



# Coherent Diffraction Imaging (CDI) with X-Rays

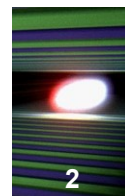
School on Synchrotron and Free-Electron-Laser Based Methods:  
Multidisciplinary Applications and Perspectives

ICTP Trieste,  
April 15 - 2016

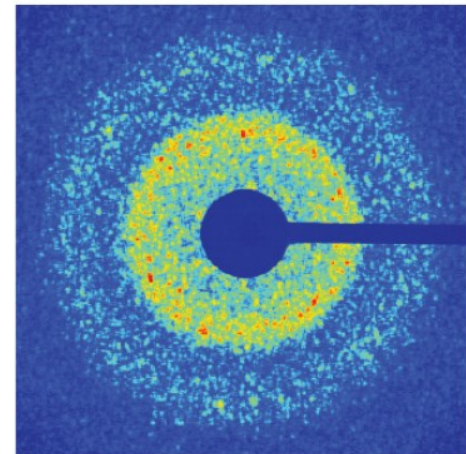
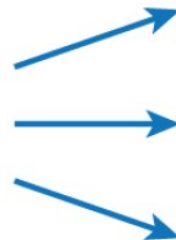
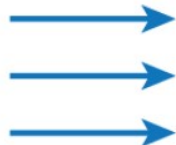
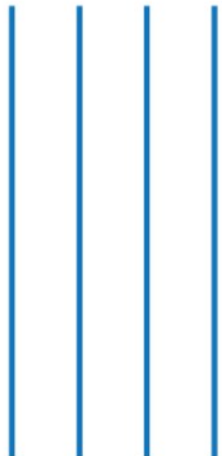
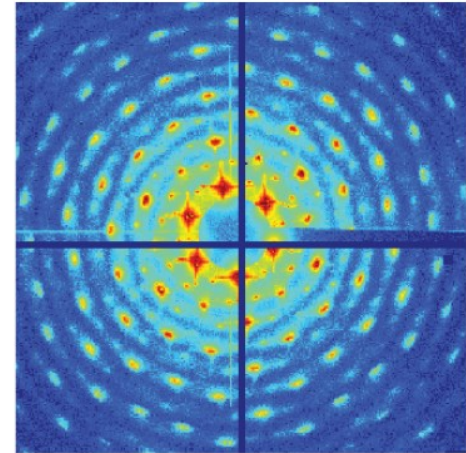
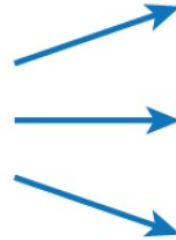
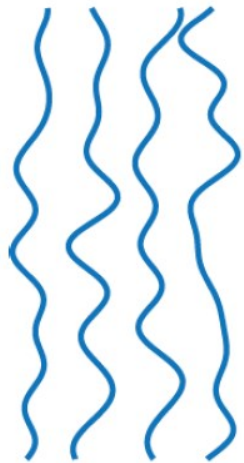
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European X-Ray Free-Electron Laser Facility  
Hamburg, Germany

[anders.madsen@xfel.eu](mailto:anders.madsen@xfel.eu)

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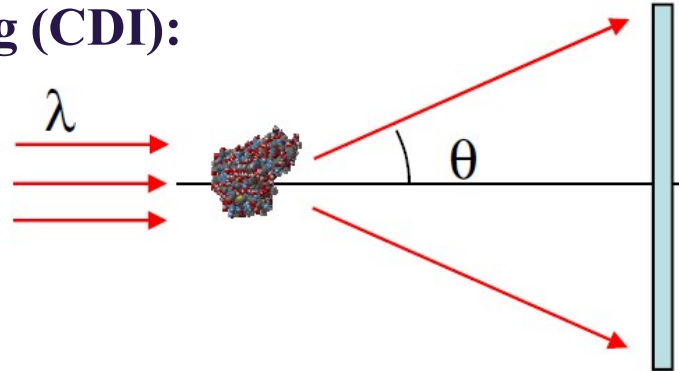


- Motivation
- X-ray Imaging
- X-ray Coherence
- All the tricks of CDI
- Image reconstruction
- Related methods
- Applications
  
- BREAK -
  
- Sources of Coherent X-rays
- The European XFEL project
- CDI science at XFELs
- Summary

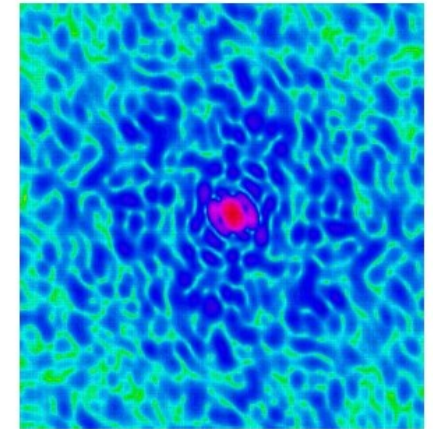


## Isolated object

**Coherent Diffraction Imaging (CDI):**



**Static scattering**

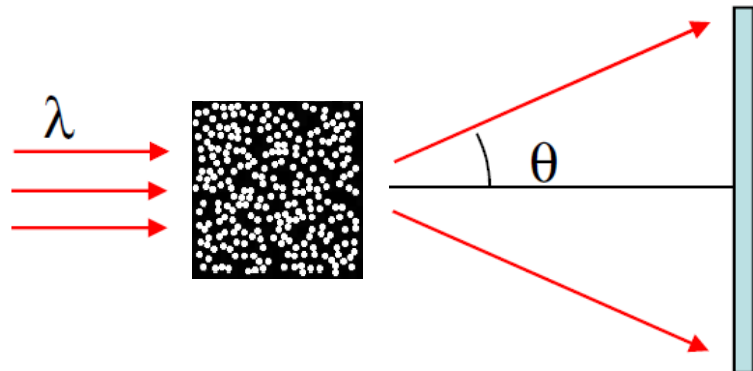


## Ensemble of objects

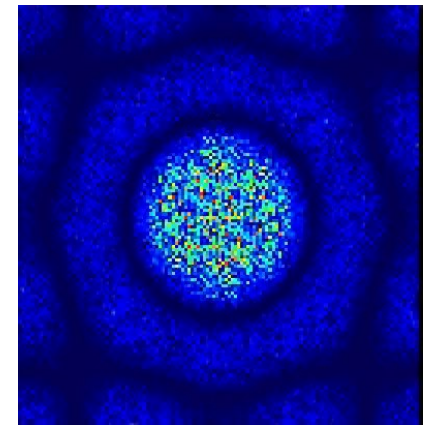
**Correlation spectroscopy:**

Temporal: XPCS

Spatial: XCCA



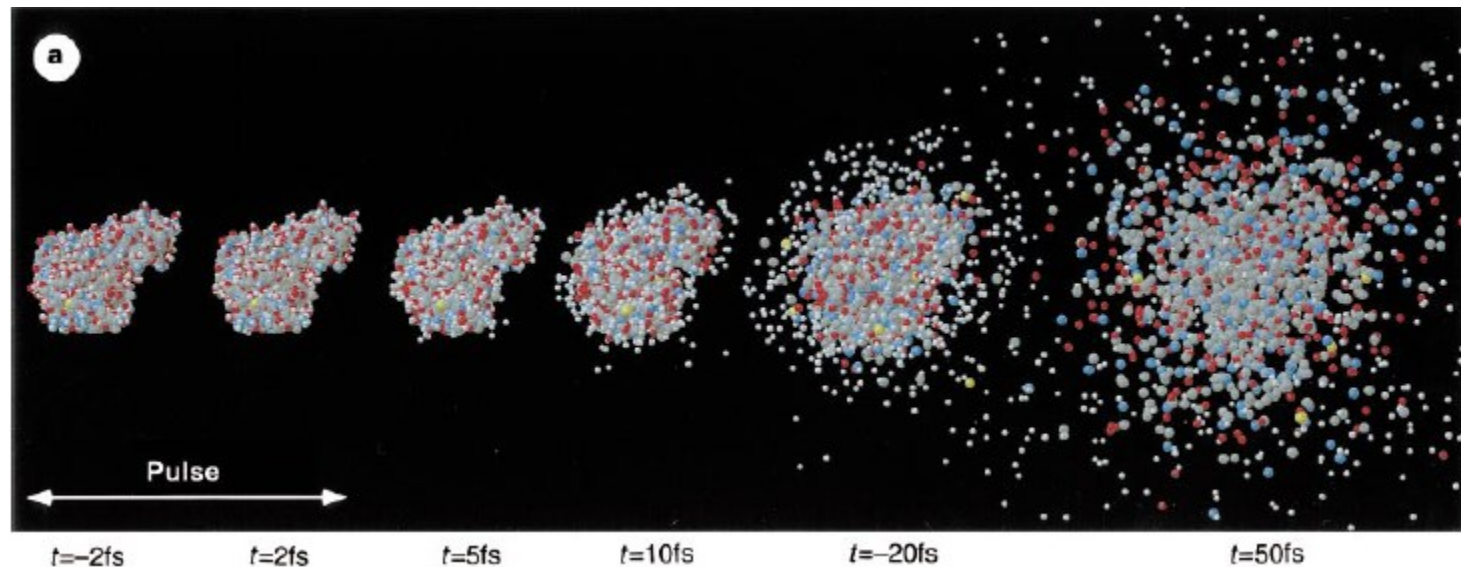
**Dynamic scattering**





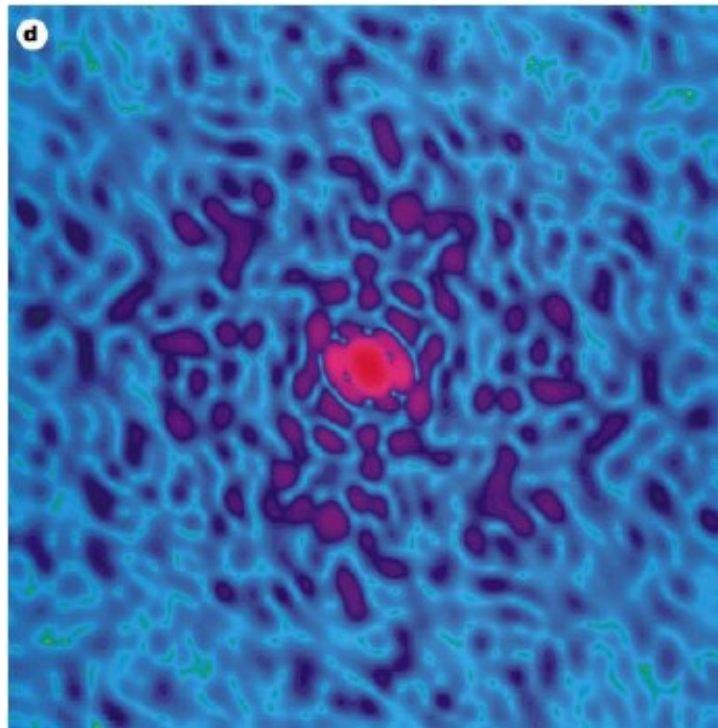
## Diffraction imaging of biomolecules with coherent femtosecond X-FEL pulses

Very much excitement, now for >15 years:



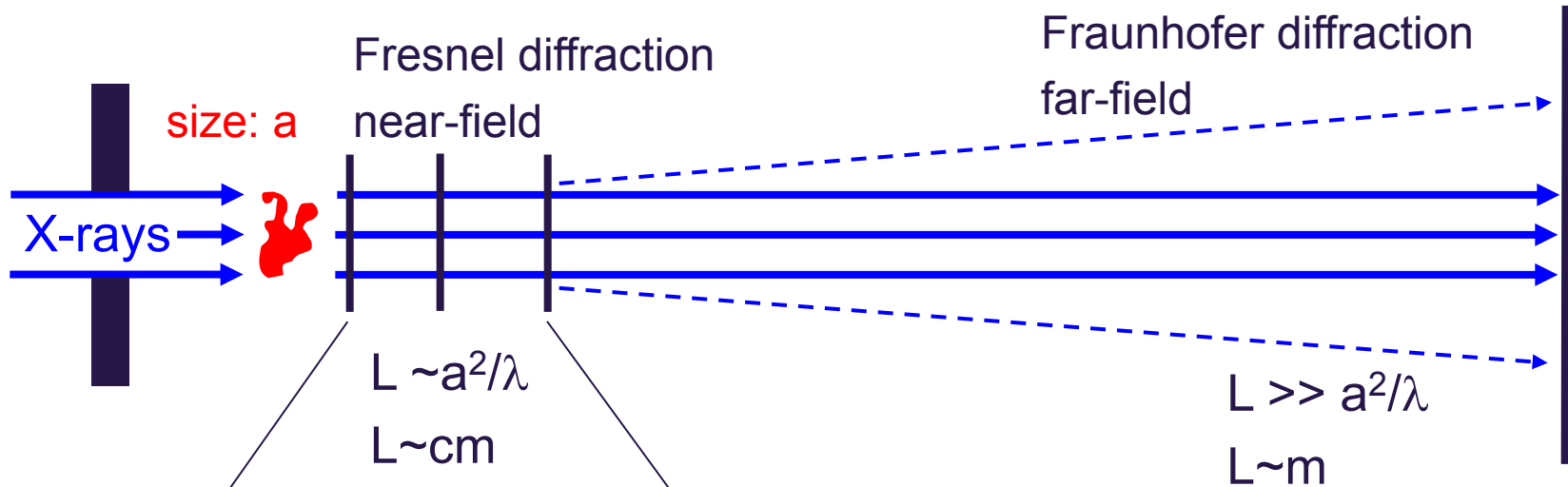
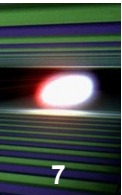
Coulomb explosion of T4 lysozyme

## Diffraction imaging of biomolecules with coherent femtosecond X-FEL pulses



Simulated coherent scattering image (**speckle**) of a T4 lysozyme molecule

# Different regimes of lensless X-ray imaging

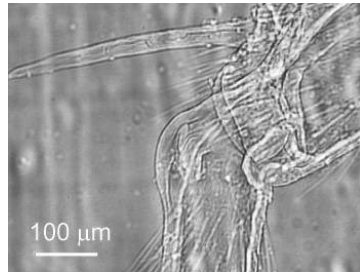


Absorption



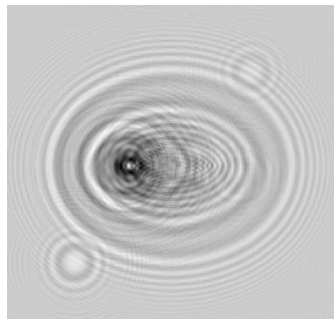
Röntgen (1895)

Phase contrast



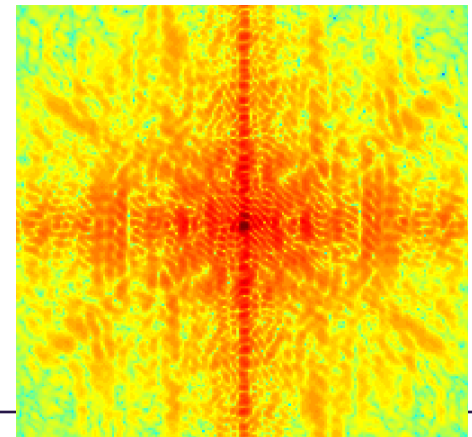
Koch *et al.* (1998)

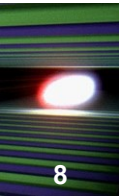
In-line holography



Zhang (2003)

Coherent Diffraction Imaging (CDI)





## Absorption regime

Easy reconstruction based on attenuation

3D tomographic reconstruction, inverse Radon transformation

## Phase contrast regime

Edge enhanced contrast

Transport-of-intensity (TIE) equation

Holotomographic reconstruction (Talbot effect)

## In-line holographic regime

Holographic reconstruction (detector dependent resolution)

Twin image problem

## Coherent diffraction imaging

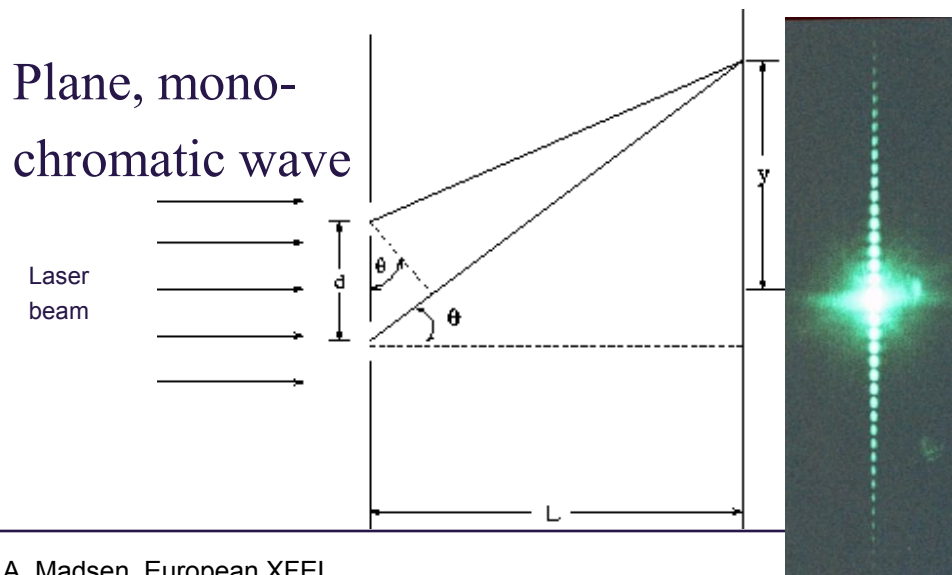
Tricky data treatment

Resolution like in scattering, i.e.  $\Delta_{\min} = 2\pi/Q_{\max}$

....

Quantum mechanics  $\rightarrow$  probability amplitudes (waves)  
 Optics  $\rightarrow$  Young's double slit experiment, interference  
 X-ray (and neutron) scattering  
 It's all about probability amplitudes and interference !!!

Example: Young's double slit experiment (Thomas Young, 1801)  
 [wave-character of quantum mechanical particles (photons)]



$$P = |\sum_j \Phi_j|^2$$

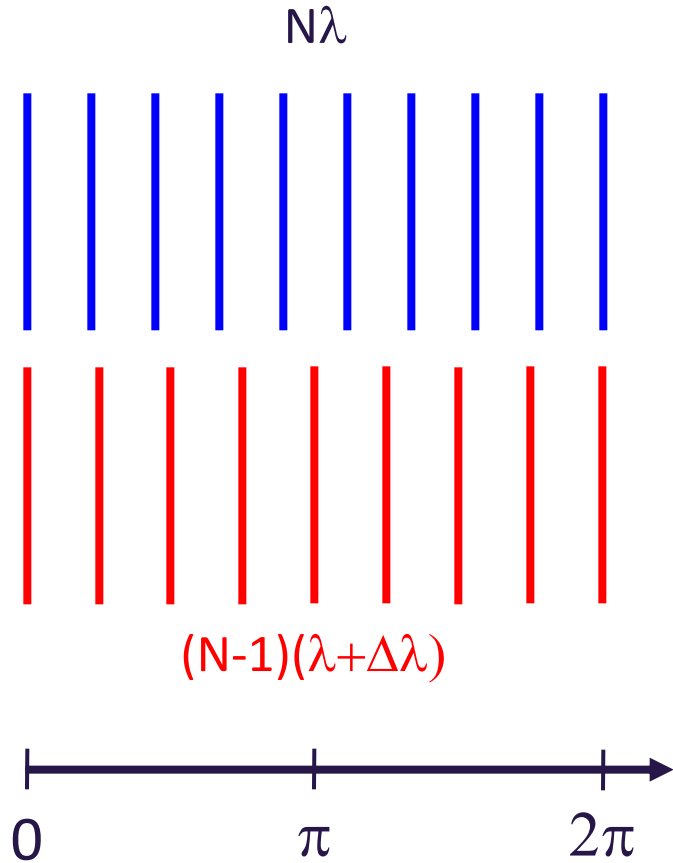
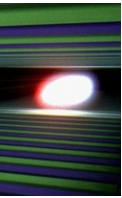
$\Phi$ : probability amplitude

$$\Phi_j \sim \exp[-i(\omega t - k l_j)]$$

$$\omega = ck, \quad k = 2\pi/\lambda, \quad l_j(L, y)$$

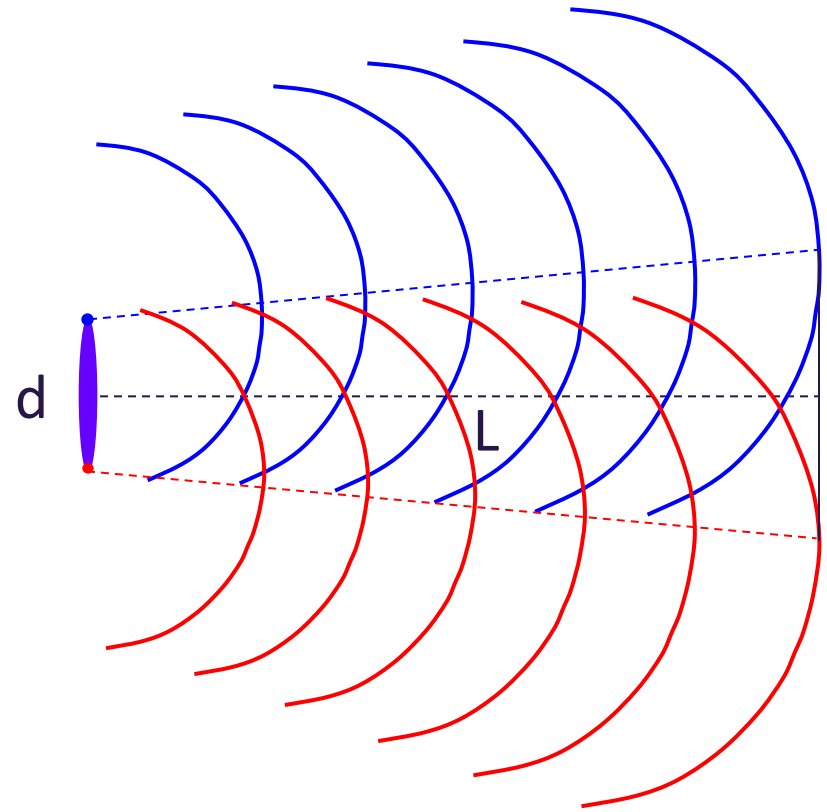
$$P(y) \sim \cos^2(\pi y d / \lambda L)$$

$$\Delta y = \lambda L / d$$



Longitudinal  
coherence length

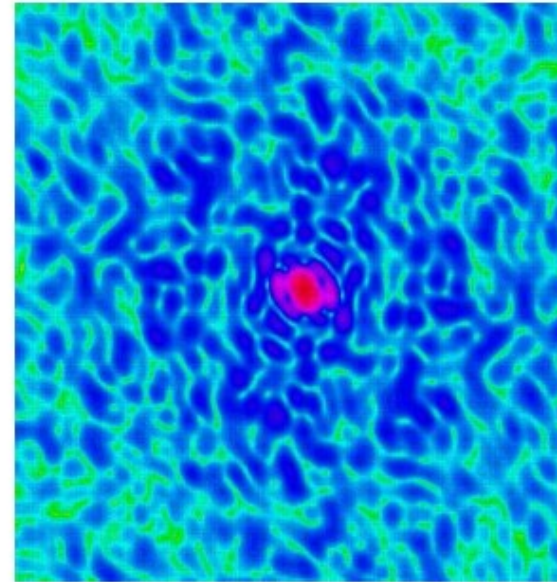
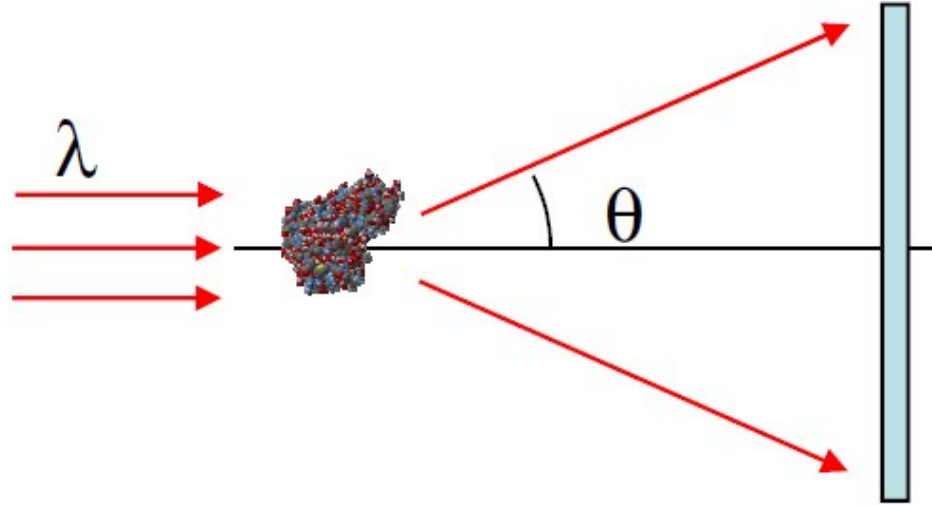
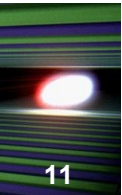
$$l_l = \lambda / 2(\Delta\lambda/\lambda)$$



Transverse  
coherence length

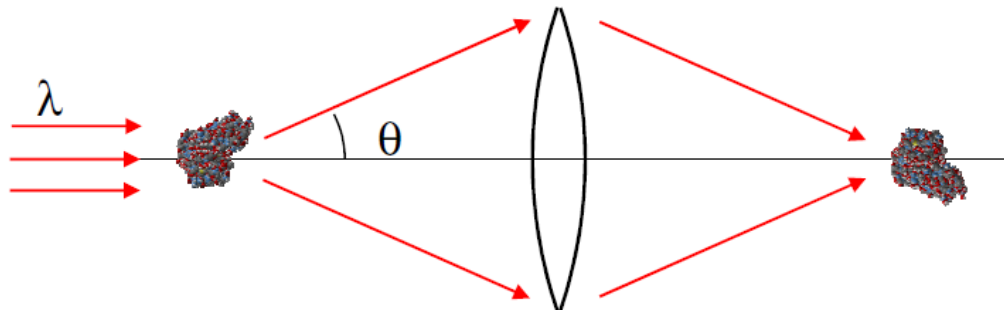
$$l_t = \lambda L / 2d$$





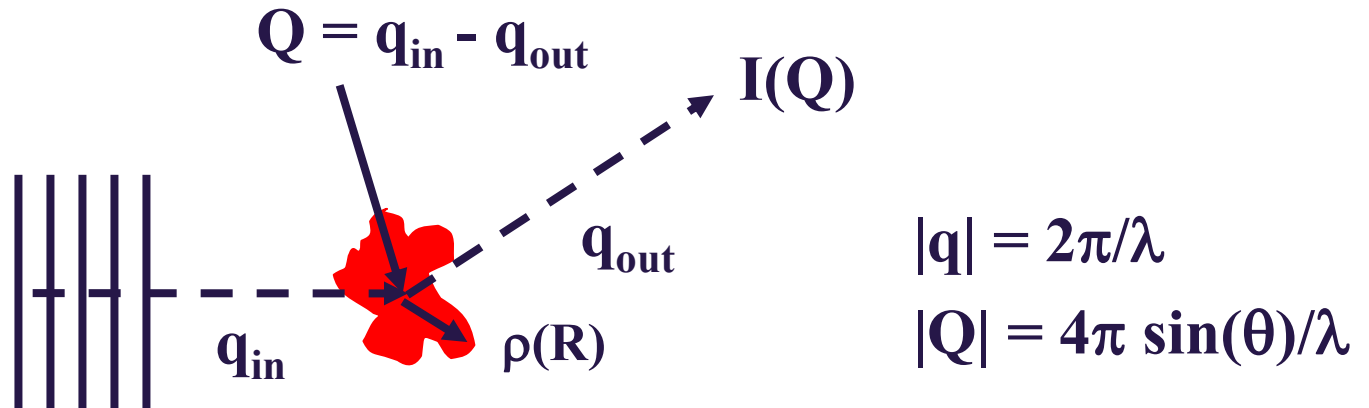
$I(q)$

Using a lens to form the image



Question

Speckle pattern does not look like sample. How to determine the sample from  $I(q)$  ?



$$E(\mathbf{Q}) \sim \int \rho(\mathbf{R}) \exp[i\mathbf{Q} \cdot \mathbf{R}] d\mathbf{R}$$

Reciprocal space  $E(\mathbf{Q}) \leftarrow \leftarrow \leftarrow \text{FT} \rightarrow \rightarrow \rightarrow \rho(\mathbf{R})$  Real space

But...  $I(\mathbf{Q}) = E(\mathbf{Q})E^*(\mathbf{Q}) = |E(\mathbf{Q})|^2$

Aim: To find  $E(Q)$  from measurements of  $I(Q) = |E(Q)|^2$

But  $E(Q)$  is a complex number with both phase and amplitude

$$E(Q) = A \exp(i\phi)$$

Measurement:  $I(Q) = |E(Q)|^2 = A^2$

No direct access to phase....

## Exercise

FT of XFEL logo  $\rightarrow E(Q)$

$I(Q) = |E(Q)|^2$  (simulation of coherent scattering)

Construct  $E(Q)$ :

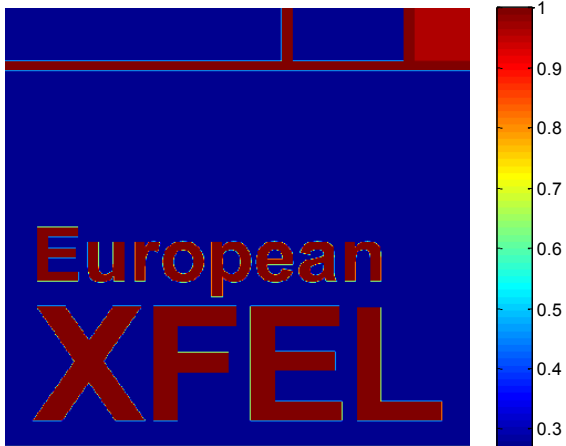
$$A = \sqrt{I(Q)}$$

Take random phases  $\phi$

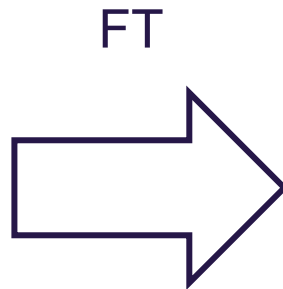
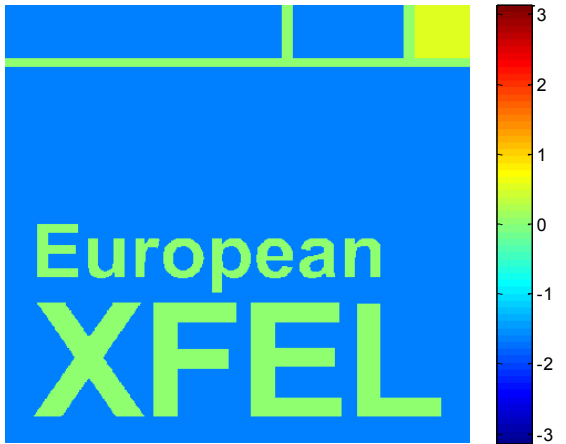
Inverse FT transform of  $A \exp(i\phi)$

$\rho(\mathbf{R})$

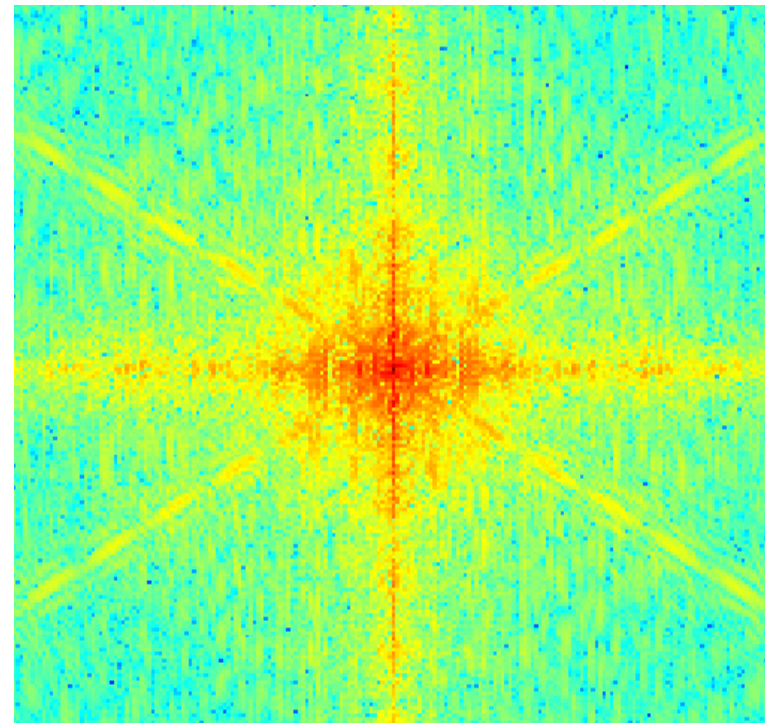
ampl  
A

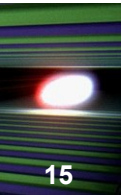


phase  
 $\phi$



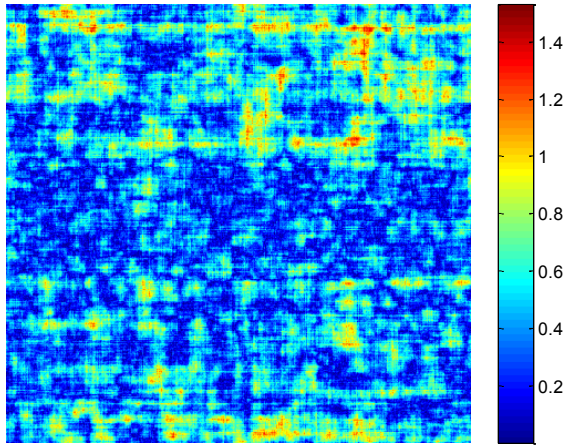
$$|\text{FT}\{\rho(\mathbf{R})\}|^2 = |\mathbf{E}(\mathbf{Q})|^2 = \mathbf{I}(\mathbf{Q})$$



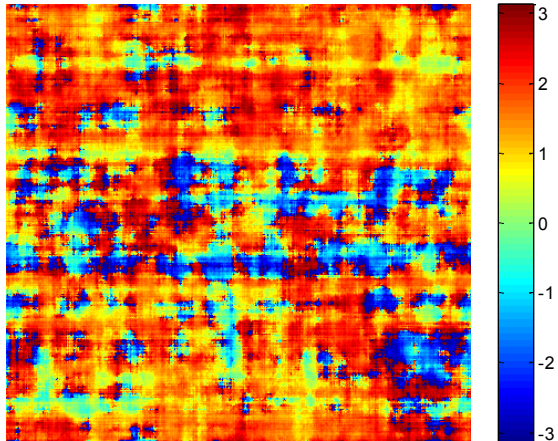


$\rho(\mathbf{R})$

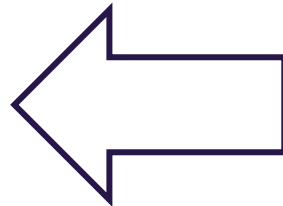
ampl



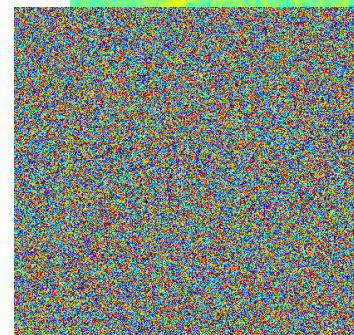
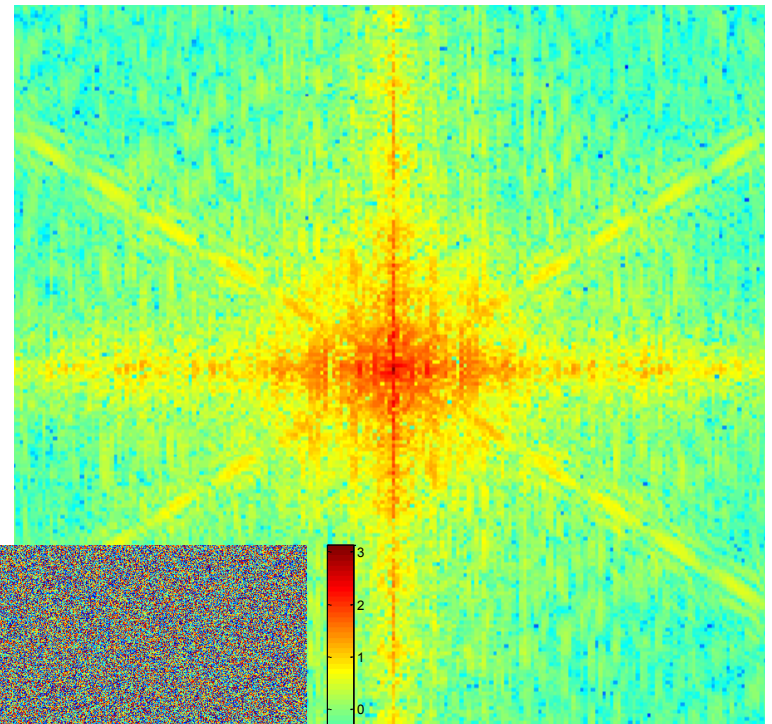
phase



$FT^{-1}\{E(\mathbf{Q})\}$

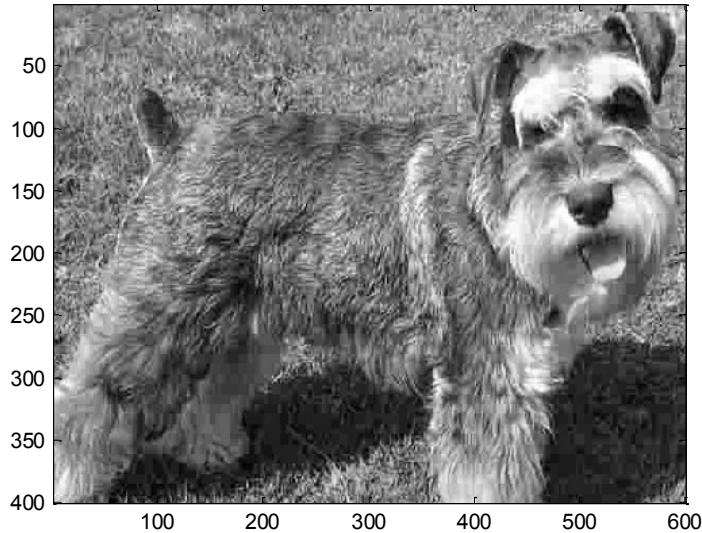
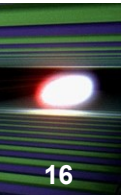


$\sqrt{I(\mathbf{Q})}$  as amplitude



random phases



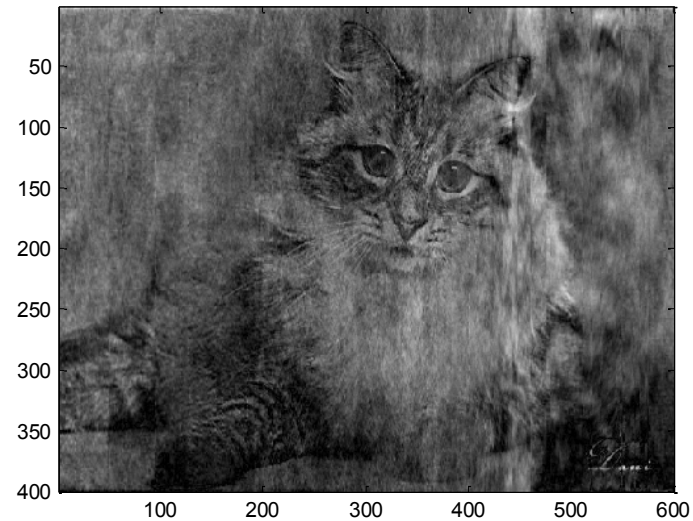
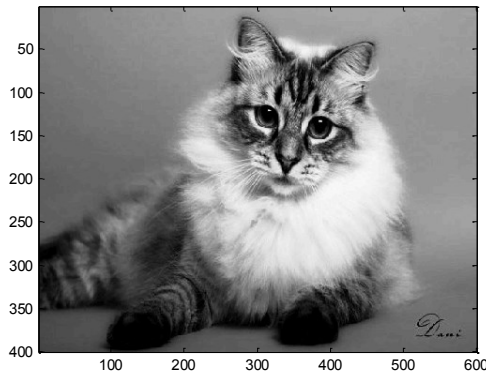


Fourier transform my dog  $\rightarrow A e^{i\phi}$   
 Keep amplitudes  $A$   
 Substitute with another image's phases  $\phi$

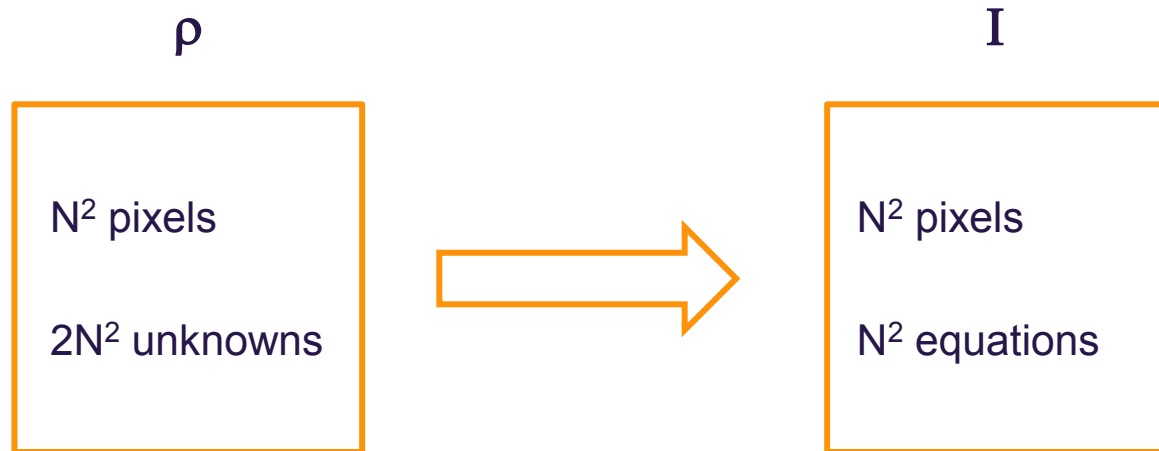
Inverse Fourier transform



The phases came from a cat...







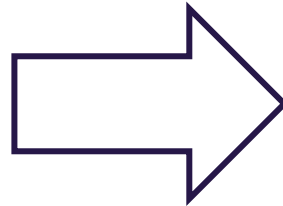
Question

How can we make this solvable?

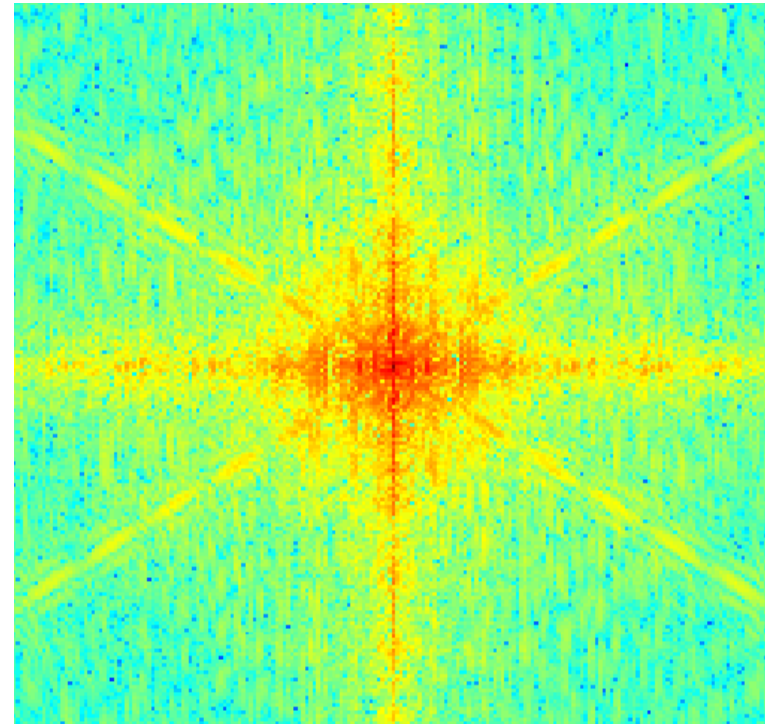
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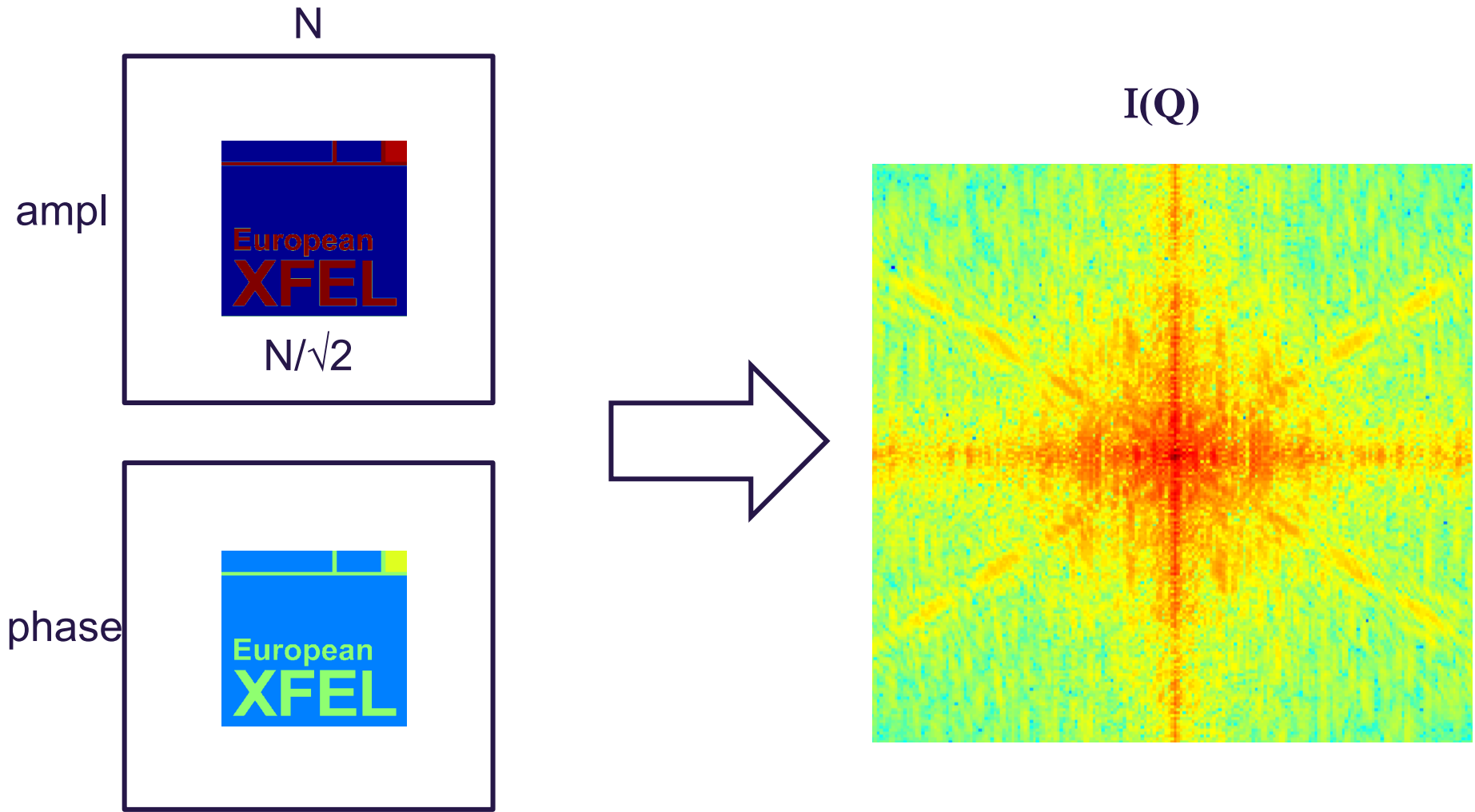
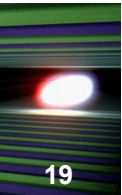


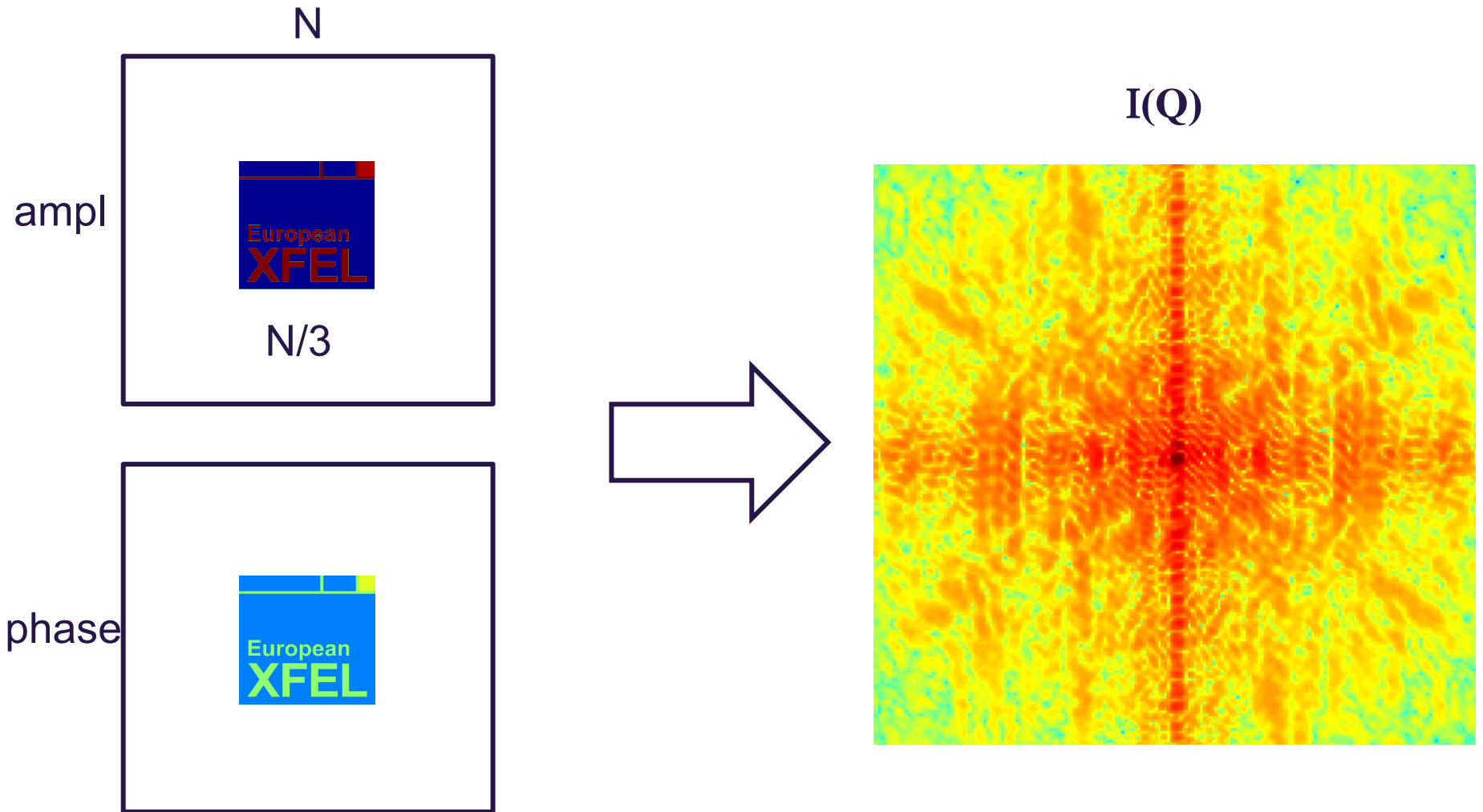
phase

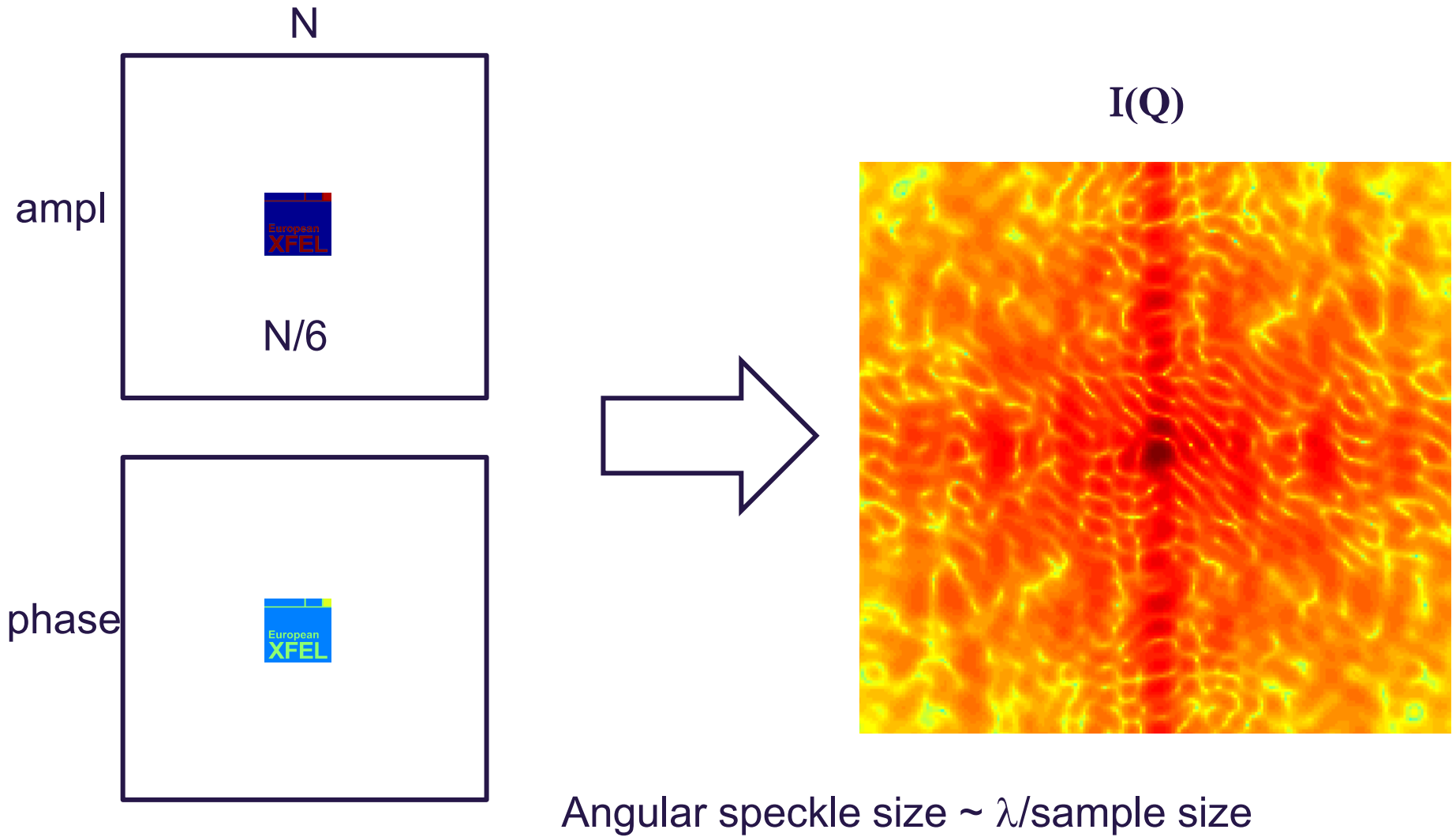
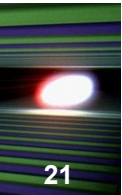


$I(Q)$









## David Sayre (1952)

*Acta Cryst.* (1952). 5, 843

**Some implications of a theorem due to Shannon.** By D. SAYRE, *Johnson Foundation for Medical Physics, University of Pennsylvania, Philadelphia 4, Pennsylvania, U. S. A.*

(Received 3 July 1952)

Shannon (1949), in the field of communication theory, has given the following theorem: If a function  $d(x)$  is known to vanish outside the points  $x = \pm a/2$ , then its Fourier transform  $F(X)$  is completely specified by the values which it assumes at the points  $X = 0, \pm 1/a, \pm 2/a, \dots$ . In fact, the continuous  $F(X)$  may be filled in merely by laying down the function  $\sin \pi a X / \pi a X$  at each of the above points, with weight equal to the value of  $F(X)$  at that point, and adding.

Now the electron-density function  $d(x)$  describing a single unit cell of a crystal vanishes outside the points  $x = \pm a/2$ , where  $a$  is the length of the cell. The reciprocal-lattice points are at  $X = 0, \pm 1/a, \pm 2/a, \dots$ , and hence the experimentally observable values of  $F(X)$  would suffice, by the theorem, to determine  $F(X)$  everywhere, if the phases were known. (In principle, the necessary points extend indefinitely in reciprocal space, but by using, say, Gaussian atoms both  $d(x)$  and  $F(X)$  can be effectively confined to the unit cell and the observable region, respectively.)

For centrosymmetrical structures, to be able to fill in the  $|F|^2$  function would suffice to yield the structure, for sign changes could occur only at the points where  $|F|^2$  vanishes. The structure corresponding to the  $|F|^2$  function is the Patterson of a single unit cell. This has

twice the width of the unit cell, and hence to fill in the  $|F|^2$  function would require knowledge of  $|F|^2$  at the half-integral, as well as the integral  $h$ 's. This is equivalent to a statement made by Gay (1951).

I think the conclusions which may be stated at this point are:

1. Direct structure determination, for centrosymmetric structures, could be accomplished as well by finding the sizes of the  $|F|^2$  at half-integral  $h$  as by the usual procedure of finding the signs of the  $F$ 's at integral  $h$ .
2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where  $|F|^2$  was observed at non-integral  $h$ , it would suffice to have only the values at half-integral  $h$ .

The extension to three dimensions is obvious.

### References

- BOYES-WATSON, J., DAVIDSON, E. & PERUTZ, M. F. (1947). *Proc. Roy. Soc. A*, **191**, 83.
- GAY, R. (1951). Paper presented at the Second International Congress of Crystallography, Stockholm.
- SHANNON, C. E. (1949). *Proc. Inst. Radio Engrs., N.Y.* **37**, 10.

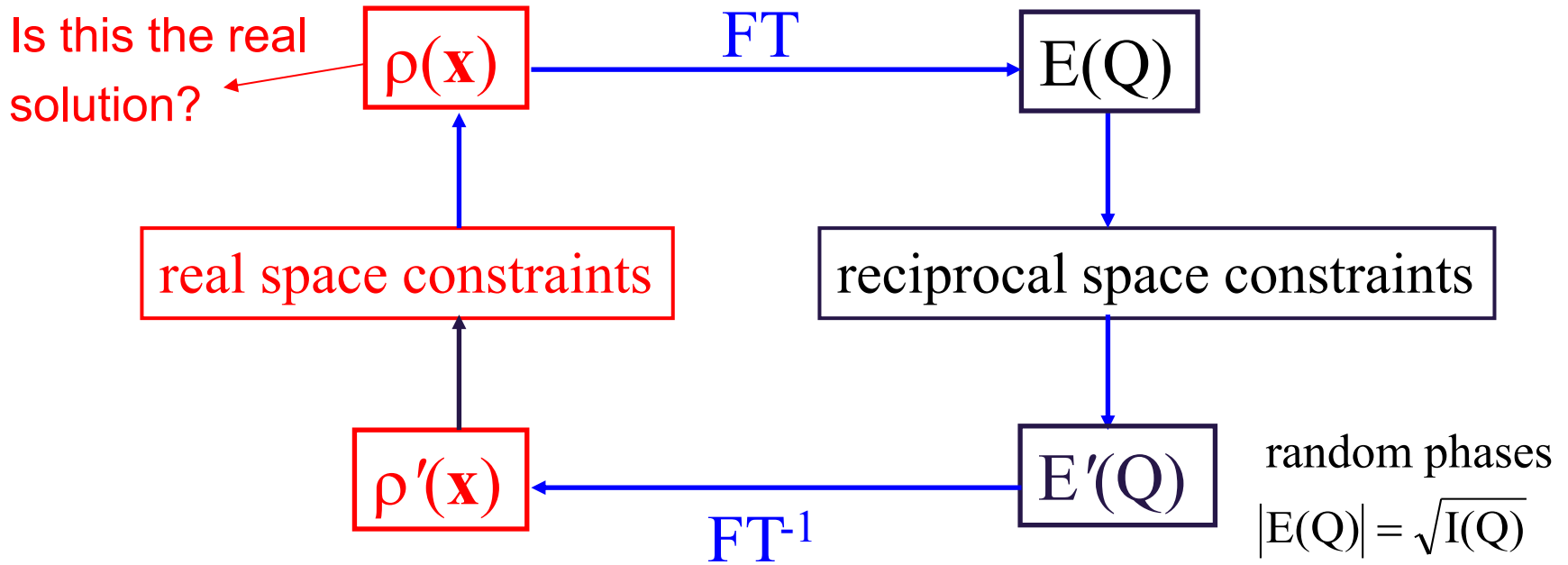
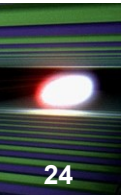


In 2D:

- Need that sample size  $a$  is  $\sqrt{2}$  smaller than beam size  $D$ :  
 $a < D/\sqrt{2}$  (**reduce number of unknowns**)
- Need to measure the speckle pattern with a resolution that is at least  $\sqrt{2}$  finer than speckle size in both dimensions. Therefore, the pixel size  $\Delta p$  must fulfil:  $\Delta p < L\lambda/(a\sqrt{2})$ , where  $L$  is the sample-detector distance (**increase number of equations**)
- Beam must be coherent over the sample size  $a$ , **otherwise the FT relationship does not hold**

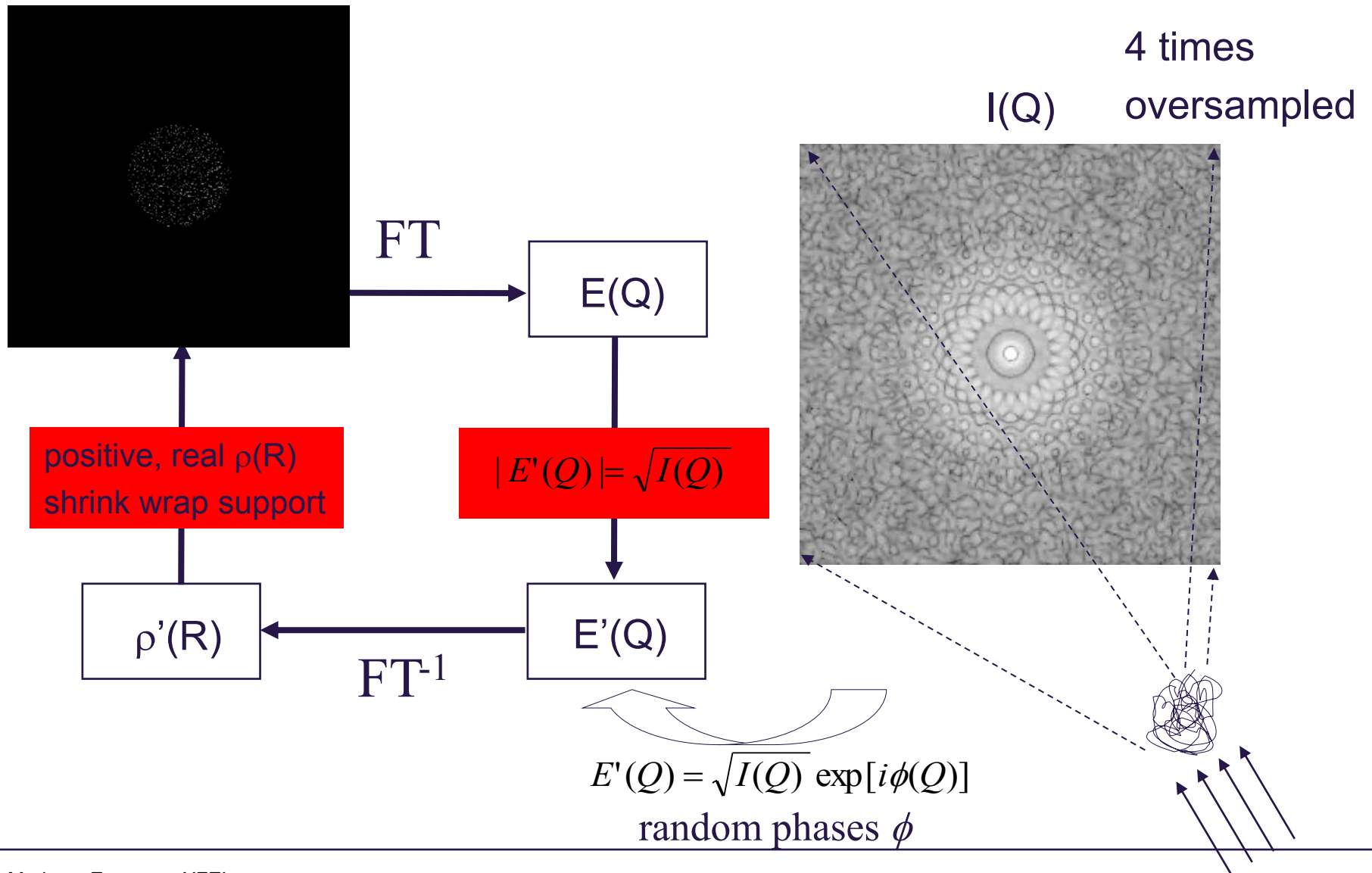
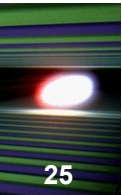
### Question

How to solve the non-linear system of  $N^2$  equations and  $M$  unknowns ( $M < N^2$ ) to find  $\rho(R)$ ?



Real space constraints:  
 finite support ( $\rho=0$  outside sample)  
 real  $\rho$  ? positive  $\rho$  ? other?

Reciprocal space constraints  
 $|E(Q)| \rightarrow \sqrt{I(Q)}$

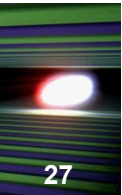


R. W. Gerchberg and W. O. Saxton, *Optik* **35**, 237 (1972)

J.R. Fienup, *Appl. Opt.* **21**, 2758 (1982)

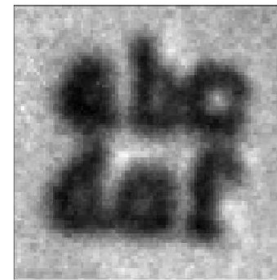
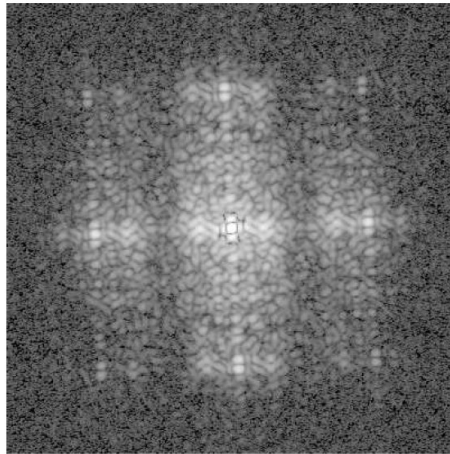
Review: R. Millane *et al.*, *J. Opt. Soc. Am.* **A14**, 568 (1997)

Difference map: V. Elser, *J. Opt. Soc. Am.* **A20**, 40 (2003)



Data collected at NSLS beamline X1B

$\lambda = 1.8$  nm  
soft x-ray  
diffraction  
pattern



Low angle data  
From optical  
micrograph

Scanning  
electron  
micrograph  
of object

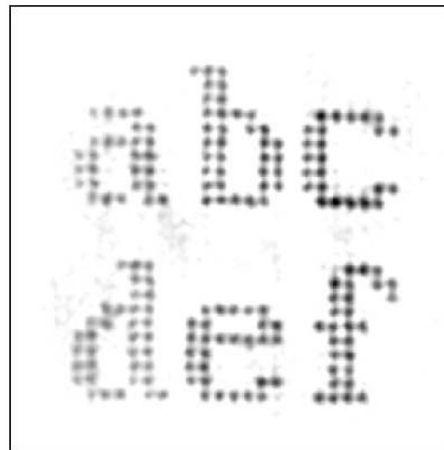
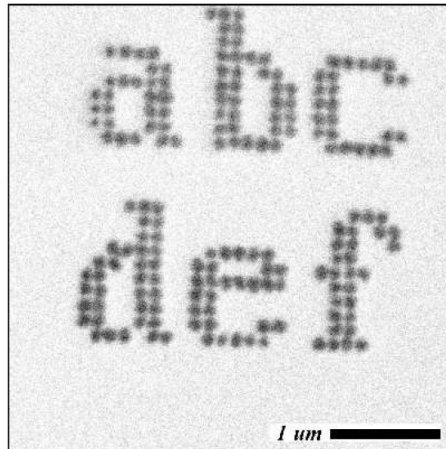
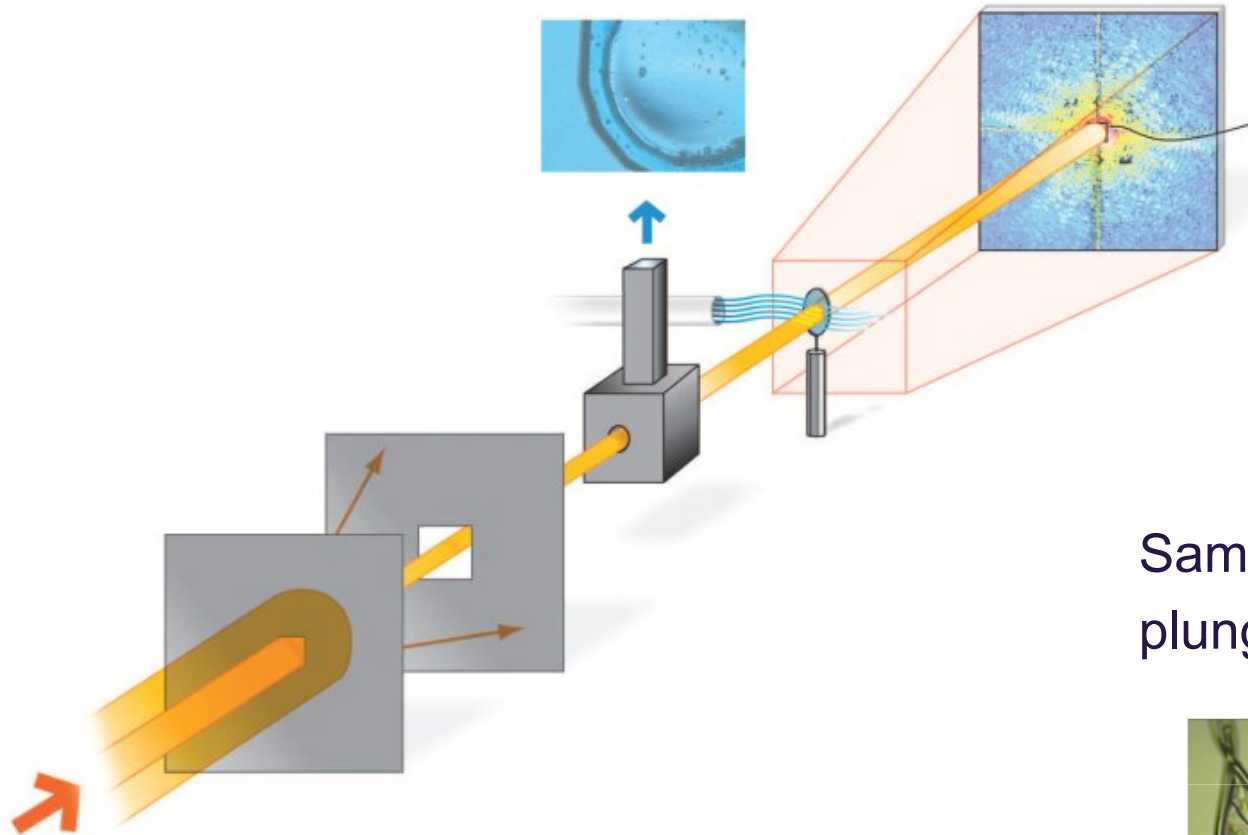
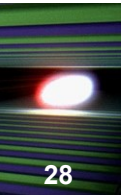
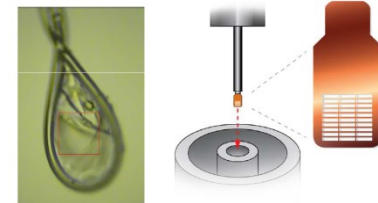


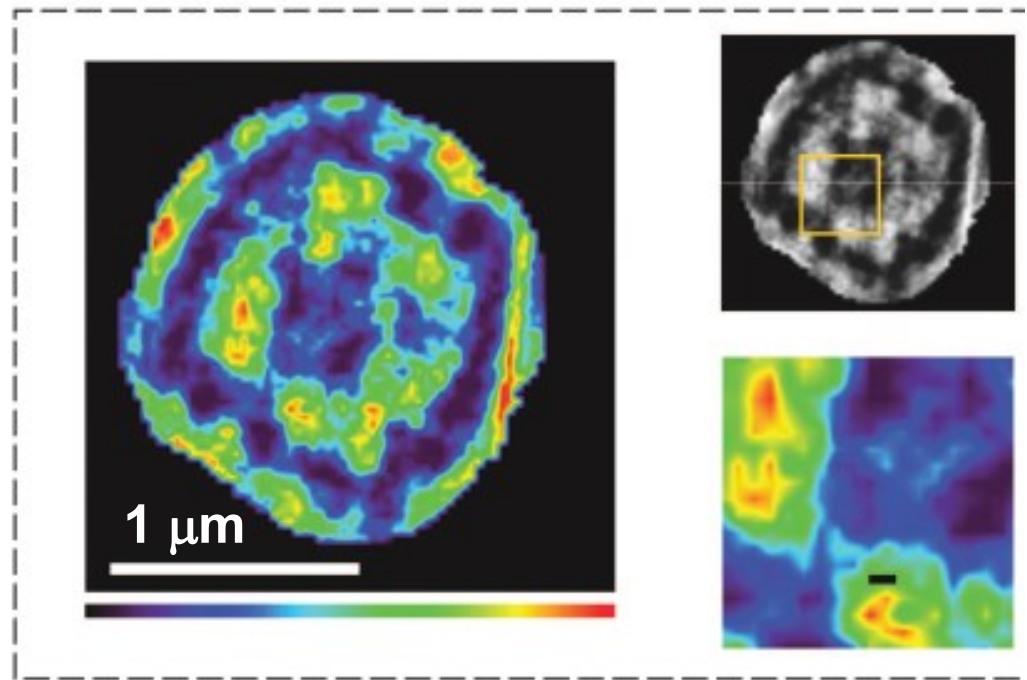
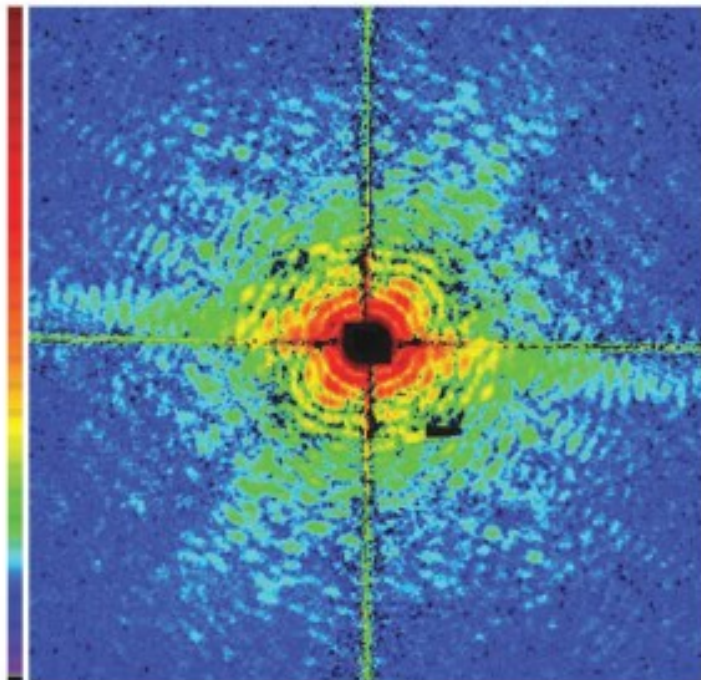
Image  
reconstructed from  
diffraction pattern  
( $\theta_{\max}$  corresponds to  
80 nm). Assumed  
positivity



Sample preparation  
plunge-freezing





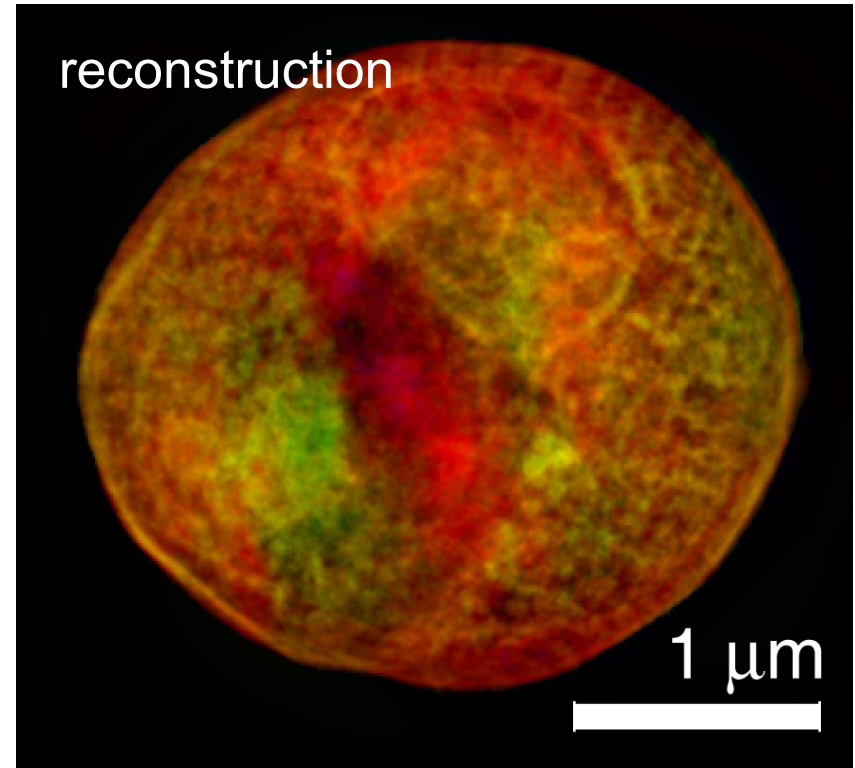
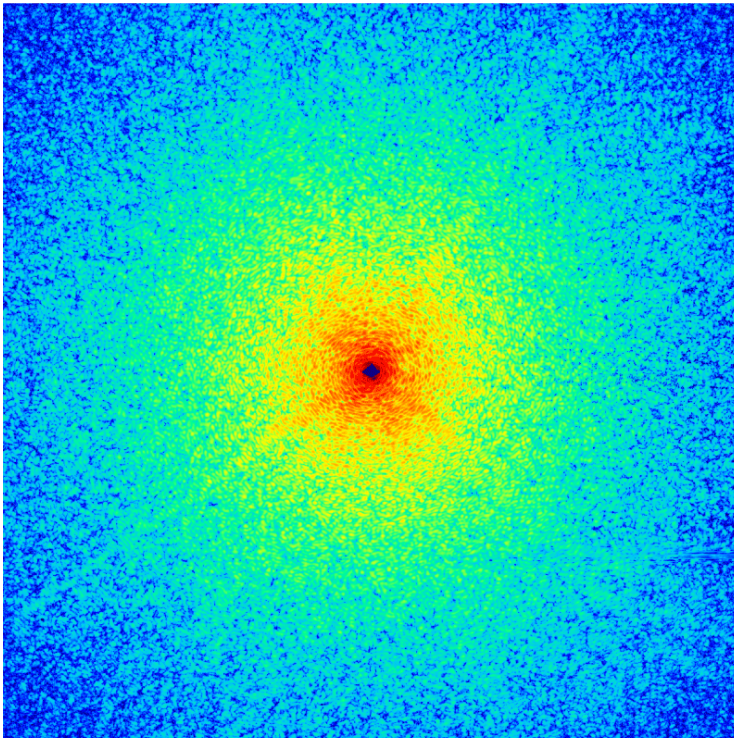
*D. Radiodurans cell*

Resolution about 30 nm

Goal: ~10 nm

CDI from a yeast cell.

Speckle pattern,  $\lambda=16.5$  Å (ALS)



No shrink warp, “hand drawn” support

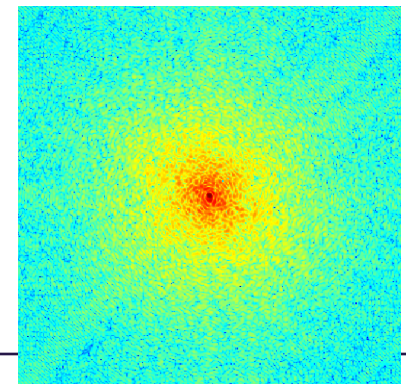
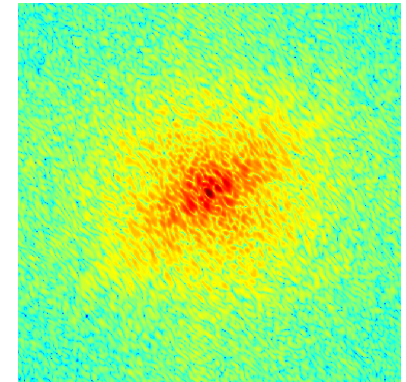
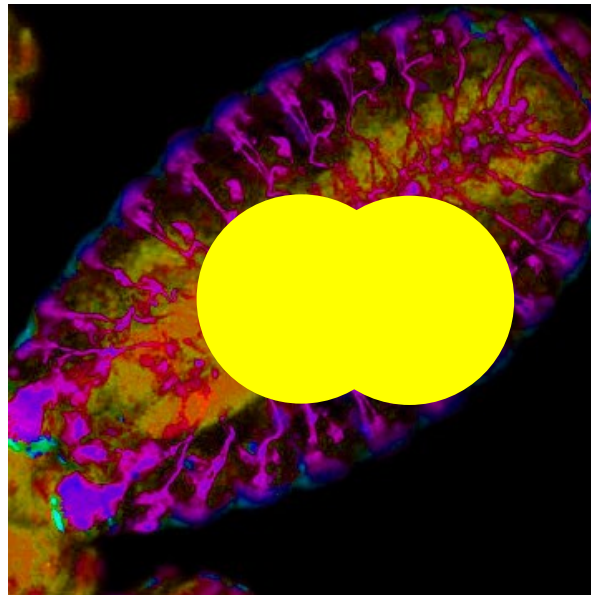
Difference map algorithm

Averaging iterates (Elser & Thibault)

Resolution ~ 30 nm

- The requirement that sample  $<$  beam is a limitation for many practical purposes
- Can we find another constraint so the  $2N^2$  unknowns can be determined?
- The answer is : Ptychography!

Ptych- :  
(to) fold (from Greek)





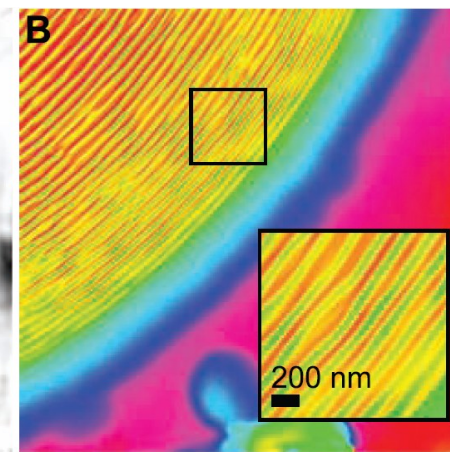
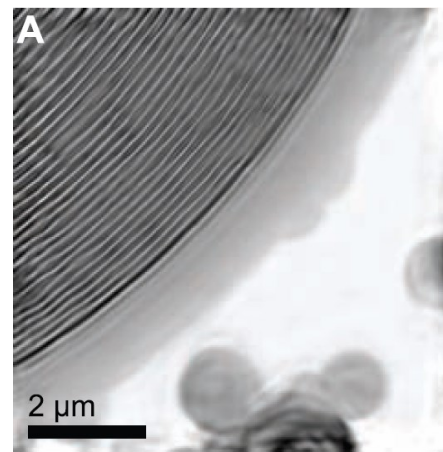
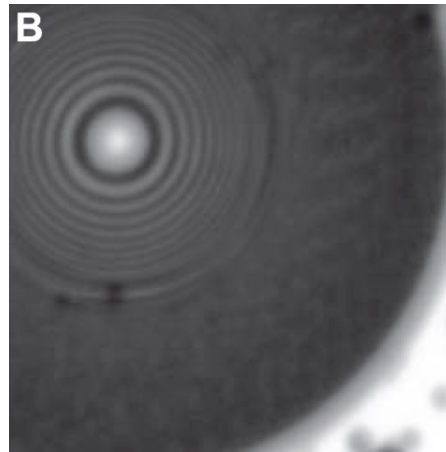
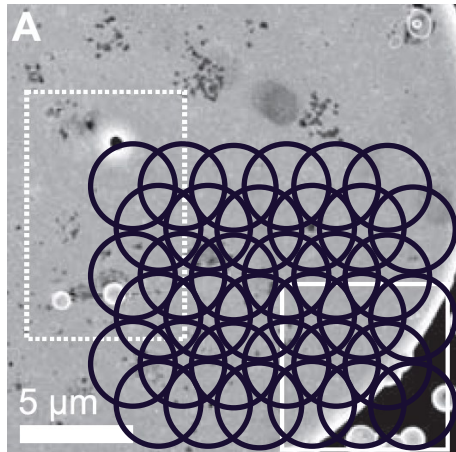
# High-Resolution Scanning X-ray Diffraction Microscopy

Pierre Thibault,<sup>1\*</sup> Martin Dierolf,<sup>1</sup> Andreas Menzel,<sup>1</sup> Oliver Bunk,<sup>1</sup> Christian David,<sup>1</sup> Franz Pfeiffer<sup>1,2</sup>

Science, **321**, 379-382 (2008)

SEM

absorption



0.15 0.85

$-\pi$   $\pi$

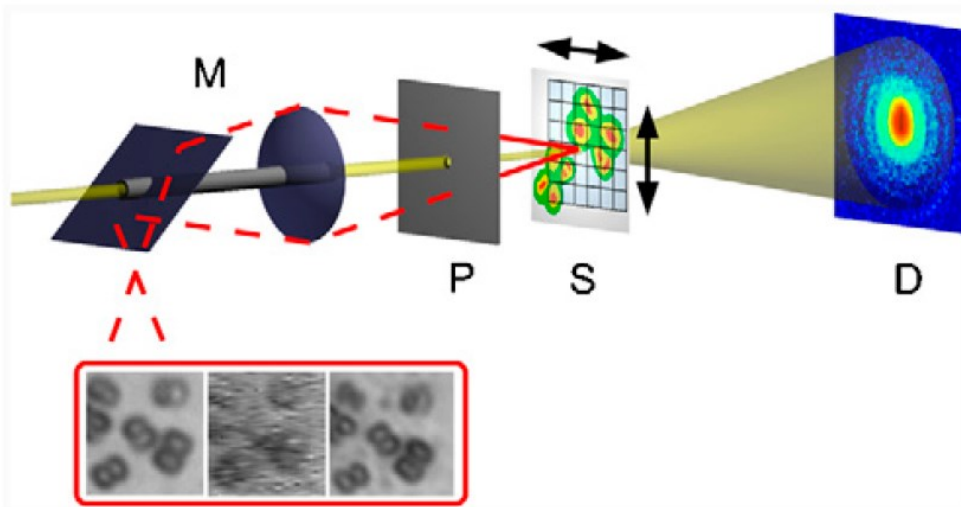
Buried zone plate

# Quantitative biological imaging by ptychographic x-ray diffraction microscopy

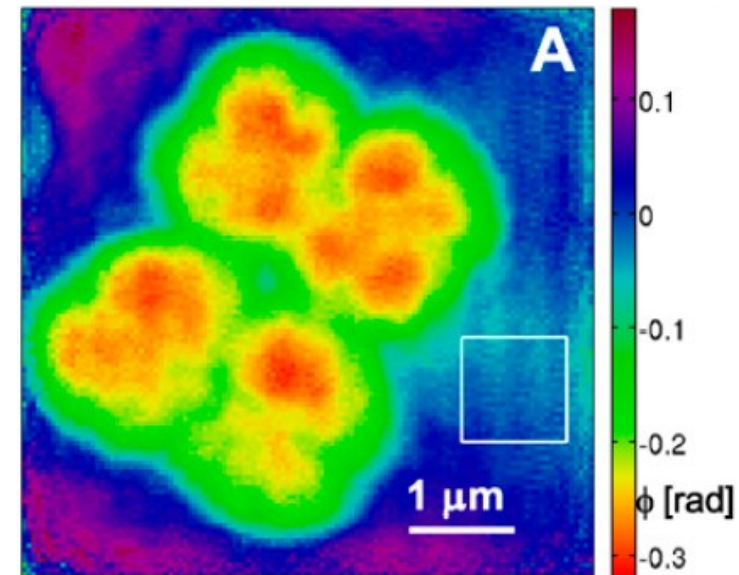
Klaus Giewekemeyer<sup>a,1</sup>, Pierre Thibault<sup>b</sup>, Sebastian Kalbfleisch<sup>a</sup>, André Beerlink<sup>a</sup>, Cameron M. Kewish<sup>c</sup>, Martin Dierolf<sup>b</sup>, Franz Pfeiffer<sup>b</sup>, and Tim Salditt<sup>a,1</sup>

Proc. Natl. Acad. Sci. USA 107, p. 529-534 (2010)

Setup at cSAXS beamline, SLS



D. Radiodurans



## Question

Do you know another method where the phases are encoded, i.e. easy reconstruction?

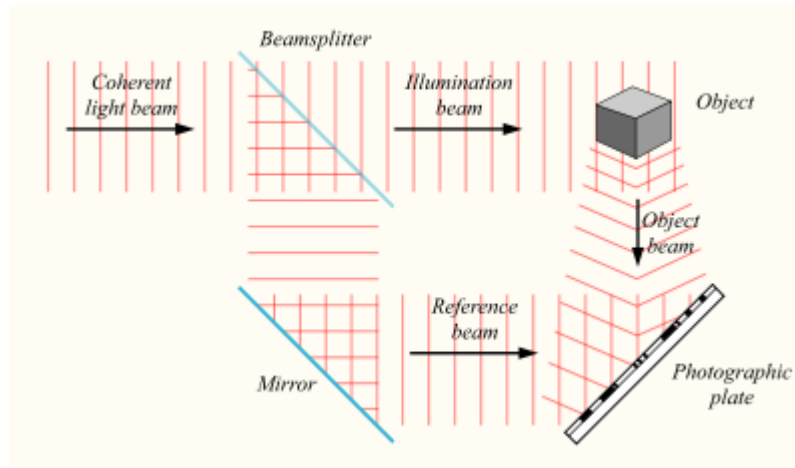
Famous method to encode the phases in the intensity pattern



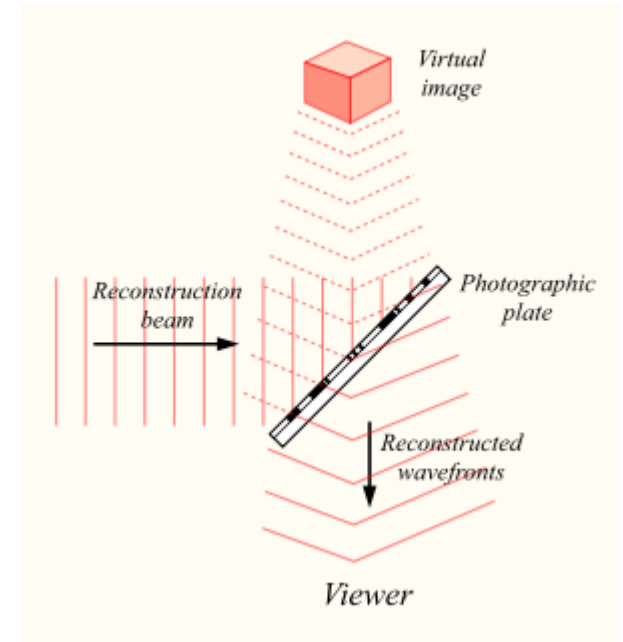
Dennis Gabor  
Nobel prize 1971

In-line holography (electrons, Gabor 1947);  
Laser (1960), 1<sup>st</sup> optical hologram ~1962

### Recording



### Holographic reconstruction



First SR hologram:

Aoki et al. Jap. J. Appl. Phy 11,  
1857 (1972)



## Fourier transform holography

- Spherical reference wave ( $r$ ) spreads speckles and encodes phases of object wave ( $o$ )
- Simple reconstruction by FT:

$$I_{\text{holo}} = |\text{FT}\{o+r\}|^2 = |\text{FT}\{o\} + \text{FT}\{r\}|^2 = |O + R|^2 = |O|^2 + |R|^2 + OR^* + RO^*$$

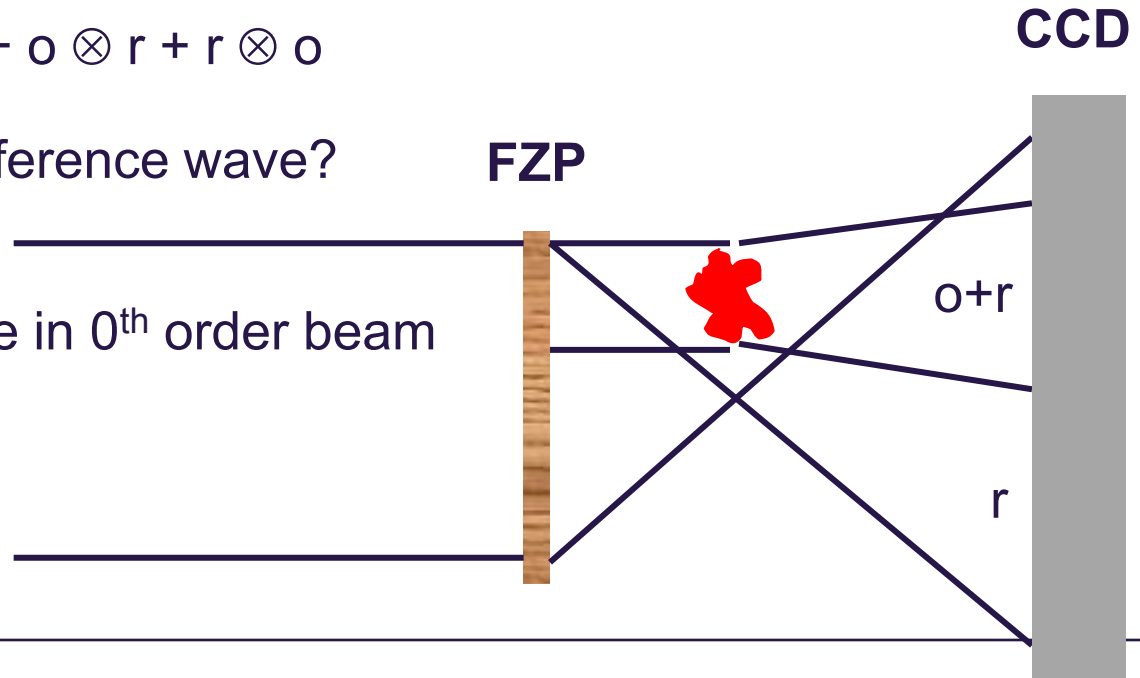
$$\text{FT}\{I_{\text{holo}}\} = o \otimes o + r \otimes r + o \otimes r + r \otimes o$$

- How to get a spherical reference wave?

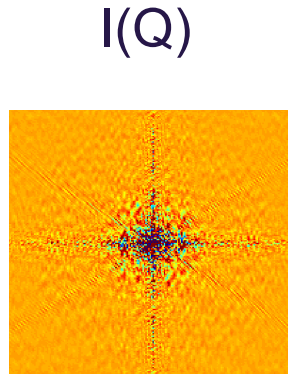
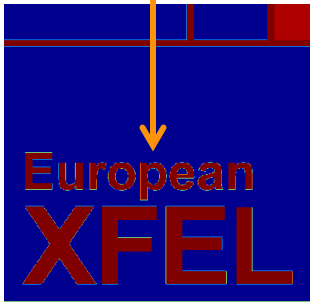
1<sup>st</sup> order from a FZP, sample in 0<sup>th</sup> order beam

McNulty et al,

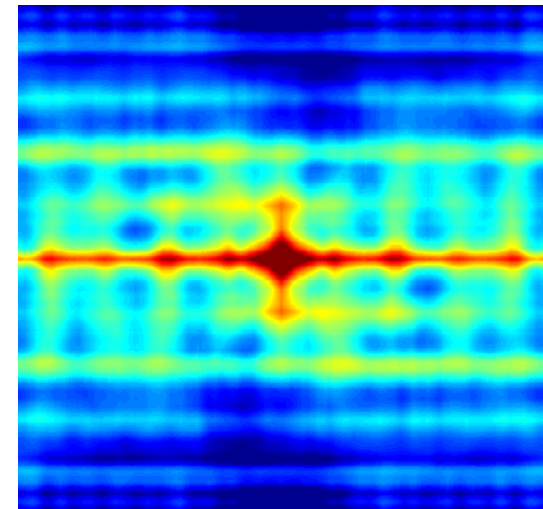
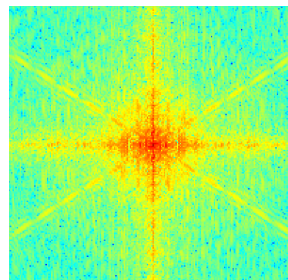
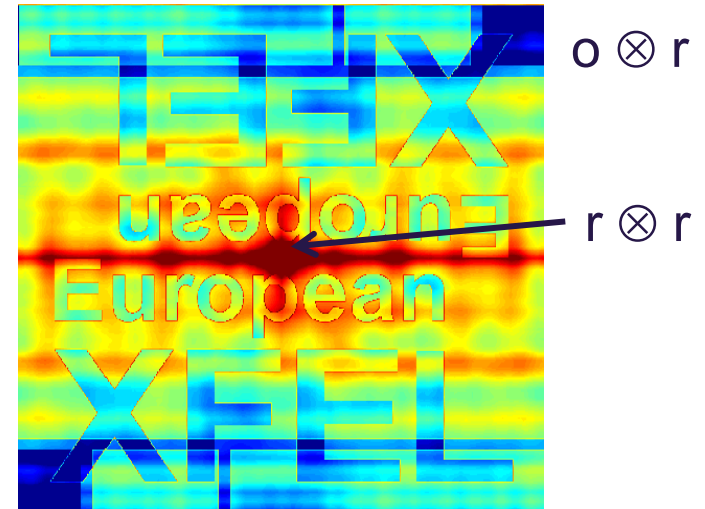
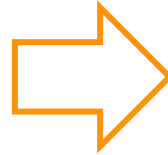
Science **256**, 1009 (1992)

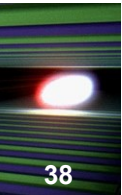


Strong reference  
scatterer

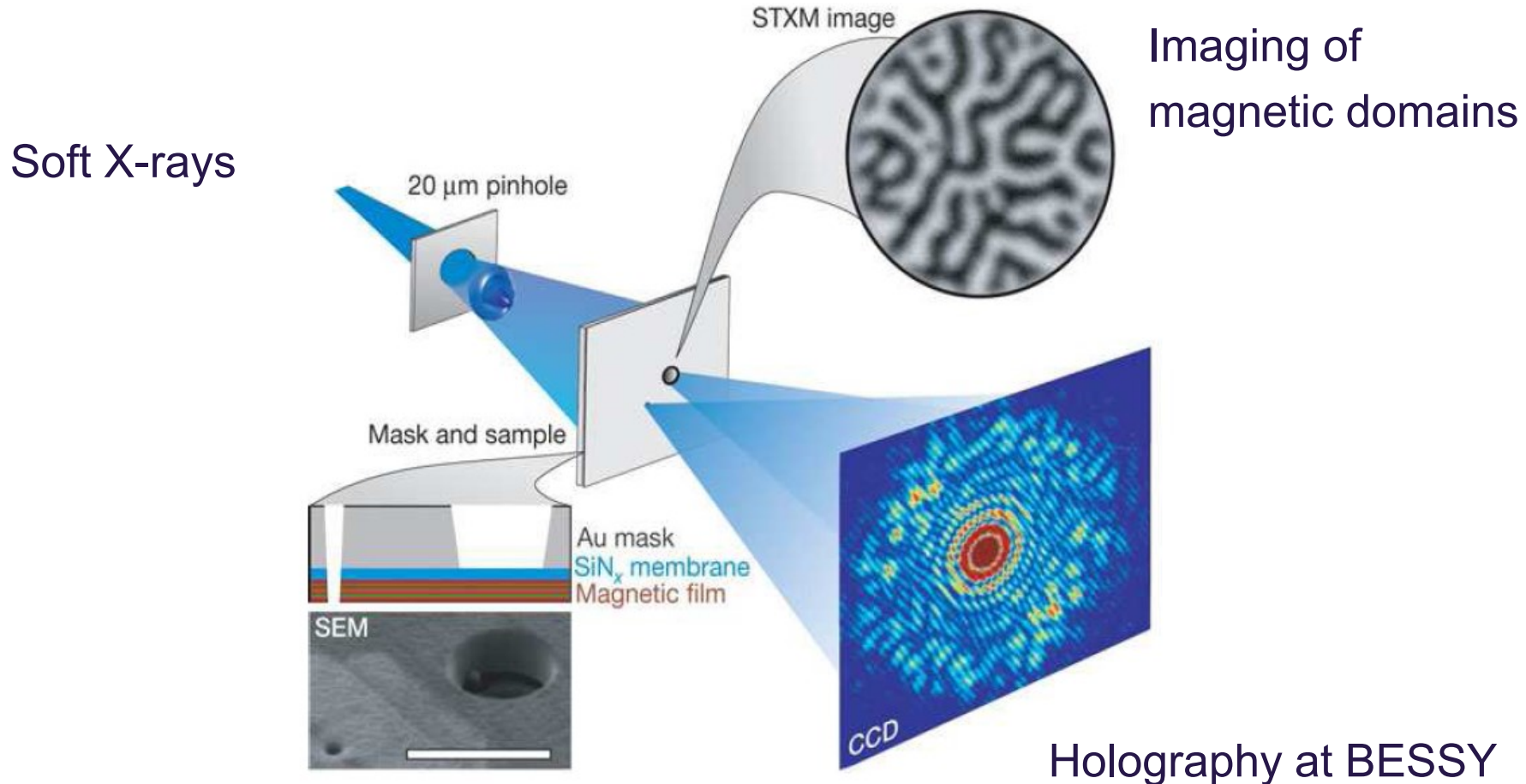


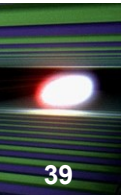
FT  $\{I(Q)\}$



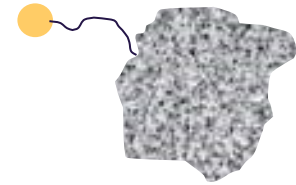


S. Eisebitt, J. Lüning, W. F. Schlotter, M. Lörger, O. Hellwig, W. Eberhardt and J. Stöhr Nature 432, 885-888(2004)

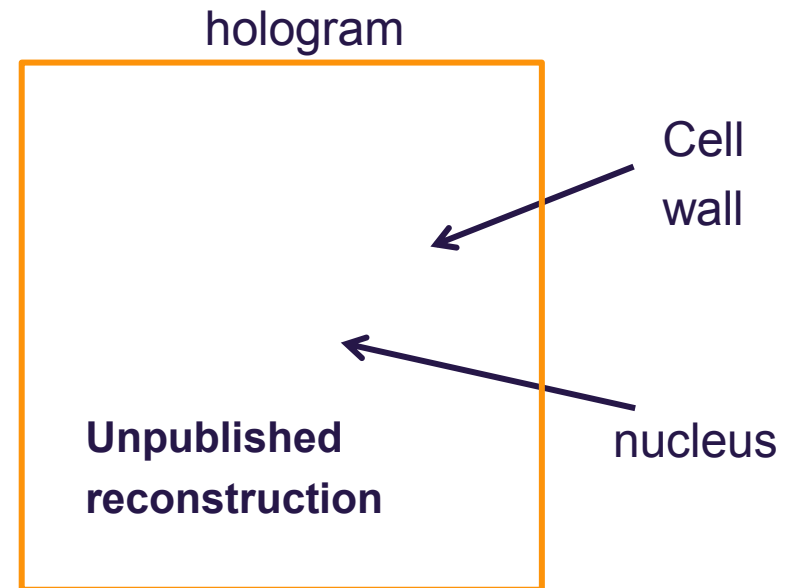
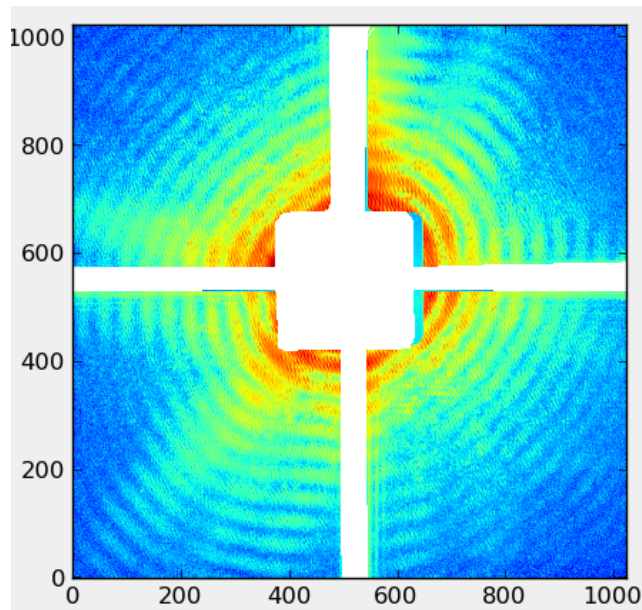




Holography of *Pichia Pastoris* (yeast) cell + 250 nm Au particle

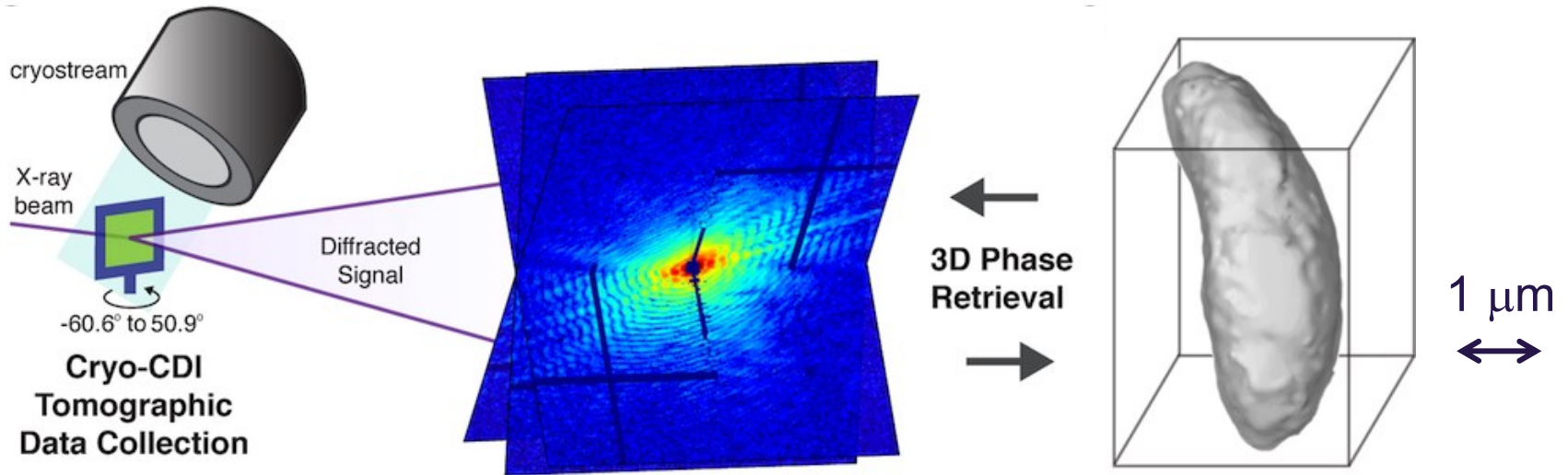


1<sup>st</sup> results from ID10, ESRF @ 8 keV

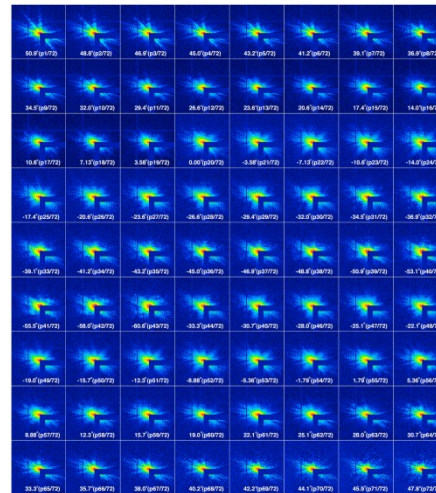


Shadow sculptures, Tim Noble and Sue Webster

<http://www.thisismarvelous.com/amazing-shadow-sculptures-by-tim-noble-and-sue-webster/>



More than 100 different  
2D projections necessary  
for 3D phase retrieval

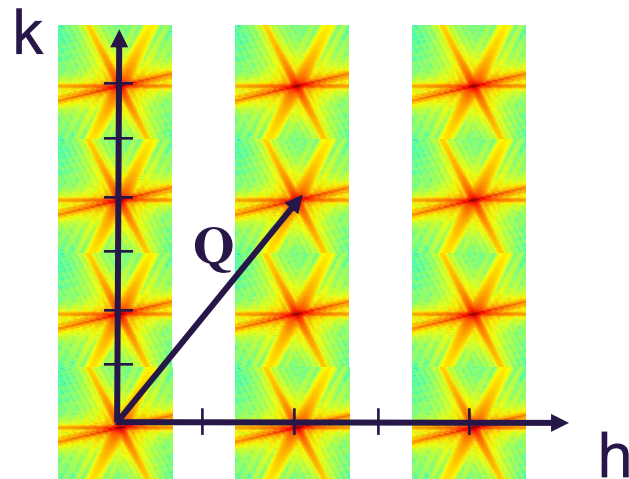
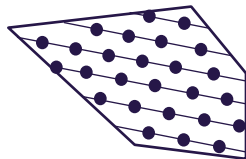
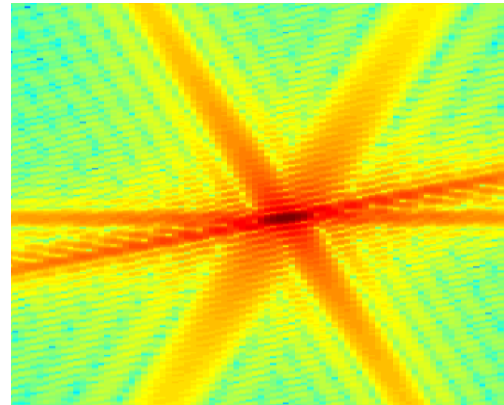
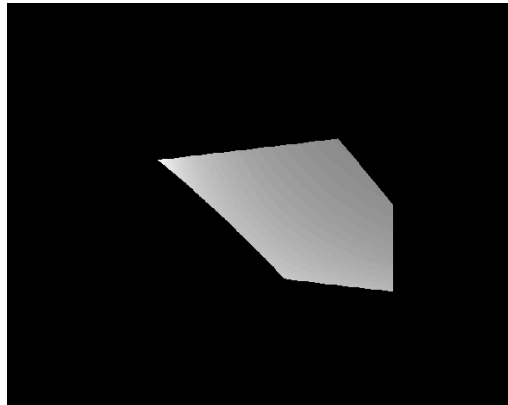
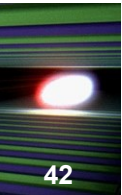


*Neospora caninum*  
parasite

Rodriguez *et al.* (2015)

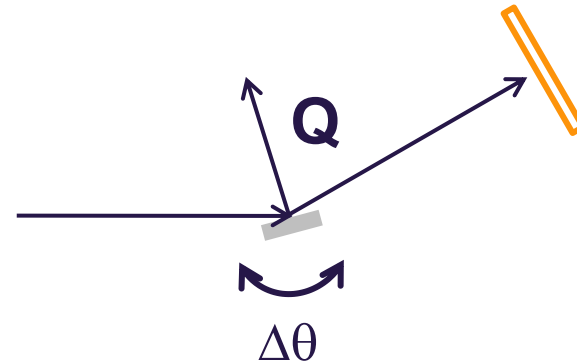
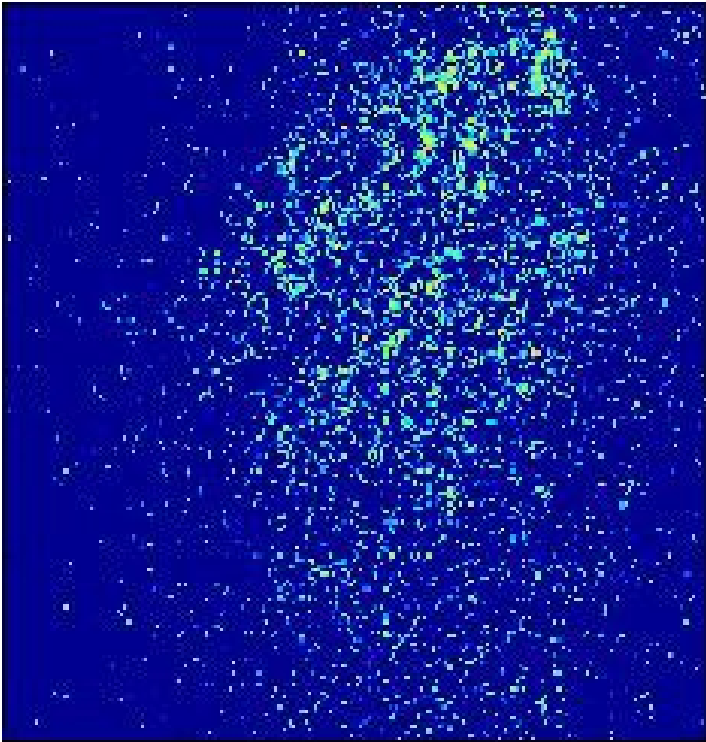
IUCrJ 2, 575

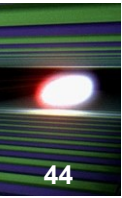




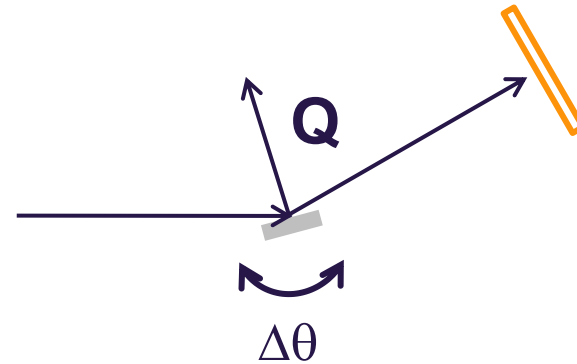


Rocking scan ( $\Delta\theta$ ) sweeps the detector-plane through reciprocal space

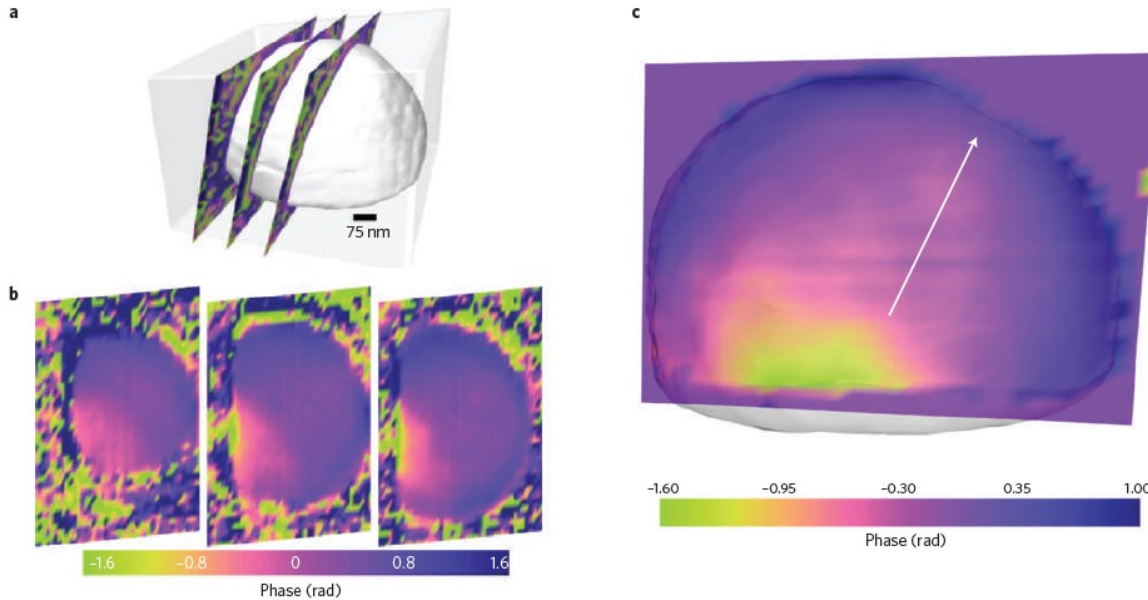




Rocking scan ( $\Delta\theta$ ) sweeps the detector-plane through reciprocal space



## Study of Pb nanocrystals



I. K. Robinson & R. Harder  
Nature Materials **8**, 291 (2009)

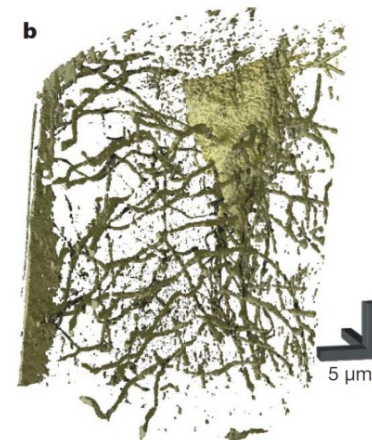
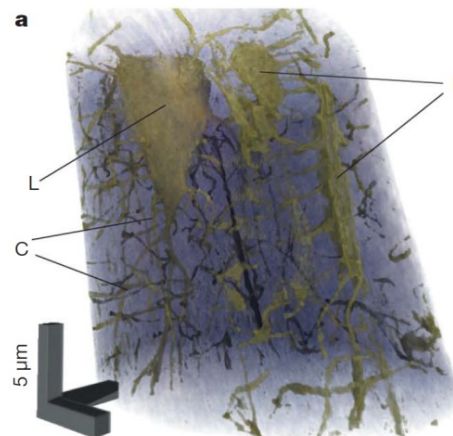
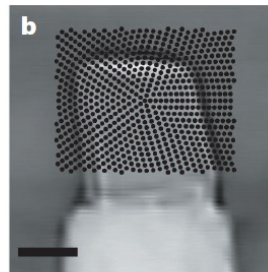
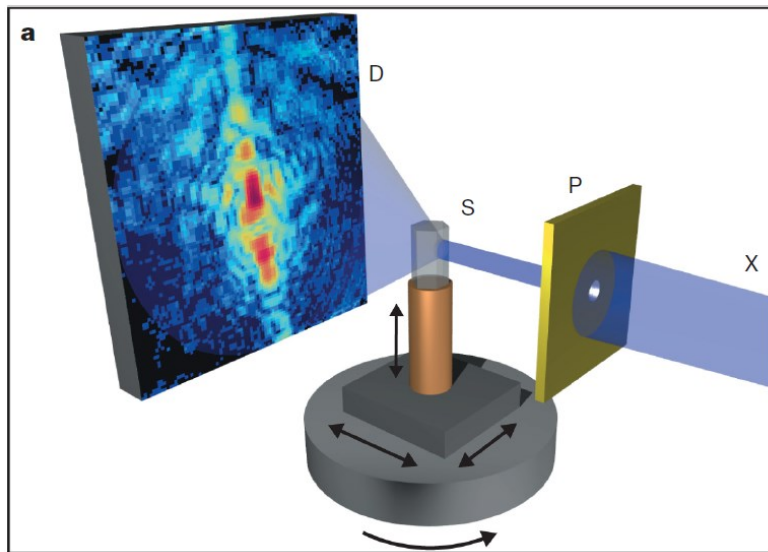
Work from APS, sector 34

# Ptychographic X-ray computed tomography at the nanoscale

Martin Dierolf<sup>1</sup>, Andreas Menzel<sup>2</sup>, Pierre Thibault<sup>1</sup>, Philipp Schneider<sup>3</sup>, Cameron M. Kewish<sup>2†</sup>, Roger Wepf<sup>4</sup>, Oliver Bunk<sup>2</sup> & Franz Pfeiffer<sup>1</sup>

Nature **467**, p. 436 (2010)

**Figure 3 | 3D rendering of the tomographic reconstruction.** **a**, Volume rendering with the bone matrix in translucent colours to show osteocyte lacunae (L) and the connecting canaliculi (C). **b**, Isosurface rendering of the lacuno-canalicular network obtained by segmenting the corresponding peak in the density on histogram shown in Fig. 4c. Morphological analysis of tomographic reconstructions is most often based on this type of segmentation, which is independent of the absolute scale of the density. Long edges of 3D scale bars, 5  $\mu\text{m}$ .



- Why is phase important
- How does phase retrieval work in coherent diffraction imaging
- How does phase retrieval work in ptychography
- How does phase retrieval work in holography
- Examples of published work
- 3D resolution is needed!

Next: X-ray sources, new opportunities with Free-electron lasers  
The European X-ray Free-Electron Laser in Hamburg

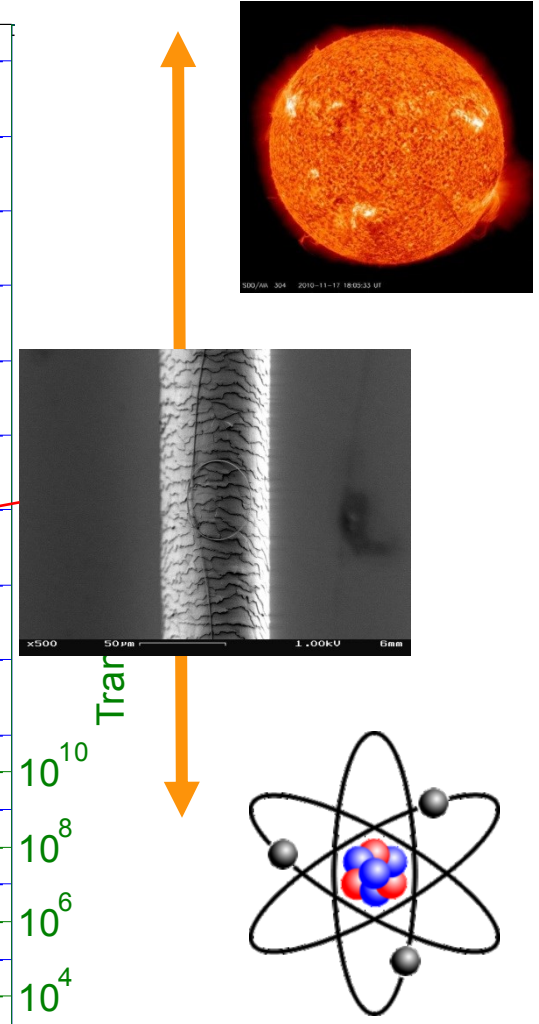
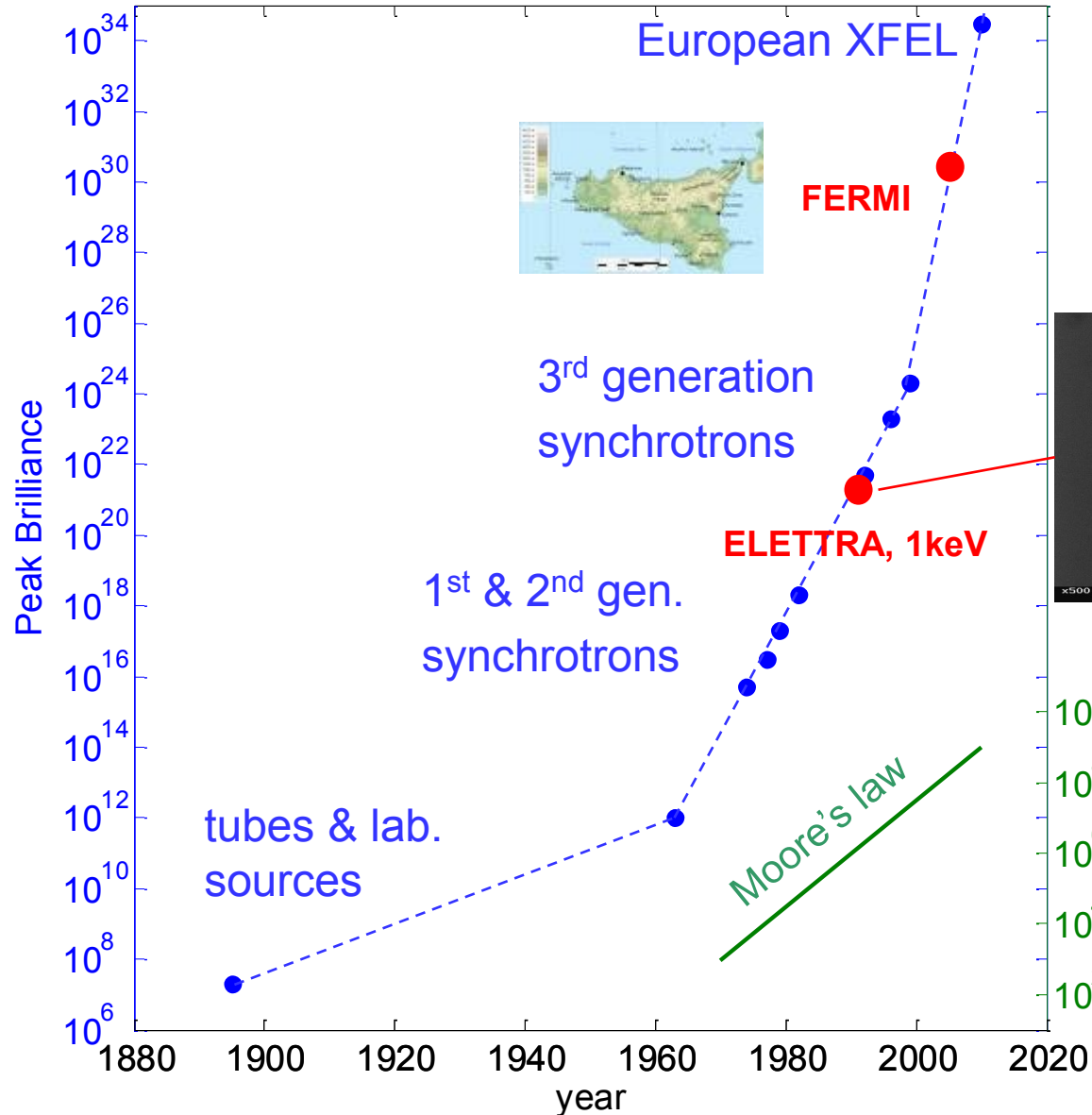
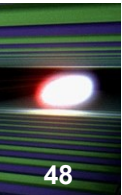
$$I_C = \lambda^2 B / 4^{(*)}$$

B: Brilliance (spectral brightness) of source

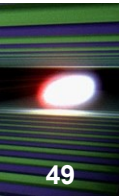
$$B: \frac{ph/s}{mm^2 mrad^2 0.1\%BW}$$



(\*) only strictly valid for chaotic sources



Trans



## Soft X-Rays:

FLASH (Hamburg, Germany)

[first x-ray laser]

FERMI (Trieste, Italy)

[first seeded x-ray laser]

...

## Hard X-Rays:

LCLS (Stanford, USA)

[first hard x-ray laser]

SACLA (Sayo, Japan)

PAL-XFEL (Pohang, Korea), first beam ~2016

SwissFEL (Villingen, Switzerland), first beam ~2016

European XFEL (Hamburg, Germany), first beam ~2017

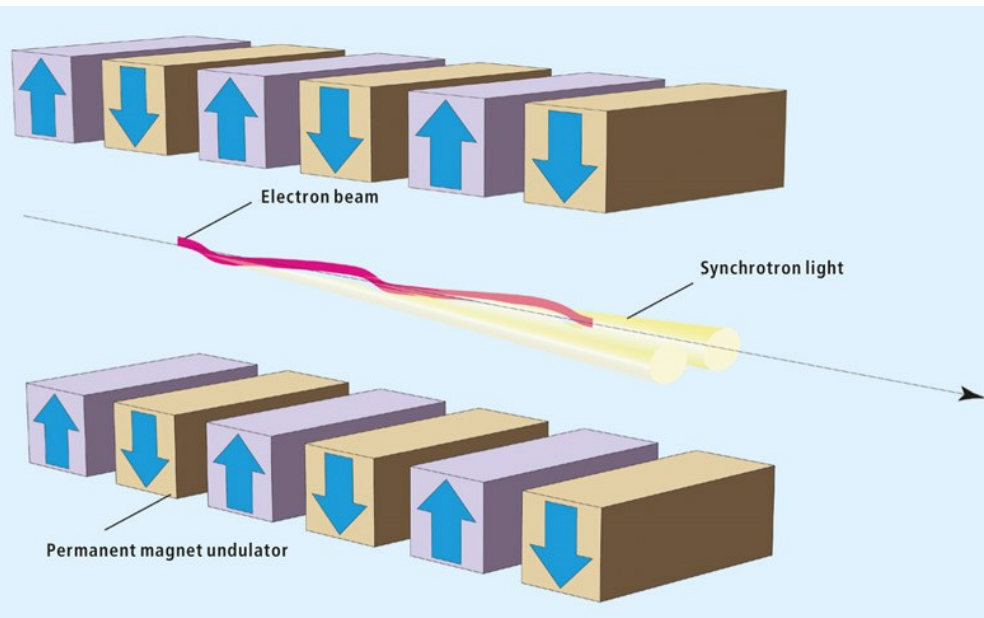
...



**Undulator:** Magnetic device installed in the straight sections of the synchrotron

$$\mathbf{F} = e(\mathbf{v} \times \mathbf{B})$$

$N \sim 100$   
magnetic poles

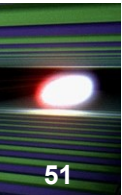


1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> generation

$I \propto N_e$  (Bending magnet)

$I \propto N_e \cdot N$  (Wiggler)

$I \propto N_e \cdot N^2$  (Undulator)

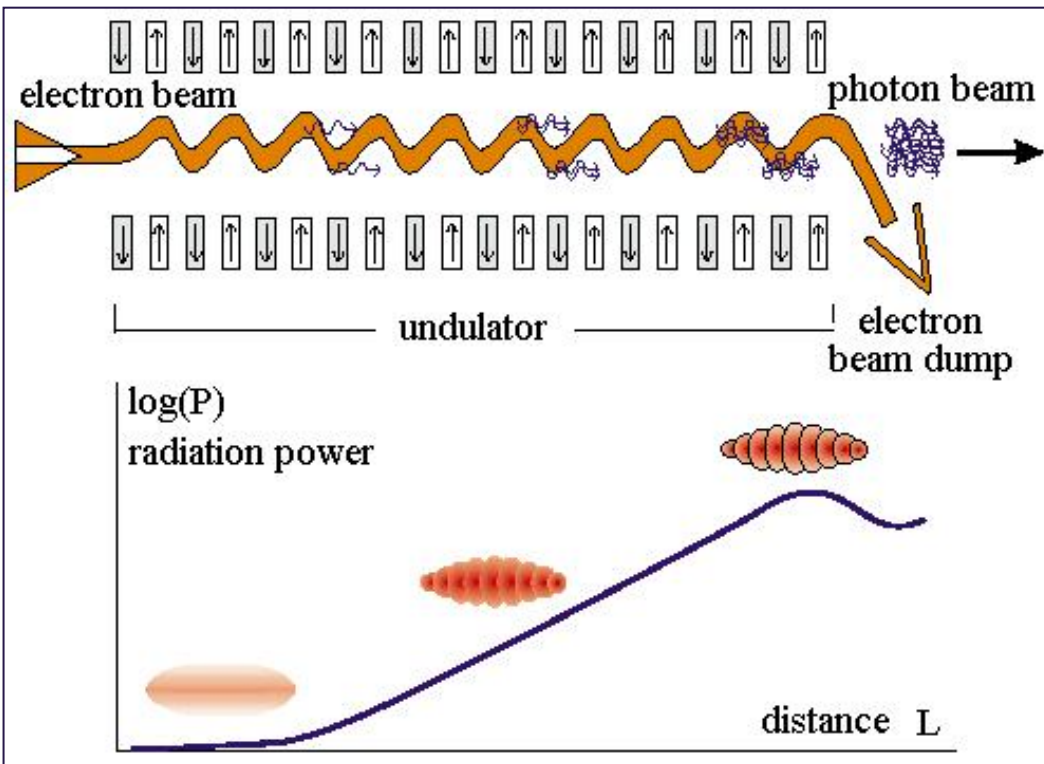


SASE: Self-Amplified Spontaneous Emission

SR undulator: **2 - 5 m**

SASE undulator at European XFEL: **175 m**

Operates with a linac feeding short (<100 fs) electron bunches into a long undulator



Interaction between intense EM-field and electrons leads to e-beam instability and micro-bunching of the electrons.

Micro-bunching gives lasing & saturation:

**Coherent sum of emitted fields from all electrons**

$$I \propto N_e^2 \text{ for SASE}$$

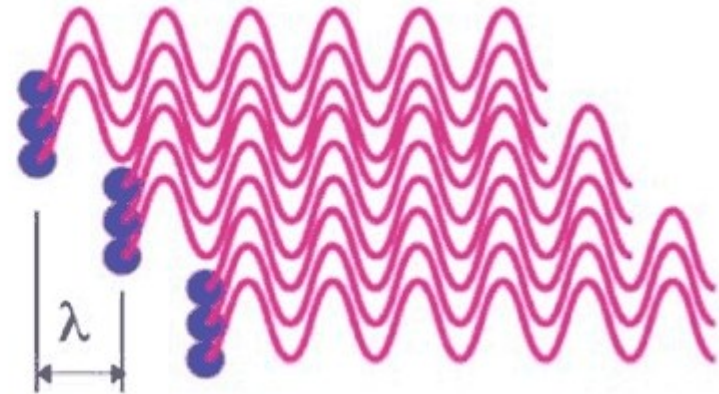
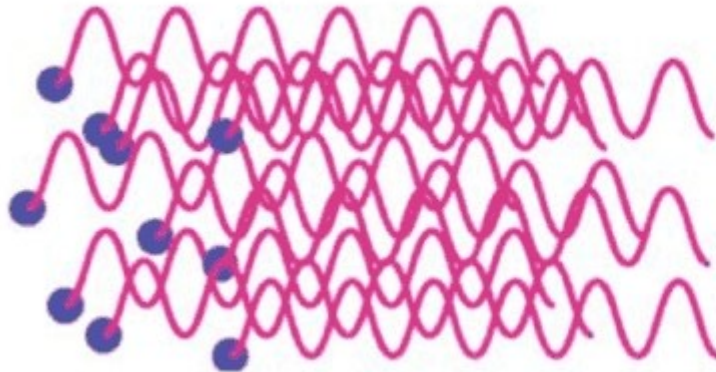
## The “trick” of Free-Electron Lasers:

Spontaneous emission (SR)

Spontaneous emission (SASE)

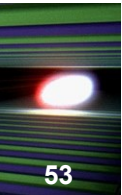
Uncorrelated X-ray emission

Correlated X-ray emission

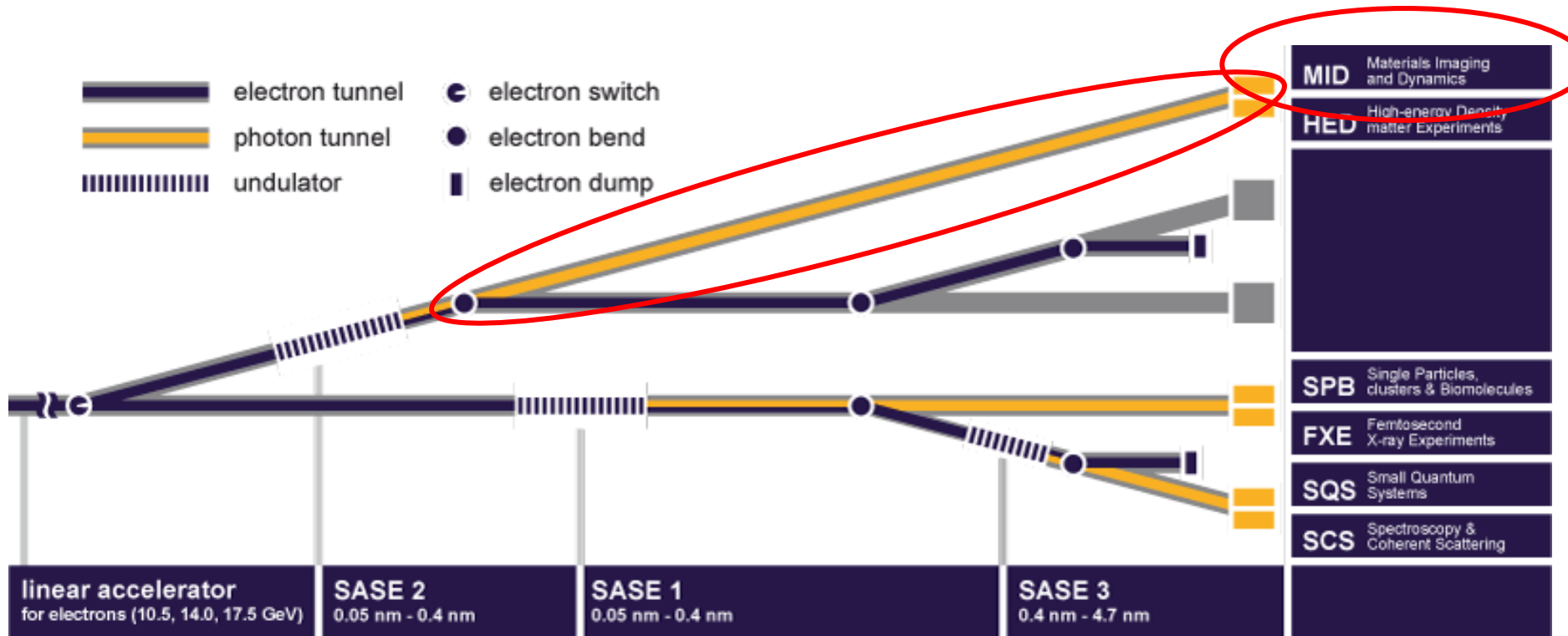


SASE: Self-Amplified Spontaneous Emission.

First demonstrated at DESY (FLASH) in the soft X-ray range



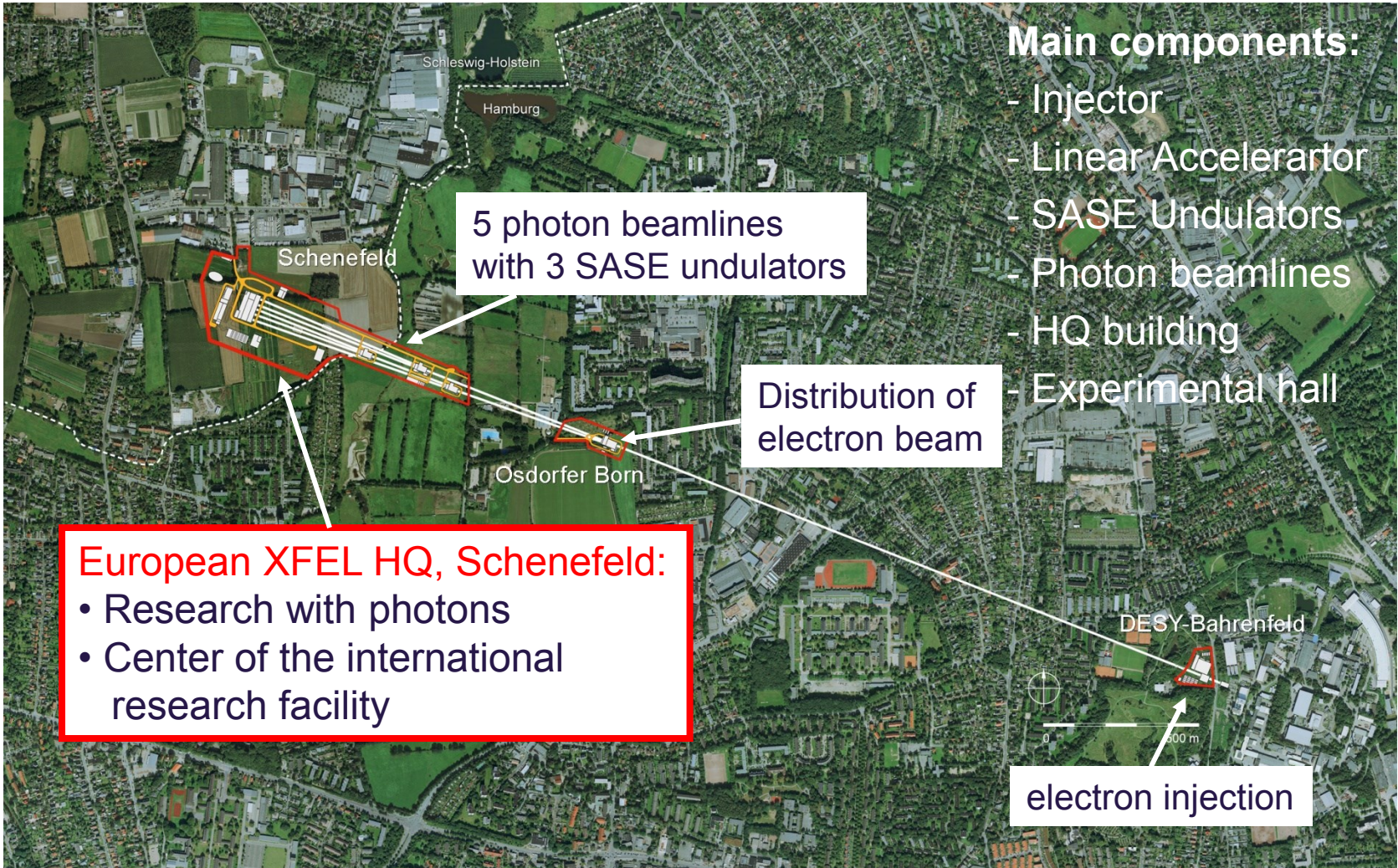
## Materials Imaging and Dynamics Instrument @ SASE-2





### Main components:

- Injector
- Linear Accelerator
- SASE Undulators
- Photon beamlines
- HQ building
- Experimental hall



5 photon beamlines with 3 SASE undulators

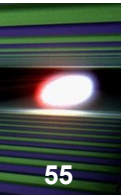
Distribution of electron beam

**European XFEL HQ, Schenefeld:**

- Research with photons
- Center of the international research facility

electron injection

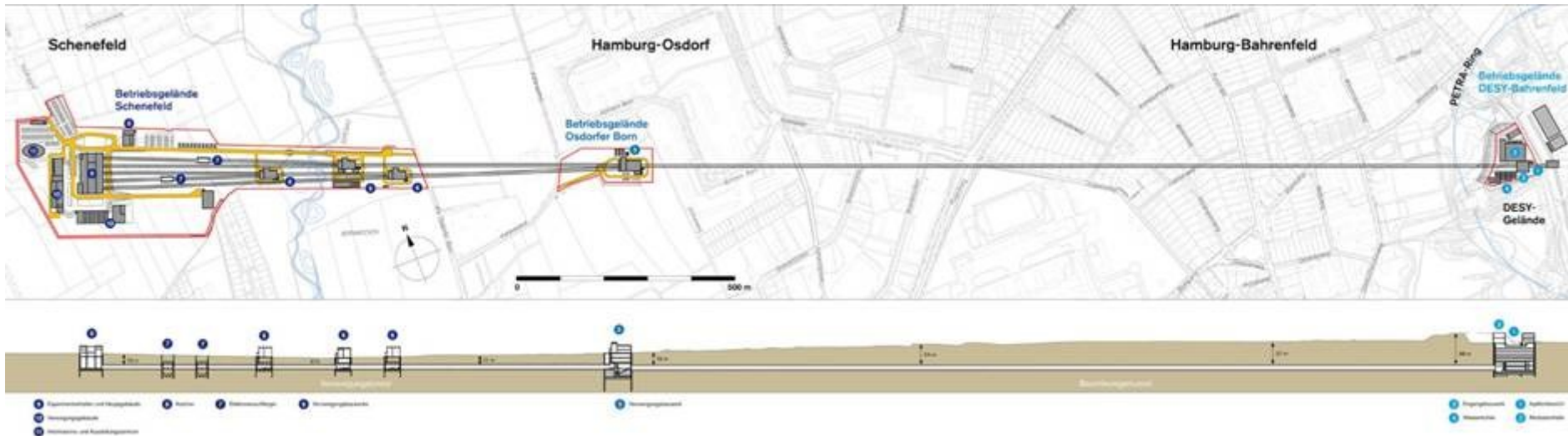




Schenefeld

Osdorfer Born

Bahrenfeld

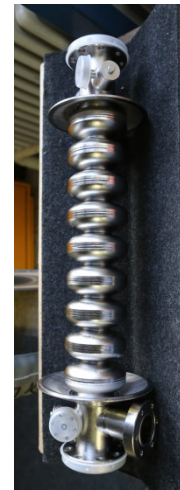
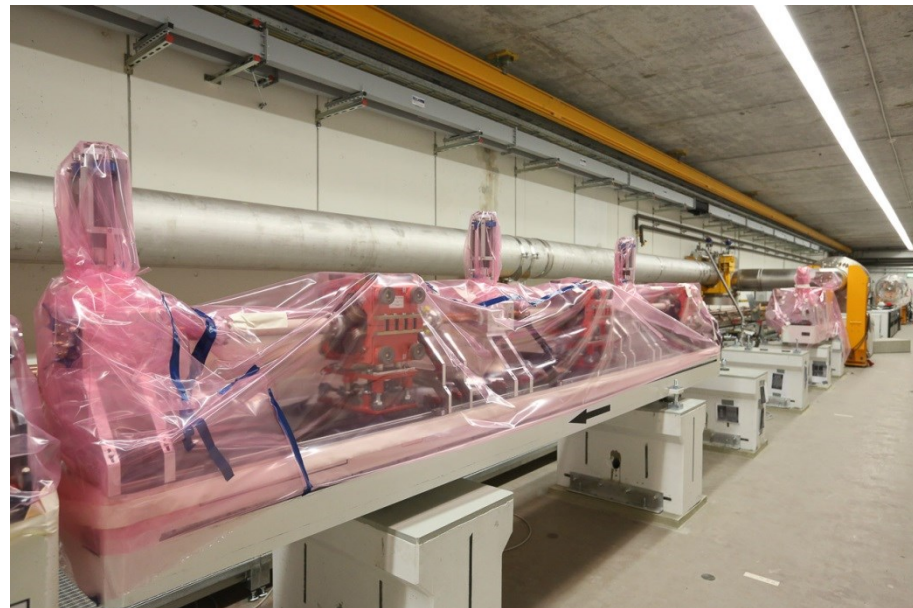


8 shafts and ca. 5.7 km tunnels, superconduction 2.1 km linac, 17.5 GeV

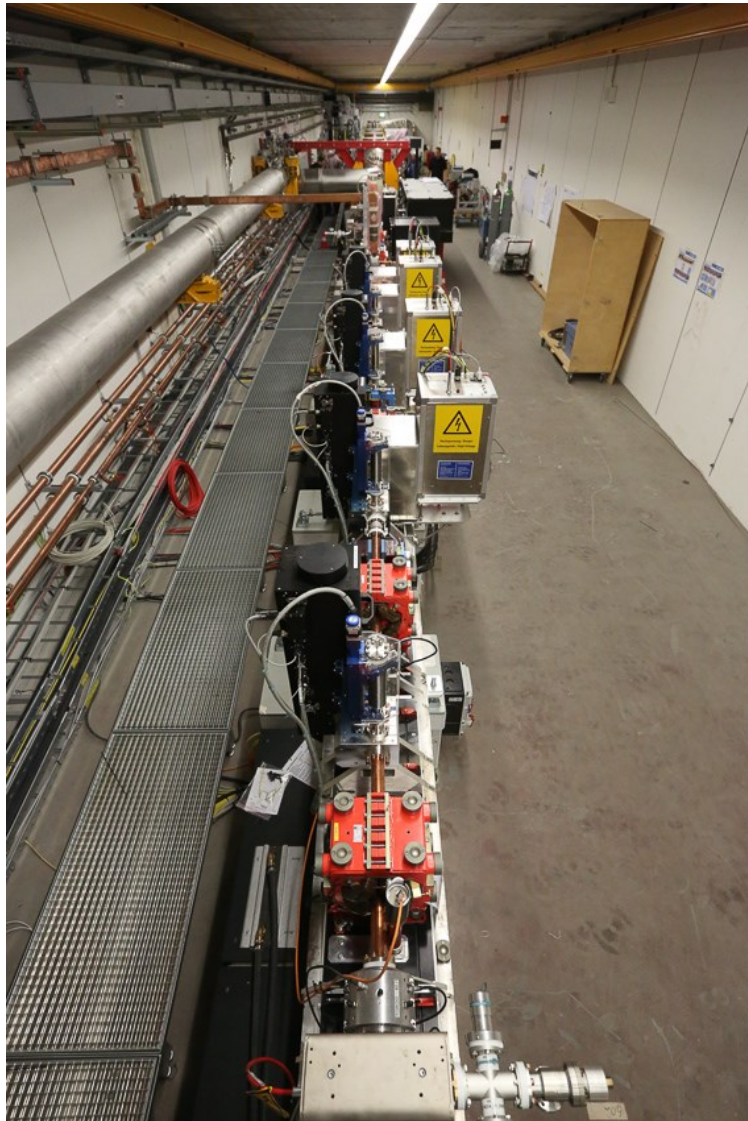
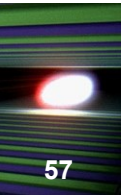
Total straight length of facility: 3.4 km

Underground experimental hall with 6 instruments, space for 6 more









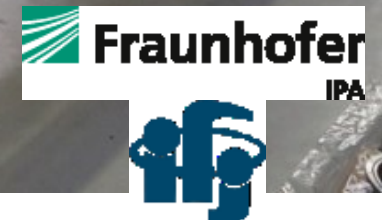
3.9 GHz module installed in 9/2015  
Welding connections finished 10/2015  
Isolation vacuum created

TÜV inspection on November 16th  
Injector cool-down started end of November

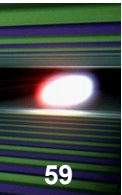
Christmas wish:  
first accelerated beam before  
end of the year



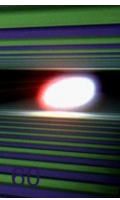
**YES, WE DID IT!**  
**Dec 21, 2015: First electrons accelerated  
by injector (first 45 m of linac)**  
**More info: [www.xfel.eu](http://www.xfel.eu)**







**Closing of tunnel: Sept 2016  
Cool down to 4K starts...**



First 5 m segment  
installed in July 2015

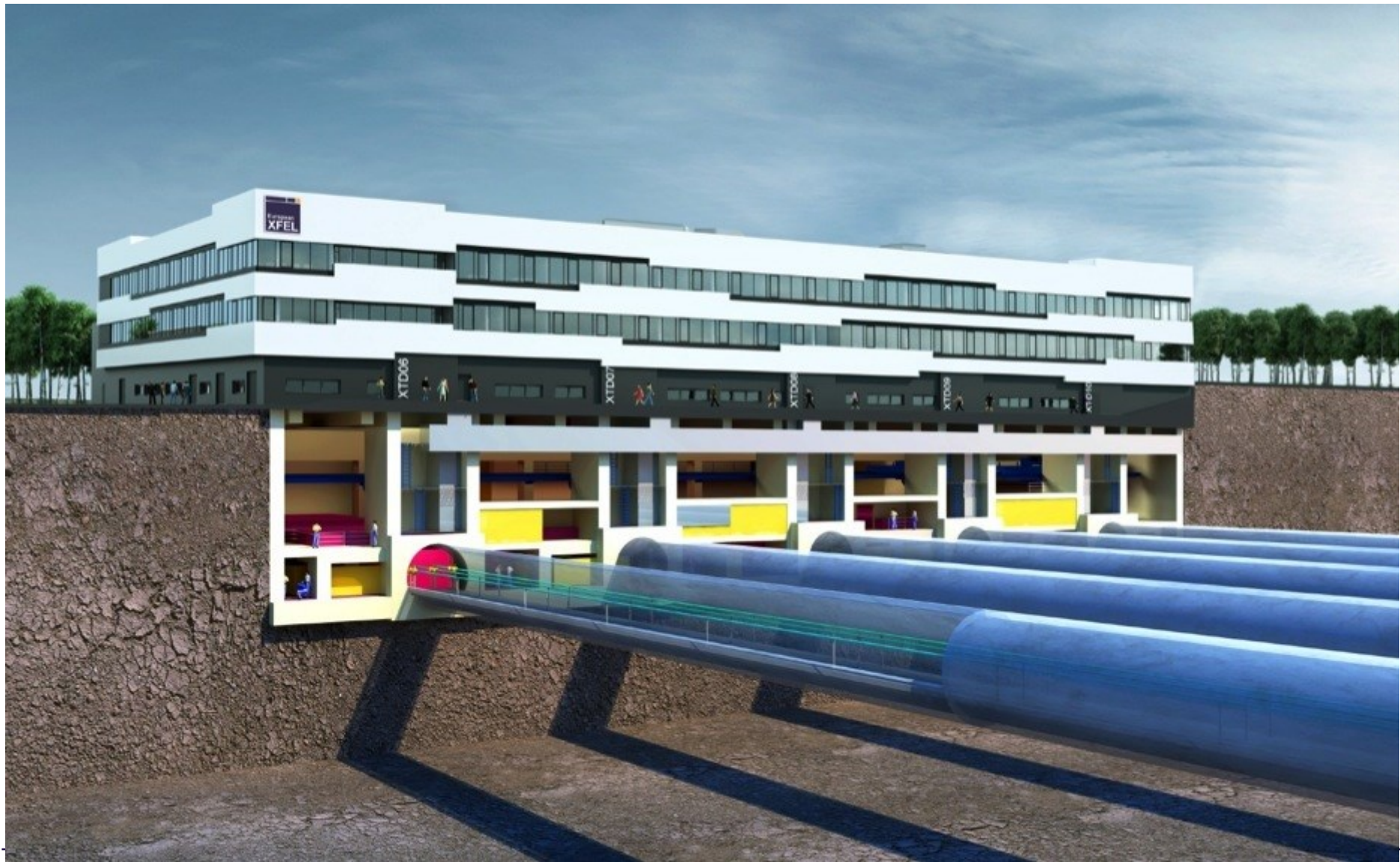
Installation of all  
segments finished  
by end of:

SASE-1: **02.2016**

SASE-3: **04.2016**

SASE-2: **10.2016**





A. Madsen, European XFEL





XHE2-4

XHPSC

XHQ

XHVAC

XHGATE

XHWS



■ Status September 2015



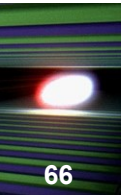




XHQ – moving-in date: 4. June 2016

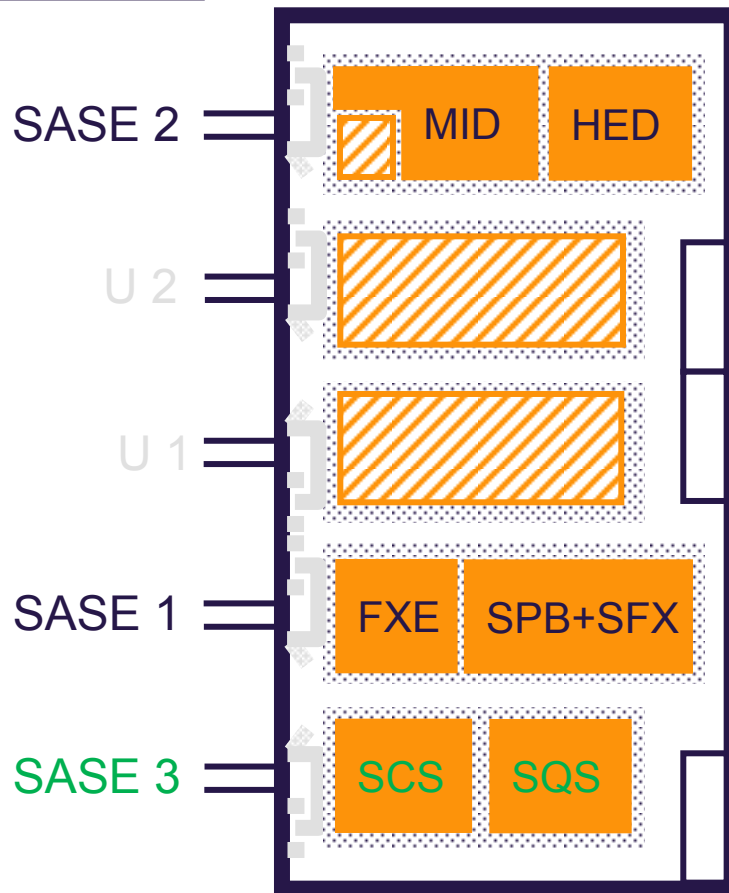




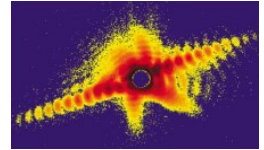


Experimental hall  
~ 90 x 50 m

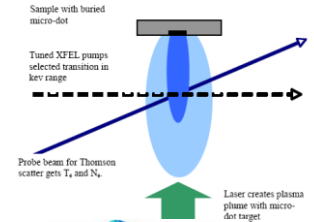
[Link to webcams](#)



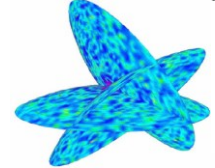
**MID** Materials Imaging & Dynamics



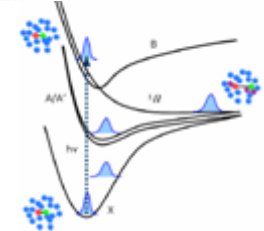
**HED** High Energy Density Science



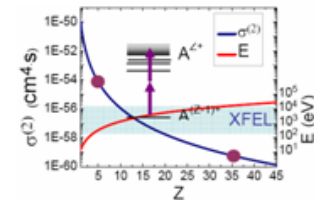
**SPB** Single Particles & Biomolecules



**FXE** Femtosecond X-ray Experiments



**SQS** Small Quantum Systems

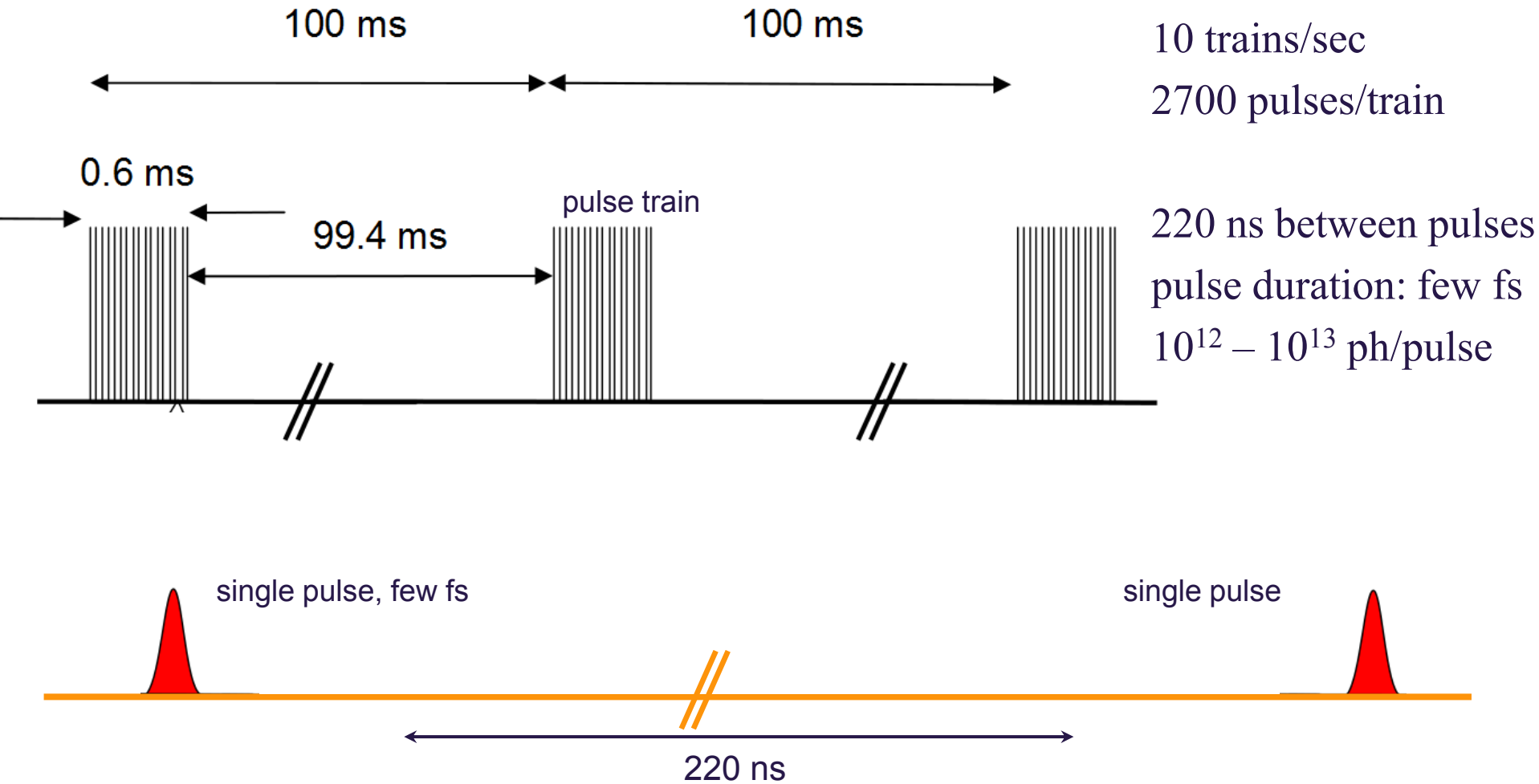
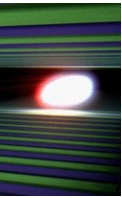


**SCS** Spectroscopy & Coherent Scattering



Source: [www.xfel.eu](http://www.xfel.eu)

# Time-structure of European XFEL



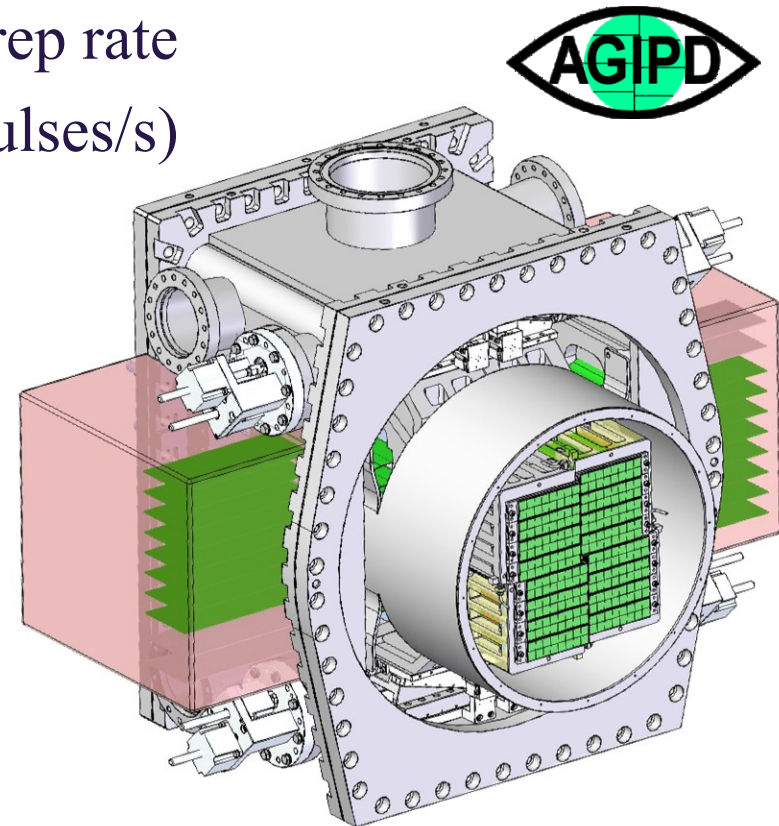
European XFEL repetition rate: 4.5 MHz, most other FEL sources  $\sim 100$  Hz

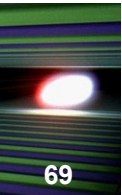


The unique properties:

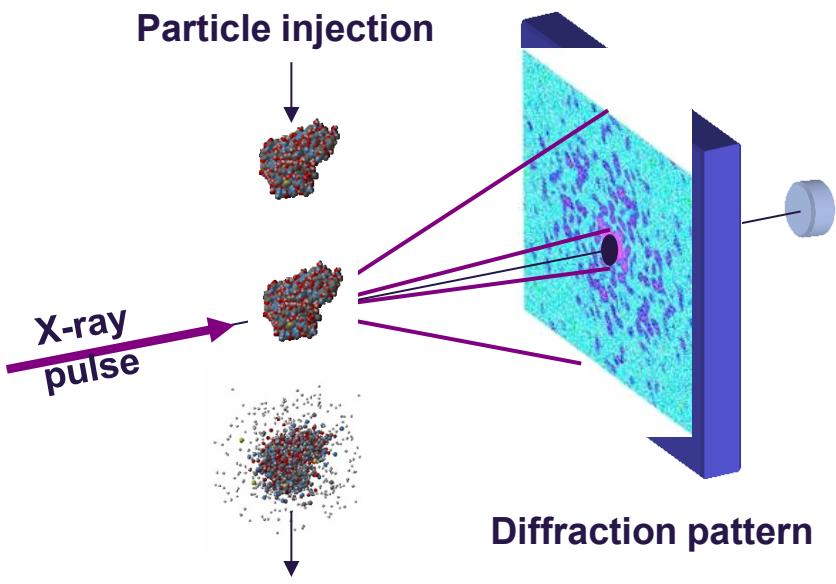
- Ultrafast time resolution
- Ultrahigh peak Brilliance at 4.5 MHz rep rate
- Ultrahigh average Brilliance (27000 pulses/s)
- Coherence of the XFEL beam

will enable completely new experiments  
to study structure and dynamics of  
materials

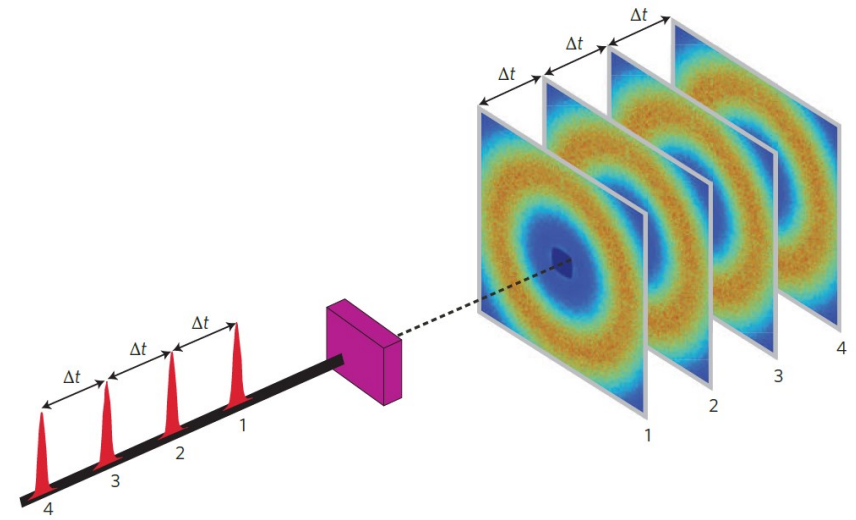




- Imaging of single molecules
- Ultra-fast dynamics of molecules and materials



Gaffney and Chapman,  
Science **316**, 1444 (2007)



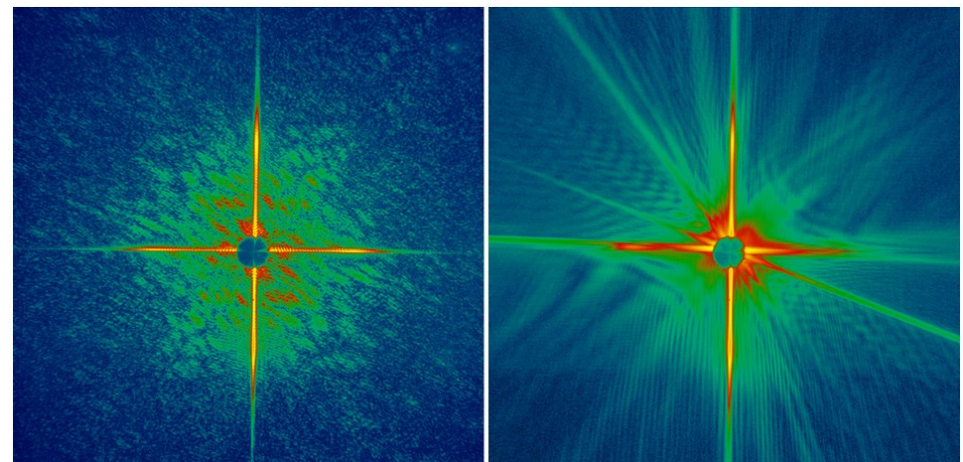
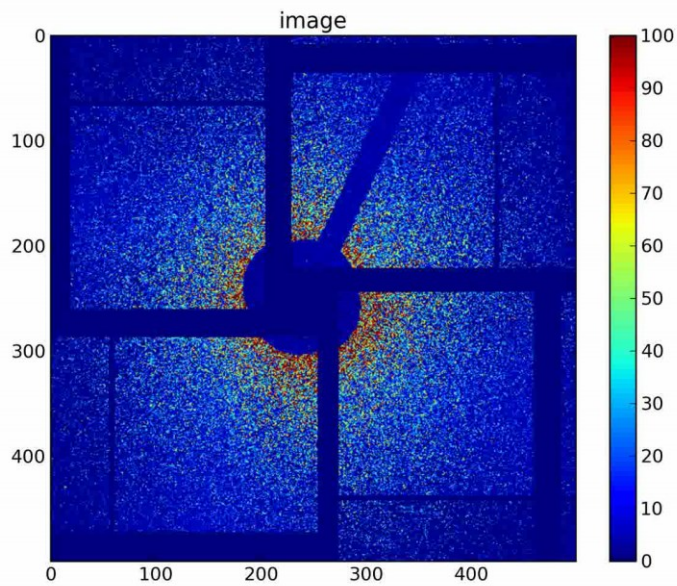
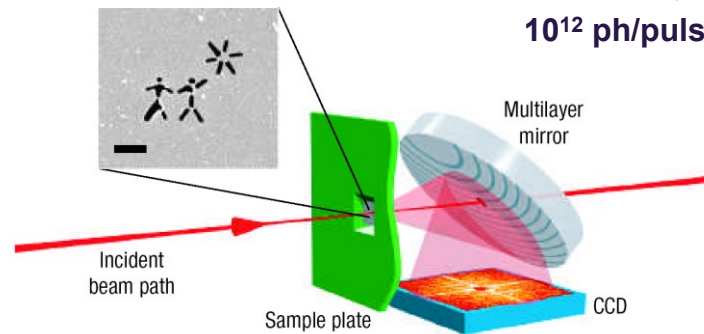
Stephenson *et al*,  
Nature Materials **8**, 702 (2009)

XFEL experiments can be destructive...

but not necessarily

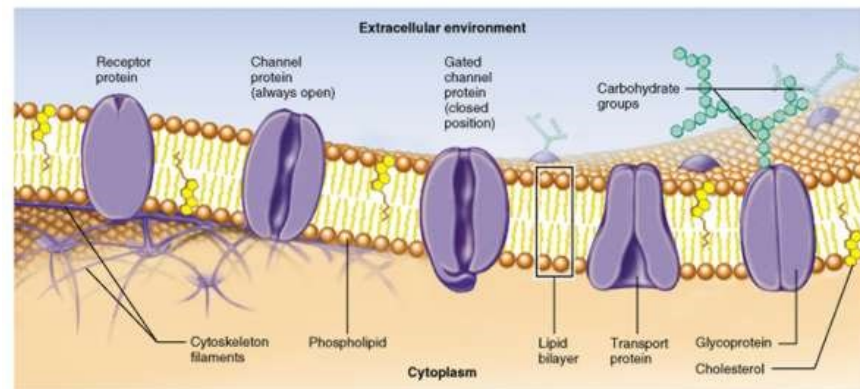
FLASH (DESY)

$\Lambda = 32$  nm, 25 fs pulse duration,  
 $10^{12}$  ph/pulse



H. Chapman *et al*, Nature Physics **2**, 839 (2006)

- Serial crystallography (sample injector)
- Femtosecond pulses (diffraction before destruction)
- Nanocrystals formed by most proteins



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## Serial femtosecond crystallography: the first five years

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\*Correspondence e-mail: [ilme.schlichting@mpimf-heidelberg.mpg.de](mailto:ilme.schlichting@mpimf-heidelberg.mpg.de)

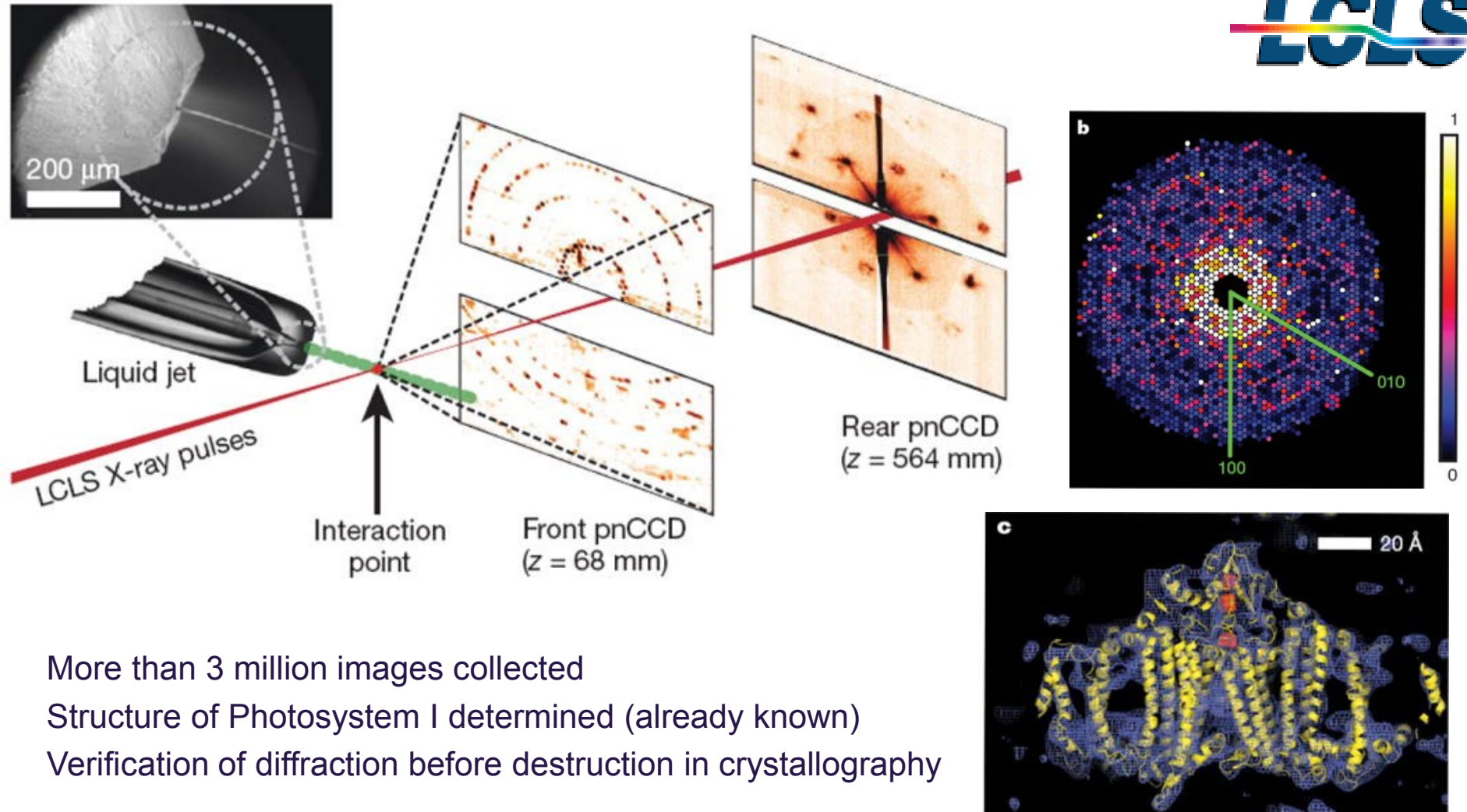
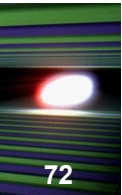
Edited by T. Ishikawa, Harima Institute, Japan (Received 6 August 2014; accepted 9 December 2014; online 3 February 2015)



CrossMark



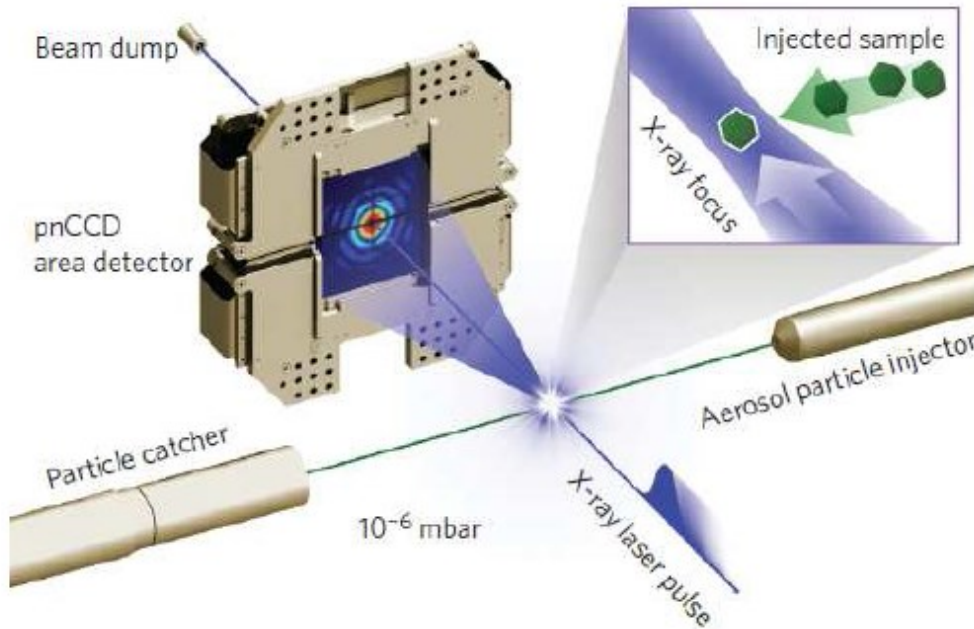
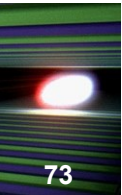
# Diffraction before destruction: Femto-second crystallography (destructive)



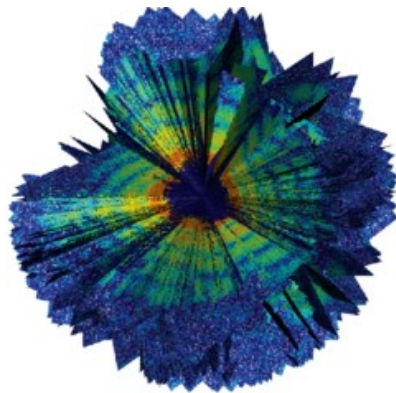
More than 3 million images collected  
 Structure of Photosystem I determined (already known)  
 Verification of diffraction before destruction in crystallography



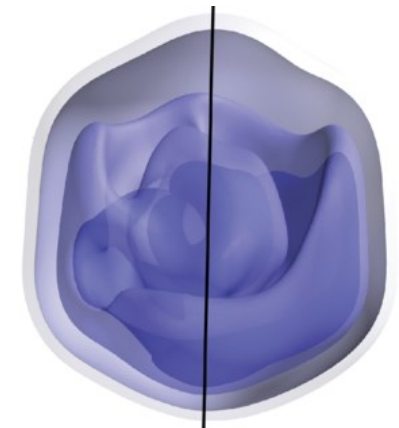
# Diffraction before destruction: CDI using single shot exposures



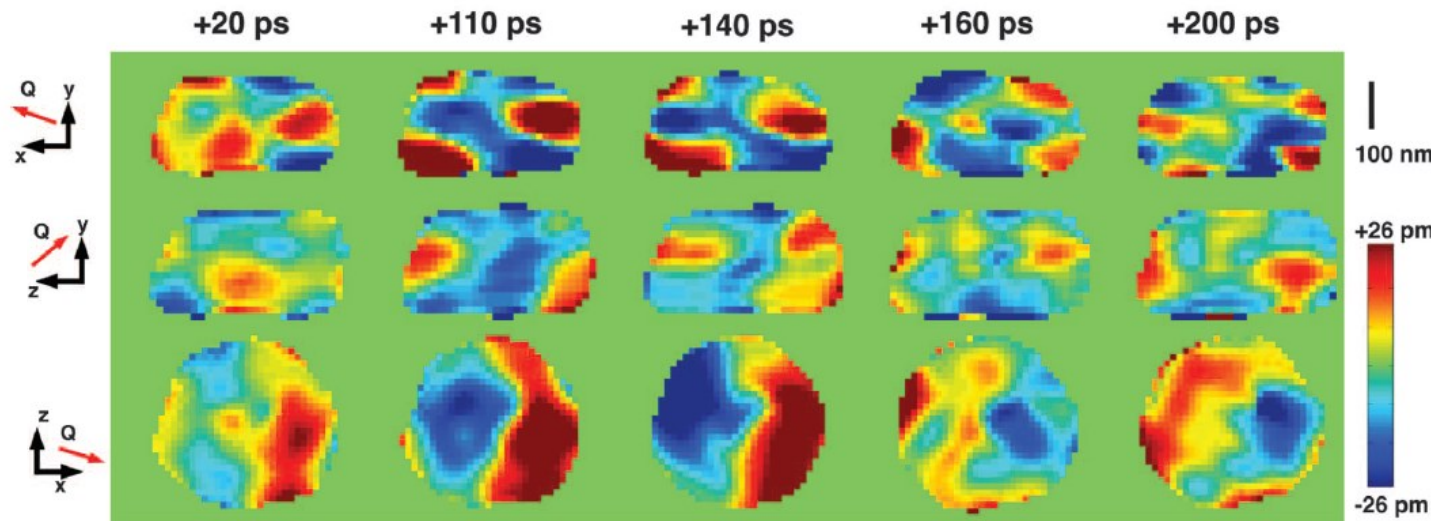
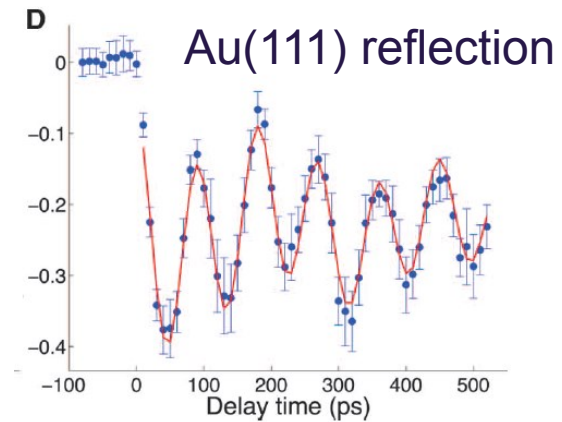
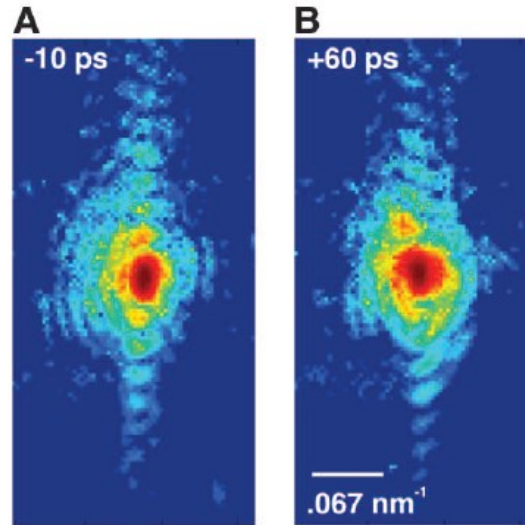
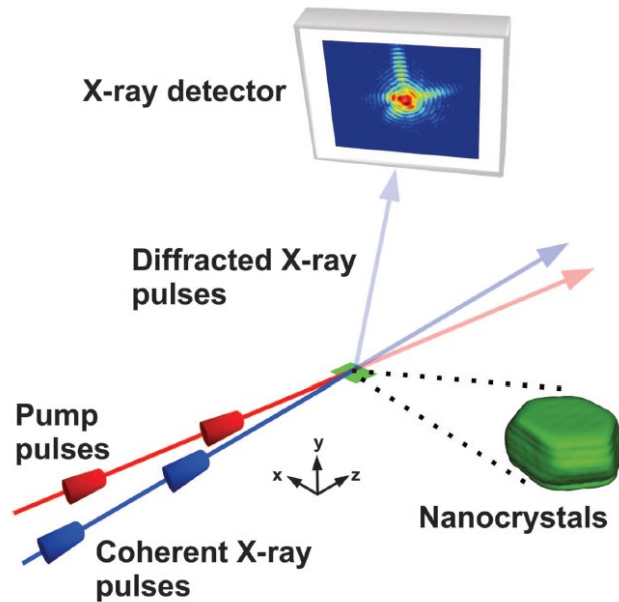
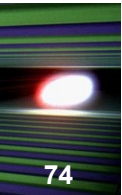
X-ray Imaging of a virus in 3D  
Ekeberg et al, PRL **114**, 098102 (2015)  
Particle injector at AMO, LCLS



Phase retrieval  
Tomographic reconstruction  
3D resolution

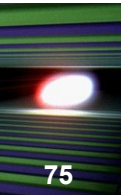


# Non-destructive XFEL Imaging: Combining CDI and pump-probe



Measuring phonons in Au nanocrystals by PP CDI at LCLS

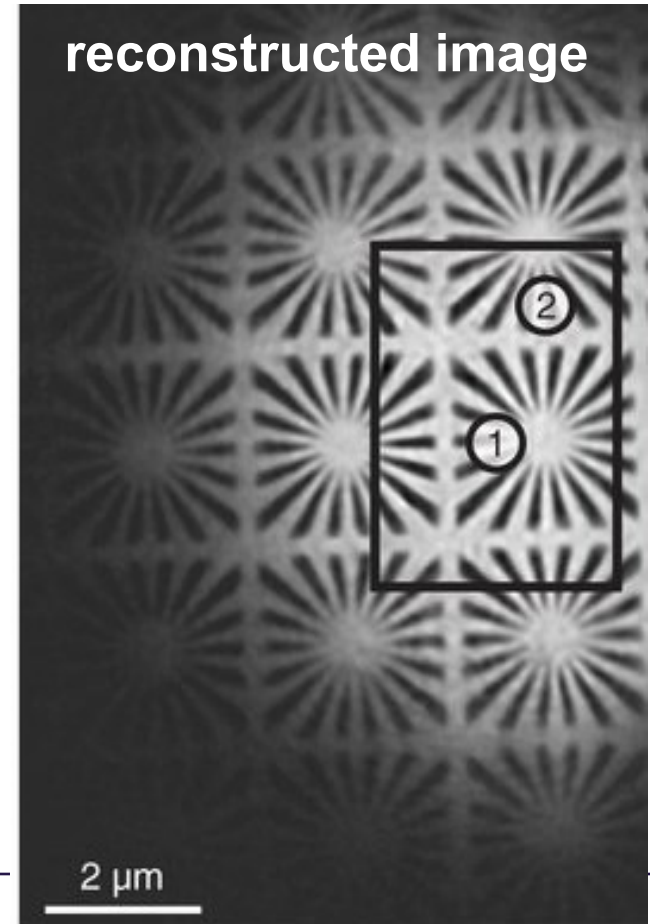
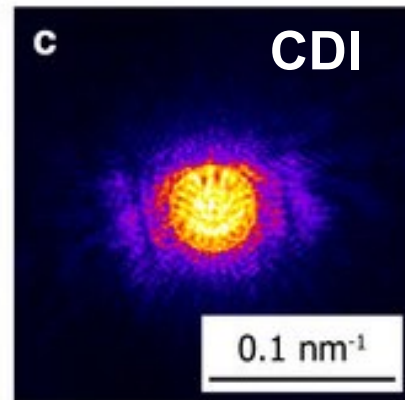
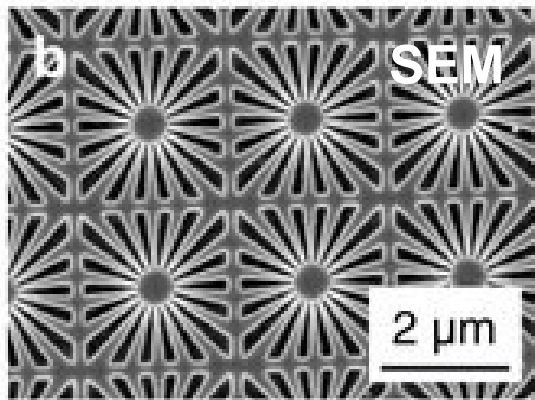
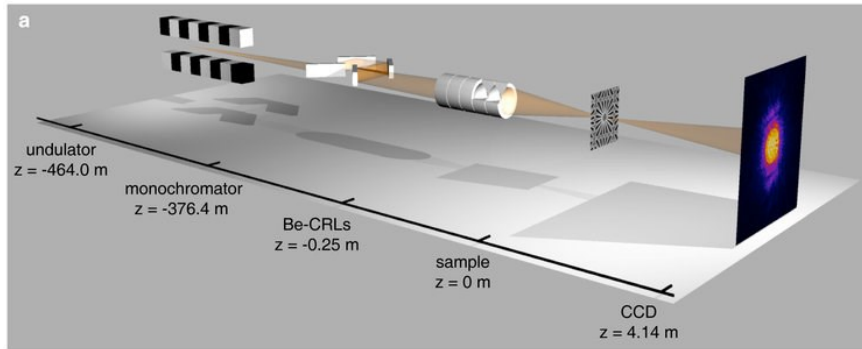
J. Clark, ... & I. Robinson, Science **341**, 56 (2013)



## Full spatial characterization of a nanofocused x-ray free-electron laser beam by ptychographic imaging

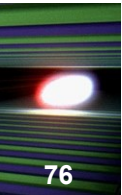
*Sci. Rep.* 3, 1633 (2013)

Andreas Schropp<sup>1,2</sup>, Robert Hoppe<sup>1</sup>, Vivienne Meier<sup>1</sup>, Jens Patommel<sup>1</sup>, Frank Seiboth<sup>1</sup>, Hae Ja Lee<sup>2</sup>, Bob Nagler<sup>2</sup>, Eric C. Galtier<sup>2</sup>, Brice Arnold<sup>2</sup>, Ulf Zastra<sup>2</sup>, Jerome B. Hastings<sup>2</sup>, Daniel Nilsson<sup>3</sup>, Fredrik Uhlén<sup>3</sup>, Ulrich Vogt<sup>3</sup>, Hans M. Hertz<sup>3</sup> & Christian G. Schroer<sup>1</sup>

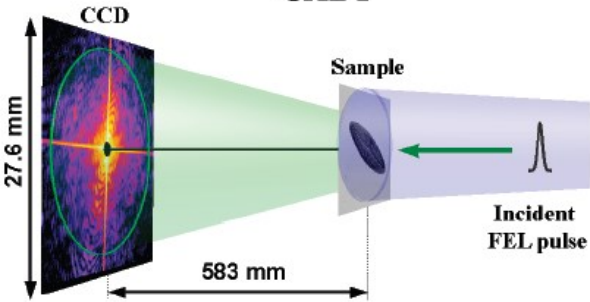




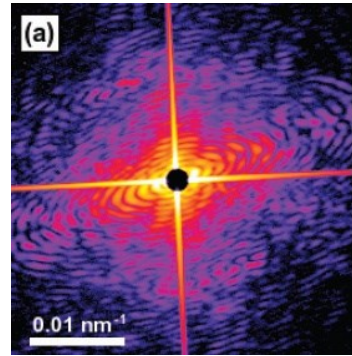
# Non-destructive XFEL Imaging: comparison of Bio CXDI and Holography at FLASH



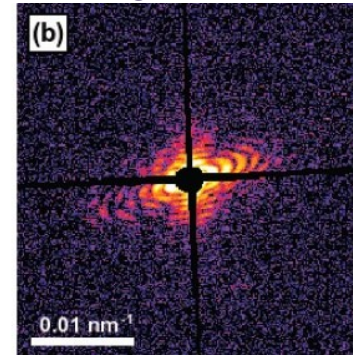
## CXDI



## integrated

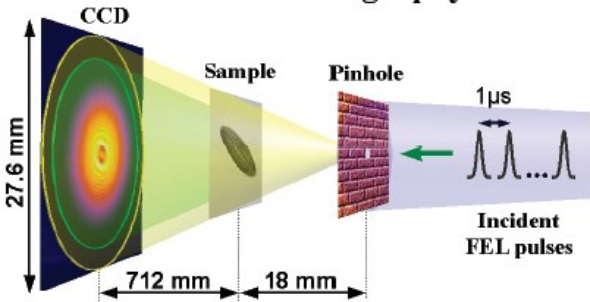


## single pulse

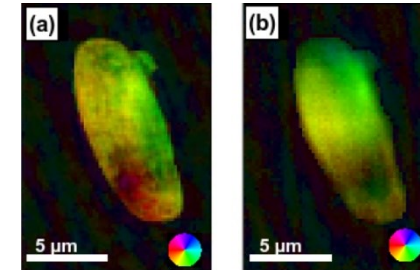


Unicellular algae  
(*Navicula perminuta*)  
10 fs pulses,  $\lambda=8$  nm  
 $\sim 1e10$  ph/pulse

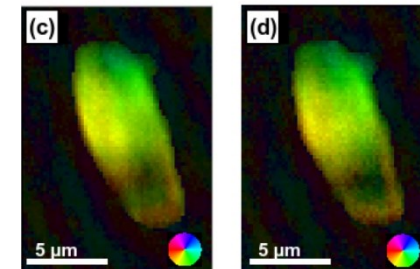
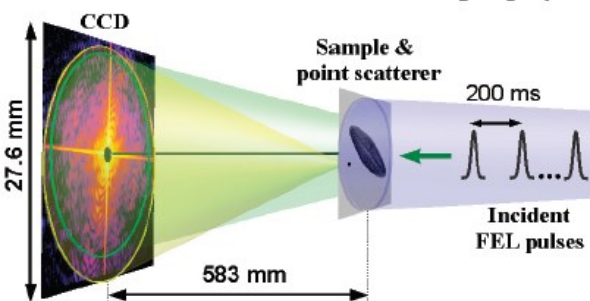
## In-line Holography



Integrated vs. single-shot  
reconstructions



## Fourier Transform Holography



- Coherent Diffraction Imaging is a method developed at synchrotron sources to overcome limitations of optics
- The phase retrieval is difficult but necessary to reconstruct the image from the measured Intensities
- Related methods exist that sometimes can make the phase retrieval easier
- 3D resolution is of course desired in many cases
- Novel X-ray laser sources promise a bright future for coherent imaging techniques but new experimental strategies are needed
- Femtosecond nano-crystallography is, until now, the biggest success of XFELs overall
- The combination of CDI and ultrafast science (fs-ns) is promising but only few experiments so far...

**?? QUESTIONS ??**



[www.xfel.eu](http://www.xfel.eu)

[lcls.slac.stanford.edu/](http://lcls.slac.stanford.edu/)

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## Materials science in the time domain using Bragg coherent diffraction imaging

Ian Robinson<sup>1,2</sup>, Jesse Clark<sup>3</sup> and Ross Harder<sup>4</sup>

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*Journal of Optics*, Volume 18, Number 5

K. A. Nugent, Coherent methods in the X-ray sciences

<https://arxiv.org/ftp/arxiv/papers/0908/0908.3064.pdf>

# The End