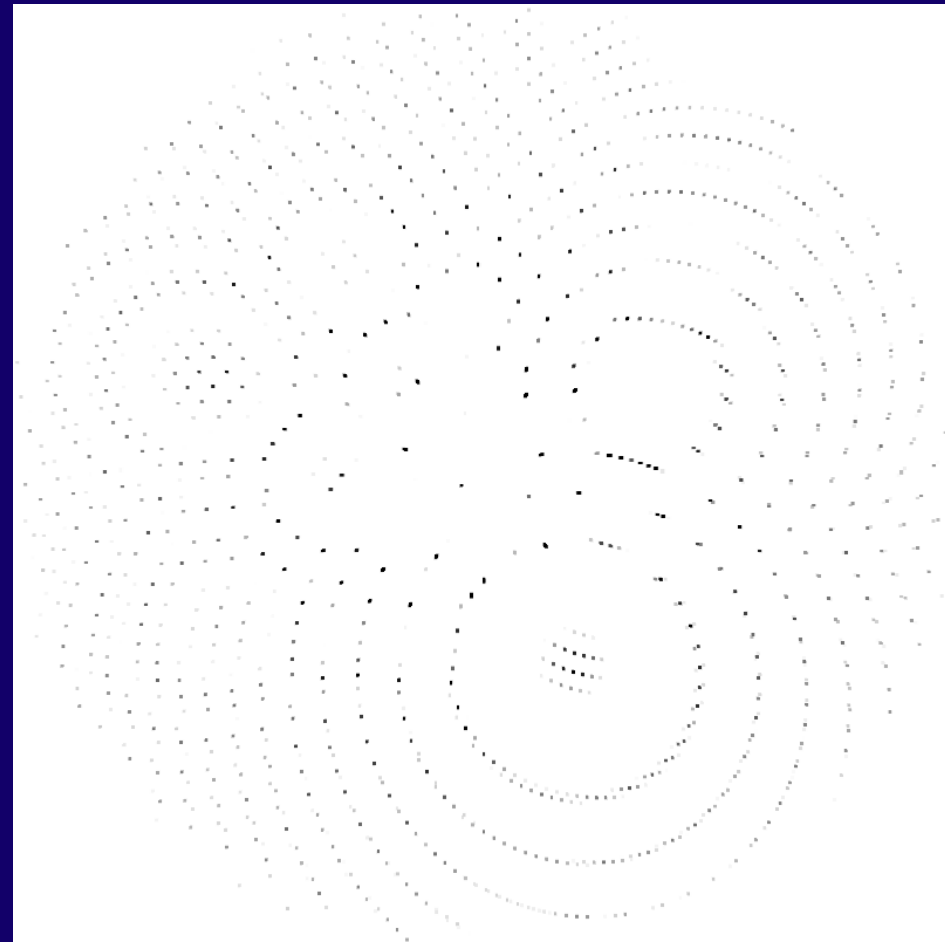


Pink vs mono

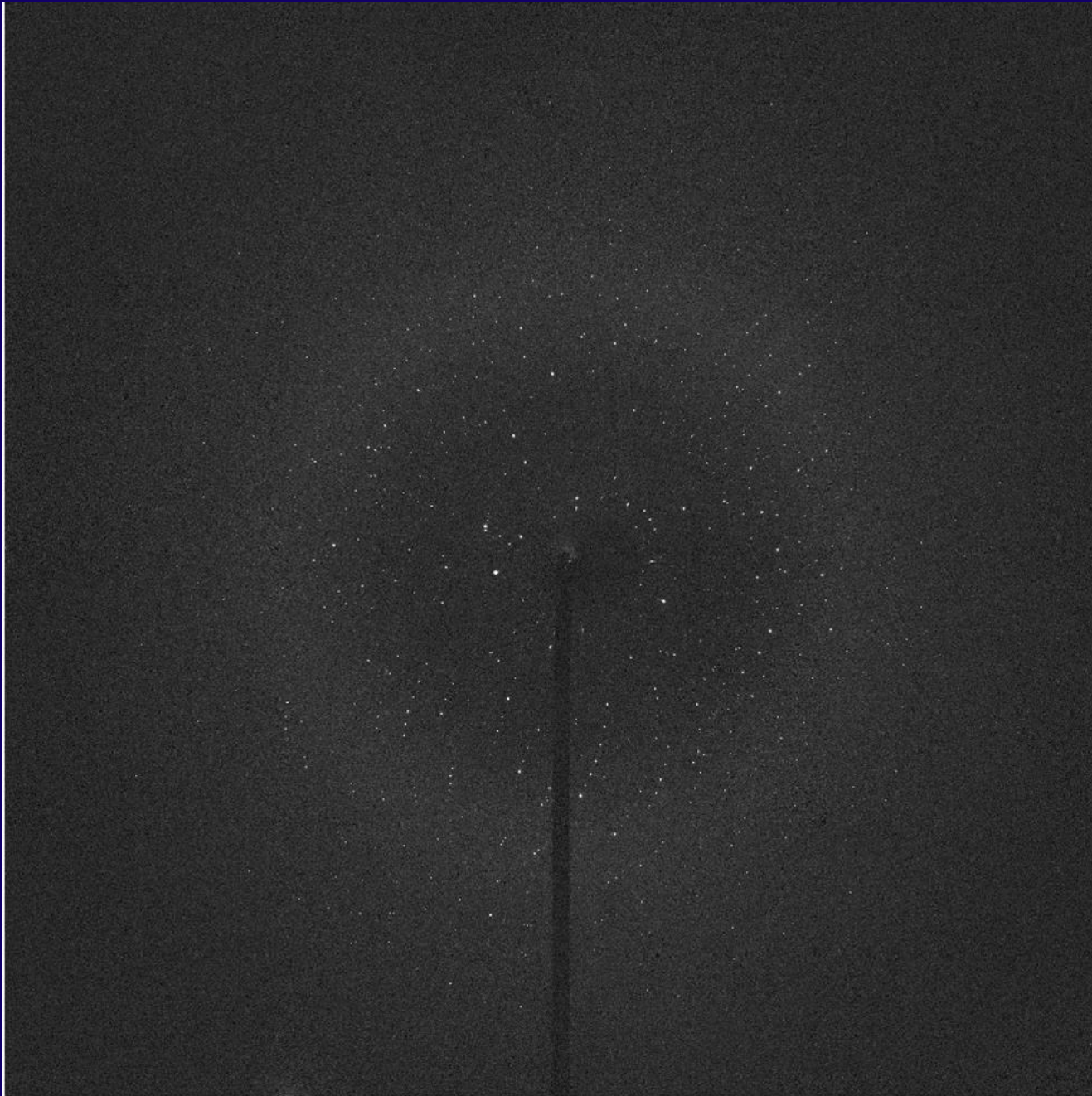
Monochromatic beam



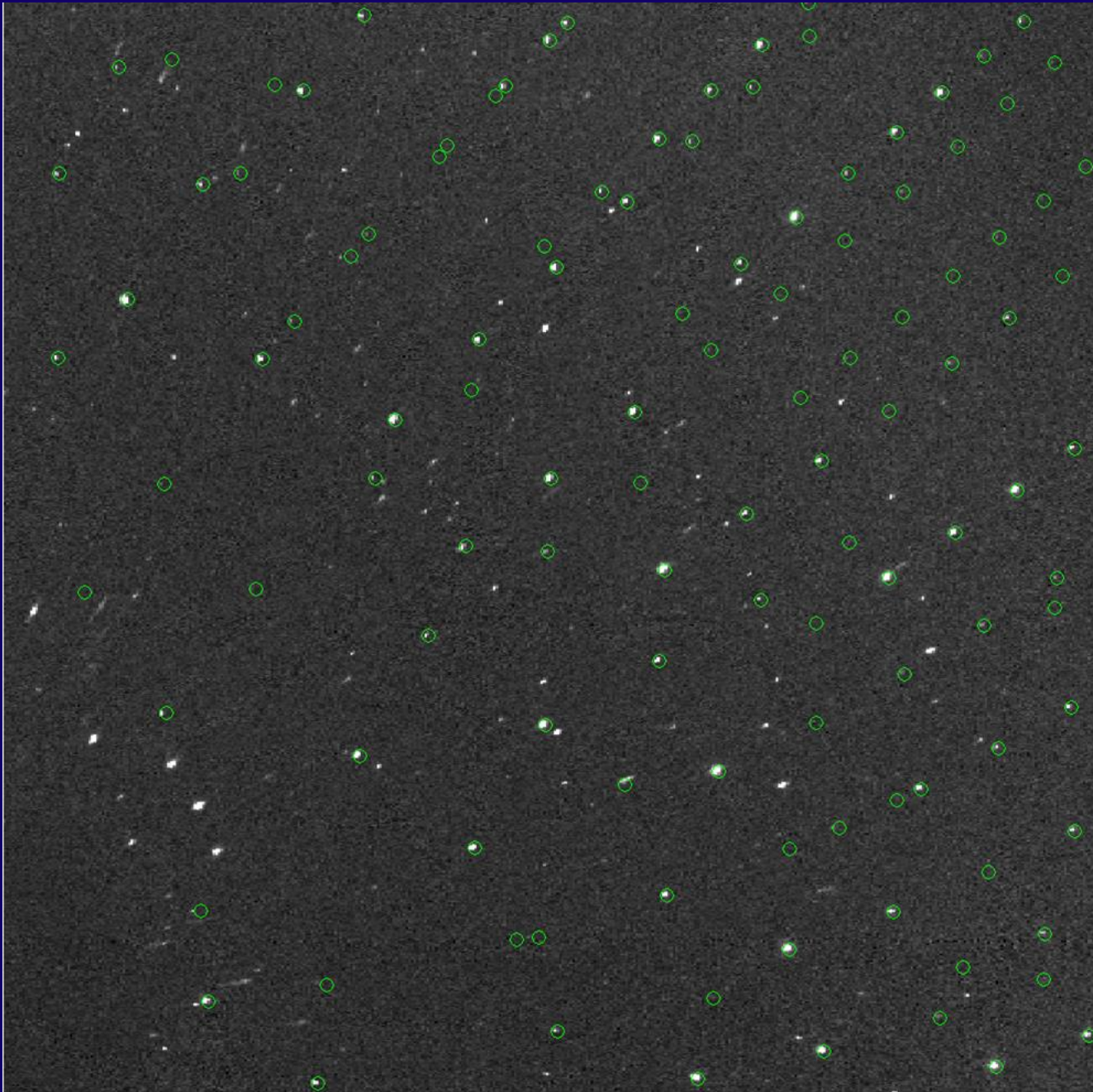
Pink beam



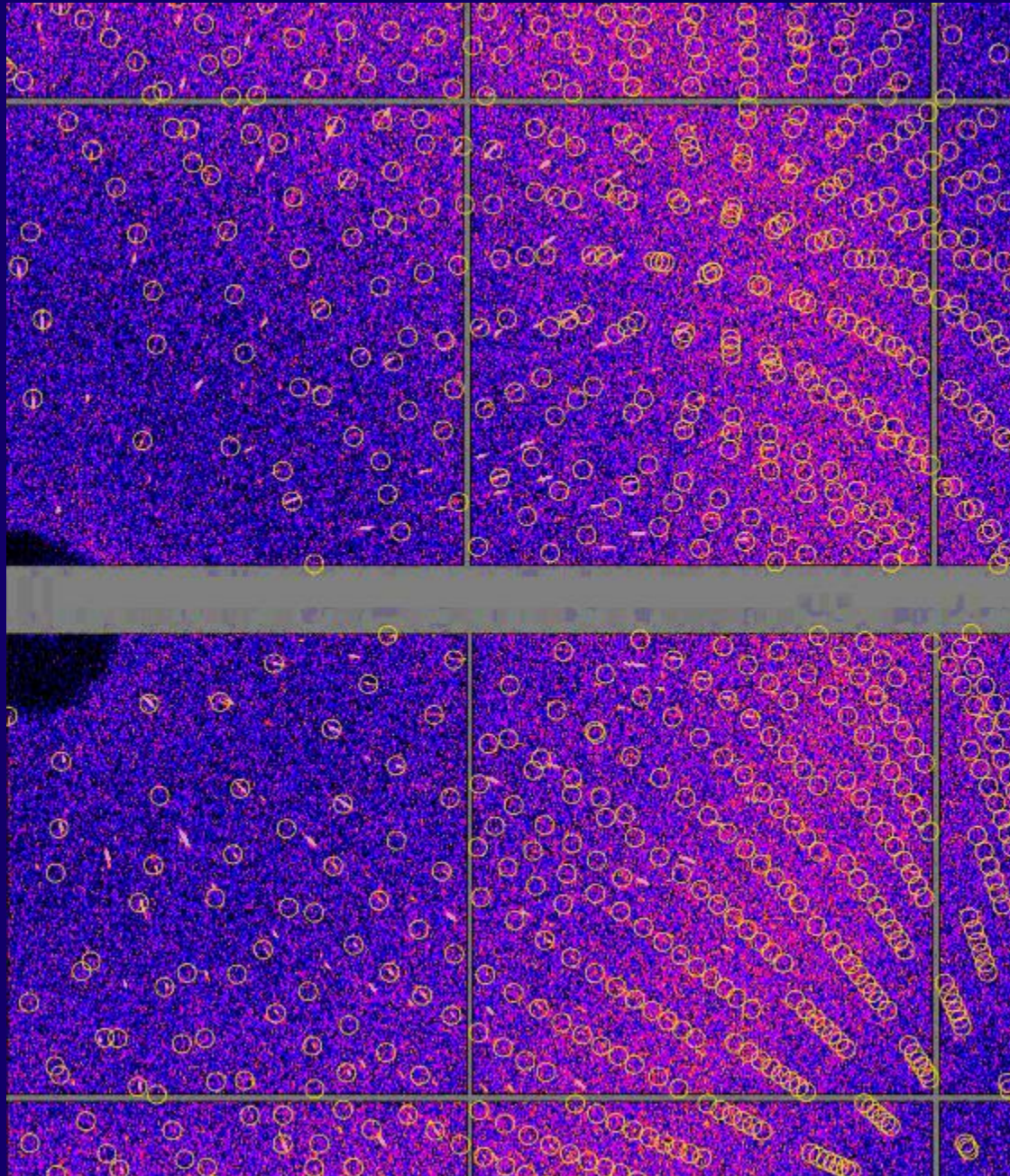
Indexing



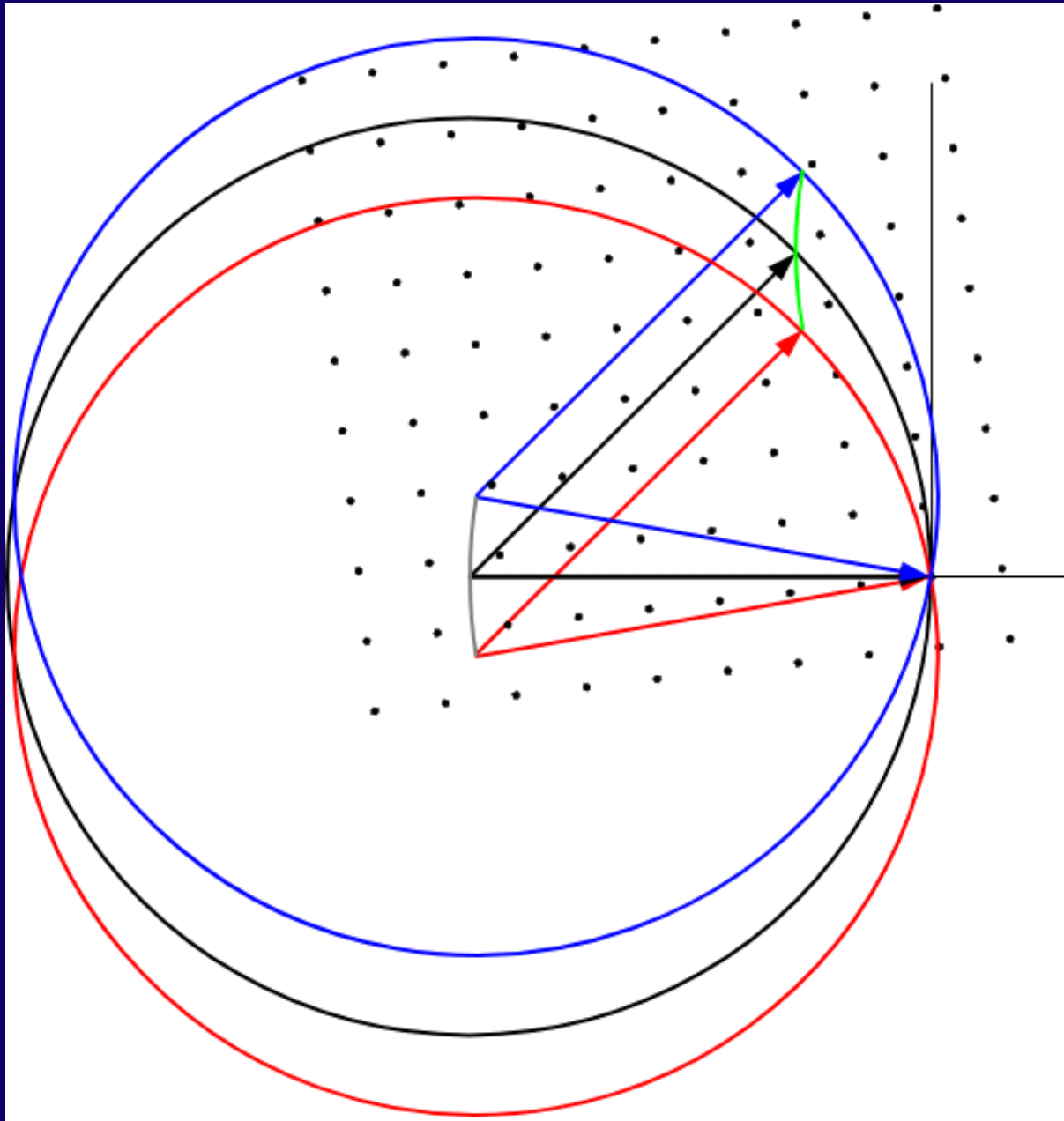
Indexing



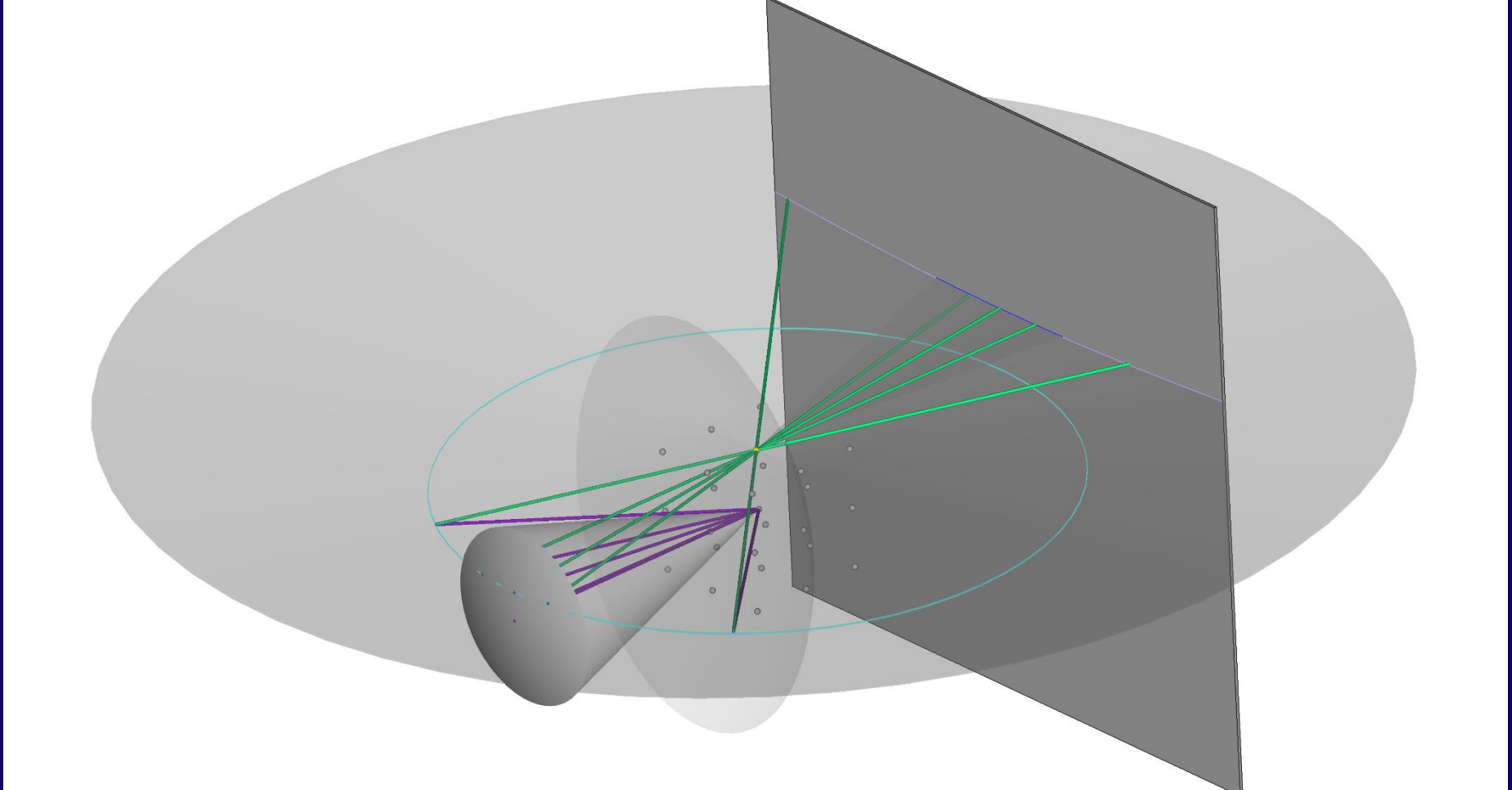
Indexing



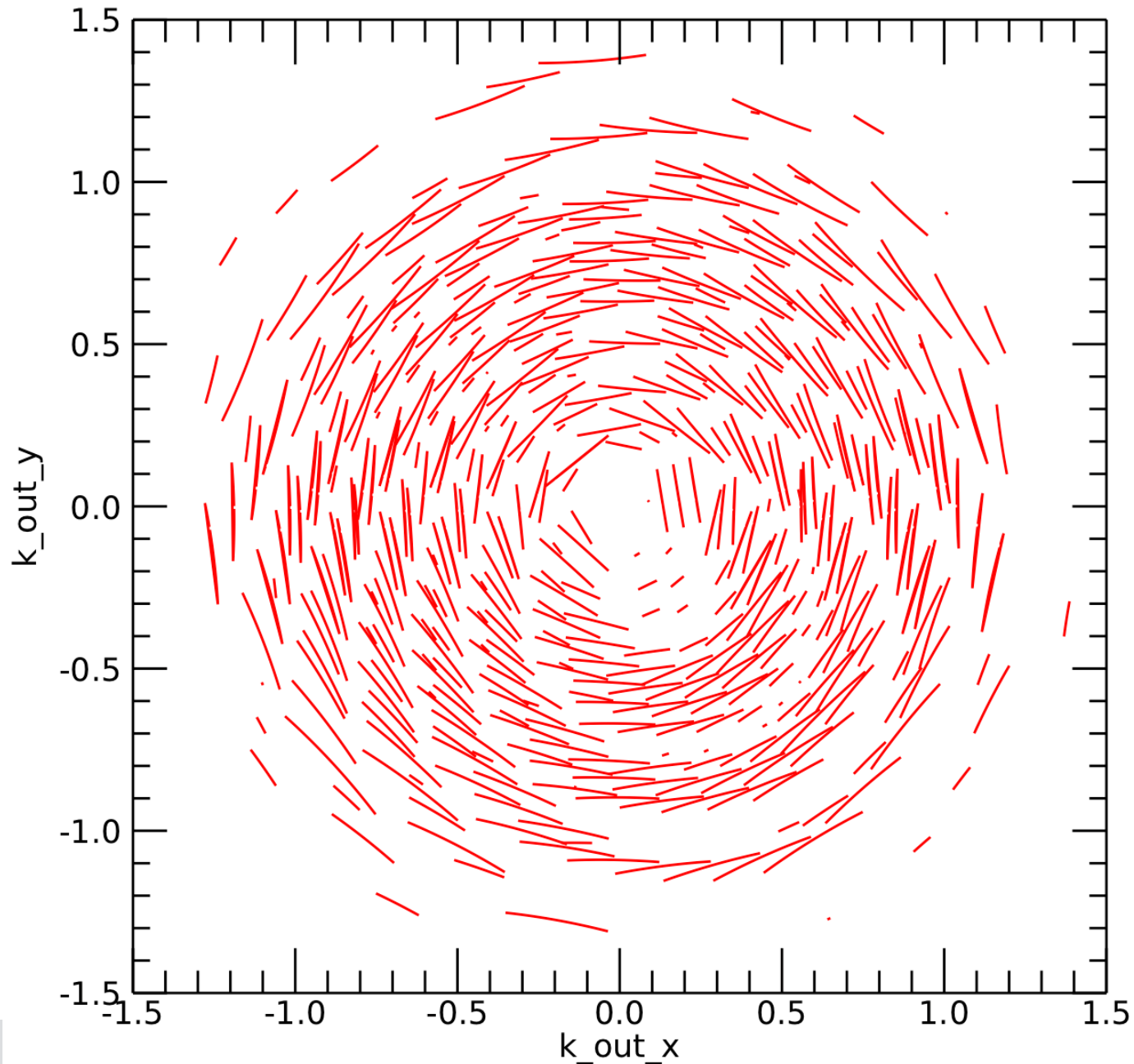
Divergent beam in reciprocal space



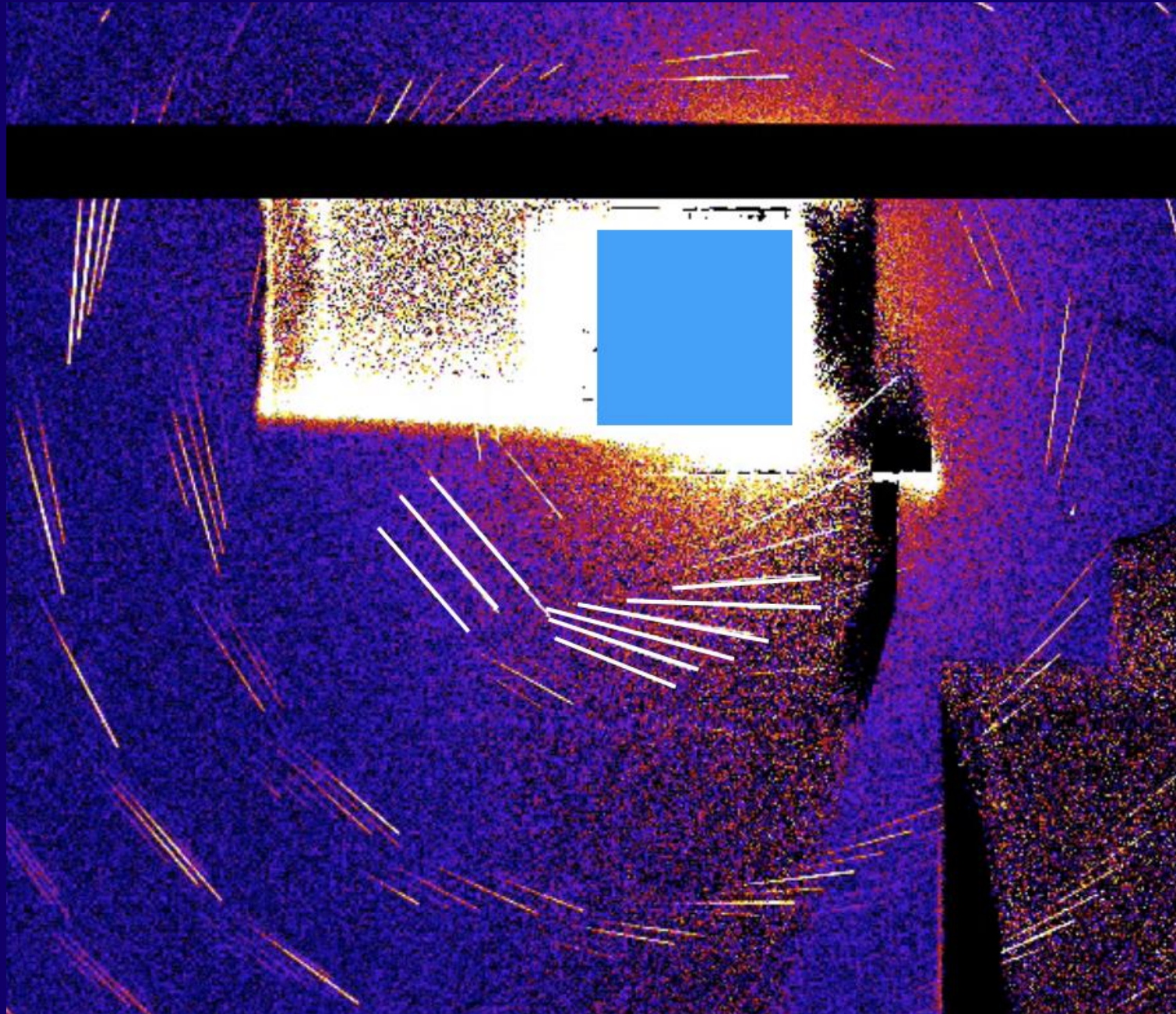
Divergent beam in reciprocal space (3D)



Diffraction pattern with big divergence



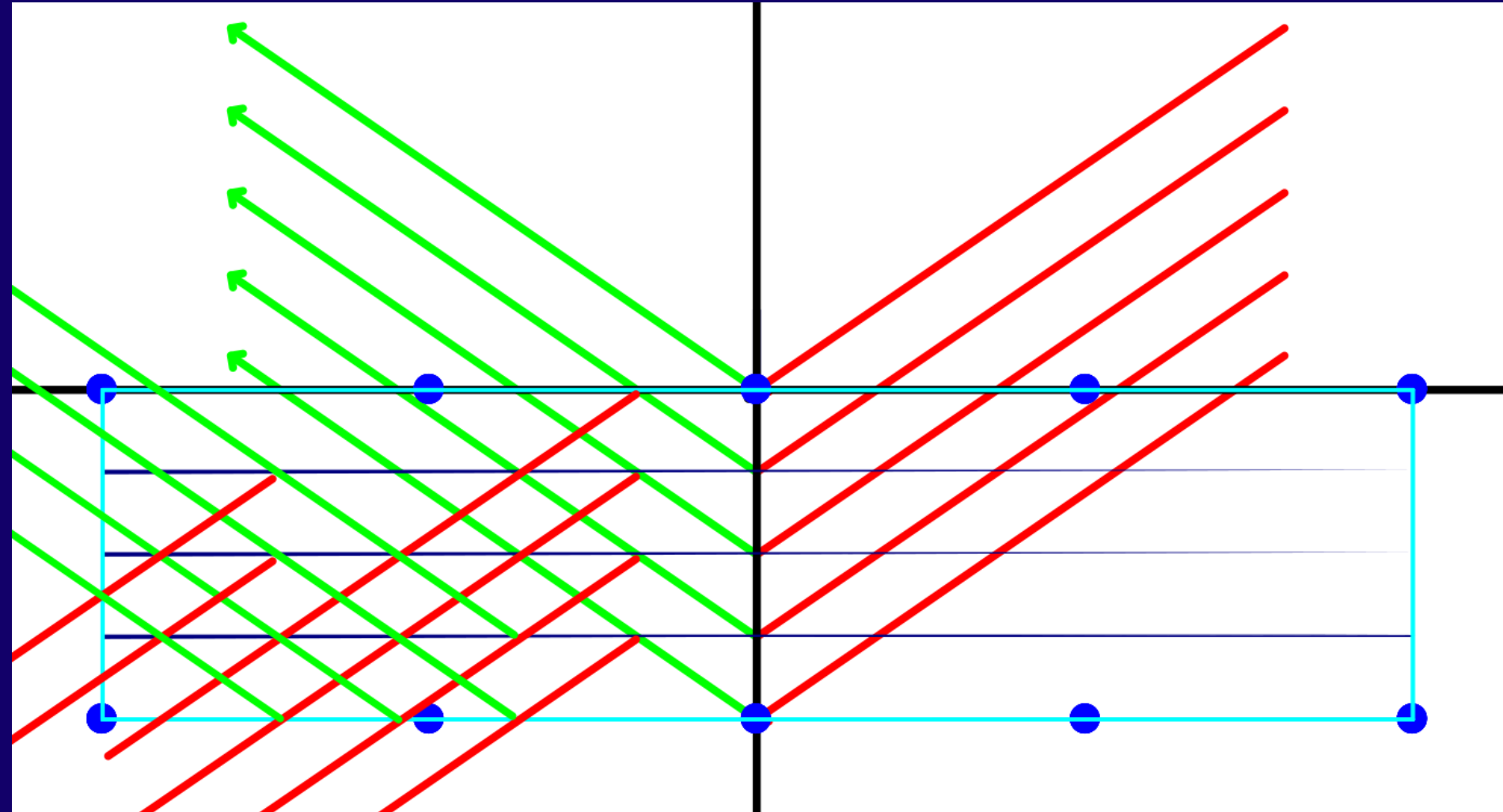
Experimental diffraction pattern





Multiple scattering (dynamical diffraction theory)

Dynamical diffraction



Propagation equation:

$$\text{rot } \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\text{rot } \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\text{div } \vec{D} = 0$$

$$\text{div } \vec{B} = 0$$

$$\vec{D} = \varepsilon_0 \varepsilon \vec{E}$$

$$\vec{B} = \mu_0 \mu \vec{H}$$

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r}) \exp(2\pi i \nu t)$$

$$\Delta \vec{E} - \text{grad div } \vec{E} + 4\pi^2 K^2 (1 + \chi) \vec{E} = 0$$

$$\vec{E}(\vec{r}) = \sum_h \vec{E}_h \exp(2\pi i \vec{k}_h \cdot \vec{r}) \quad \vec{H}_h = [\vec{k}_h \times \vec{E}_h]$$

$$\chi = \sum_h \chi_h \exp(2\pi i \vec{h} \cdot \vec{r}) \quad \vec{D}_h = \vec{E}_h + \sum_{h'} \chi_{h-h'} \vec{E}_{h'}$$

$$\frac{(k_h^2 - K^2)}{K^2} \vec{E}_h = \frac{(\vec{k}_h \cdot \vec{E}_h) \vec{k}_h}{K^2} + \sum_{g \neq h} \chi_{h-g} \vec{E}_g$$

$$\Delta_E = 0$$

Dispersion equation

Boundary conditions

$$E_t = \text{const}$$

$$D_n = \text{const}$$

$$H_t = \text{const}$$

$$B_n = \text{const}$$

$$\sum_h (\vec{E}_h)_t = \text{const}$$

$$\sum_h [\vec{k}_h \times \vec{E}_h]_t = \text{const}$$

$$\sum_h \left((\vec{E}_h)_n + \sum_{h'} \chi_{h-h'} (\vec{E}_{h'})_n \right) = \text{const}$$

2-beam case: $\vec{E}(\vec{r}) = \vec{E}_0 \exp(2\pi i \vec{k}_0 \cdot \vec{r}) + \vec{E}_h \exp(2\pi i \vec{k}_h \cdot \vec{r})$

$$= \text{const}$$

$$\begin{cases} \frac{(k_0^2 - (1 + \chi_0) * K^2)}{K^2} \vec{E}_0 = C \chi_h \vec{E}_h \\ \frac{(k_h^2 - (1 + \chi_0) * K^2)}{K^2} \vec{E}_h = C \chi_0 \vec{E}_0 \end{cases}$$

$$(k_0^2 - (1 + \chi_0) K^2)(k_h^2 - (1 + \chi_0) K^2) = C^2 K^4 \chi_h \chi_0$$

$$\vec{k}_h = \vec{K}_0 + \vec{h} + K \varepsilon \vec{n}$$

$$\varepsilon^4 + A_3 \varepsilon^3 + A_2 \varepsilon^2 + A_1 \varepsilon + A_0 = 0$$



Processing “big” SX data

Data rates at modern sources

LCLS (CS-PAD):

$4.6\text{Mb} * 120\text{Hz} * 3600\text{sec} * 10\text{hours} * 5\text{days} = 95\text{Tb}$

PINK beam at APS (JoungFrau 1M):

$2\text{Mb} * 1000\text{Hz} * 3600\text{sec} * 20\text{hours} * 5\text{days} = 860\text{Tb}$

Modern synchrotron (Eiger2 XE 16M, compressed):

$16\text{Mb} * 400\text{Hz} * 3600\text{sec} * 20\text{hours} * 5\text{days} = 2.1\text{Pb}$

eXFEL now (AGIPD):

$(2+2)\text{Mb} * 3520\text{Hz} * 3600\text{sec} * 10\text{hours} * 5\text{days} = 2.4\text{Pb}$

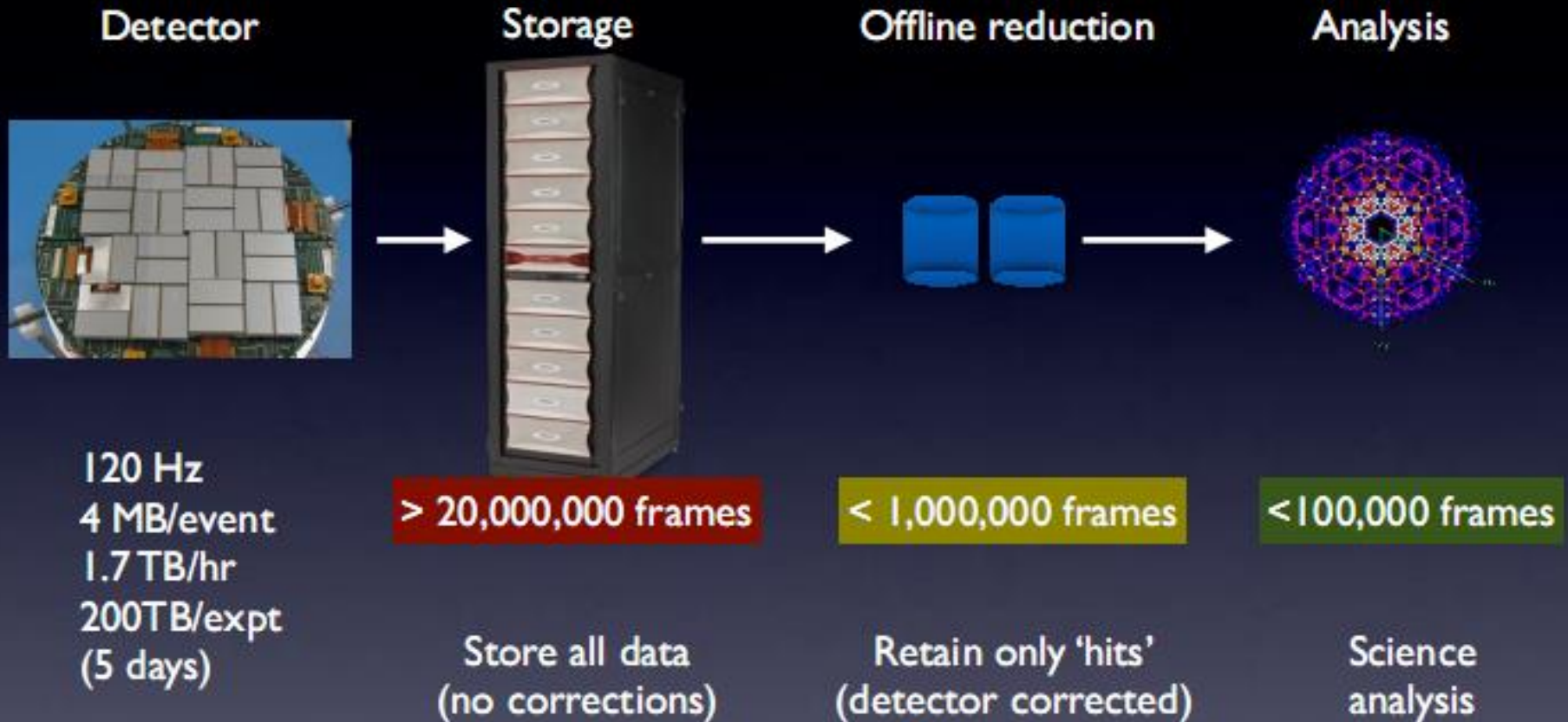
eXFEL soon (AGIPD 4M, 2023+):

$(8+8)\text{Mb} * 3520\text{Hz} * 3600\text{sec} * 10\text{hours} * 5\text{days} = 9.5\text{Pb}$

LCLS2 soon (ePix10k-HR, 2024+):

$8.4\text{Mb} * 10000\text{Hz} * 3600\text{sec} * 10\text{hours} * 5\text{days} = 14\text{Pb}$

Data rate (LCLS)



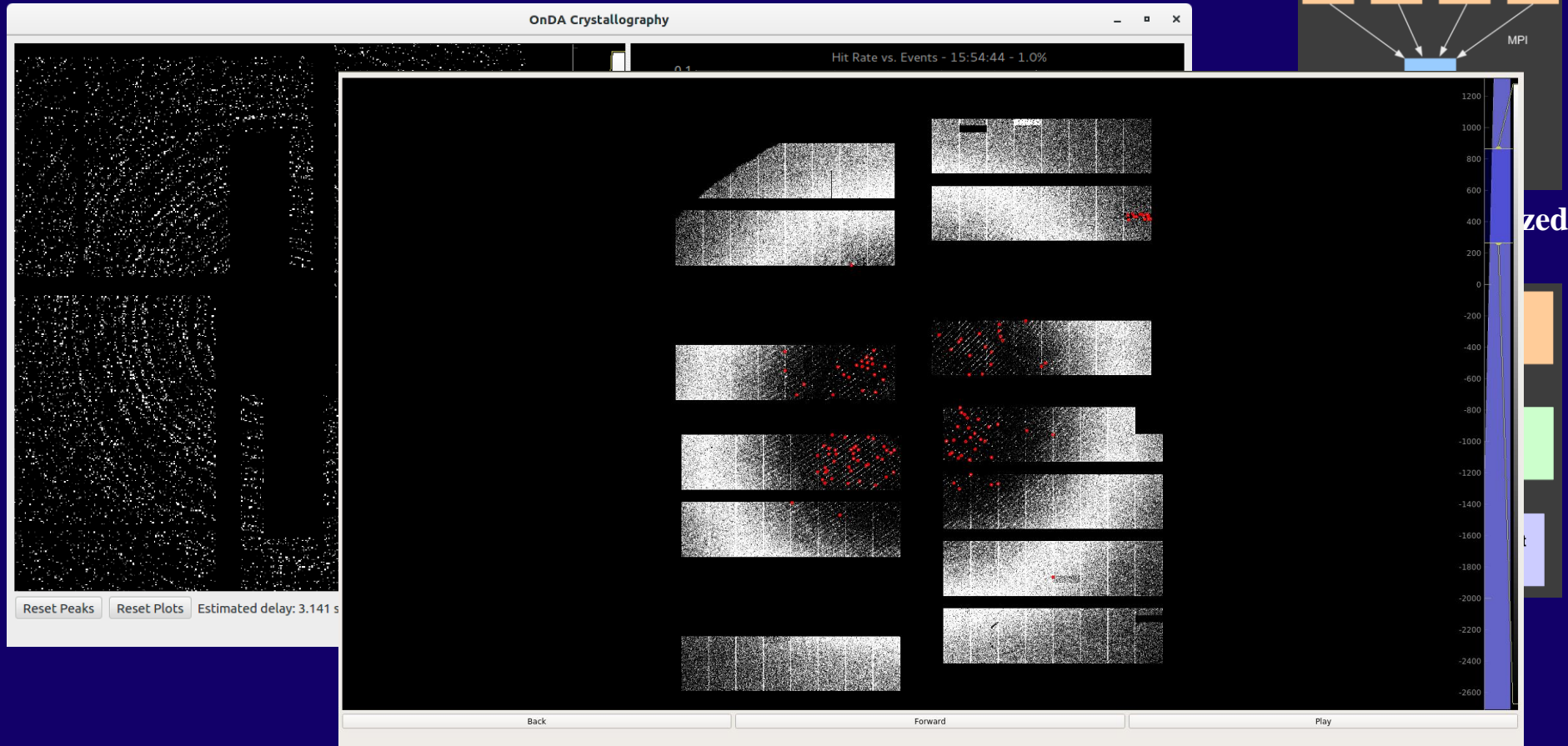
Automated high volume image processing is essential
(reliable background correction, automatic identification of useful data)

Online processing (OnDA/OM)

Up to date information > Real-time human feedback

Keep up with data flow (fresh)

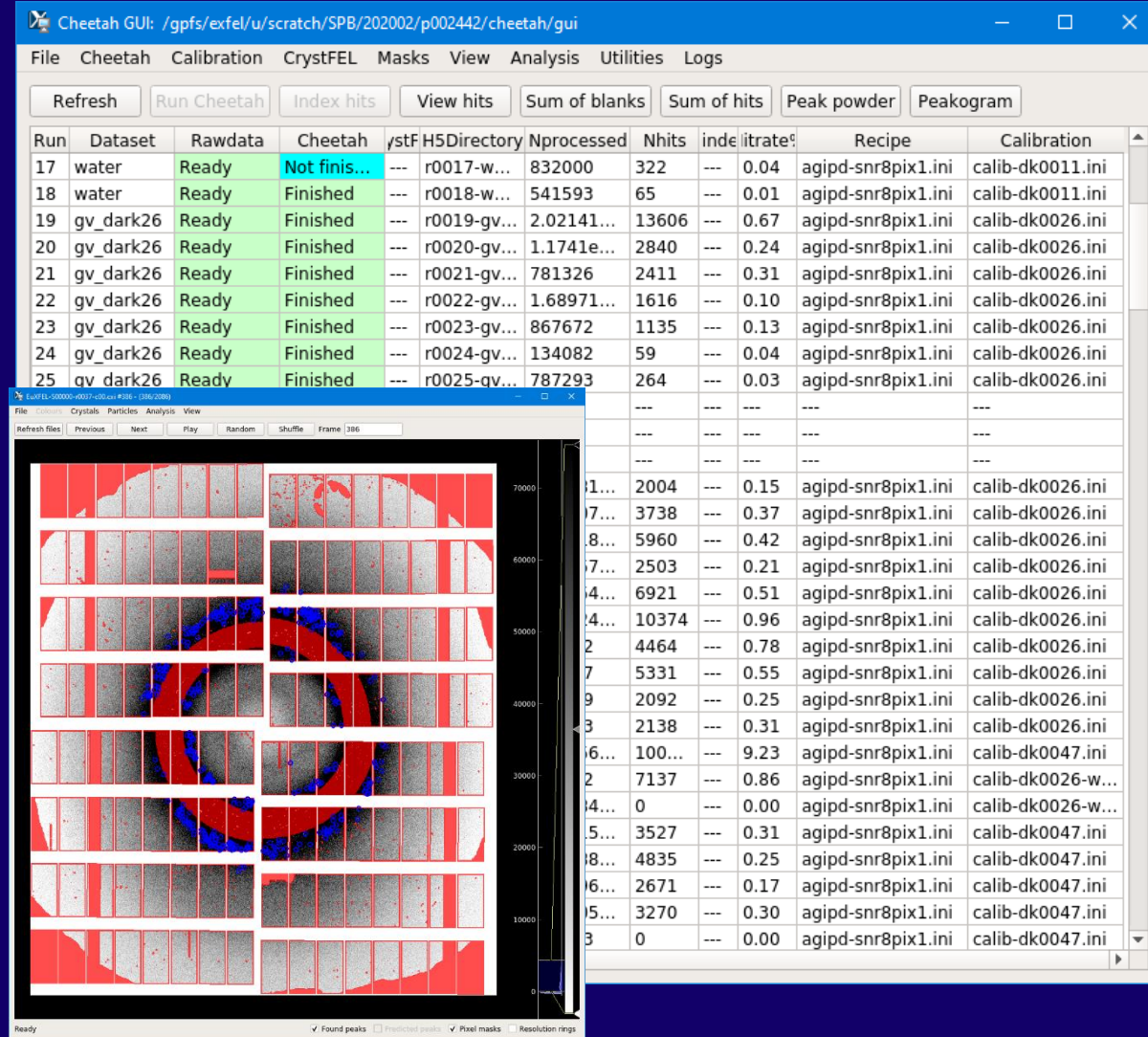
Data that help us take immediate decisions



Accuracy is not a strong requirement. Low latency is!

Offline data processing

Fast (C, Python?)
Parallelizable
Reliable
Adjustable
Tools to check results
User friendly
HDF5 compatible
Segmented detectors
AI is not always suitable



Maxwell cluster



max-exfl099	upex-beamtime upex-middle exfel upex all allrsv	80									E5-2698 v4 @ 2.20GHz	0	INTEL, V4, E5-2698, 512G
max-exfl101	exrsv upex-beamtime upex-middle exfel upex all allrsv	72									Gold 6140 CPU @ 2.30GHz	0	INTEL, Gold-6140, 768G
max-exfl102	exrsv upex-beamtime upex-middle exfel upex all allrsv	72	2	18	2	+	1728	768GB	0		Gold 6140 CPU @ 2.30GHz	0	INTEL, Gold-6140, 768G
max-exfl259	upex-high exrsv upex exfel allrsv all	72	2	18	2	+	1844	768GB	0		Gold 6240 CPU @ 2.60GHz	0	INTEL, Gold-6240, 768G
max-exfl260	upex-high exrsv upex exfel allrsv all	72	2	18	2	+	1844	991GB	0		Gold 6240 CPU @ 2.60GHz	0	INTEL, Gold-6240, 768G
max-exfl261	upex-beamtime exrsv upex-middle upex exfel	128	2	32	2	+	1740	512GB	0		AMD EPYC 7542	0	AMD, EPYC, 7542, 512G
max-exfl360	upex-beamtime exrsv upex-middle upex exfel	128	2	32	2	+	1740	512GB	0		AMD EPYC 7542	0	AMD, EPYC, 7542, 512G
max-exflg006	allgpu upex-beamtime upex-middle upex exfel	40	2	10	2	+	768	256GB	1xGV100GL		E5-2640 v4 @ 2.40GHz	7000	INTEL, V4, E5-2640, GPU, V100, GPUx1, 256G
max-exflg024	allgpu upex-beamtime upex-middle exfel upex	40	2	10	2	+	768	256GB	1xGP100GL		E5-2640 v4 @ 2.40GHz	4700	INTEL, V4, E5-2640, GPU, P100, GPUx1, 256G
Total: 354 hosts	CPU/GPU nodes: 336/18	31088	708				562 TFlops	215775GB	18		5 different CPUs	84 TFlops	

Data reduction

RAW data files (HDF5)

```
RAW-R0070-AGIPD00-S00000.h5
RAW-R0070-AGIPD01-S00000.h5
RAW-R0070-AGIPD02-S00000.h5
RAW-R0070-AGIPD03-S00000.h5
RAW-R0070-AGIPD04-S00000.h5
RAW-R0070-AGIPD05-S00000.h5
RAW-R0070-AGIPD06-S00000.h5
RAW-R0070-AGIPD07-S00000.h5
RAW-R0070-AGIPD08-S00000.h5
RAW-R0070-AGIPD09-S00000.h5
RAW-R0070-AGIPD10-S00000.h5
RAW-R0070-AGIPD11-S00000.h5
RAW-R0070-AGIPD12-S00000.h5
RAW-R0070-AGIPD13-S00000.h5
RAW-R0070-AGIPD14-S00000.h5
RAW-R0070-AGIPD15-S00000.h5
RAW-R0070-DA01-S00000.h5
```

+

Calibration data

DESY FS-DS calibration
(Aschkan, Manuela, Thorsten)

XFEL calibration data
(Steffen Hauf)

53 TB
→

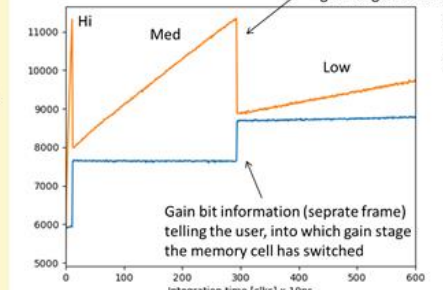
2.5 GB
→

Cheetah-AGIPD

(detector calibration, trainID matching)

https://www.cryptoolib.org/2020/03/02/cheat-catalog/										
	Refresh	Run	Details	Run	Cheatlib	Index	View	Power	Fullscreen	
		Run	Outset	HTC	Cheatlib	Cryptlib	HTC/Outset/Approved	HTCs	Minidex	HTCs/HTs
39	dark	Ready	Finished				000739-dark	0	0.00	
40	power	Ready	Finished				000400-power	0	0.00	
41	dark	Ready	Finished				00041-dark	0	0.00	
42	dark	Ready	Finished				00042-dark	0	0.00	
43	dark	Ready	Finished				00043-dark	0	0.00	
44	power	Ready	Finished				00044-power	41832	0	0.00
45	power	Ready	Finished				00045-power	41832	0	0.00
46	water	Ready	Finished				00046-water	13944	0	0.00
47	water	Ready	Finished				00047-water	13944	0	0.00
48	water	Ready	Finished				00048-water	13944	0	0.00
49	water	Ready	Finished				00049-water	13944	0	0.00
50	water	Ready	Finished				00050-water	41832	0	0.00
51	water	Ready	Finished				00051-water	41832	0	0.00
52	water	Ready	Not Done				00052-water	30000	0	0.00
53		Ready								
54		Ready								
55	yes	Ready	Finished				00055-yes	13958	0	0.00
56	yes	Ready	Finished				00056-yes	13944	0	0.00
57	yes	Ready	Finished				00057-yes	13944	0	0.00
58	yes	Ready	Finished				00058-yes	13958	0	0.00
59	yes	Ready	Finished				00059-yes	13944	0	0.00
60	yes	Ready	Finished				00060-yes	13944	0	0.00
61	yes	Ready	Finished				00061-yes	13944	0	0.00
62	yes	Ready	Finished				00062-yes	13944	0	0.00
63	no sample	Ready	Finished							
64	no sample	Ready	Finished							
65	no sample	Ready	Finished				00065-yes	13958	817	5.85
66	yes	Ready	Finished				00066-yes	13944	810	5.81
67	yes	Ready	Not Done				00067-yes	13000	762	5.60
68	yes	Ready	Finished				00068-yes	13944	684	4.91
69	yes	Ready	Finished				00069-yes	13958	619	4.43
70	yes	Ready	Finished				00070-yes	25000	914	4.07
71	yes	Ready	Not Done				00071-yes	25000	914	4.07
72	yes	Ready	Finished				00072-yes	25000	915	4.09
73	yes	Copping	Not Done				00073-yes	25000	914	3.02
74	yes	Ready	Not Done				00074-yes	25000	508	2.12
75	yes	Ready	Finished				00075-yes	27000	596	2.21
76	yes	Copping	Not Done				00076-yes			
77	yes	Ready	Finished				00077-yes	13958	401	3.30
78	yes	Ready	Finished				00078-yes	13958	405	3.34
79	yes	Ready	Finished				00079-yes	13958	405	3.34
80	yes	Ready	Finished				00080-yes	13958	401	3.30
81	yes	Ready	Finished				00081-yes	13944	791	5.87
82	yes	Ready	Finished				00082-yes	13944	172	1.29
83	yes	Ready	Finished				00083-yes	13944	815	5.84
84	yes	Ready	Finished				00084-yes	13944	608	4.23
85	yes	Ready	Finished				00085-yes	13944	404	3.30
86	yes	Ready	Finished				00086-yes	13944	925	6.61
87	yes	Ready	Finished				00087-yes	13944	925	6.61
88	yes	Ready	Finished				00088-yes	13958	461	3.30
89	yes	Copping	Finished				00089-yes	12348	0	0.00
90	yes	Ready	Finished				00090-yes	13944	0	0.00
91	yes	Ready	Finished				00091-yes	13944	0	0.00
92	yes	Ready	Finished				00092-yes	13944	0	0.00
93	yes	Ready	Finished				00093-yes	13944	0	0.00
94	power	Ready	Finished				00094-power	13944	0	0.00
95	power	Ready	Finished				00095-power	13944	0	0.00
96	power	Ready	Finished				00096-power	13944	0	0.00
97	power	Ready	Finished				00097-power	13944	0	0.00
98	power	Ready	Finished				00098-power	13944	0	0.00
99	power	Ready	Finished				00099-power	13944	0	0.00

Analog information from which offset and gain for each gain stage are extracted



CrystFEL

Detector
geometry

160 GB

411 kB

MTZ file



Phenix,
CCP4

Thank you for attention!

