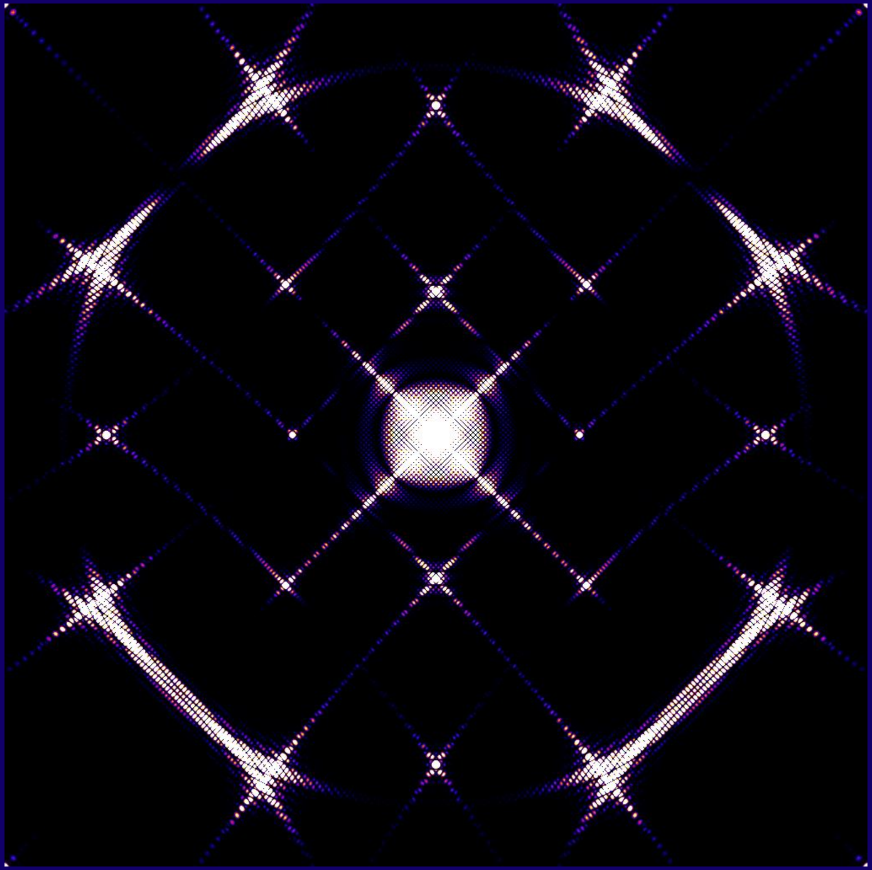
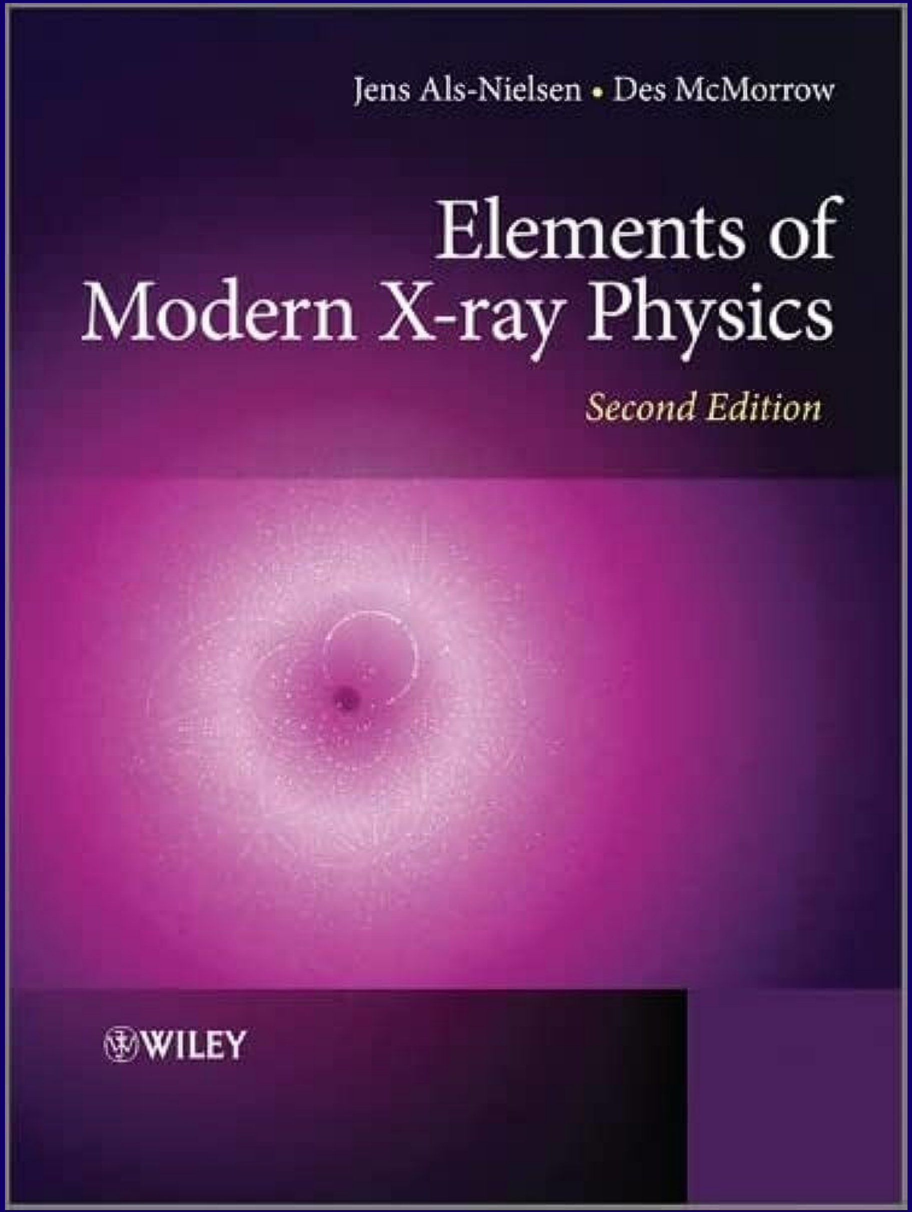
Reciprocal space. Part 2



O. M. Yefanov

CFEL at DESY, Hamburg, Germany

To read


Jens Als-Nielsen • Des McMorrow
Elements of Modern X-ray Physics
Second Edition
WILEY

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

H = h**a***+k**b***+l**c***

h, k, l – Miller indexes

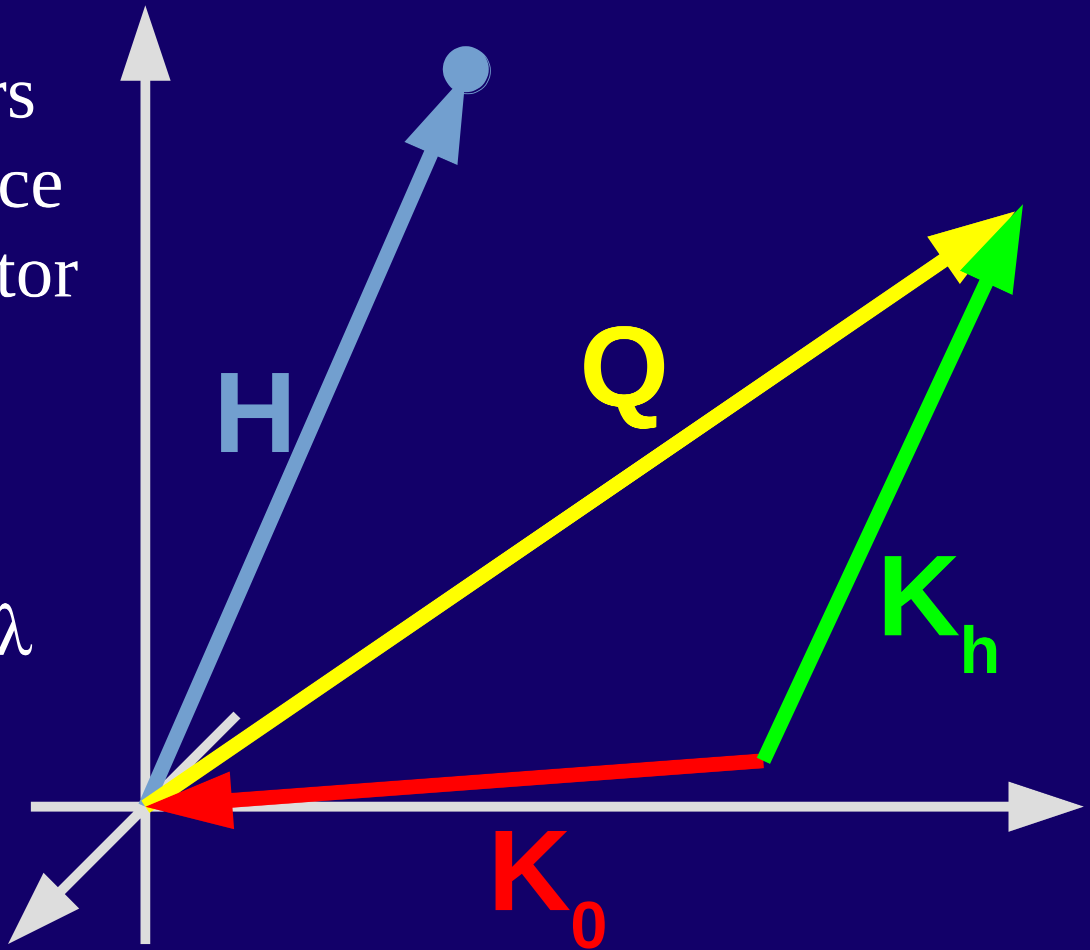
λ – wavelength (~1Å)

K – wavevector, |**K**| = 1/ λ

Q – scattering vector

$\mathbf{Q} = \mathbf{K_h} - \mathbf{K_0}$

H = Q – Bragg's law



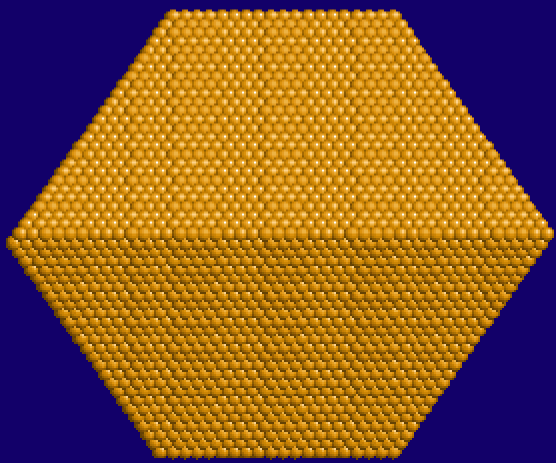
Non-crystalline objects

Reciprocal space in 3D

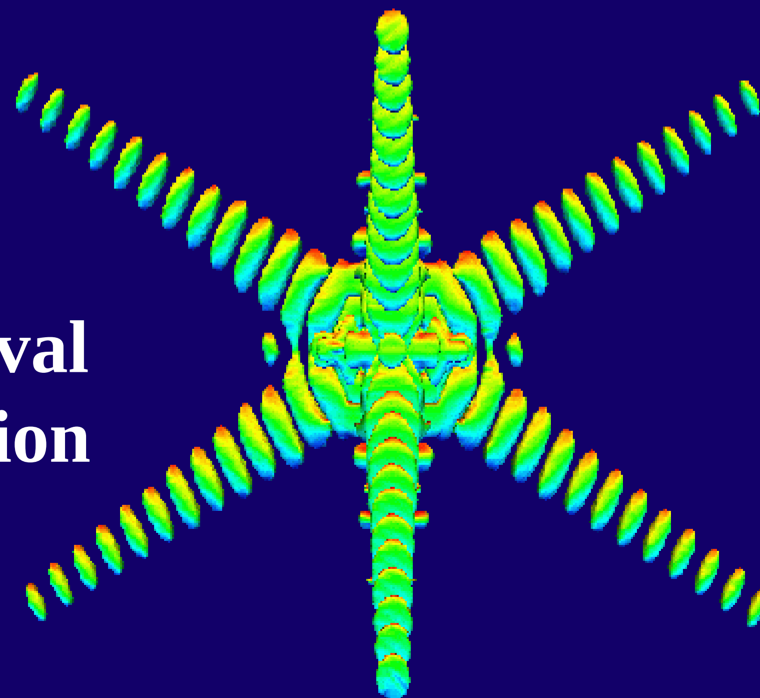
Real (object)

Fourier transform

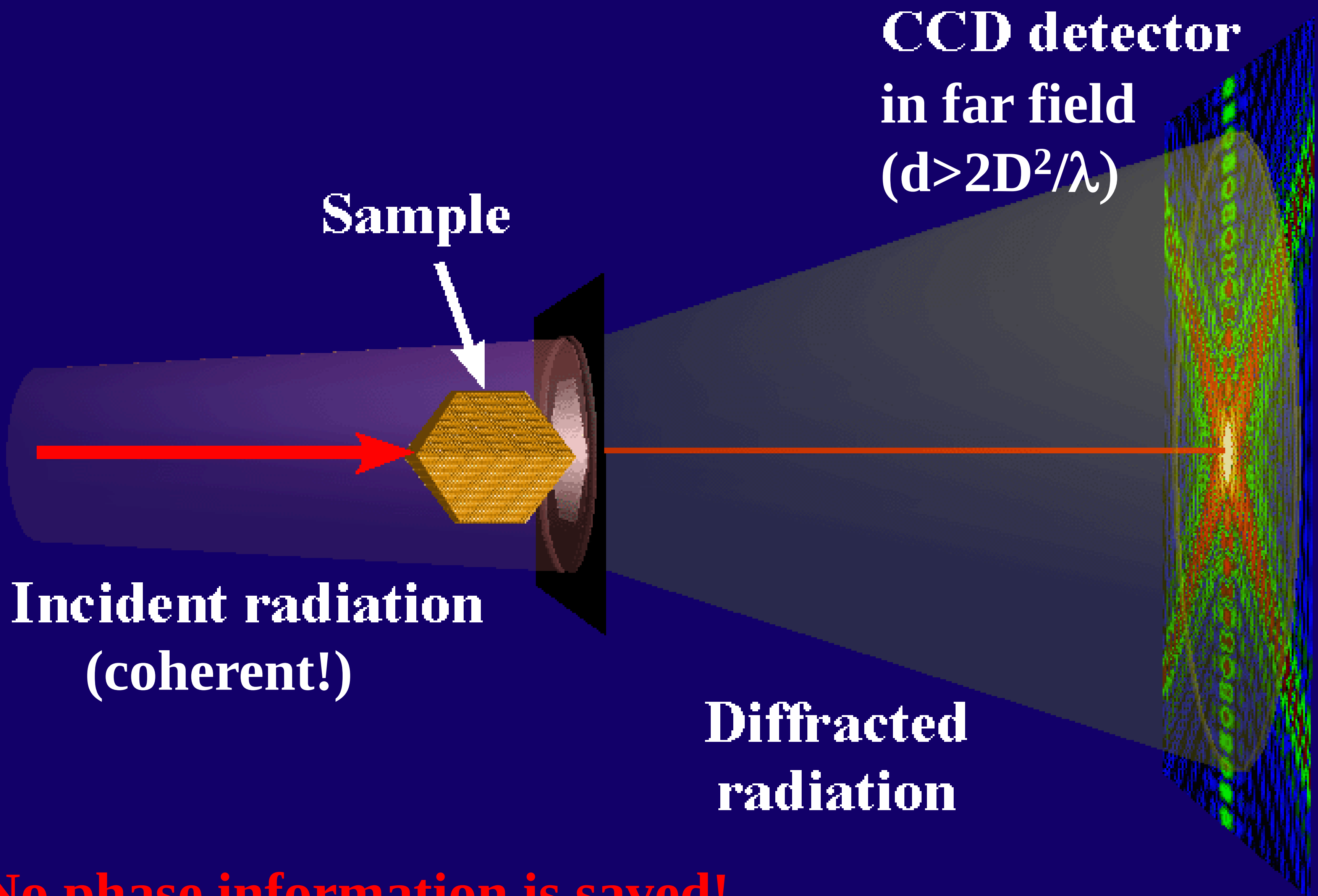
Reciprocal (object)



Phase retrieval reconstruction



Coherent X-ray Diffraction Imaging



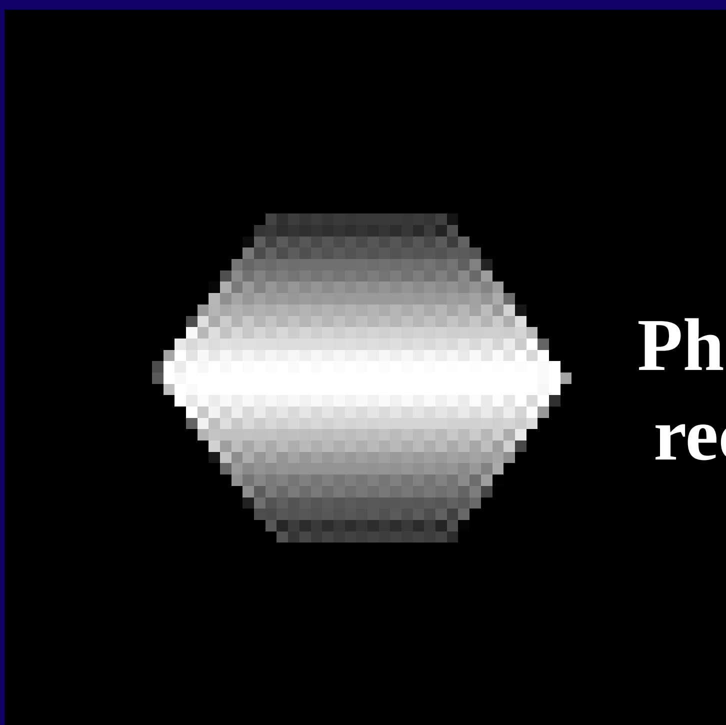
No phase information is saved!

Reciprocal space in 2D

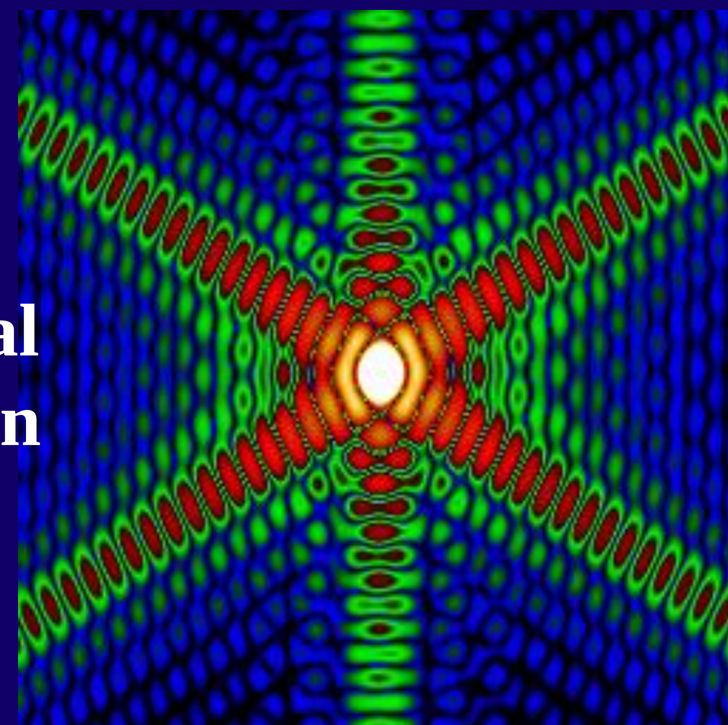
Projection of the object

Section through reciprocal space

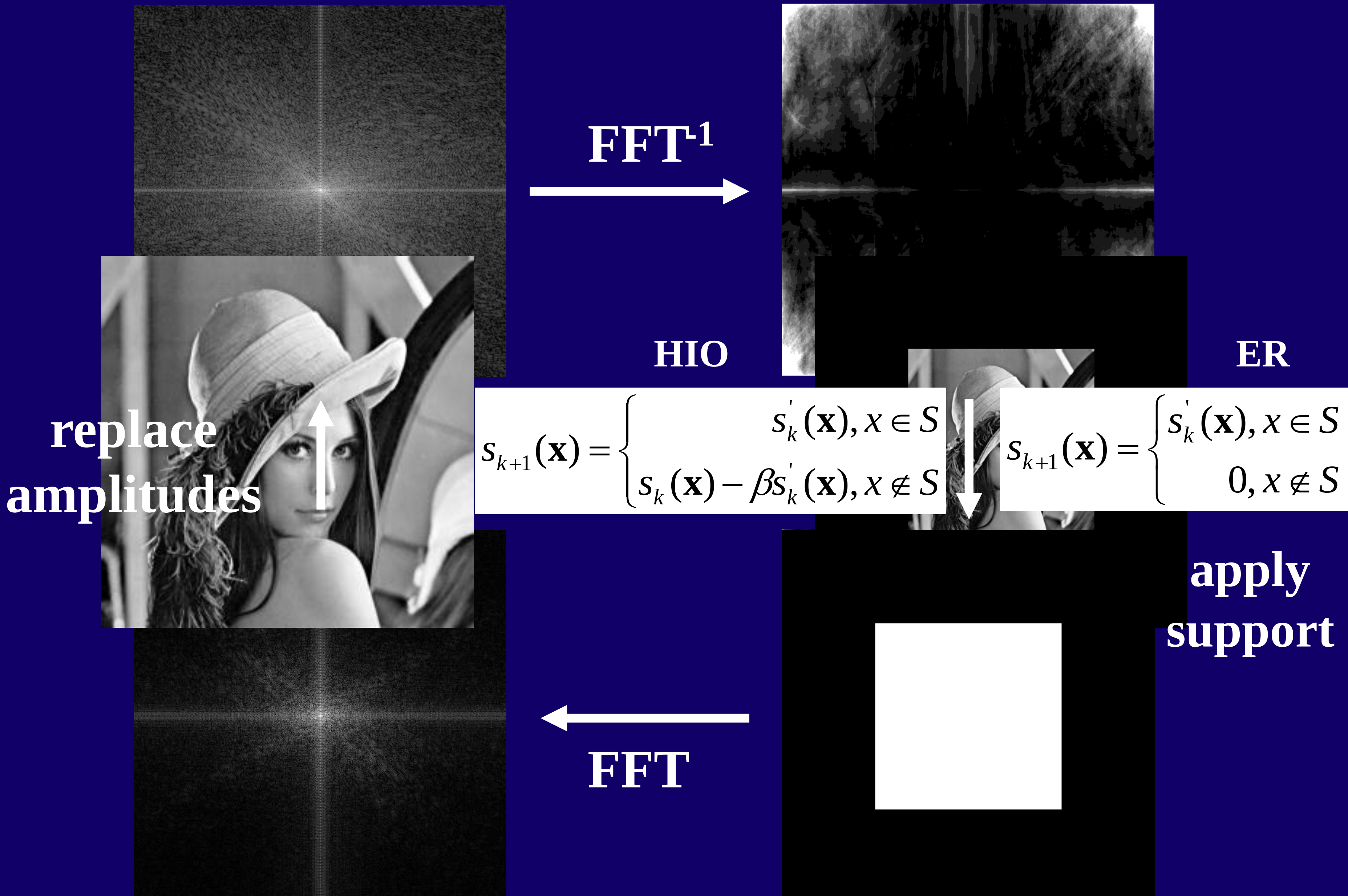
Fourier transform



Phase retrieval reconstruction



Phase retrieval algorithm:



HIO:

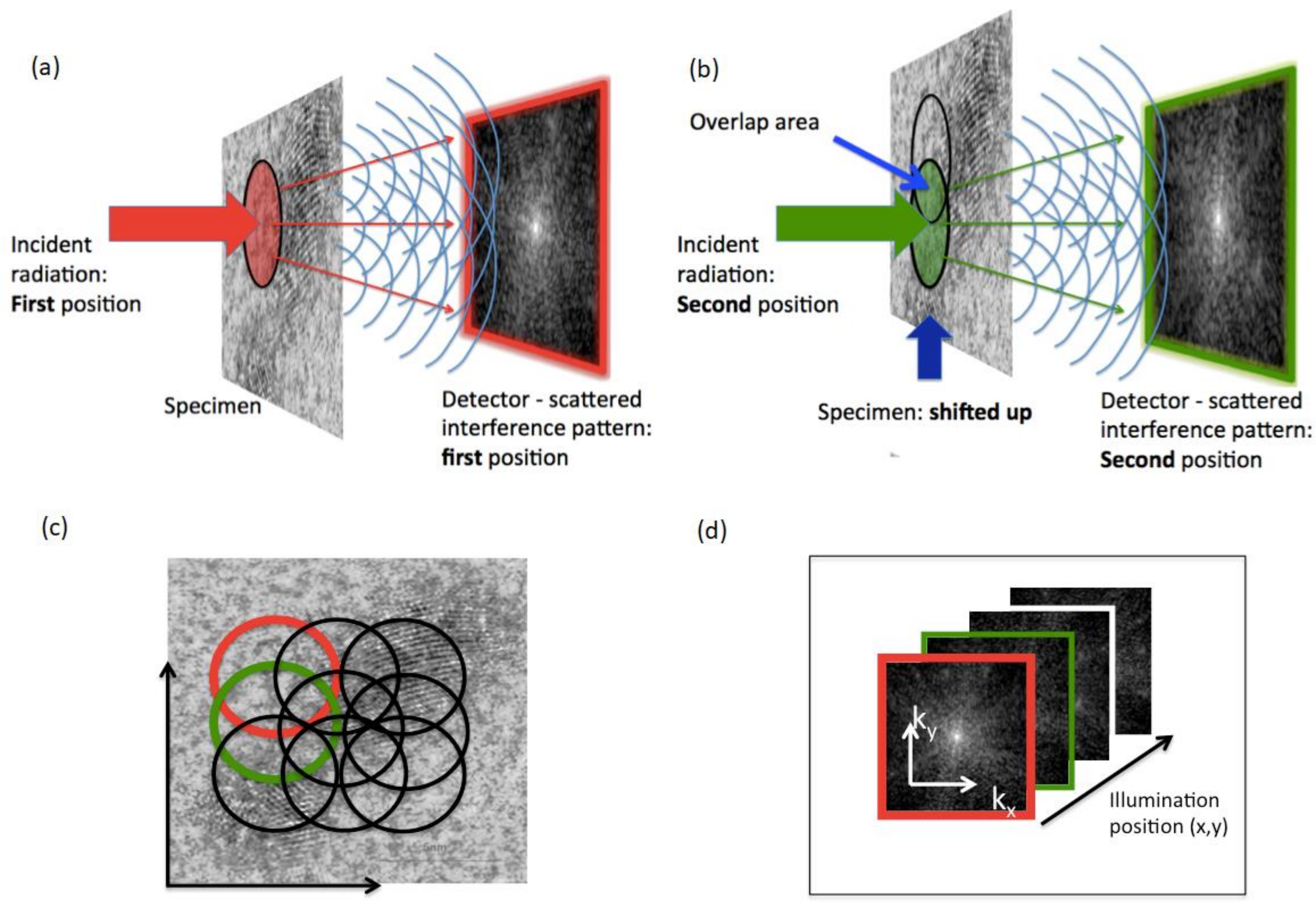
$$s_{k+1}(\mathbf{x}) = \begin{cases} s_k^{'}(\mathbf{x}), x \in S \\ s_k(\mathbf{x}) - \beta s_k^{'}(\mathbf{x}), x \notin S \end{cases}$$

ER:

$$s_{k+1}(\mathbf{x}) = \begin{cases} s_k^{'}(\mathbf{x}), x \in S \\ 0, x \notin S \end{cases}$$

Phase retrieval algorithm:

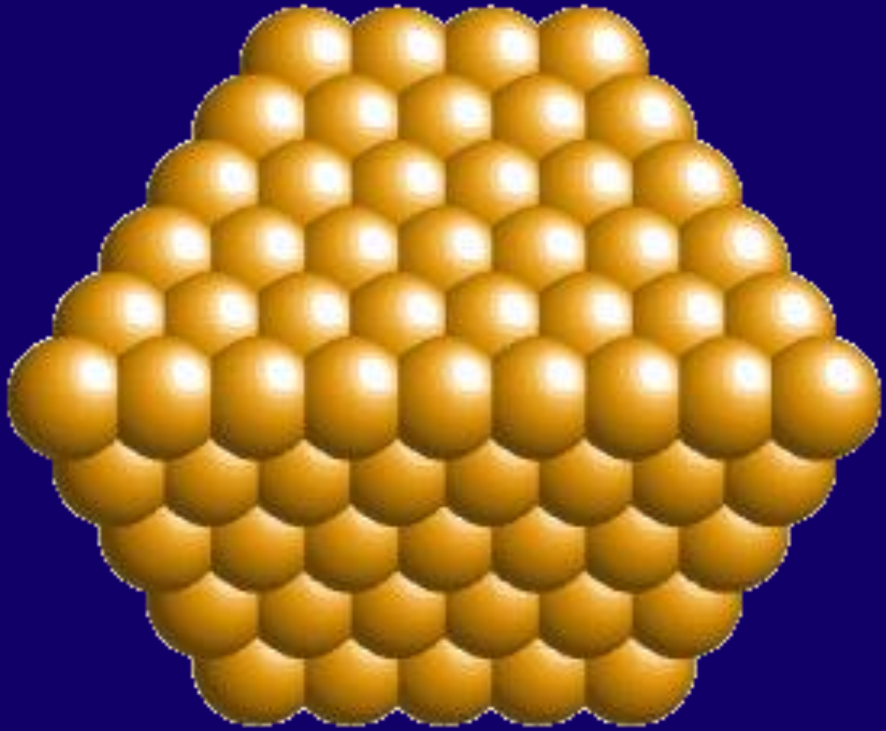
Ptychography



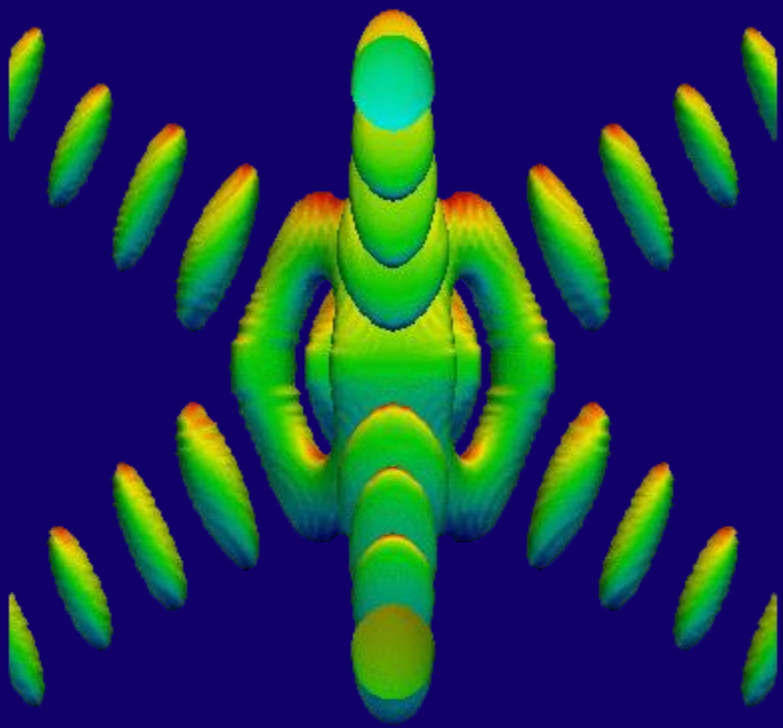
From Wiki

Why do we need high resolution?

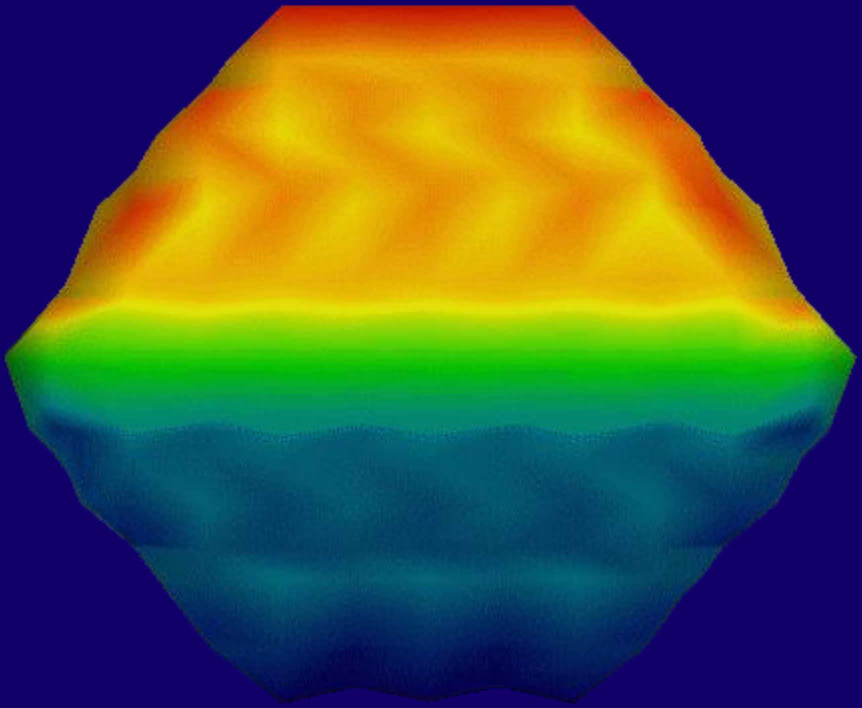
3D crystalline sample



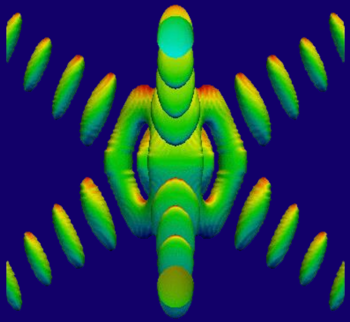
Reciprocal space for low Q

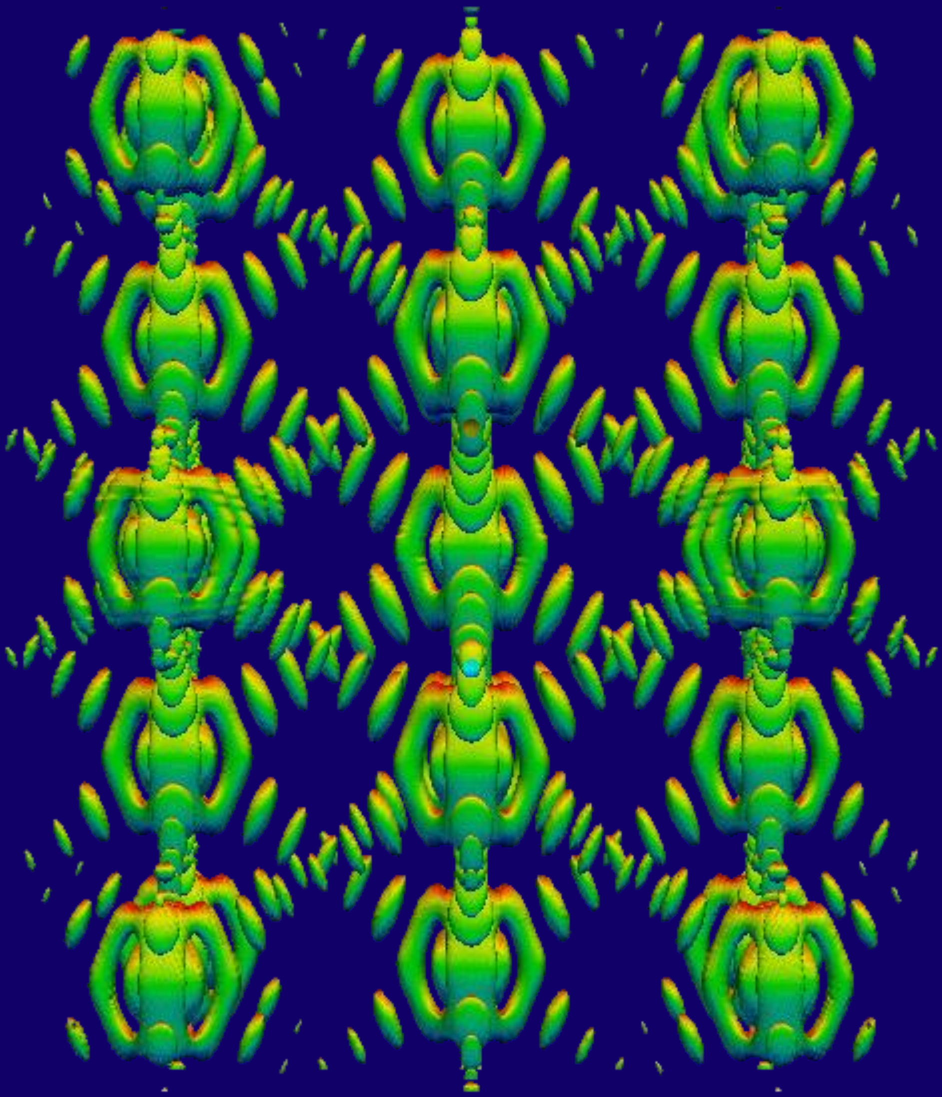


Reconstruction for low Q

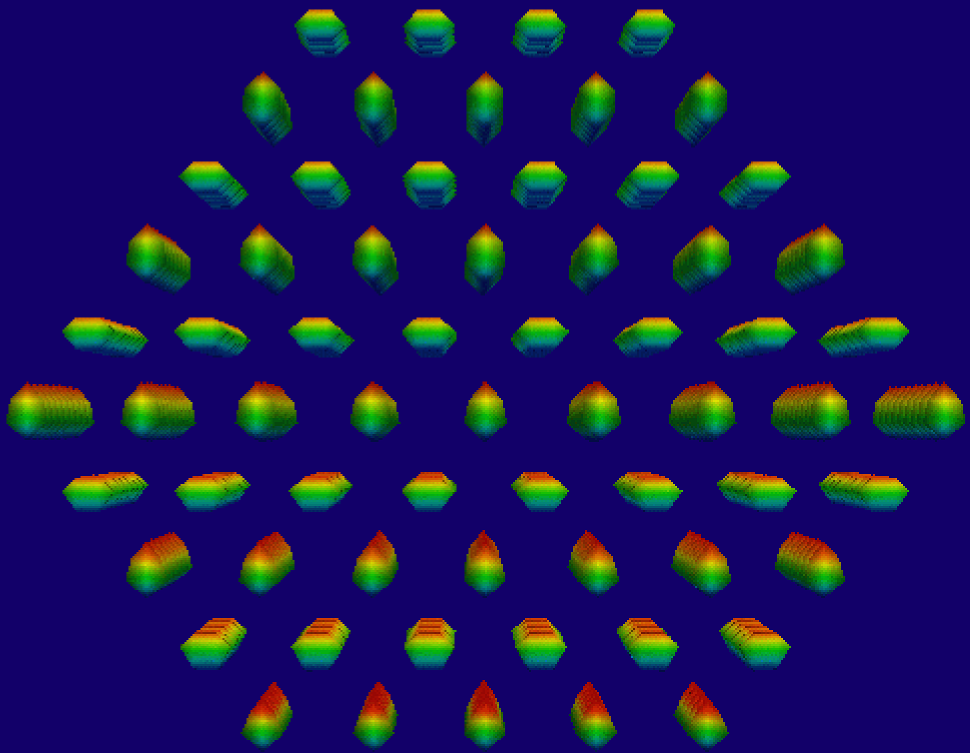


Reciprocal space for high Q



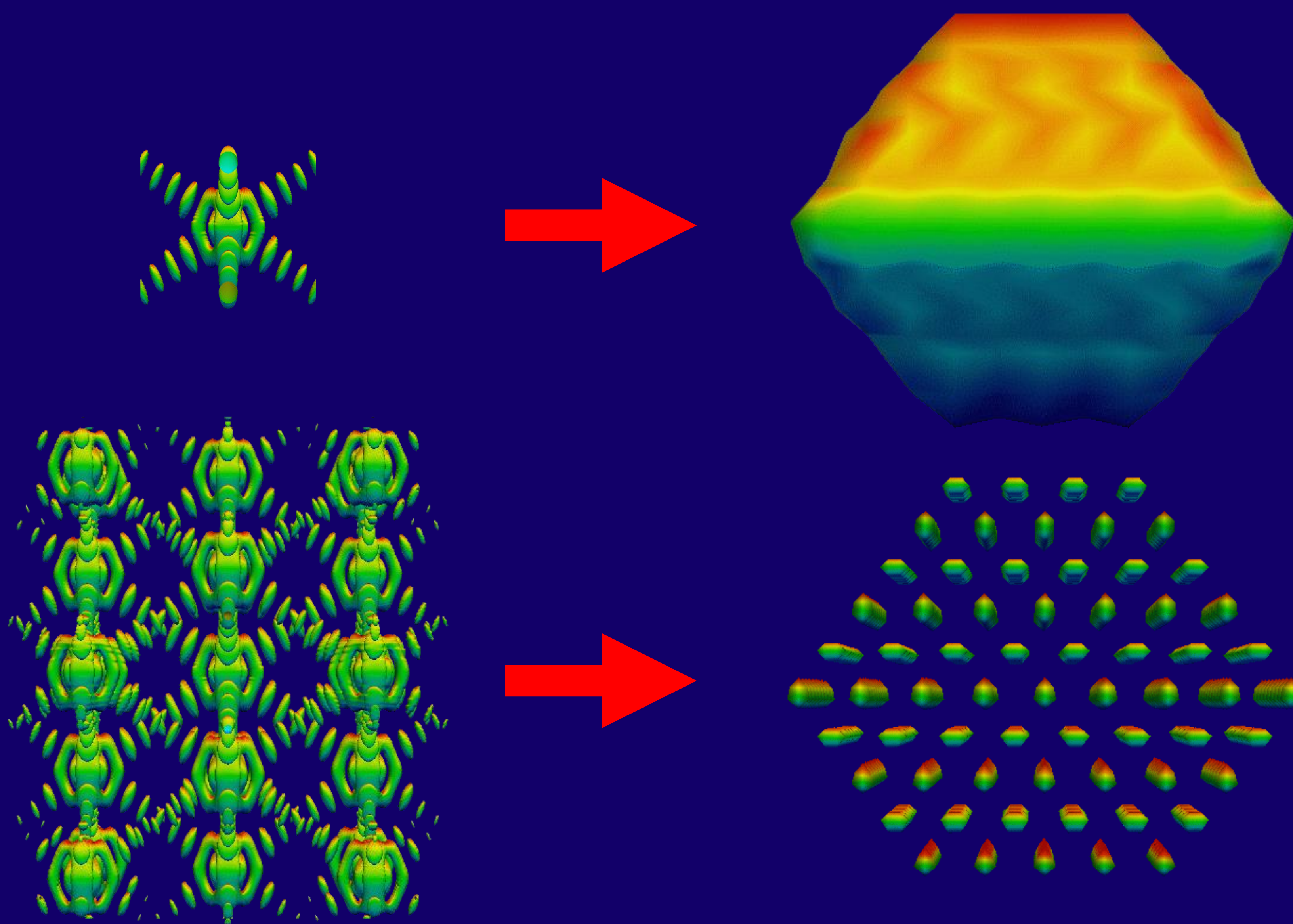


Reconstruction for high Q



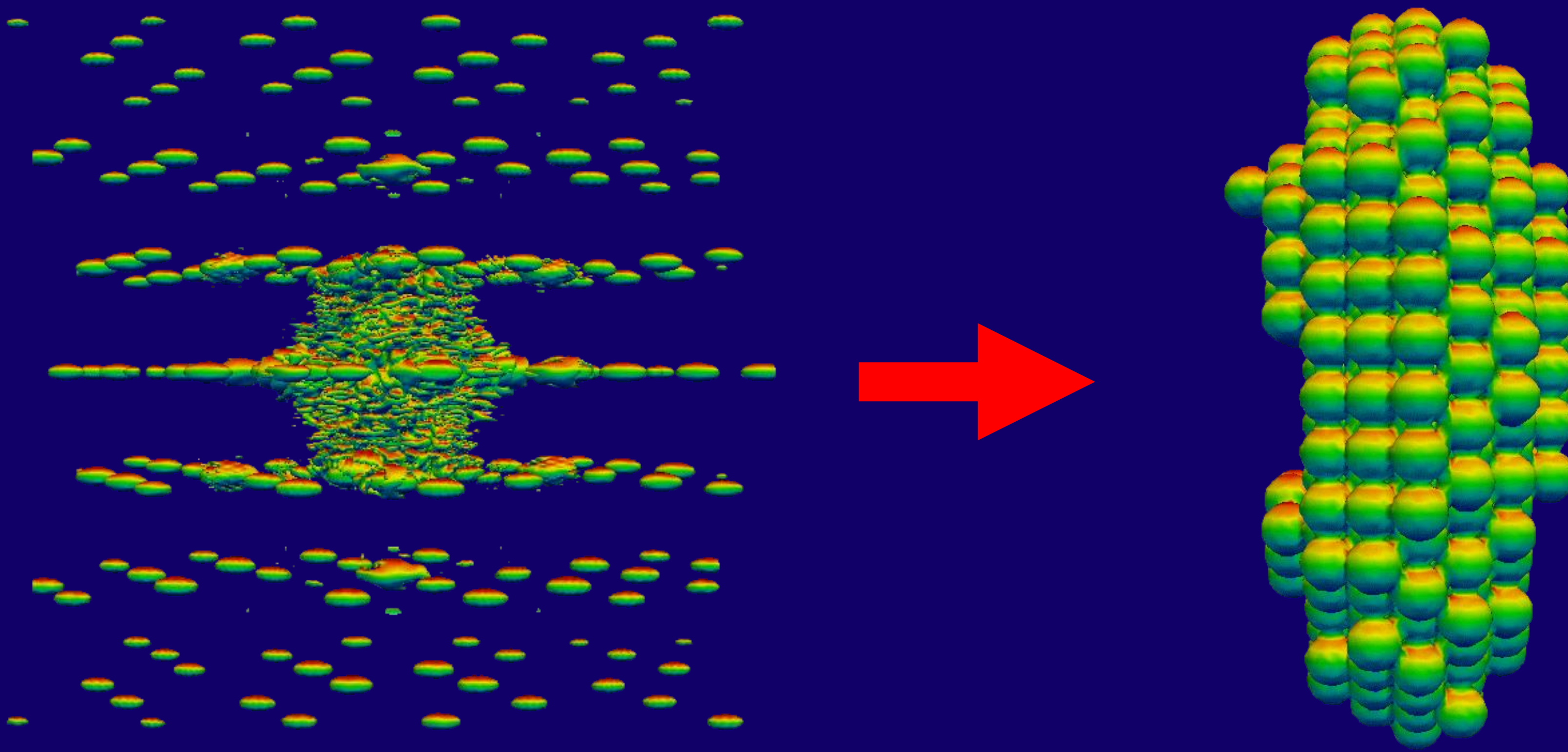
High vs low Q:

Reciprocal space **Real space**



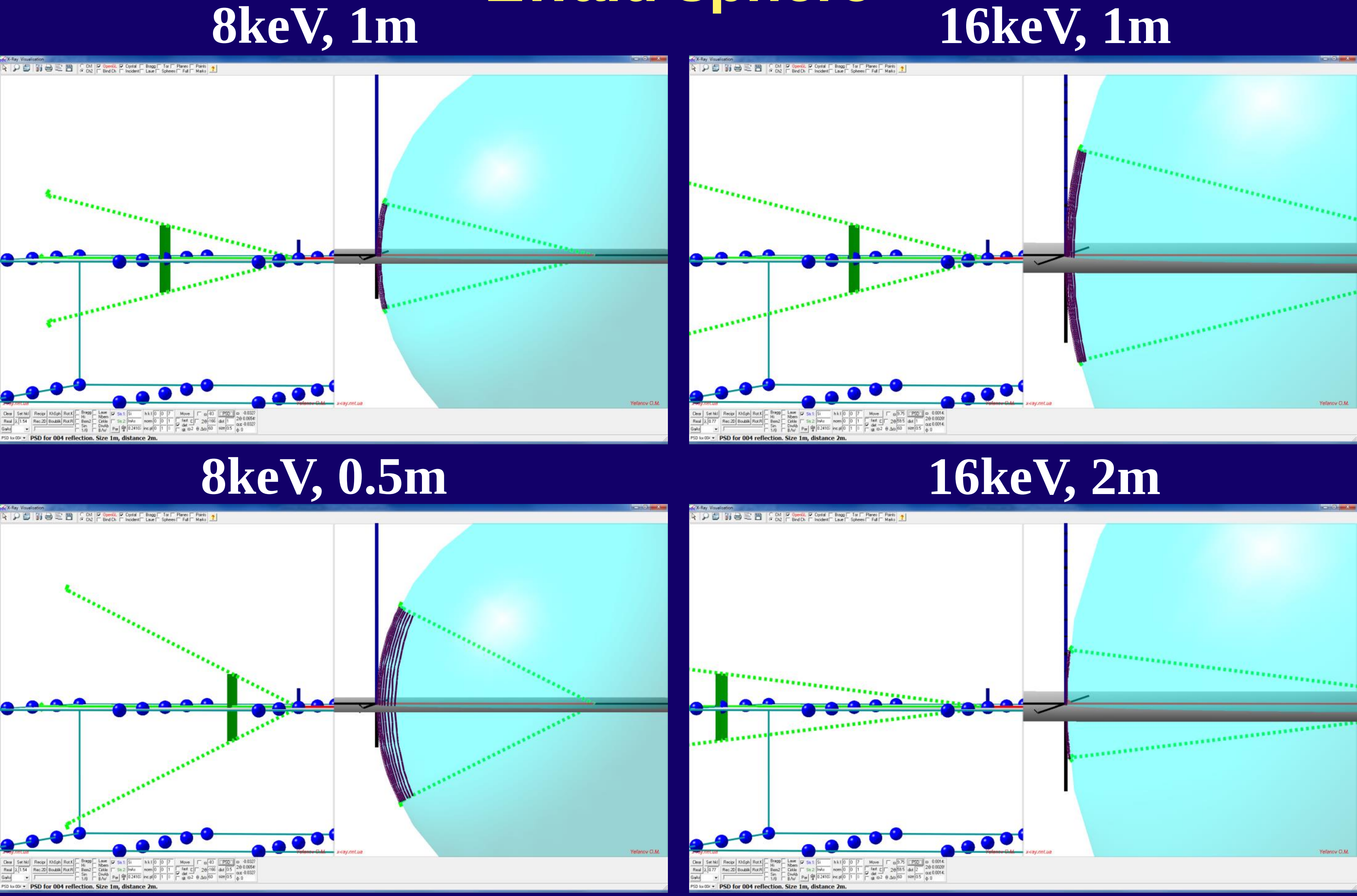
Another example

Reciprocal space **Real space**



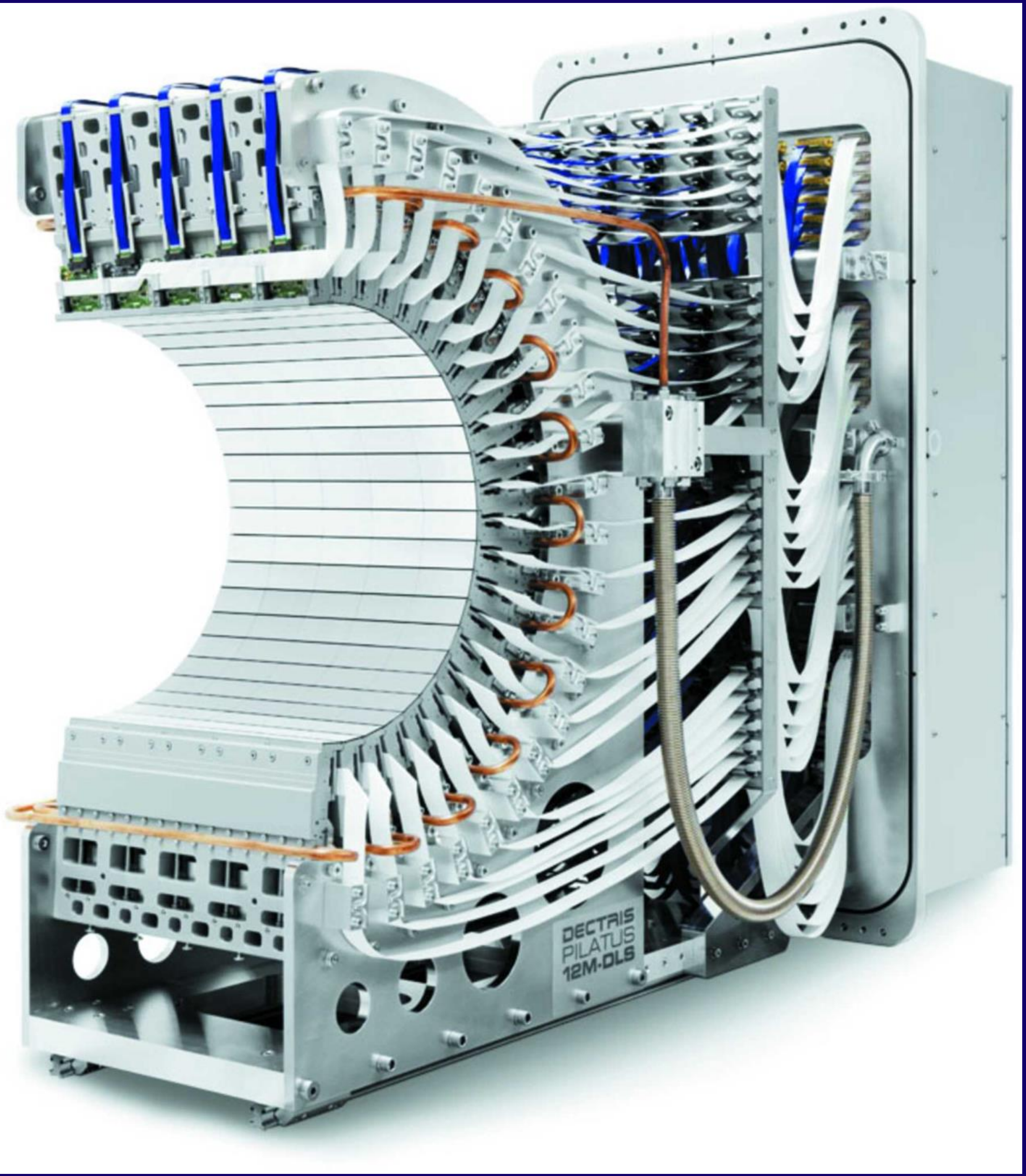
Ewald sphere

Ewald sphere



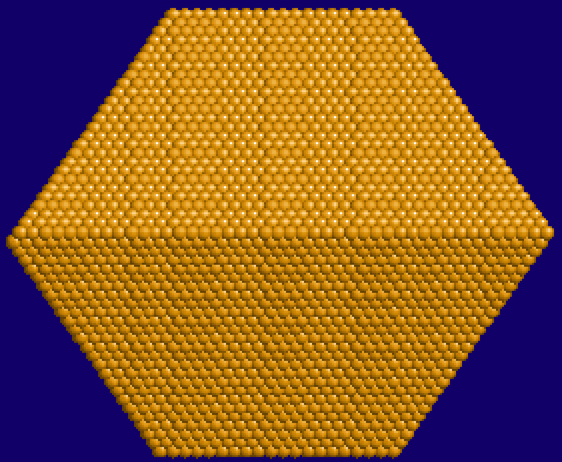
Soft x-rays are difficult for high resolution

Ewald sphere, low energy



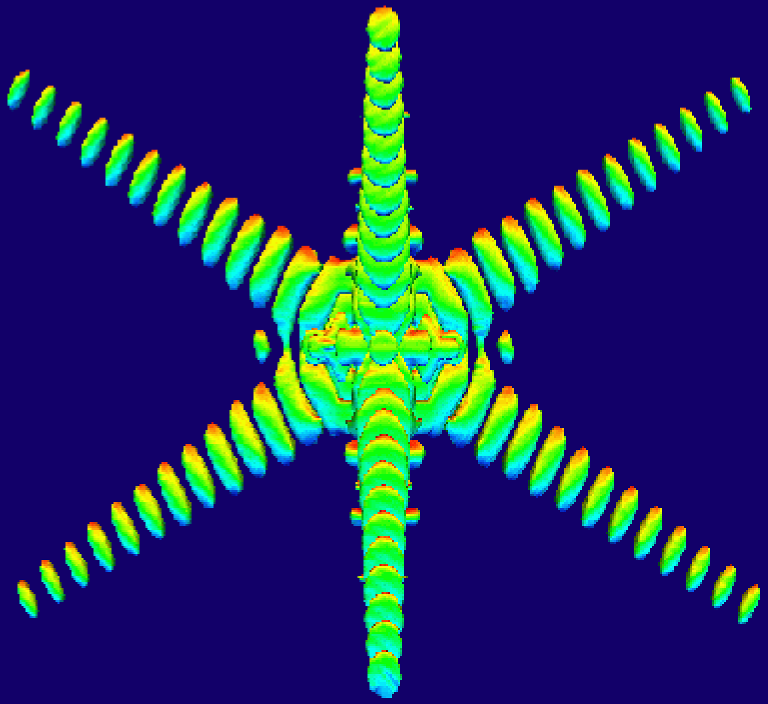
Reciprocal space in 3D

Real (object)



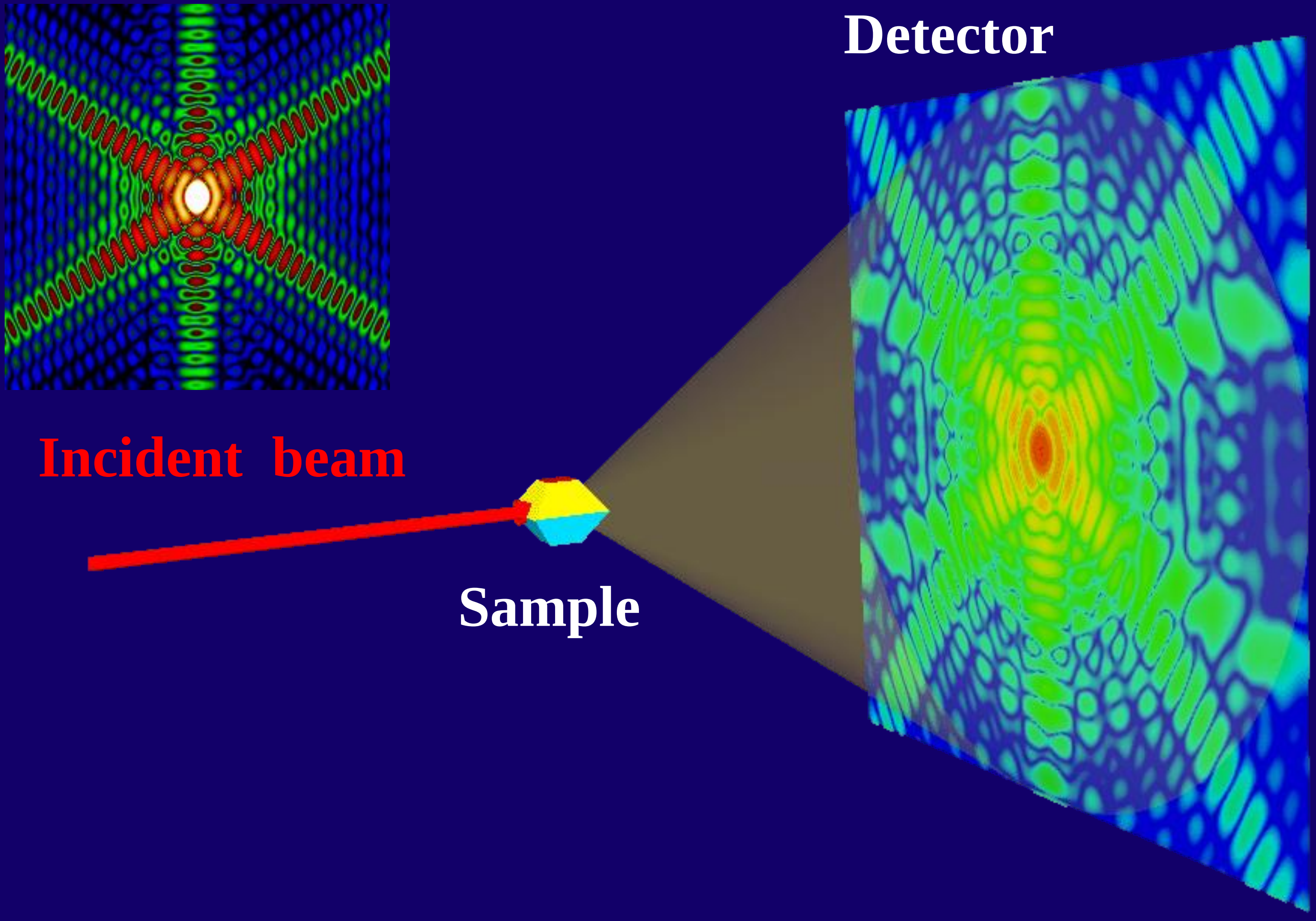
≈ Fourier transform

Reciprocal (object)

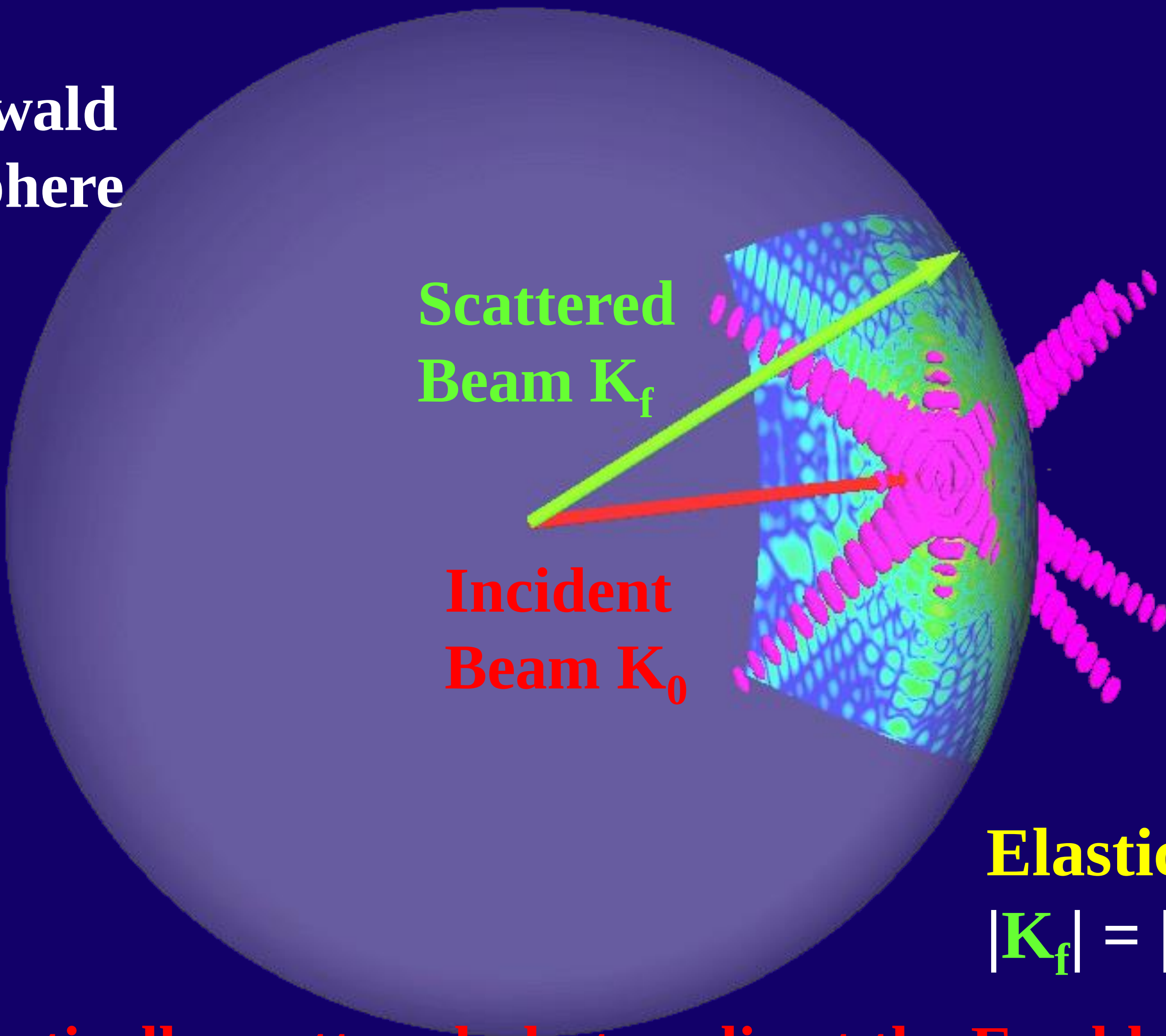


Truncation rods

Diffraction in real space



Diffraction in reciprocal space



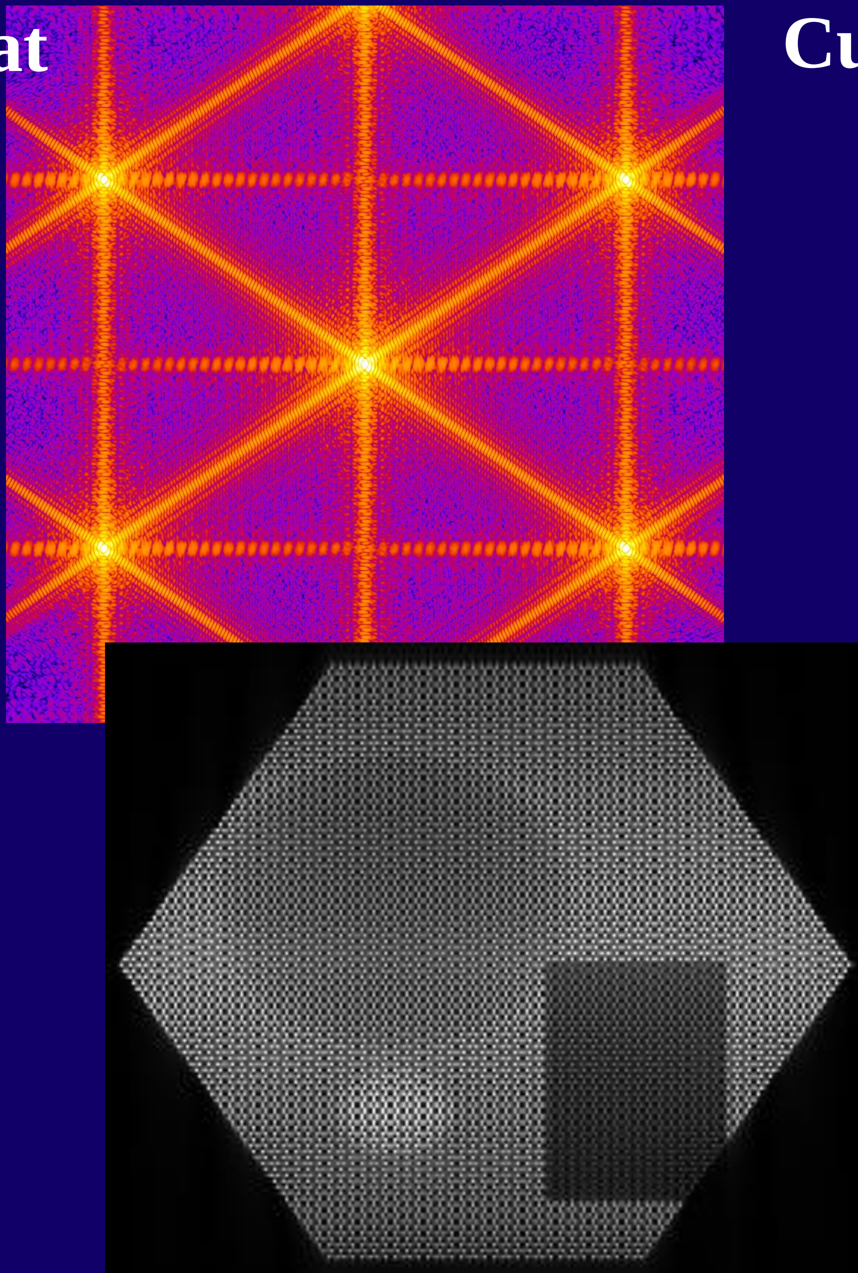
Elastic scattering:

$|K_f| = |K_0| = 2\pi/\lambda$

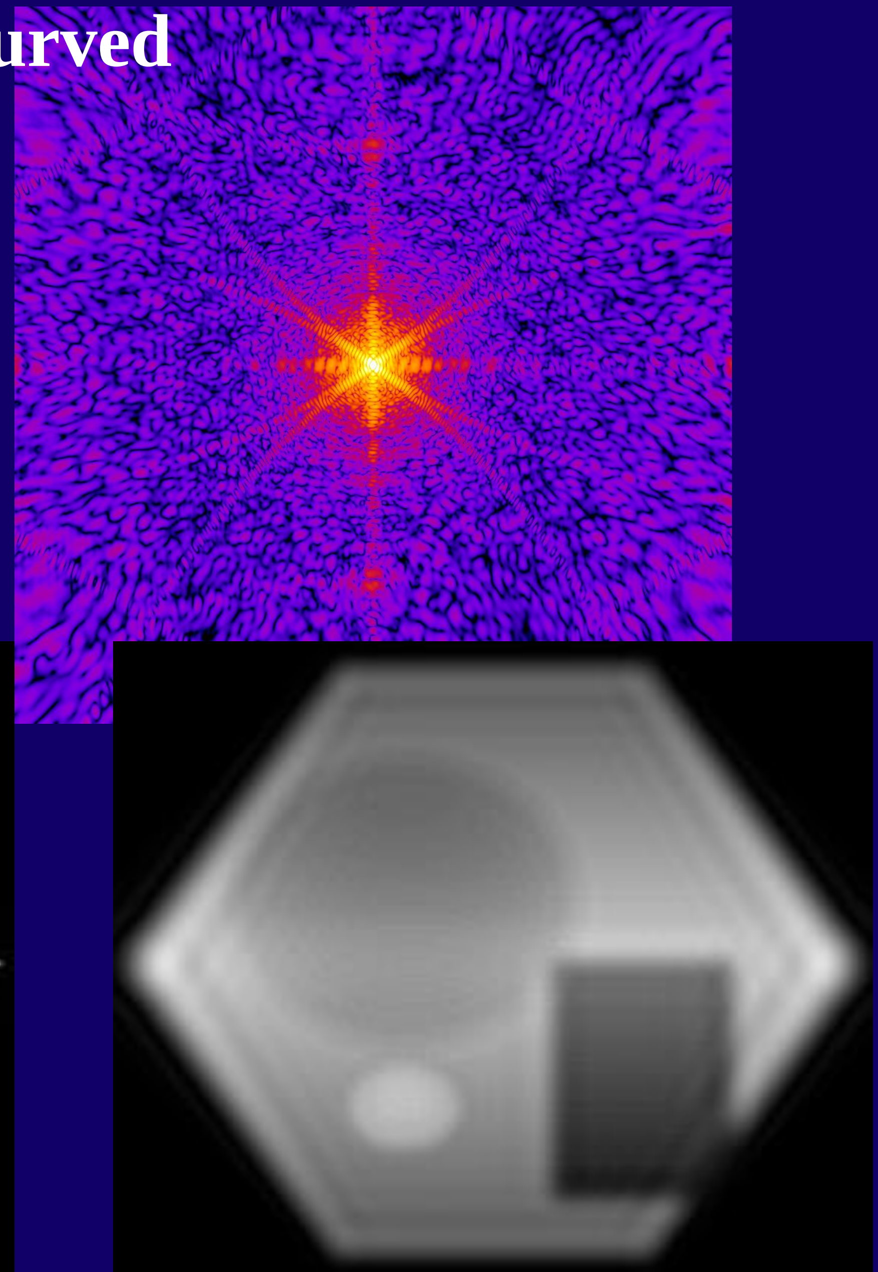
Elastically scattered photons lie at the Ewald sphere

Ewald sphere "effects"

Flat

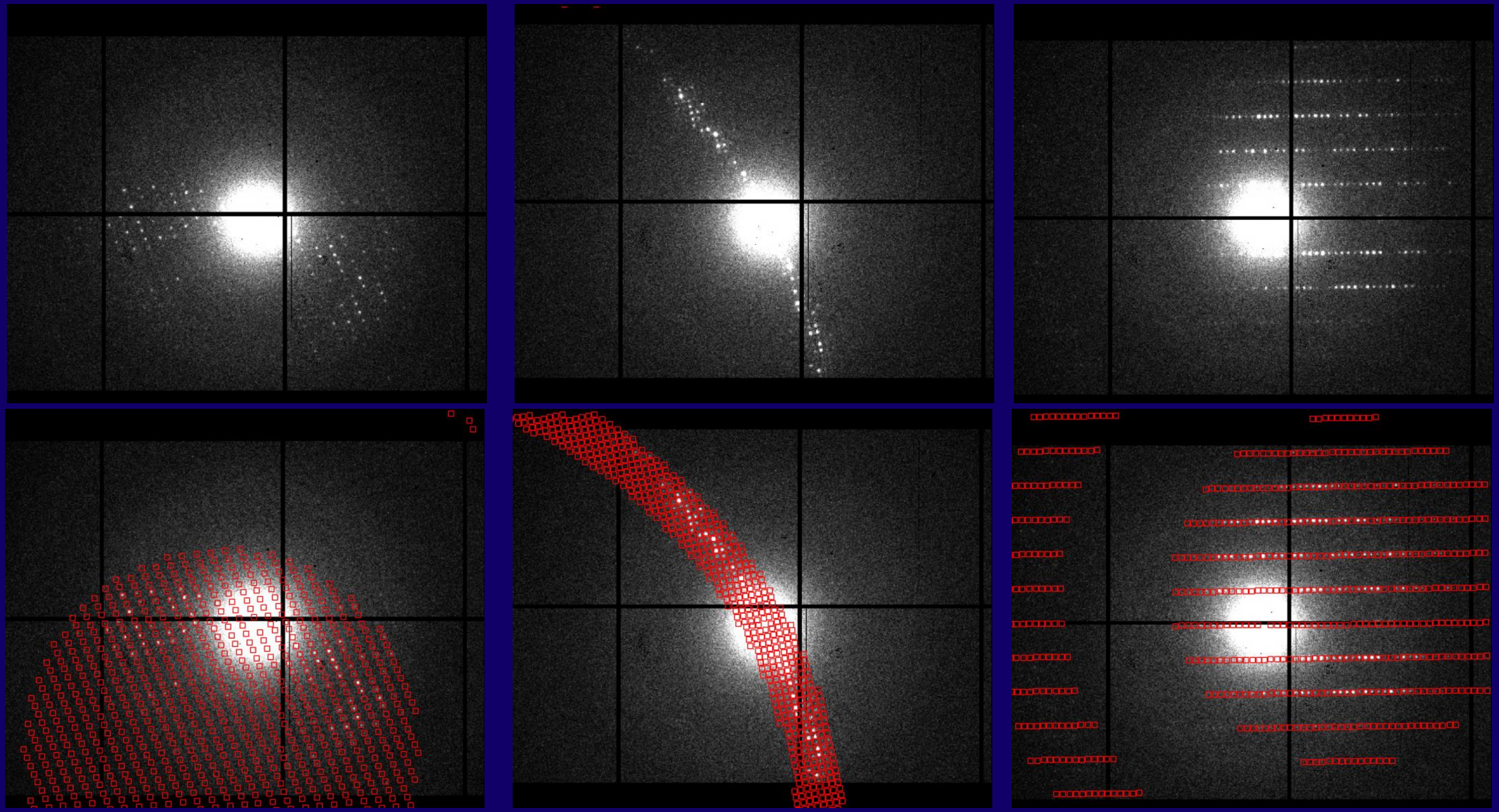


Curved



Electron Diffraction

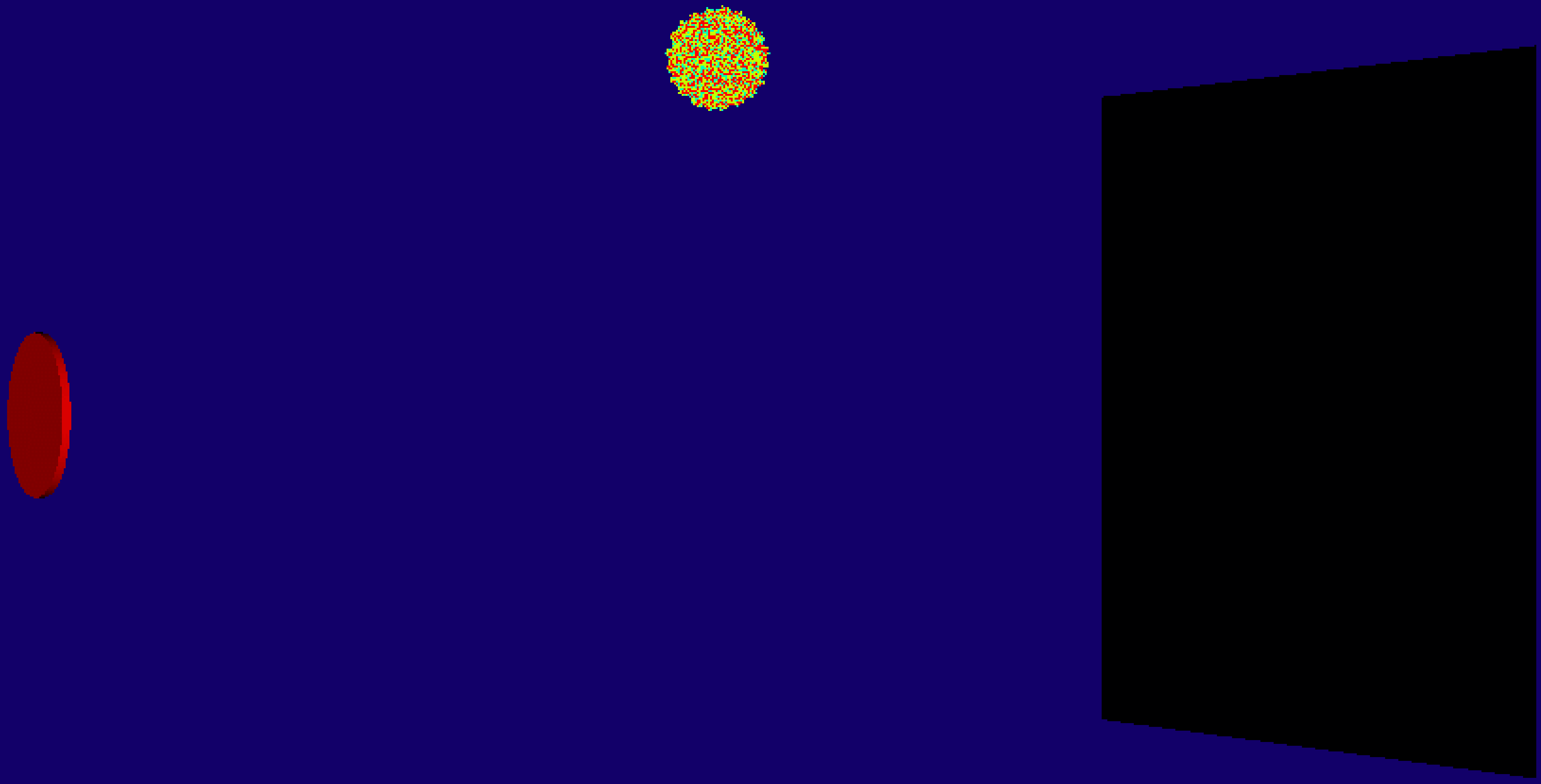
500keV, L = 1570mm, D (vert) = 34mm, so L/D = 50!



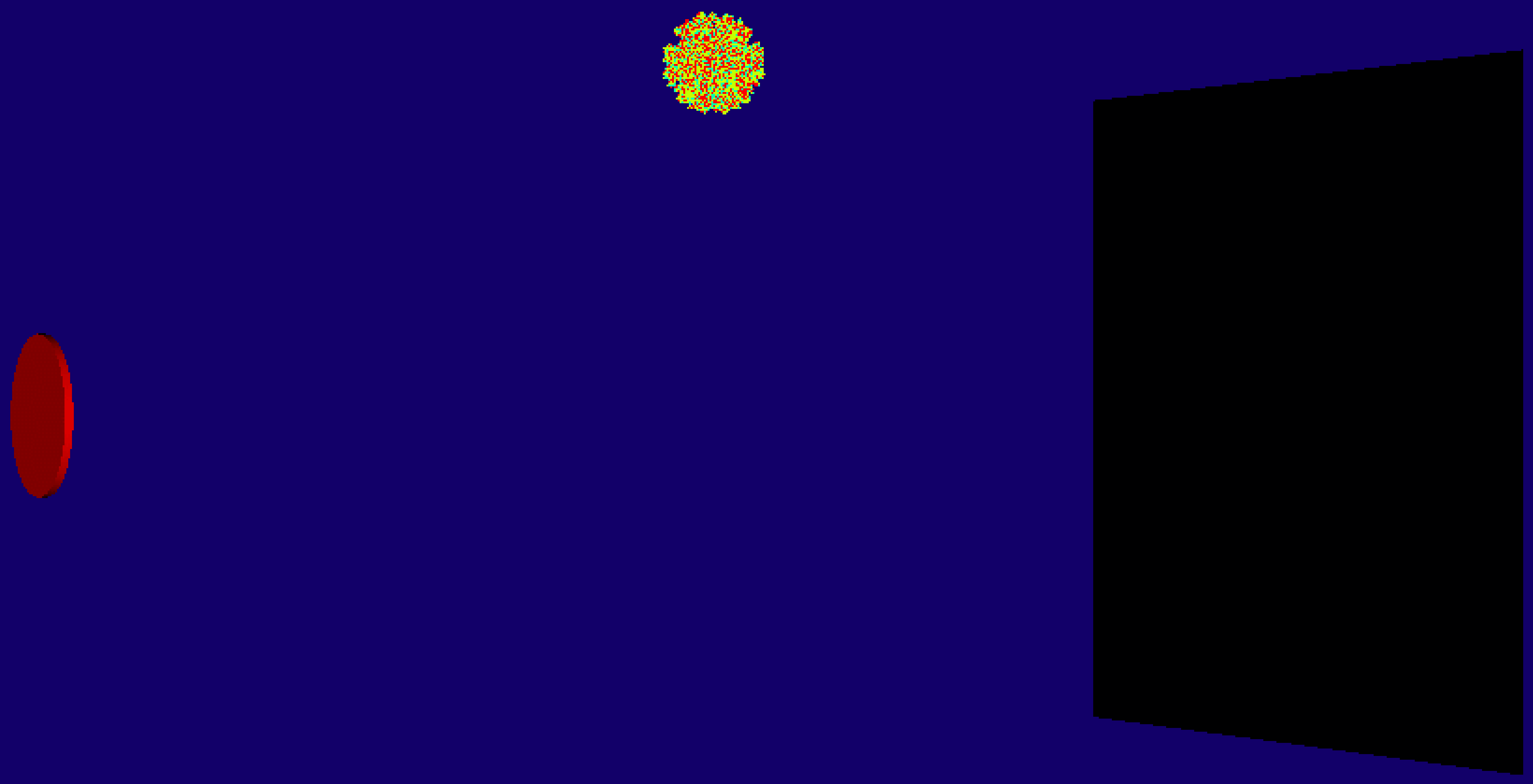
Even for electrons Ewald sphere is not "flat"!

Single Particle Imaging (SPI)

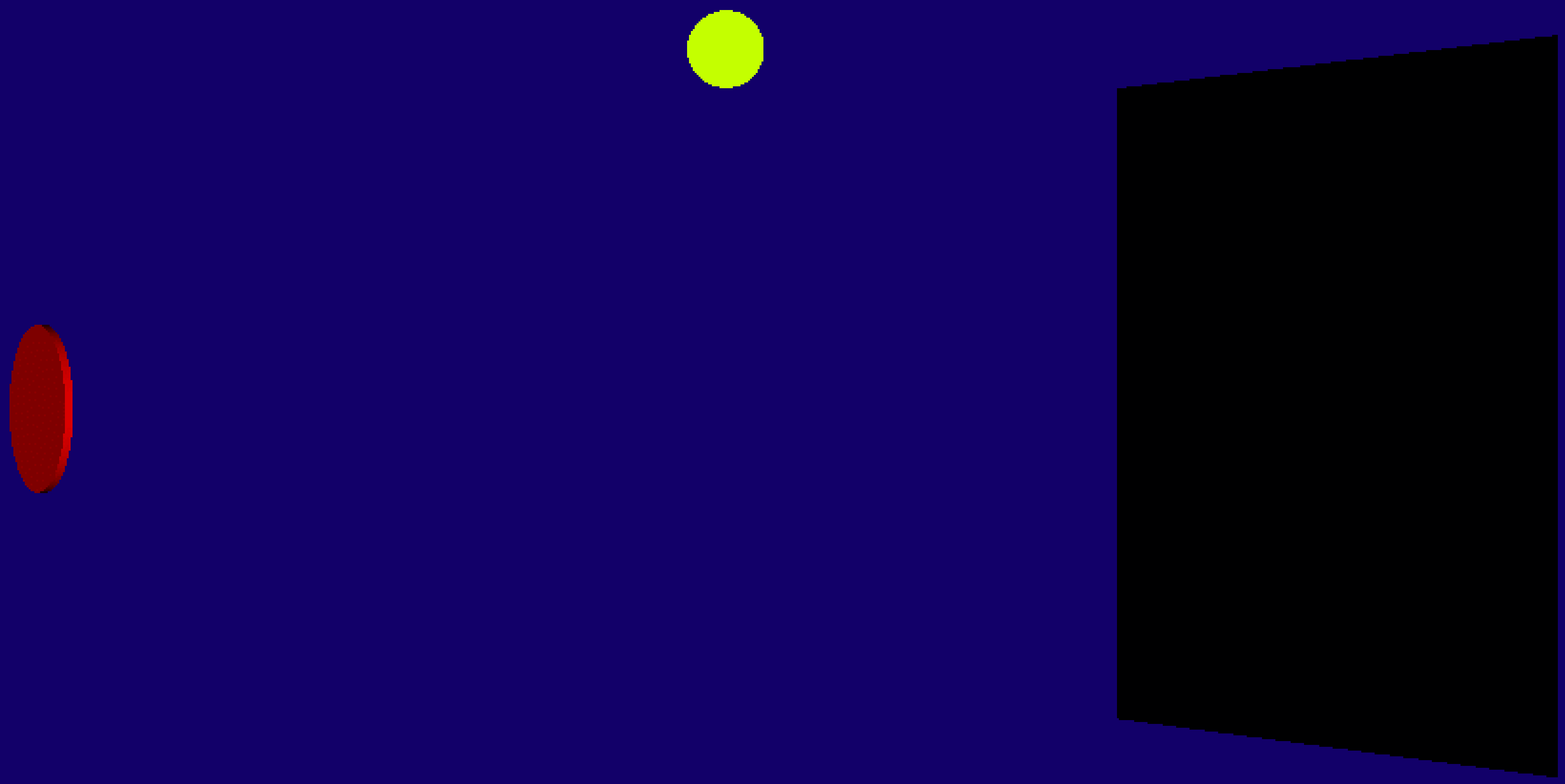
Diffraction on a single virus



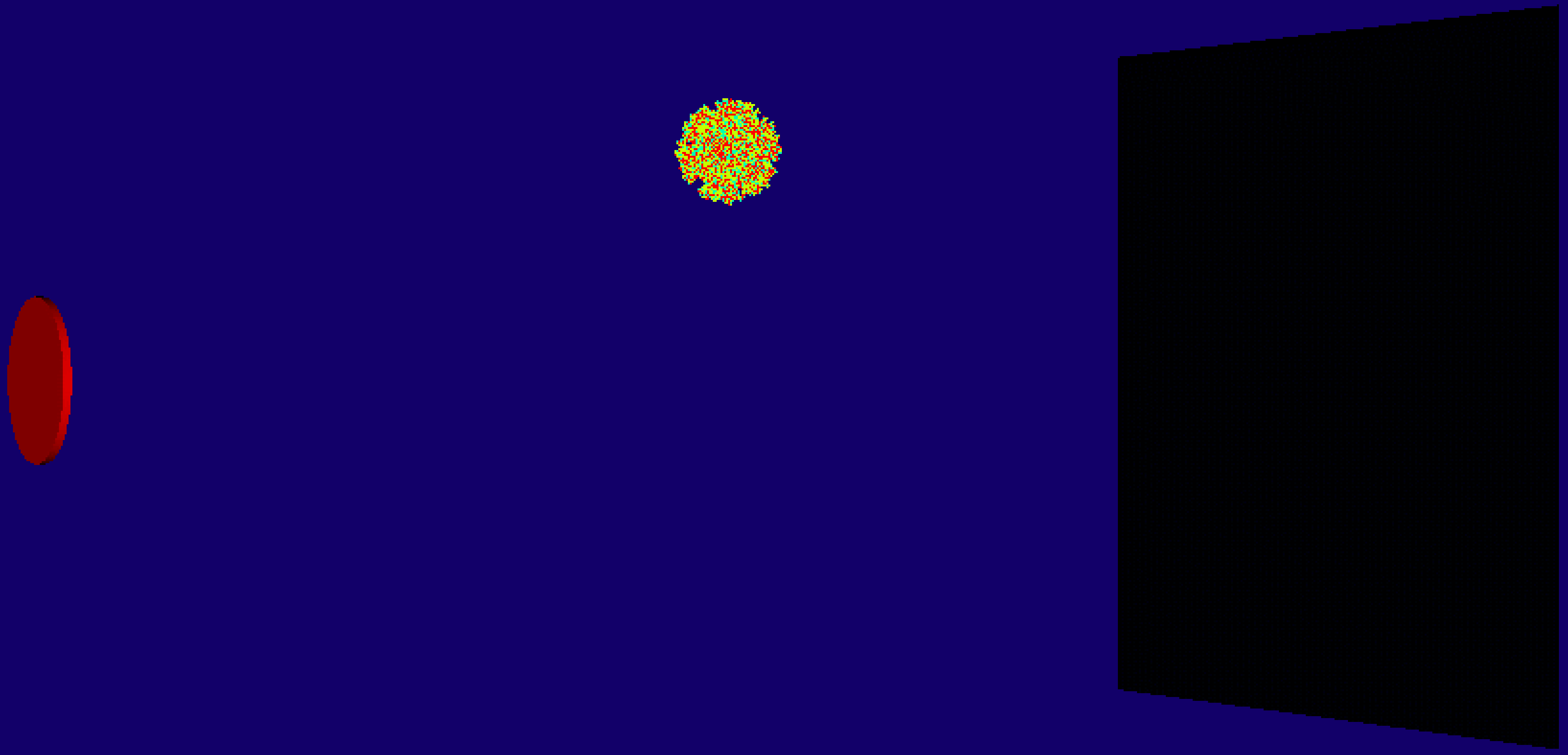
Diffraction on a single virus



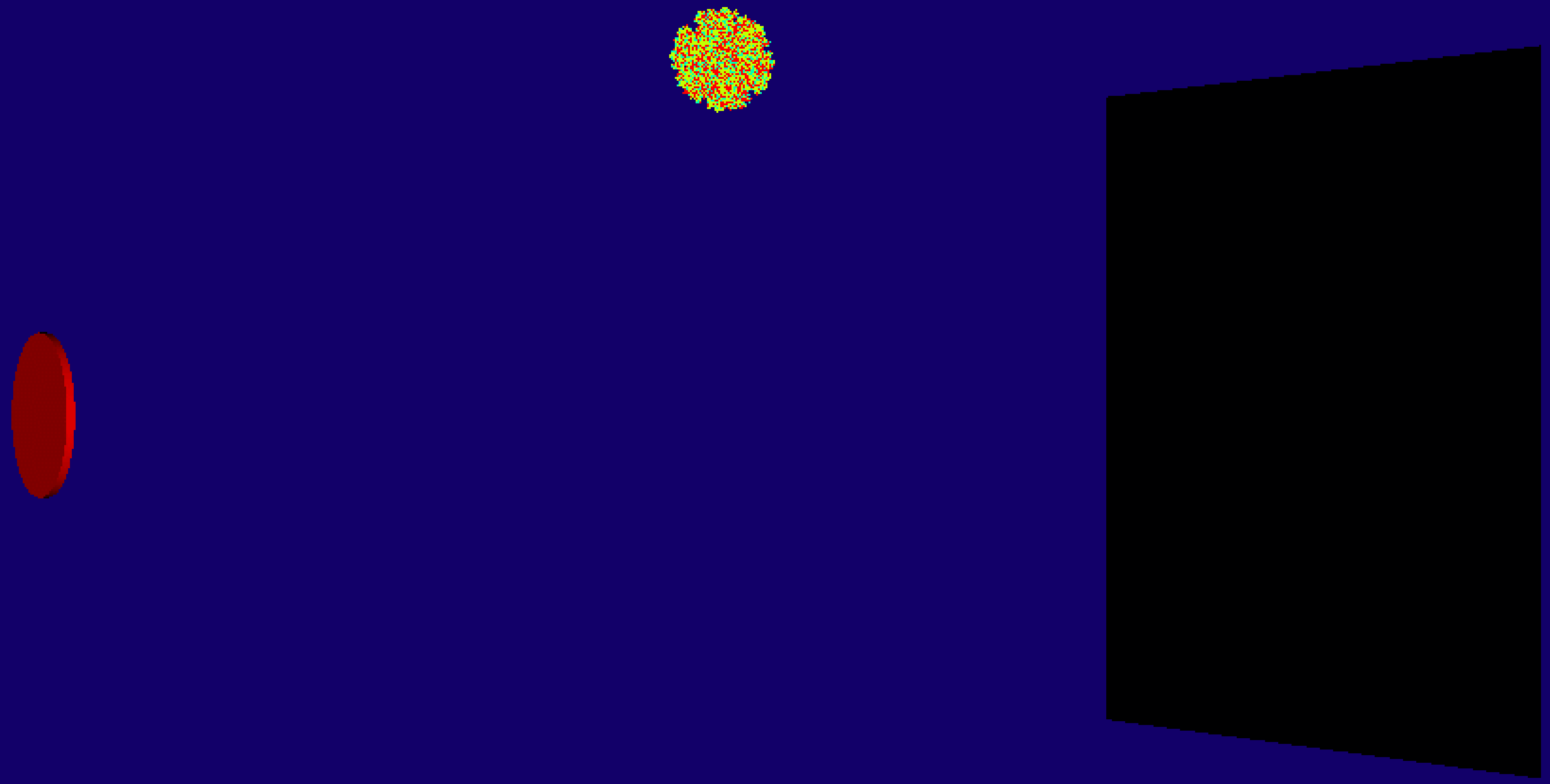
Diffraction on a a drop of water



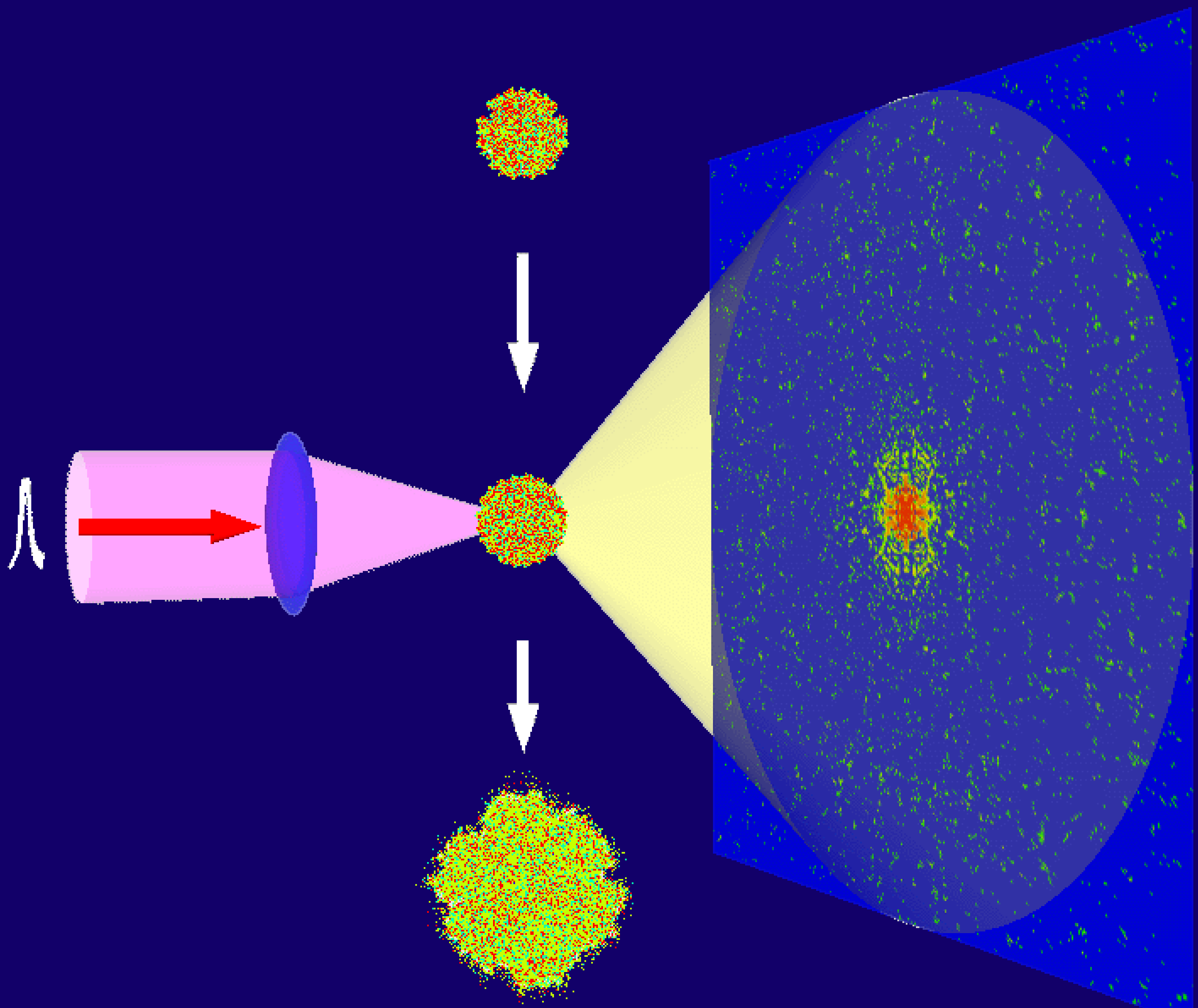
Miss the target



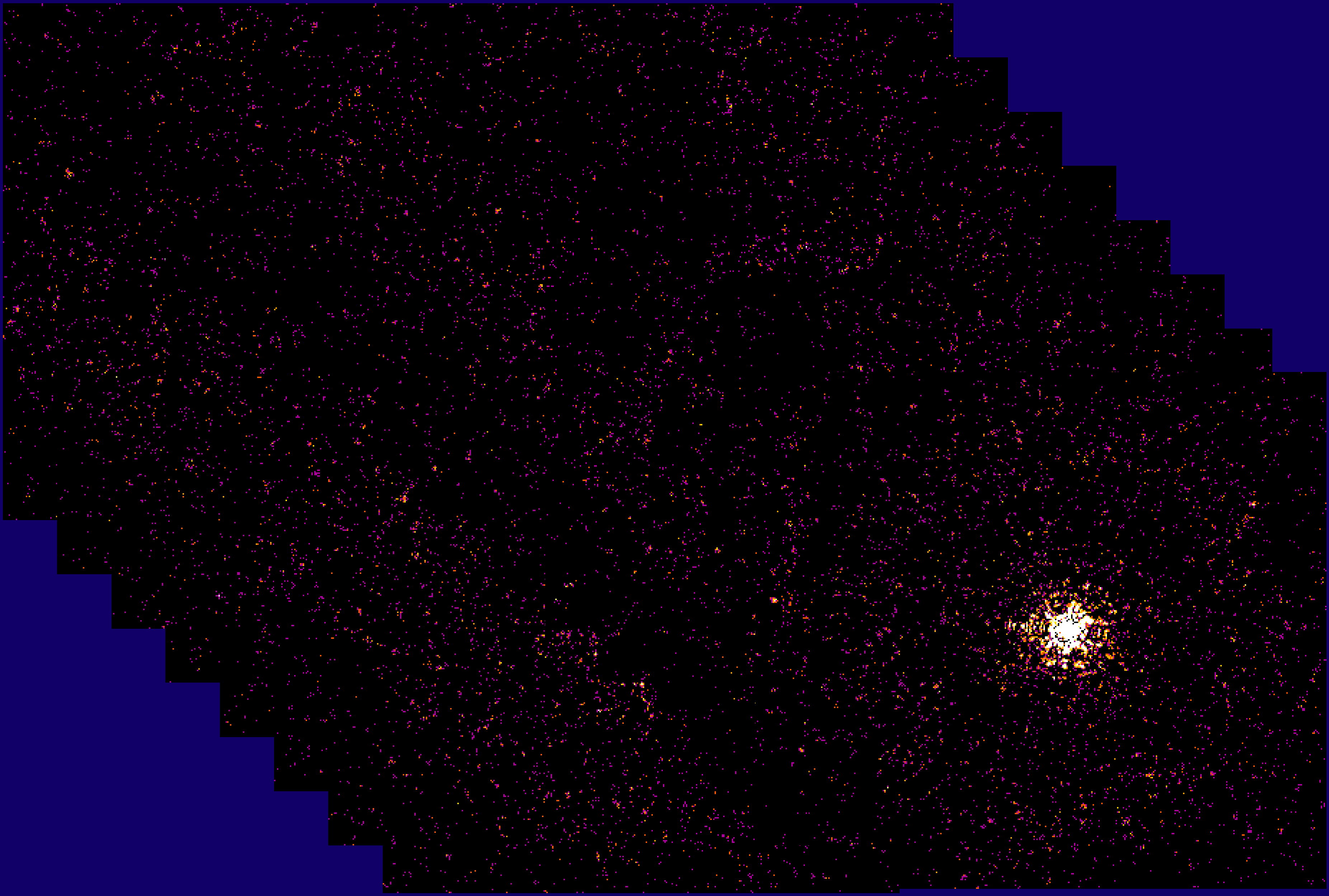
Diffraction on a single virus



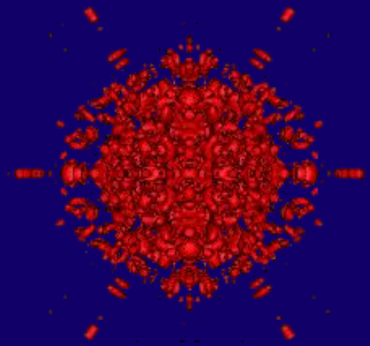
Real experiment schematic



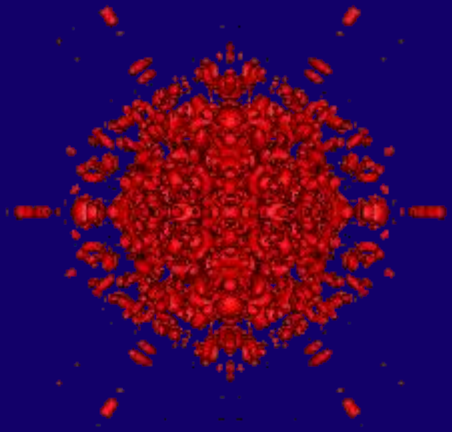
Single shot diffraction patterns



SPI, 3D merging

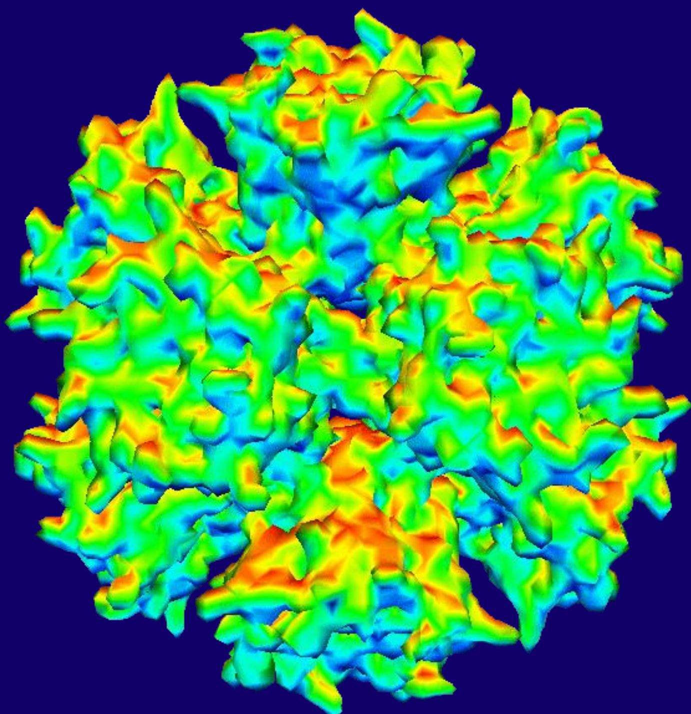


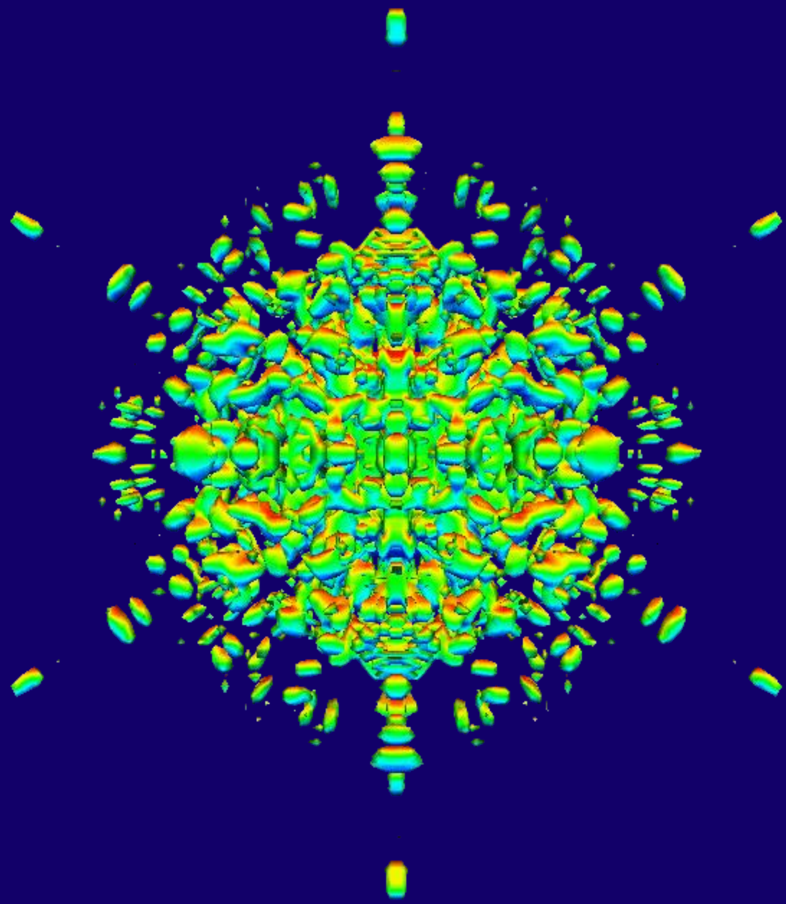
SPI, orientation refinement



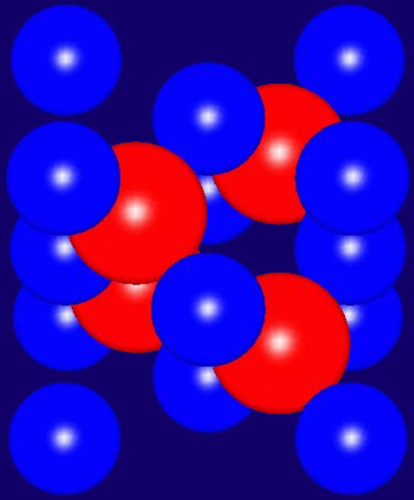
Virus 2c6s (200k atoms), 27nm
12000 random oriented patterns

Real space | **Reciprocal space**



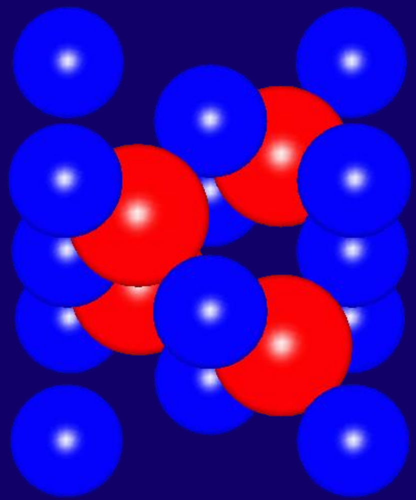


Why crystals?

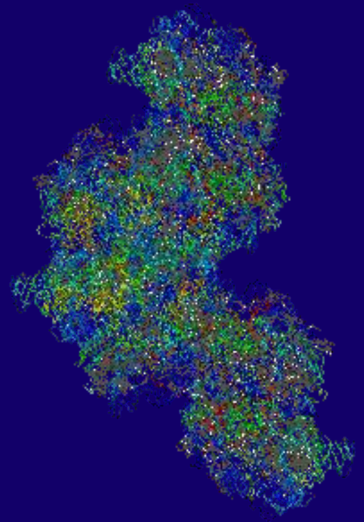


Unit cells

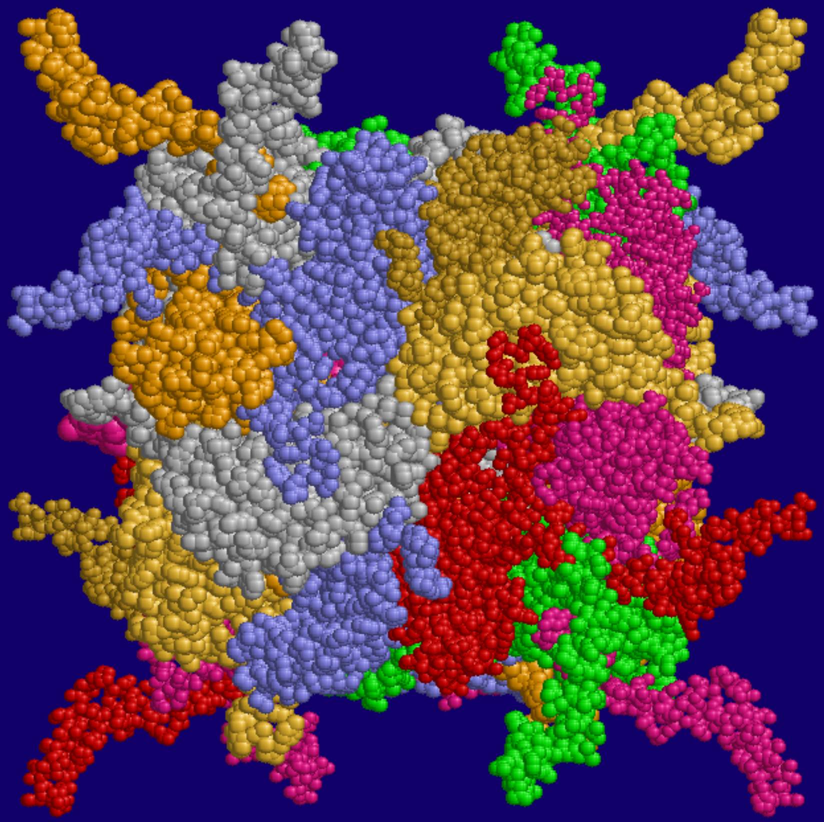
GaAs



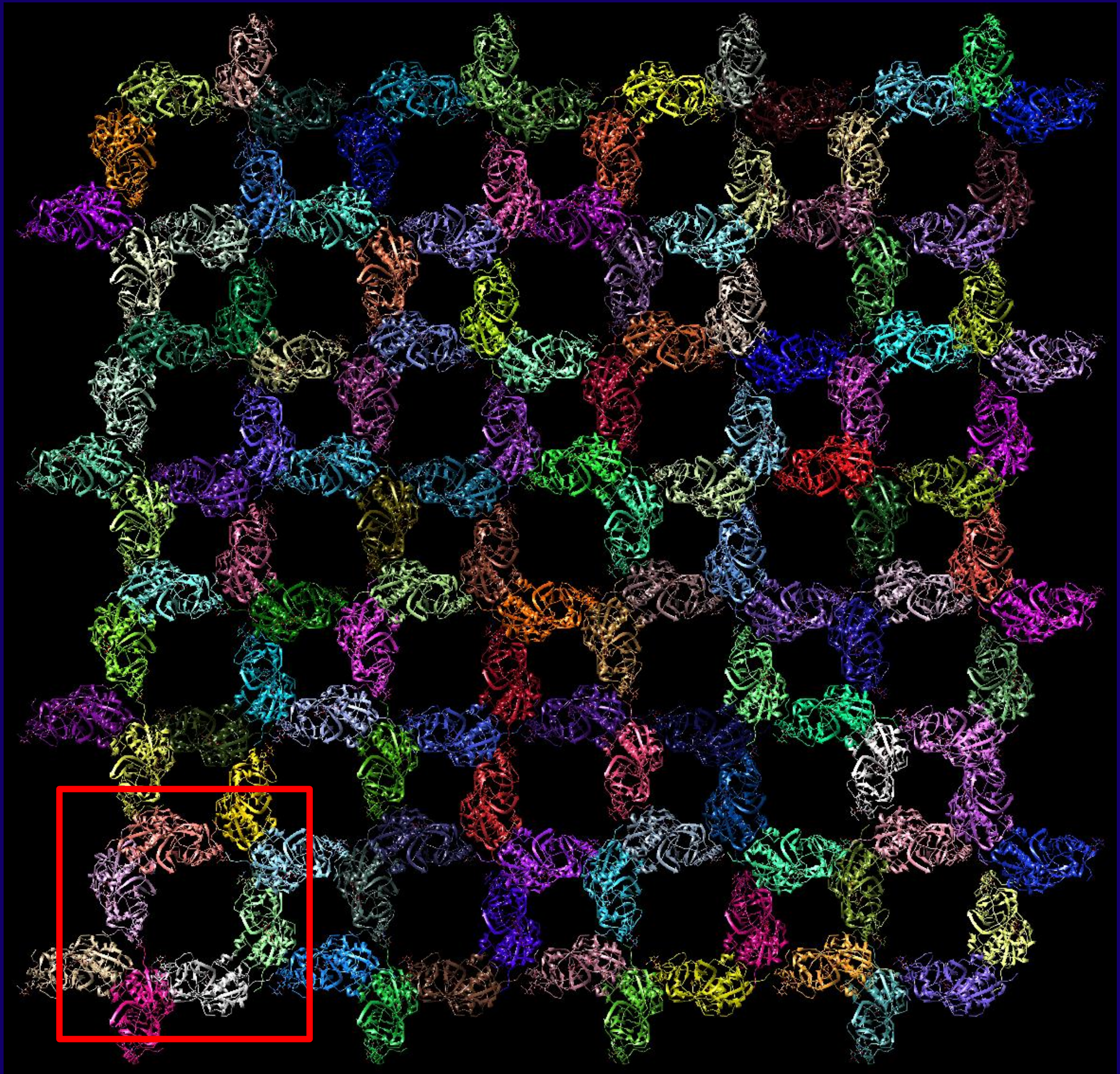
PS2



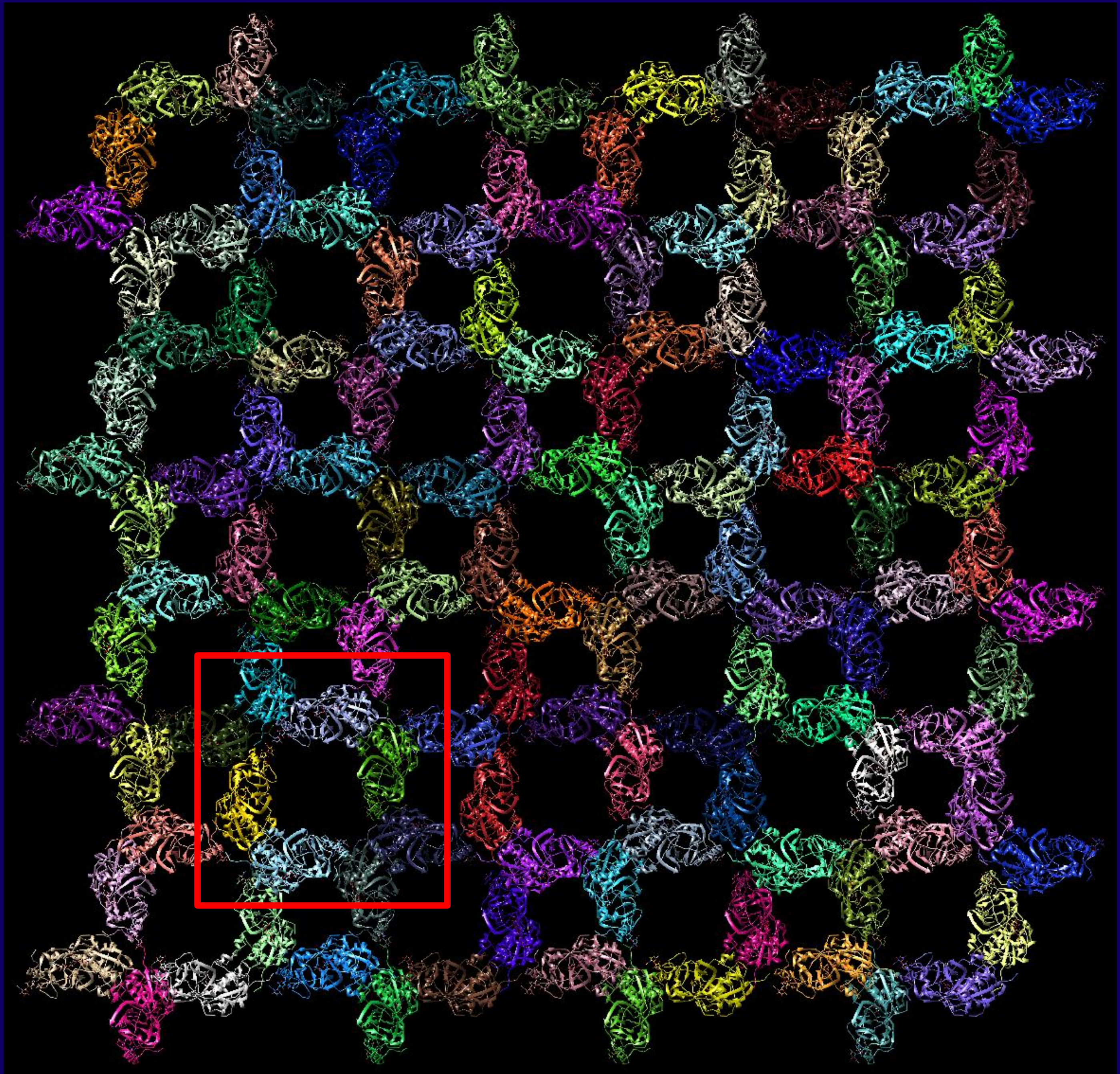
GV



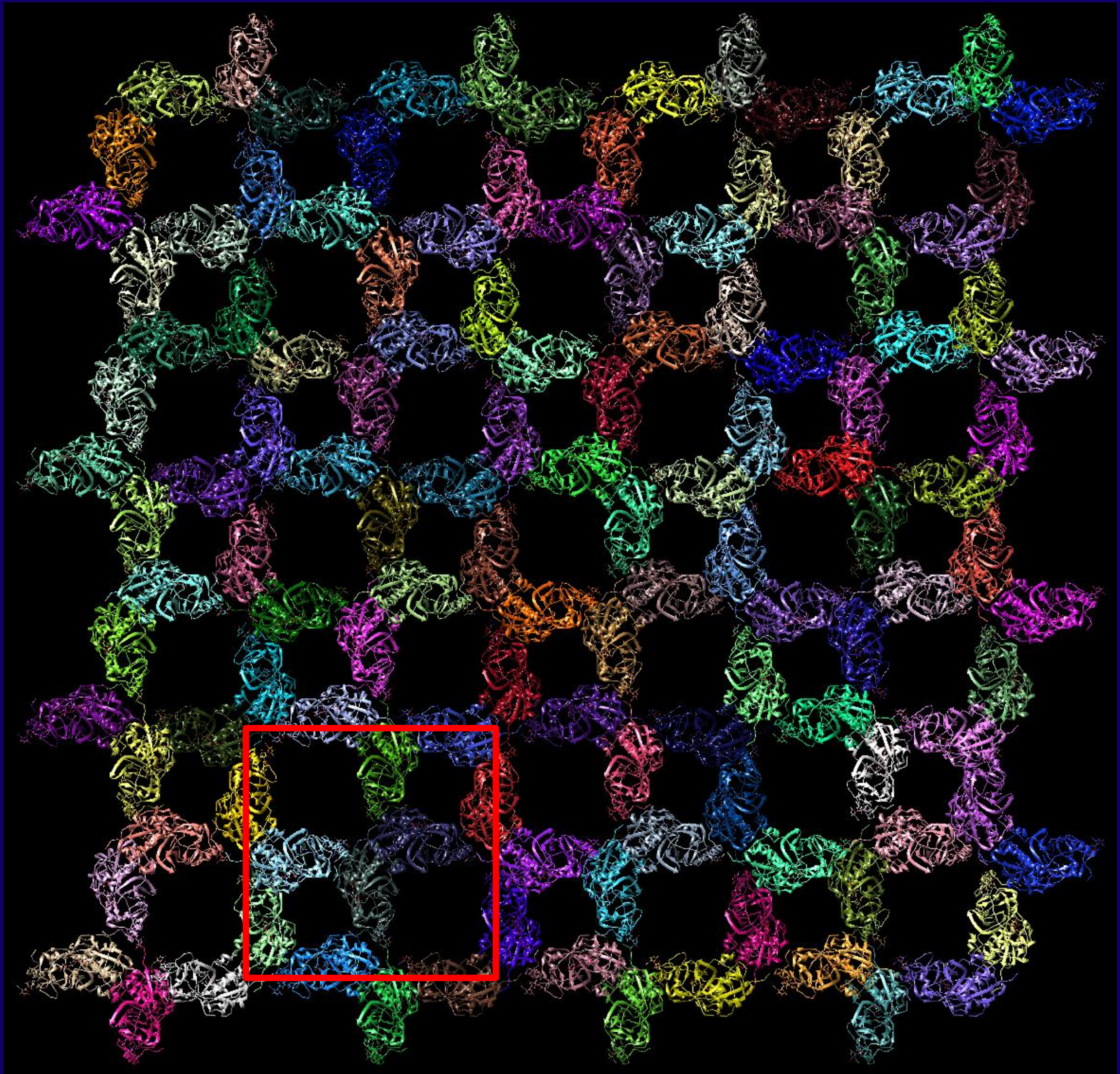
The choice of a unit cell



The choice of a unit cell

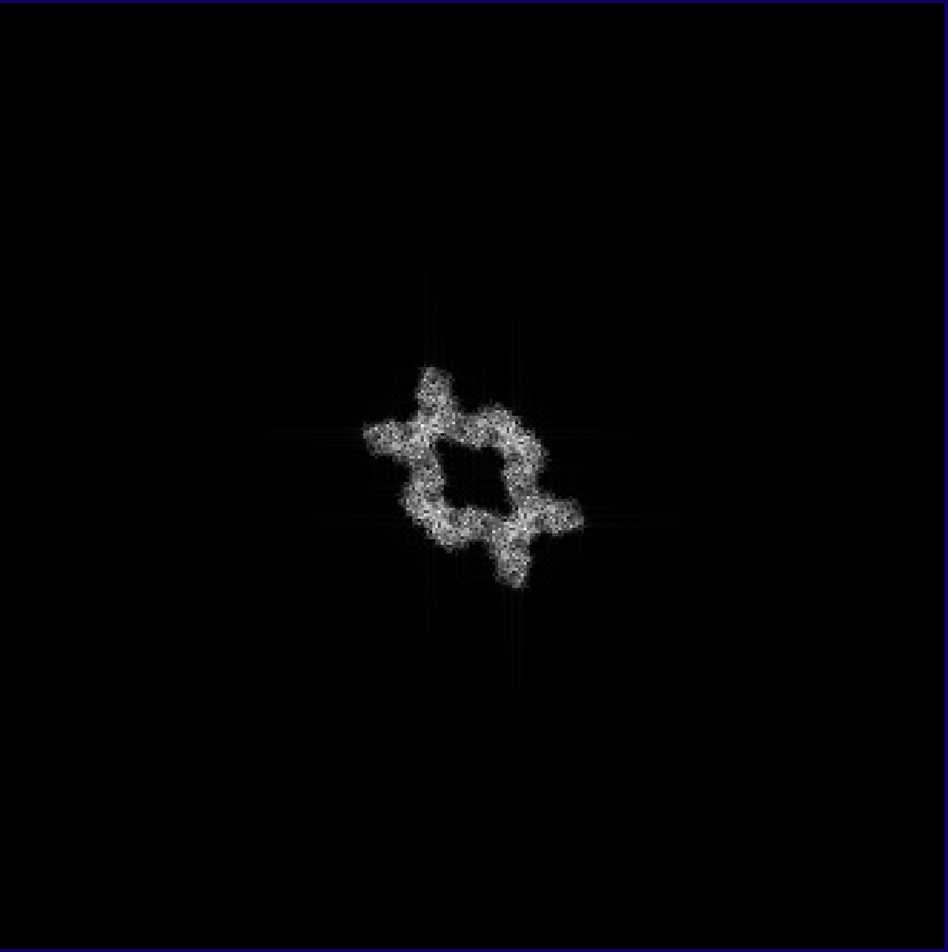


The choice of a unit cell

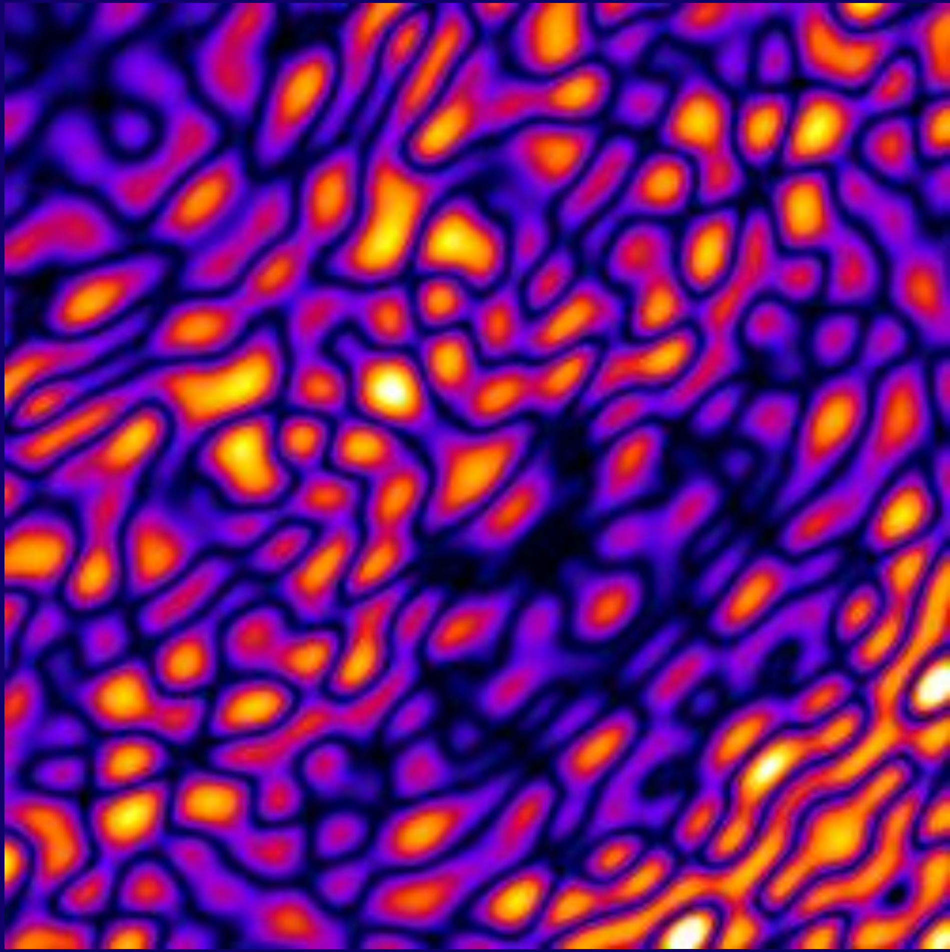


Introduction into crystallography

1 unit cell (CatB)



Ideal diffraction pattern

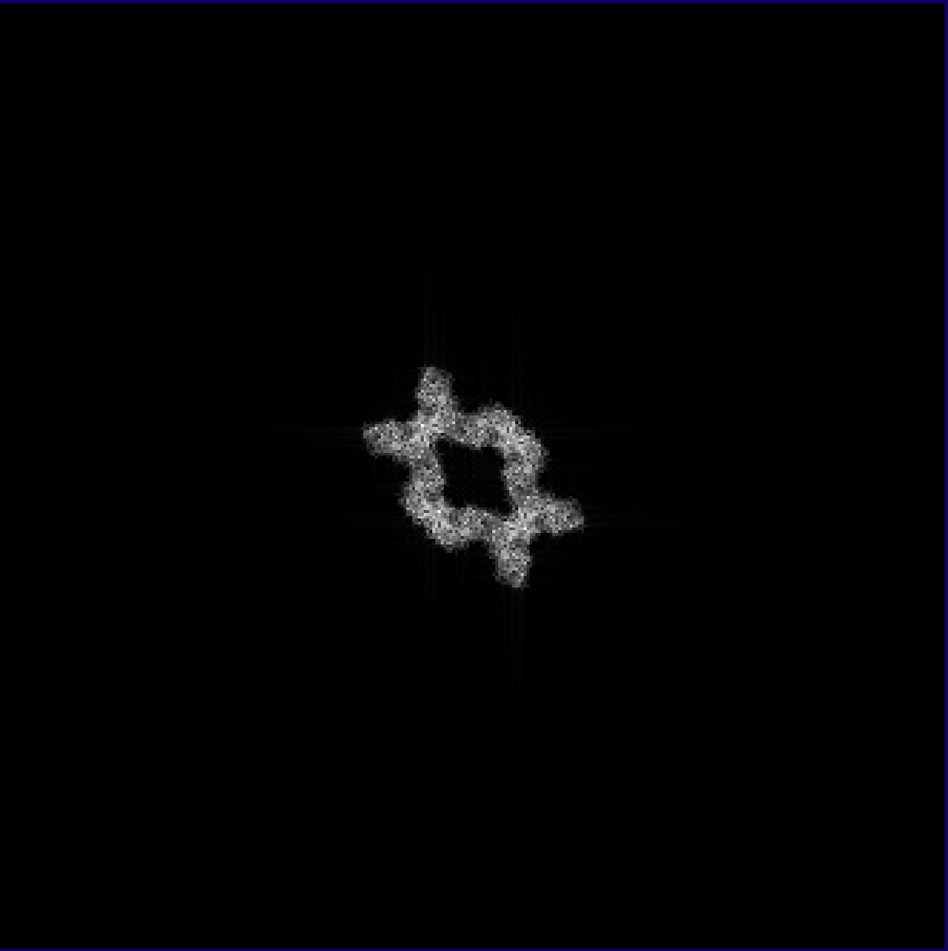


All simulations made with Moltrans

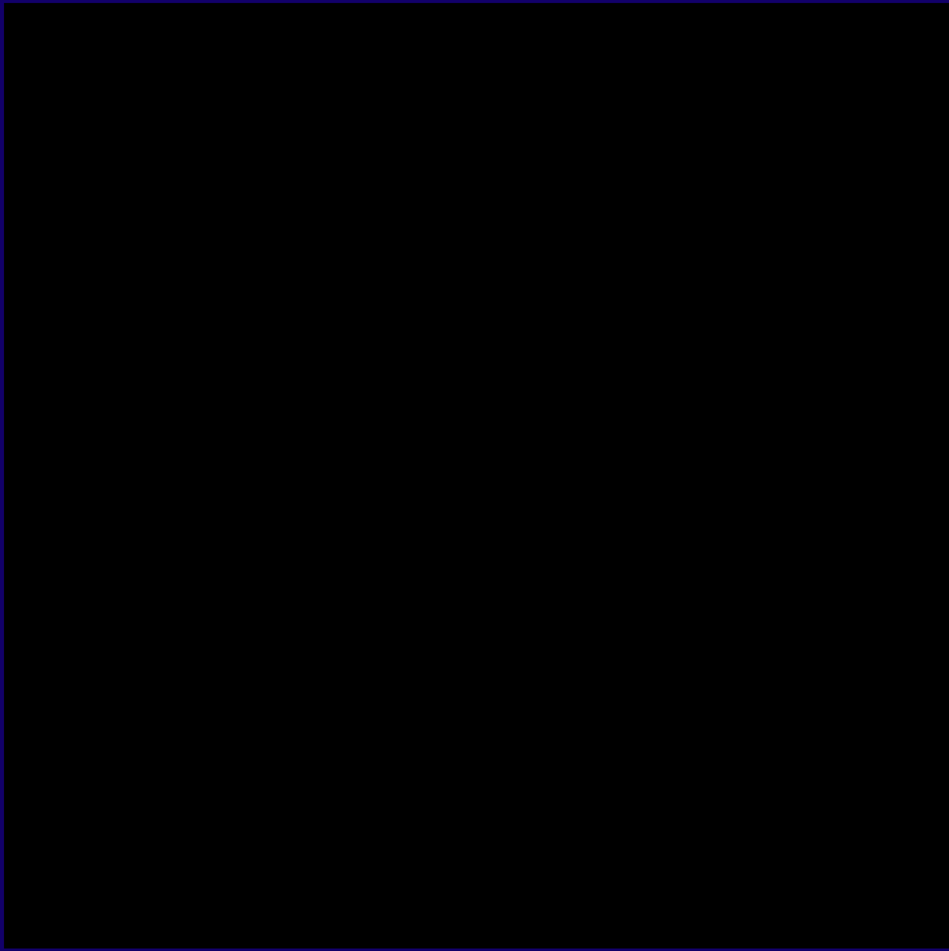
Again, why crystals?

Introduction into crystallography

1 unit cell (CatB)



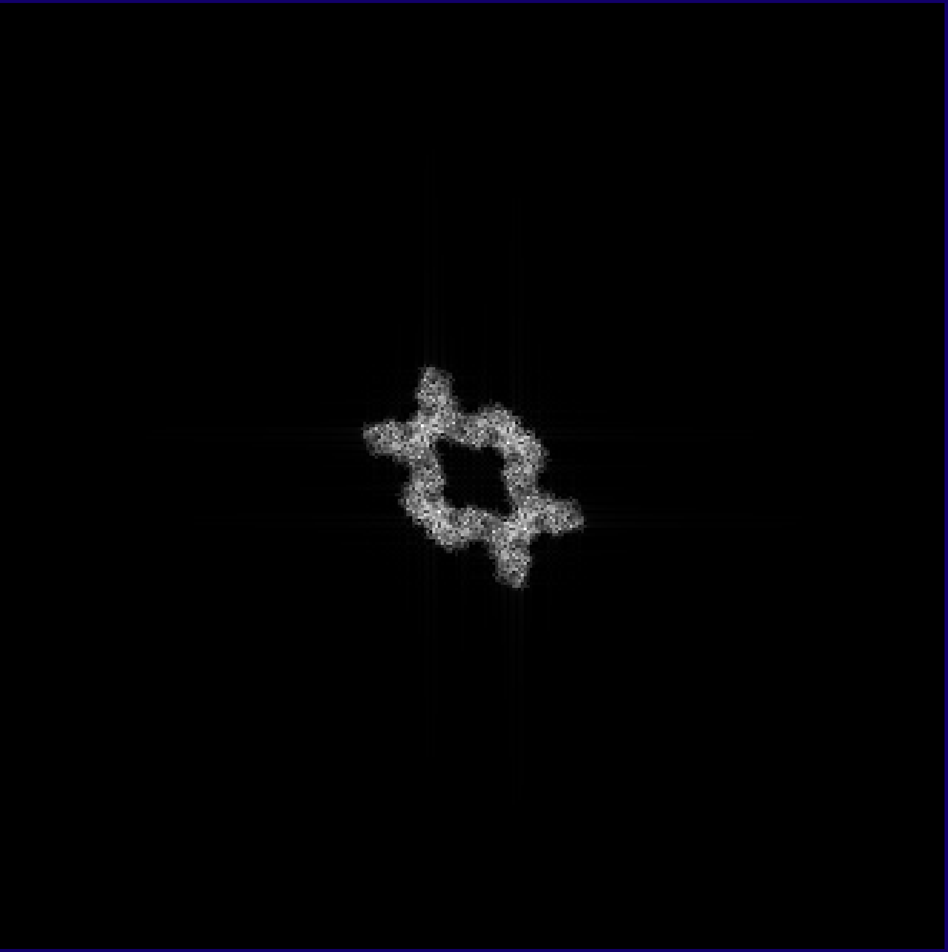
Realistic diffraction pattern



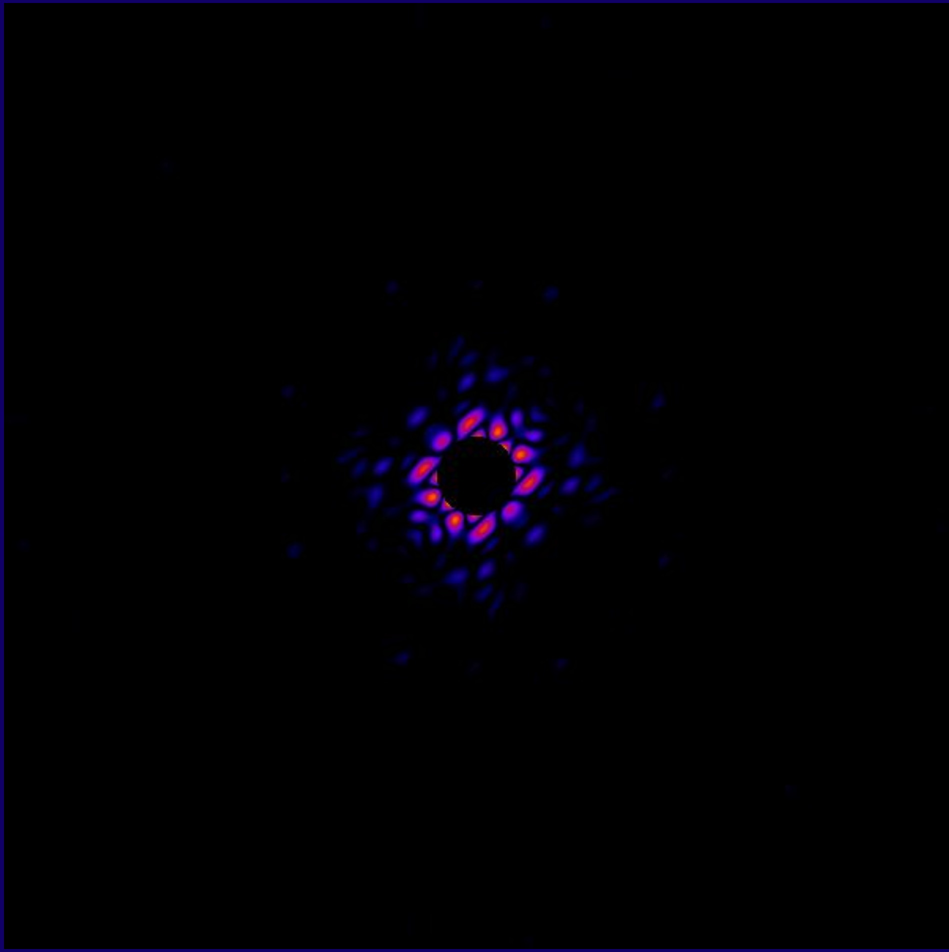
All simulations made with Moltrans

Introduction into crystallography

1 unit cell (CatB)



Diffraction pattern

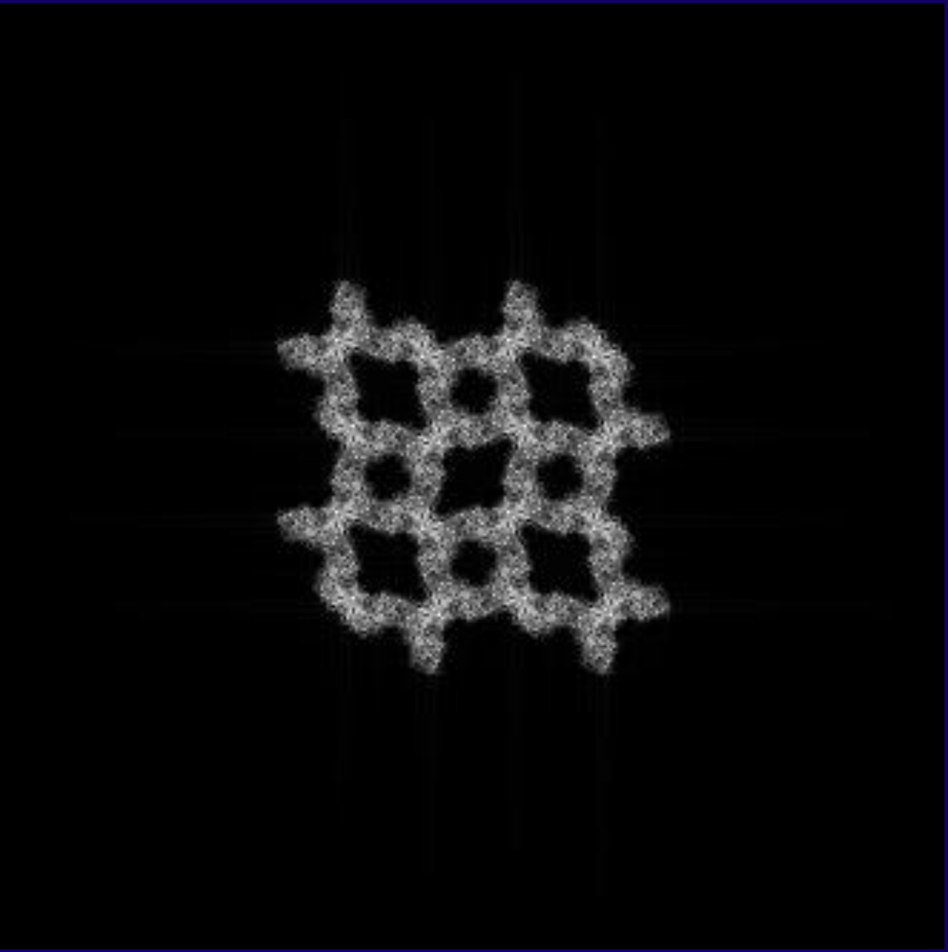


All simulations made with Moltrans

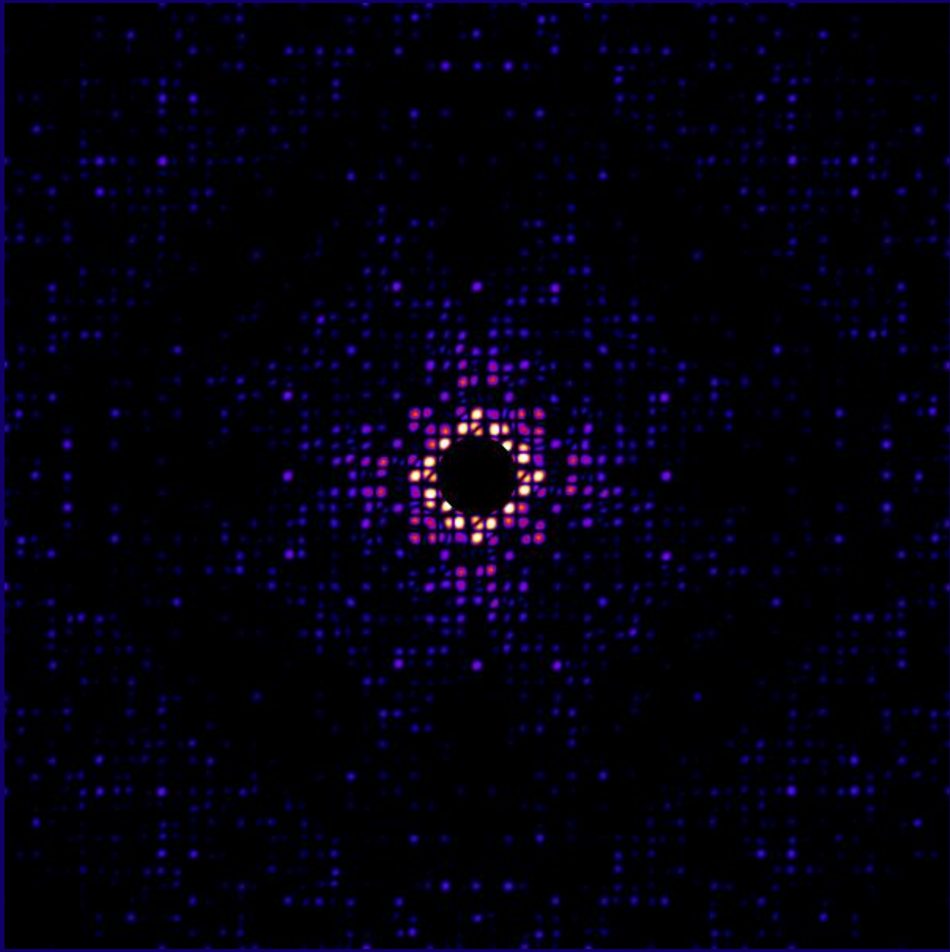
Unreal flux (1e20 photons)

Introduction into crystallography

2x2 unit cells (CatB)



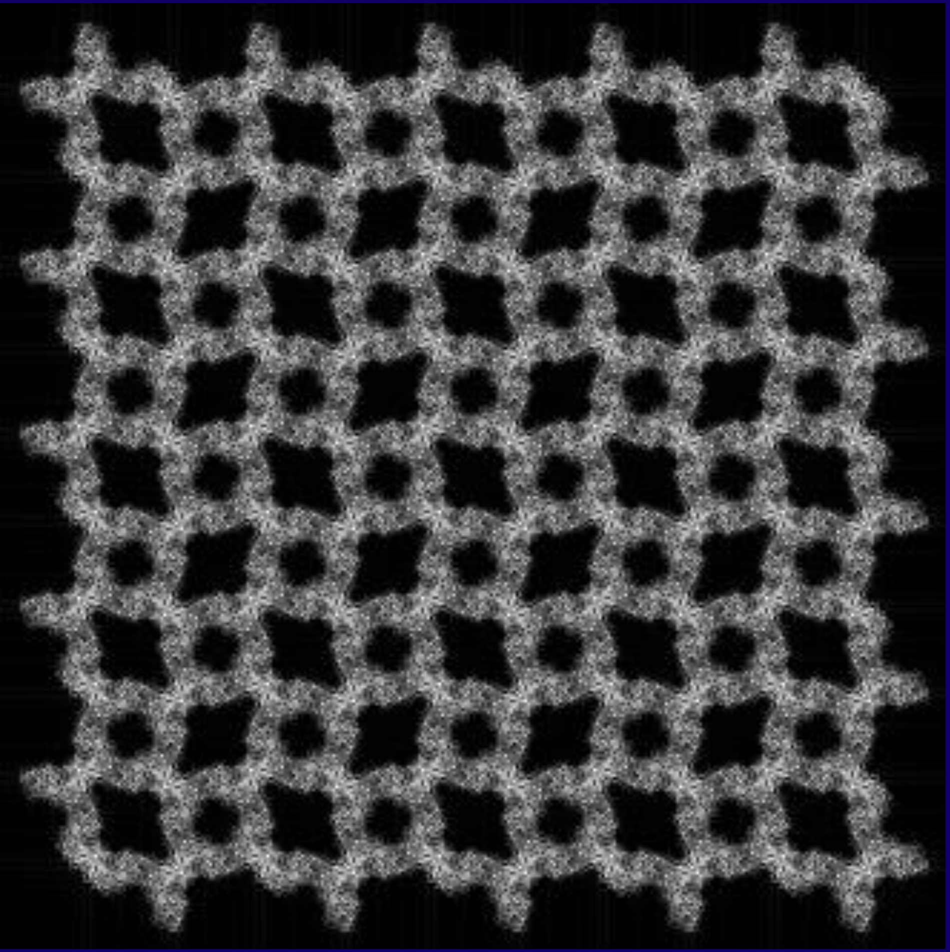
Diffraction pattern



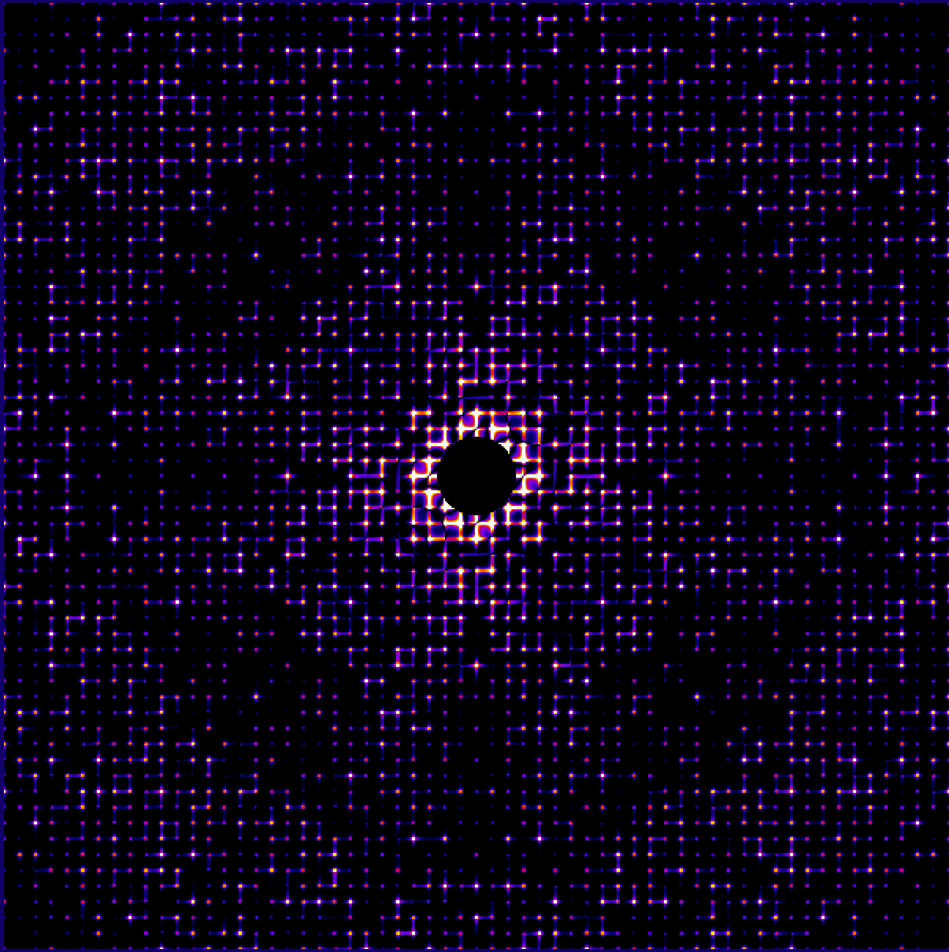
All simulations made with Moltrans

Introduction into crystallography

5x5 unit cells (CatB)



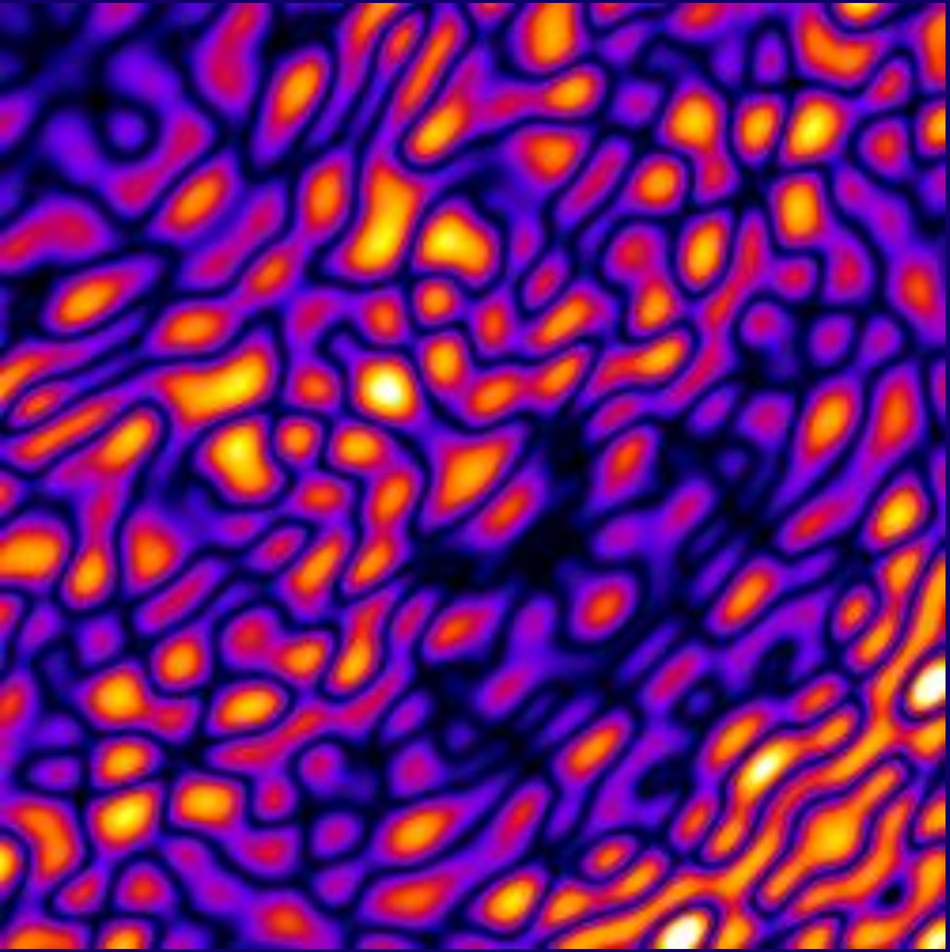
Diffraction pattern



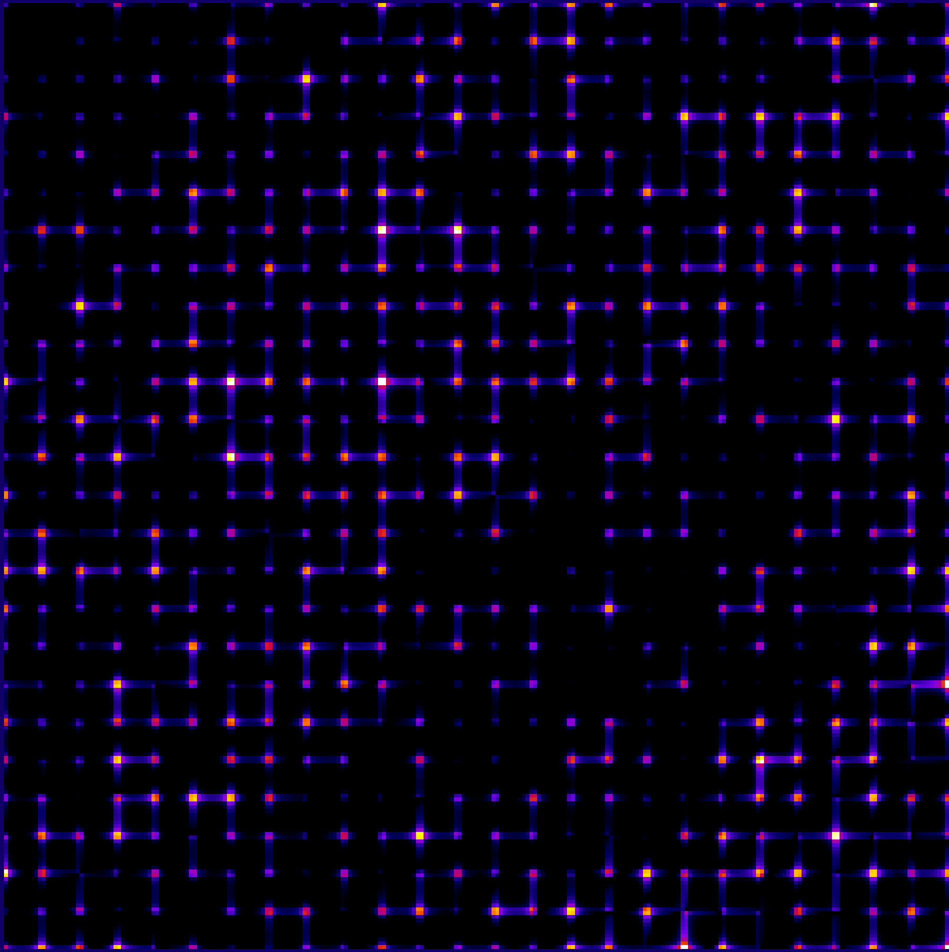
All simulations made with Moltrans

Introduction into crystallography

Pattern of 1 unit cell (CatB)



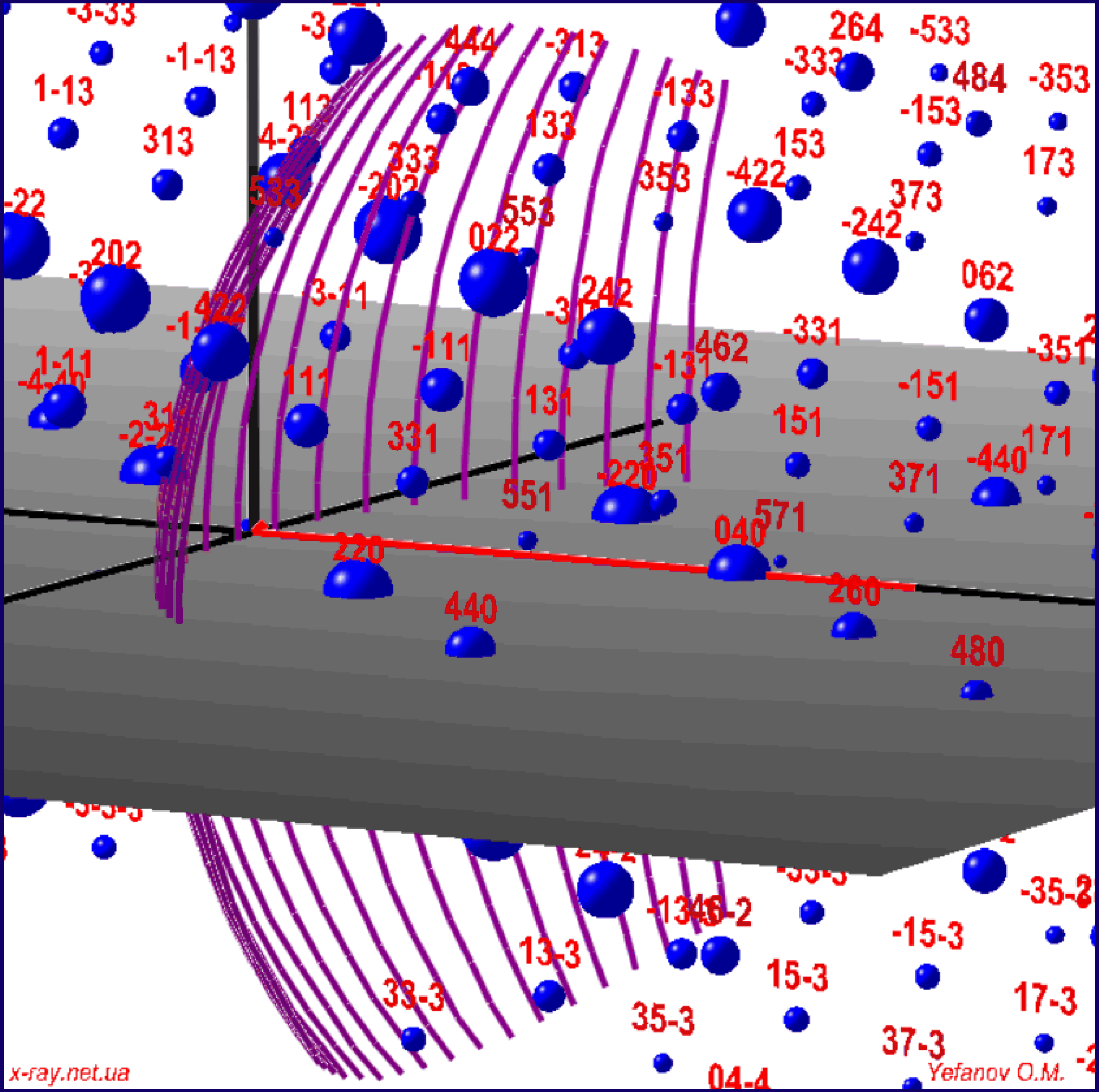
Pattern of 5x5 unit cells



Bragg peaks intensities are modulated by the FFT of the UC

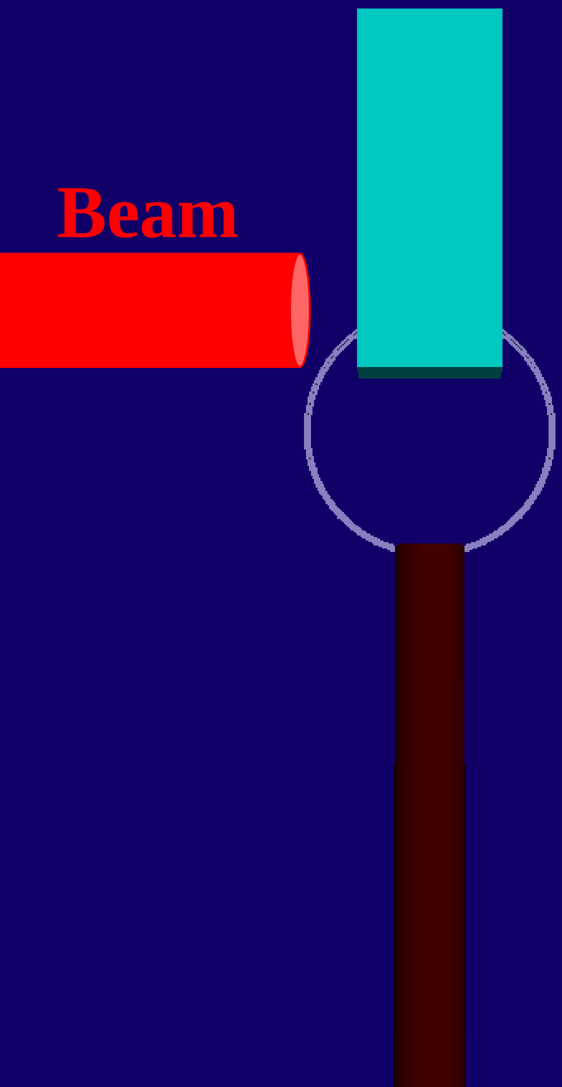
Measuring protein crystals

Typical “tomographic” measurement

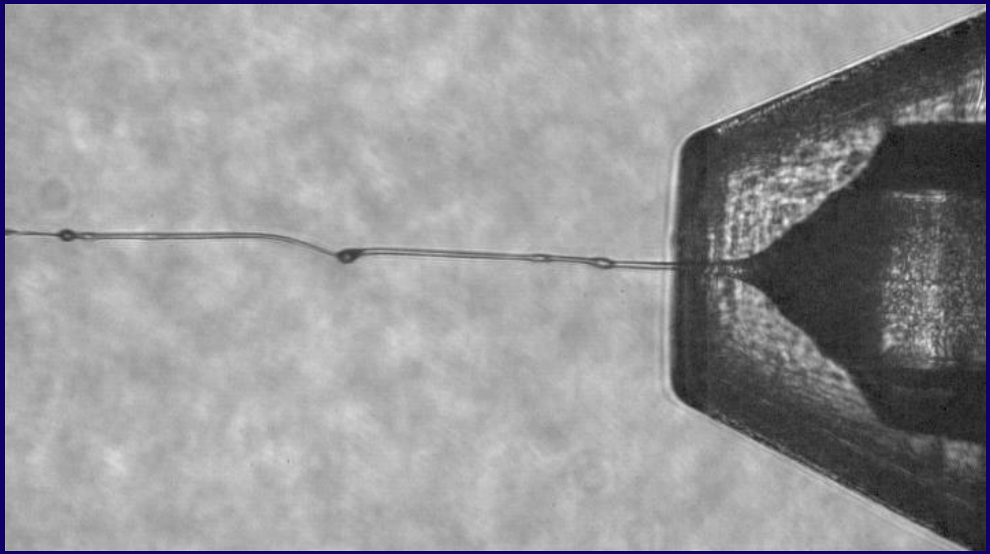


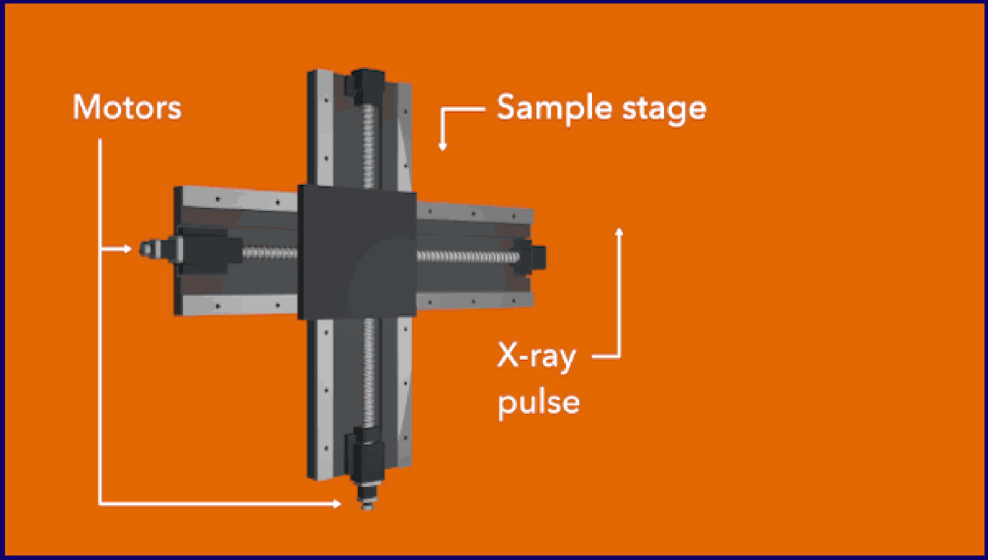
Single crystal and serial crystallography

Single crystal



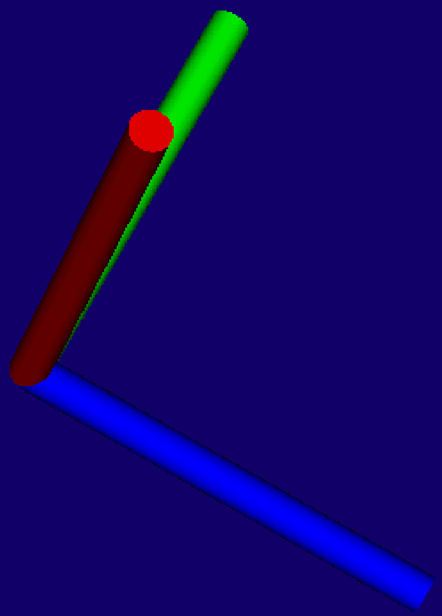
Serial



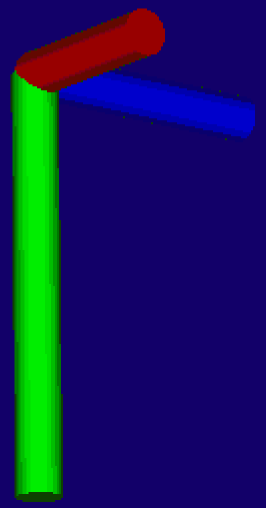


Unit cell vectors

Single crystal



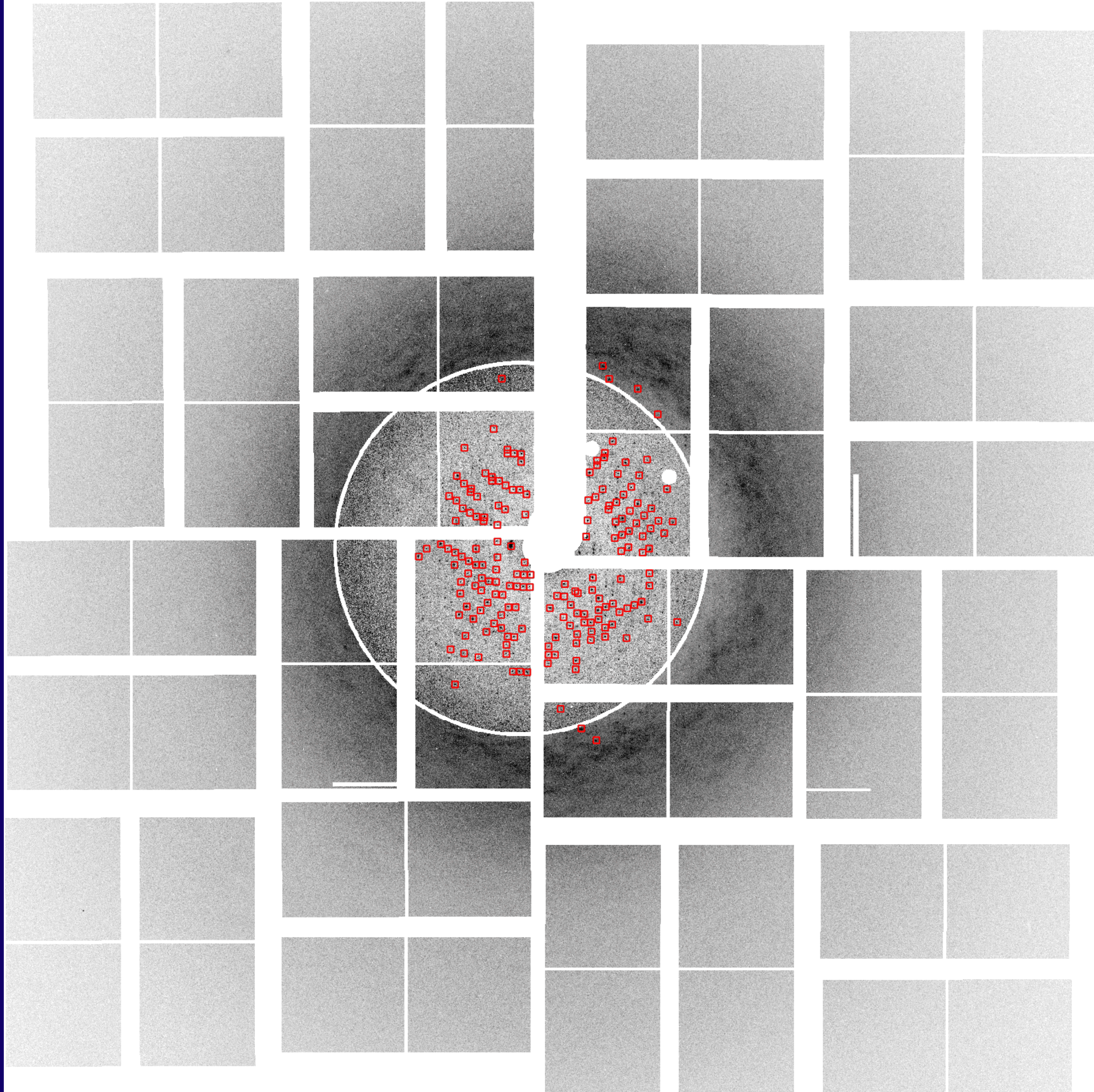
Serial

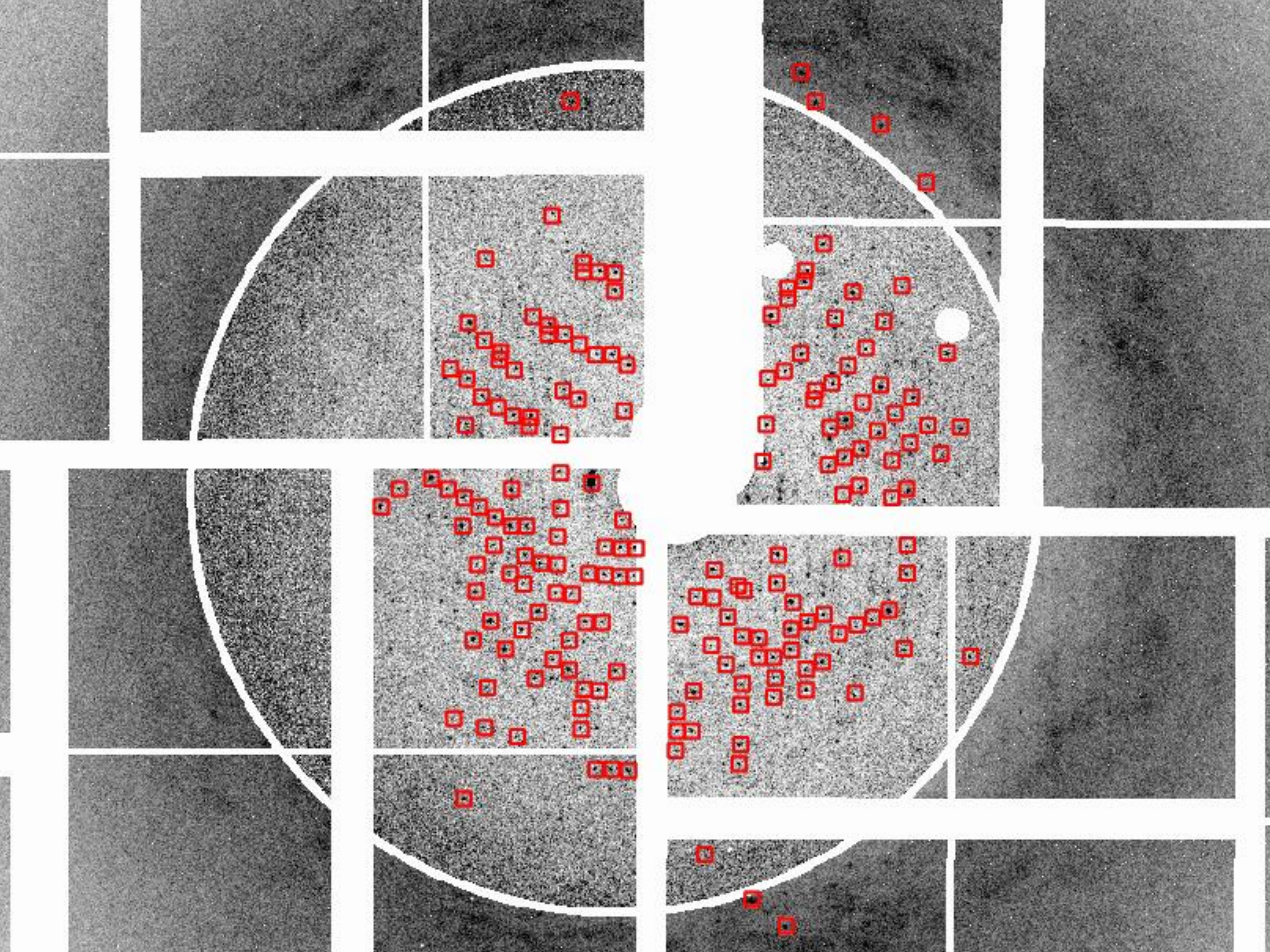


Measured patterns

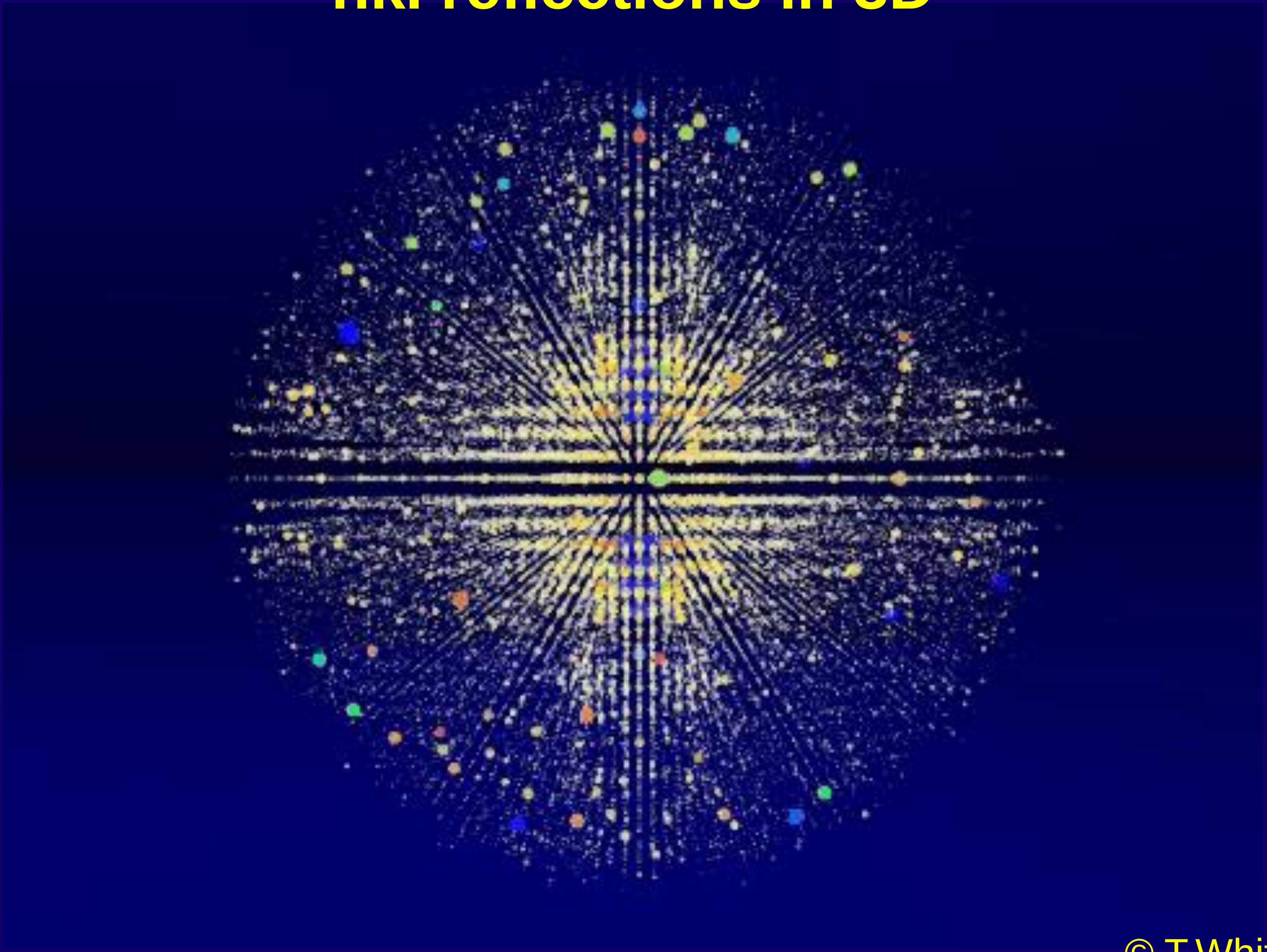
Single crystal | **Serial**

An indexed pattern (CS-PAD detector)





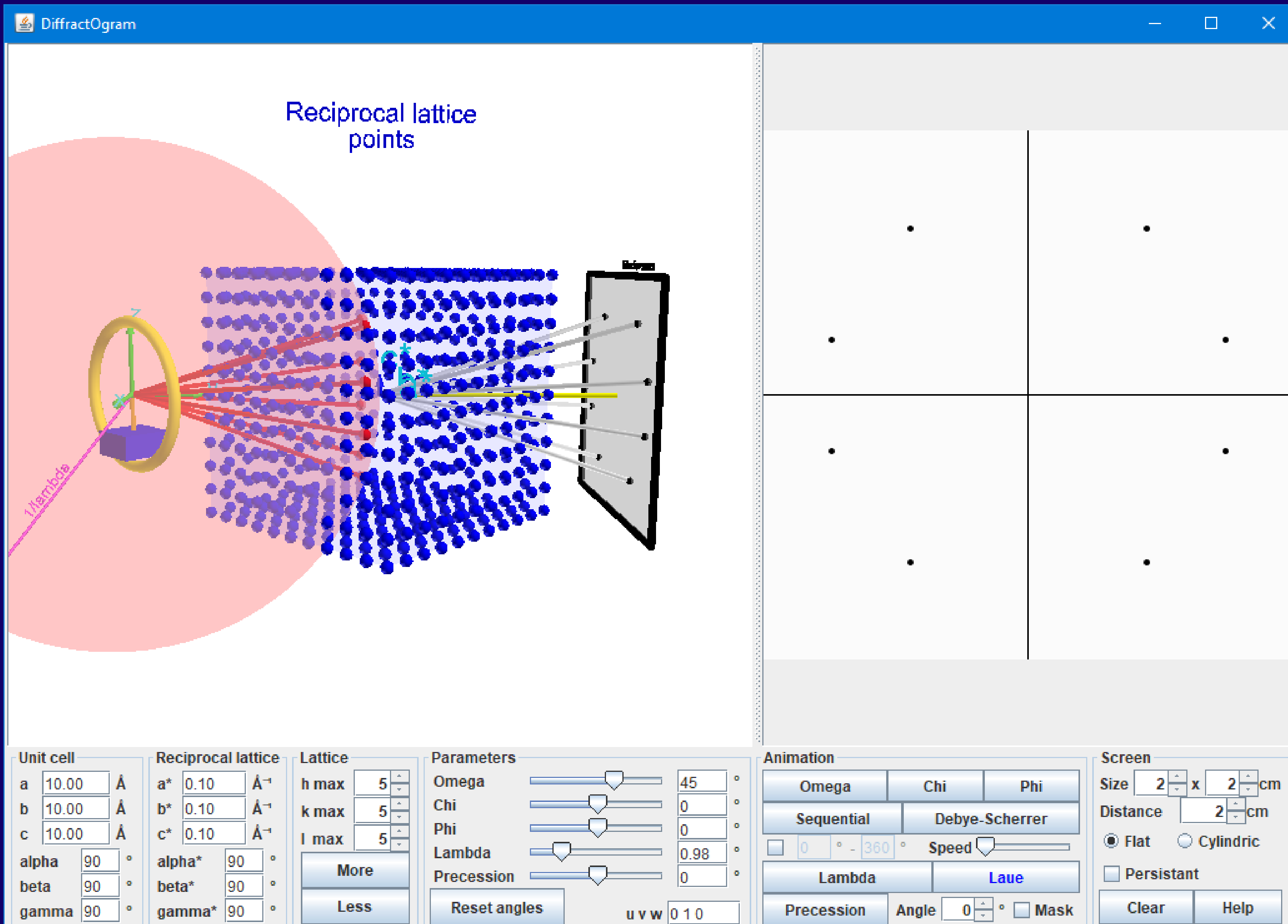
hkl reflections in 3D



DiffractOrgam

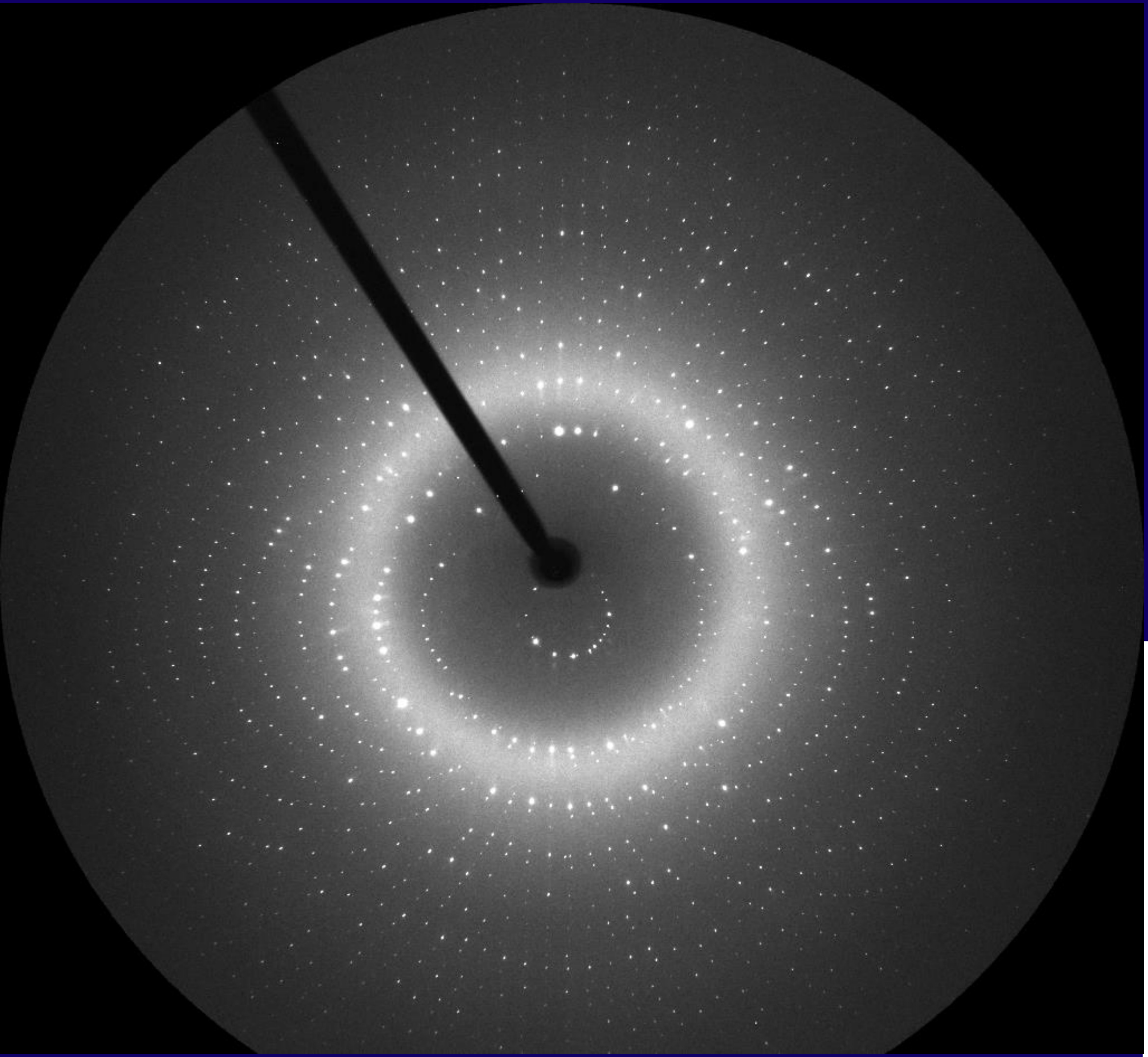
Diffractogram

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

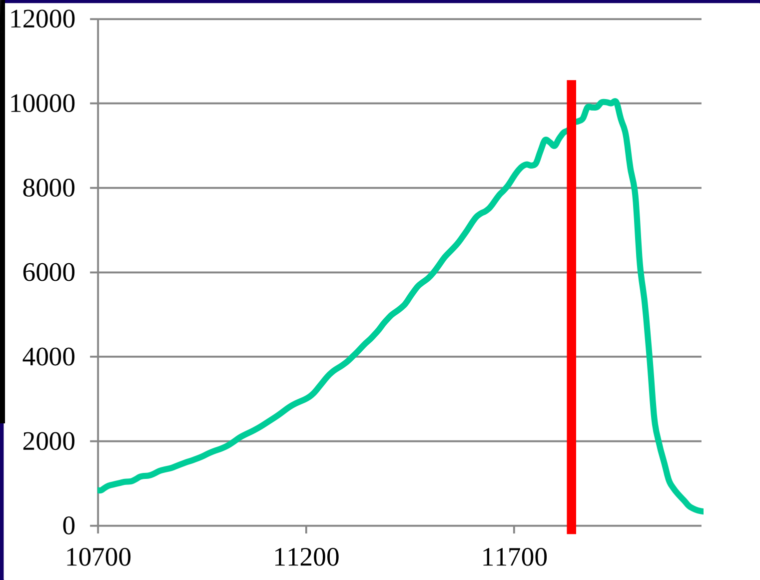


Pink and Convergent beams

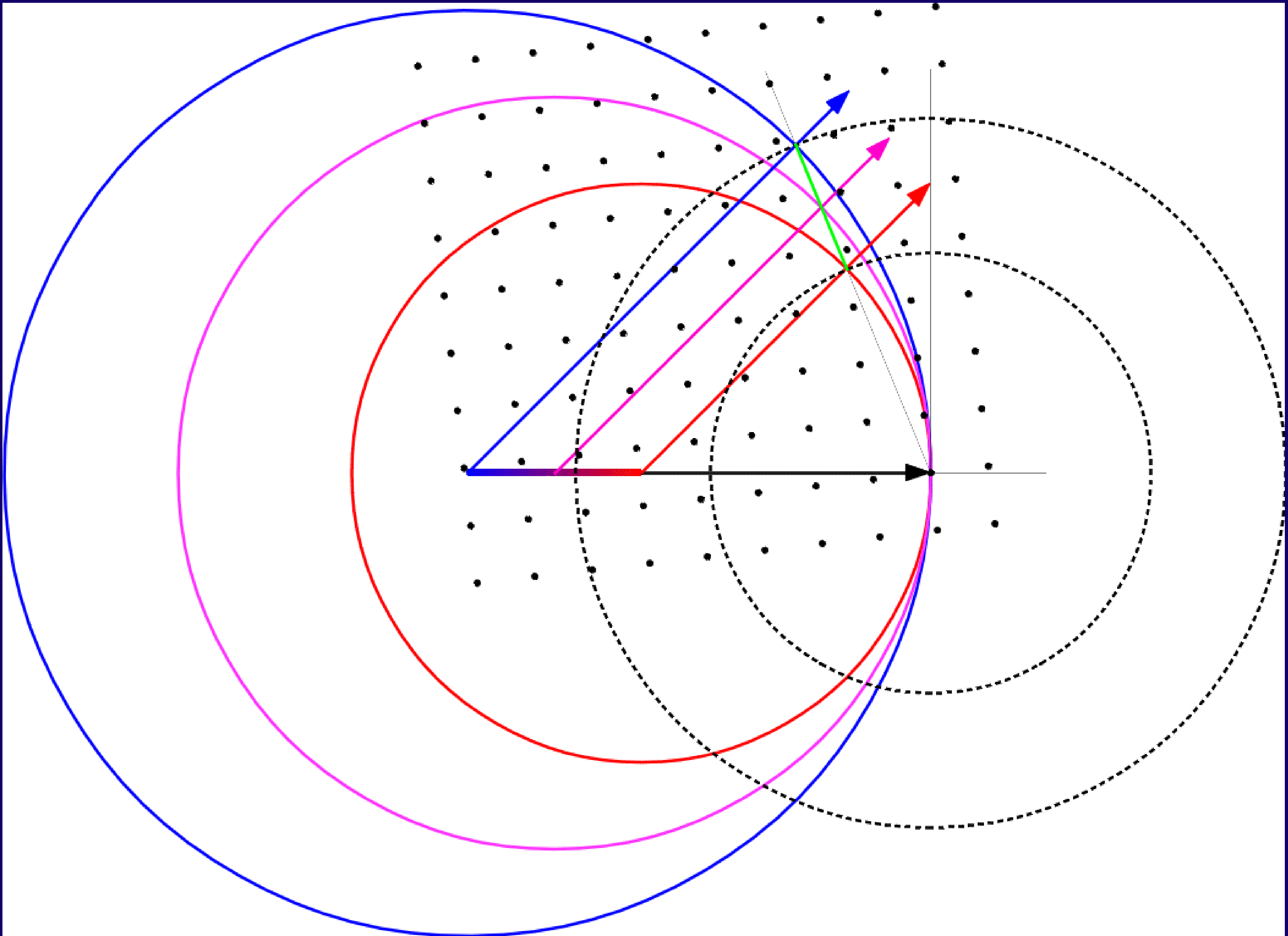
Pink beam (Laue diffraction)



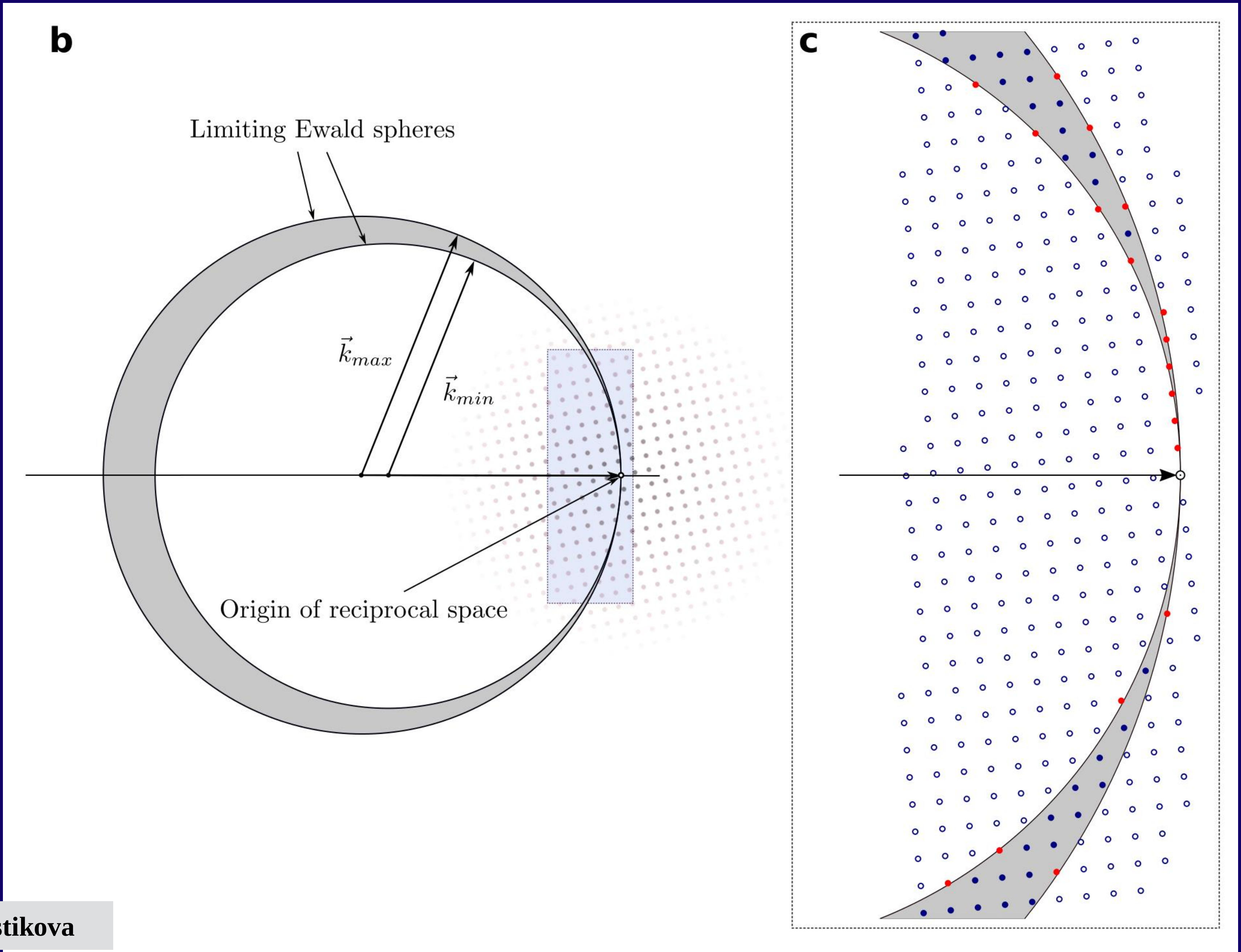
- 1e15 ph/sec
- Single 100ps bunch from sync. is enough
- 5% bandwidth
- New algorithms needed



Pink beam in reciprocal space



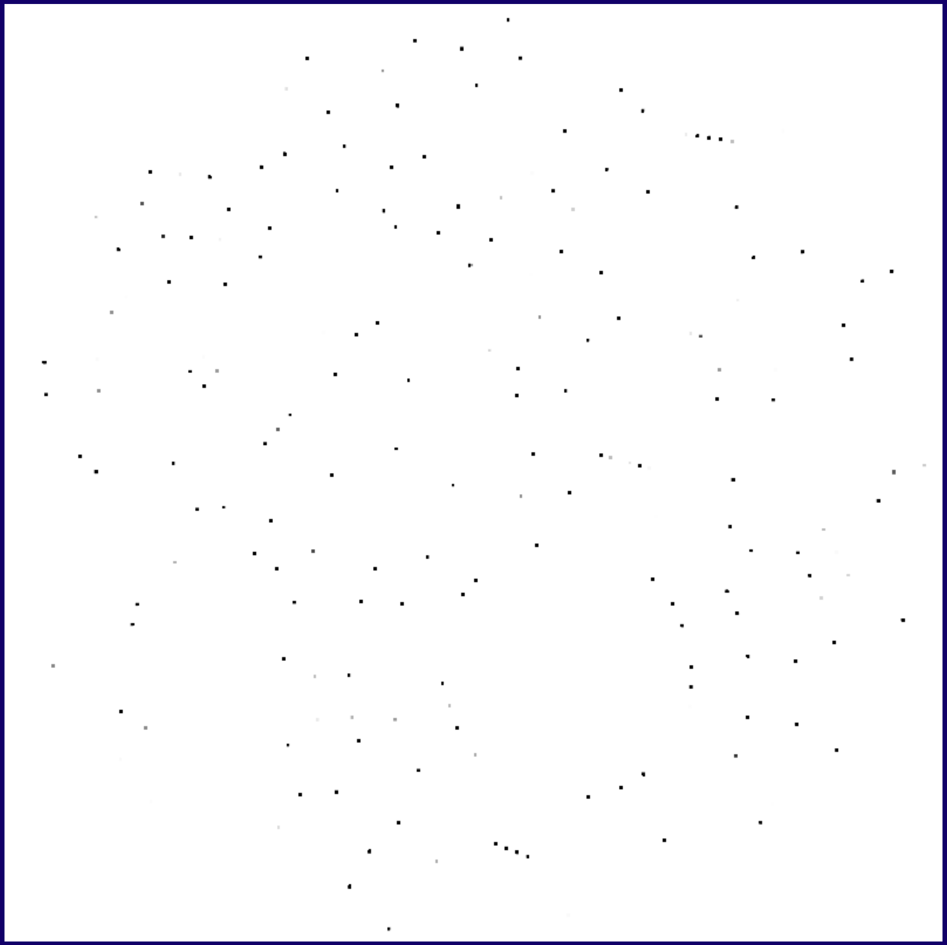
Partiality with pink beam



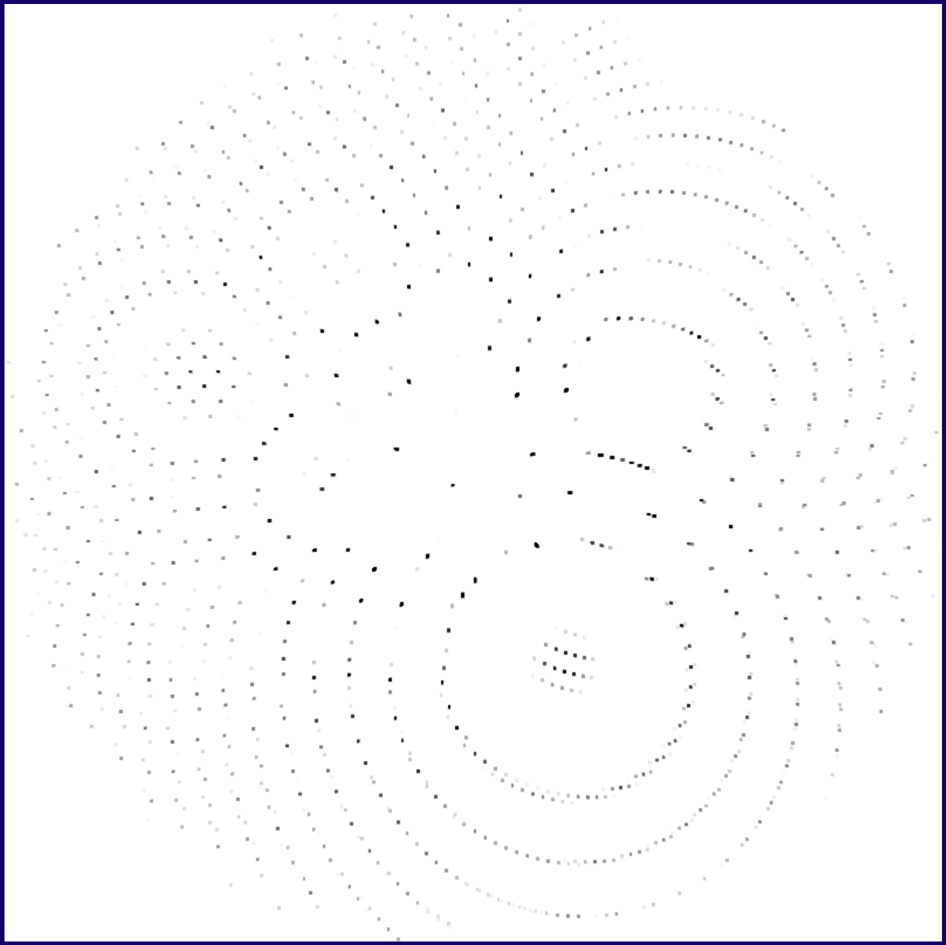
A.Tolstikova

Pink vs mono

Monochromatic beam

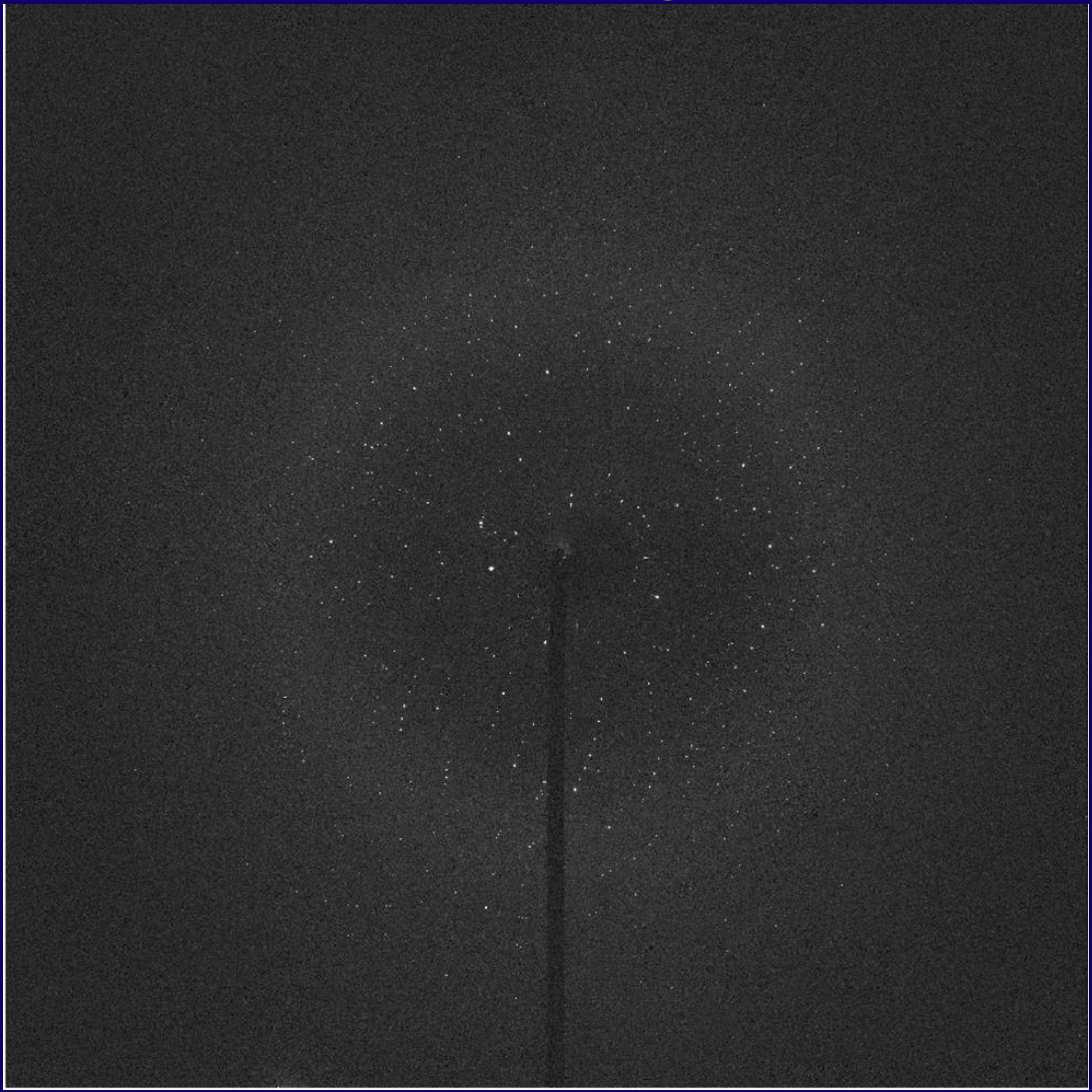


Pink beam



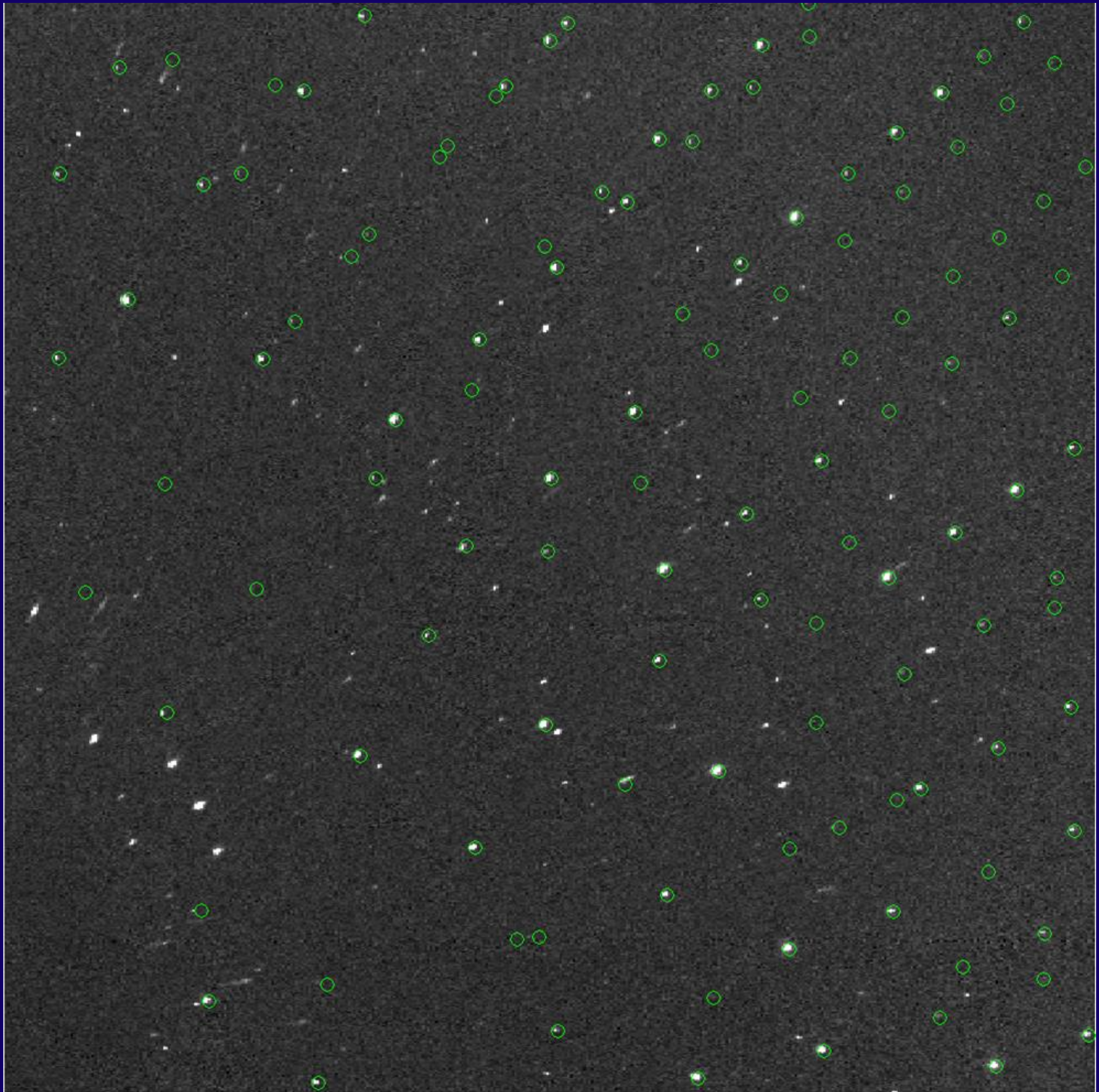
Y.Gevorkov

Indexing



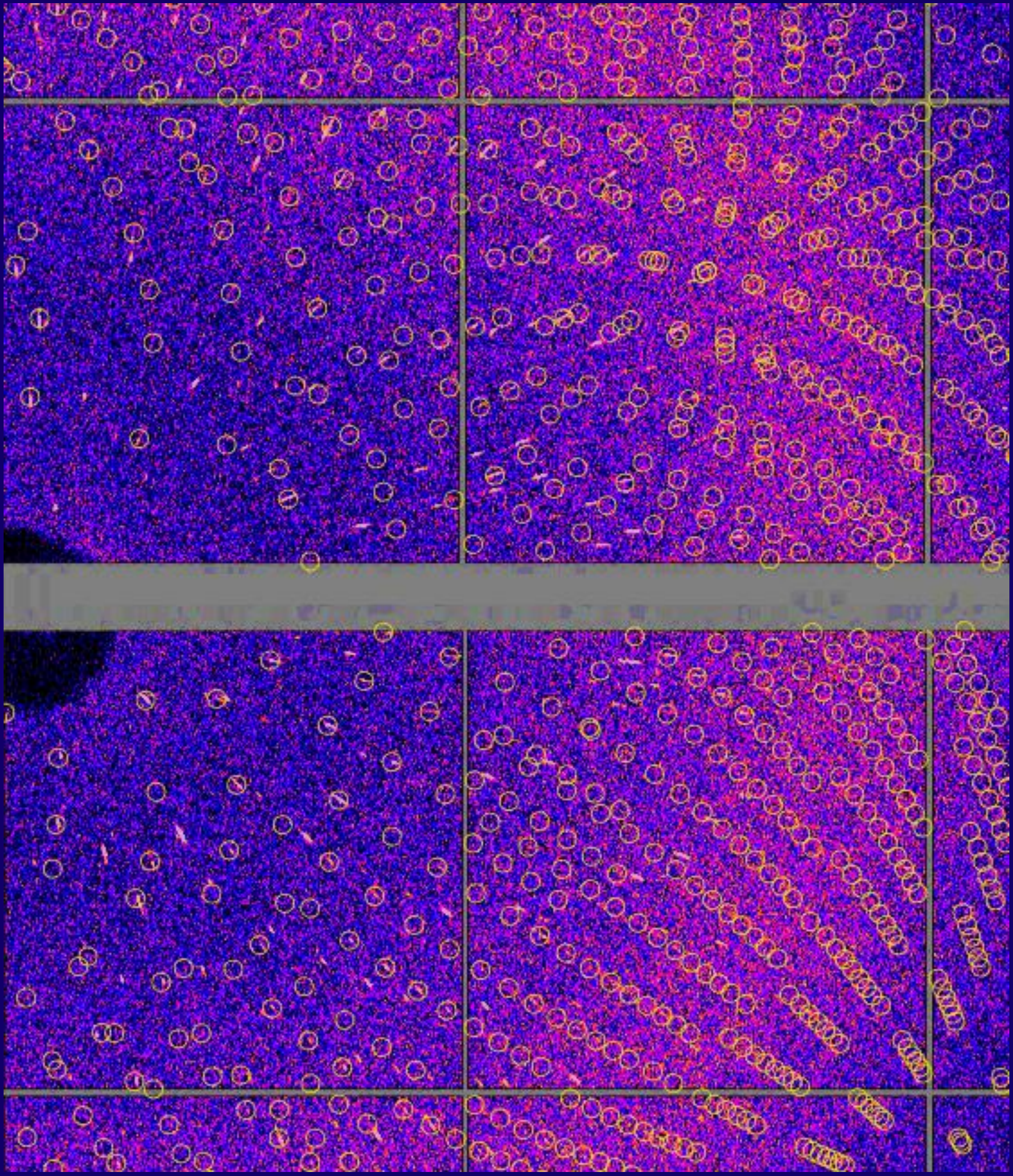
Y.Gevorkov

Indexing



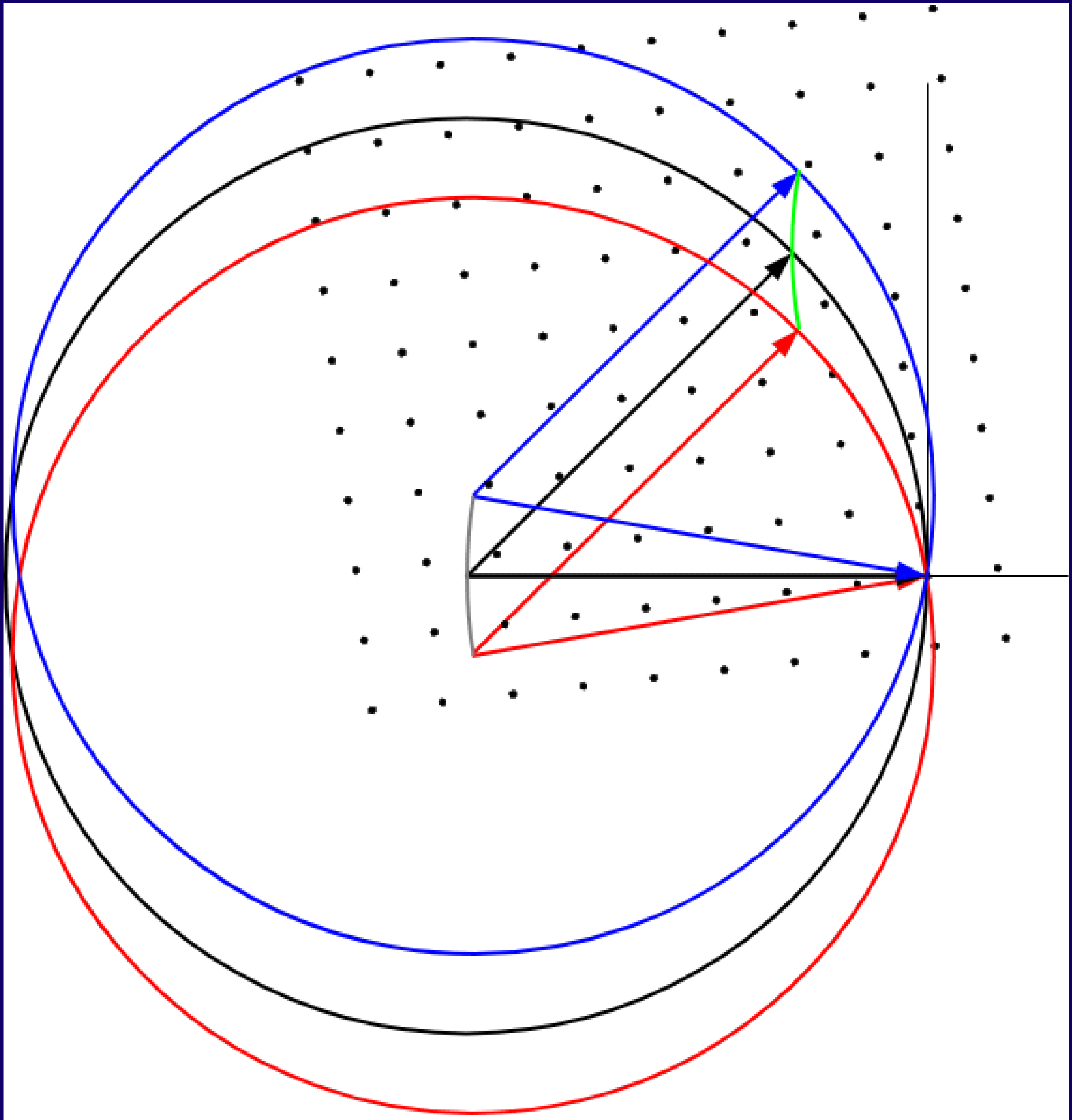
Y.Gevorkov

Indexing

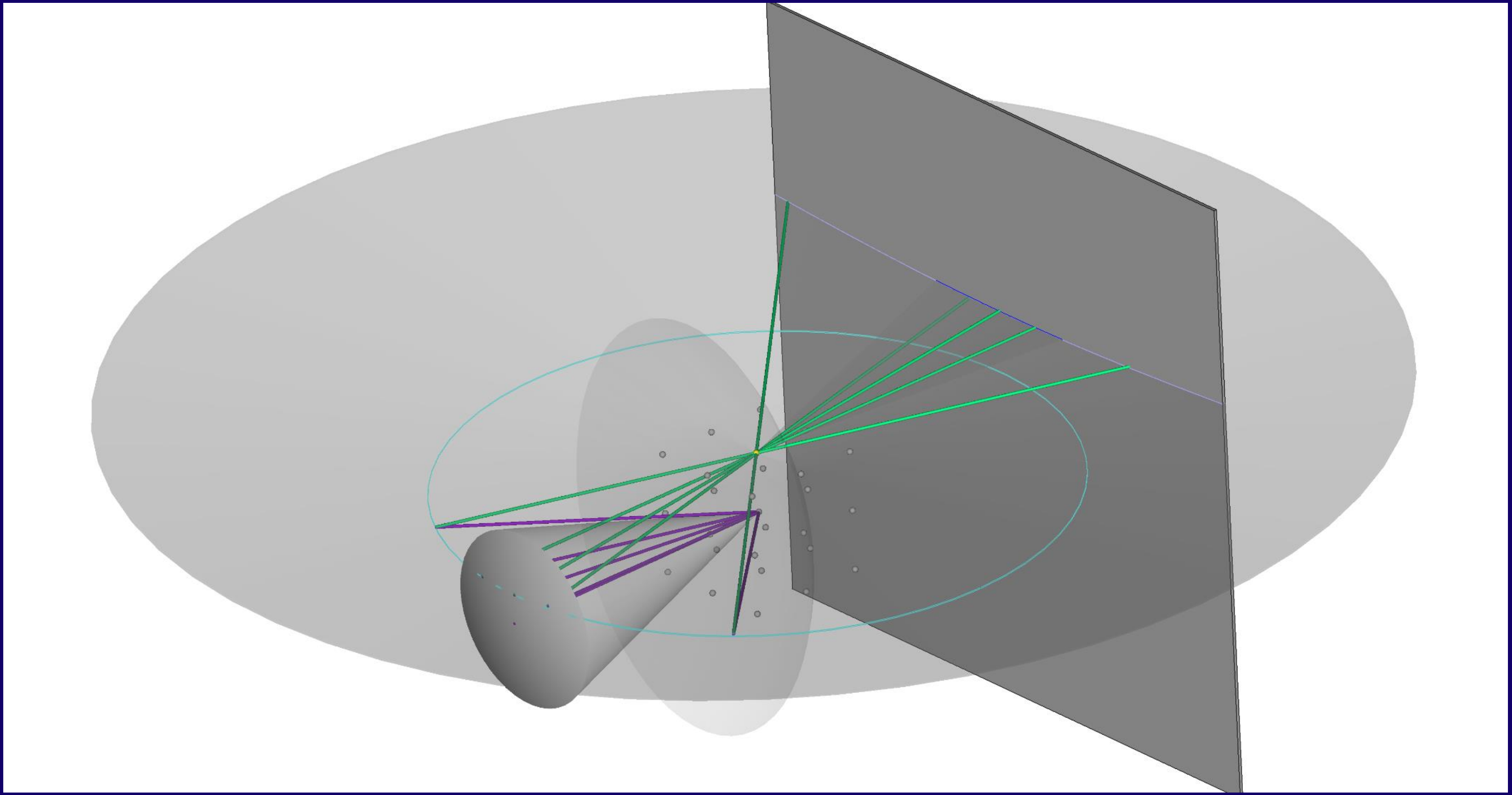


Y.Gevorkov

Divergent beam in reciprocal space

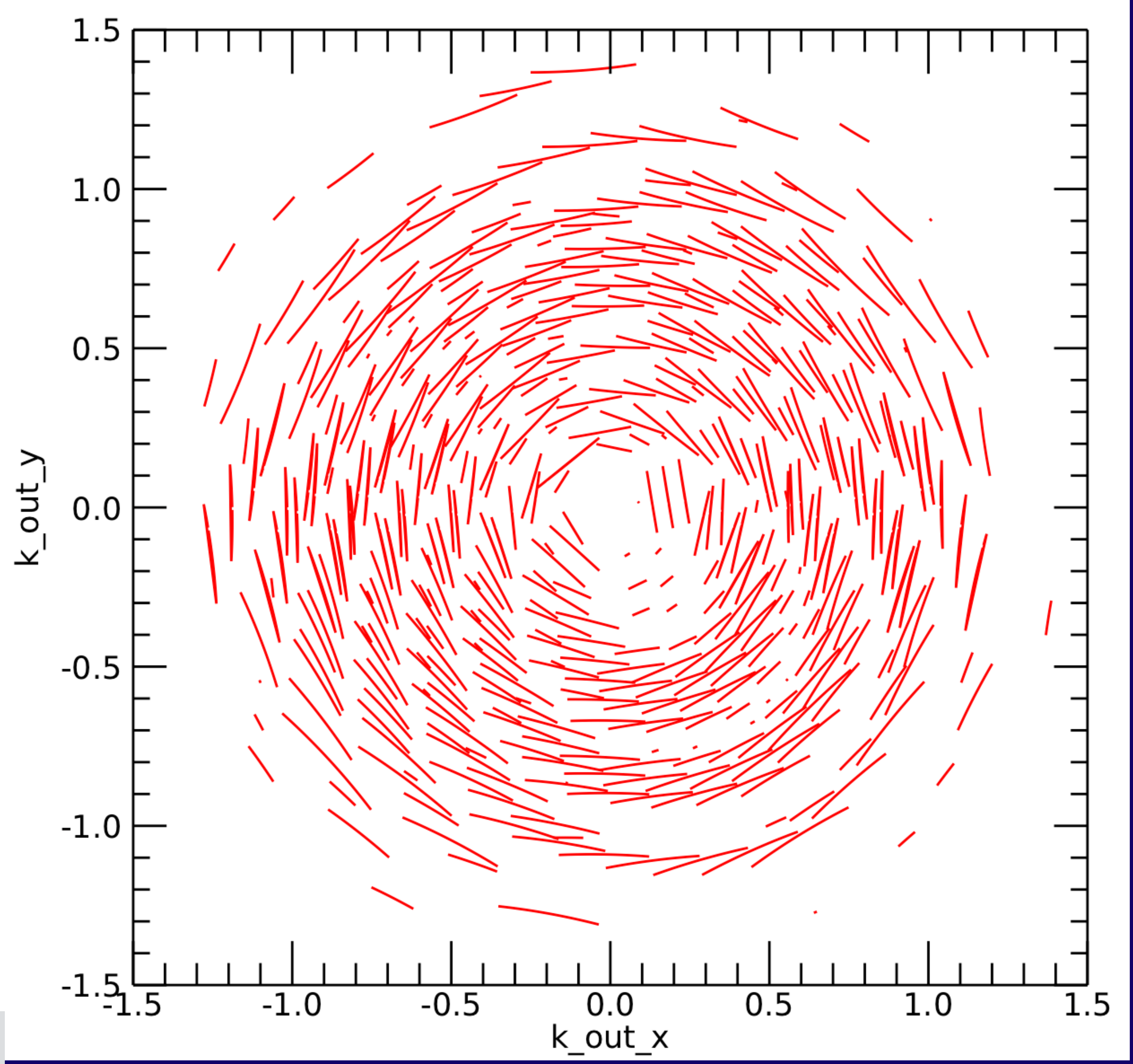


Divergent beam in reciprocal space (3D)



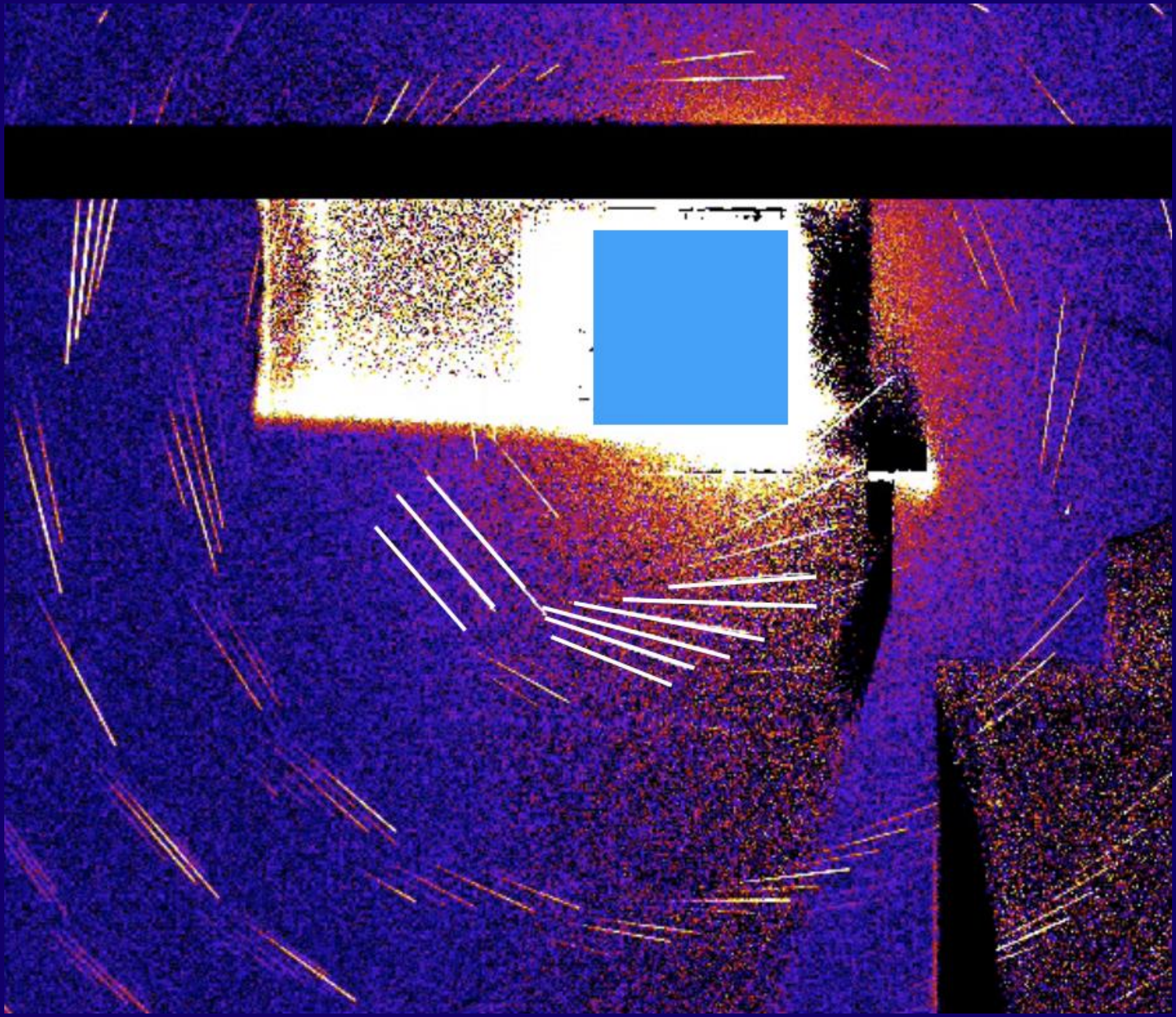
Y.Gevorkov

Diffraction pattern with big divergence



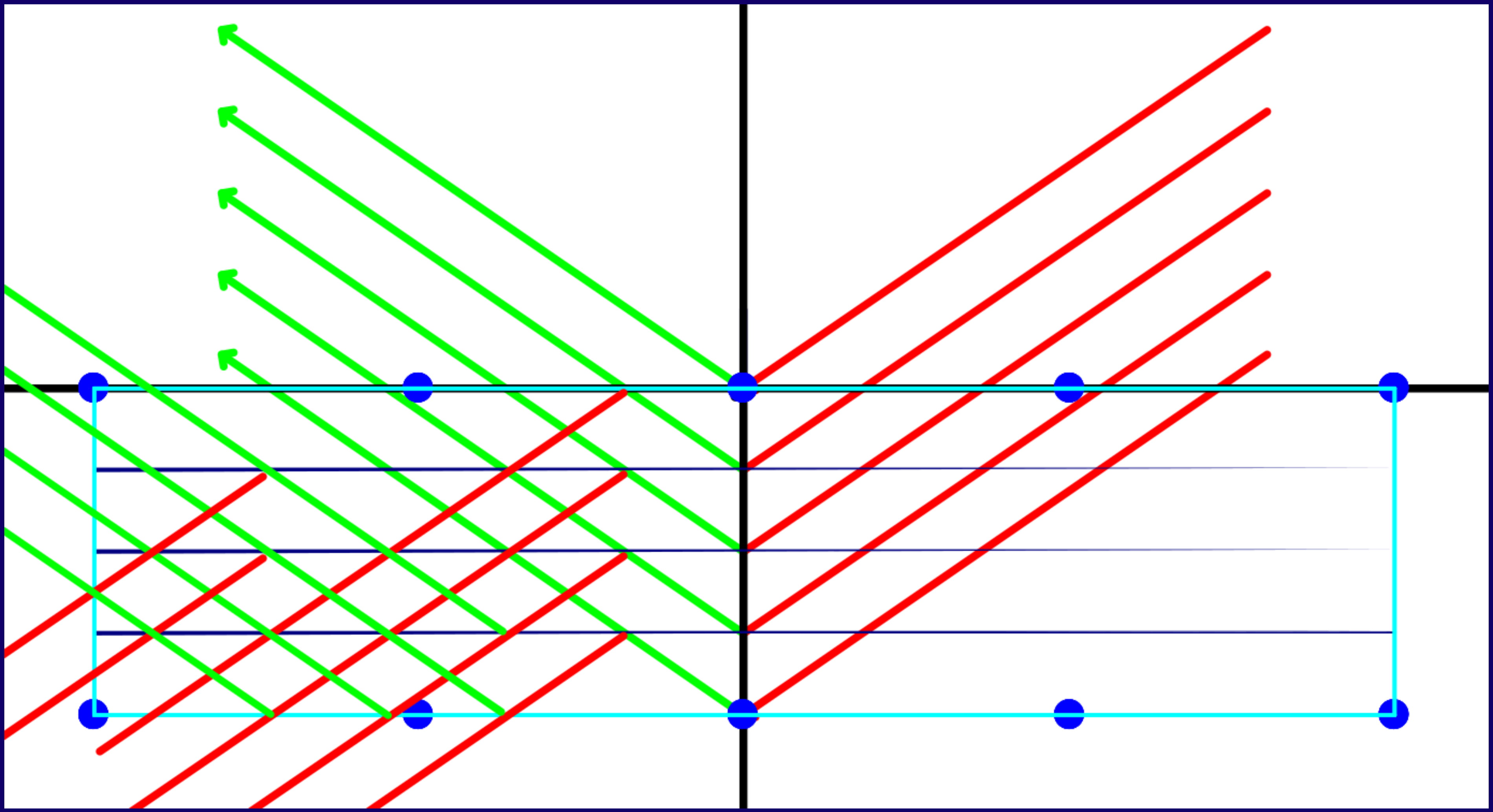
H.Chapman

Experimental diffraction pattern



Multiple scattering
(dynamical diffraction theory)

Dynamical diffraction



Propogation equation:

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

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

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

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

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

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

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

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

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

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

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

$$\Delta_E = 0$$

Dispersion equation

Boundary conditions

$$E_t = const$$

$$D_n = const$$

$$H_t = const$$

$$B_n = const$$

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

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

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

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

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

$$(k_0^2 - (1+\chi_0)K^2)(k_h^2 - (1+\chi_0)K^2) = C^2 K^4 \chi_{\bar{h}} \chi_h$$

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

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

Processing “big” SX data

Data rates at modern sources

LCLS (CS-PAD):

4.6Mb * 120Hz * 3600sec * 10hours * 5days = 95Tb

PINK beam at APS (JoungFrau 1M):

2Mb * 1000Hz * 3600sec * 20hours * 5days = 860Tb

Modern synchrotron (Eiger2 XE 16M, compressed):

16Mb * 400Hz * 3600sec * 20hours * 5days = 2.1Pb

eXFEL now (AGIPD):

(2+2)Mb * 3520Hz * 3600sec * 10hours * 5days = 2.4Pb

eXFEL soon (AGIPD 4M, 2023+):

(8+8)Mb * 3520Hz * 3600sec * 10hours * 5days = 9.5Pb

LCLS2 soon (ePix10k-HR, 2024+):

8.4Mb * 10000Hz * 3600sec * 10hours * 5days = 14Pb

Data rate (LCLS)

Detector

120 Hz
4 MB/event
1.7 TB/hr
200TB/expt
(5 days)

Storage

> 20,000,000 frames

Store all data
(no corrections)

Offline reduction

< 1,000,000 frames

Retain only 'hits'
(detector corrected)

Analysis

<100,000 frames

Science analysis

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

CFEL SCIENCE

Online processing (Onda/OM)

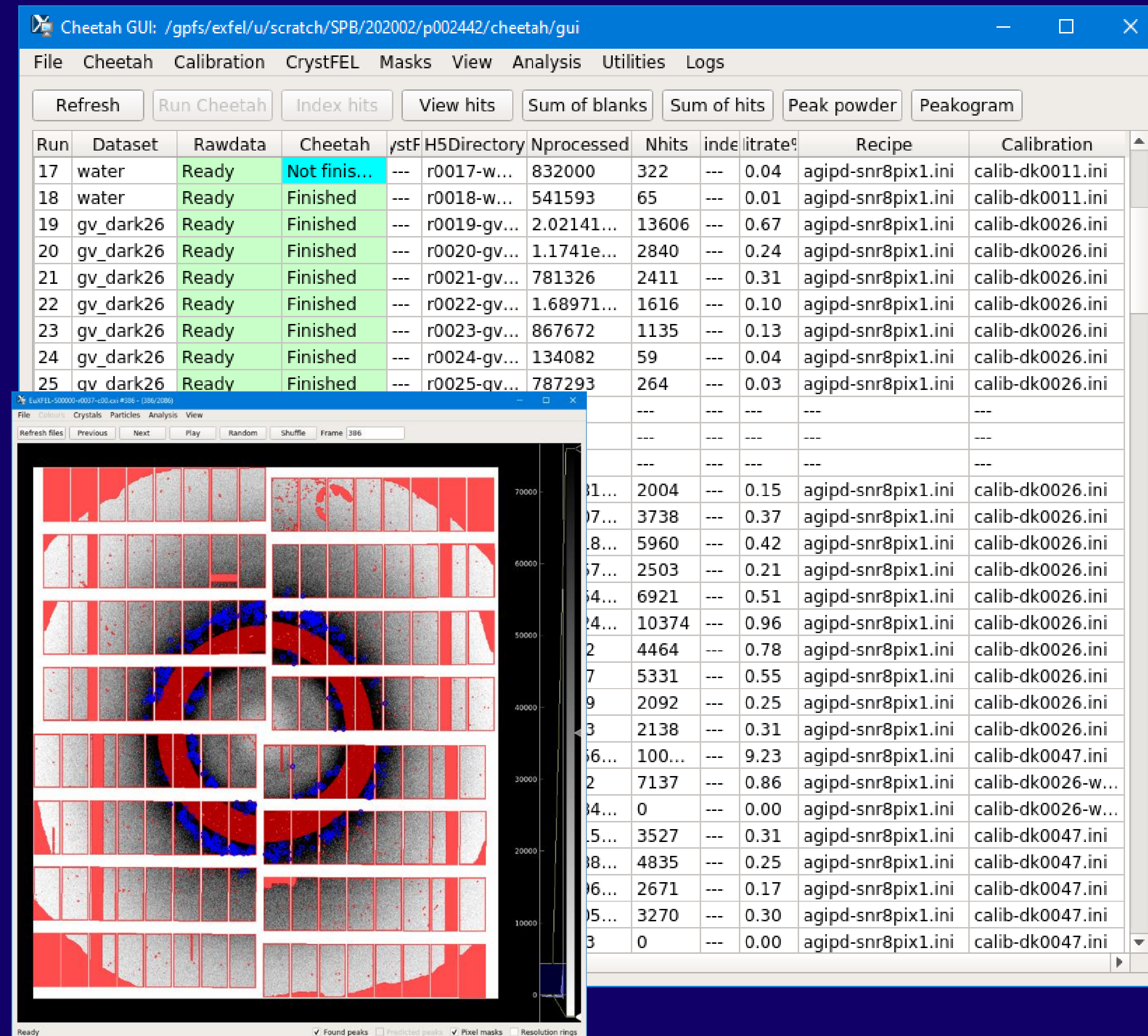
Up to date information > Real-time human feedback
Keep up with data flow (fresh)
Data that help us take immediate decisions

Accuracy is not a strong requirement. Low latency is!

Mariani et al., "OnDA: online data analysis and feedback for serial X-ray imaging", J. Appl. Cryst. (2016)

Offline data processing

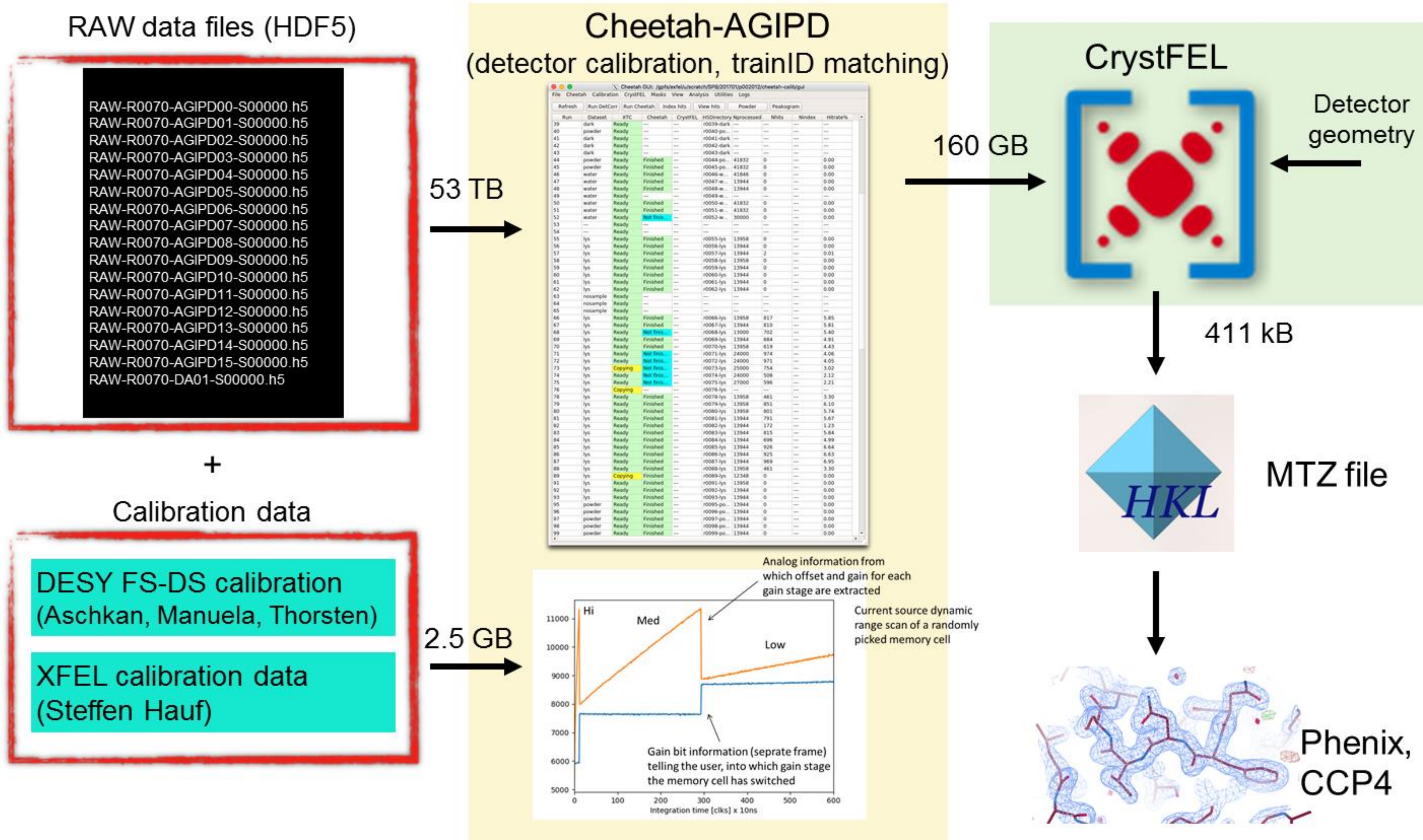
Fast (C, Python?)
Parallelizable
Reliable
Adjustable
Tools to check results
User friendly
HDF5 compatible
Segmented detectors
AI is not always suitable



Maxwell cluster

max-exfl099	upex-beamtime upex-middle exfel upex all allrsv	80	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	5-2698 v4 @ 2.20GHz	0	INTEL, V4, E5-2698, 512G
max-exfl101	exrsv upex-beamtime upex-middle exfel upex all allrsv	72	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	d 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



Thank you for attention!