Coherent X-rays & applications

ESRF | The European Synchrotron

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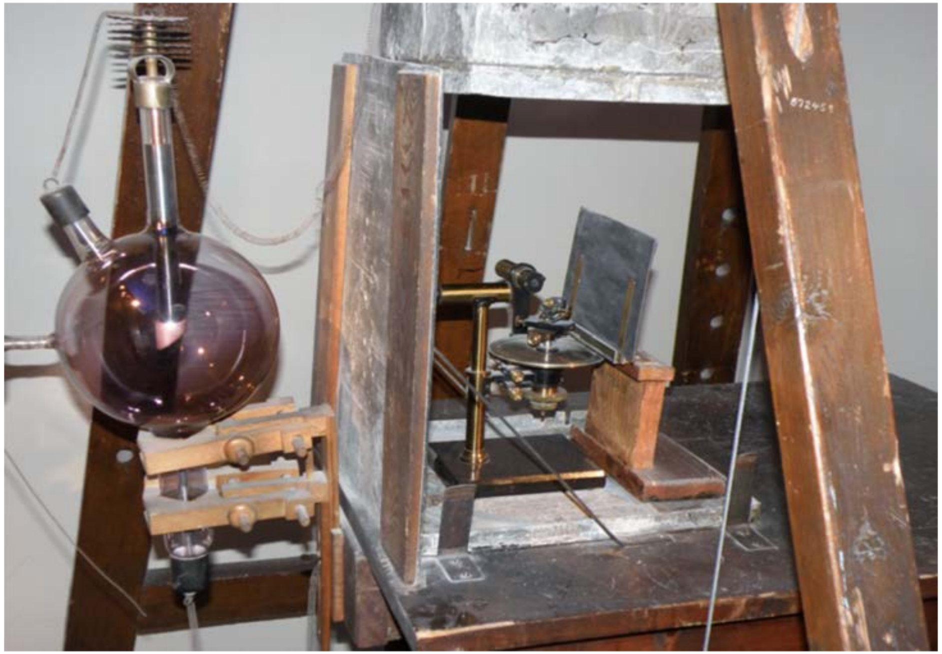
Algorithms & scientific Data Analysis

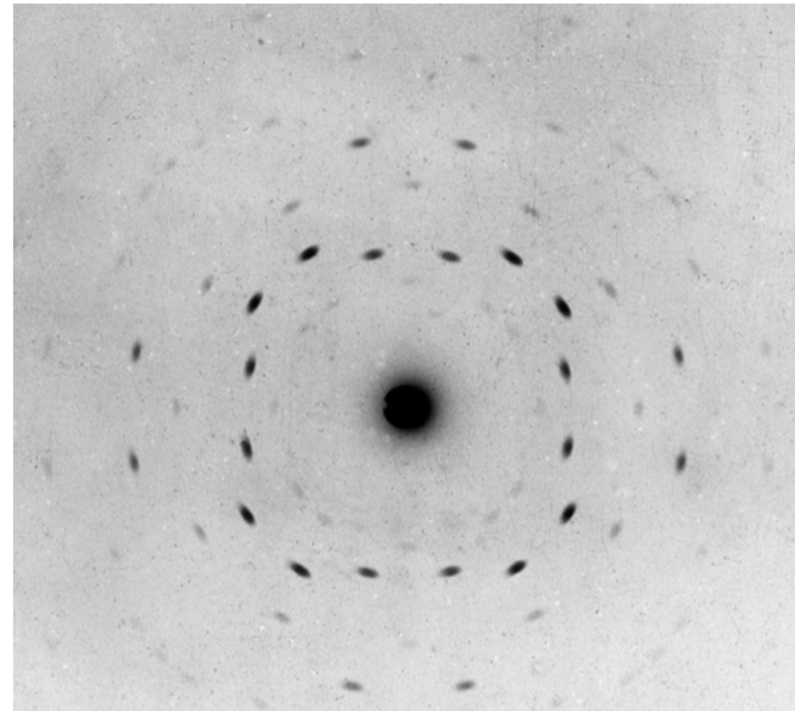
on leave from Univ. Grenoble Alpes

UNIVERSITÉ Grenoble Alpes

COHERENT X-RAYS ?



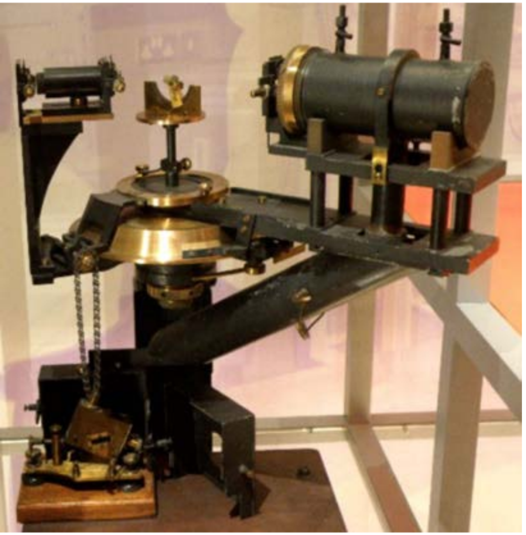
Friedrich, Knipping, Laue

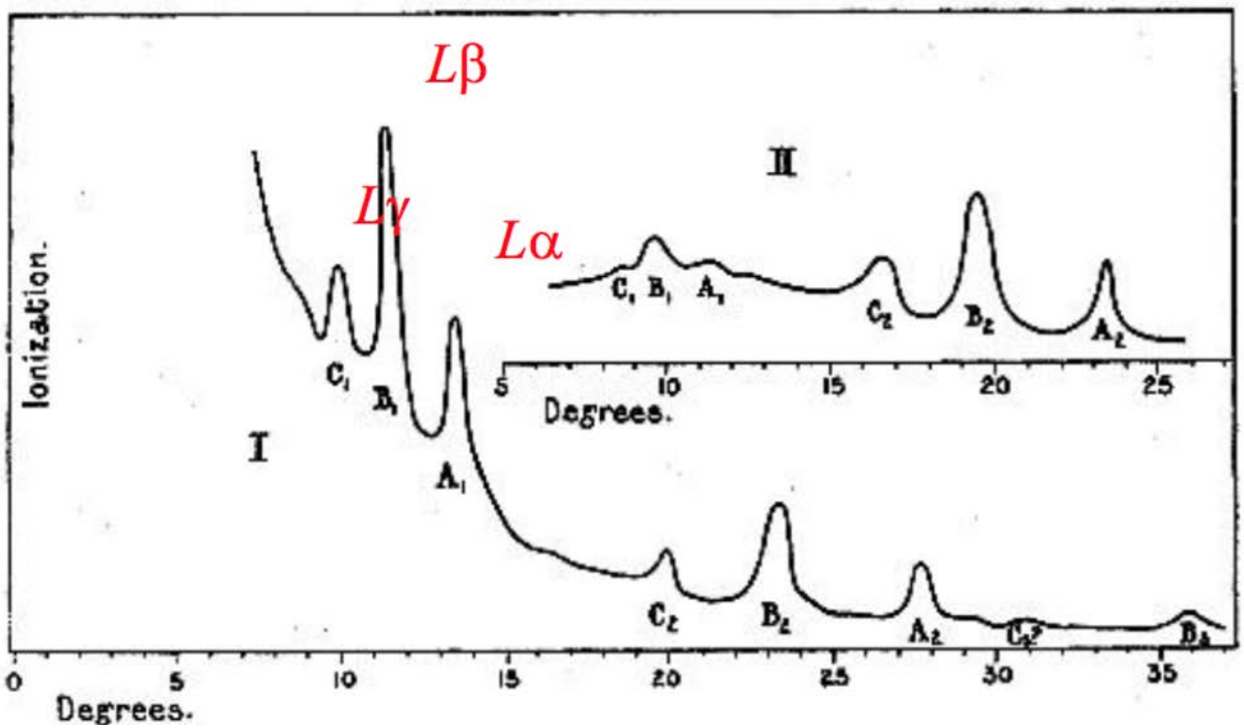


ZnS (blende)

Illustrations from Authier « Early days of crystallography, Oxford University Press

COHERENT X-RAYS ?





W & H Bragg : first X-ray spectrum : NaCl diffraction from Pt radiation

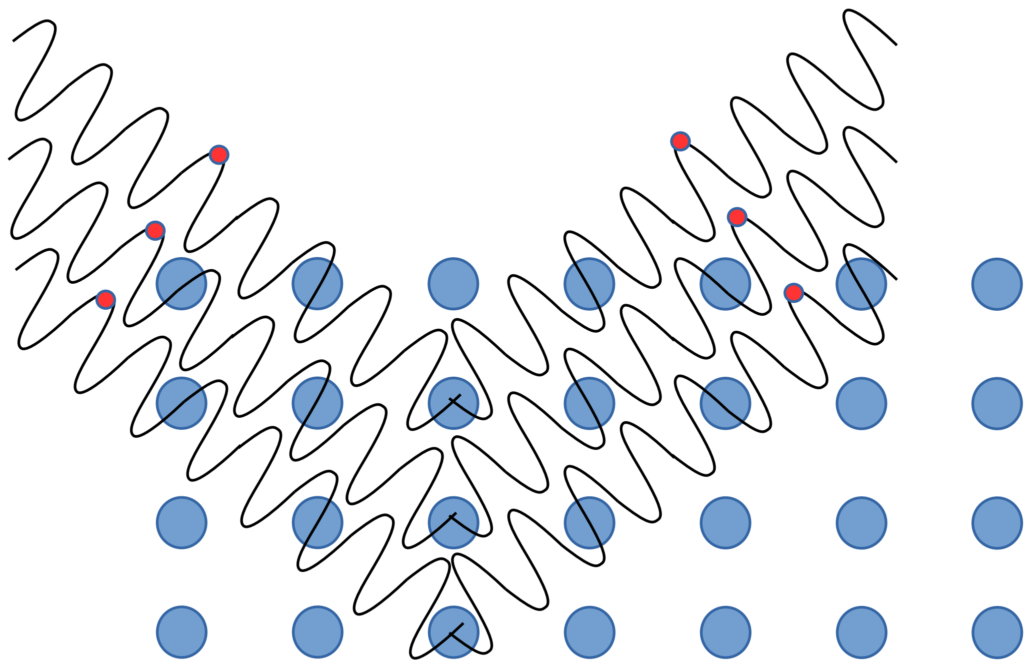
Illustrations from Authier « Early days of crystallography, Oxford University Press

COHERENT X-RAYS ?

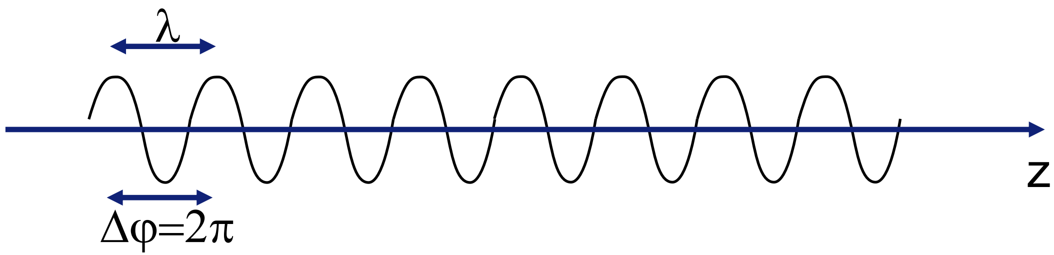
X-rays can produce (Bragg) diffraction even from "low-quality" X-ray sources :

- Large source size
- Non-monochromatic (but discrete spectrum)

Diffraction implies interferences => coherence



WAVE PROPAGATION BASICS



$$A_0 \cos(\omega t - kz) = A_0 \cos\left(\omega t - \frac{2\pi z}{\lambda}\right) = A_0 \cos(\varphi)$$

- λ: wavelength (0.01 to 1 nm for X-rays)
- ω: pulsation = $2\pi/\nu$
- ν: frequency
- φ: phase

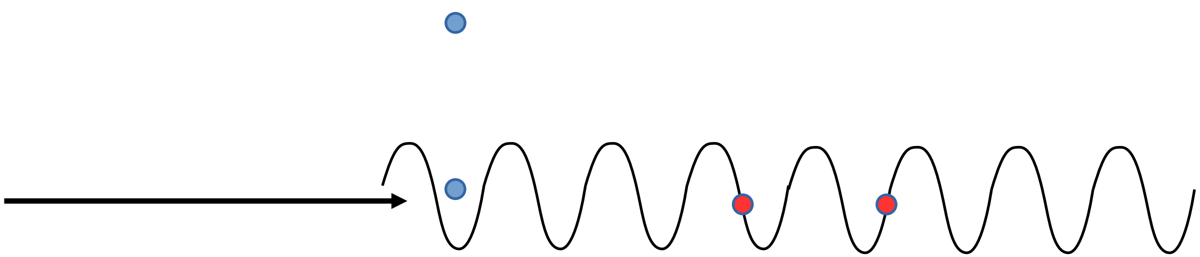
COHERENT XRAYS ?

Definition (from Malcolm Howells):

- "Optical coherence exists in a given radiating region if the **phase differences between all pairs of points** in that region have definite values which are constant with time"

Two types of coherence must be considered:

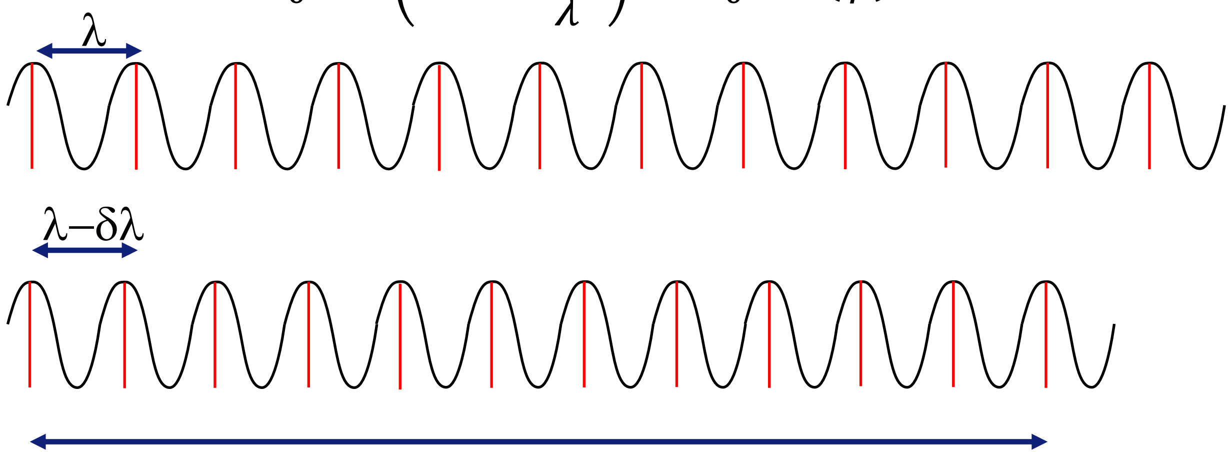
- Transverse coherence, between points in plane perpendicular to the wavevector
- Longitudinal (temporal) coherence between points along the wavevector



LONGITUDINAL COHERENCE

- Longitudinal (temporal) coherence
- Related to the monochromaticity
- For a beam with $\delta\lambda$ spectrum width (typical $\delta\lambda/\lambda=10^{-4}$: for Si 111 monochromator)

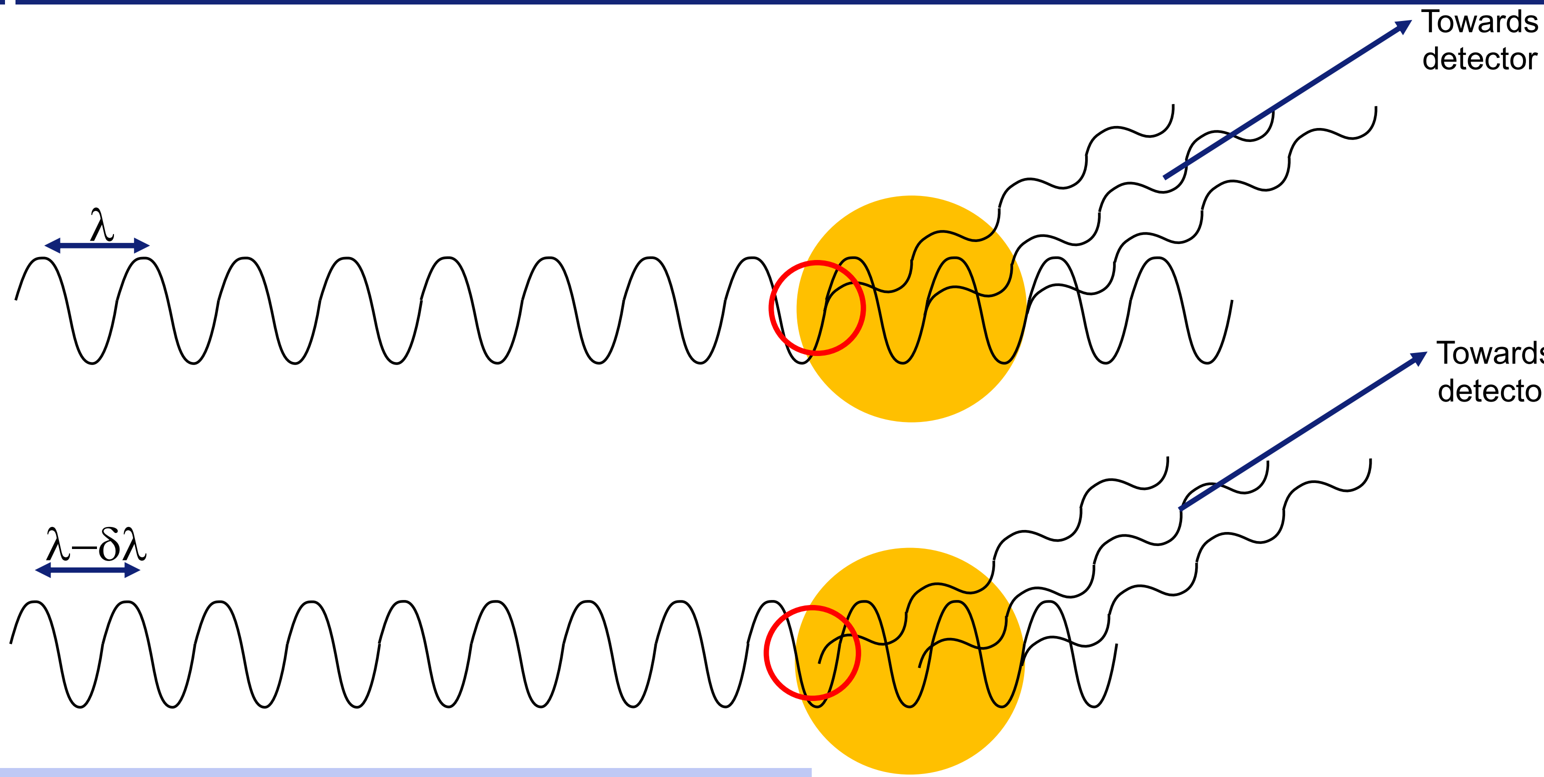
$$A_0 \cos\left(\omega t - \frac{2\pi z}{\lambda}\right) = A_0 \cos(\varphi)$$



Longitudinal coherence length = length for a 2π shift due to $\delta\lambda$.

$$\Lambda_{long} = \lambda \frac{\lambda}{\delta\lambda} = \frac{\lambda^2}{\delta\lambda}$$ => typically 0.5 to 1 µm

LONGITUDINAL COHERENCE & SCATTERING



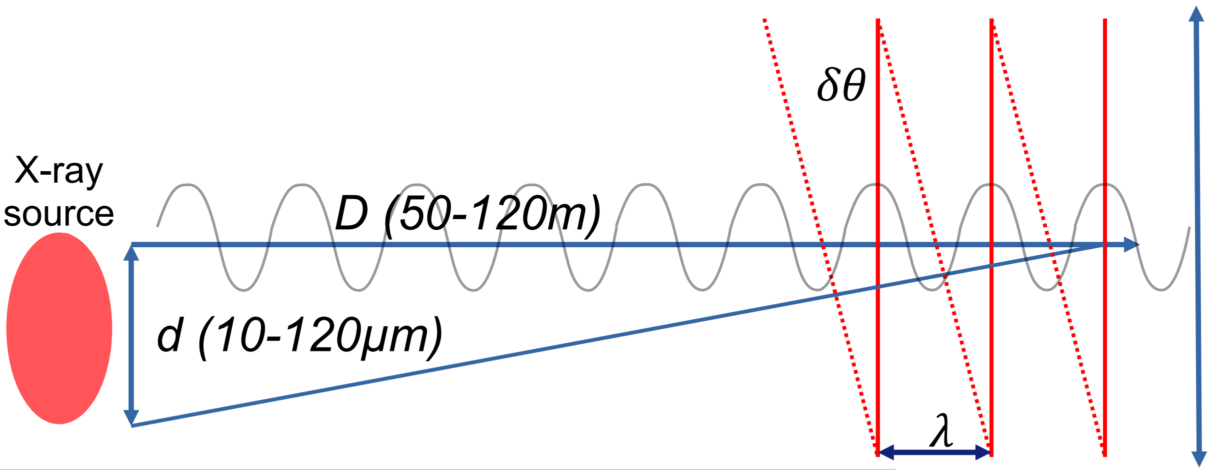
There is a phase difference between the beginning and the end of the particle.

As long as this difference is small, it does not affect the scattering signal

For crystallography, the coherence length is much larger than a unit cell (~1nm), which is why we can always see Bragg diffraction with 'low' coherence

TRANSVERSE COHERENCE

- Transverse coherence, between points in plane perpendicular to the wavevector
- Related to the source size
- X-ray sources (tubes, bending magnet, undulators, ~~XFEL~~) are incoherent (different points within the source emit with random phase shifts)
- For a source width d (a few 10's of µm), seen from a distance D (50-120m):



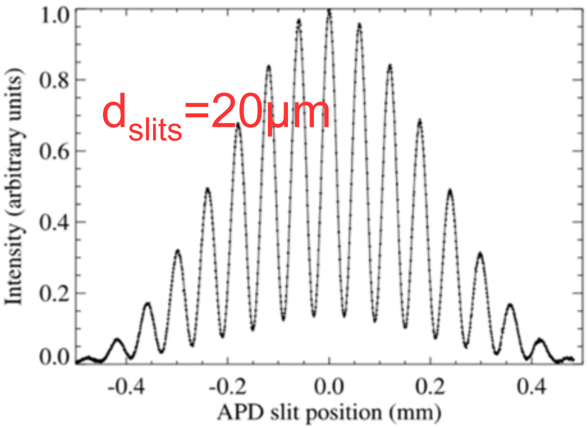
$$L_{trans} = \frac{\lambda \cdot D}{2d} \approx 20 - 100\mu m$$

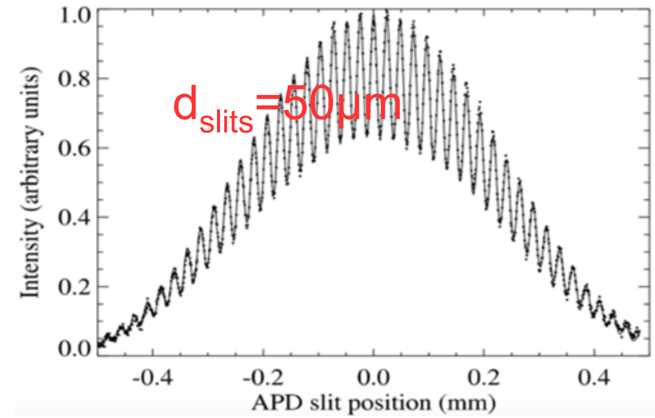
There is a phase difference between incident waves emited by different parts of the source.

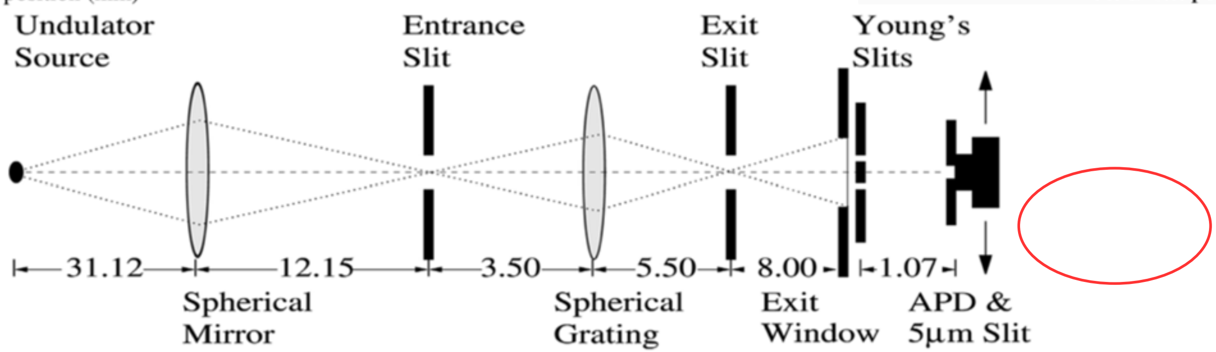
As long as this difference is small, it does not affect the scattering signal

High coherence implies:
- Small sources
- Long beamlines

- Transverse coherence can be evaluated by fringe visibility:



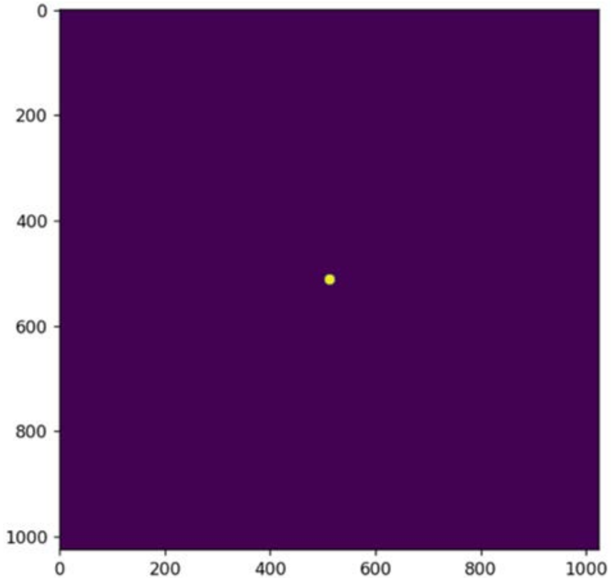




Fringes for a Young double-slit experiment @1.1 keV, 8m from the source

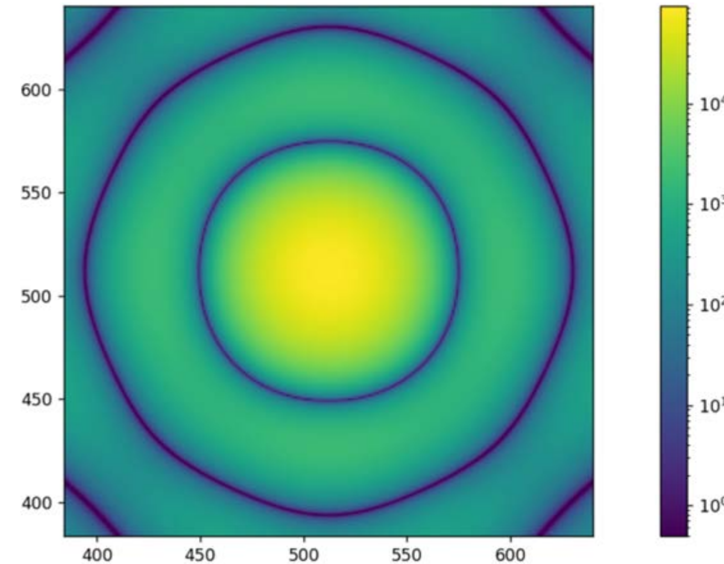
Optics Communications 195, 79 (2001)

COHERENT SCATTERING: 1 PARTICLE



Circular particle
(**r=10** pixels)

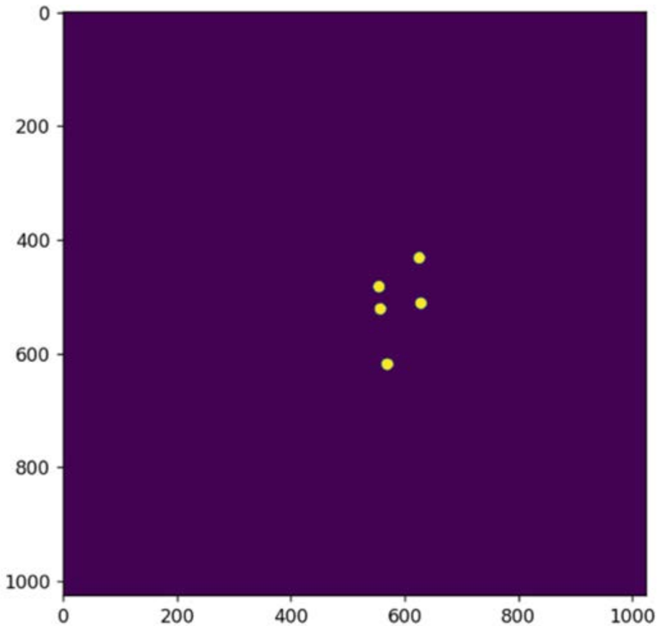
Fourier
transform



Detector (20 cm to a few m away)
Oscillations with a period in 1/r

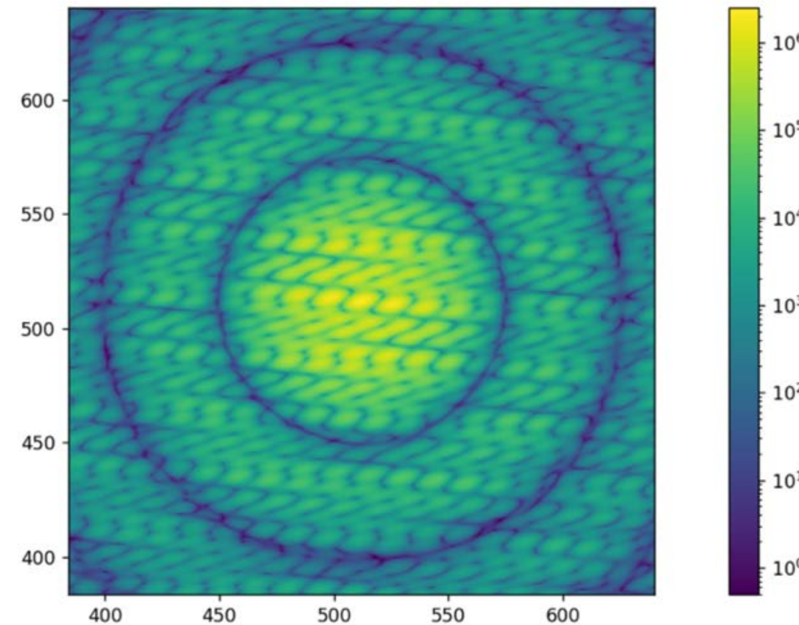
The scattering from a **coherently illuminated** particle can be simply computed using a Fourier transform

COHERENT SCATTERING: 5 PARTICLES



N=100 circular particles
(**r=10** pixels)

Fourier transform

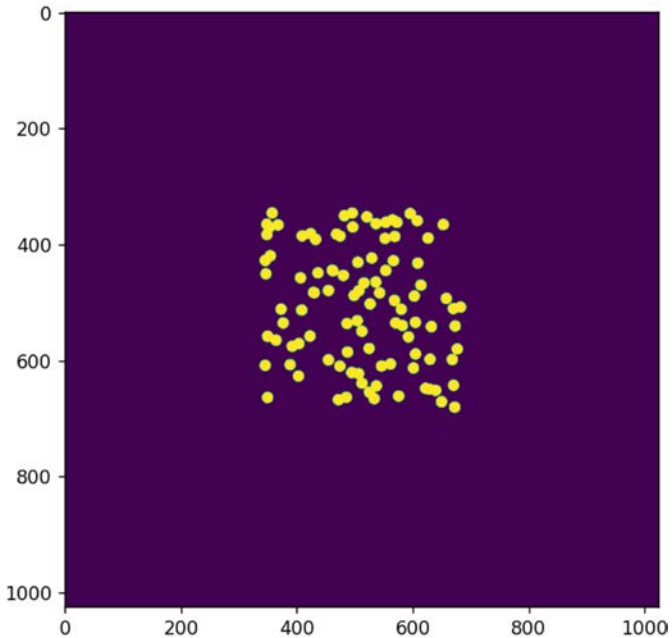


Detector (20 cm to a few m away)
Oscillations with a period in 1/r

+ 'speckles' due to interferences between the scattering of all particles

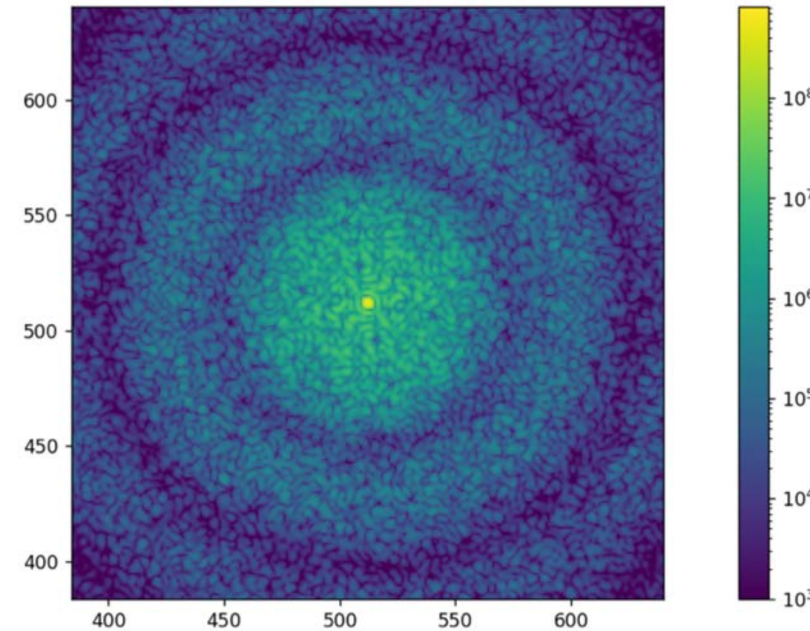
If the particles were ***not*** coherently illuminated, the detector image would be exactly the same as for a single particle.

COHERENT SCATTERING: 100 PARTICLES



N=100 circular particles
(**r=10** pixels)

Fourier transform

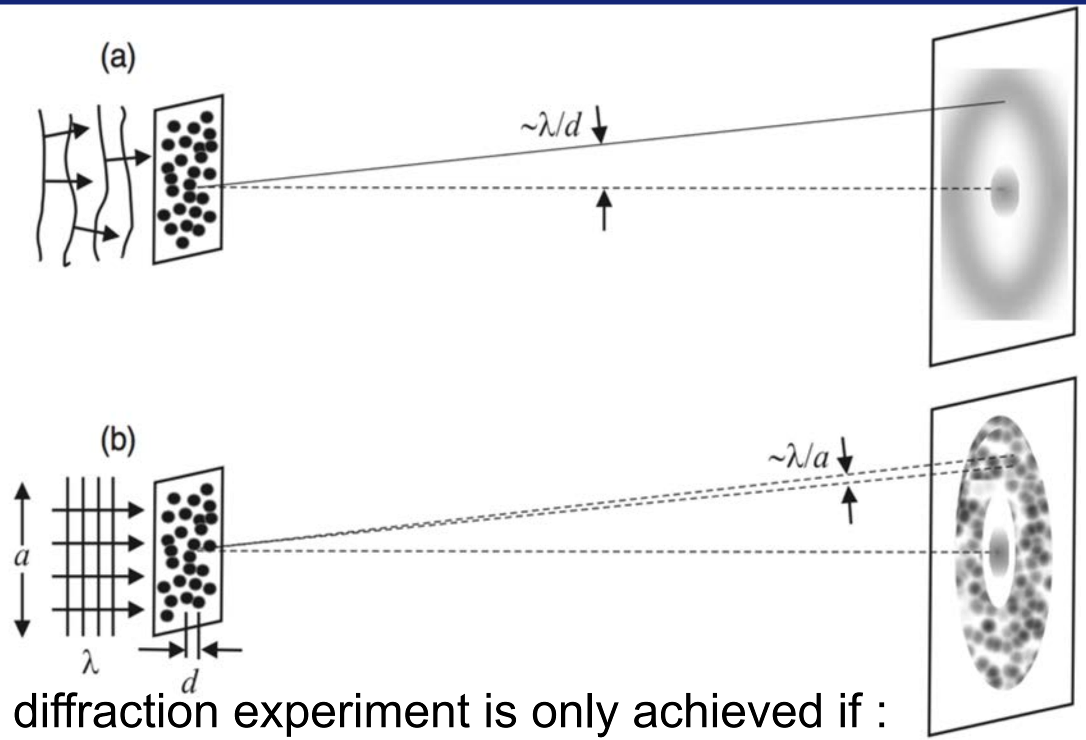


Detector (20 cm to a few m away)
Oscillations with a period in 1/r
+ 'speckles' due to interferences between the scattering of all particles

Features which can be extracted:

- Average particle size from oscillations
- Average distance between particles from speckles
- Time evolution

COHERENT ILLUMINATION

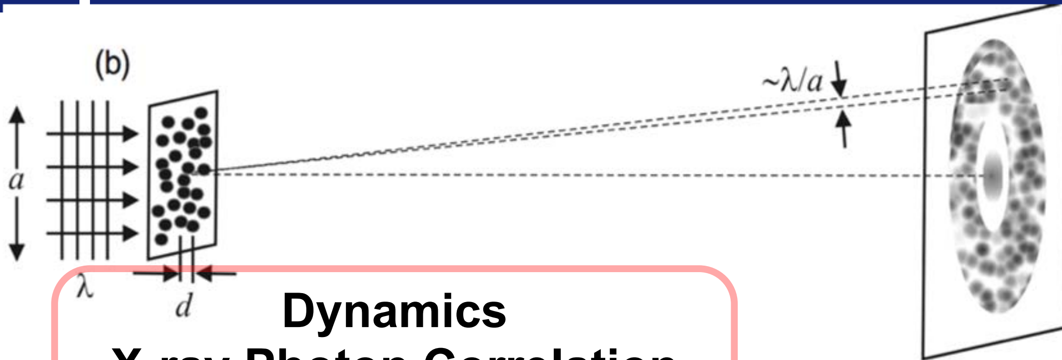


A coherent diffraction experiment is only achieved if :

- The sample is smaller than the coherent length
- Or the beam is collimated to a smaller size than the coherent length

In 3D, the term ‘coherent volume’ can be used

J. Phys.: Condens. Matter 16, 5003 (2004)



The diffraction pattern is the sum of the interference of the scattering from all particles

$$A(\vec{s}) = \sum \rho_i e^{2i\pi\vec{s}.\vec{r}_i}$$

Dynamics
X-ray Photon Correlation Spectroscopy

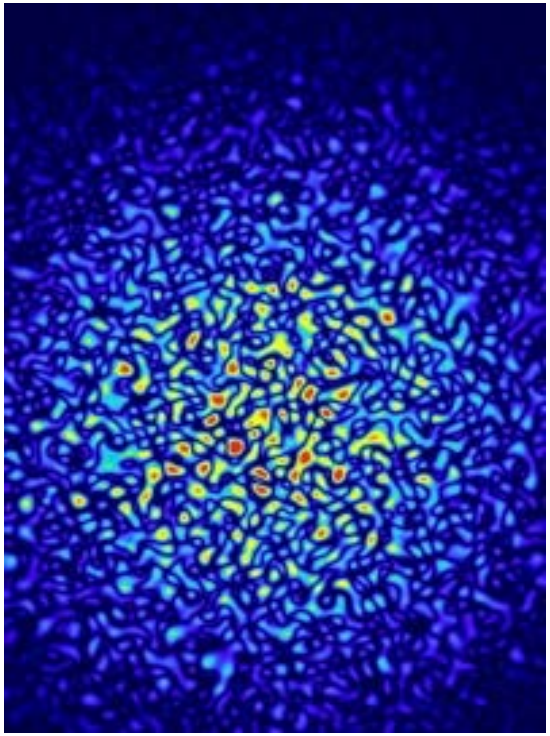
- Study the frame-by frame evolution of the diffraction pattern (image cross-correlation)
- Information about the evolution of relative position between particles
- Study **diffusion coefficients**, from atomistic to mesoscopic to length scales (colloids, glasses, magnetic systems, etc…)

High-resolution imaging

- The diffraction image obtained by **Fourier Transform(s)** of the illuminated object
- Once the phase has been recovered (algorithms), the **object can be reconstructed** (in **2D** or **3D**)
- The **resolution** is inversely proportional to the angular extent of the scattering (far field)

COHERENT ILLUMINATION

If the object is too complex (too many parameters vs available information), then the experiment will only at best yield a ‘speckle pattern’



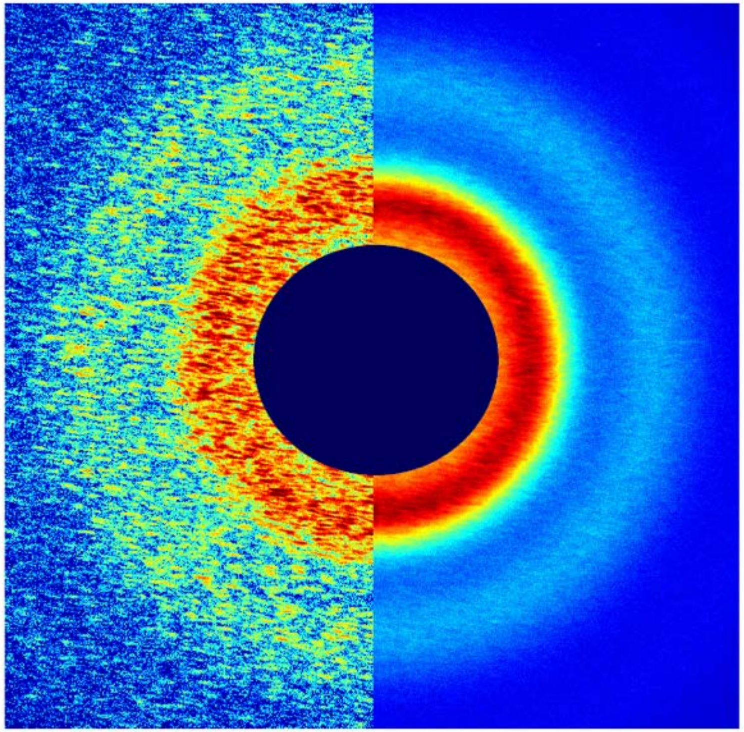
From Oleg Shpyrko web page

Statistical information :

- Width of speckle pattern ↔ average particle size
- Number of speckles peaks along one
  - dimension ↔ number of particles

Time-resolved experiments : XPCS

X-RAY PHOTON CORRELATION SPECTROSCOPY (XPCS)



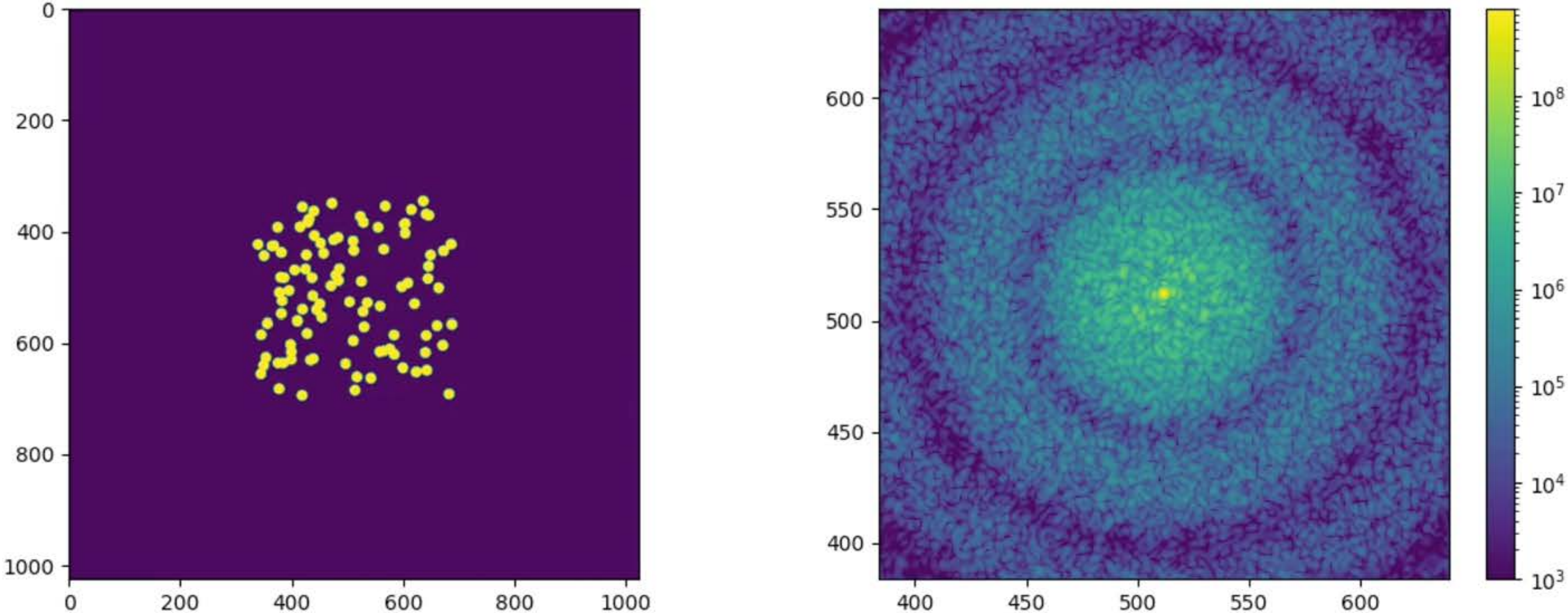
High coherence Low coherence

C. Gutt

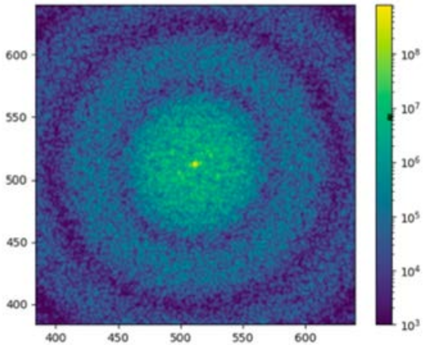
XPCS:

- Measure the correlation of the scattered intensity as a function of time
- *Not* a spectroscopy technique

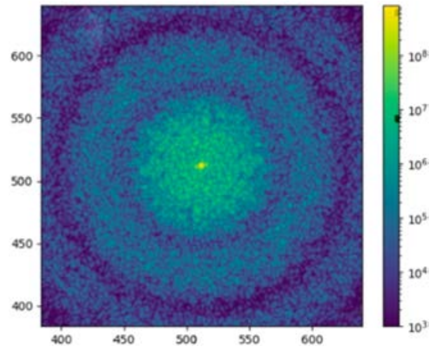
X-RAY PHOTON CORRELATION SPECTROSCOPY (XPCS)



- Movement of particles (molecules, atoms..) induce changes in the speckles
- Higher angular momentum (far from the centre) are more sensitive to smaller displacements
- Movement (diffusion) can be quantified by correlation



$I(\boldsymbol{Q},\tau)$



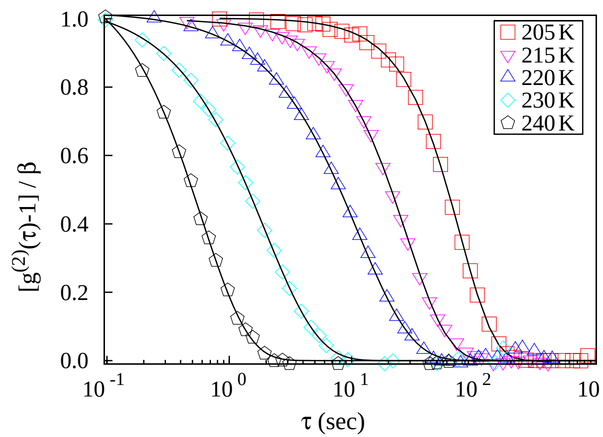
$I(\boldsymbol{Q},\tau+t)$

Temporal intensity auto-correlation function:

$$g^{(2)}(\boldsymbol{Q},t) = \frac{\langle I(\boldsymbol{Q},\tau) I(\boldsymbol{Q},\tau+t)\rangle}{\langle I(\boldsymbol{Q},\tau)\rangle^2}$$

Example 1: Dynamics of silica colloidal nano-particles in super-cooled propanediol

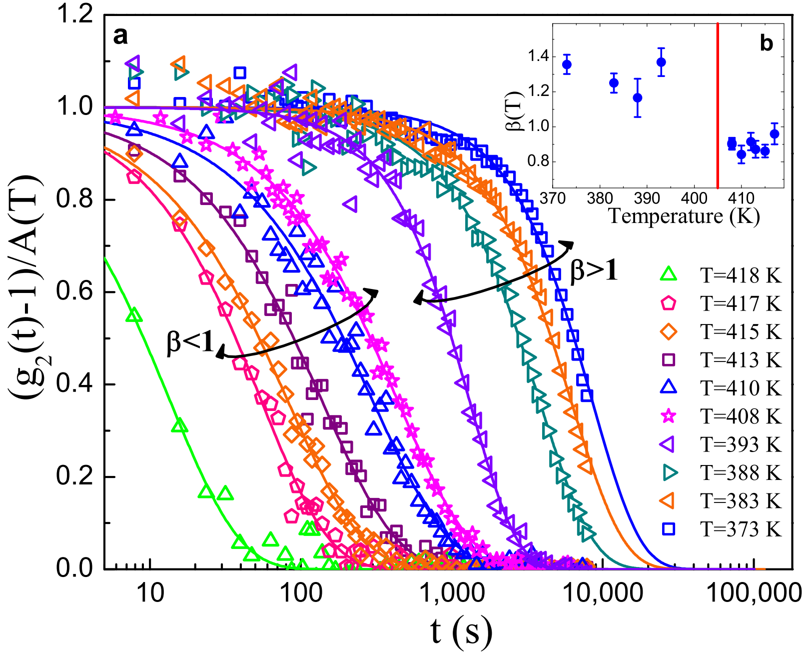
- Tf = 245K for propanediol
- T<Tf => supercooled liquid, towards a glass transition



PRL 100, 055702 (2008)

X-RAY PHOTON CORRELATION SPECTROSCOPY (XPCS)

Example 2: atomic-scale dynamics & in a metallic glass ($Mg_{65}Cu_{25}Y_{10}$)

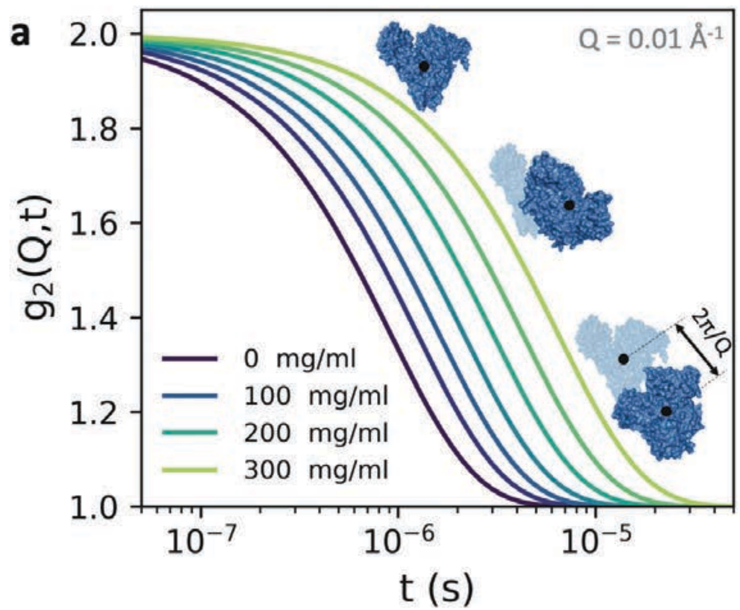


Phys. Rev. Lett. 109, 165701 (2012)

- Glasses are seen as ‘frozen liquids’
- … they are *still* liquids, but with a *very* large viscosity
- Tg = 405K
- There is still atomic motion below Tg
- The ß value changes between above and below Tg – different motion regimes

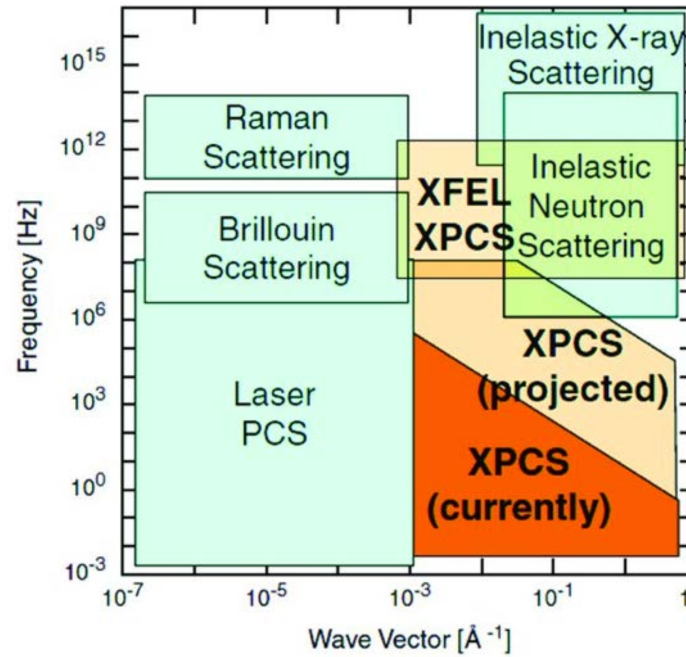
$$g^{(2)}(\boldsymbol{Q},t) = 1 + Ae^{-2\left(\frac{t}{\tau}\right)^{\beta}}$$

X-RAY PHOTON CORRELATION SPECTROSCOPY (XPCS)



XPCS also applies to protein solutions

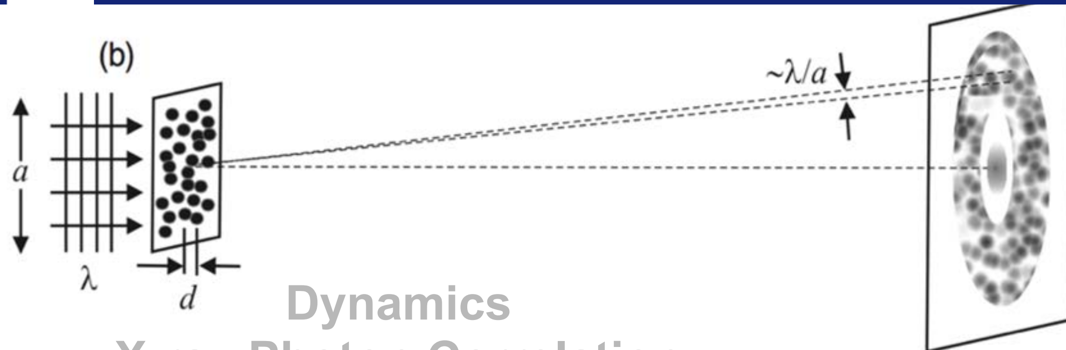
Phys. Chem. Chem. Phys. **22**, 19443 (2020)



Dynamics can be probed on a wide range of time-scales, which increases with modern synchrotron sources and XFEL

Pawel Kwasniewski PhD (Grenoble)

COHERENT X-RAYS: DYNAMICS & IMAGING



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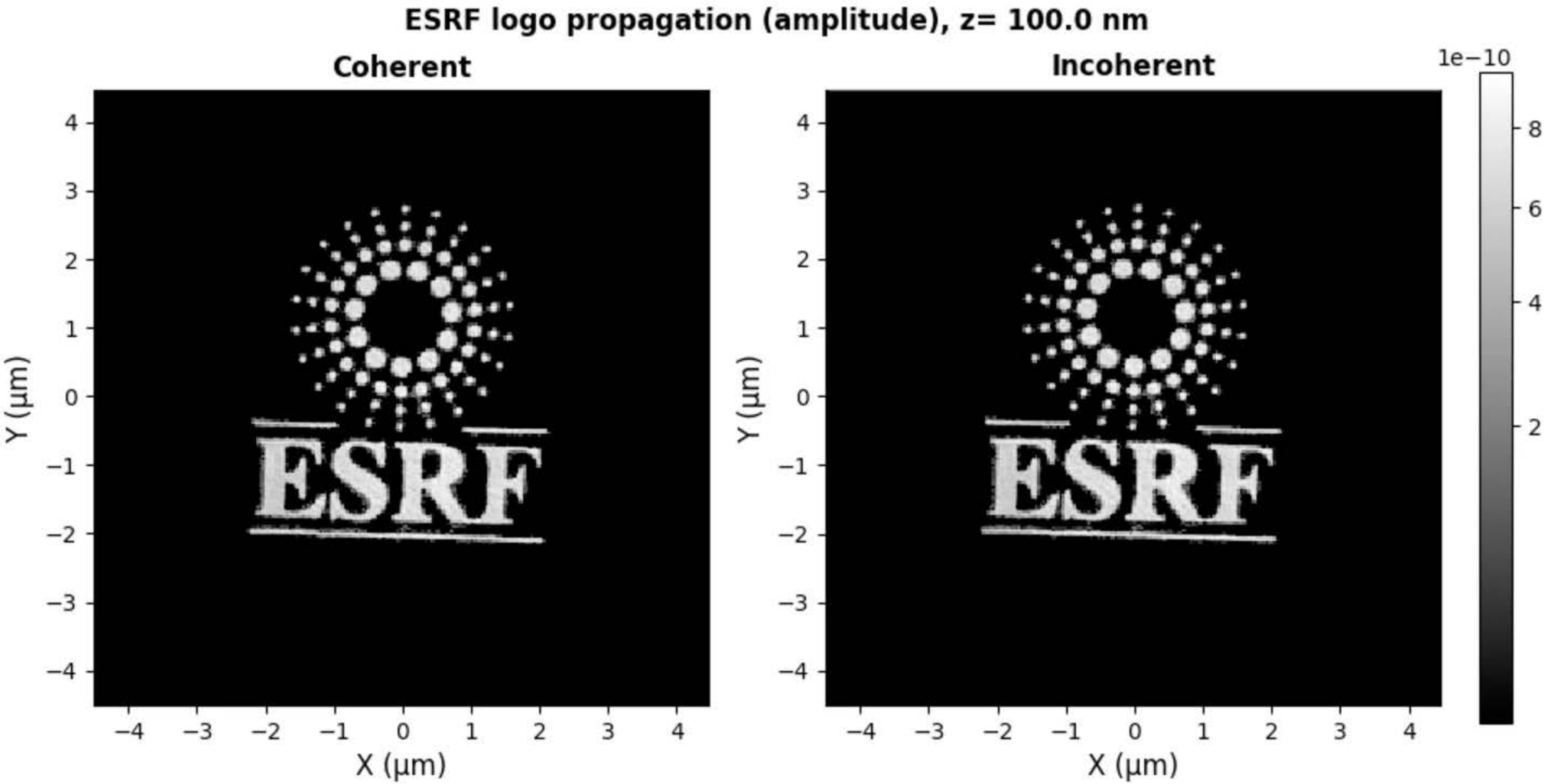
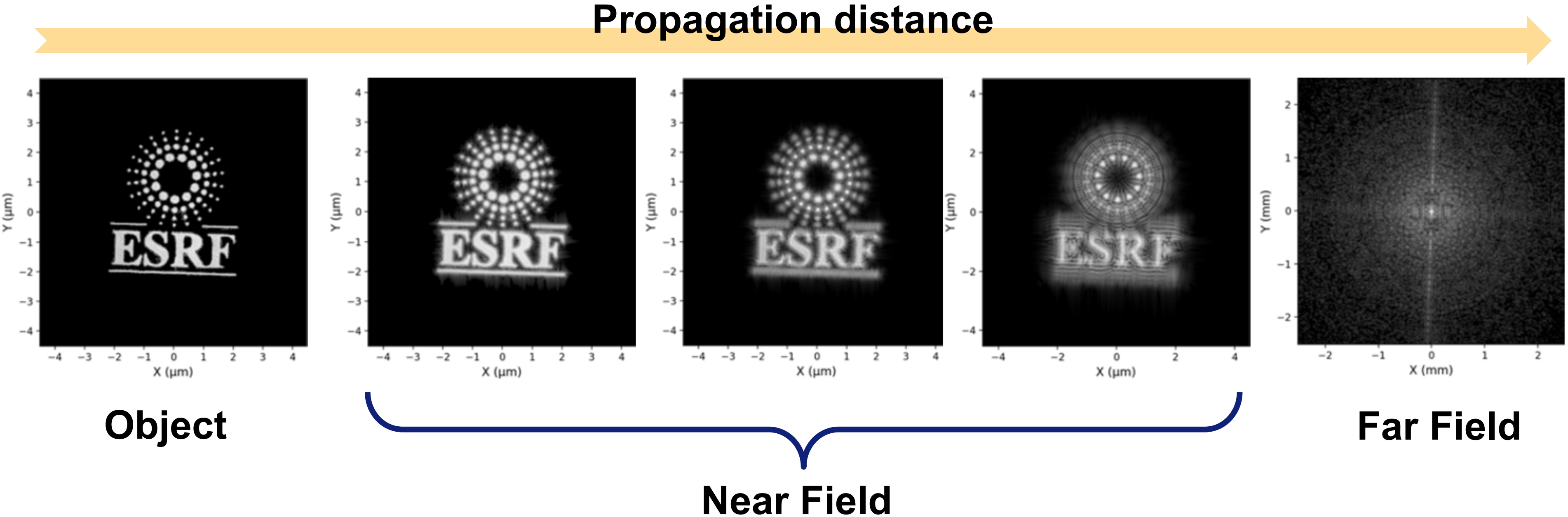
COHERENT VS INCOHERENT IMAGING

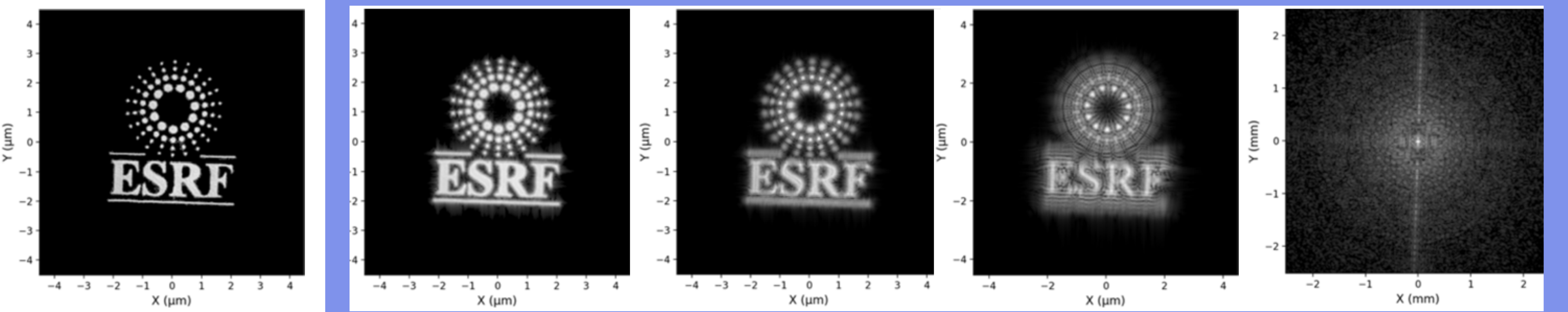


COHERENT X-RAY IMAGING TECHNIQUES



COHERENT X-RAY IMAGING: ALGORITHMS ?

Propagation distance

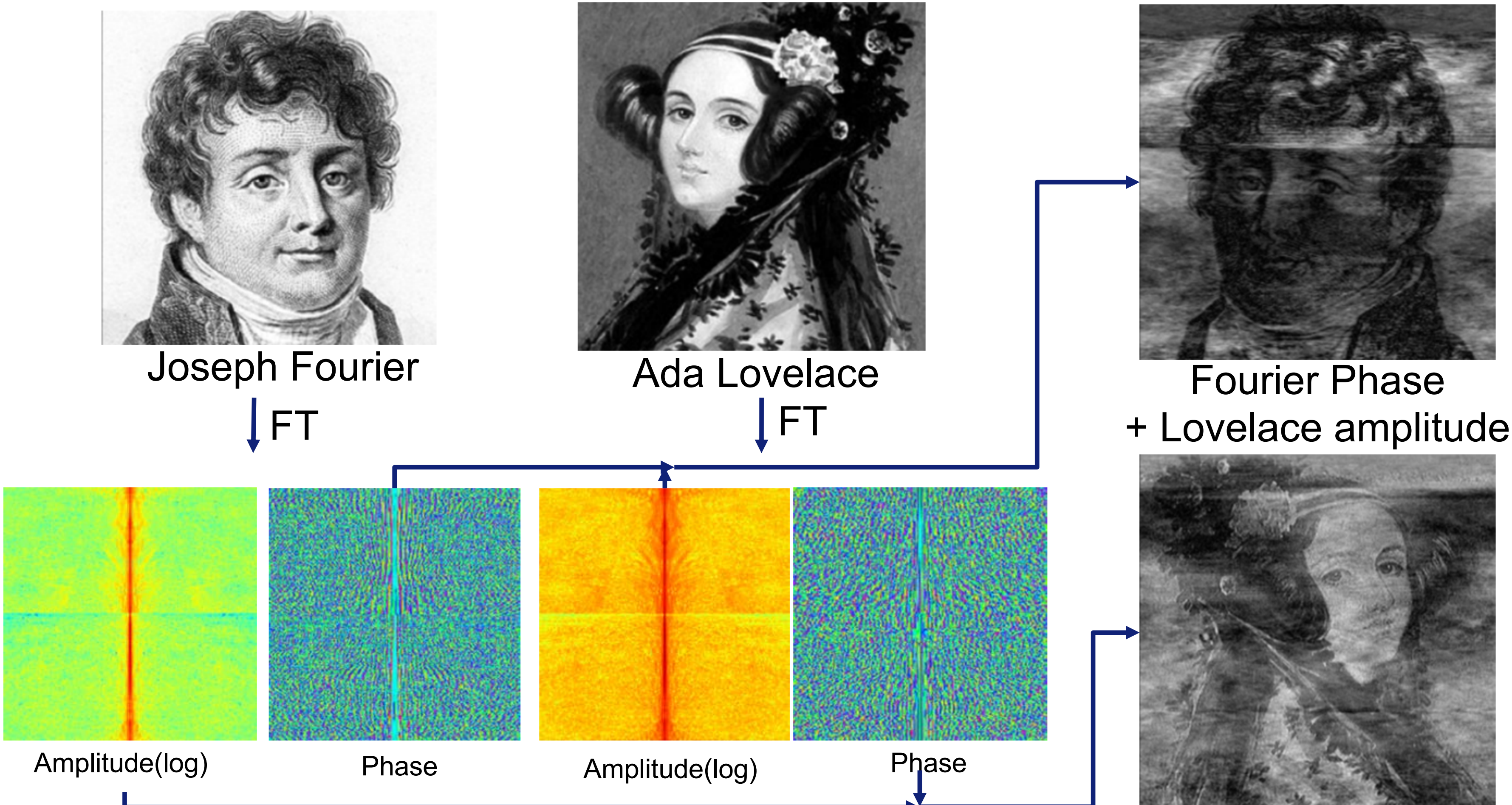


Object

The Phase problem

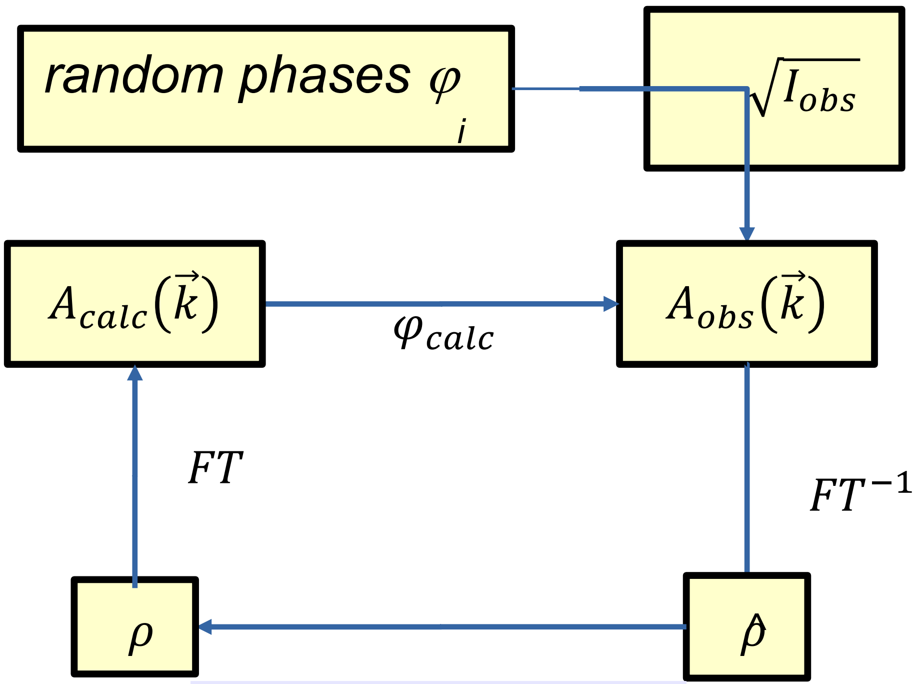
- Only the intensity is measured
- Complex algorithms required to reconstruct the object
- Iterative processes are used to yield the highest resolution

AMPLITUDE & PHASE



THE PHASE PROBLEM

To compute the inverse Fourier Transform, both the phase and the amplitude are needed
→ Phase Retrieval algorithms are required

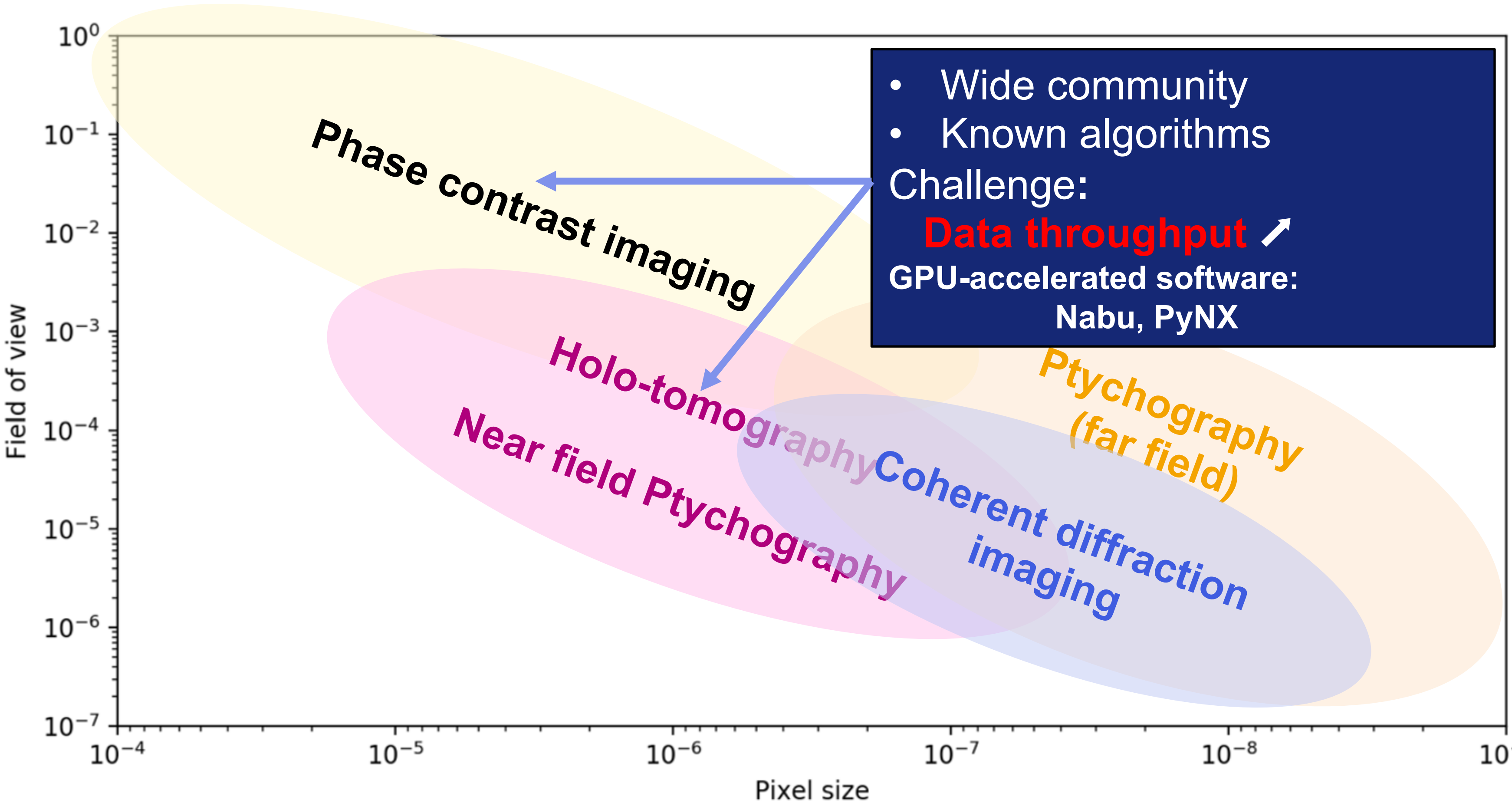


Density modification:
- Positivity (*)
- Finite support

Algorithms:
Hybrid Input/Output (HIO)
Error Reduction
Charge Flipping
....

NB : the **'Fourier recycling' algorithms** are essentially the same as those used to obtain electronic density from anomalous (or isomorphous) diffraction data for macromolecular crystallography.

IMAGING: FIELD-OF VIEW VS RESOLUTION



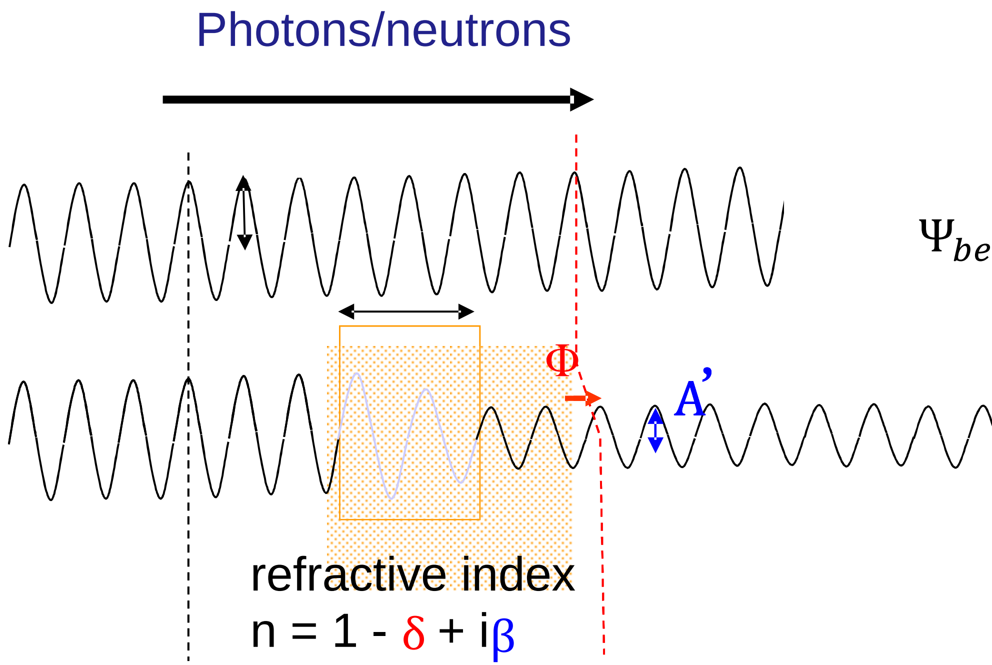
- Wide community
- Known algorithms

Challenge:

Data throughput ↗

GPU-accelerated software:
Nabu, PyNX

ATTENUATION VS PHASE CONTRAST

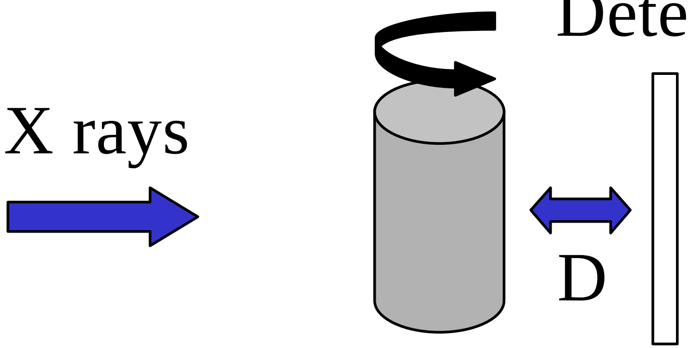


$$\Psi_{before} = Ae^{i\omega t-kx}$$

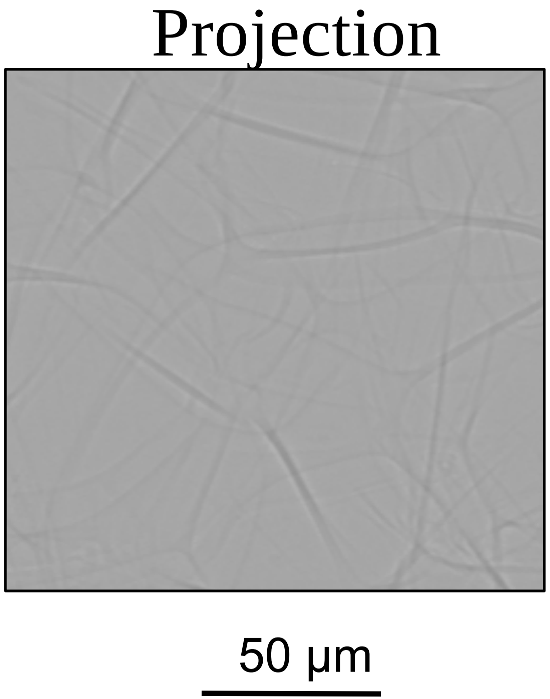
$$\Psi_{after} = \underbrace{Ae^{-2i\pi\frac{\delta}{\lambda}s}}_{\Phi}\ \underbrace{e^{-2\pi\frac{\beta}{\lambda}s}}_{A'/A}\ \Psi_{before}$$

real life:

PHASE CONTRAST IMAGING (NEAR FIELD / FRESNEL REGIME)



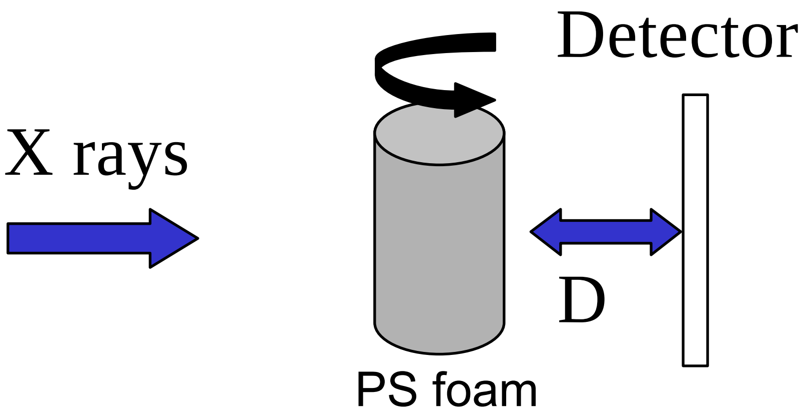
D increases → edge detection



Only absorption, faint contrast

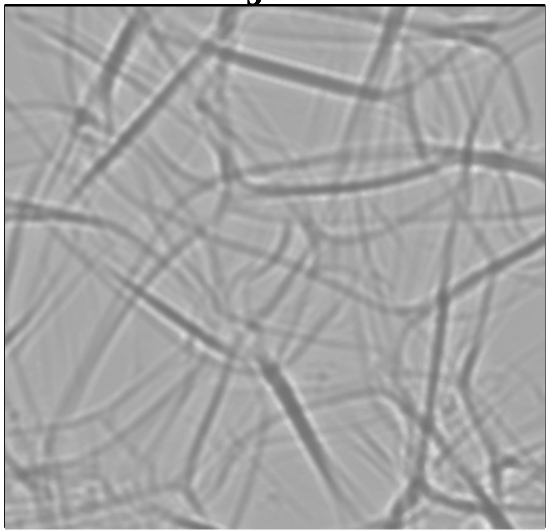
Slide from JY Buffiere

PHASE CONTRAST IMAGING (NEAR FIELD / FRESNEL REGIME)



D increases → edge detection

Projection

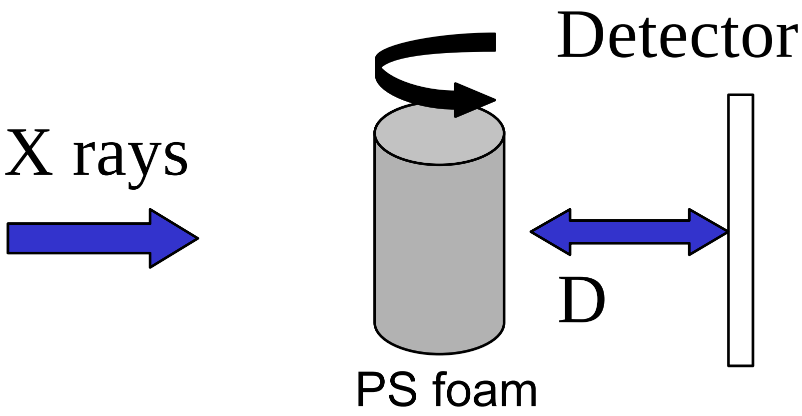


50 µm

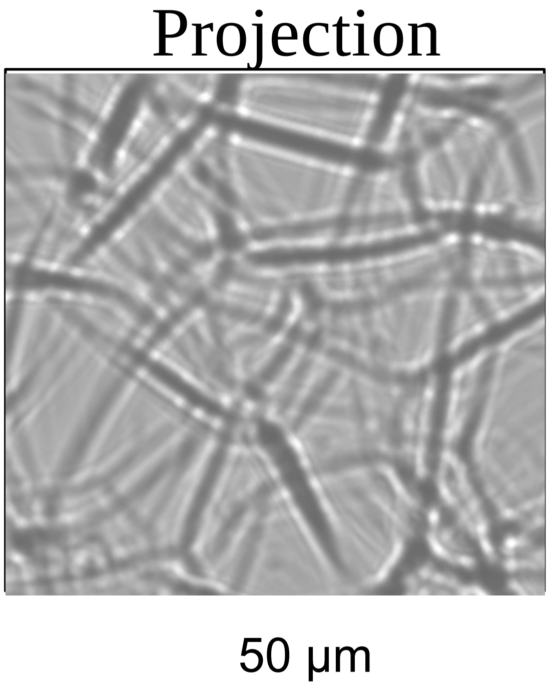
Better contrast

Slide from JY Buffiere

PHASE CONTRAST IMAGING (NEAR FIELD / FRESNEL REGIME)



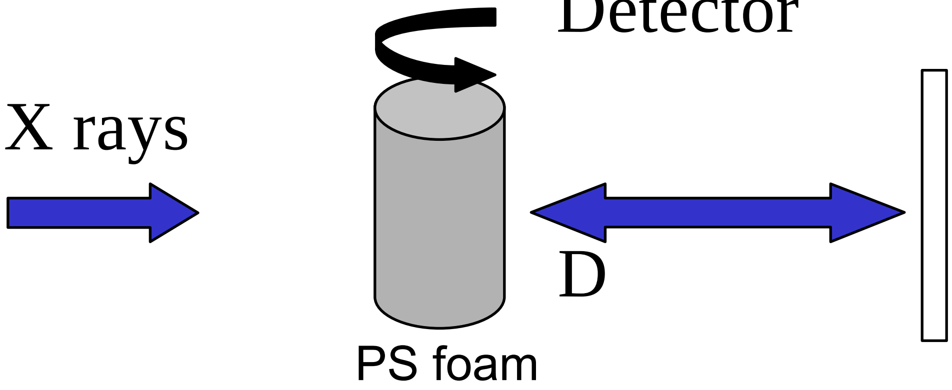
D increases → edge detection



Stronger contrast

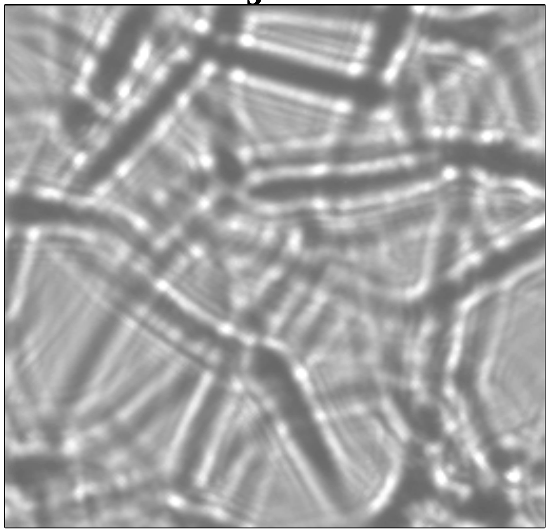
Slide from JY Buffiere

PHASE CONTRAST IMAGING (NEAR FIELD / FRESNEL REGIME)



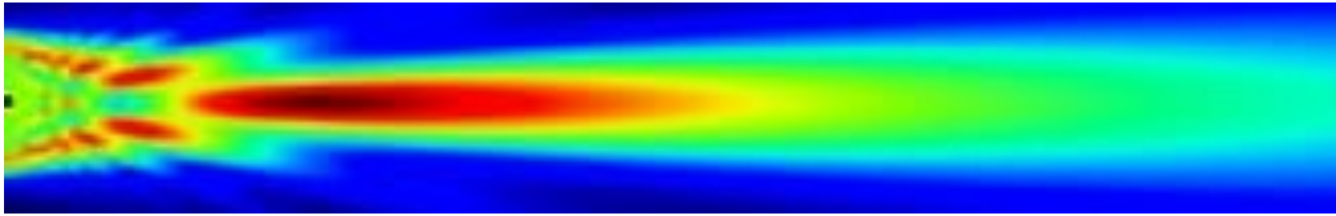
D increases → edge detection

Projection



Most contrast from phase

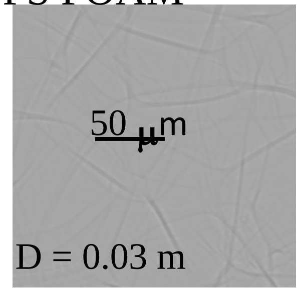
50 µm

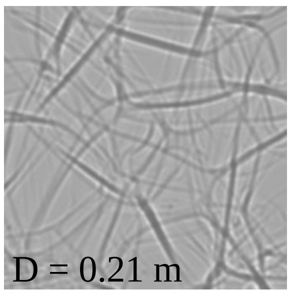


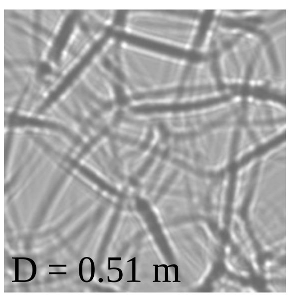
Slide from JY Buffiere

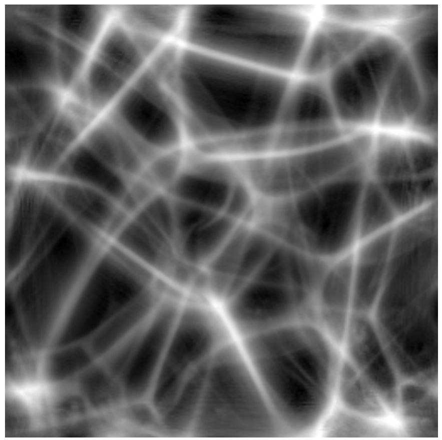
PHASE CONTRAST IMAGING: HOLOTOMOGRAPHY

PS FOAM









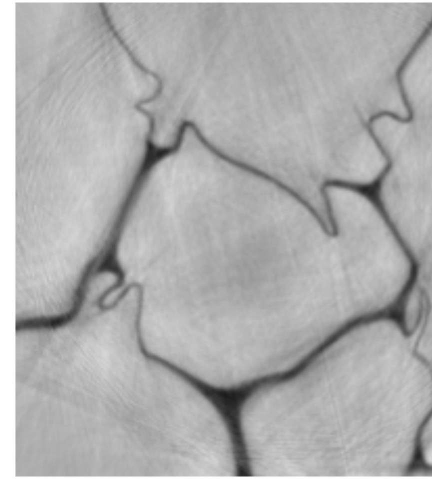
Phase retrieval

$\Delta\varphi = 2\pi\delta t/\lambda$

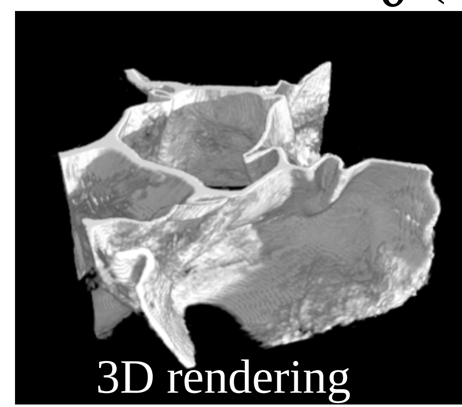
t : thickness

N projections →

tomographic reconstruction



Reconstruction of δ (r)



Cloetens et al, Applied Physics Letters 75, 2912 (1999)

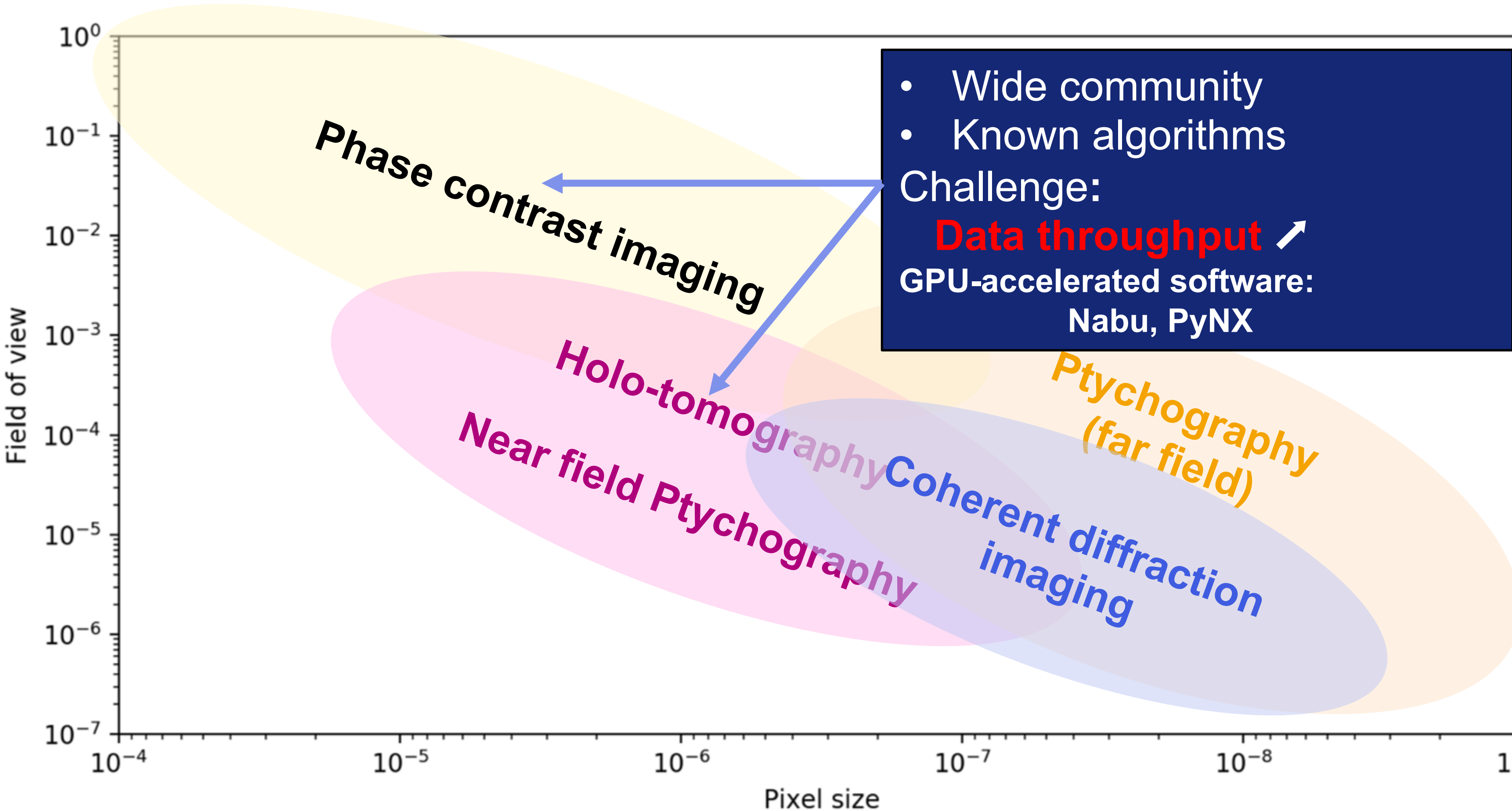
IMAGING: FIELD-OF VIEW VS RESOLUTION

- Wide community
- Known algorithms

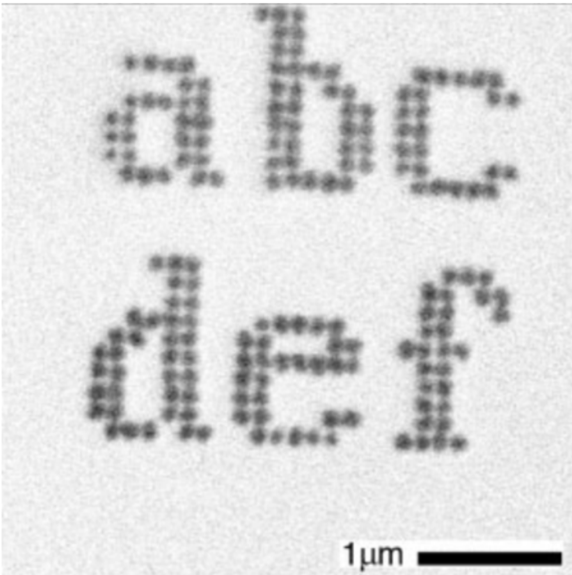
Challenge:

Data throughput ↗

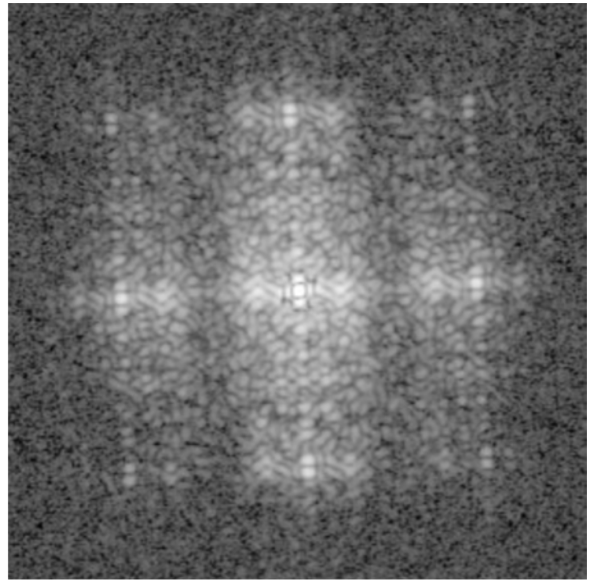
GPU-accelerated software:
Nabu, PyNX



COHERENT DIFFRACTION IMAGING



Gold dots



Diffraction image

Reconstruction

J. Miao, P. Charalambous, J. Kirz, and D. Sayre, Nature 400, 342 (1999).

WHY COHERENT DIFFRACTION IMAGING

?

Why use a method :

- Which is complex (experimentally : coherence)
- Where more than half the information (phase) is lost
- Where algorithms are not always robust

When there are simpler methods :

- Absorption imaging
- Phase contrast imaging
- Scanning microscopy

RESOLUTION

For scanning microscopy :

- Resolution = beam size

For phase contrast/absorption imaging :

- Resolution = pixel size
- With focusing optics (projection microscopy), down to a few 10’s of nm

WHY COHERENT DIFFRACTION IMAGING

?

Why use a method :

- Which is complex (experimentally : coherence)
- Where more than half the information (phase) is lost
- Where algorithms are not always robust

When there are simpler methods :

- Absorption imaging
- Phase contrast imaging
- Scanning microscopy

For CDI

The smaller the object, the wider its Fourier Transform !

→ The resolution is inversely proportionnal to the extent of the measured scattering in reciprocal space

→ lower current limit : 5-10 nm for CDI at 8-15 keV

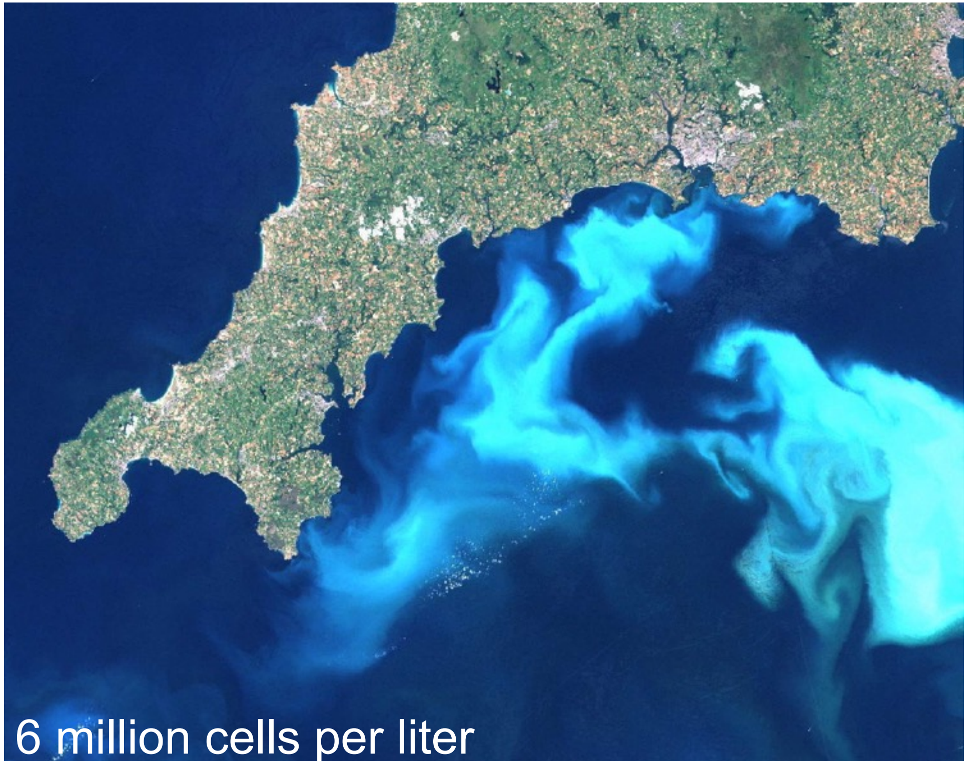
The resolution is smaller than the beam size → " **super-resolution** "

→ **High resolution studies and/or nano-objects**

MORPHOLOGY OF COCCOLITHS USING CDI

T. Beuvier[a,b], I. Probert[c], L. Beaufort[d], B. Suchéras-Marx[d], Y. Chushkin[b], F. Zontone[b] and A. Gibaud[a]

[a] LUNAM, IMMM, UMR 6283 CNRS, Faculté des Sciences 72085 Le MANS Cedex 09, France,
[b] EuropeanSynchrotron Radiation Facility, 71, avenue des Martyrs, 38000 Grenoble, France,
[c] CNRS, Sorbonne Uni-versité Pierre et Marie Curie (UPMC) Paris 06, FR2424, Roscoff Culture Collection, Station Biologiquede Roscoff, Place Georges Teissier, 29680 Roscoff, France,
[d] Aix Marseille Univ, CNRS, IRD, CollFrance, CEREGE, Aix-en-Provence, France.



Emiliania Huxleyi bloom south of cornwall (UK)

single-celled phytoplankton covered with calcite disks (coccoliths)

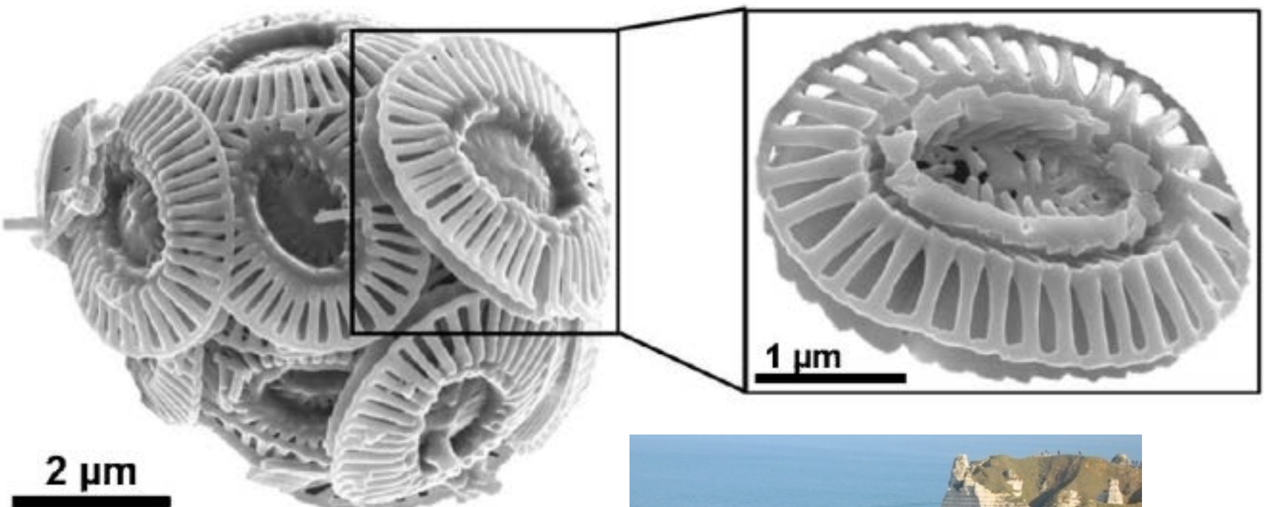
Landsat image from 24th July 1999, courtesy of Steve Groom, Plymouth Marine Laboratories.

MARINE ALGAE - COCCOLITHOPHORES

Emiliania huxleyi

Coccosphere

Coccolith



Hoffmann et al (2014)

Production is light dependent

1 per 2 hours

Calcite crystals $CaCO_3$

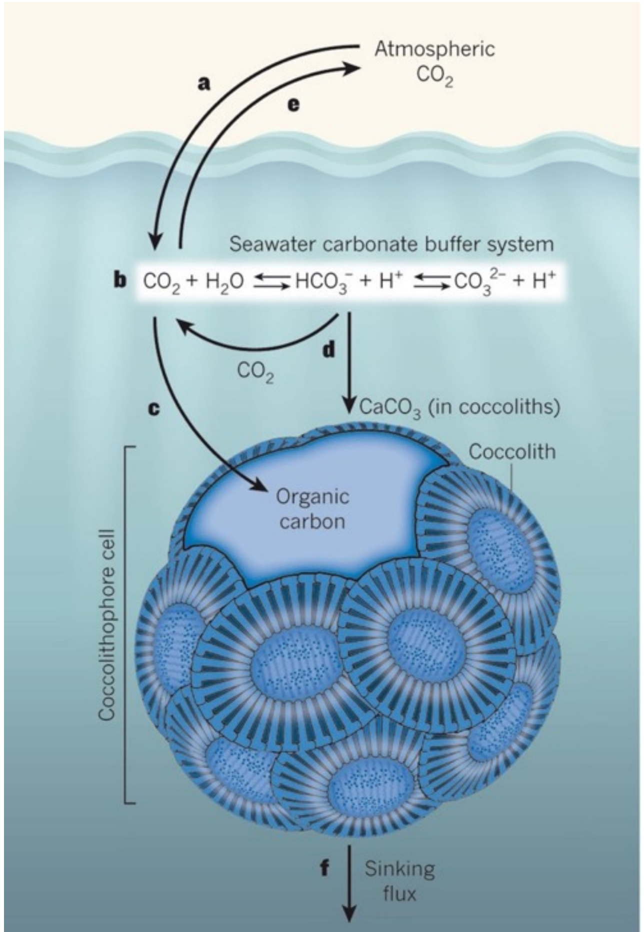
Coccoliths 1-10 µm big

10-20 coccoliths per coccosphere

Most important calcifying organisms

Slide: Y. Chushkin

COCCOLITHOPHORE CARBON CHEMISTRY



D. A. Hutchins Nature **476**, 41, (2011)

Transfer of CO_2 from atmosphere to limestone

Last 200 years absorbed 50% of CO_2 emitted by human activities (>500 Gt CO_2)

Pre-industrial atmospheric CO_2 280 ppm

Today atmospheric CO_2 380 ppm

pH decreased of 0.1 units since pre-industrial times
pH of sea water today 8.2±0.3

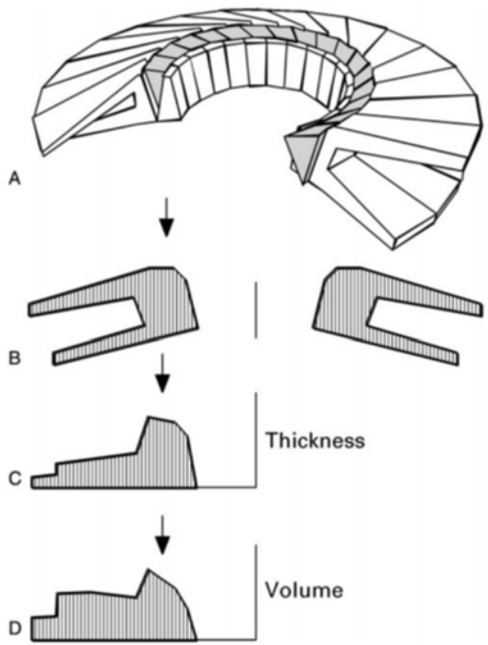
Calculating mass fluxes is major endeavour

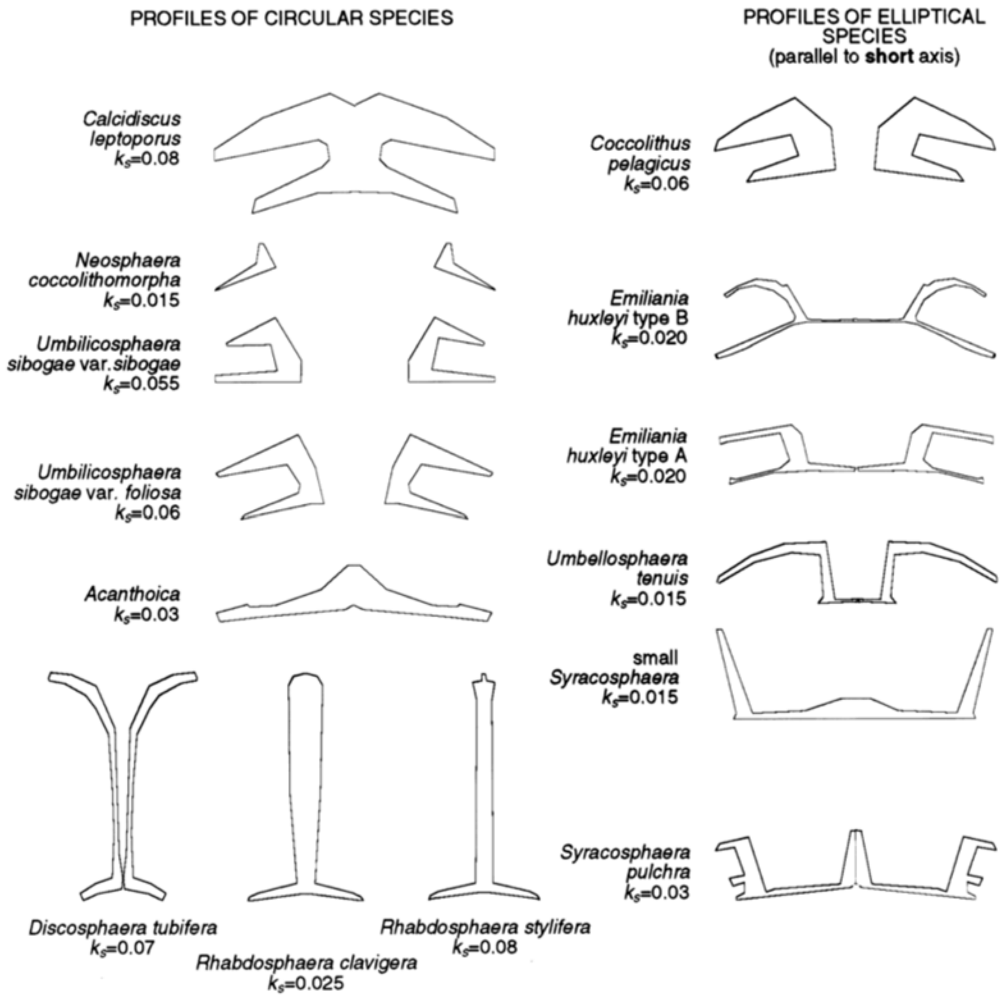
Slide: Y. Chushkin

COCCOLITHS MASS DETERMINATION – OPTICAL METHOD

$$m = \rho \cdot V \quad V = k_s \cdot l^3 \quad m = 2.7 \cdot k_s \cdot l^3$$

J.R. Young, P. Ziveri, Deep-Sea Research II, **47**, 1679, (2000)





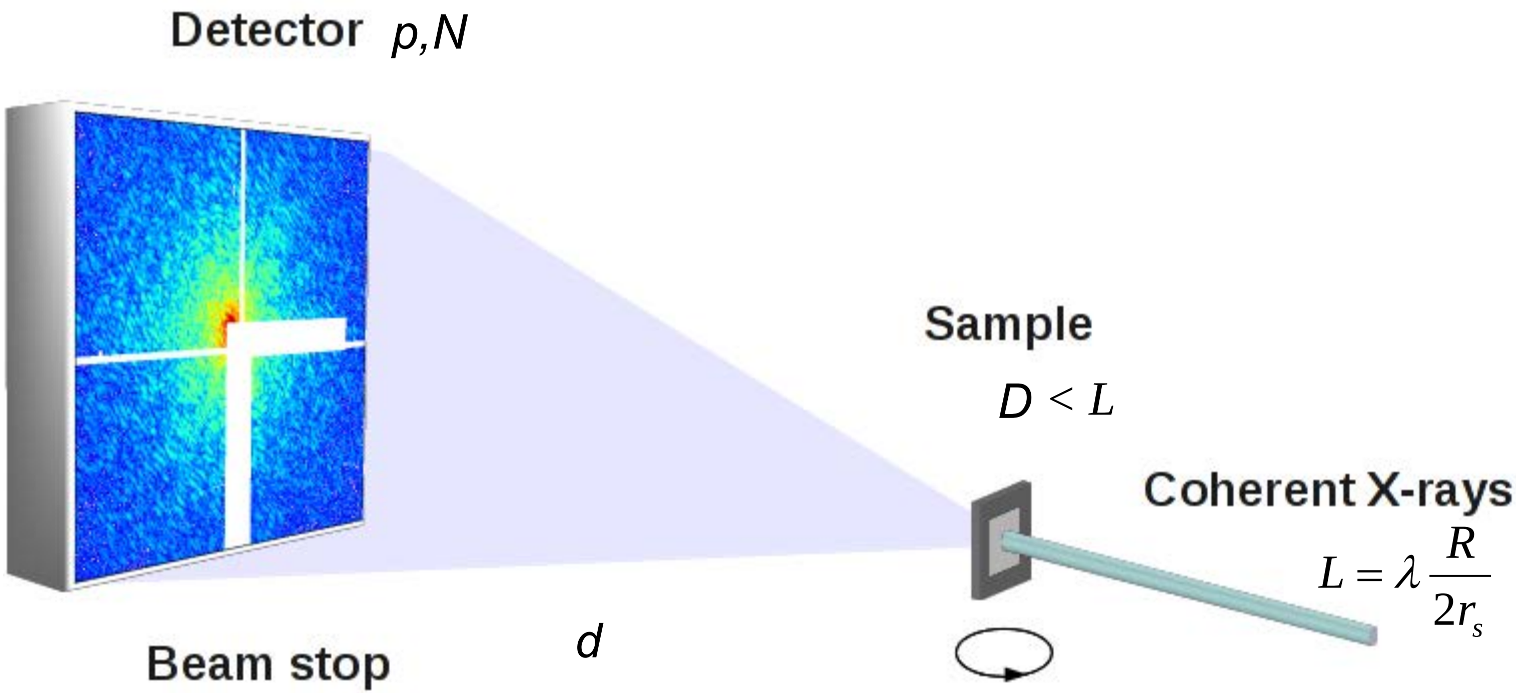
Cross-section determination

Mass estimation 50% accuracy

Slide: Y. Chushkin

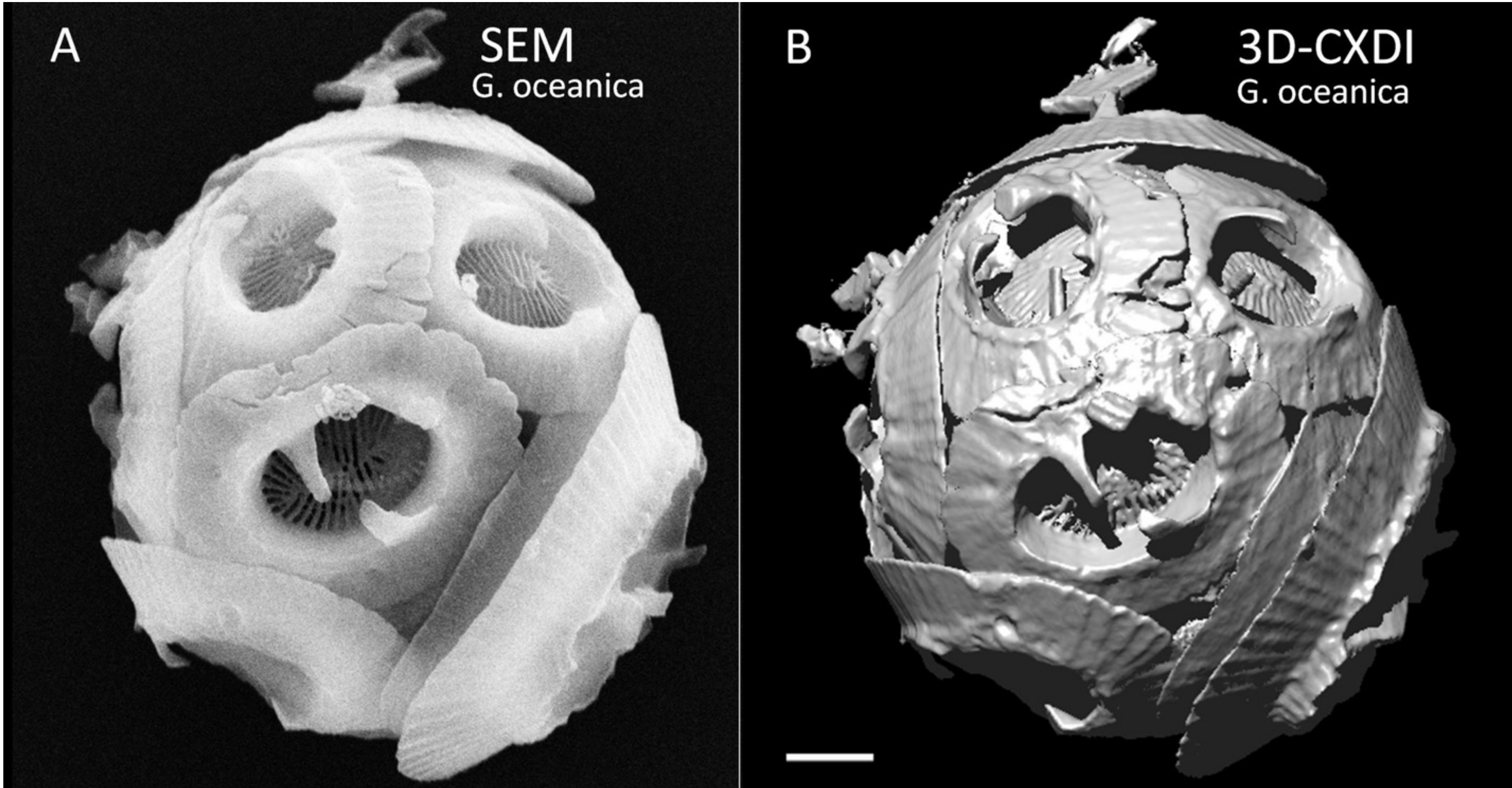
CXDI – ID1O BEAMLINE

Isolated sample <7 µm is illuminated with coherent plane wave
Voxel size < 32nm



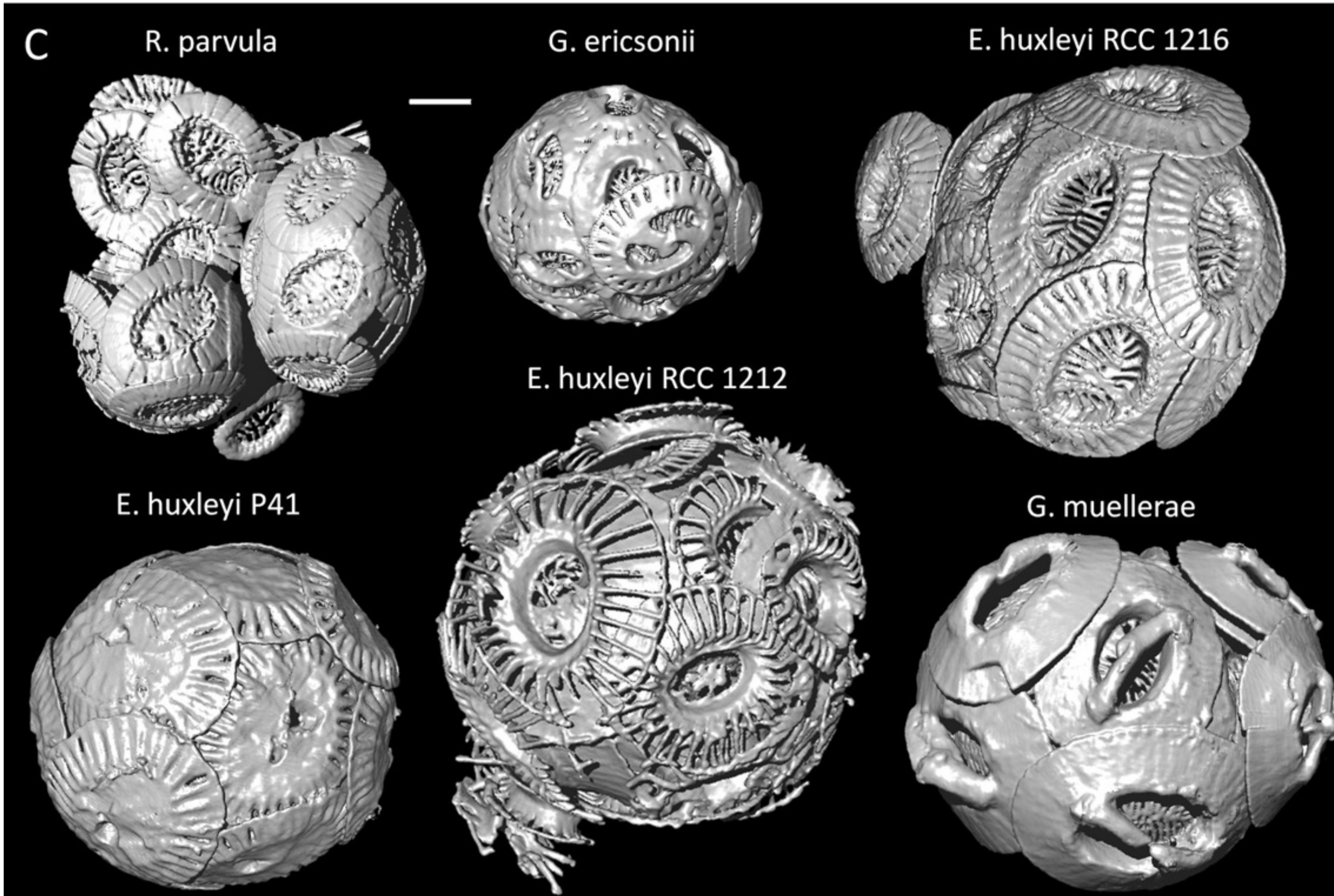
Slide: Y. Chushkin

3D-CXDI



Slide: Y. Chushkin

3D-CXDI

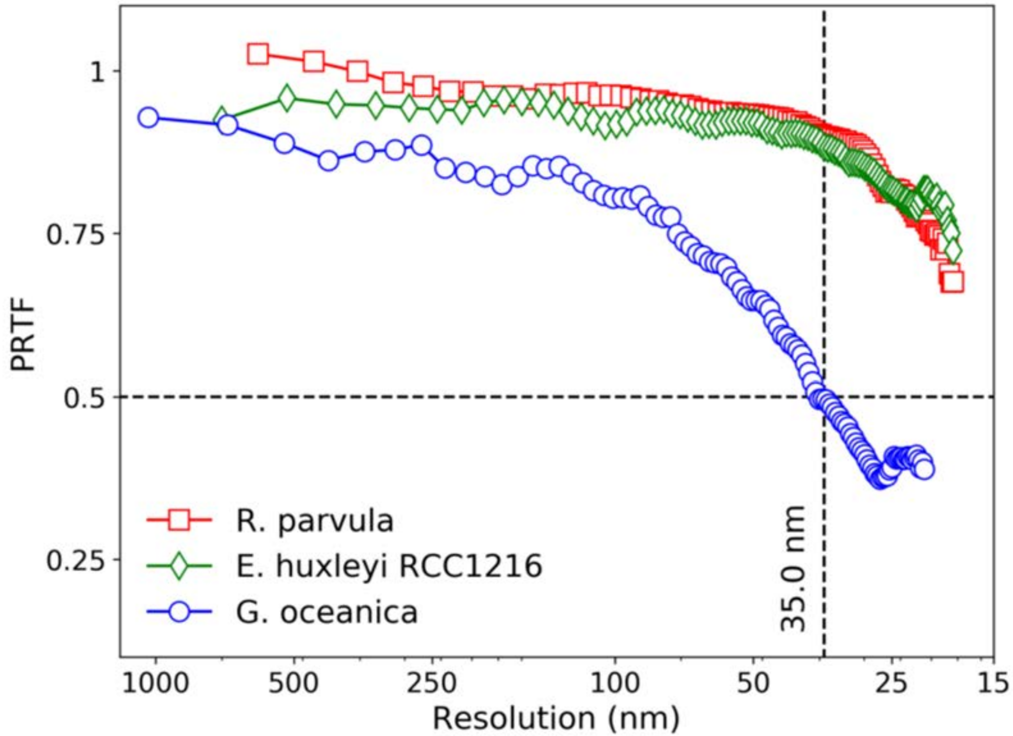


Slide: Y. Chushkin

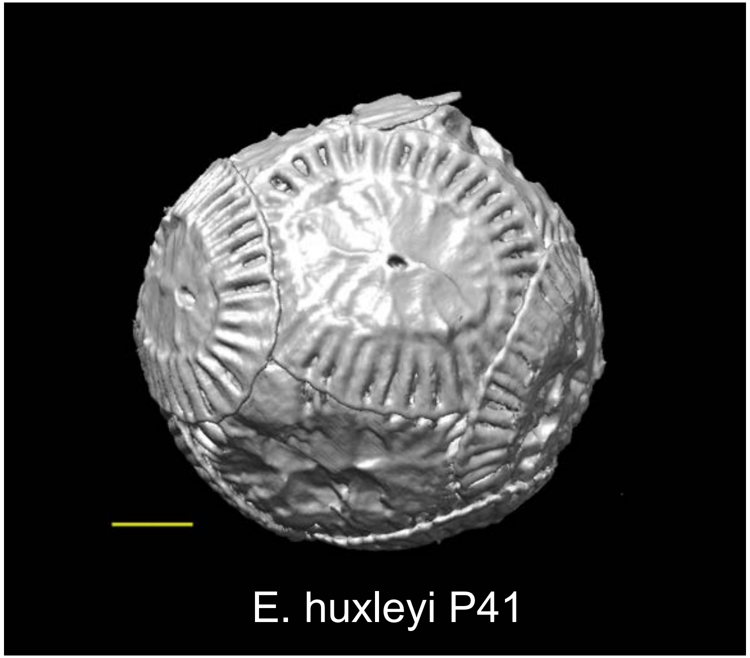
RESOLUTION

Phase retrieval transfer function

$$PRTF(f) = \frac{\sum_{f=const} A(f)}{\sum_{f=const} \sqrt{I(f)}}$$



Att 1 - 2 s exposure 1h full 3D data

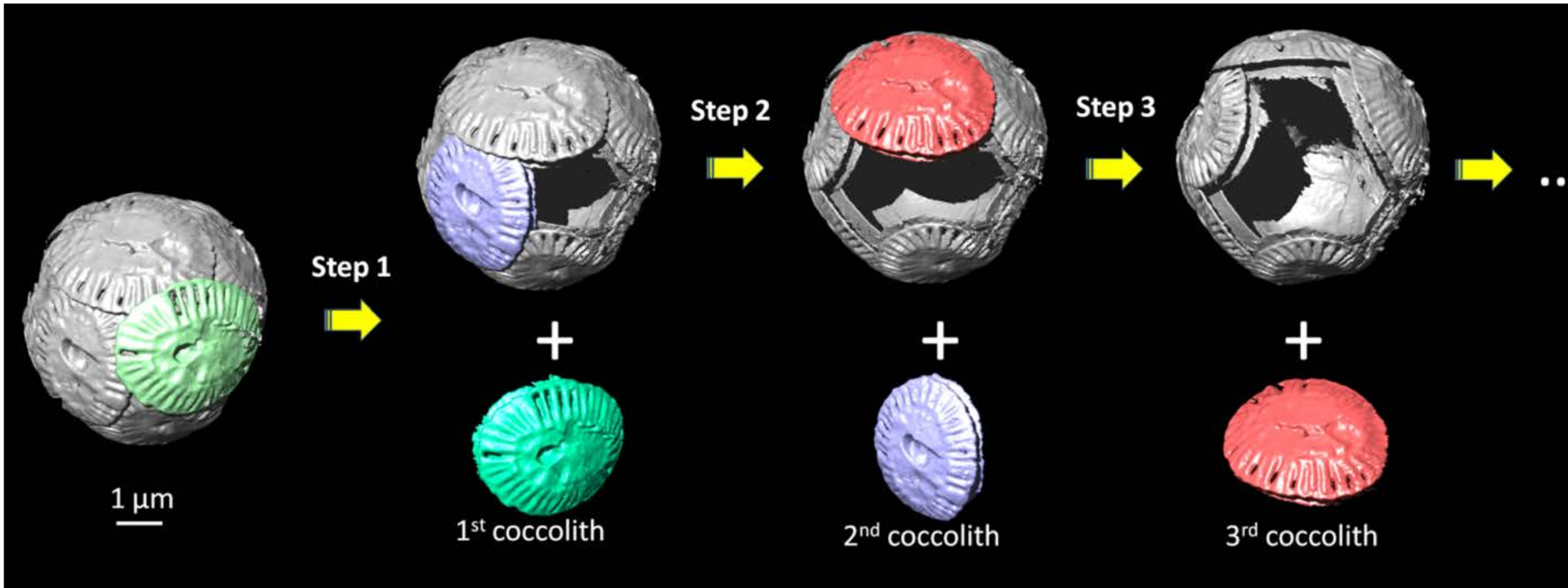


Voxel size 26-32 nm

Slide: Y. Chushkin

SEGMENTATION

E. Huxleyi RCC1216

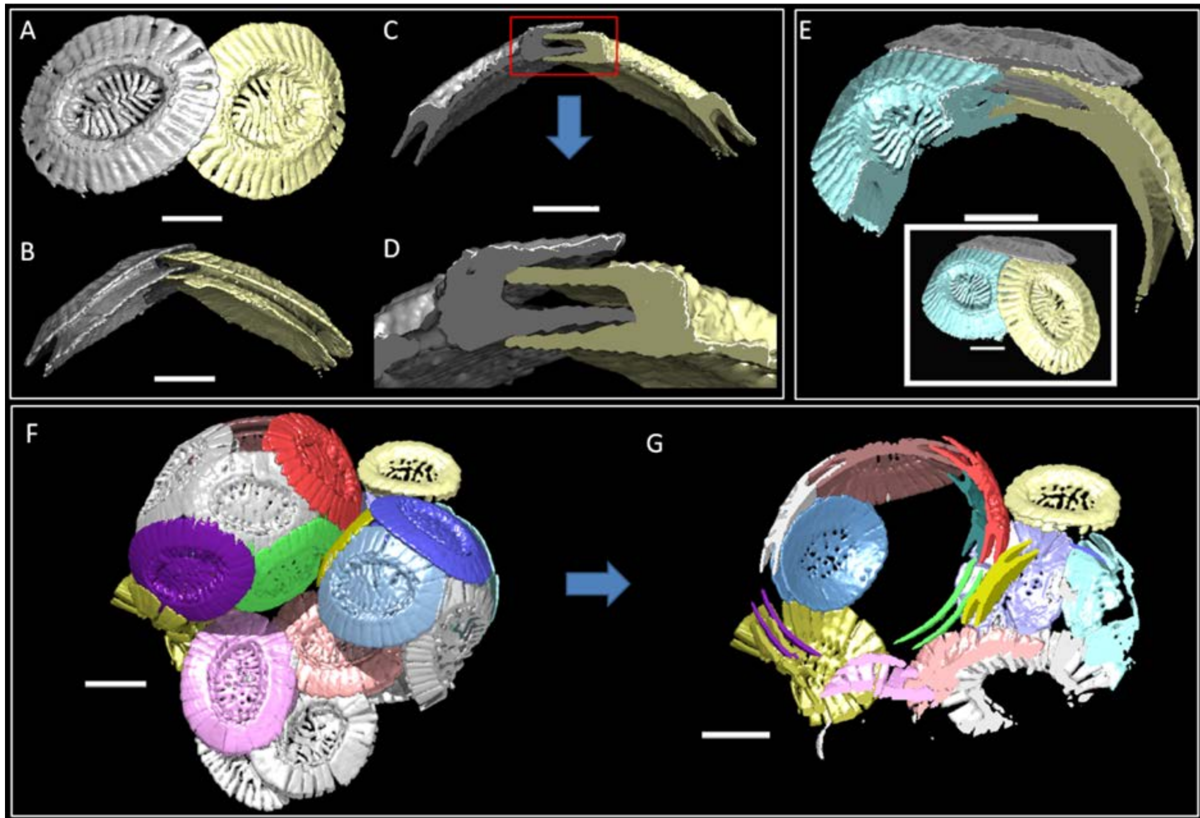


The European Synchrotron | ESRF

Slide: Y. Chushkin

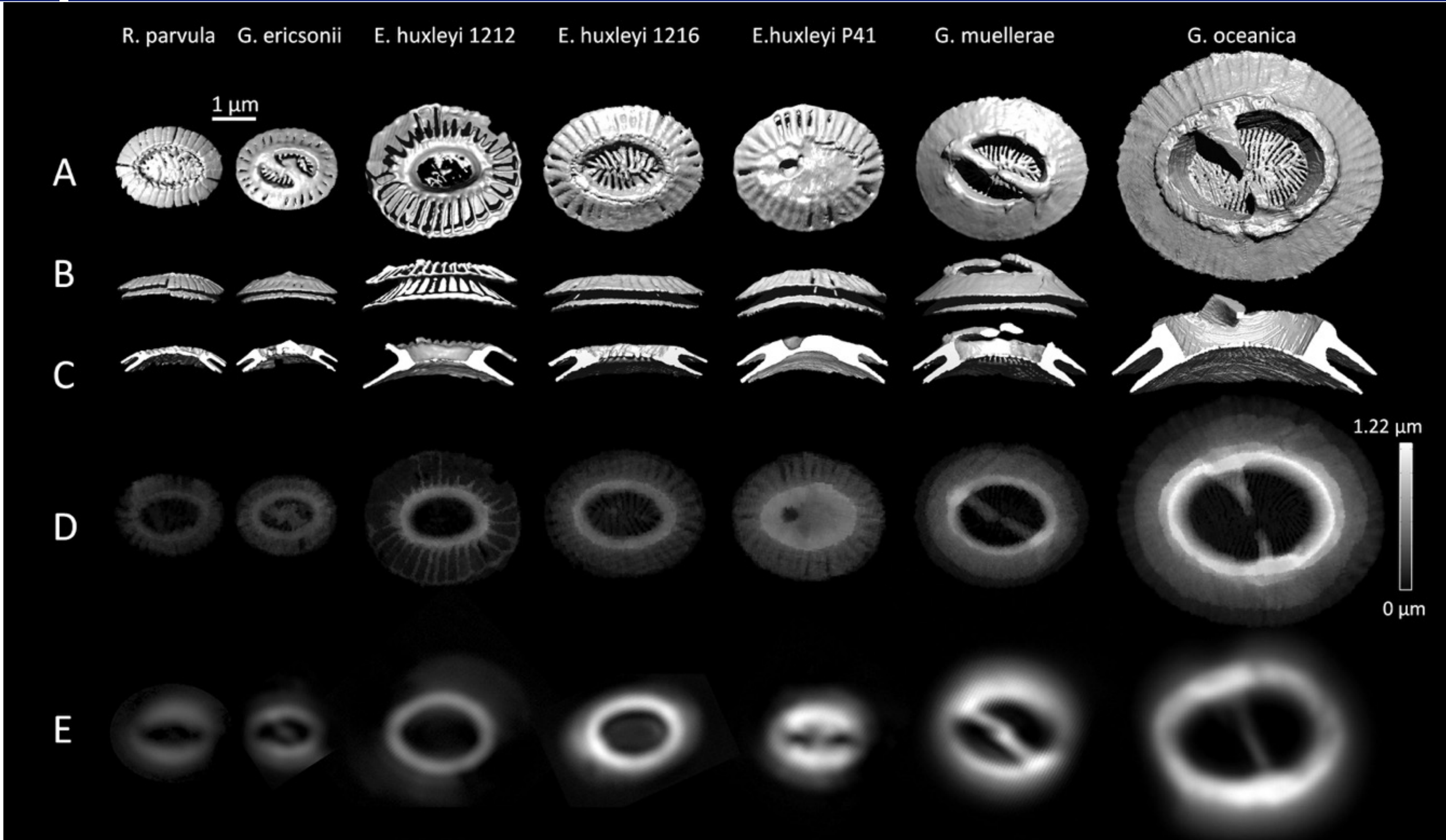
SEGMENTATION

E. Huxleyi RCC1216



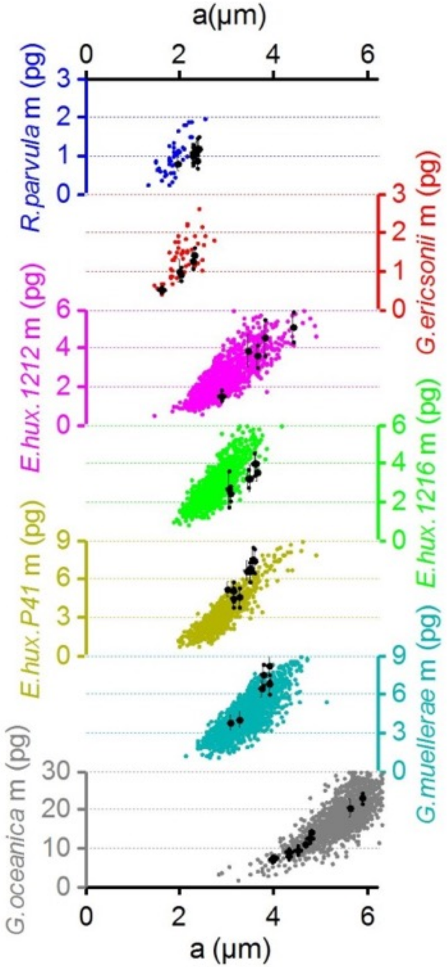
Slide: Y. Chushkin

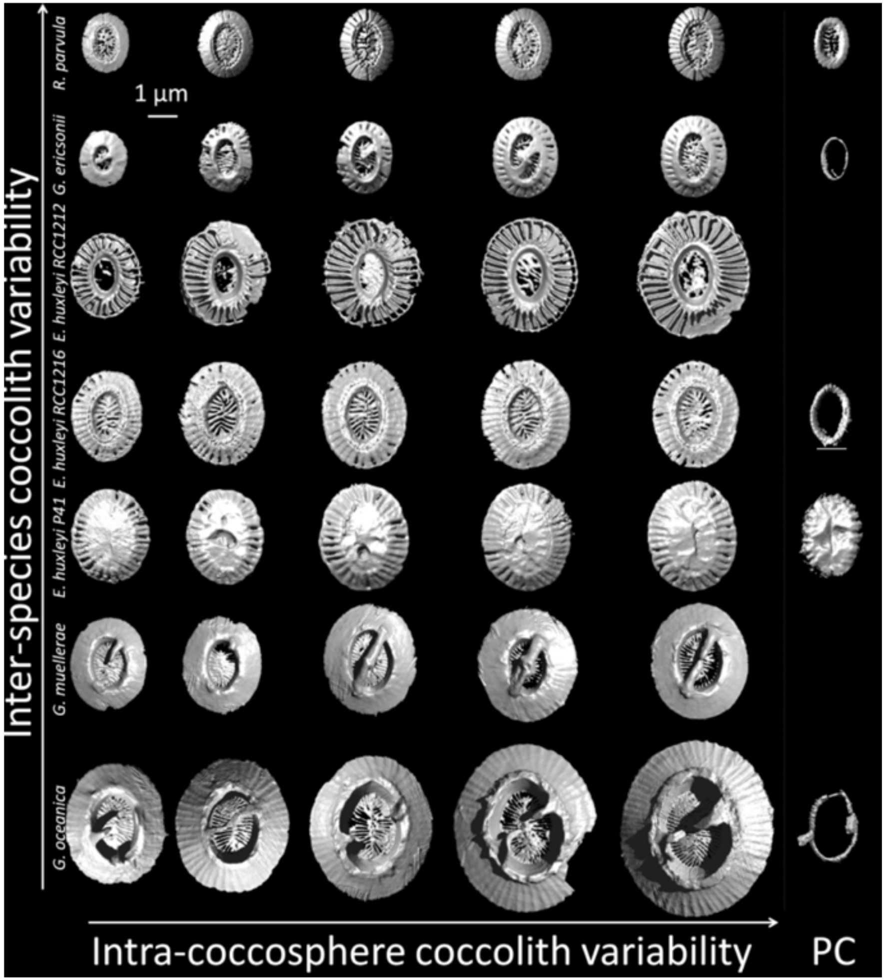
COCCOLITHS



Slide: Y. Chushkin

COCCOLITHS - MASS

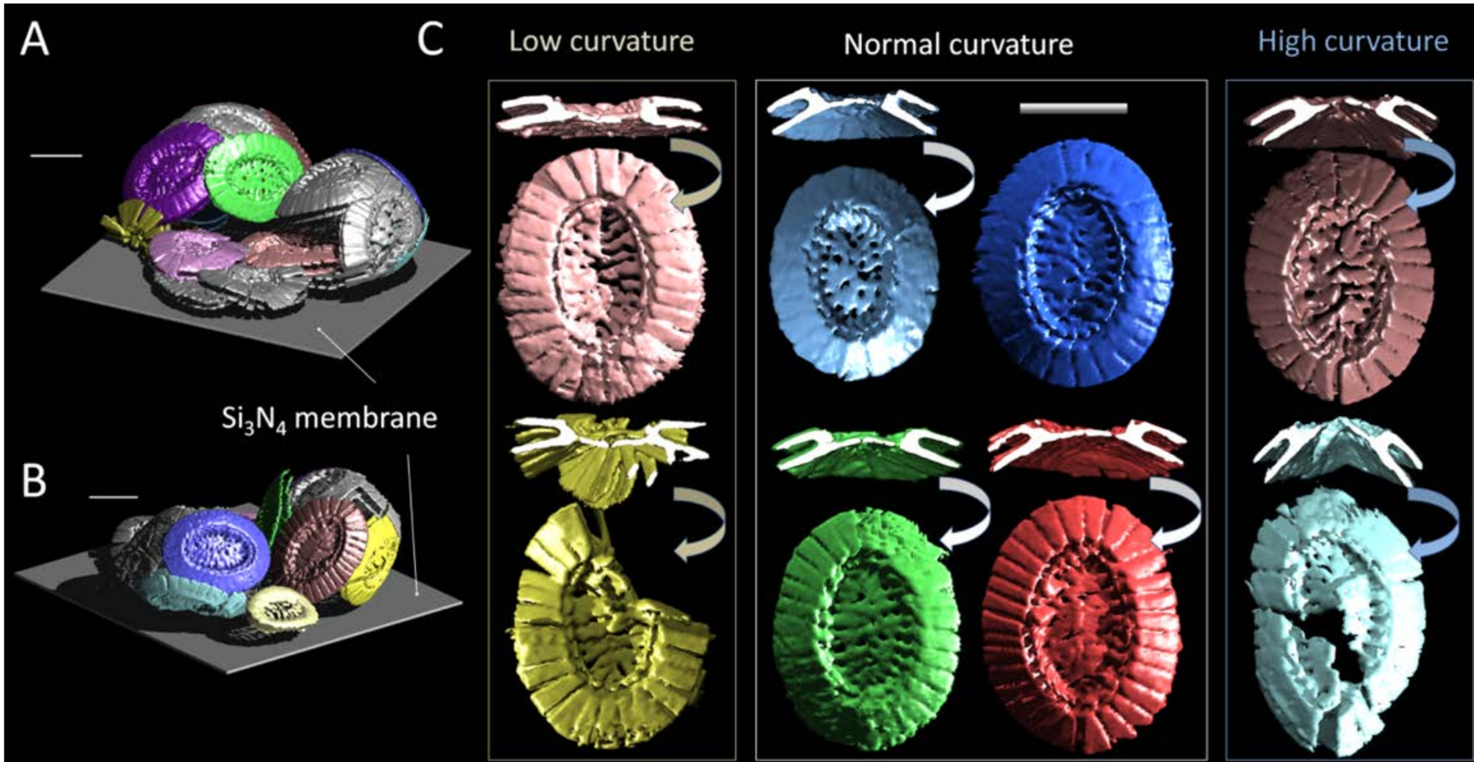




Slide: Y. Chushkin

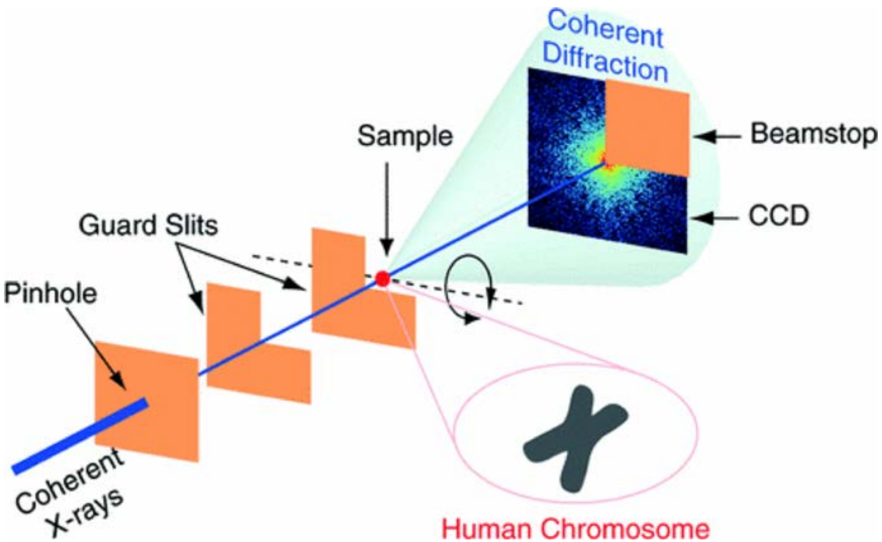
COCCOLITHS DEFORMATION

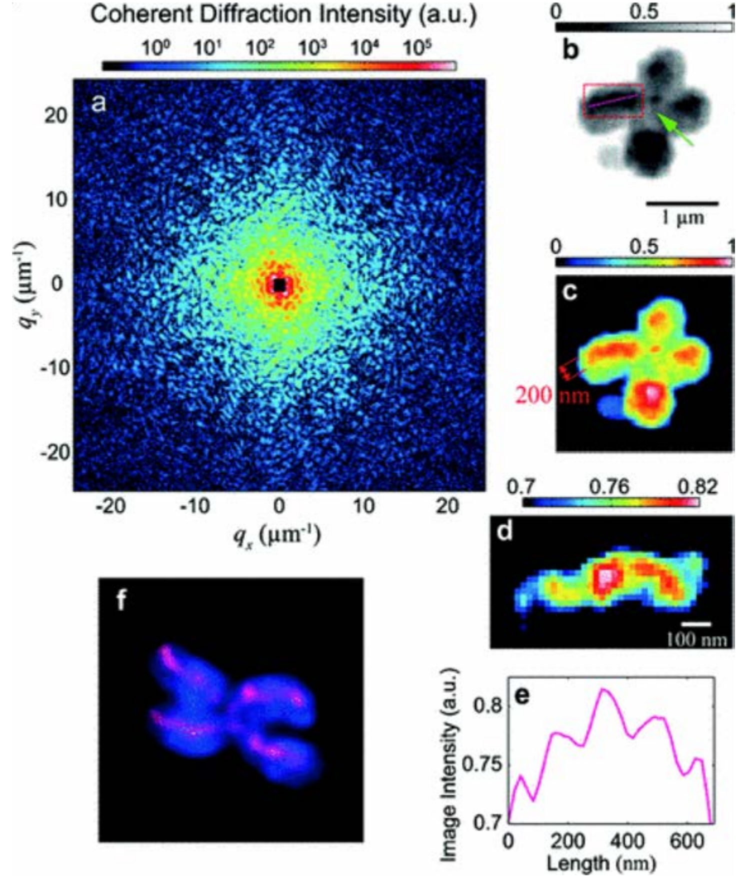
R. parvula



Slide: Y. Chushkin

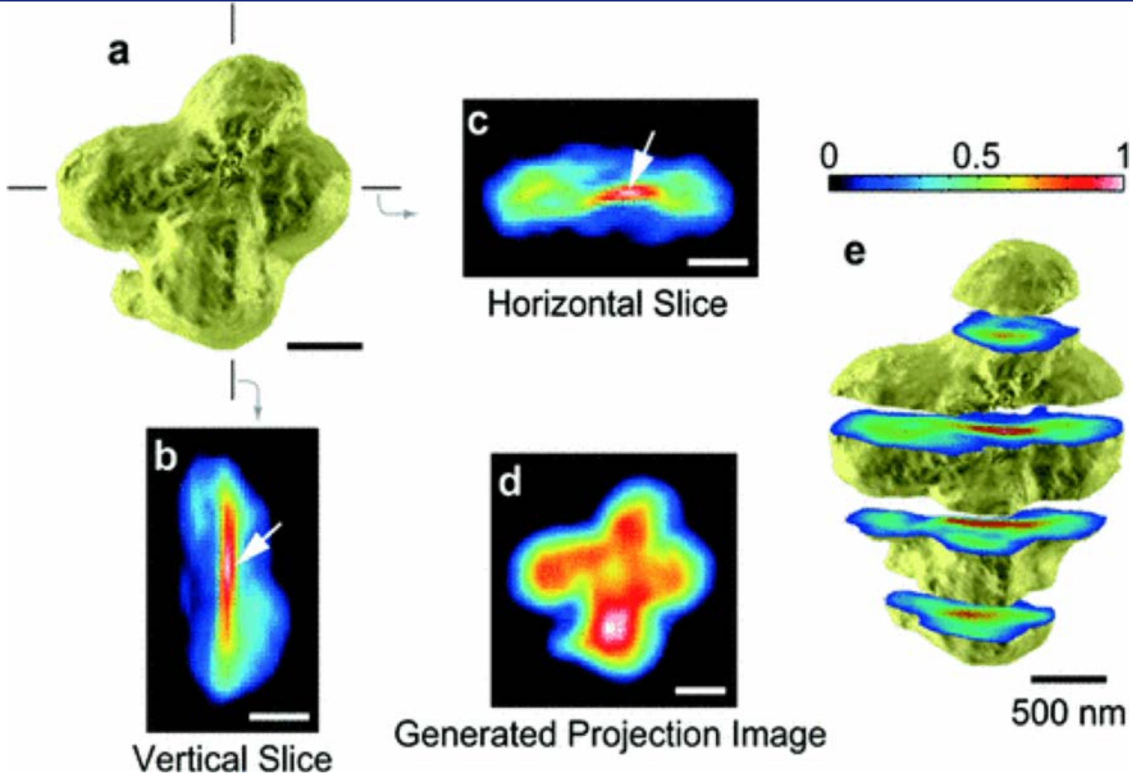
CDI: CHROMOSOME





Y. Nishino et al, Physical Review Letters 102, (2009).

CDI: CHROMOSOME



Reconstructed 3D structure :

- 2D resolution : 38 nm
- 3D resolution : 120 nm
- Dose : 2x10^10 Gy

Y. Nishino et al, Physical Review Letters 102, (2009).

Limitations of CDI :

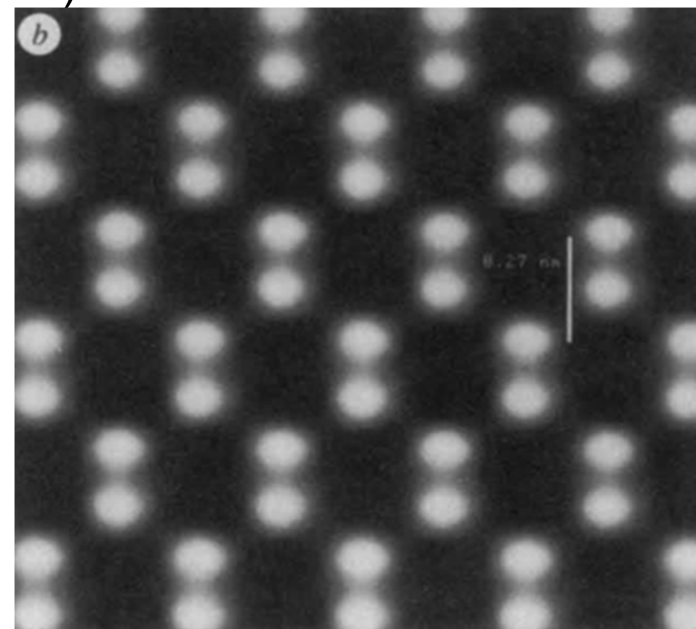
- No imaging of extended objects (limited to the coherent volume of the beam)
- Need oversampled diffraction data
- Convergence of the algorithm can be difficult (support evaluation)
- The probe (amplitude and phase of the incoming beam) is unknown
- Non-unicity of the solution

First experiments from electron microscopy :

Hoppe, Acta Cryst. A25 (1969) 459
Hoppe, Ultramicroscopy 10, 187 (1982)

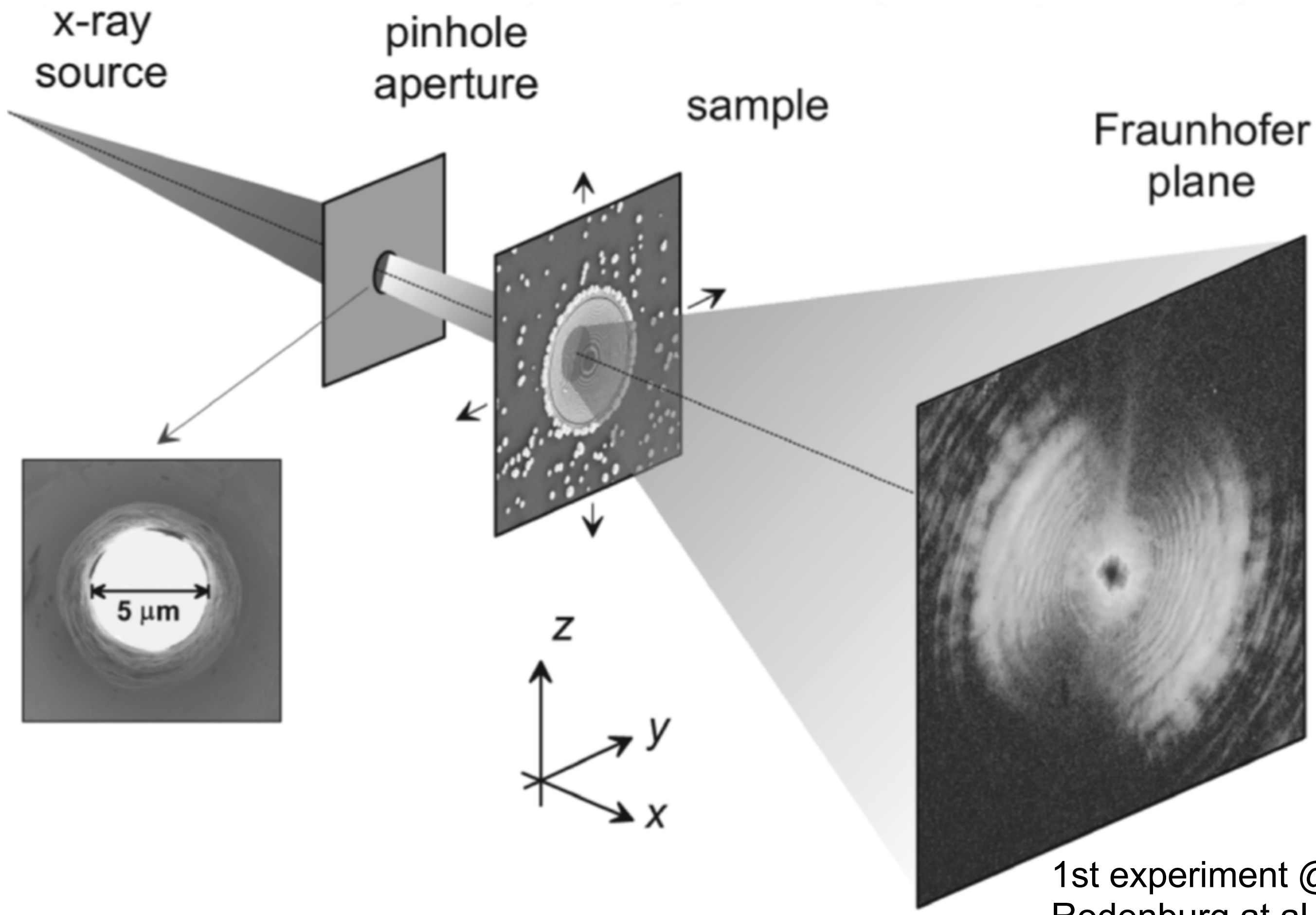
Nellist, McCallum & Rodenburg Nature A54 (1995) 49

“ Resolution beyond the 'information limit' in transmission electron microscopy ”



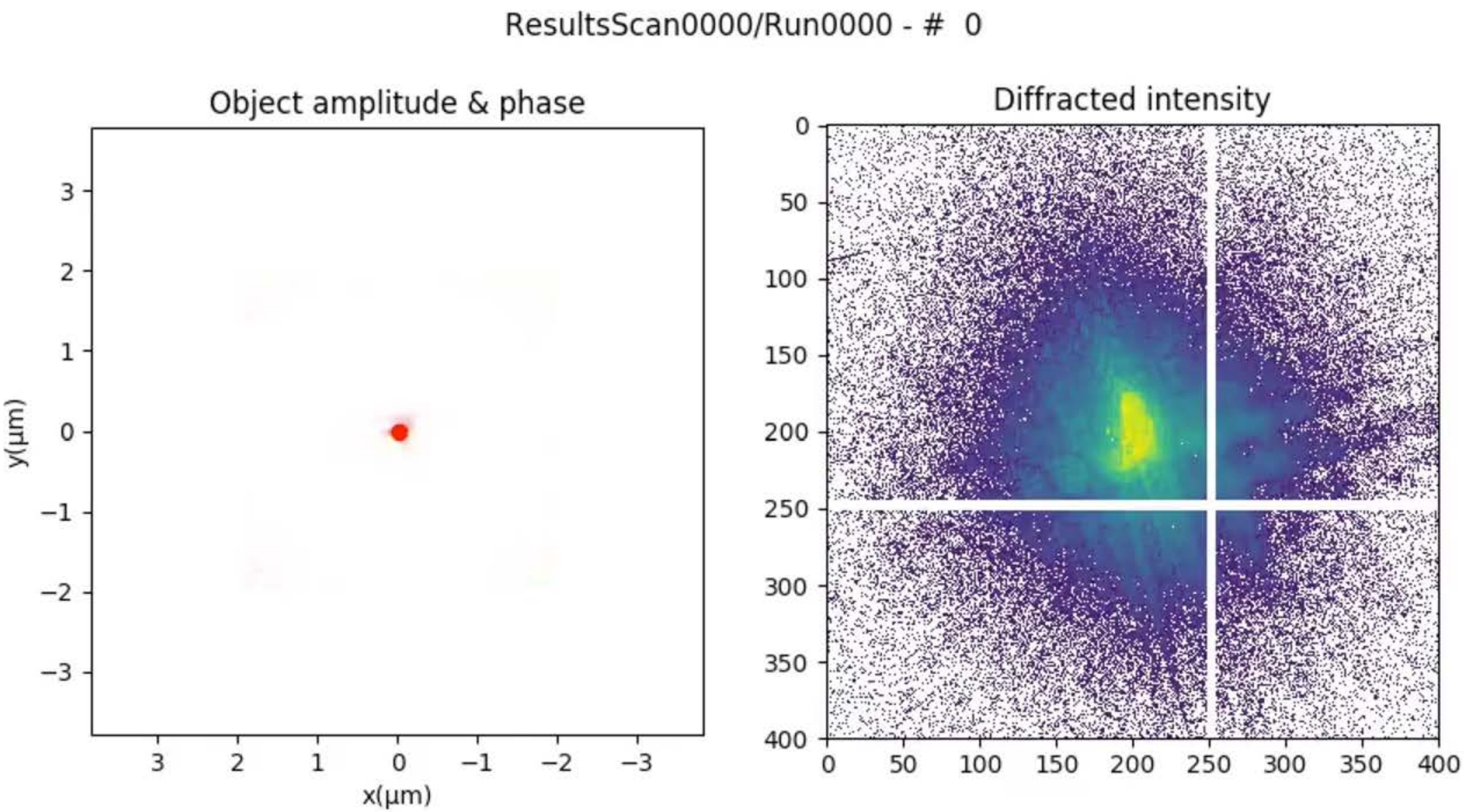
Silicon reconstruction along [110]

X-RAY PTYCHOGRAPHY



1st experiment @PSI
Rodenburg at al, PRL 98, 034801 (200

PTYCHOGRAPHY



PTYCHOGRAPHY ANALYSIS WITH PYNX

Analysis is possible using https://jupyter-slurm.esrf.fr
Remote access to notebooks & compute cluster

jupyter-slurm.esrf.fr/user/favre/notebooks/pynx-private/pynx/ptycho/examples/position-optim-CXI-Copy1.ipynb

jupyterhub position-optim-CXI-Copy1 Last Checkpoint: 34 minutes ago (autosaved)

File Edit View Insert Cell Kernel Widgets Help

Run Code

Notebook: Ptychography reconstruction with positions update from a CXI dataset

This notebook uses the the runner API (`pynx.ptycho.runner`) to load the data and prepare the optimisation.

This is what is used for the command-line scripts, here we just grap the Ptycho object from the runner.

This uses a dataset recorded on id01@ESRF, which exhibits some position distortions near the ceneter of the spiral scan.

In [ ]:

```
# Select language and/or GPU name or rank through environment variable (optional)
#import os
#os.environ['PYNX_PU'] = 'cuda.0'

%matplotlib notebook
import matplotlib.pyplot as plt
from pynx.ptycho import simulation, shape

# Import Ptycho, PtychoData and operators (automatically selecting OpenCL or CUDA)
from pynx.ptycho import *

# Import CXI runner
from pynx.ptycho.runner.cxi import PtychoRunnerScanCXI
from pynx.ptycho.runner.runner import params_generic as params

# This can be used to have a wide screen for the notebook
from IPython.core.display import display, HTML
display(HTML("<style>.container { width:90% !important; }</style>"))
```

Load CXI data

dataset is available from the PyNX ESRF public folder

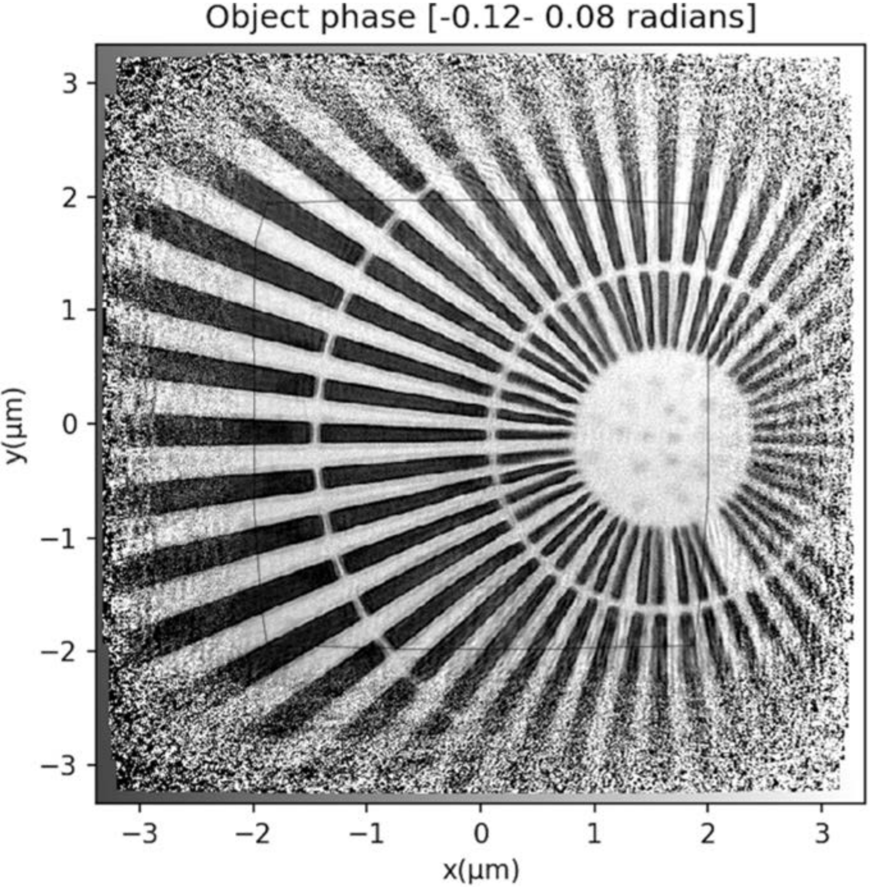
In [ ]:

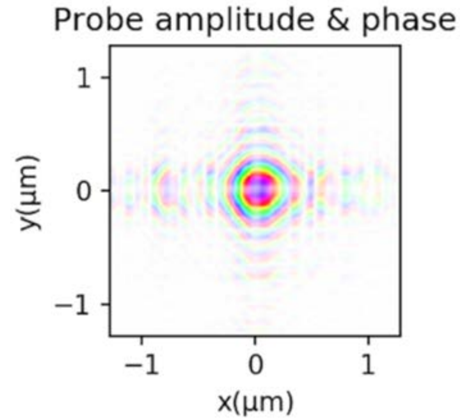
```
if not os.path.exists('ptycho-siemens-star-id01.cxi'):
    os.system('curl -O http://ftp.esrf.fr/pub/scisoft/PyNX/data/ptycho-siemens-star-id01.cxi')
```

Load the data & setup the runner parameters

As we are using the `pynx.ptycho.runner` API, we can setup the parameters exactly as for the command-line scripts

PTYCHOGRAPHY: PHASE & AMPLITUDE

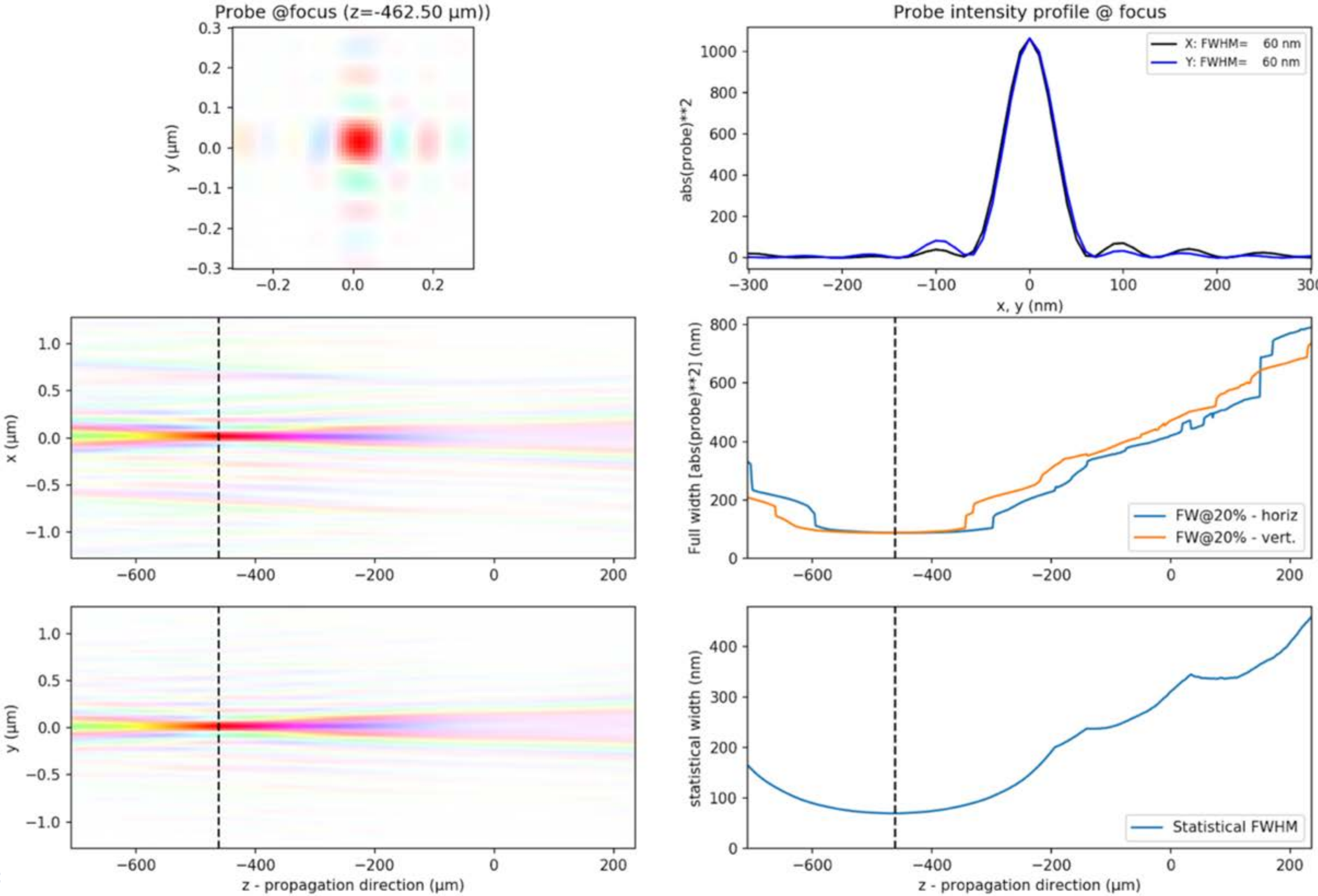




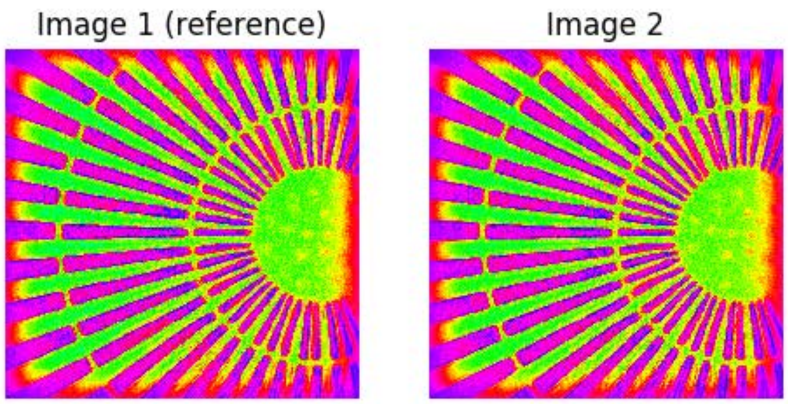
id16A @17keV
Lambda detector 256x256 GaAs
150 nm step, 125 ms/frame, 566 frames
With filters (~20x) ☹

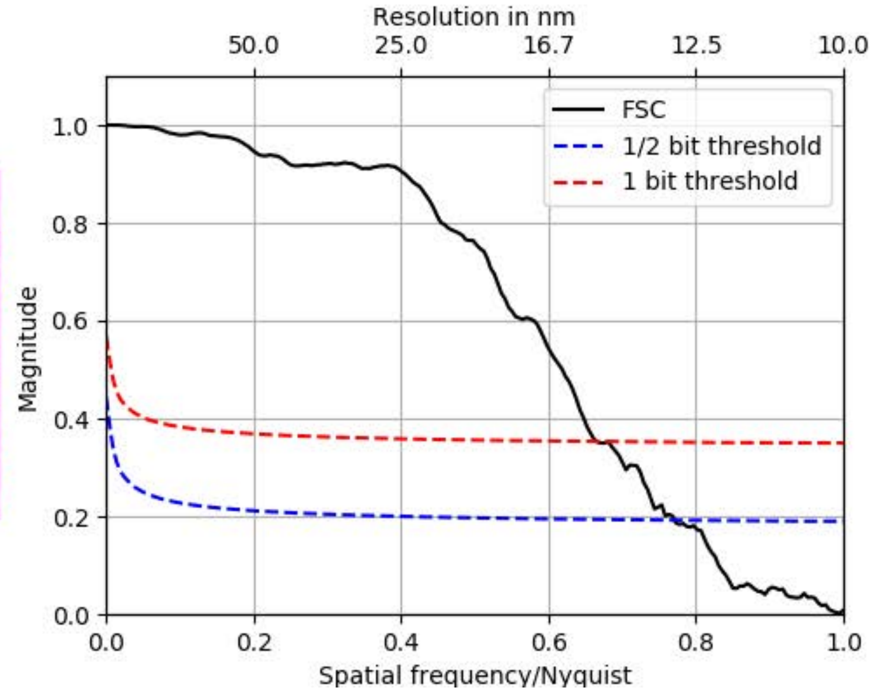
Both object and probe, amplitude and phase are recovered at the same time

PTYCHO: PROBE PROPAGATION



RESOLUTION: FOURIER SHELL (RING) CORRELATION



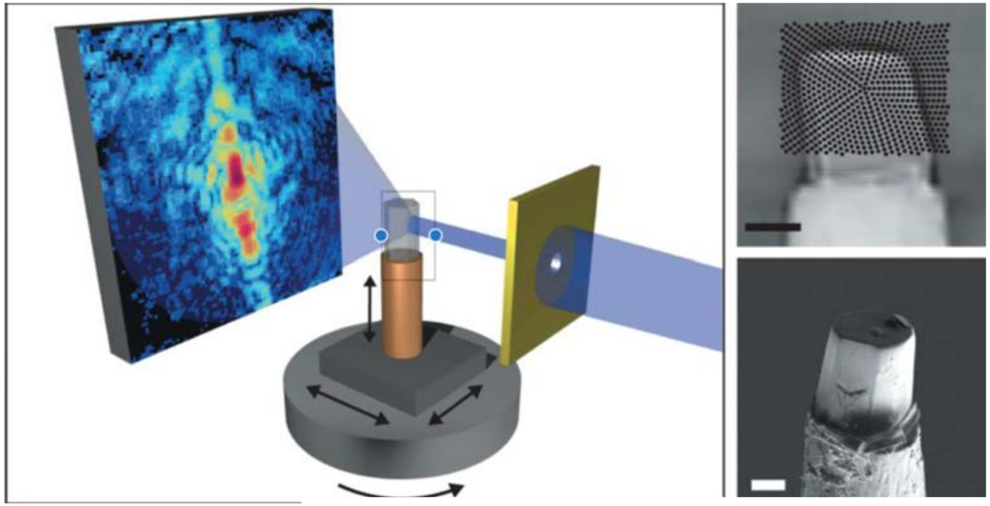


Resolution from Fourier shell (ring) correlation: ~15nm

(comparing two scans from the same area with different positions)

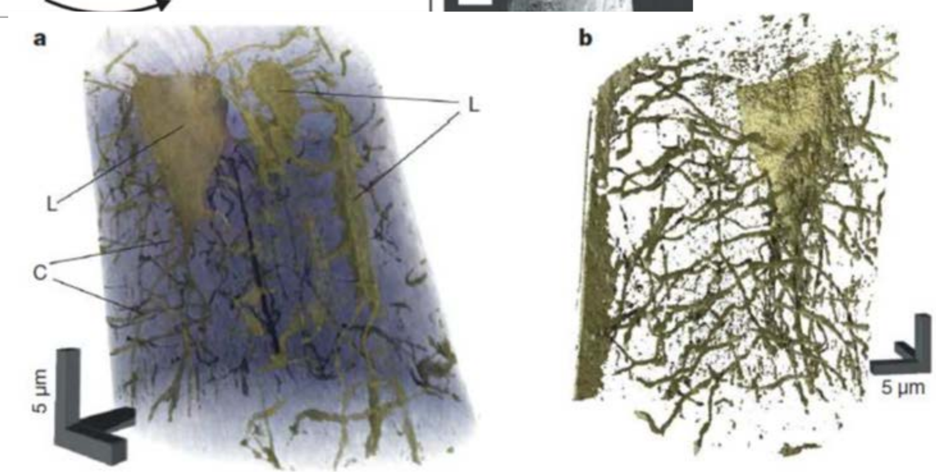
van Heel & M. Schatz, J. Struct. Biol. 151(2005), 250

PTYCHOGRAPHY-TOMOGRAPHY

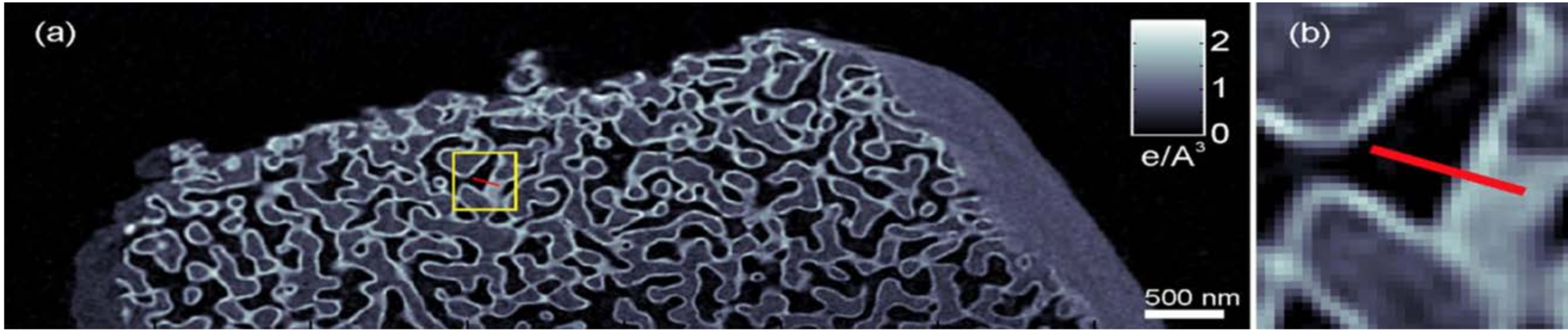


Experiments at cSAXS beamline SLS
Dierolf et al
Nature, 467, 436-439 (2010)

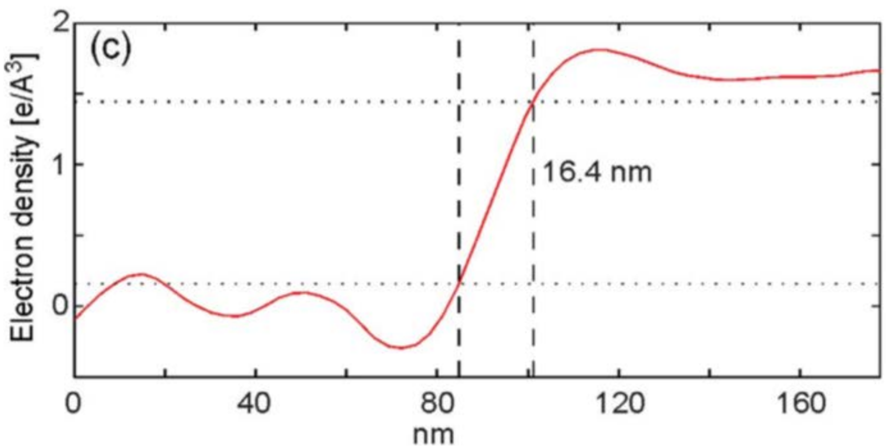
Mouse femur bone, imaged in 3D at 120nm resolution
Voxel size : 65 nm



PTYCHOGRAPHY: 3D HIGH RESOLUTION



Test object : porous SiO_2 structure of 139 nm mean pore size + Ta_2O_5 coating



3D reconstruction resolution : 16 nm

From :

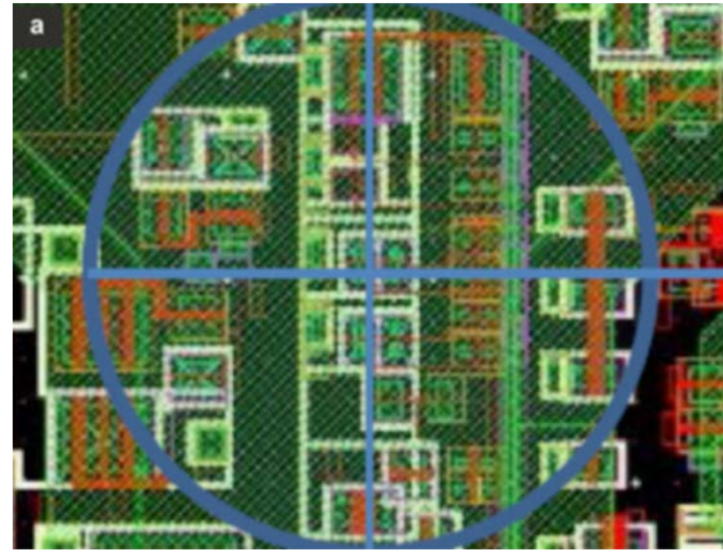
- 720 angular positions
- For each angle, 180 CDI images
- → 129600 images

Holler al. , Sci. Rep. 4 (2014), 3857

HIGH RESOLUTION IMAGING WITH PTYCHO-(TOMO)

Sample: micro-processor:

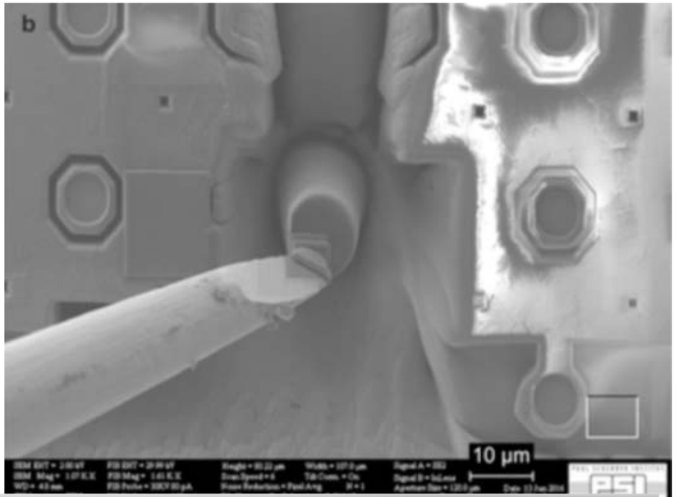
Socket LGA 1150, 3MB Cache, **22nm**

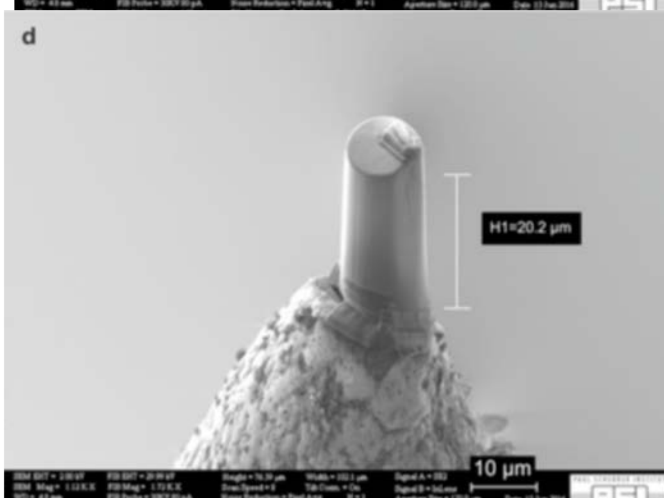


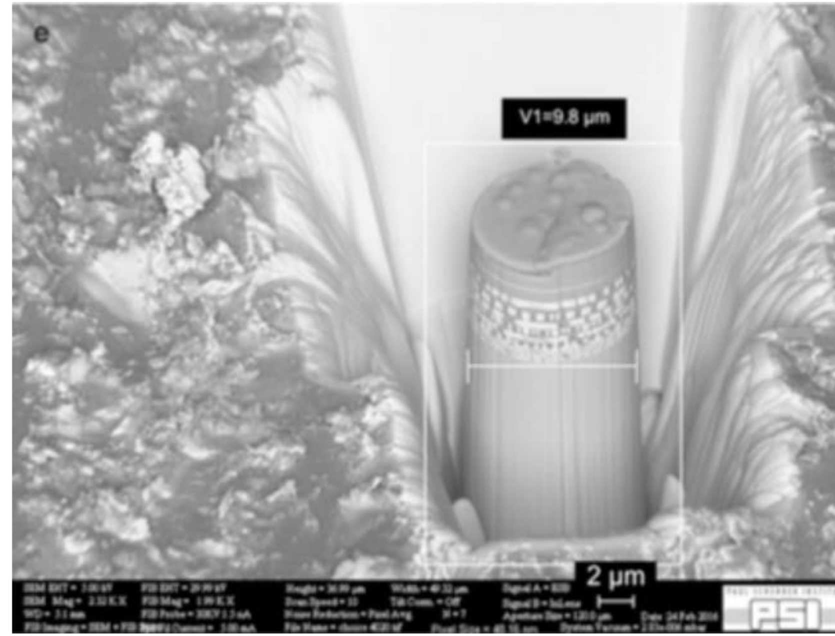
Select an area from the processor schematics

Holler et al, Nature 543, 402–406 (2017)

PTYCHO-TOMO OF INTEGRATED CIRCUITS



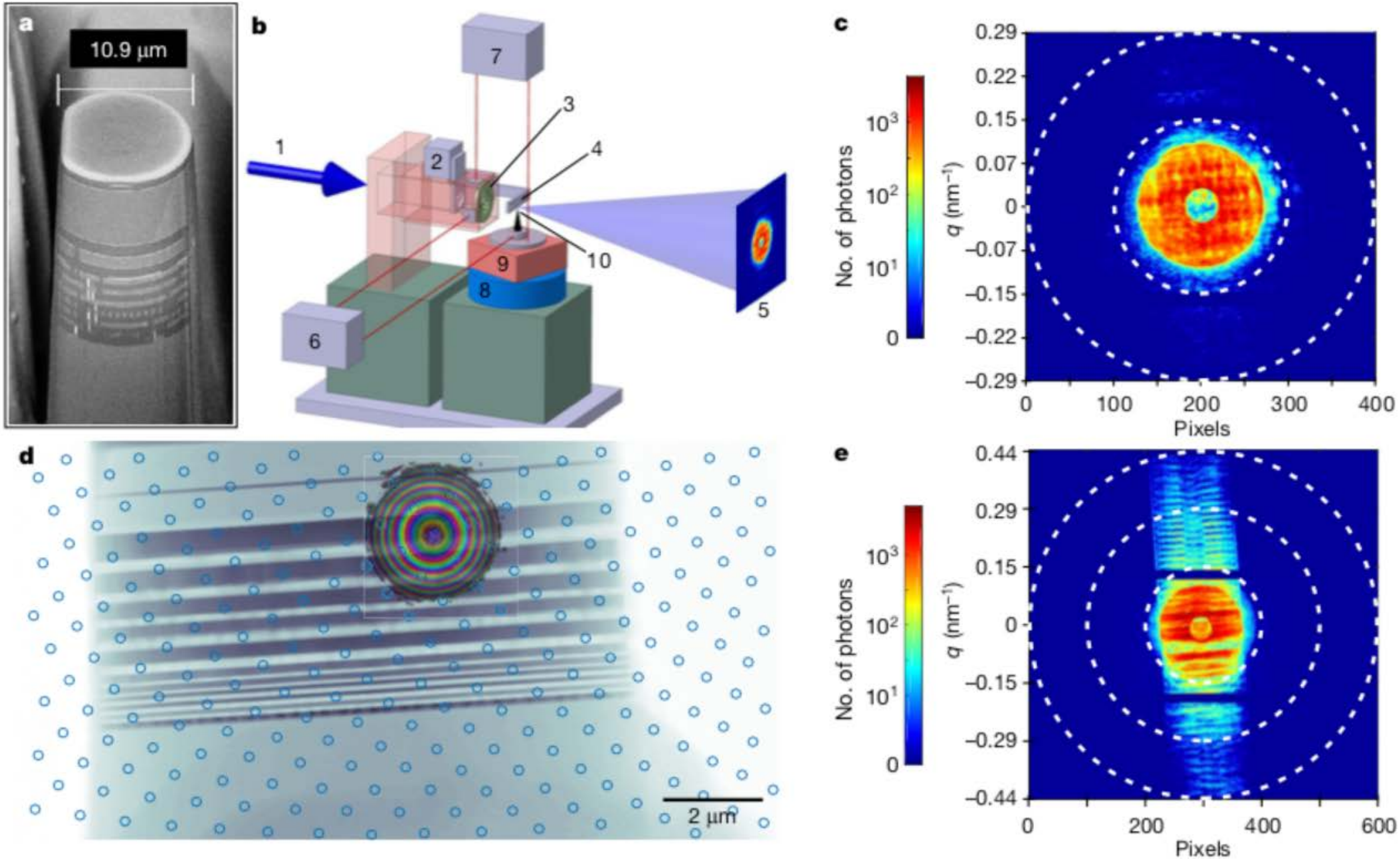




Extraction of a 10 µm pillar
Mount on a sample holder

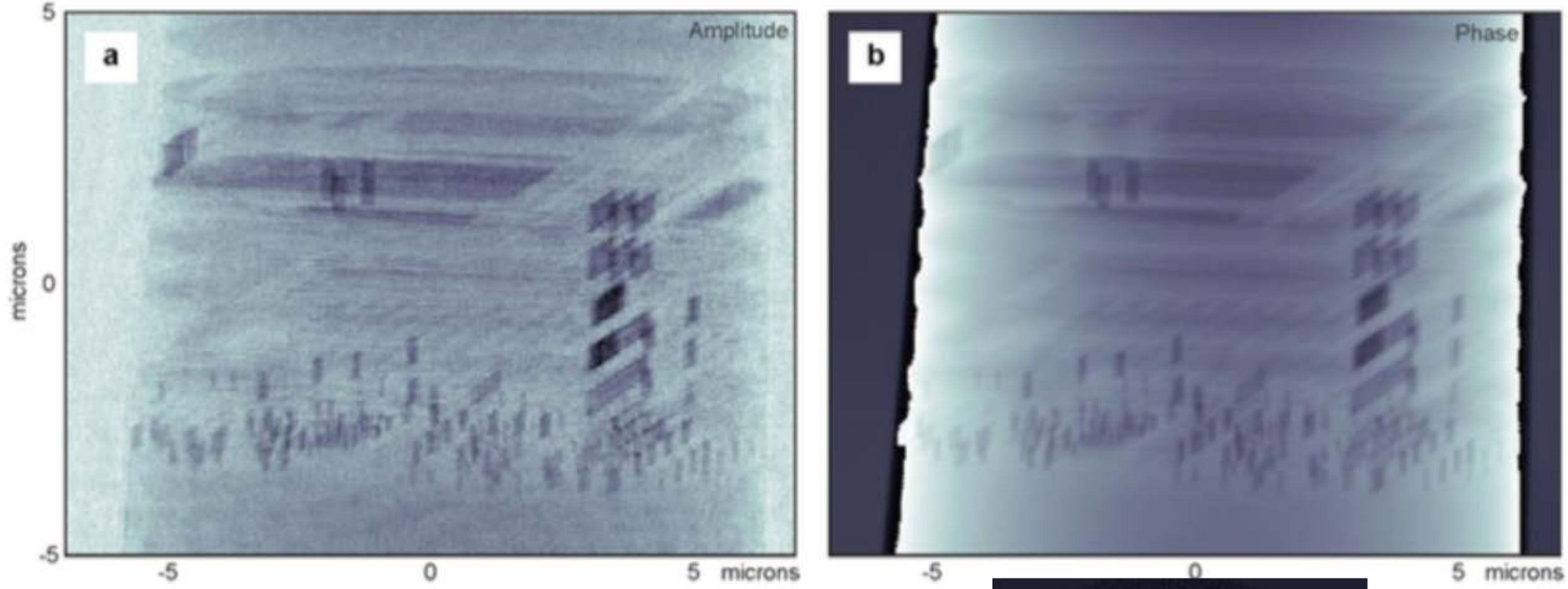
Holler et al, Nature 543, 402–406 (2017)

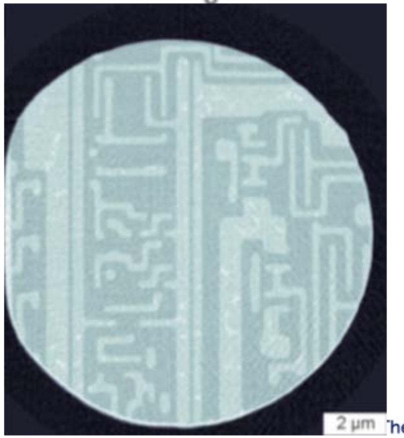
PTYCHO-TOMO OF INTEGRATED CIRCUITS



Holler et al, Nature 543, 402–406 (2017)

PTYCHO-TOMO OF INTEGRATED CIRCUITS



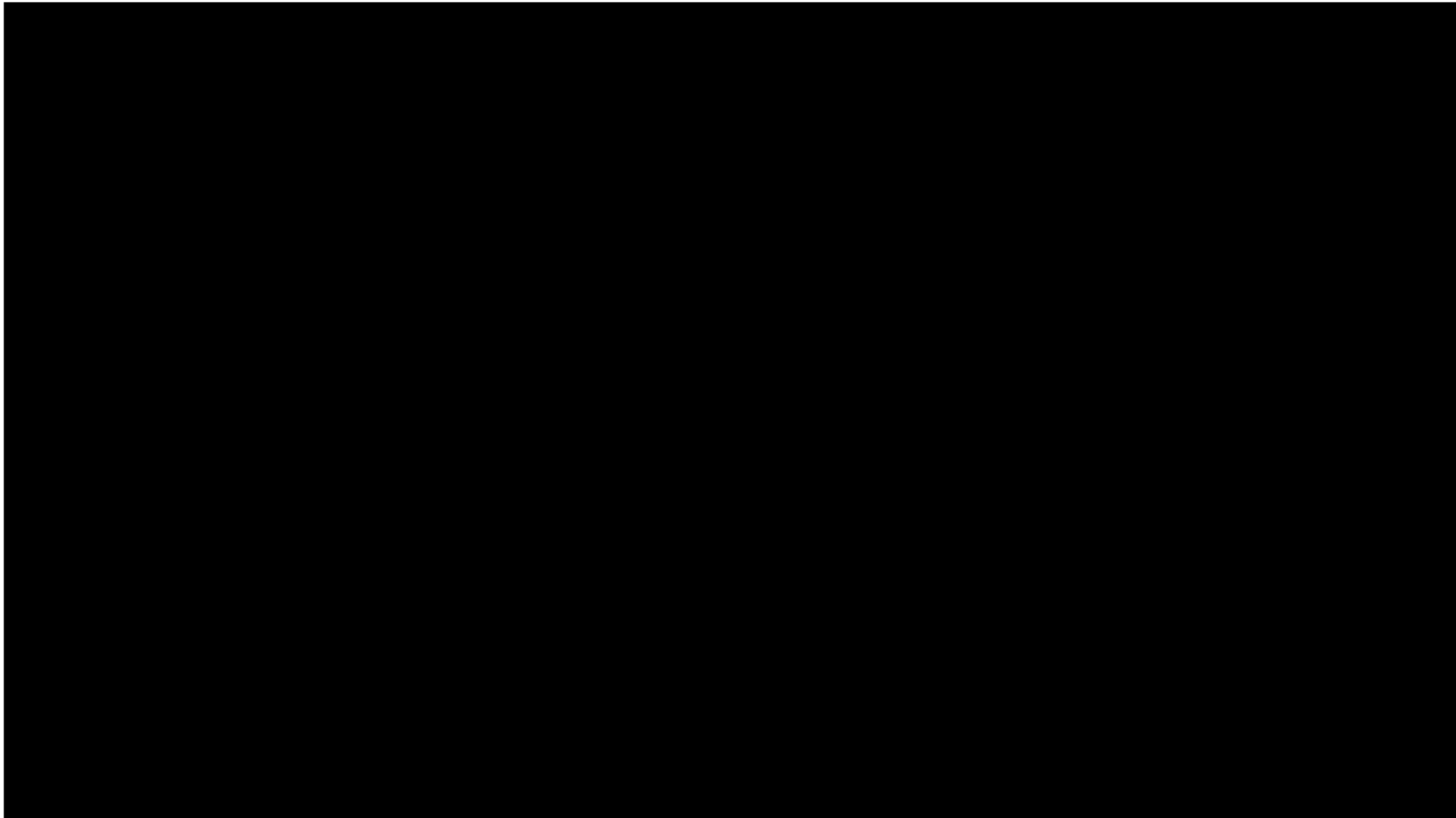


Result:

- 14.6 nm 3D resolution
- 1200 projections
- 24 hours
- 5850 resolution elements per second

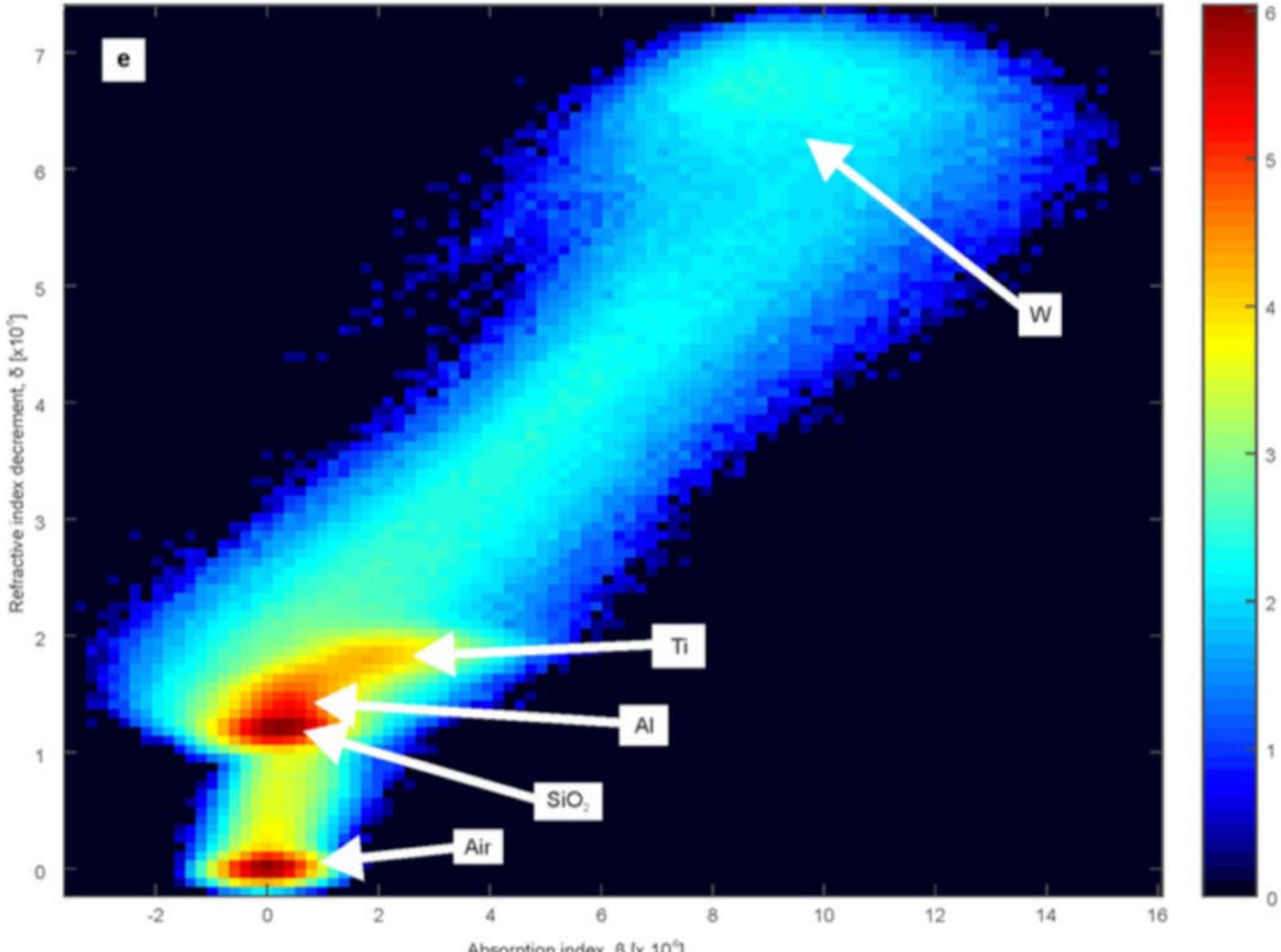
Holler et al, Nature 543, 402–406 (2017)

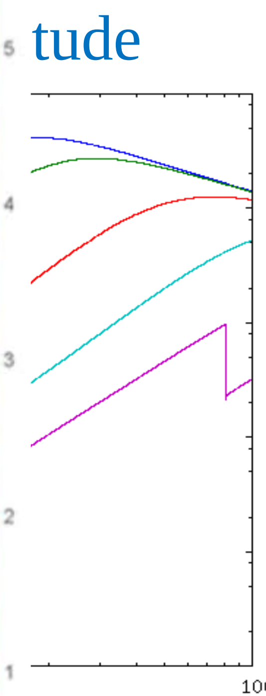
PTYCHO-TOMO OF INTEGRATED CIRCUITS



Holler et al, Nature 543, 402–406 (2017)

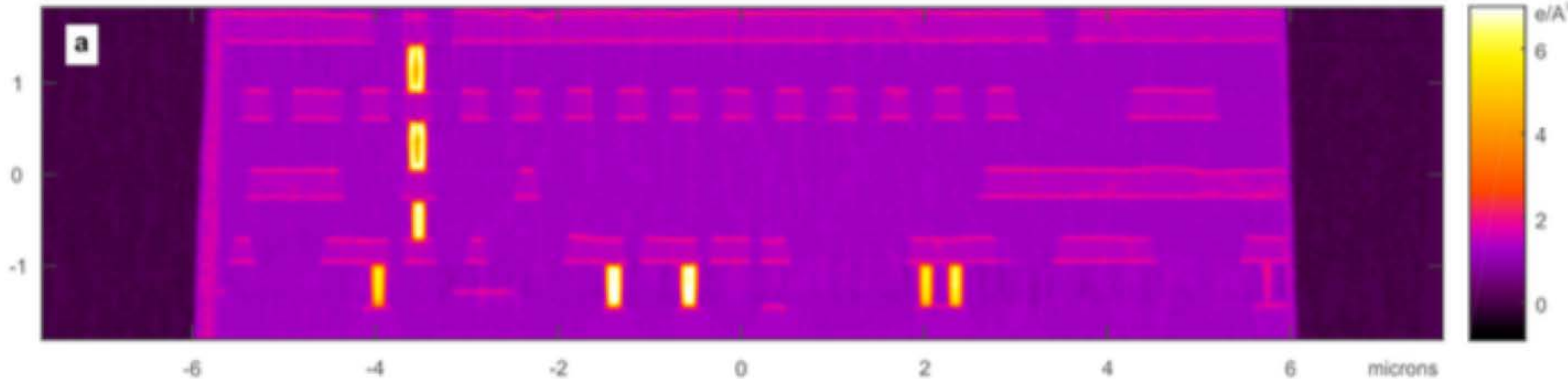
PTYCHO-TOMO OF INTEGRATED CIRCUITS

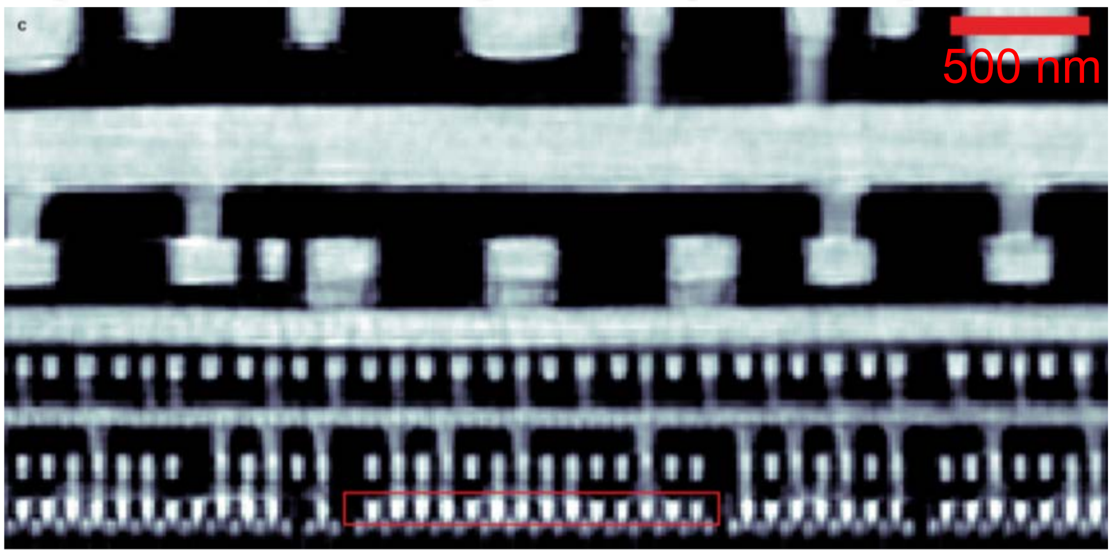




Holler et al, Nature 543, 402–406 (2017)

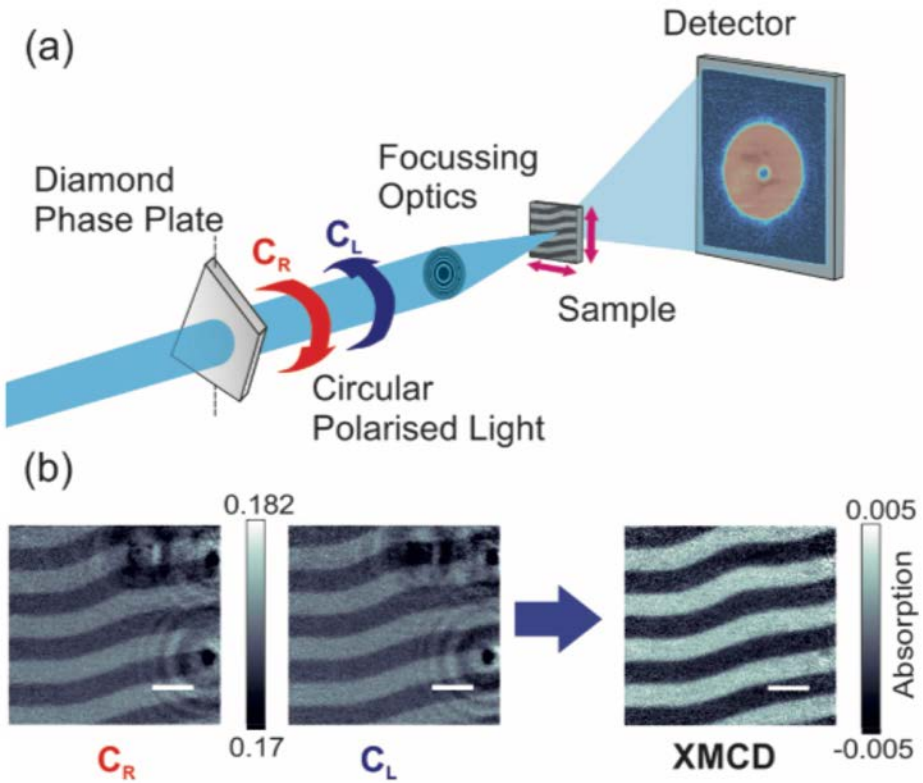
PTYCHO-TOMO OF INTEGRATED CIRCUITS





Holler et al, Nature 543, 402–406 (2017)

IMAGING MAGNETIC NANO-STRUCTURES WITH PTYCHO-TOMOGRAPHY



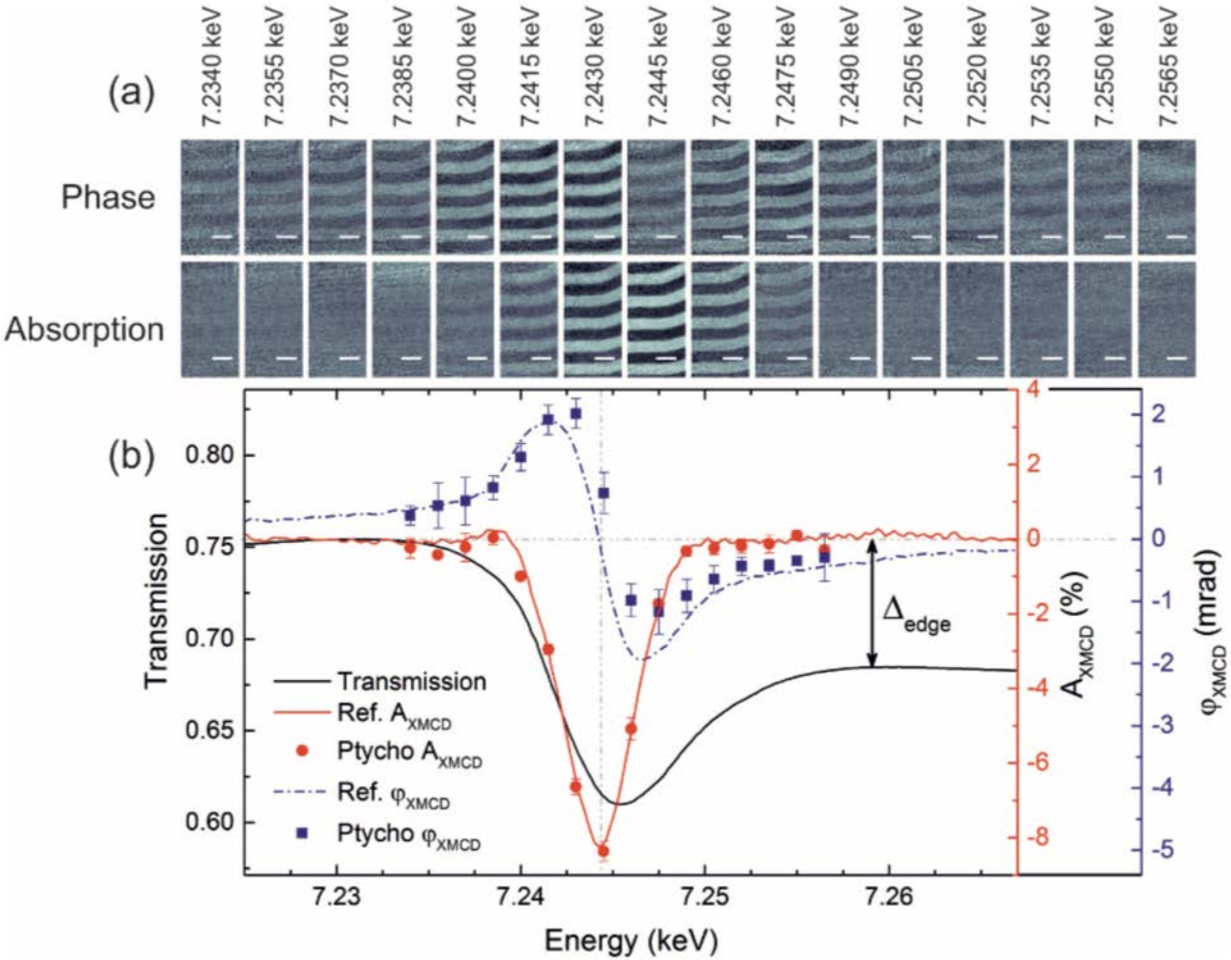
Synchrotron X-rays are normally (*) linearly polarised

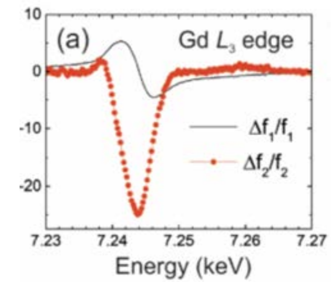
A phase plate can be used to transform this into a circularly-polarised X-ray beam

Sensitivity is maximal when magnetic moment is // to X-ray photon wavevector

Donnelly et al, Phys. Rev. B (2016)

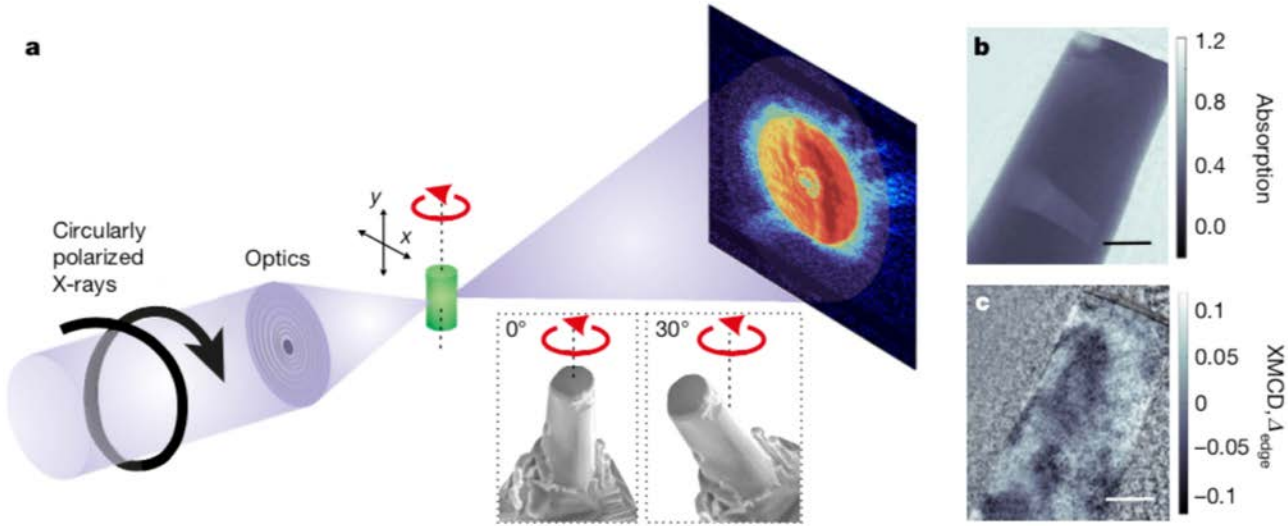
IMAGING MAGNETIC NANO-STRUCTURES WITH PTYCHO-TOMOGRAPHY





Donnelly et al, Phys. Rev. B (2016)

IMAGING MAGNETIC NANO-STRUCTURES WITH PTYCHO-TOMOGRAPHY



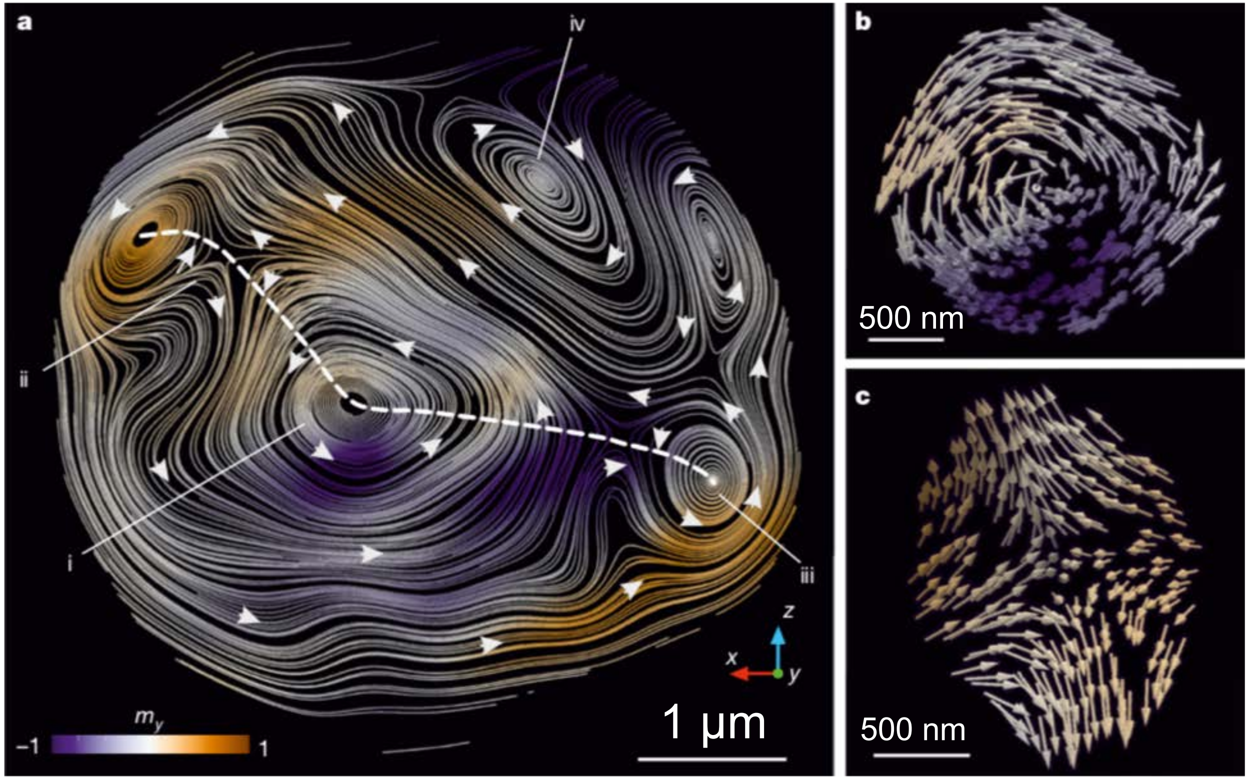
Setup for a ptycho-tomography setup

Using two tilt angles to be sensitive to the 3D orientation of magnetic domain

!! Magnetic structure is a **3D vector field**, not a 3D scalar !!

Donnelly et al, Nature 547, 328–331(2017)

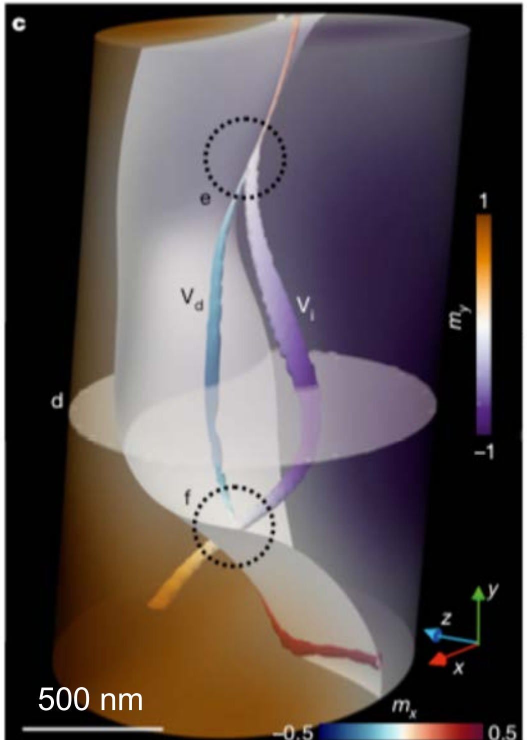
IMAGING MAGNETIC NANO-STRUCTURES WITH PTYCHO-TOMOGRAPHY

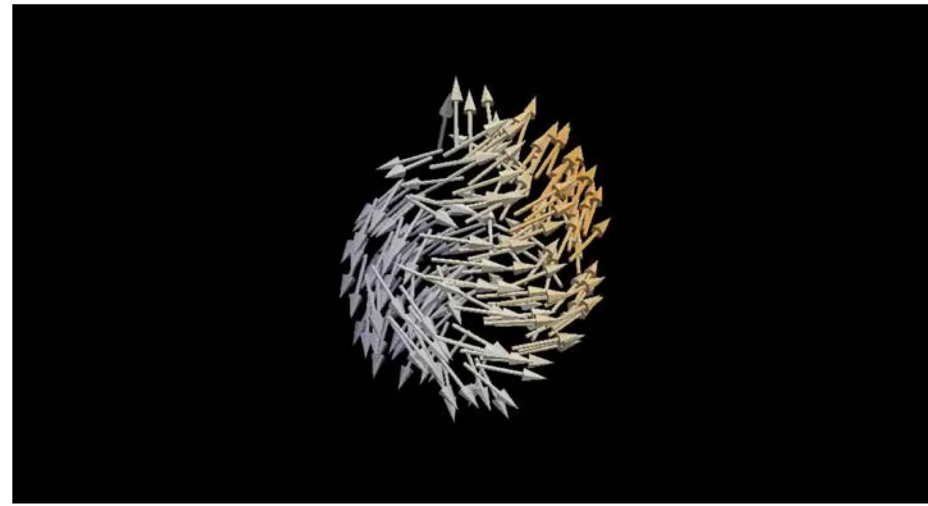


Axial tomographic slice of the reconstructed magnetization vector field
Note the anti- and clockwise vortices
Spatial resolution ~100-200 nm

Donnelly et al, Nature 547, 328–331(2017)

IMAGING MAGNETIC NANO-STRUCTURES WITH PTYCHO-TOMOGRAPHY



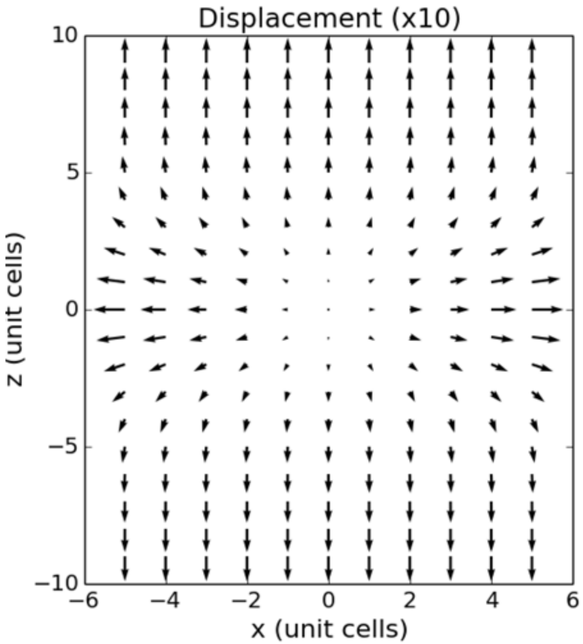


3D view of the magnetic reconstruction with two main domains
Two vortices Vi and Vd intersect at two Bloch points (m=0)

Donnelly et al, Nature 547, 328–331(2017)

SMALL ANGLE VS BRAGG CDI

$$A(\vec{k}) \approx FT\left[\Omega(\vec{r})e^{2i\pi\vec{s}\vec{u}}\right]$$



- ***Simulated nanowire w/insertion***
- *- 2% strain along x*

SMALL ANGLE VS BRAGG CDI

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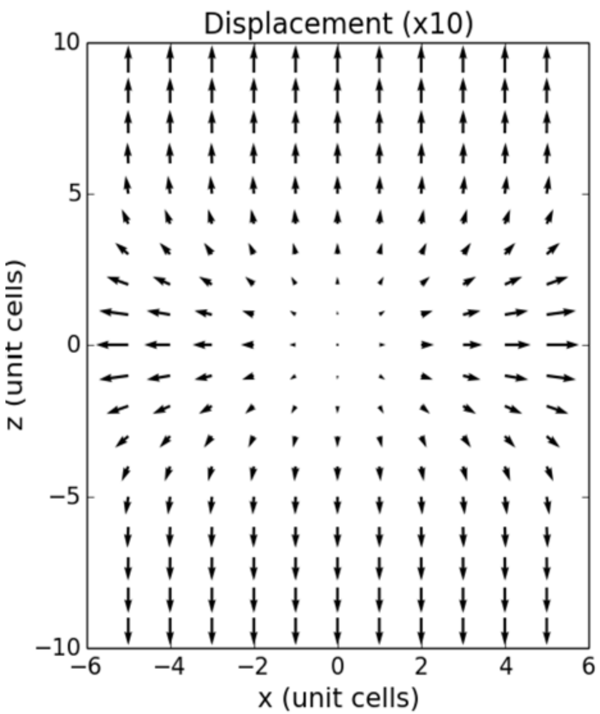
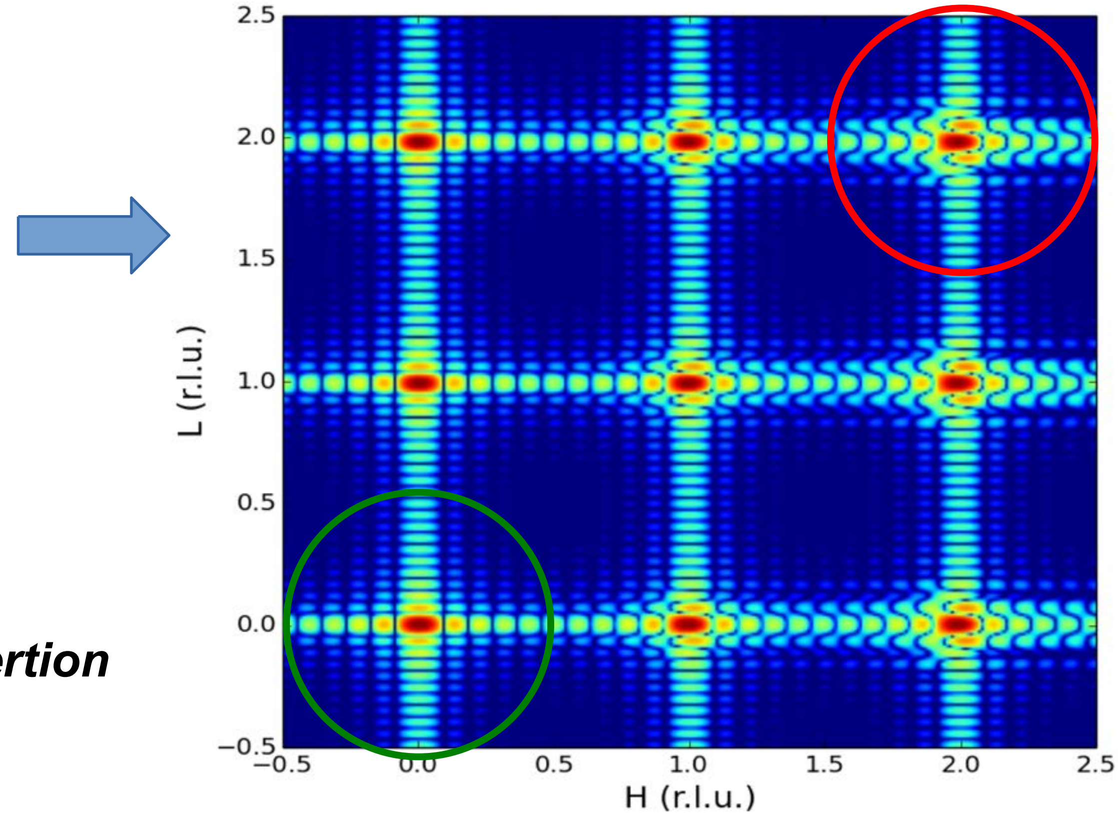


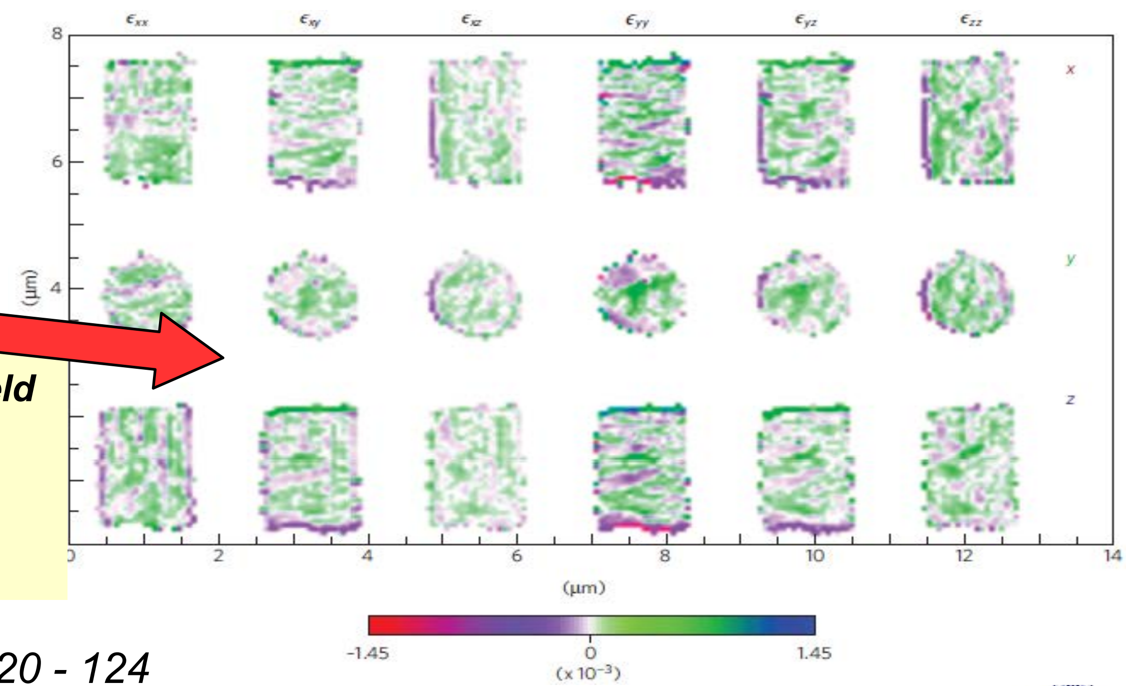


- ***Simulated nanowire w/insertion***
- *- 2% strain along x*

BRAGG CDI: STRAIN RECONSTRUCTION

$$A(\vec{k}) \approx FT\left[\Omega(\vec{r})e^{2\pi\vec{s}\vec{u}}\right]$$

- ***Measuring the CDI on at least 3 independent reflections***

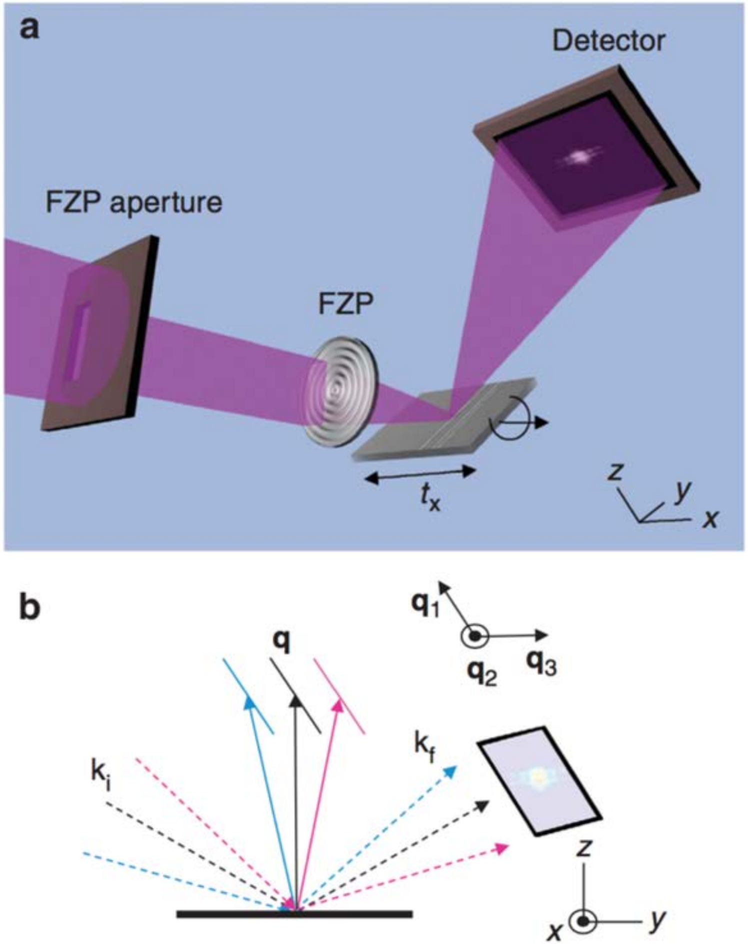


reconstruct the full 3D displacement field inside the nanocrystal

=> Access to the full strain tensor

Newton et al., Nat. Mater. ***9*** *(2010), 120 - 124*

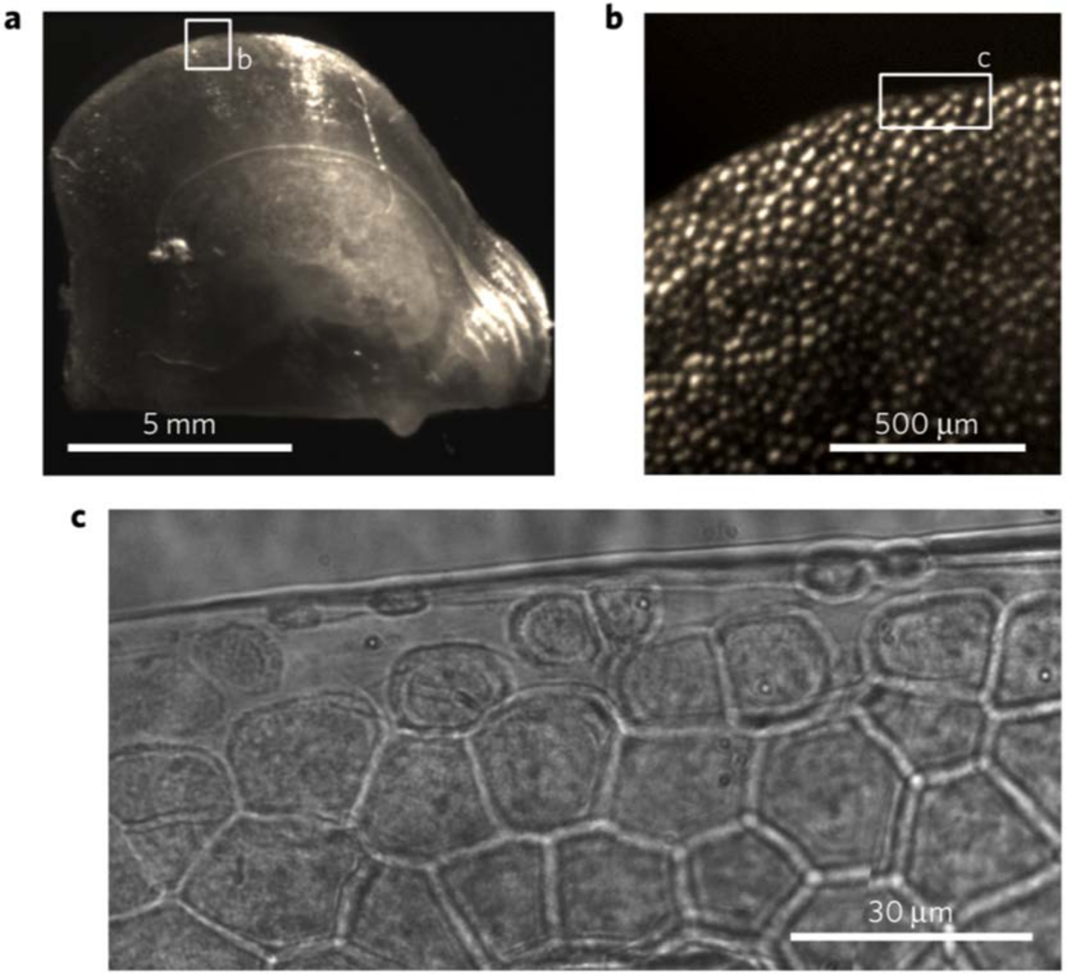
BRAGG PTYCHOGRAPHY



Bragg Ptychography :
2D Ptychography at different rotation angles
(angle step ~0.04º, ptycho step 300 nm)

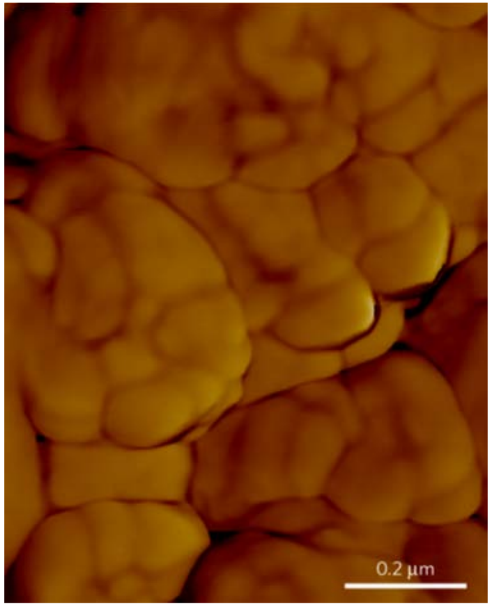
Godard et al, Nat Commun 2, 568 (2011)

BRAGG PTYCHOGRAPHY ON MOLLUSC SHELLS

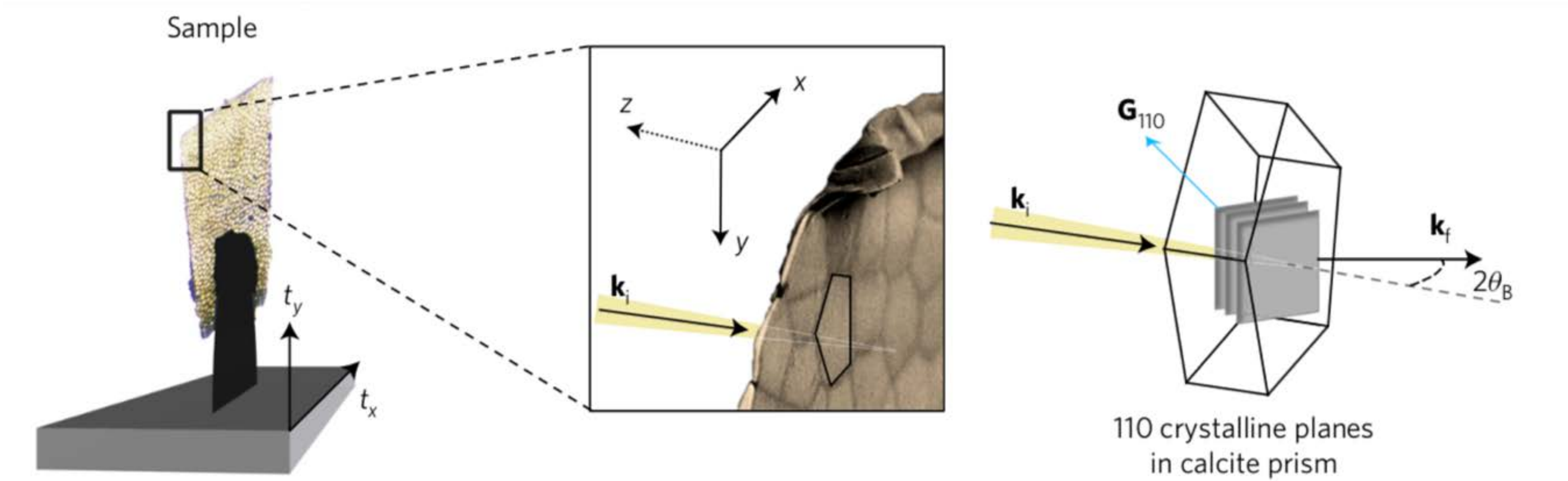


Pinctada margaritifera shell at different length scales

Calcite nano-structures

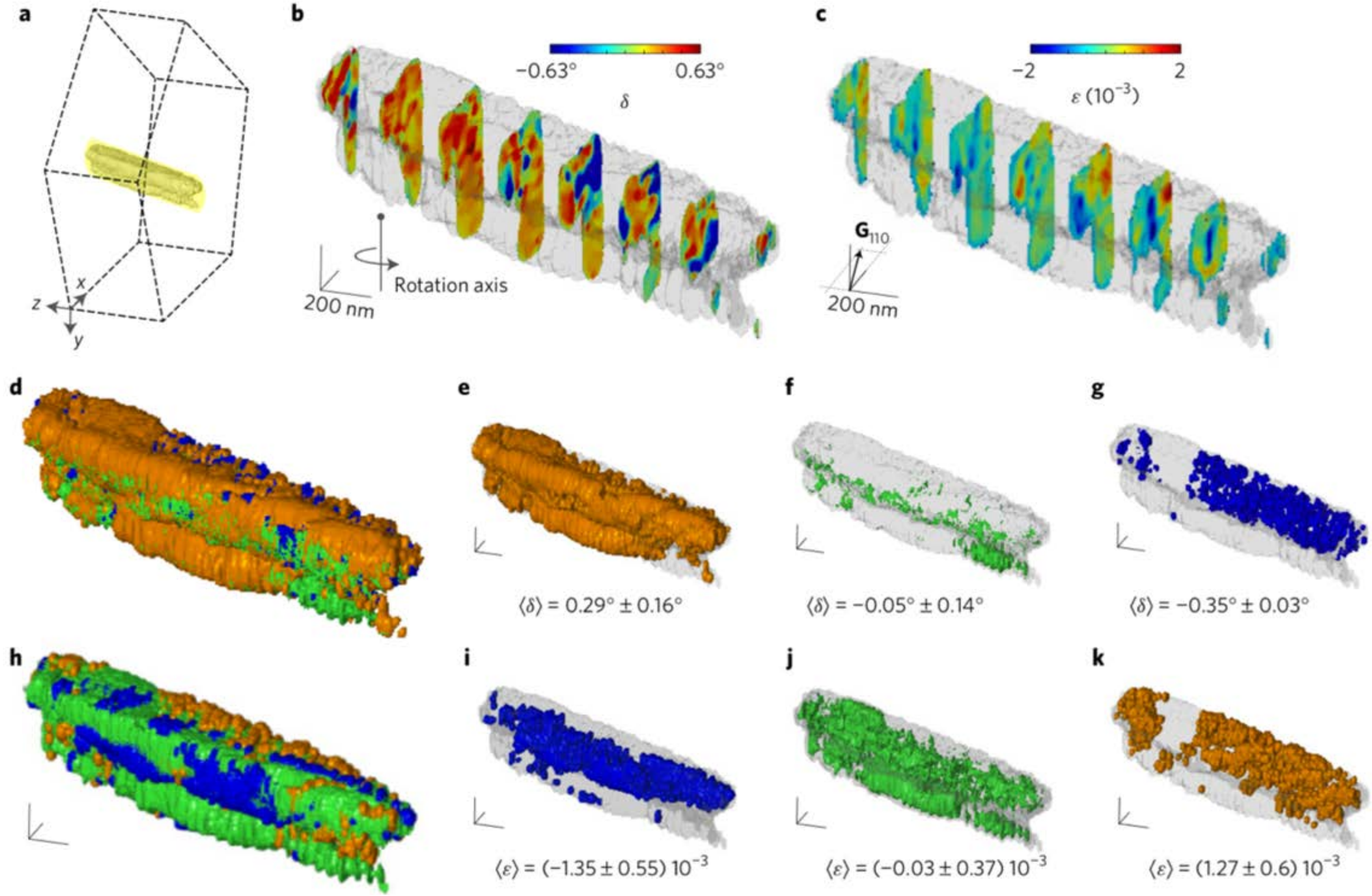


BRAGG PTYCHOGRAPHY ON MOLLUSC SHELLS



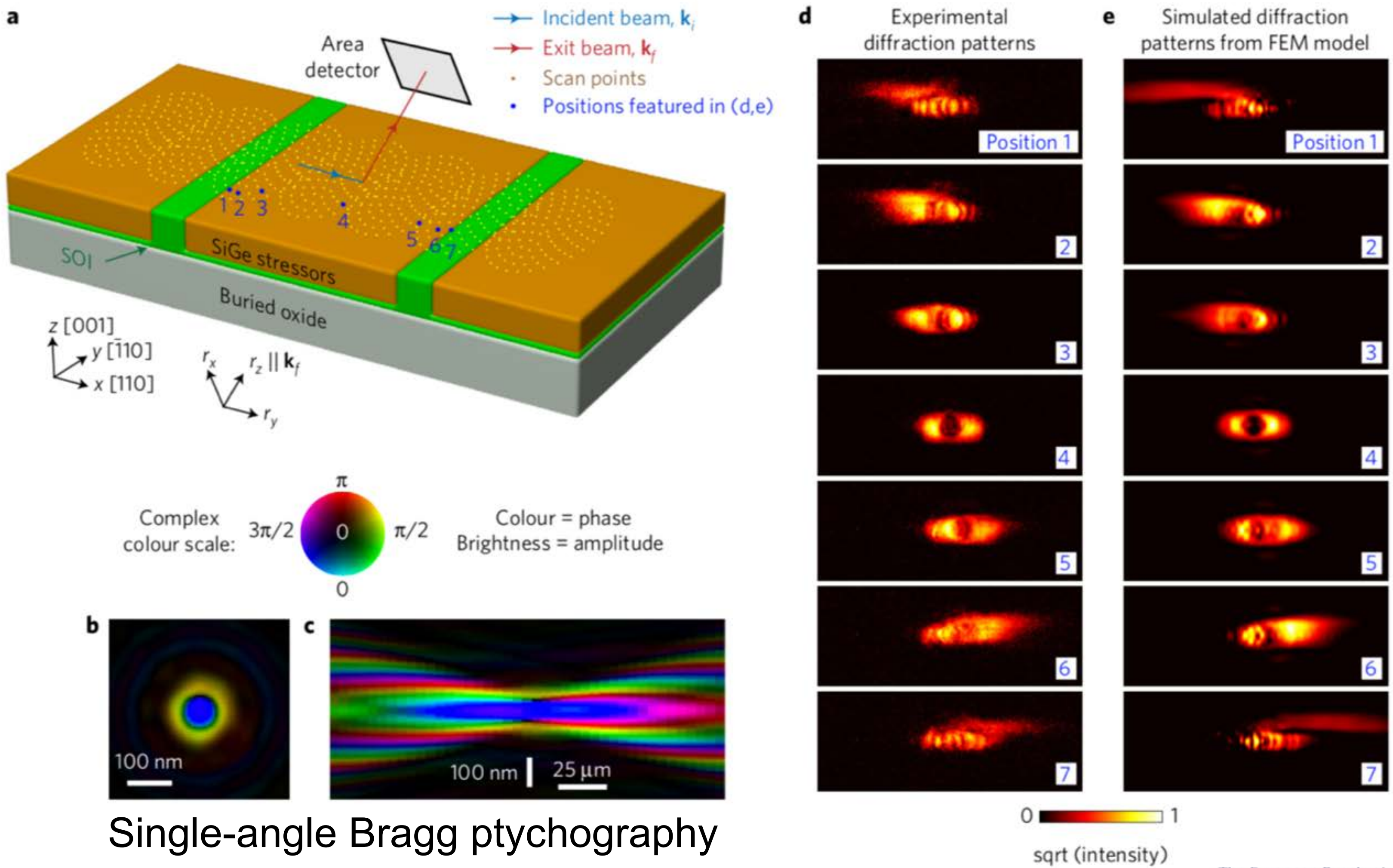
Diffraction on individual calcite prisms

BRAGG PTYCHOGRAPHY ON MOLLUSC SHELLS



Bragg ptycho yields information on tilts at a micro/nano-scale

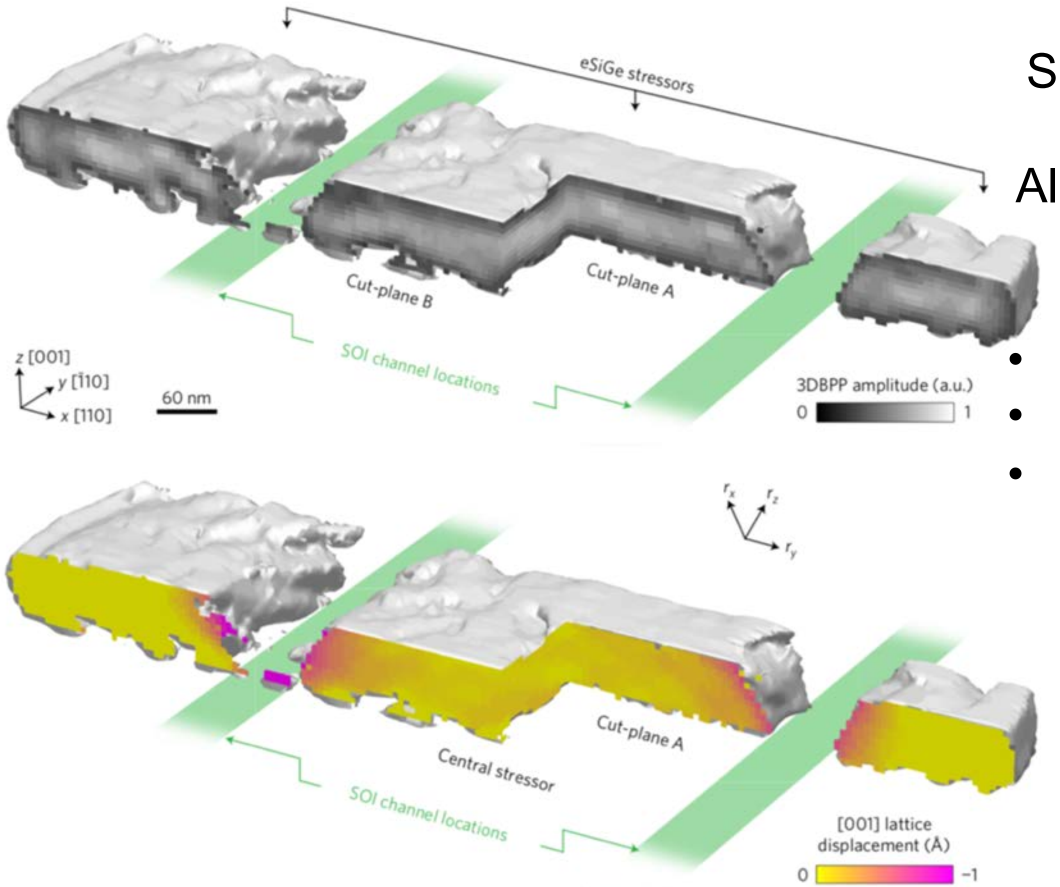
BRAGG PROJECTION PTYCHOGRAPHY



Single-angle Bragg ptychography

Hruszkewycz *et al.*, Nat Mater 16 (2016), 244

BRAGG PROJECTION PTYCHOGRAPHY

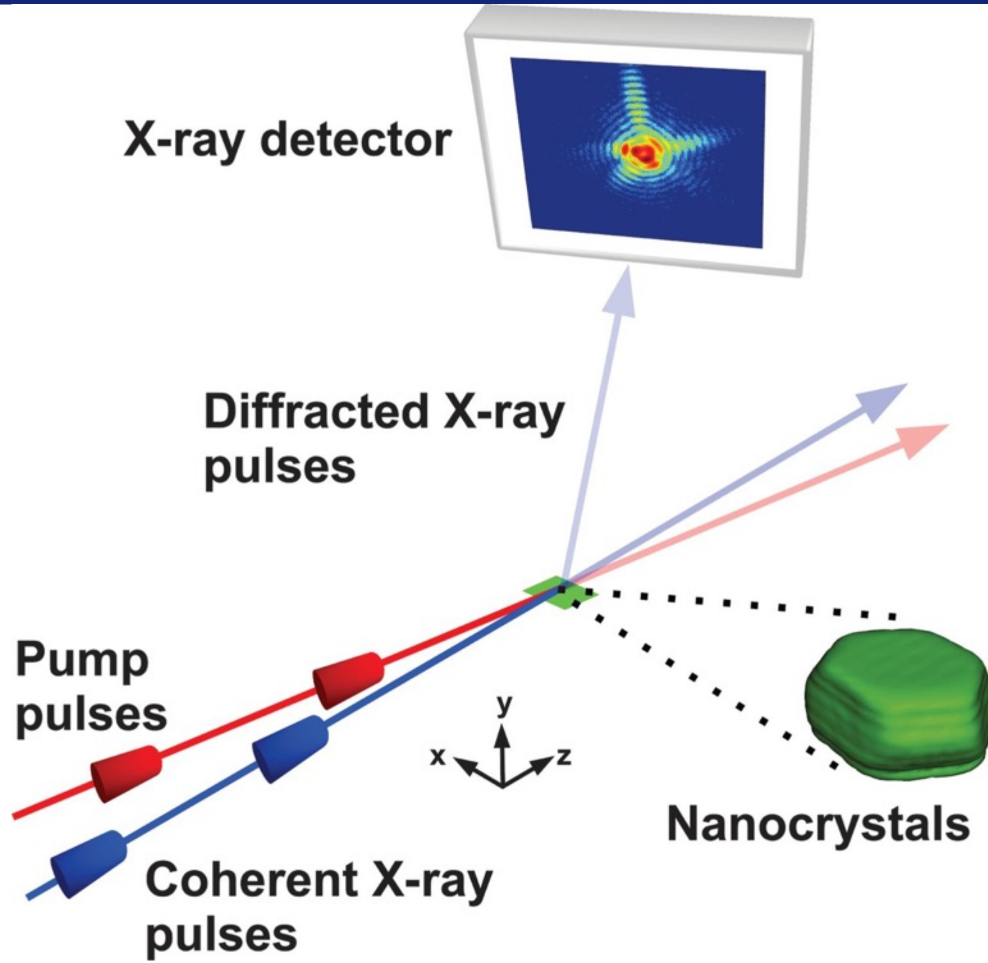


Single-angle Bragg ptychography

Allows reconstructing an extended object with limited data:

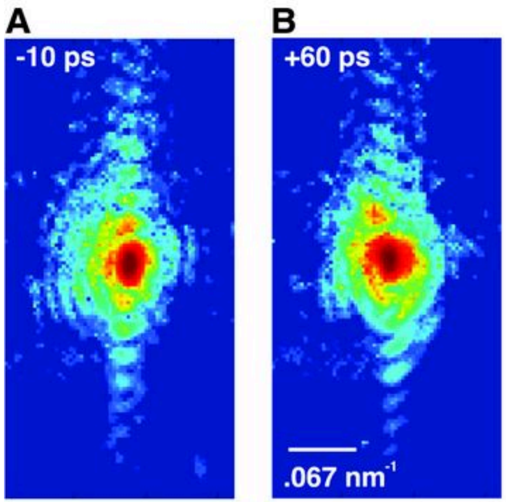
- Faster data collection
- Less radiation damage
- Only sensitive to deformation in the detector plane

XFEL LATTICE VIBRATION IMAGING USING BRAGG CDI

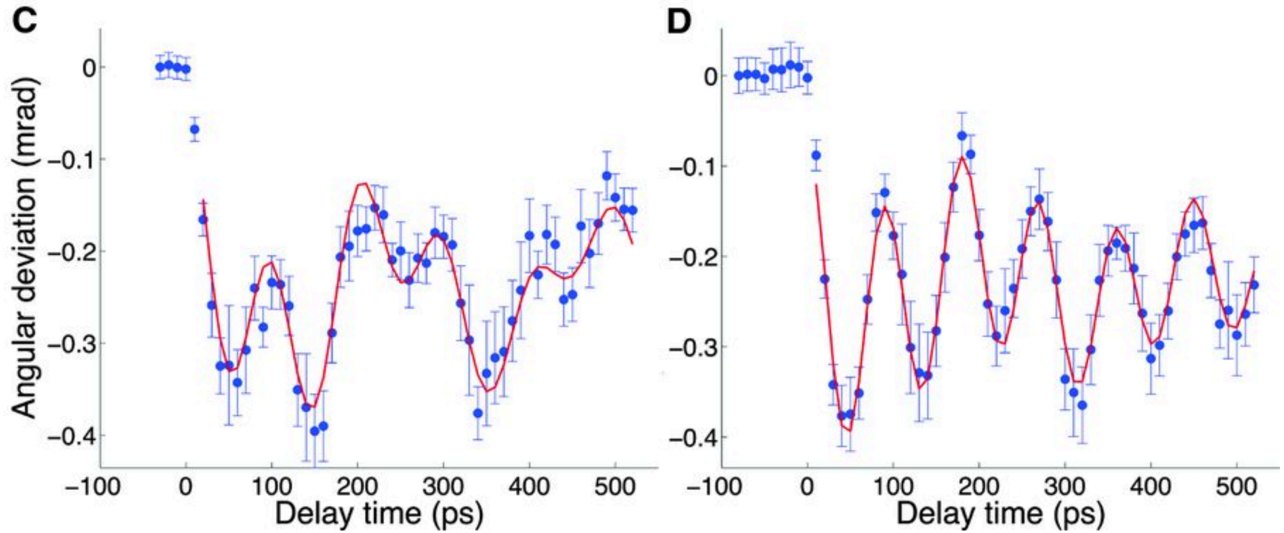


Clark et al. Science 341 (2013), 56-59

XFEL LATTICE VIBRATION IMAGING USING BRAGG CDI



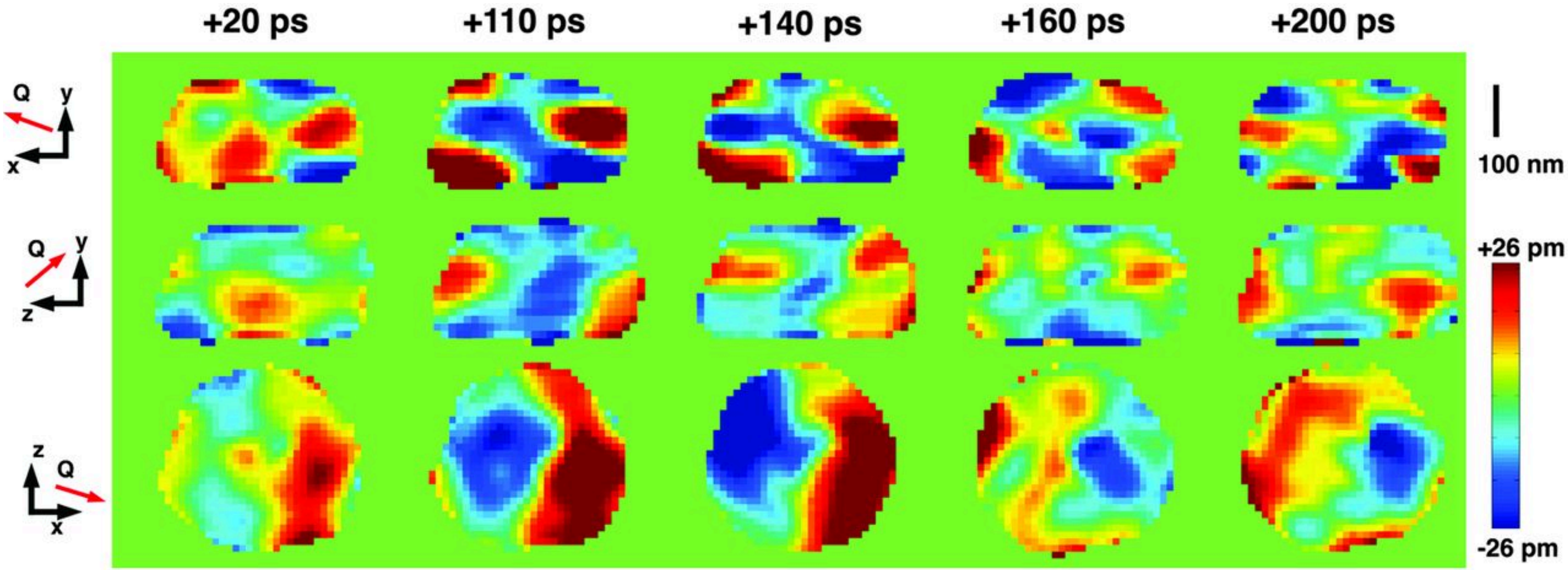
Experimentally recorded coherent diffraction patterns from a single nanocrystal for delay times of –10 and +60 ps.



Bragg peak angular shift as a function of delay time for two different nanocrystals

Clark et al. Science 341 (2013), 56-59

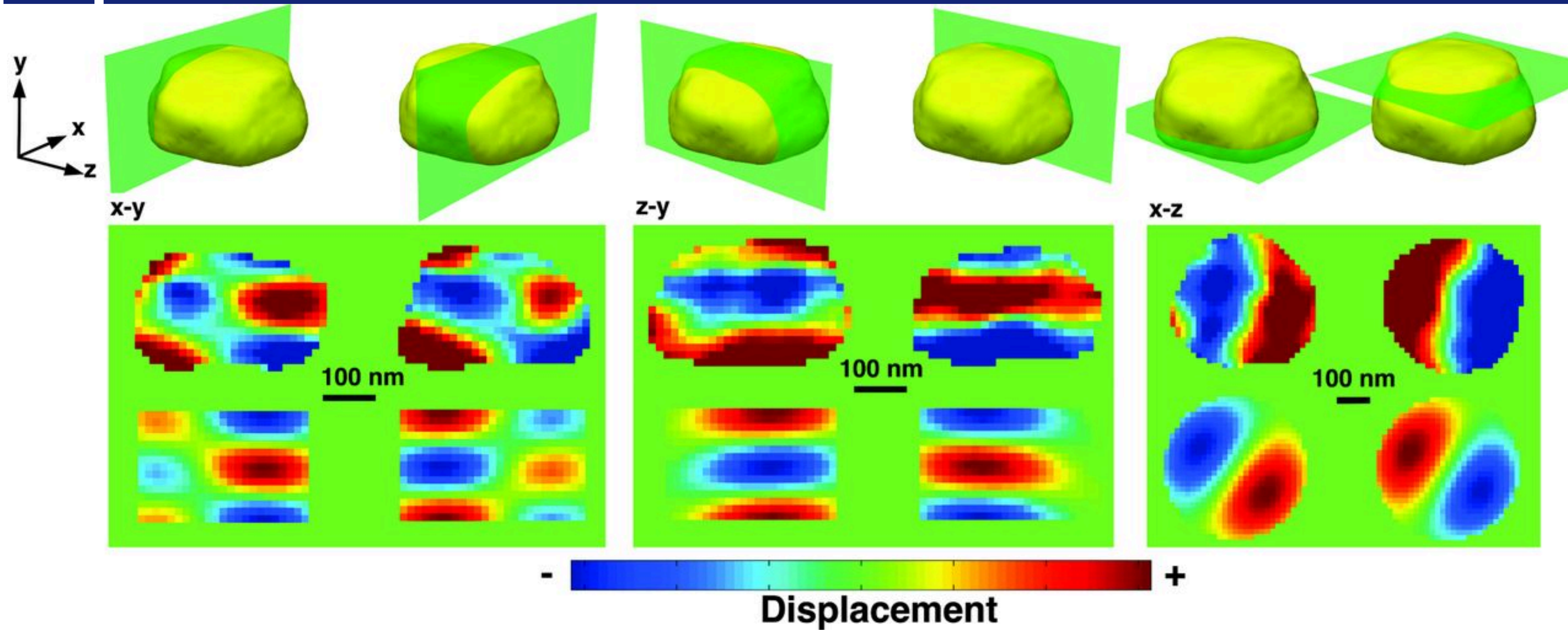
XFEL LATTICE VIBRATION IMAGING USING BRAGG CDI



Orthogonal cut planes through the center of the nanocrystal showing the projected displacement as a function of delay time

Clark et al. Science 341 (2013), 56-59

XFEL LATTICE VIBRATION IMAGING USING BRAGG CDI



Orthogonal slices taken either side of the center (top) of the nanocrystal compare the projected displacement obtained from the experiment (middle) with a simulated (1, 1) mode for a cylinder (bottom).

Clark et al. Science 341 (2013), 56-59

THANK YOU FOR YOUR ATTENTION !