9th May 2007

X-Ray Diffraction Microscopy of Extended Objects

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Swiss Light Source
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SWISS LIGHT SOURCE

SLS

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PSI

Coherent X-Ray Scattering Group

F. Pfeiffer

O. Bunk

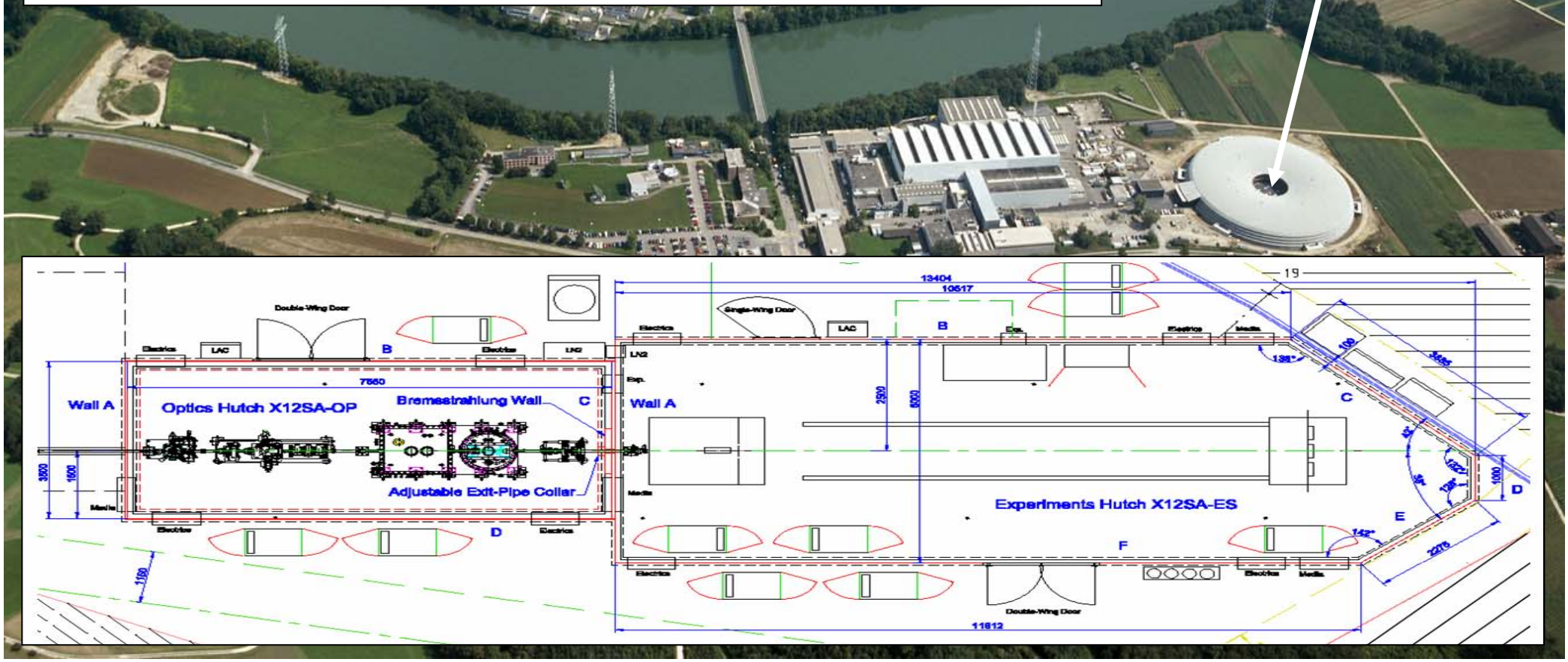
A. Menzel

X. Donath

I. Johnson

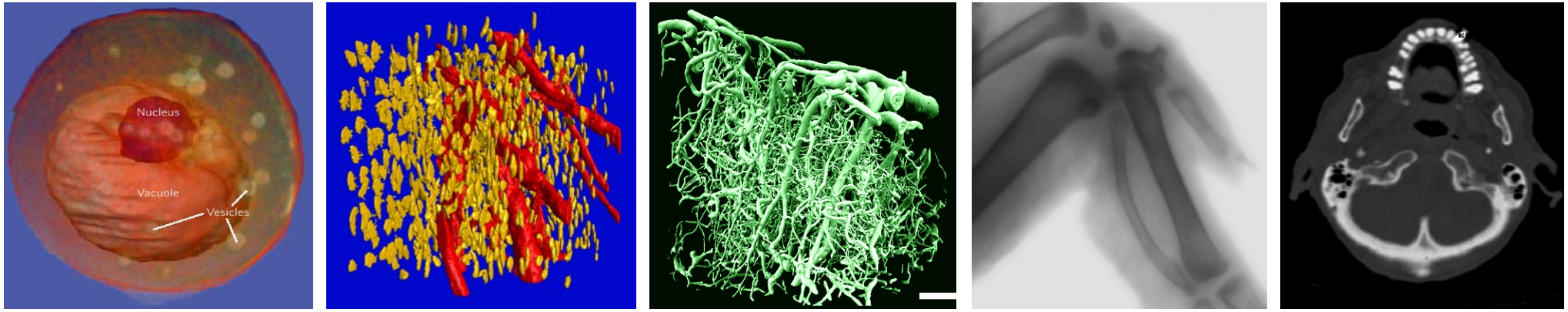
M. Dierolf

M. Bech



Coherent x-ray imaging

Synchrotron | Laboratory | Hospital



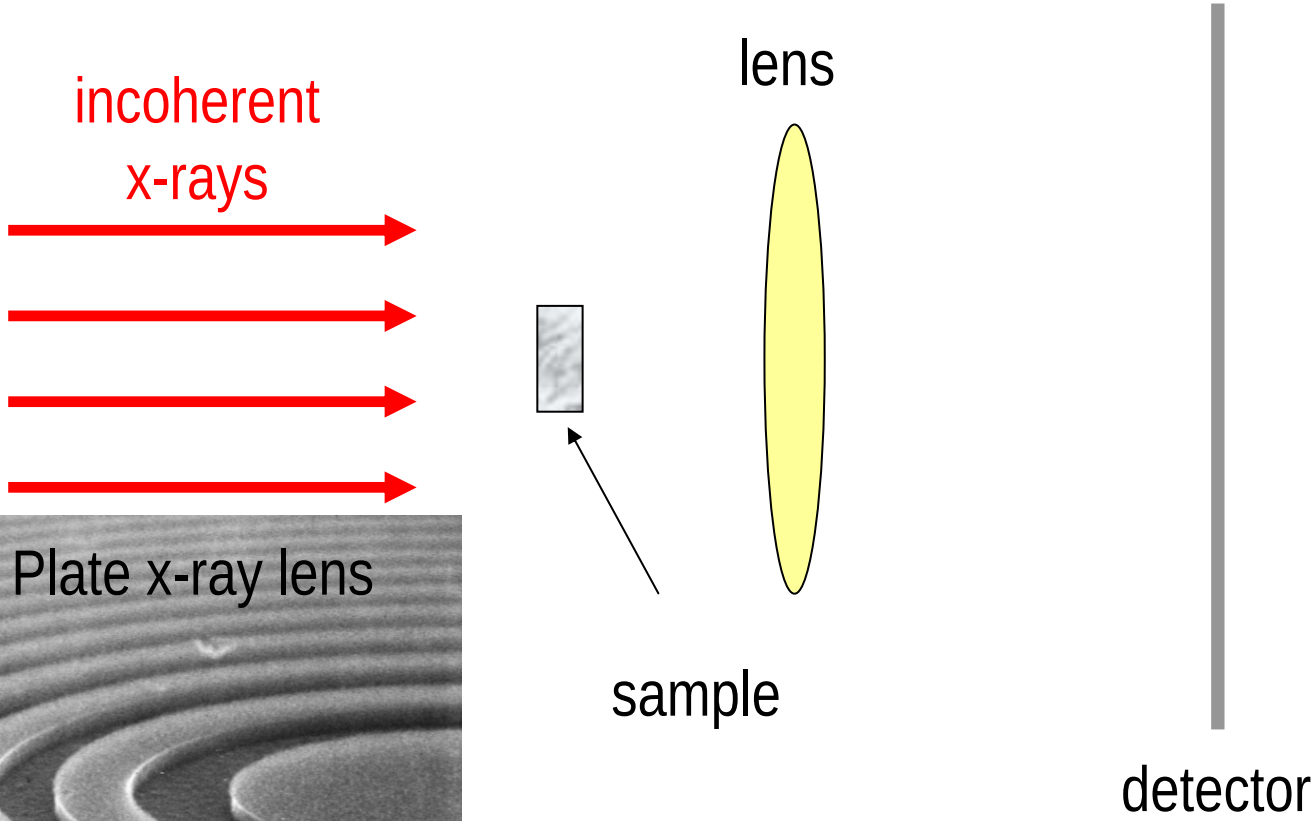
50 nm — 1 μm — 1 mm — 1 m

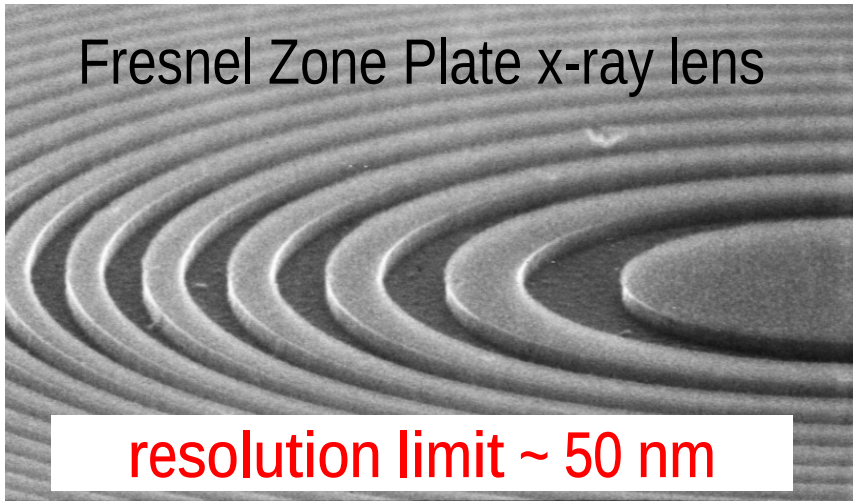
coherent diffractive imaging

lensless imaging

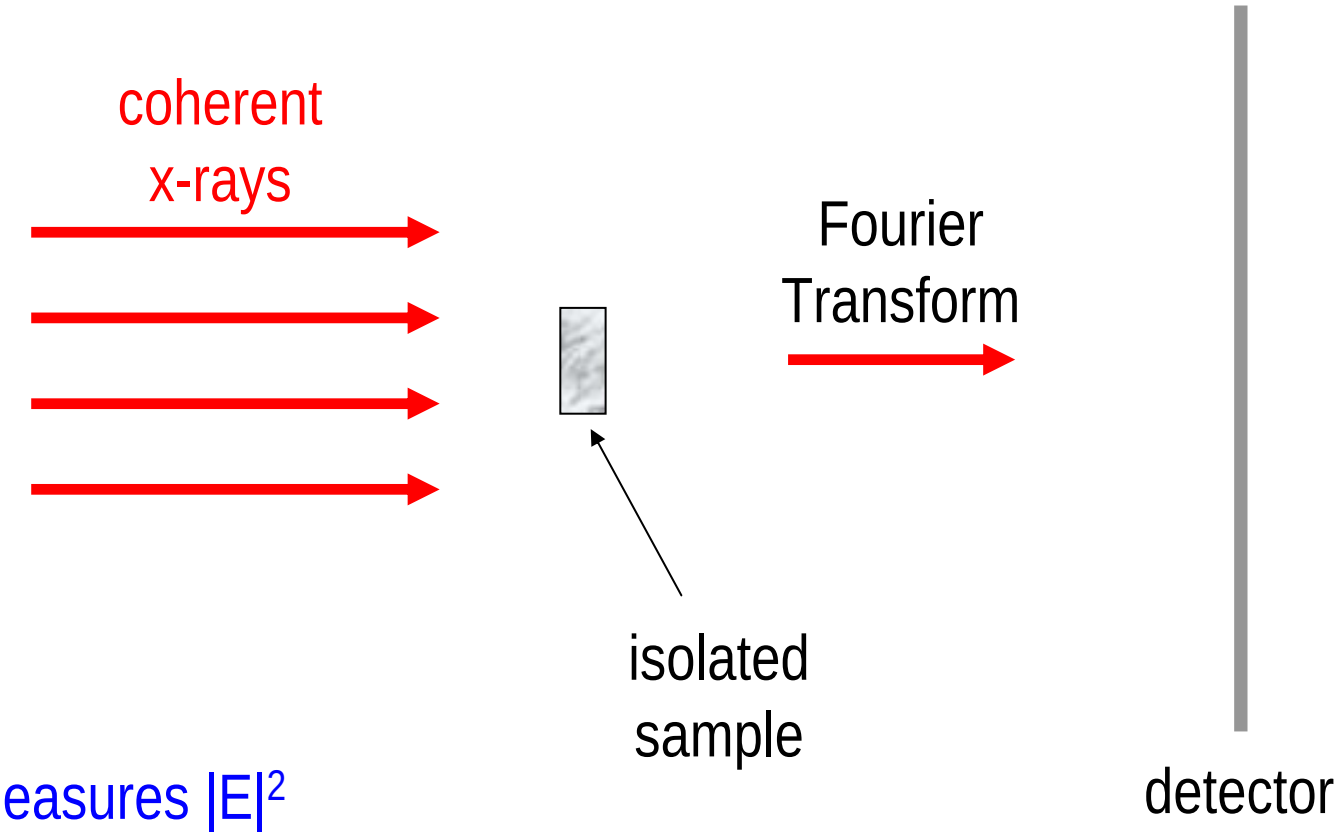
x-ray phase contrast imaging for biomedical and medical applications

‘Classical’ x-ray microscopy setup





Lensless imaging – Coherent diffractive imaging

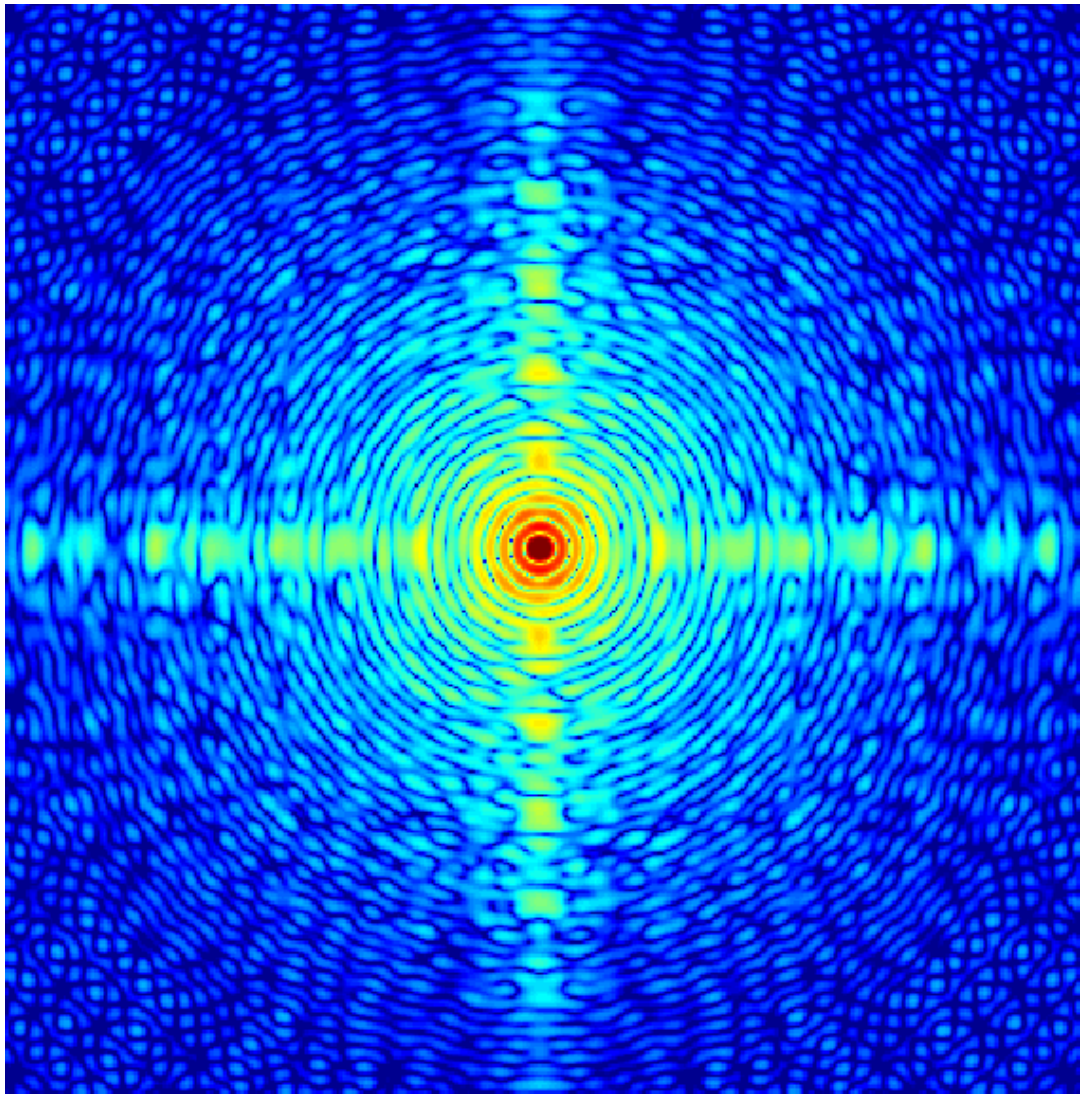


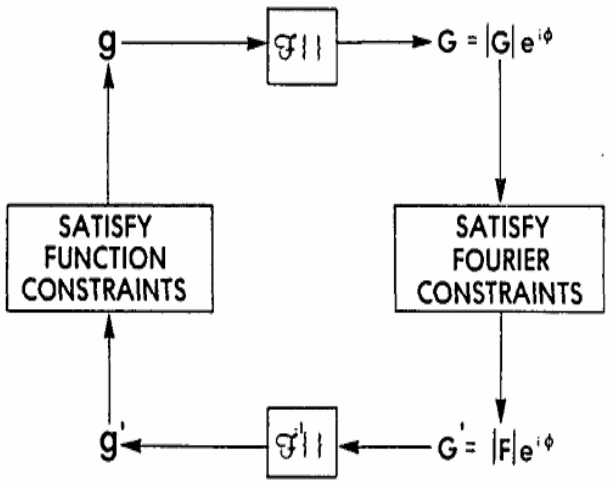
Detector measures $|E|^2$

=> phases are lost !

Iterative phase retrieval works…

Diffraction experiment (FFT)

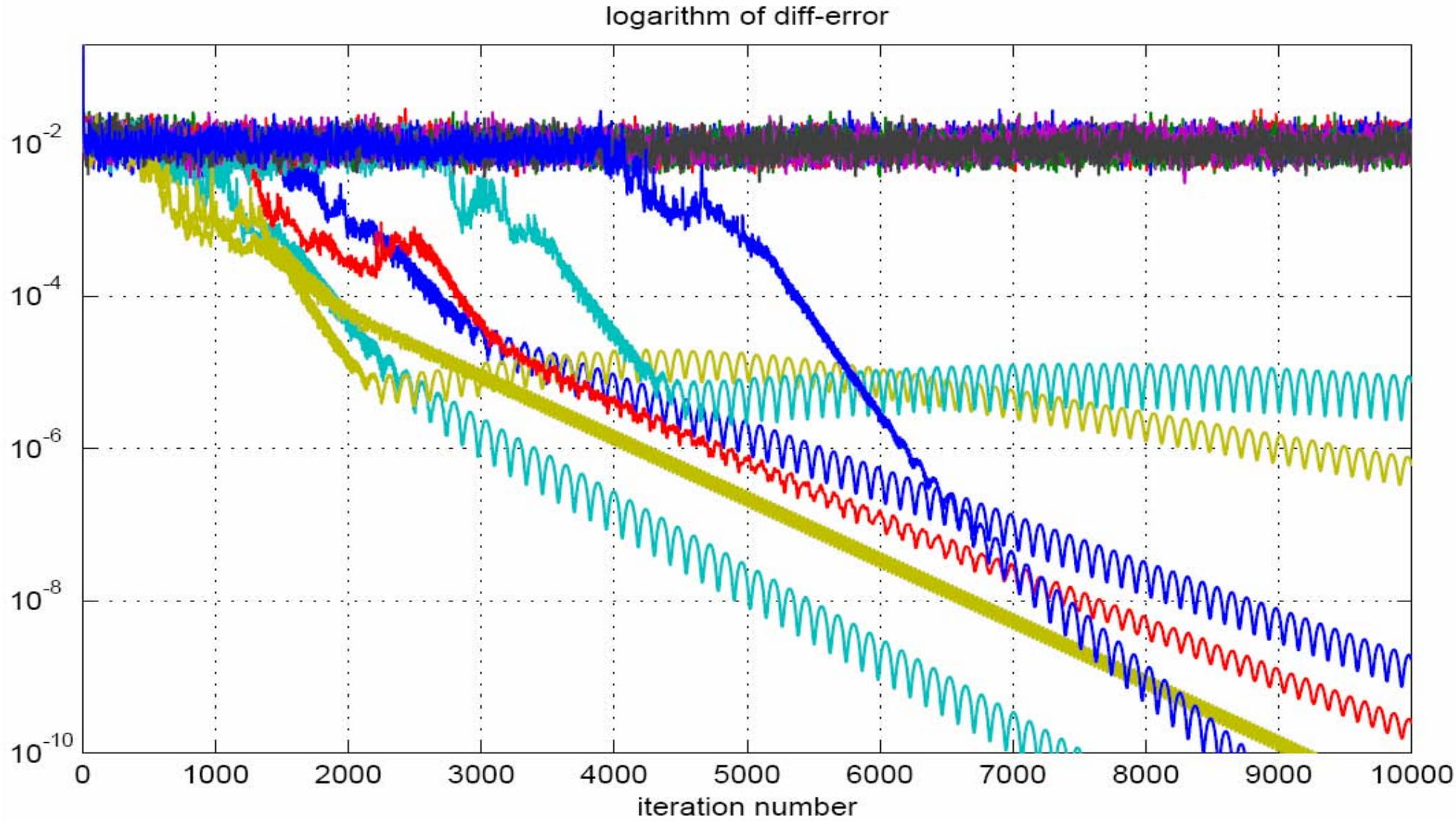




Iterative reconstruction (HIO algorithm)

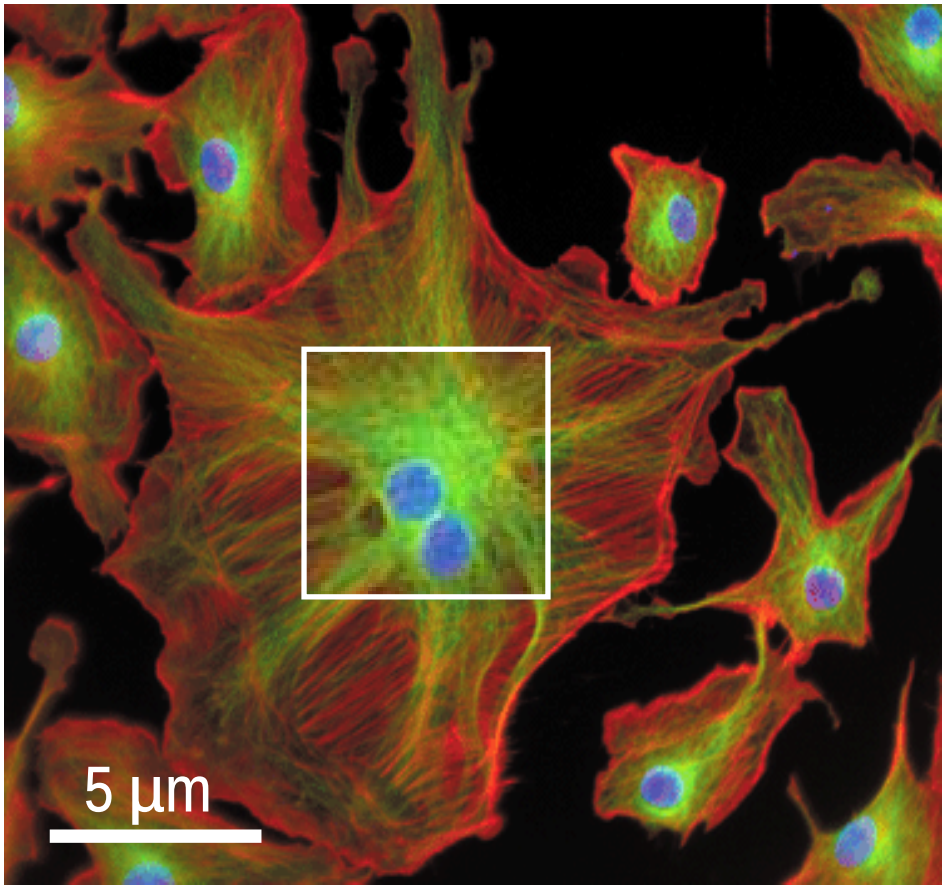
J.R. Fienup, JOSA 3, 27 (1978)

Numerous successful demonstration experiments



What cell biologists want…

- Look at large samples and screen for interesting features
- Zoom in into a region of interest
- Obtain a higher resolution than in visible light microscopy
- Obtain information more or less immediately



Fluorescence microscopy image
bovine artery cells (www.invitrogen.com)

Ptychographical iterative phase retrieval

Ptychography ‘πτυξ’

- *W. Hoppe, Acta Cryst. A 25, 508 (1969).*
- *R. Hegerl, W. Hoppe, Ber. Physik. Chemie 74, 1148 (1970).*

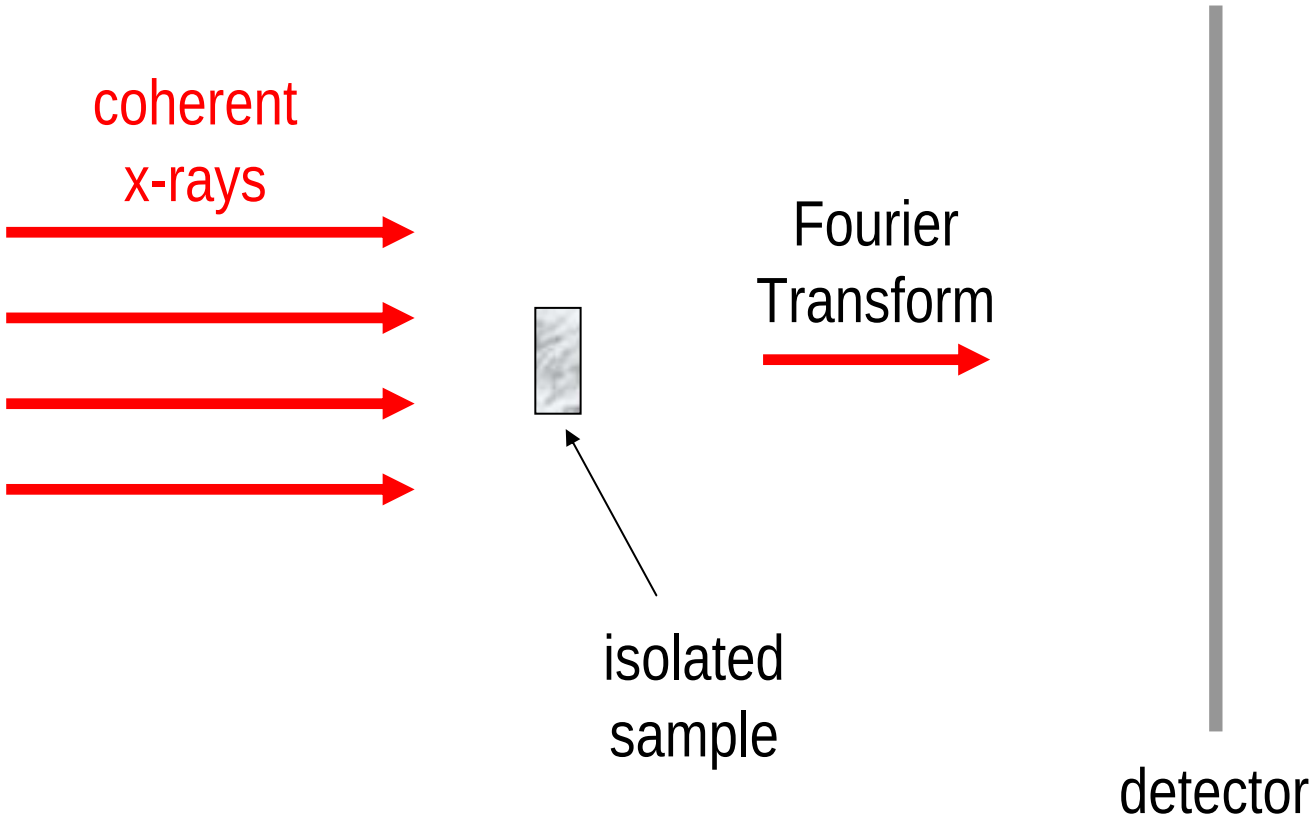
Iterative algorithms

- *R. W. Gerchberg and W.O. Saxton, Optik 35, 237 (1972).*
- *J. R. Fienup Appl. Opt. 21, 2758 (1982).*

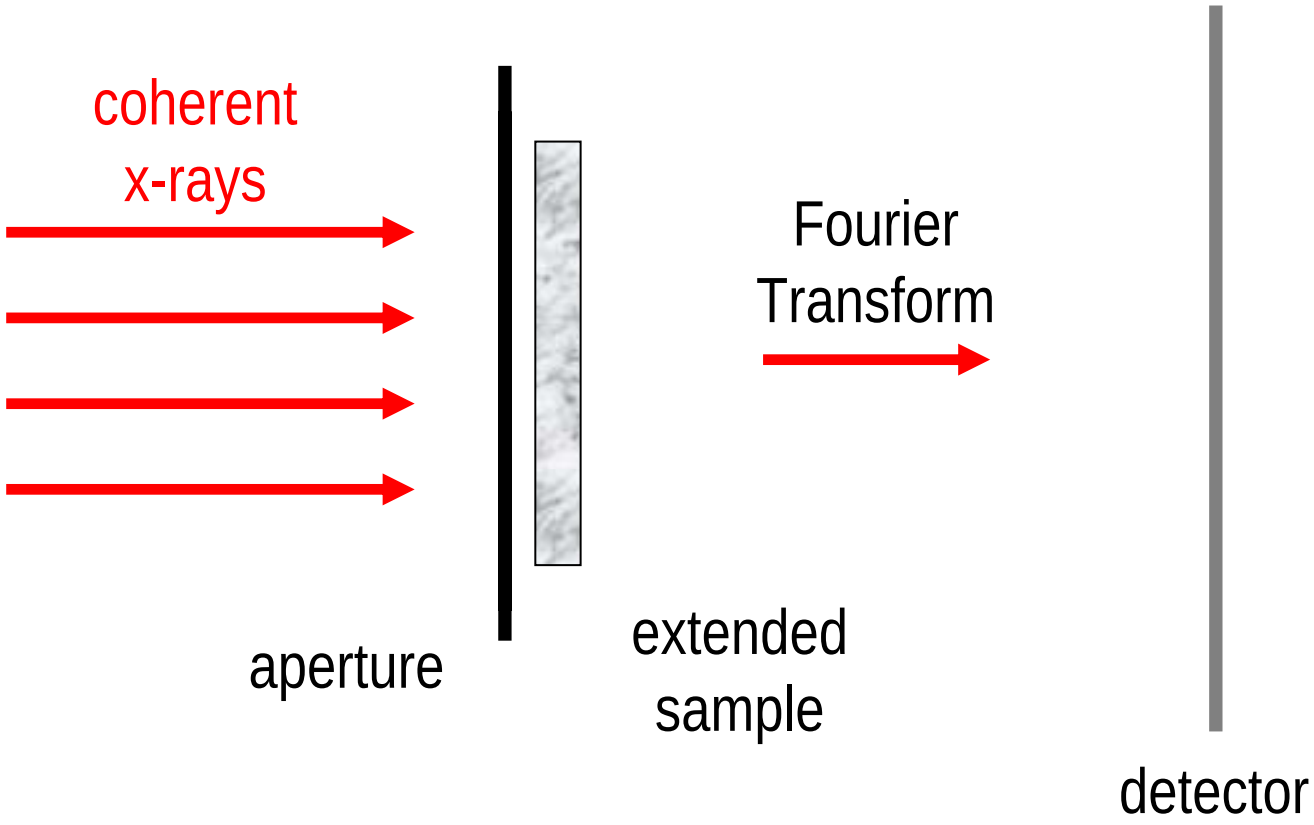
Ptychographical iterative phase retrieval

- *H. M. L. Faulkner and J. M. Rodenburg, Phys. Rev. Lett. 93, 023903 (2004).*
- *J. M. Rodenburg, A. C. Hurst and A. G. Cullis, Ultramicroscopy 107, 227 (2007).*

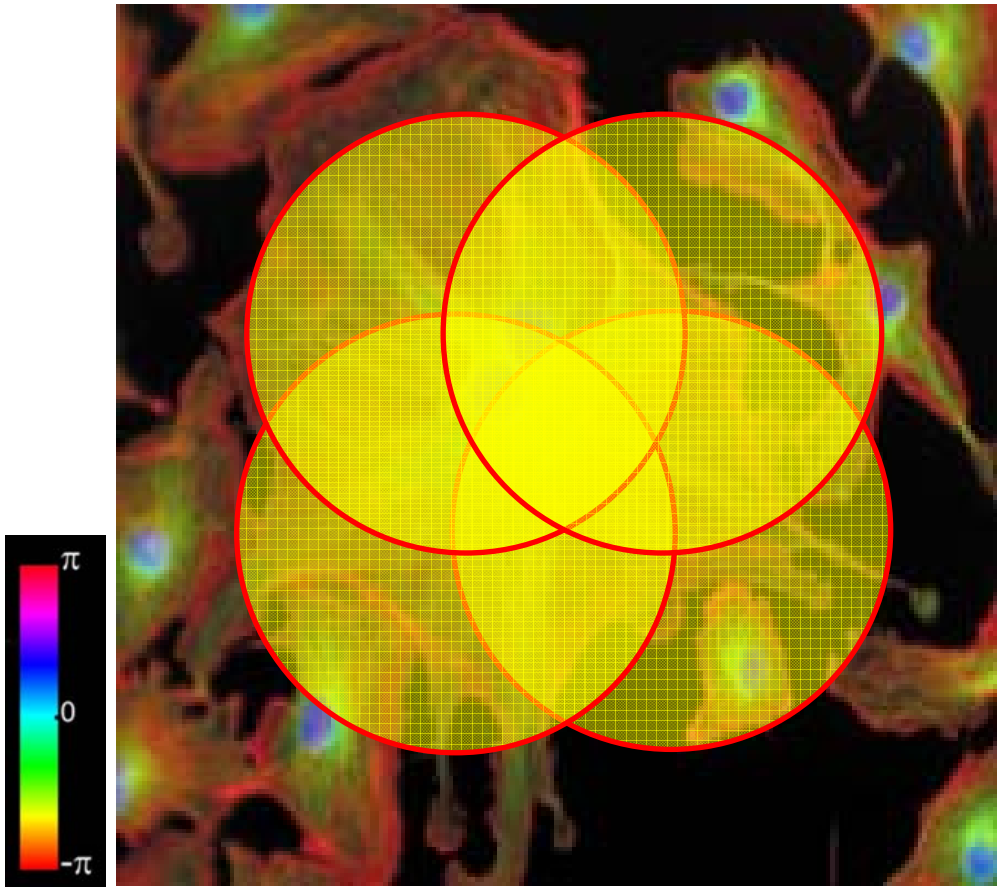
Diffractive imaging of extended objects

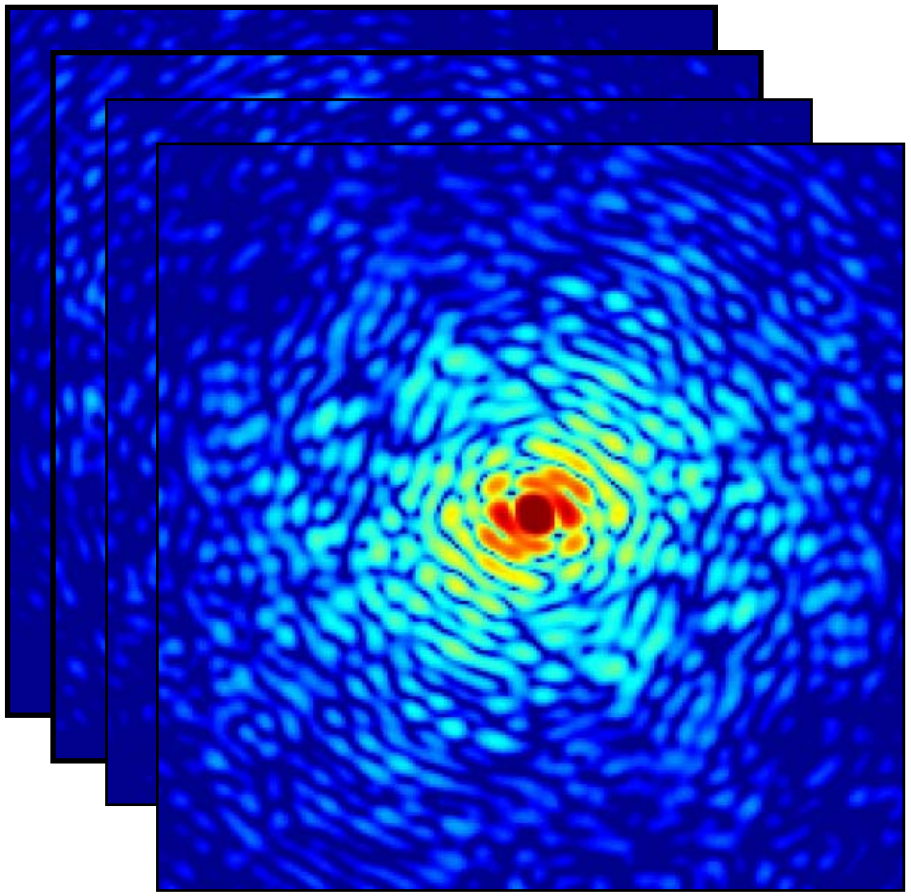


Diffractive imaging of extended objects



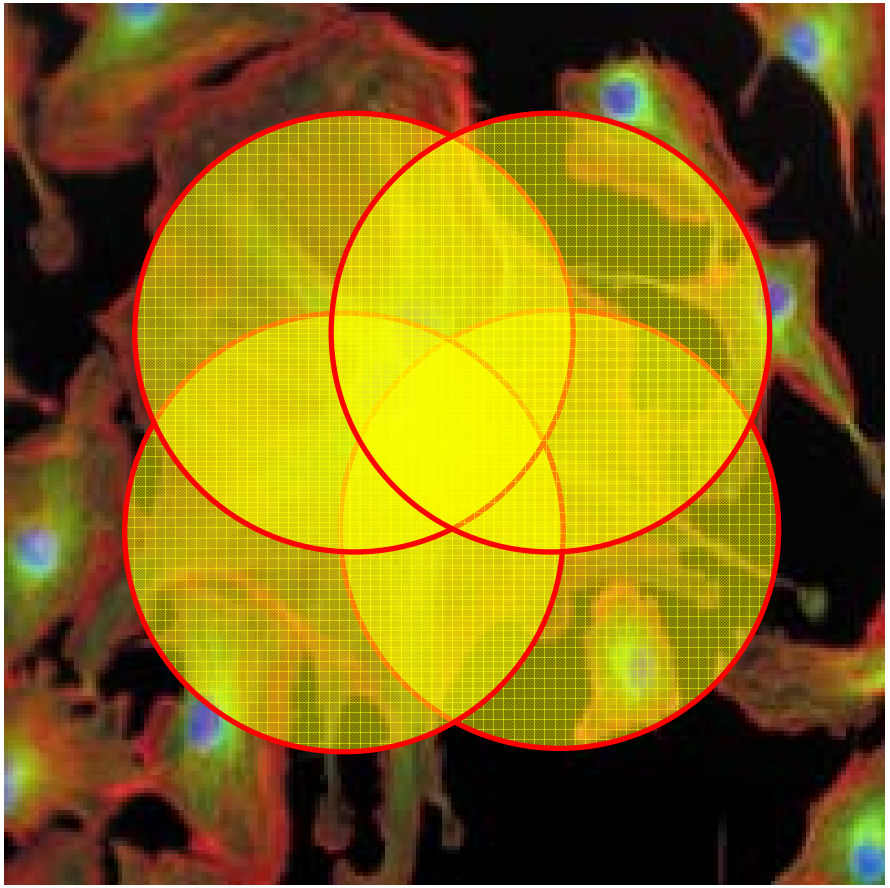
Numerical simulations



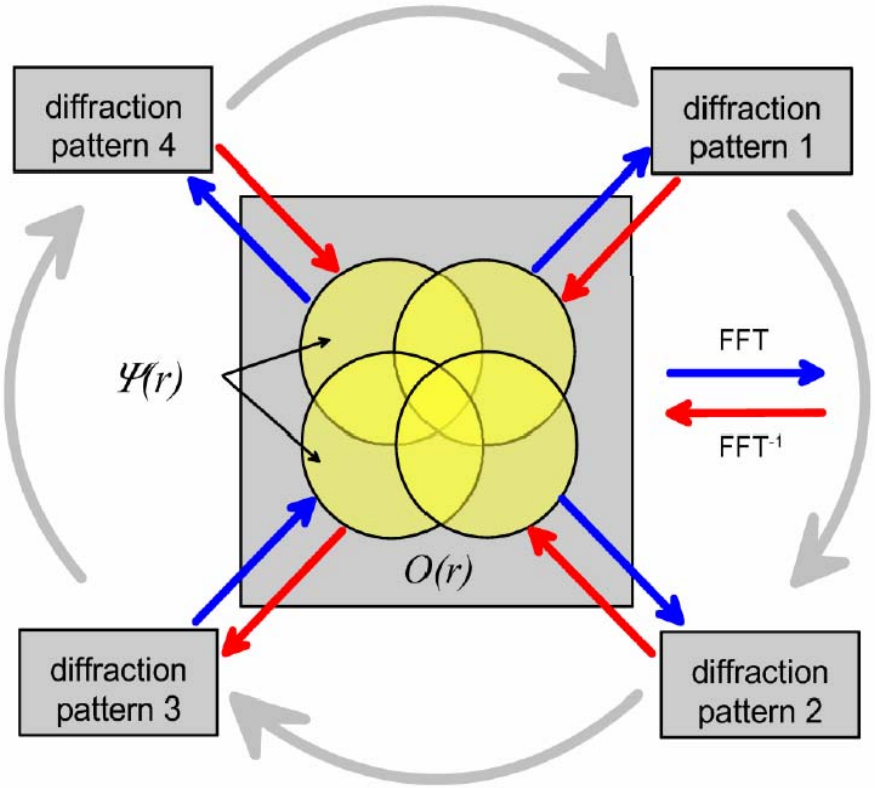


brightness => amplitude
hue => phase

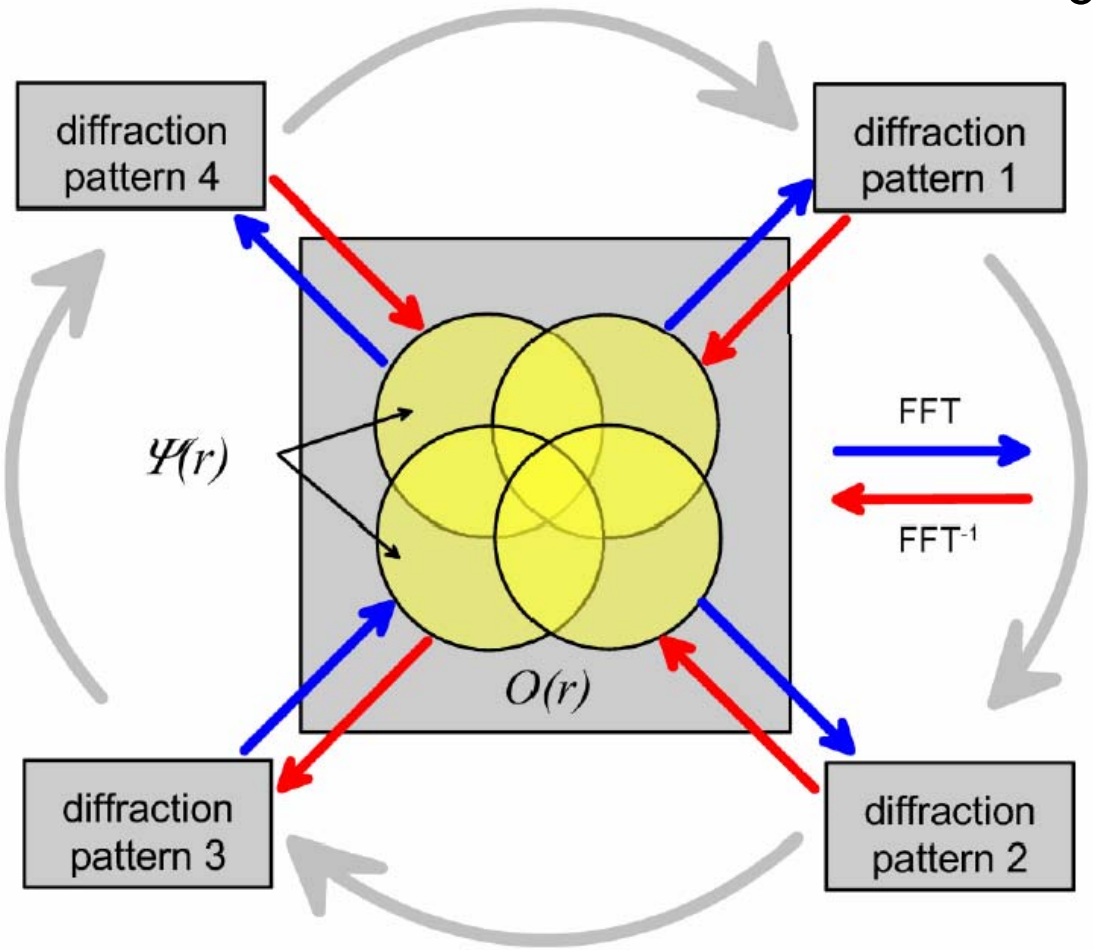
Numerical simulations



algorithm



PIE algorithm



Current object guess

Illumination function

$$\psi(\mathbf{r},\mathbf{R}) = O_n(\mathbf{r})P(\mathbf{r}-\mathbf{R})$$

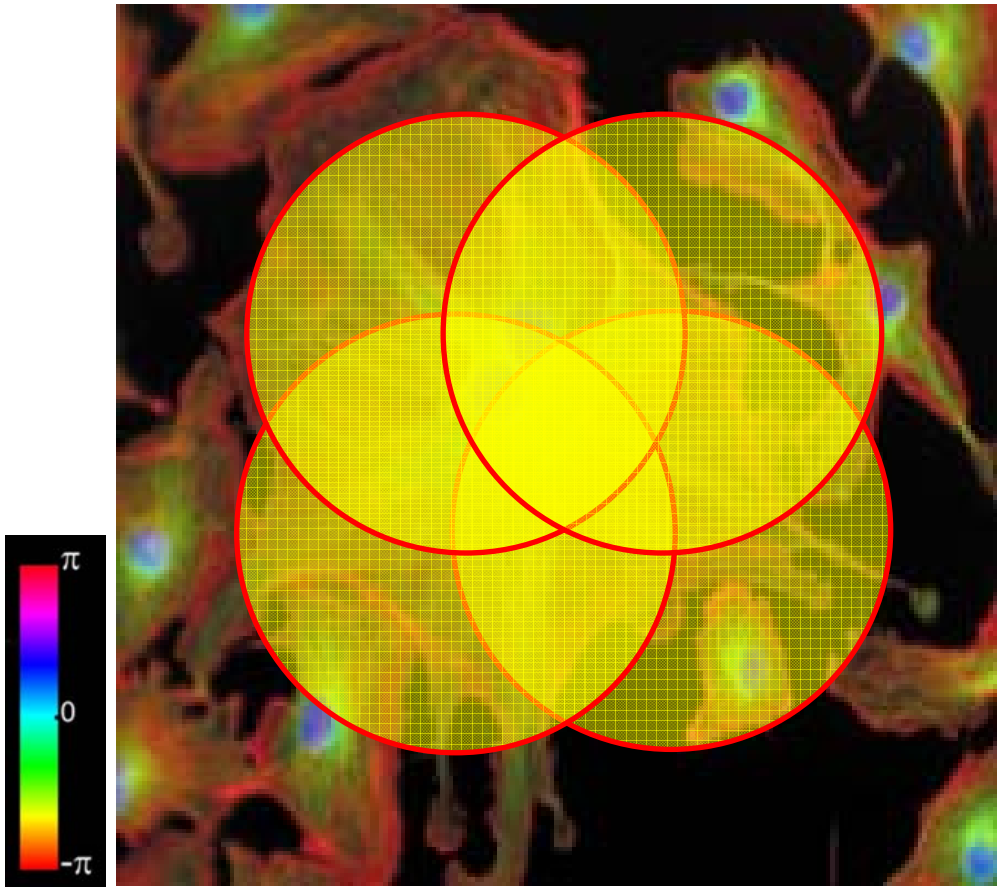
apply fourier space constraints

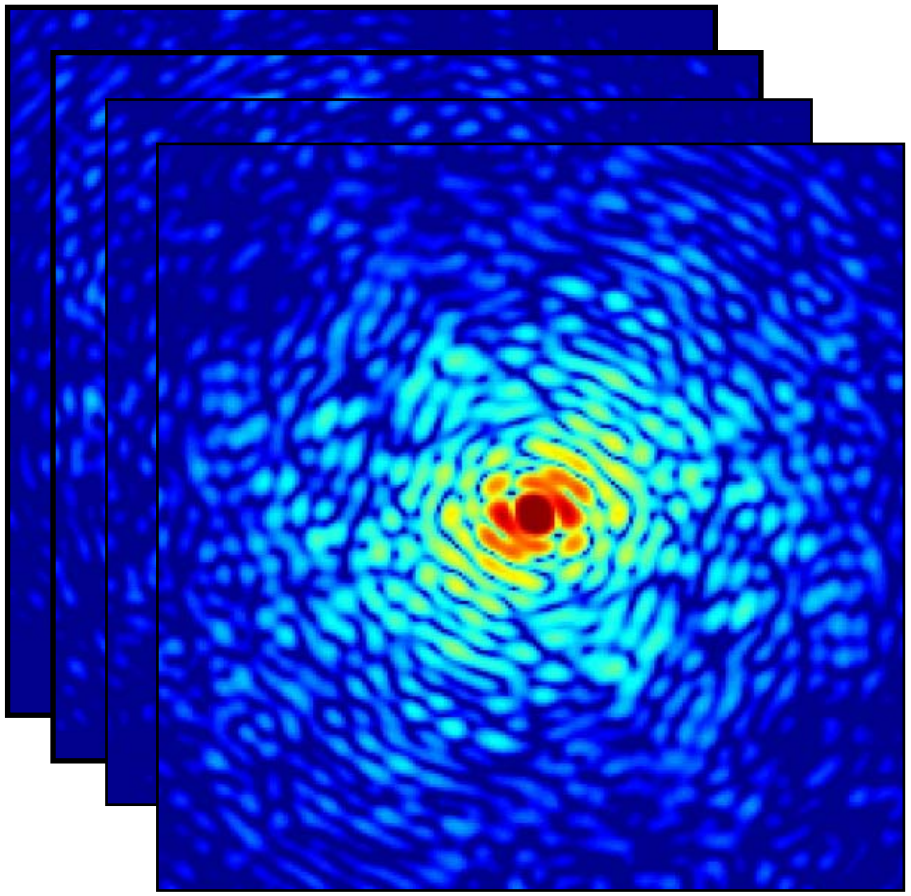
$$O_{n+1}(\mathbf{r}) = O_n(\mathbf{r}) + U(\mathbf{r}-\mathbf{R})(\psi_{c,n}(\mathbf{r},\mathbf{R}) - \psi_n(\mathbf{r},\mathbf{R}))$$

update function

move to next aperture position

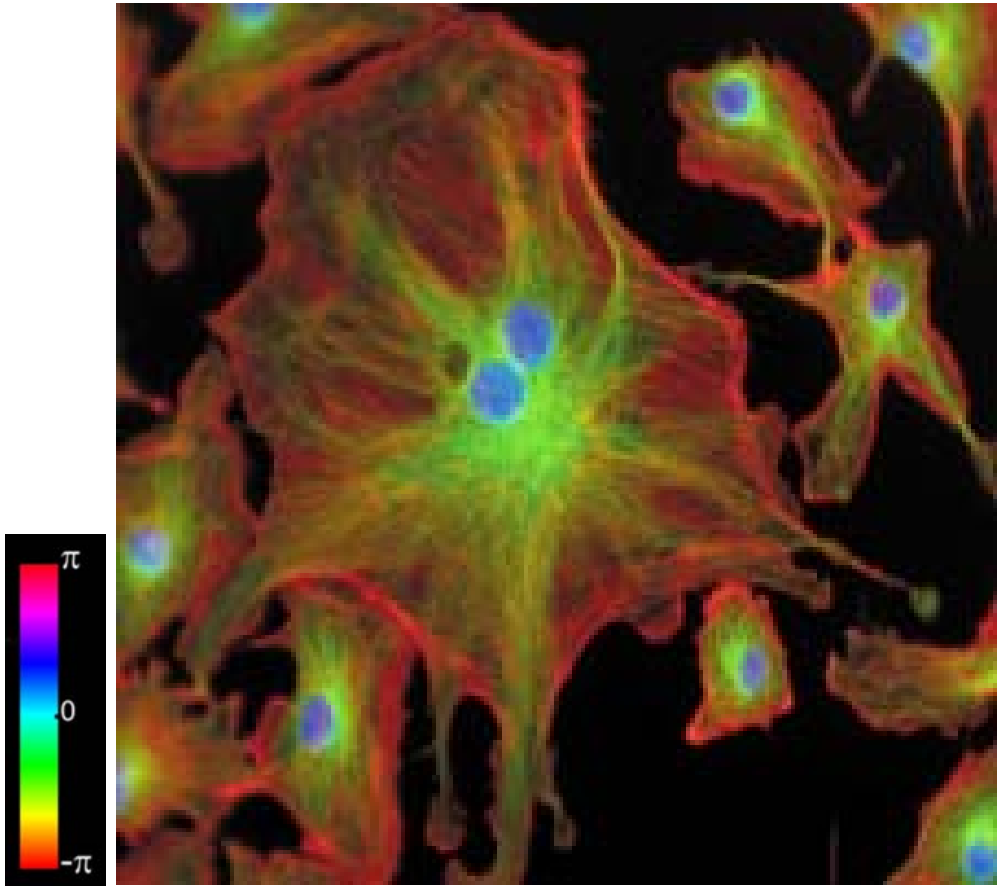
Numerical simulations

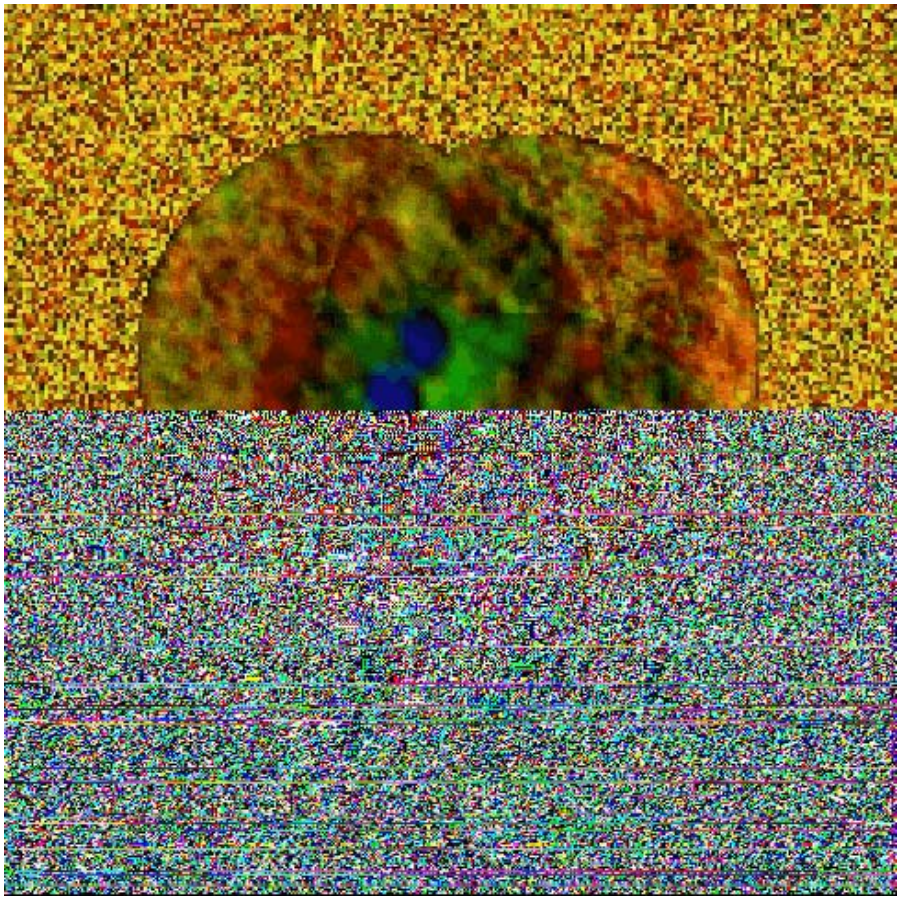




brightness => amplitude
hue => phase

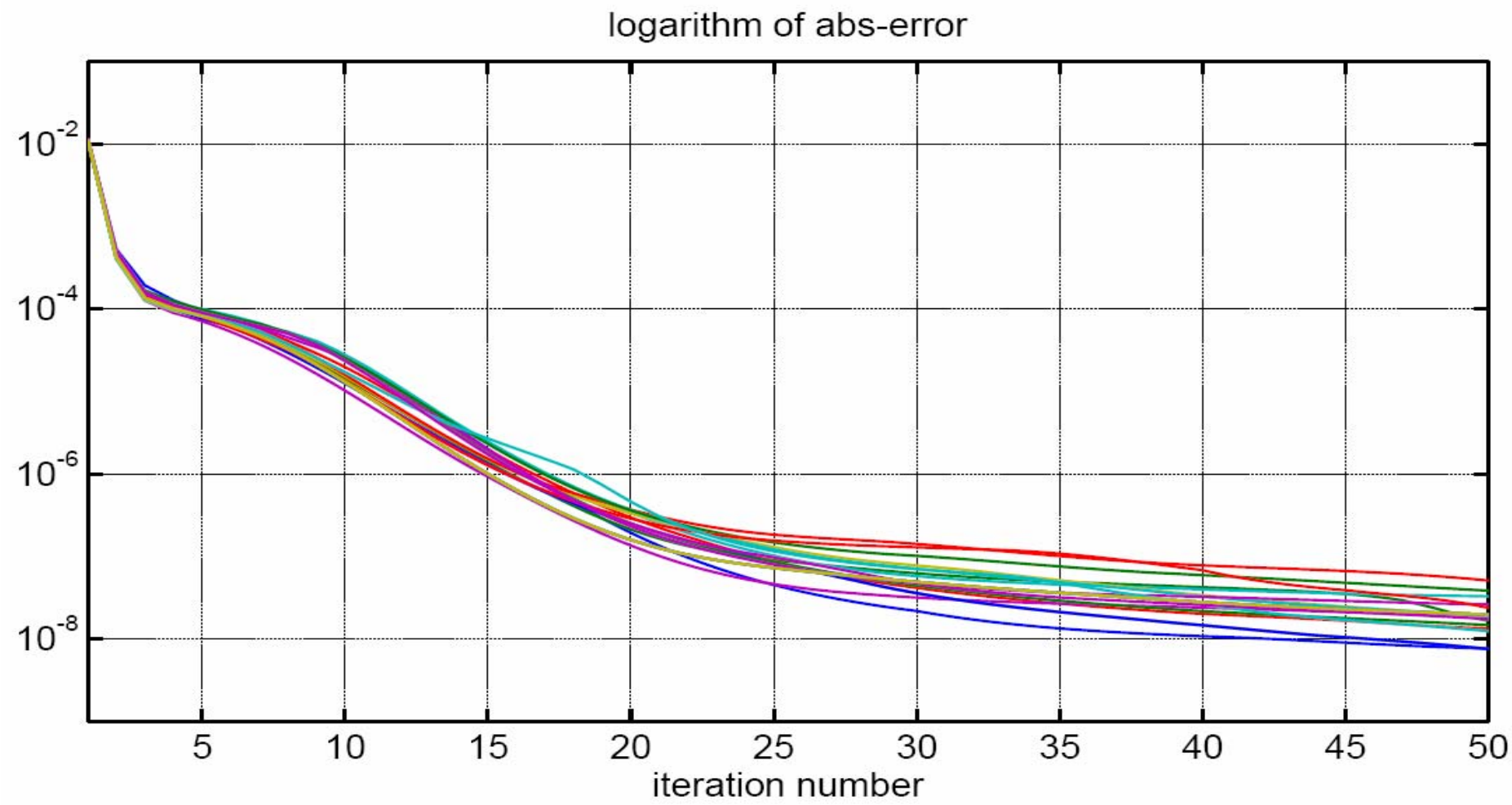
Simulations





Converges 200 x faster & works for complex extended objects

Simulations



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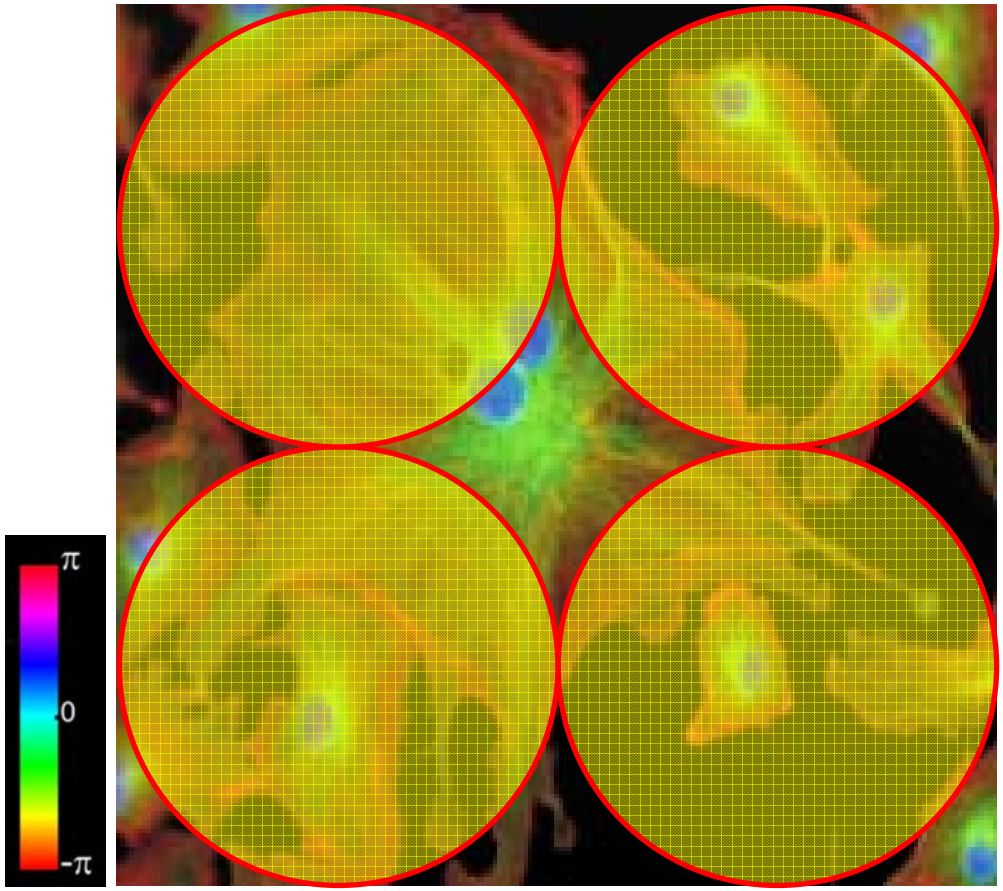
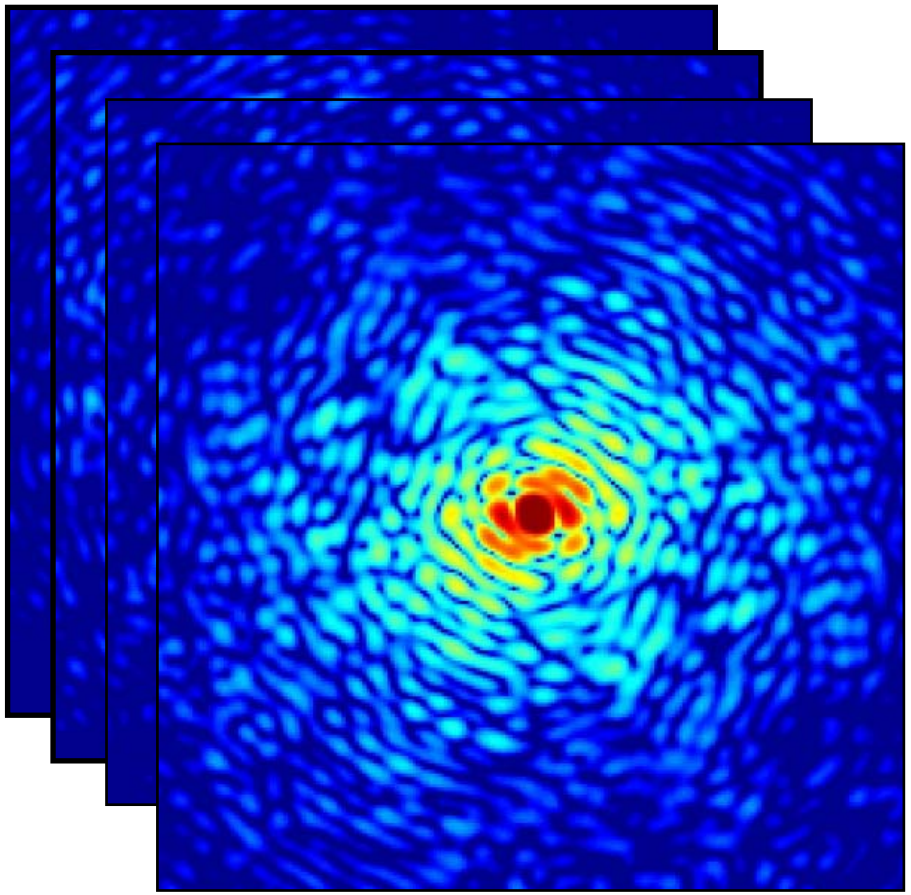
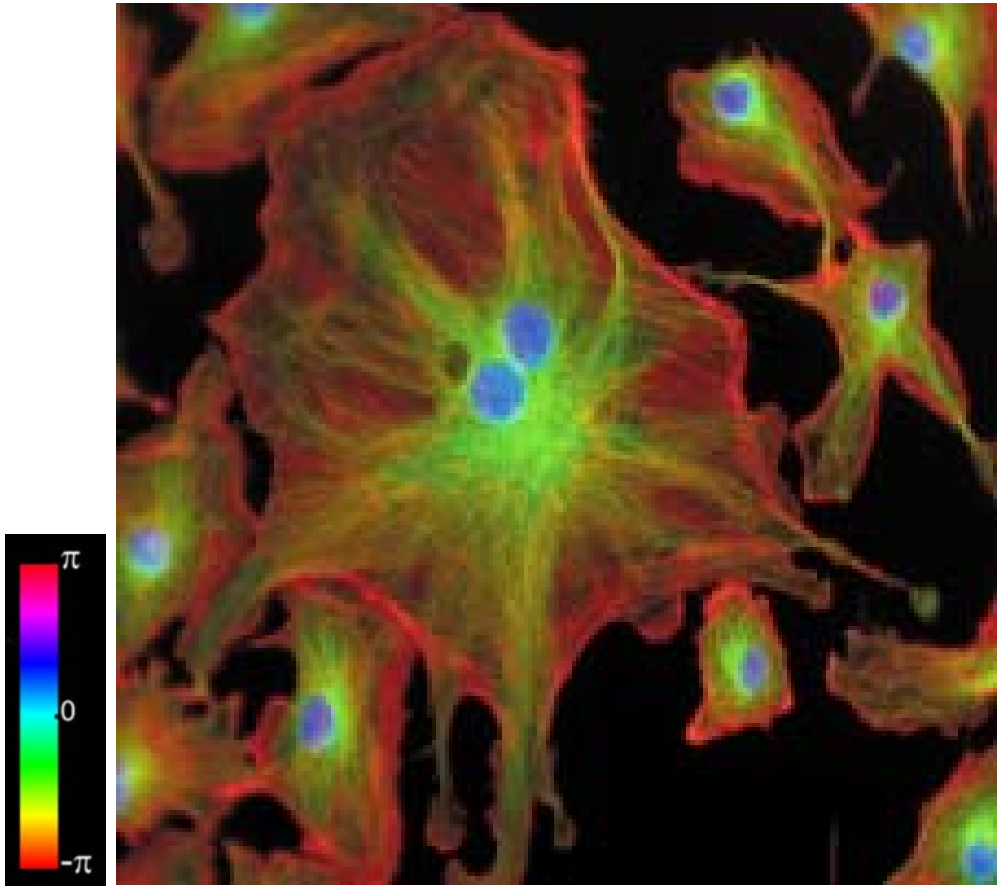
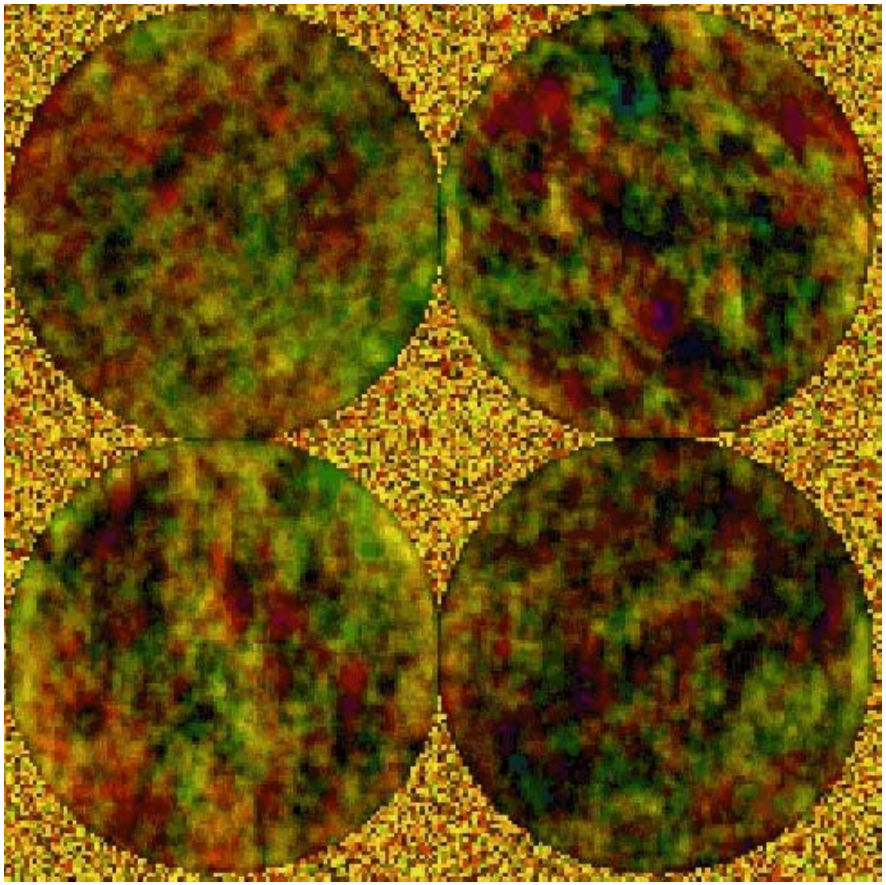
Simulations



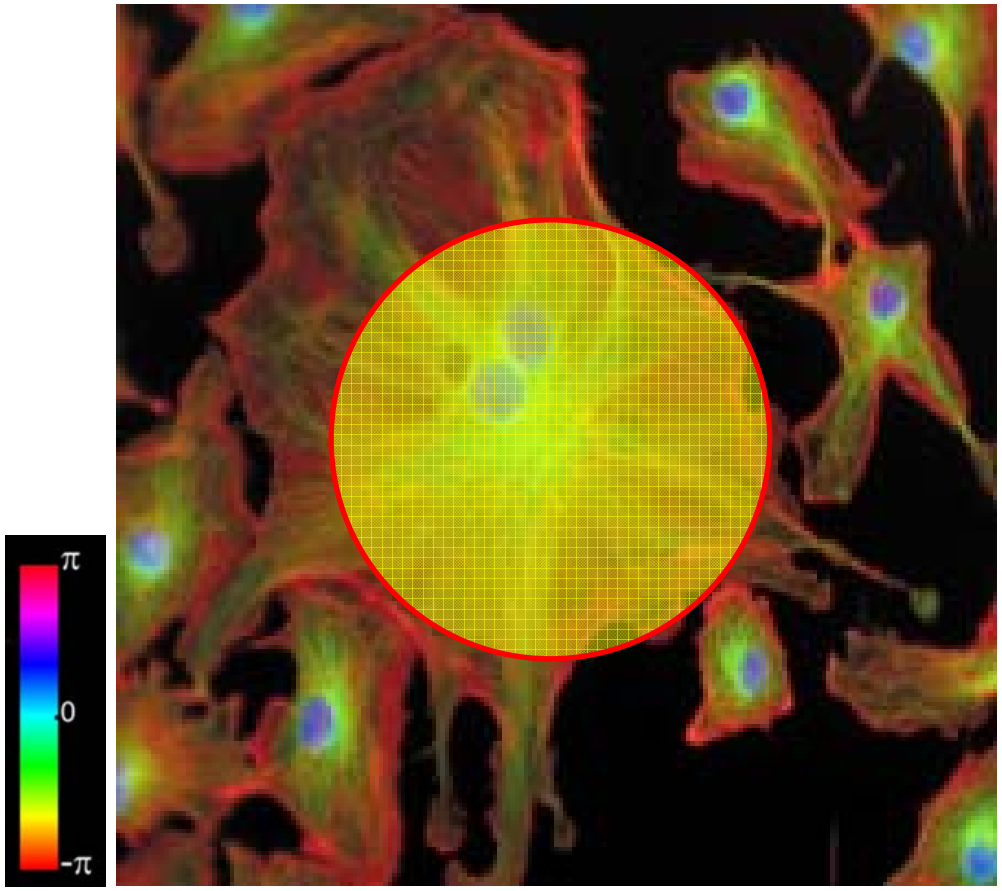


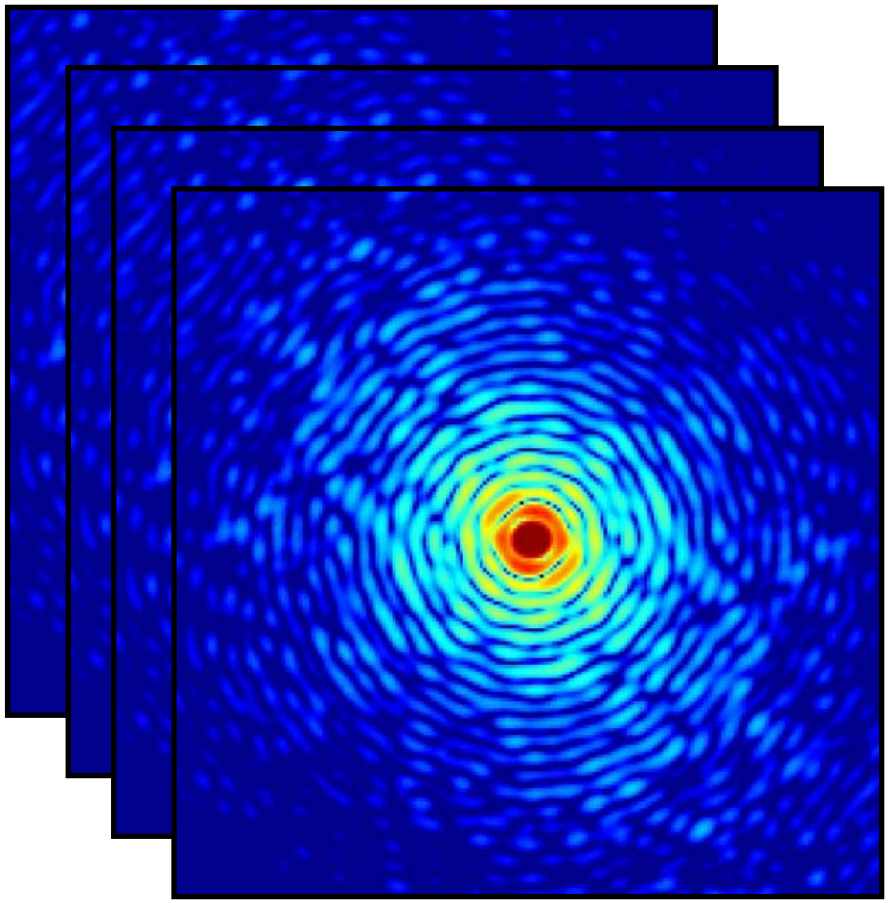
Simulations



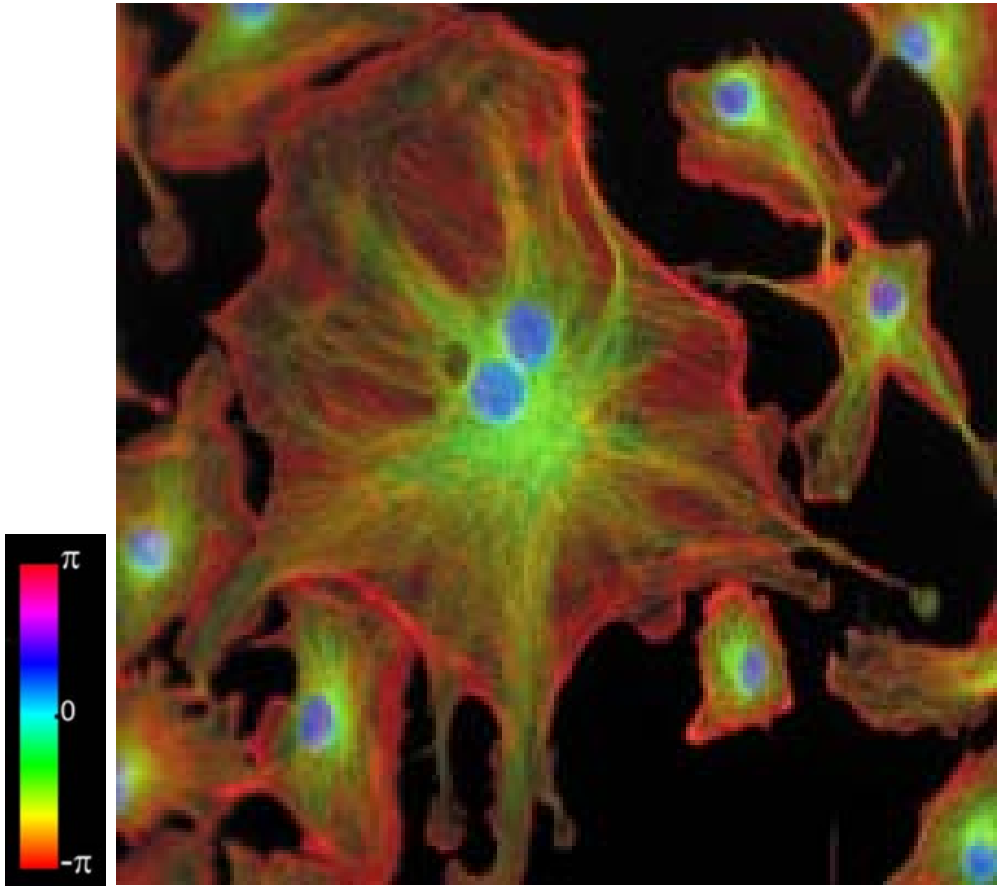


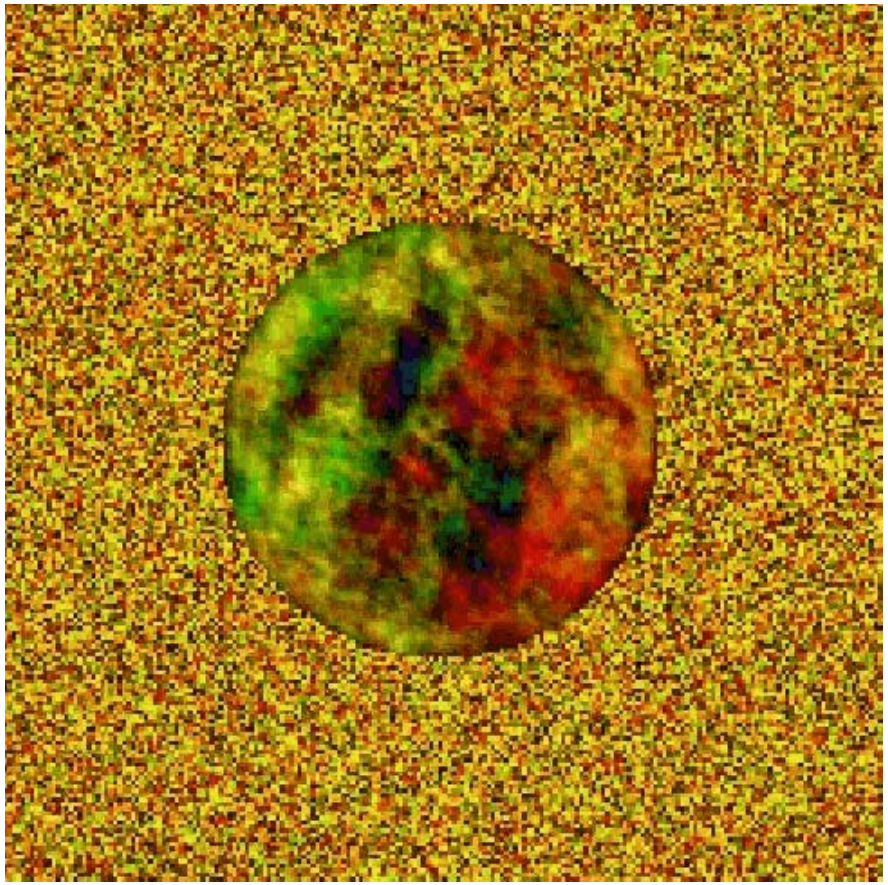
Simulations





Simulations





First experimental results with visible light

ELSEVIER

Transmission microscopy without lenses for objects of unlimited size

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ultramicroscopy

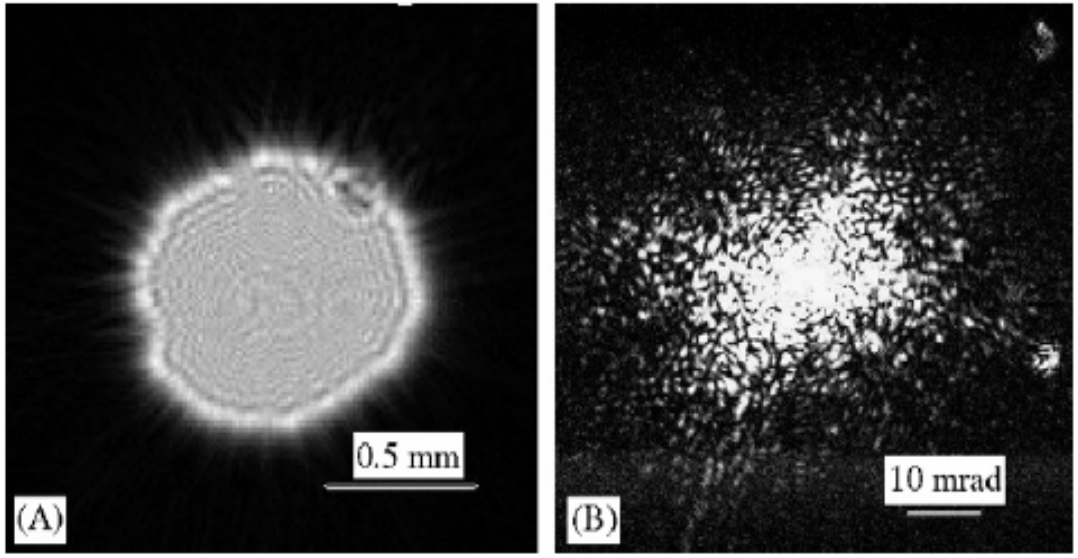
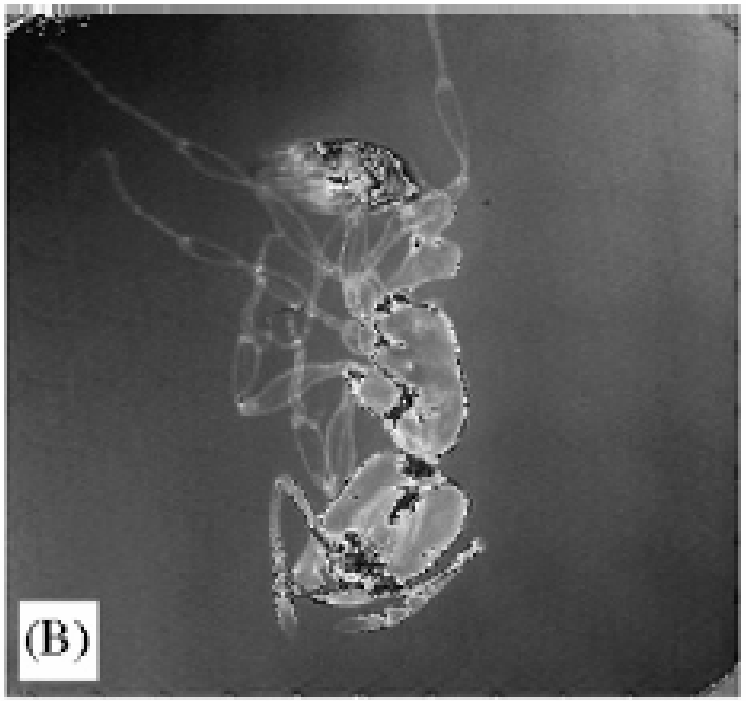
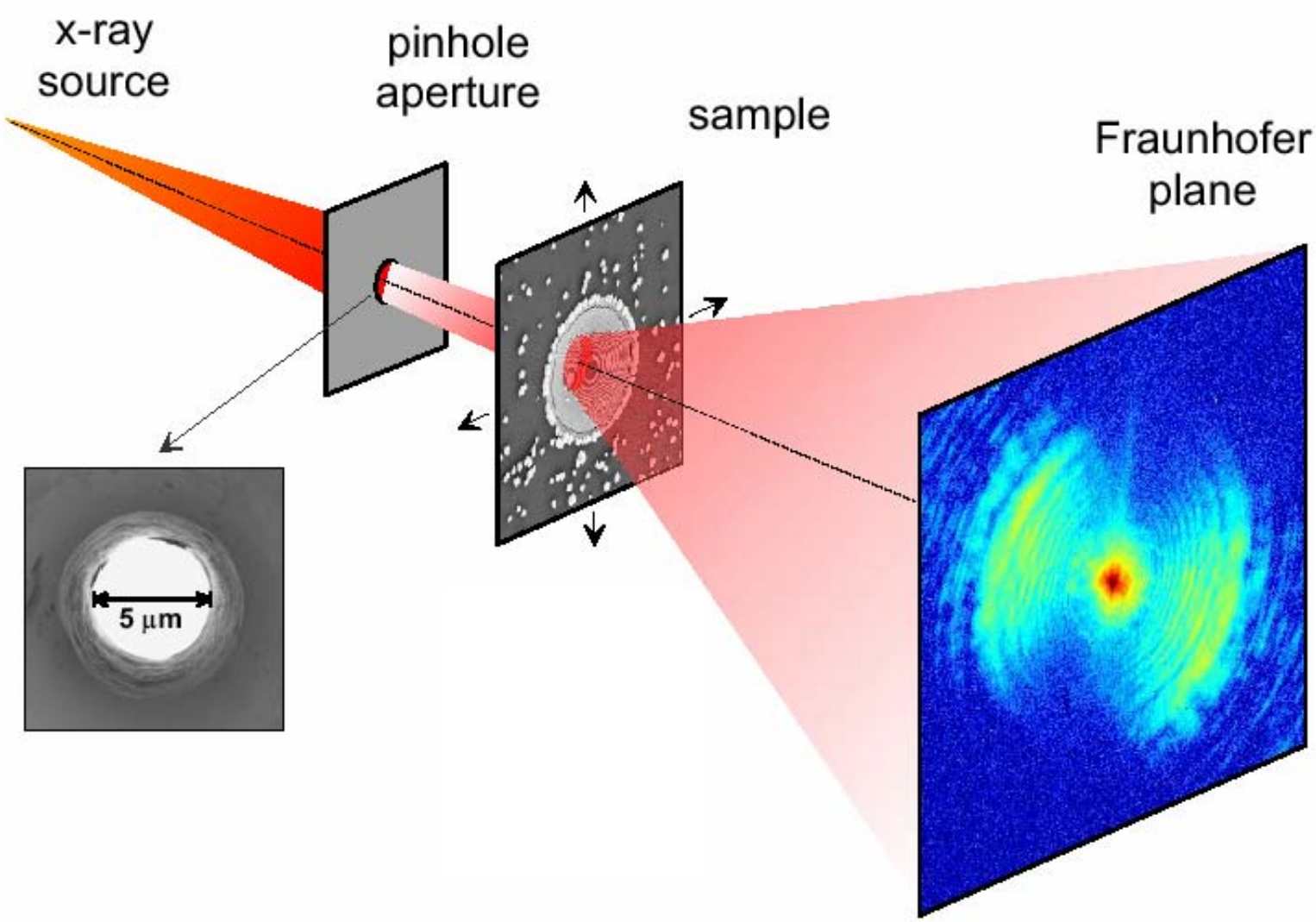


Fig. 1. Experimental data. (A) The illumination function measured in intensity at the object plane. The aperture diameter is 0.8 mm and the object plane is 1 mm downstream of this, hence we see Fresnel interference and broadening of the intensity distribution. A calculated illumination

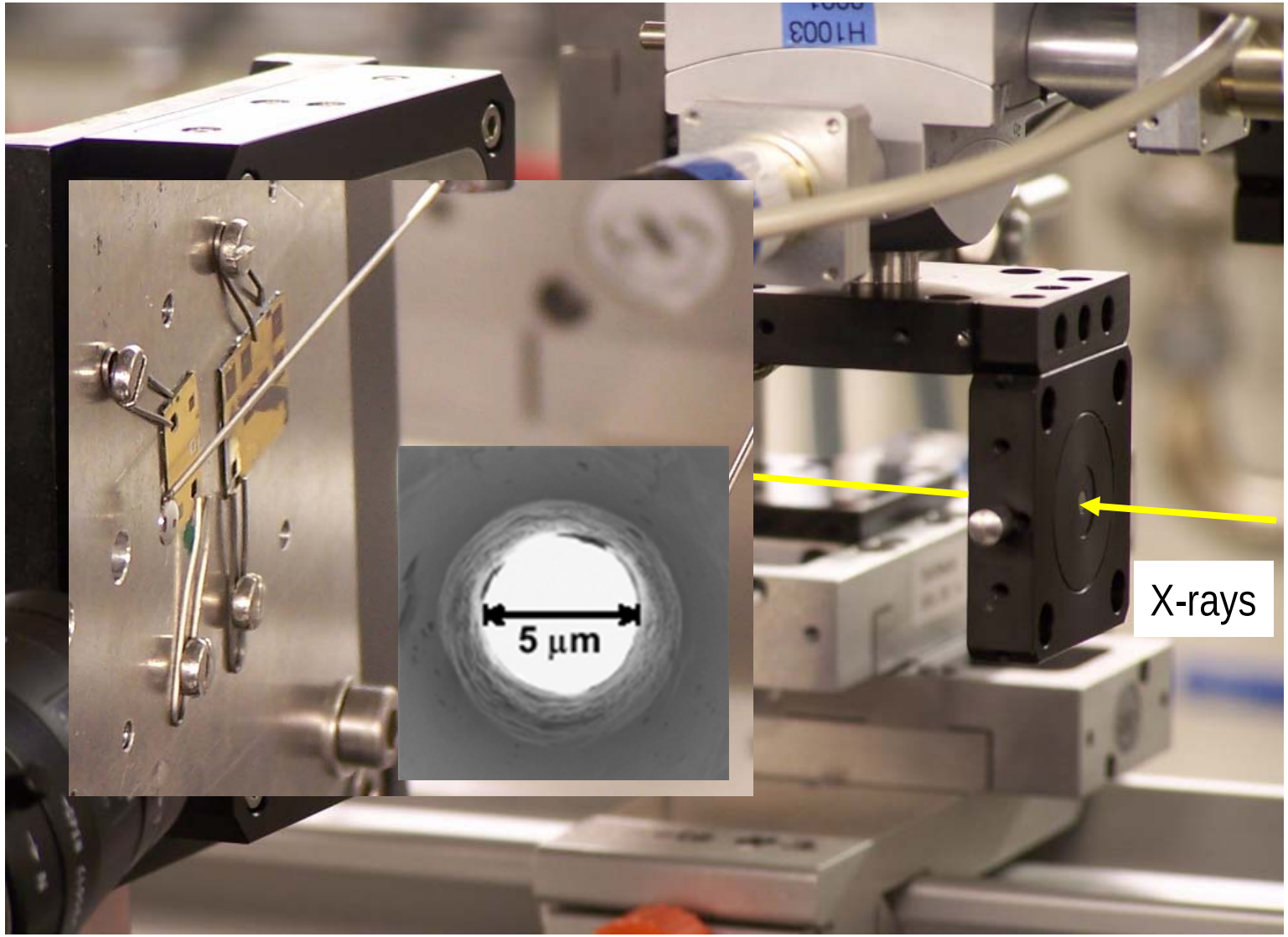


J. Rodenburg et al., Ultramicroscopy 107, 227 (2007)

First results for hard x-rays

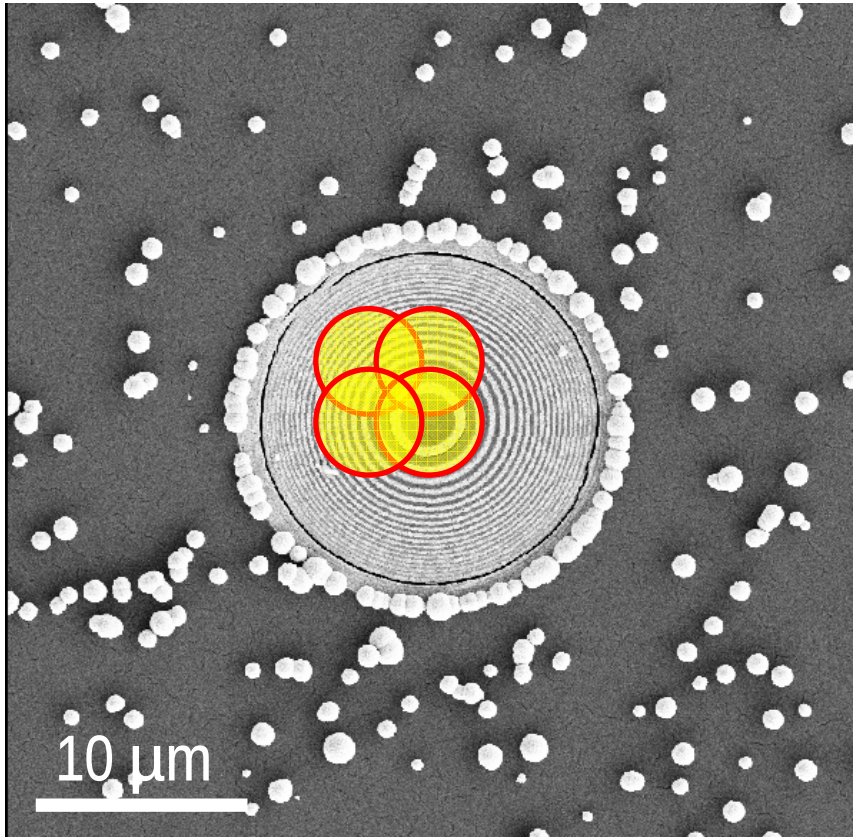


First results for hard x-rays

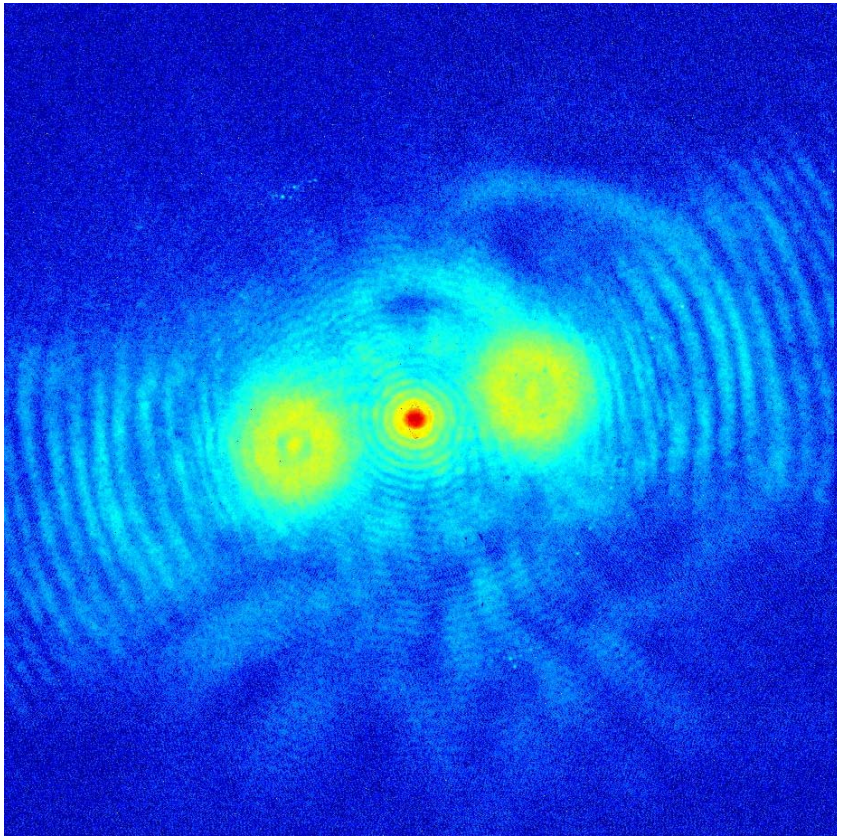


First results with hard x-rays

SEM image



measured diffraction pattern

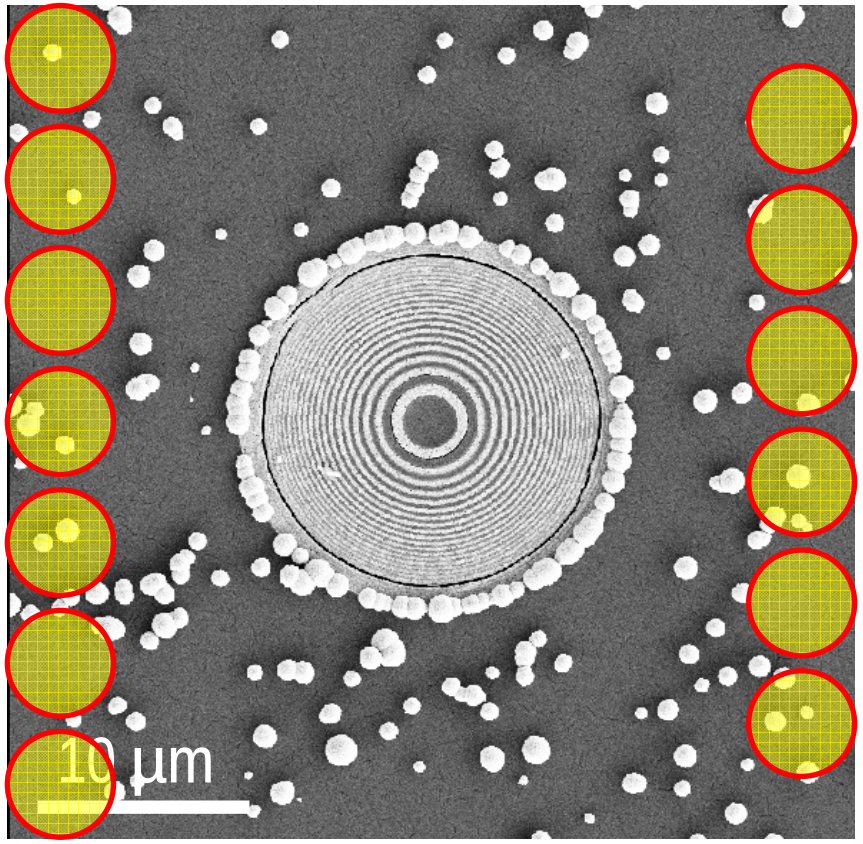


8 keV x-rays, Swiss Light Source

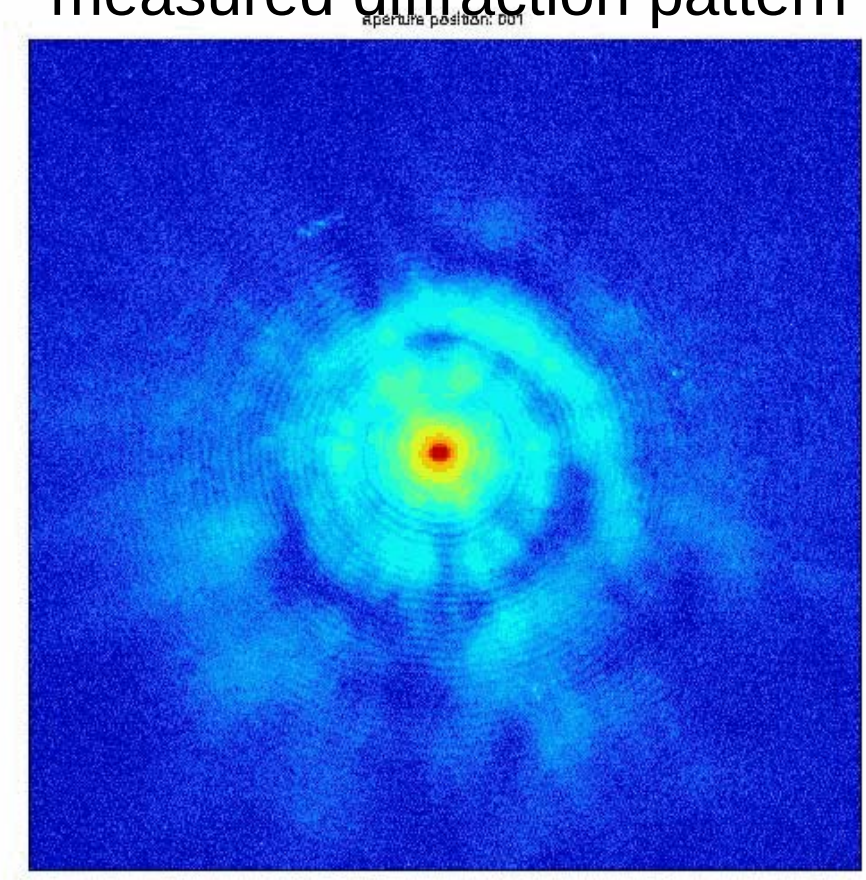
pinhole diameter: 5 µm, 17 x 17 overlapping diffraction patterns, radial overlap: 2.5 µm, 80 + 8 sec exposure time

First results with hard x-rays

SEM image



measured diffraction pattern



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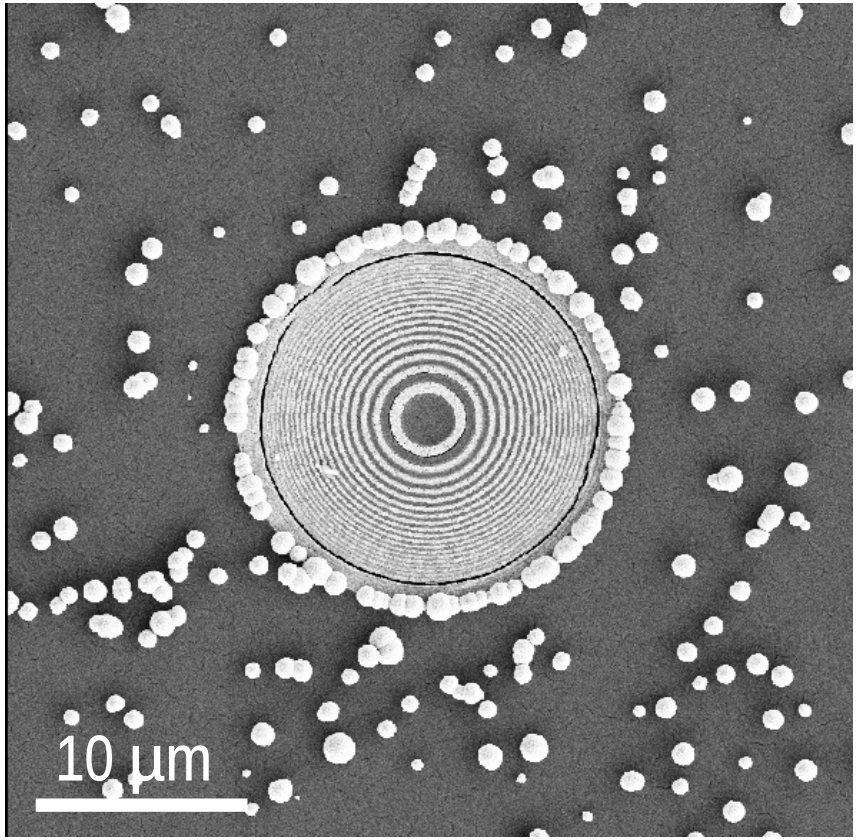
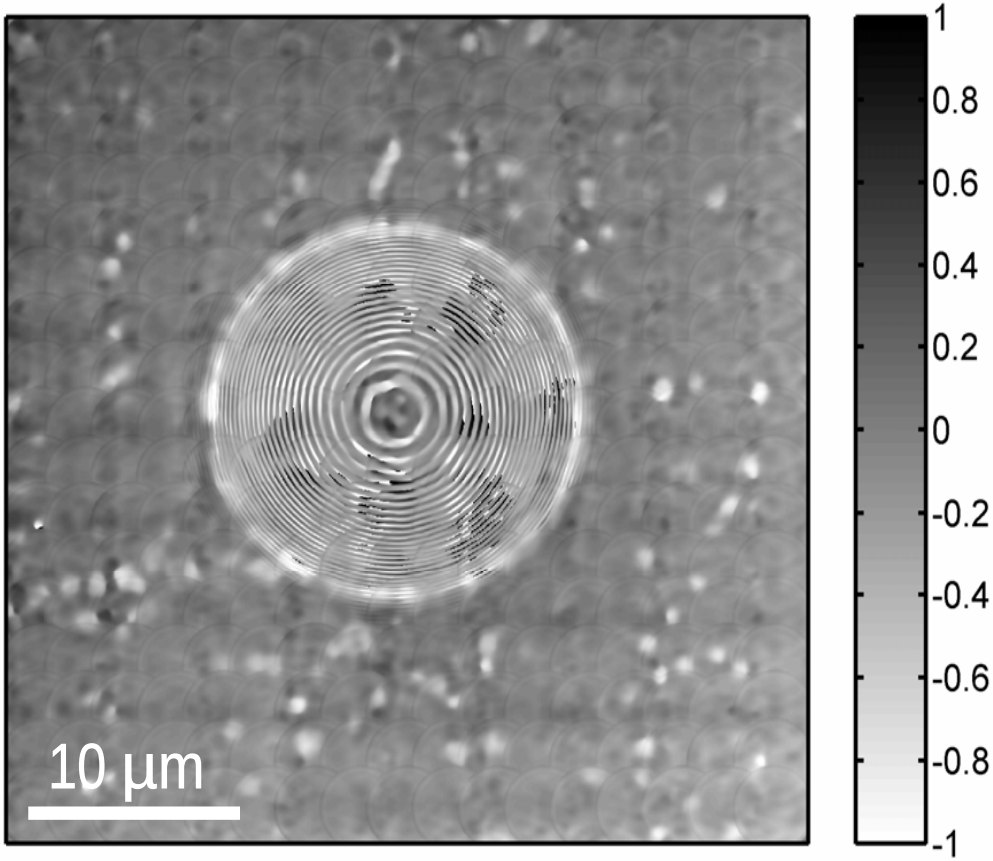
SEM image



reconstructed phase

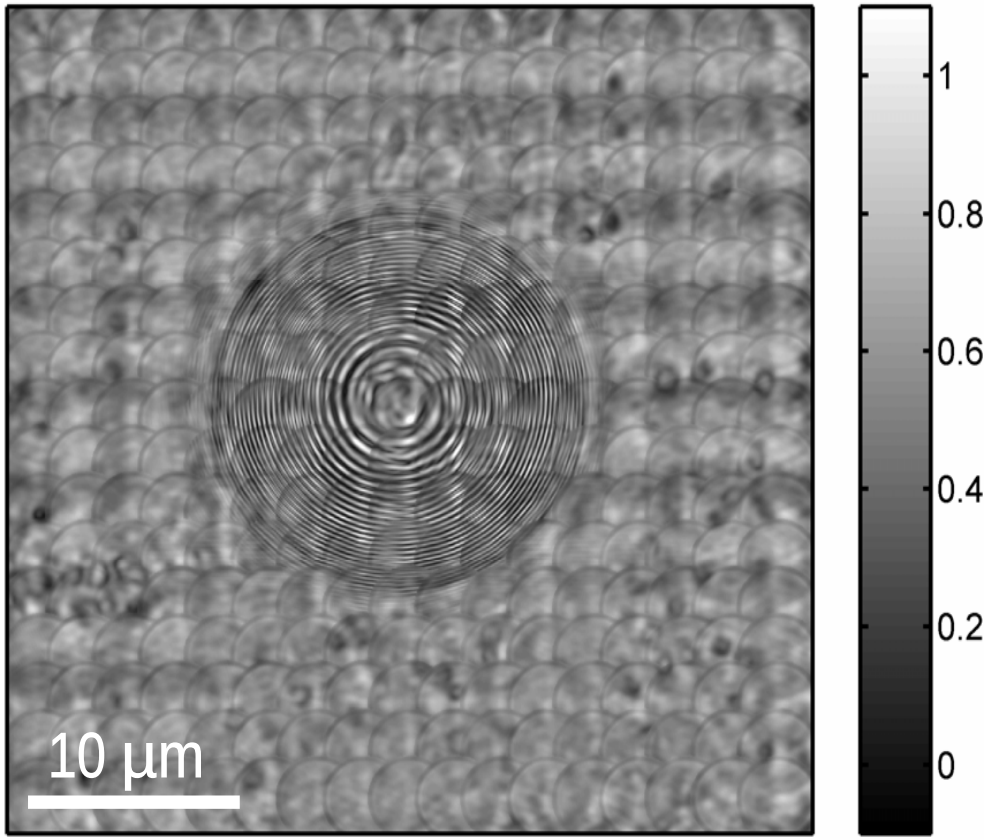


Reconstruction obtained after 20 iterations !

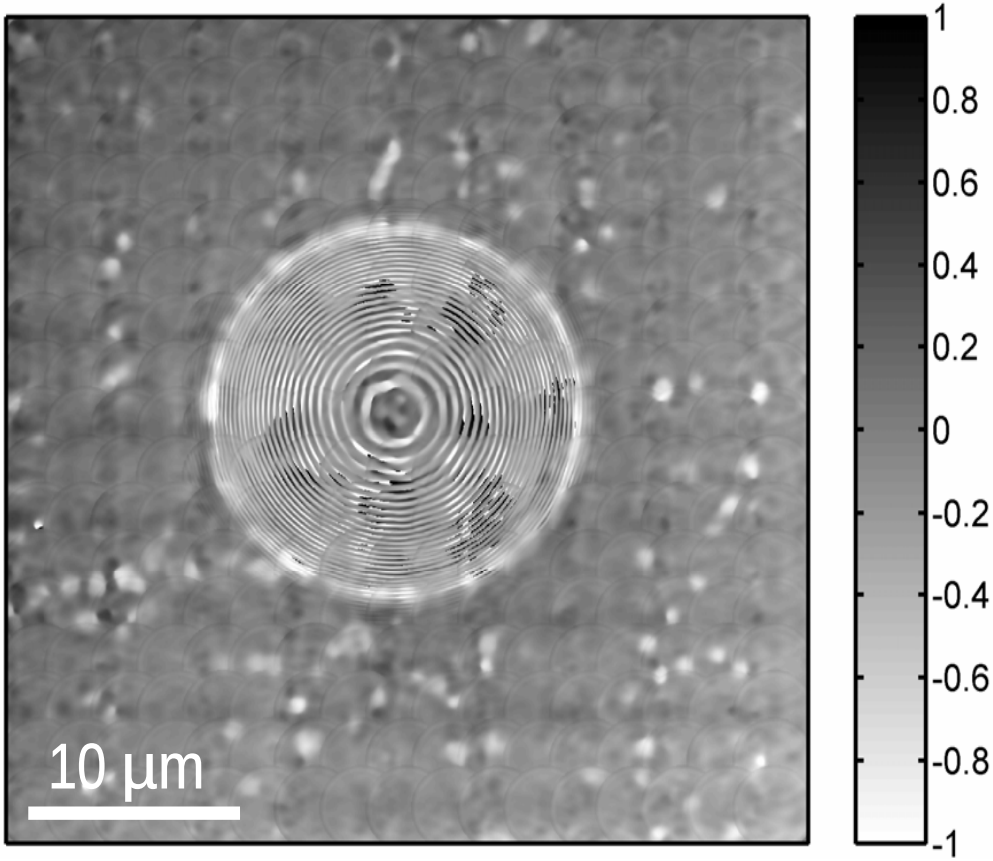
pinhole diameter: 5 µm, 17 x 17 overlapping diffraction patterns, radial overlap: 2.5 µm, 80 + 8 sec exposure time

First results with hard x-rays

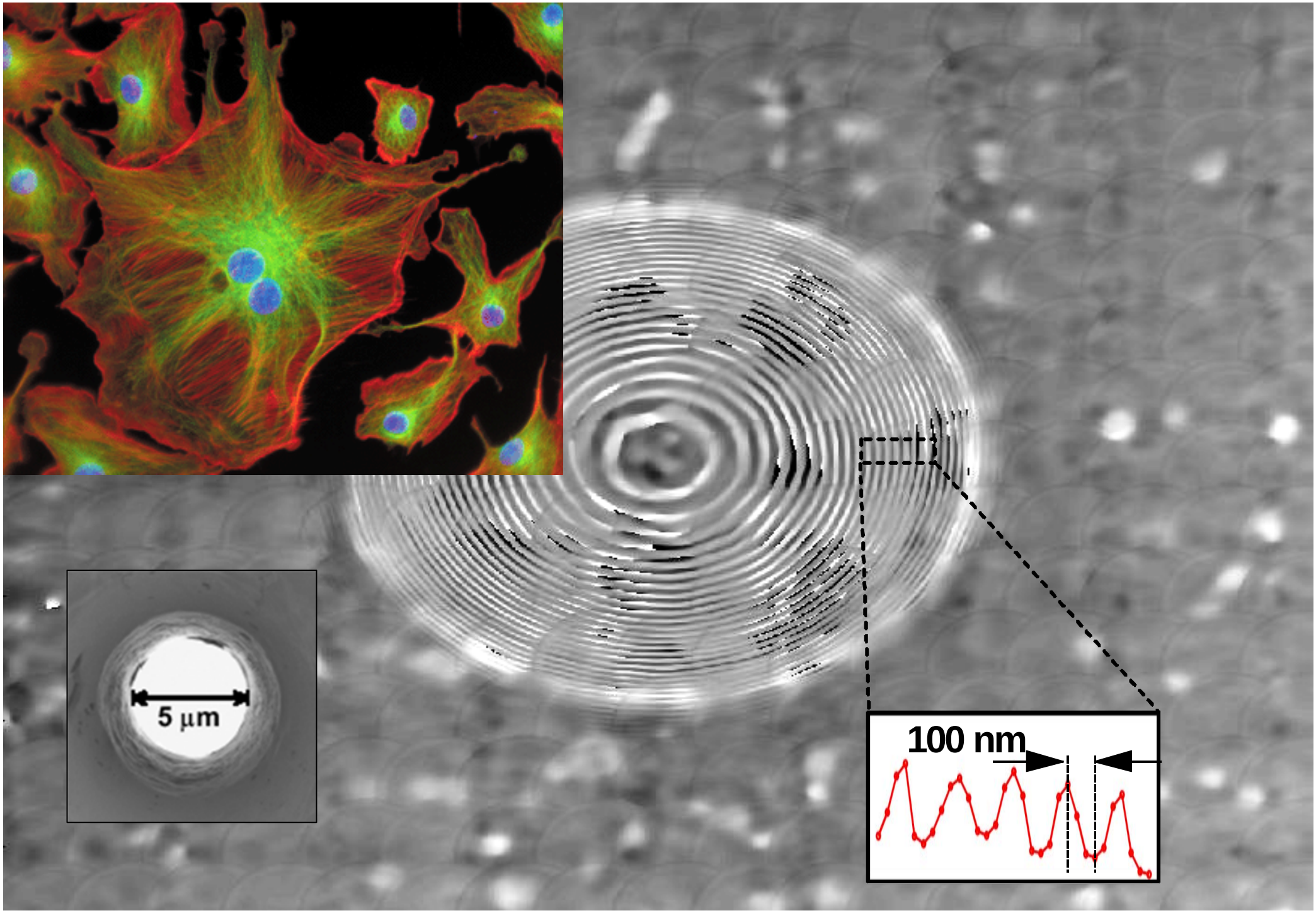
reconstructed amplitude

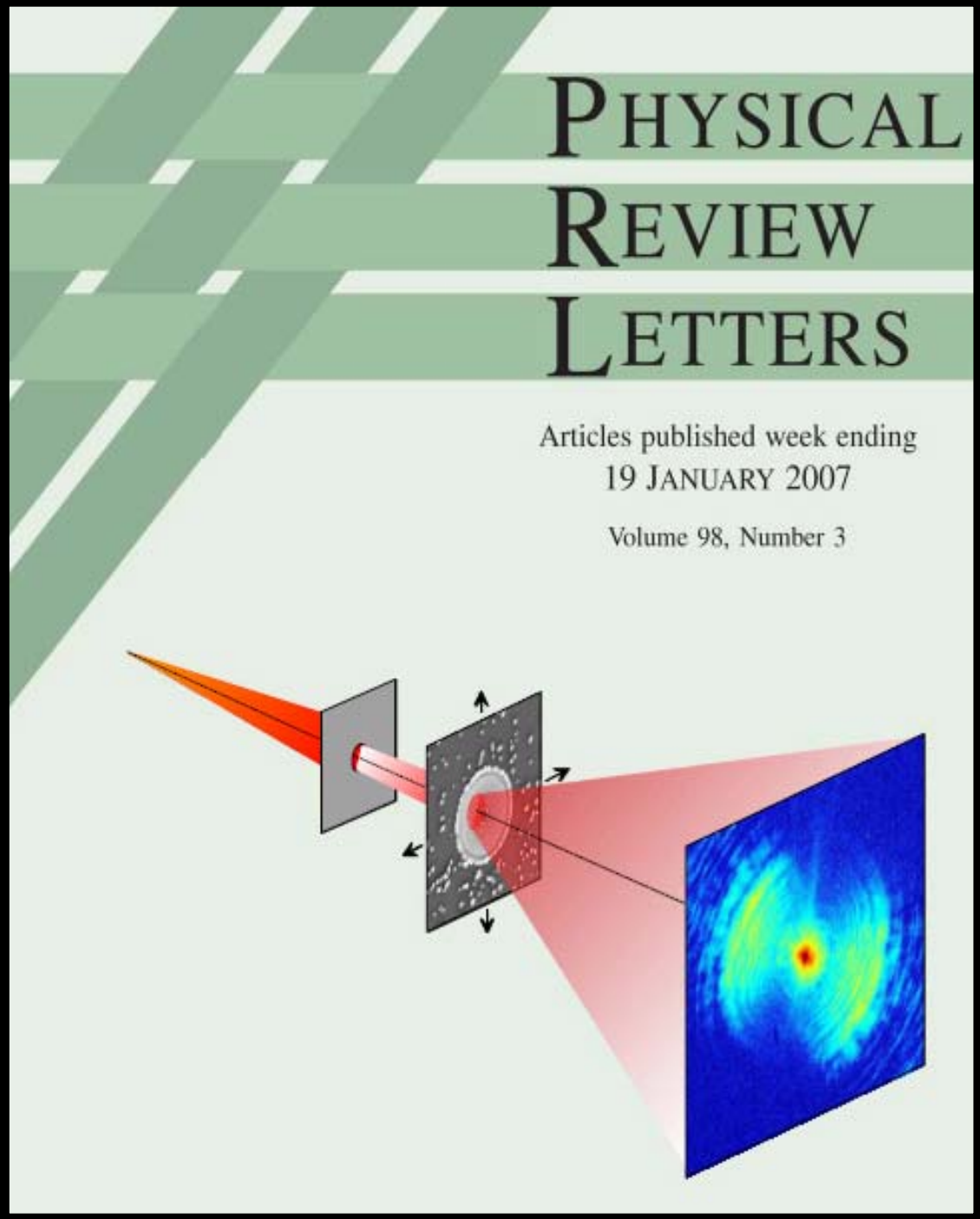


reconstructed phase



Unique solution for a complex object !

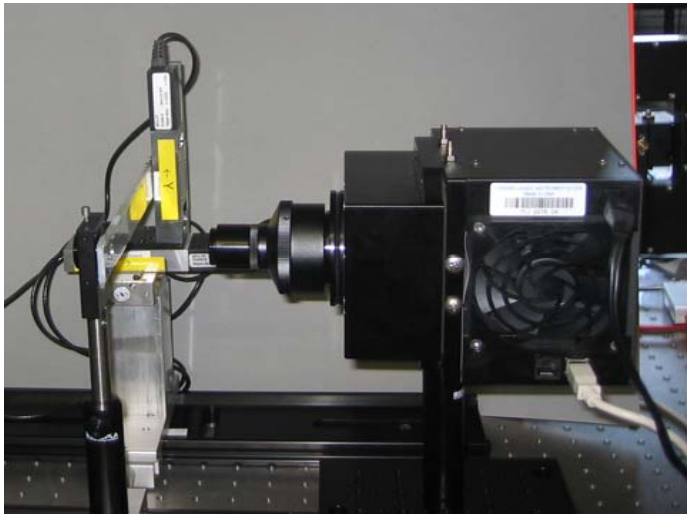

5 µm
100 nm

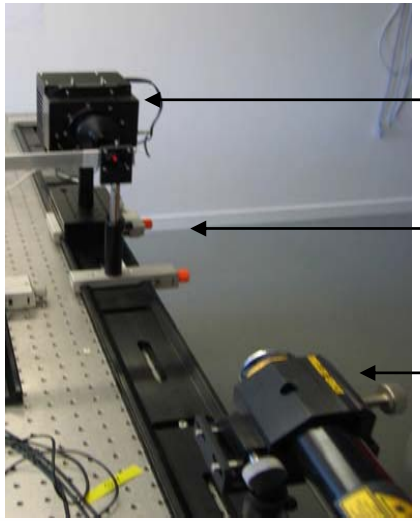


J.M. Rodenburg, A.C. Hurst, A.G. Cullis, B.R. Dobson, F. Pfeiffer, O. Bunk, C. David, K. Jefimovs, and I. Johnson

Phys. Rev. Lett. 98, 034801 (2007).

Diffractive imaging with visible laser sources

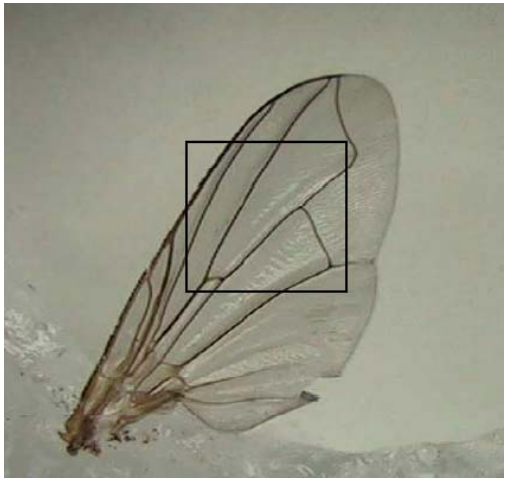


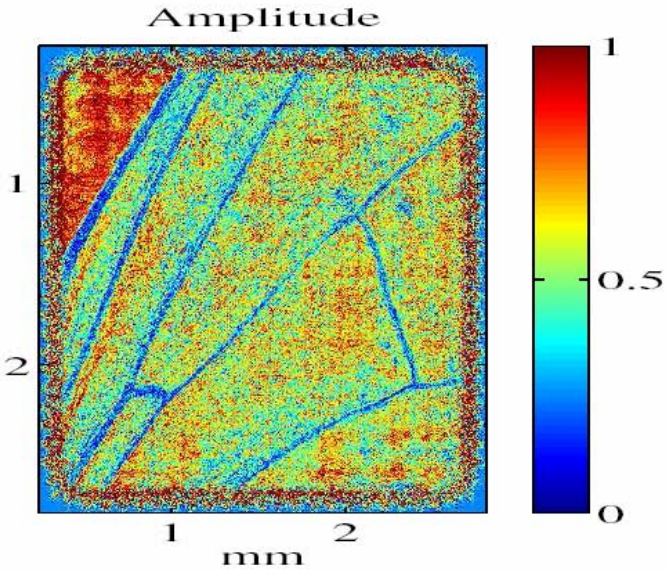


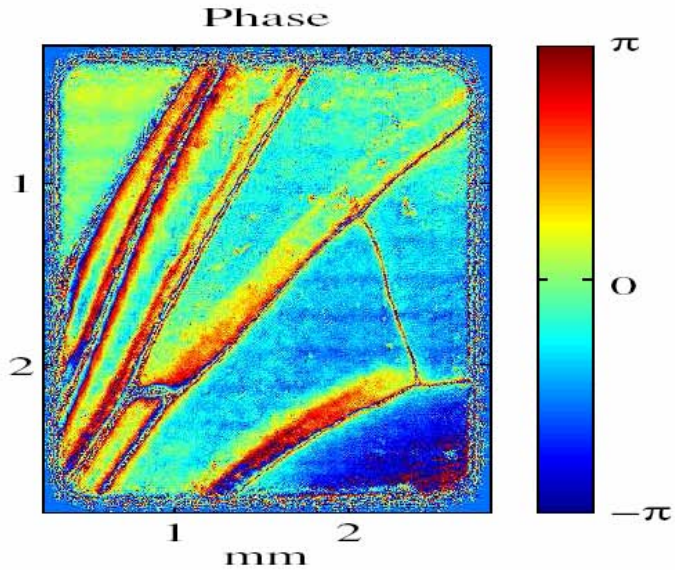
cooled CCD, 16 bit

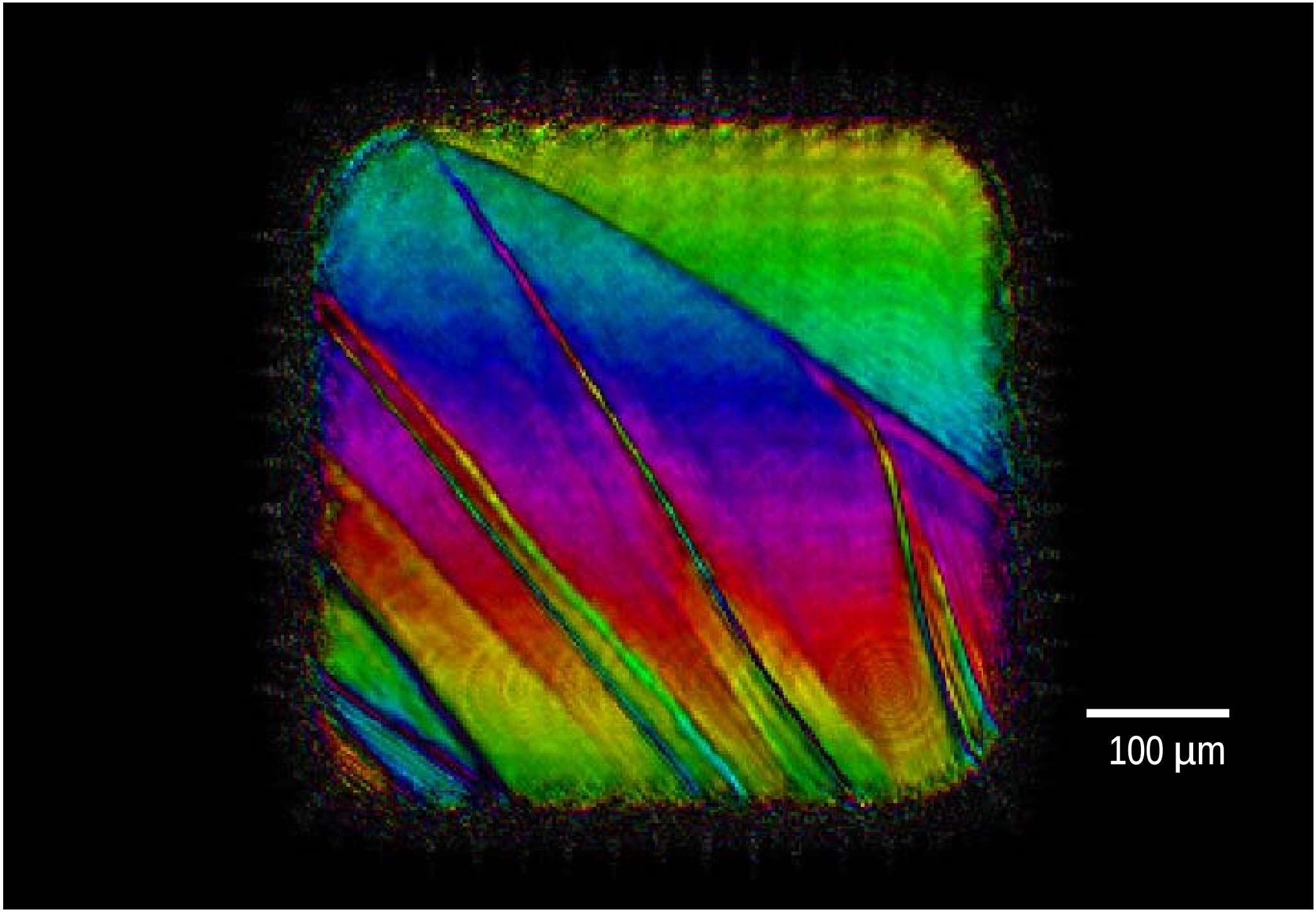
object on xy translation stage

HeNe laser, 15 mW, continuous

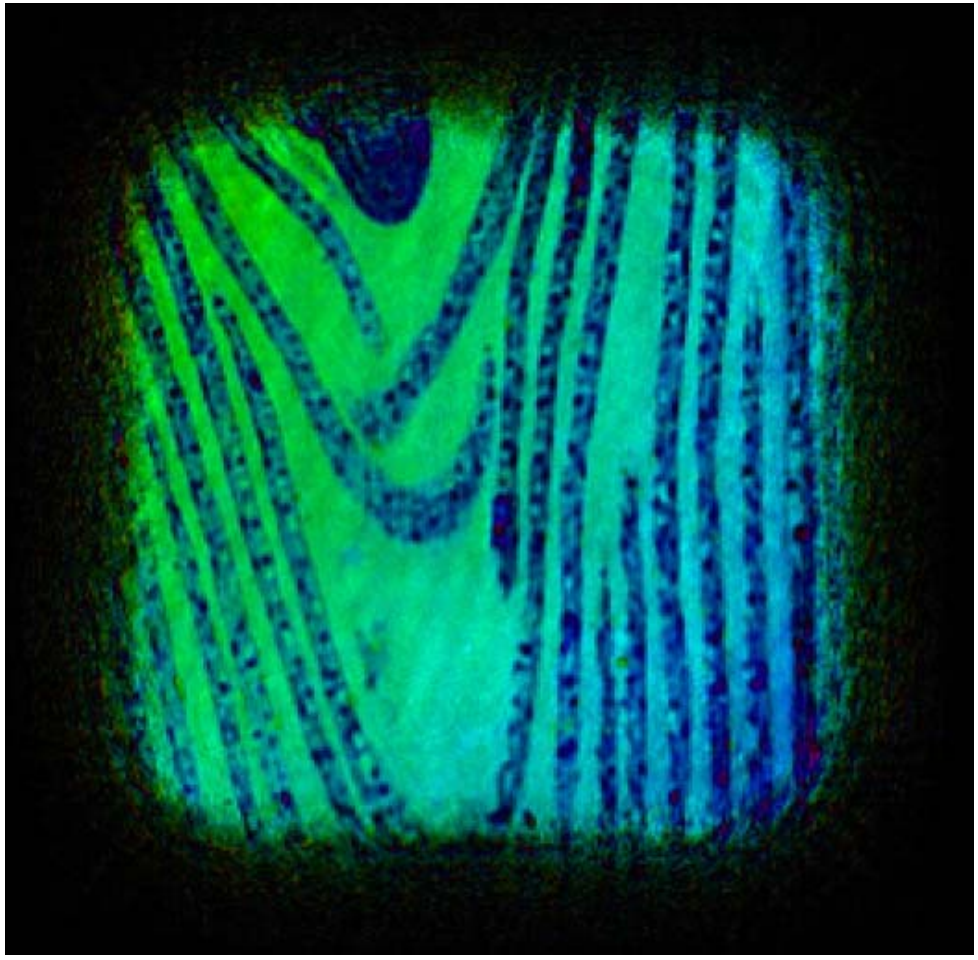






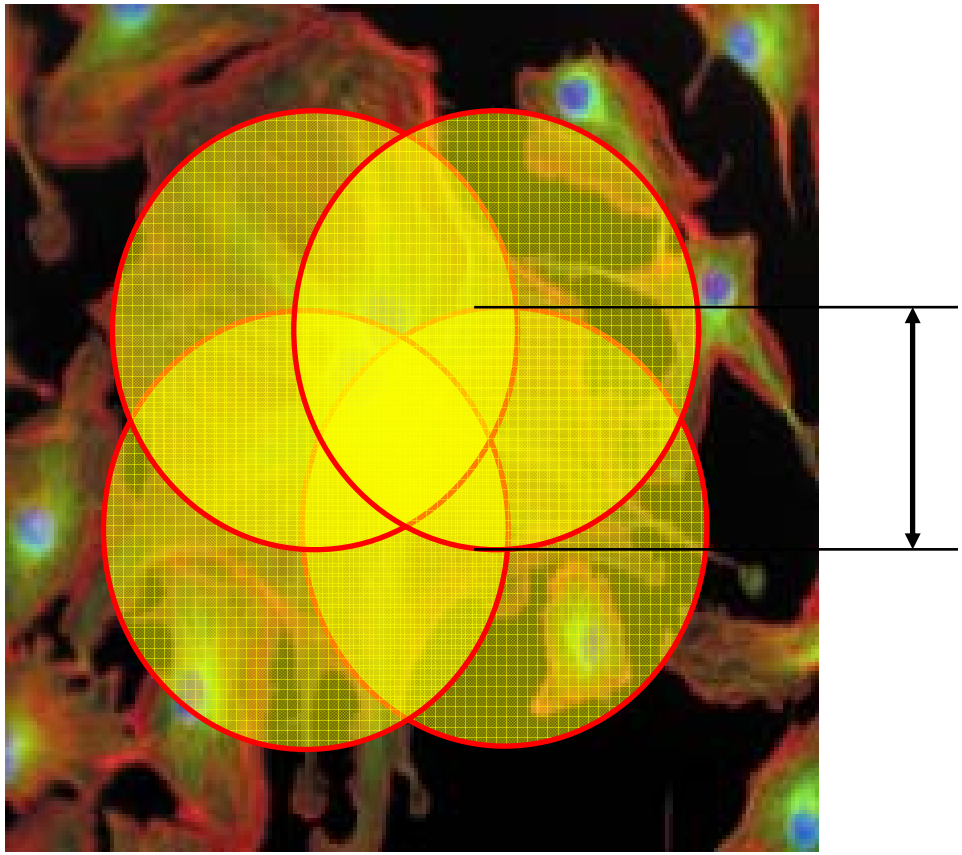

100 µm

Diffractive imaging with visible laser sources

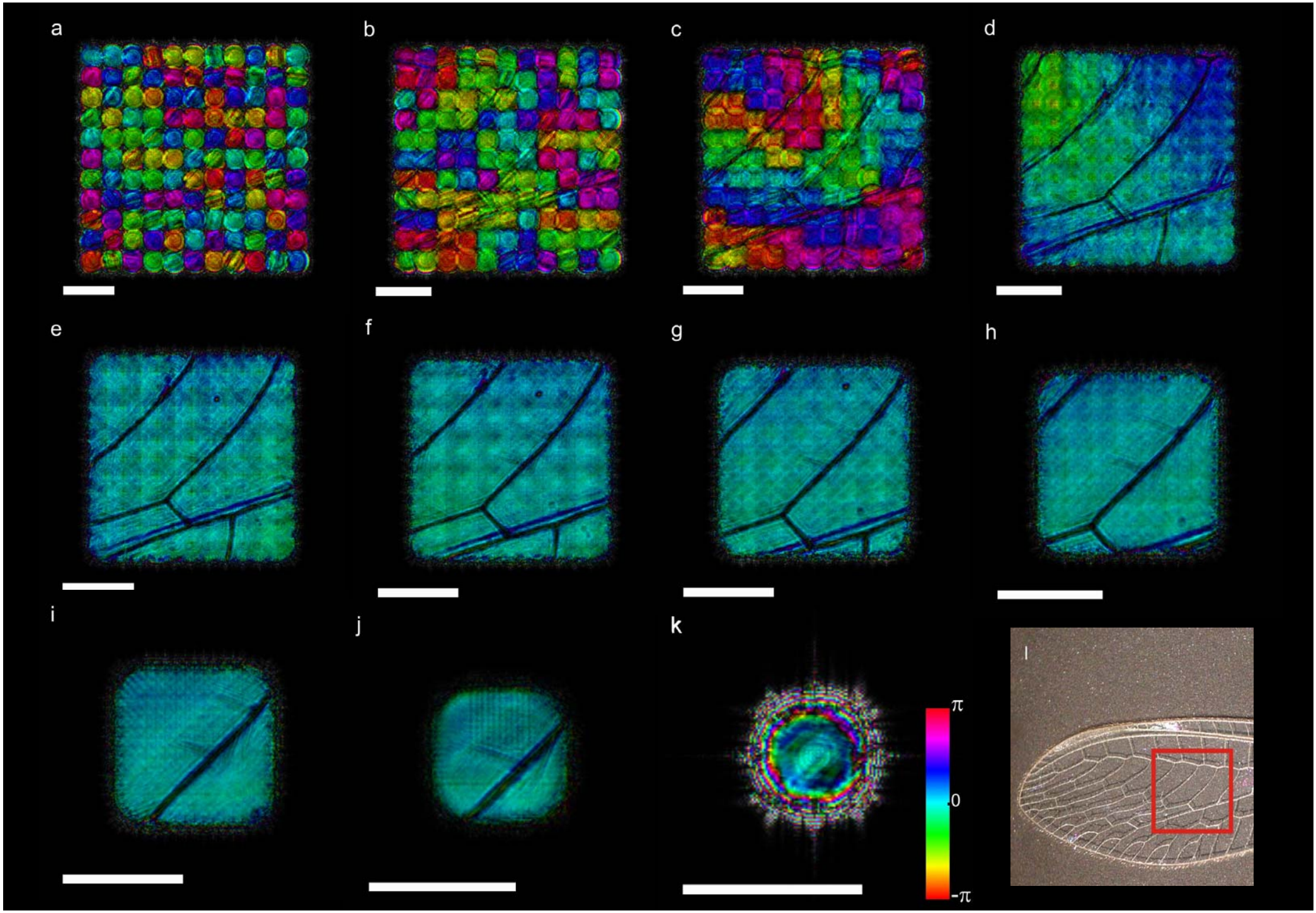


stem tip of *hydrilla vercitillata*

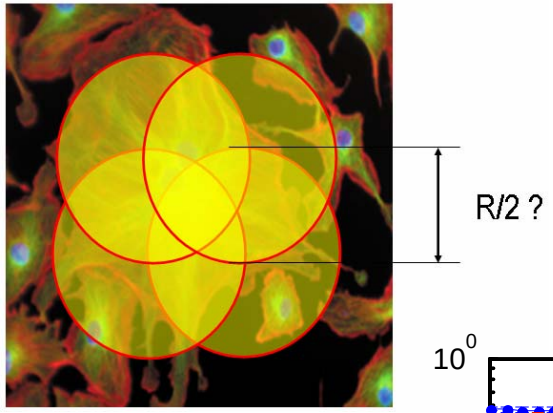
Optimization of overlap parameter



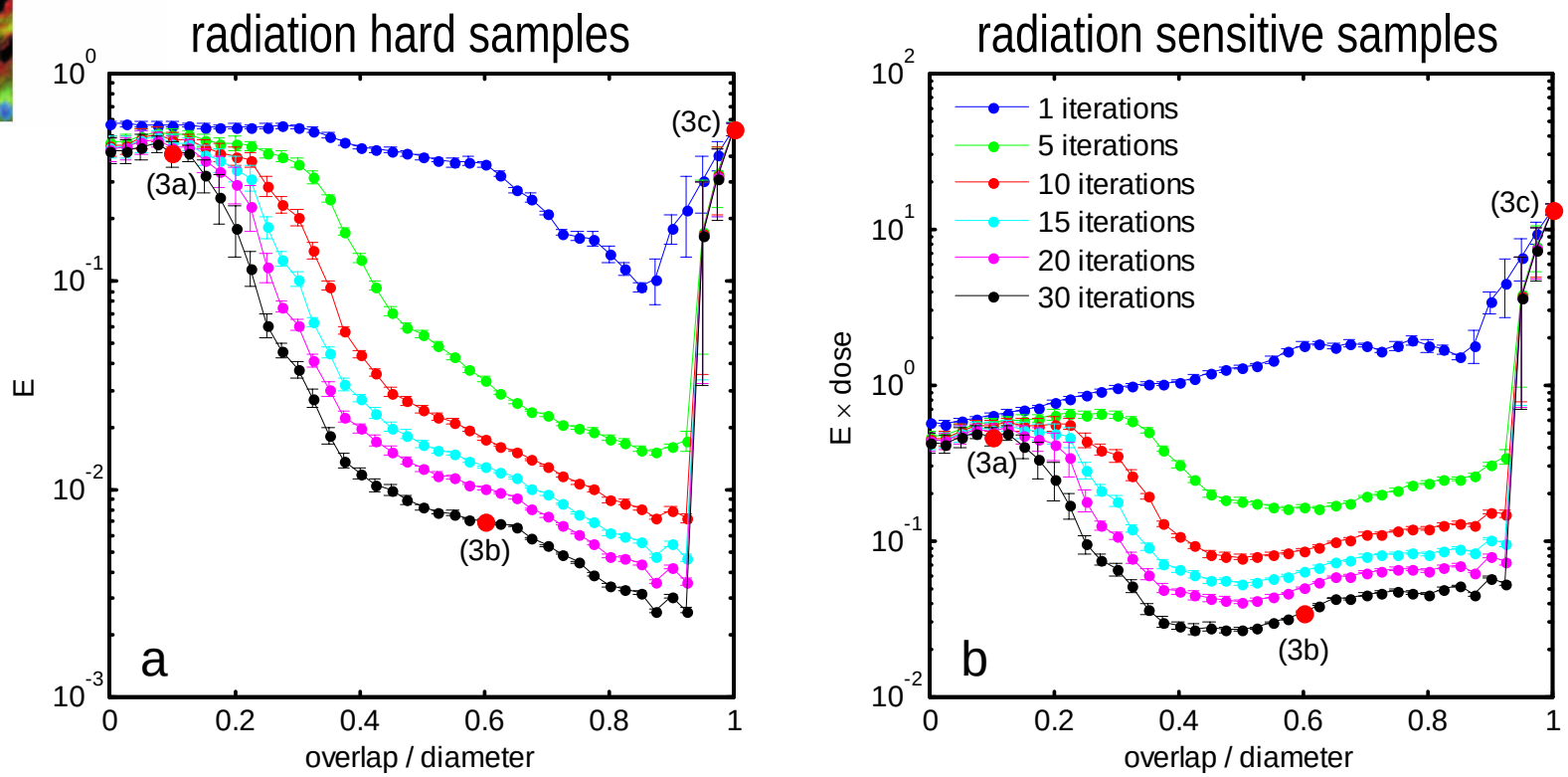
- optimum overlap parameter for best reconstruction ?
- optimum overlap for radiation sensitive samples ?


a
b
c
d
e
f
g
h
i
j
k
l
π
0
-π

Optimization of overlap parameter

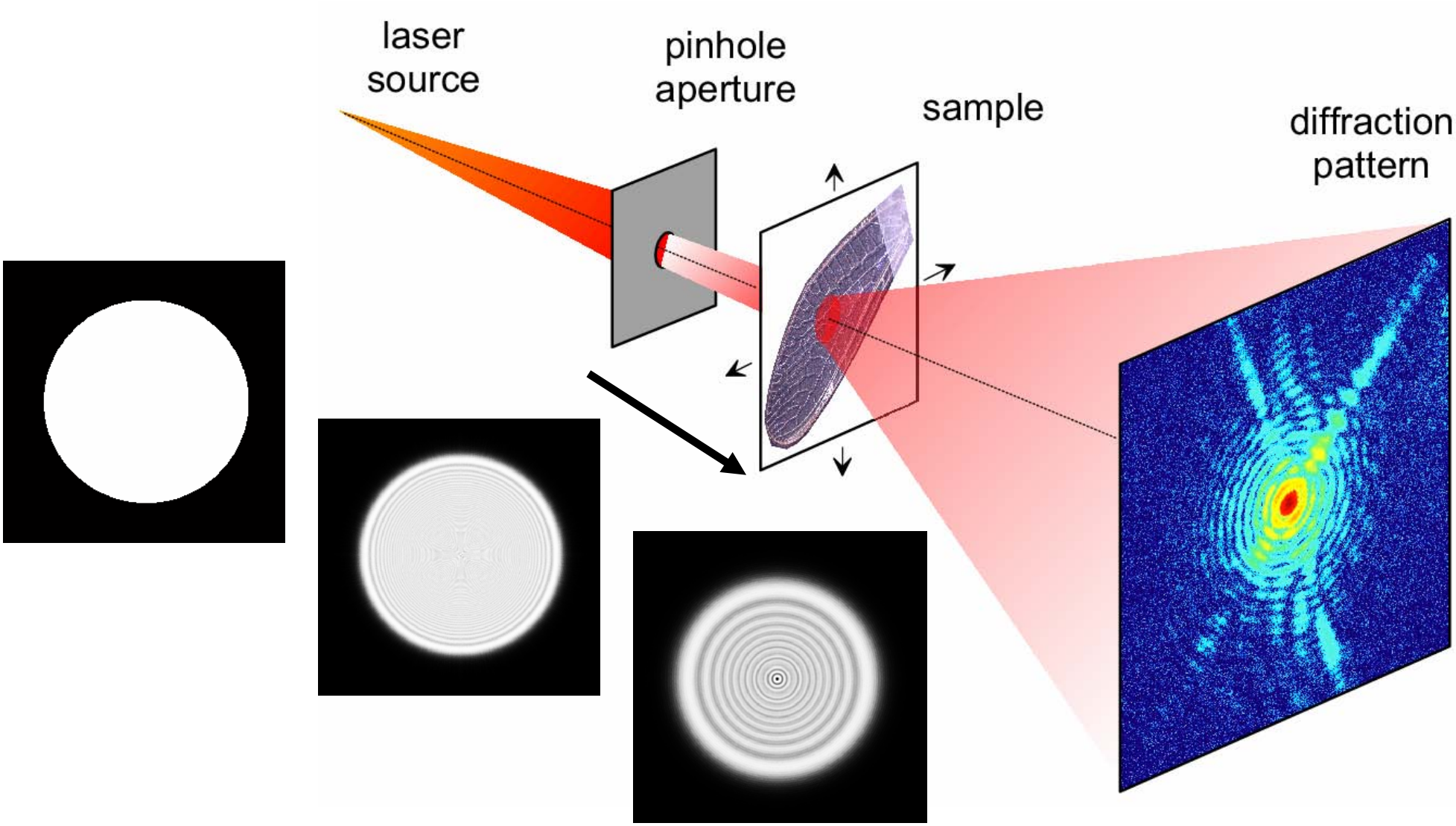


- optimum overlap parameter for best reconstruction ?
- optimum overlap for radiation sensitive samples ?

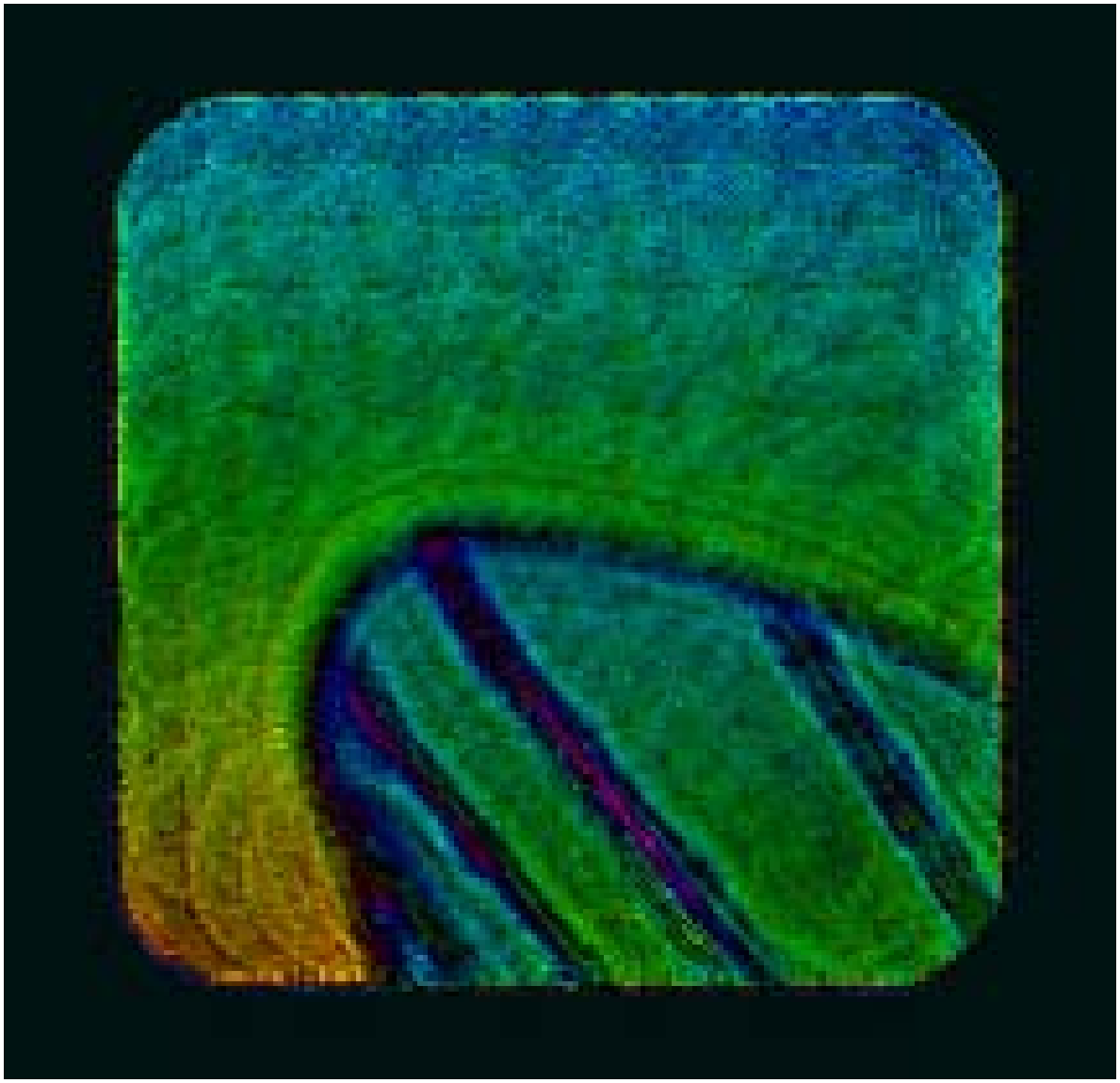


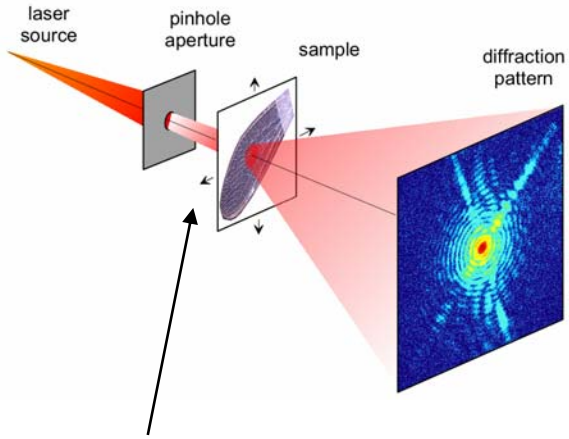
O. Bunk, M. Dierolf, F. Pfeiffer, et al., submitted

Optimization of probe defocus in reconstruction



Optimization of probe defocus in reconstruction

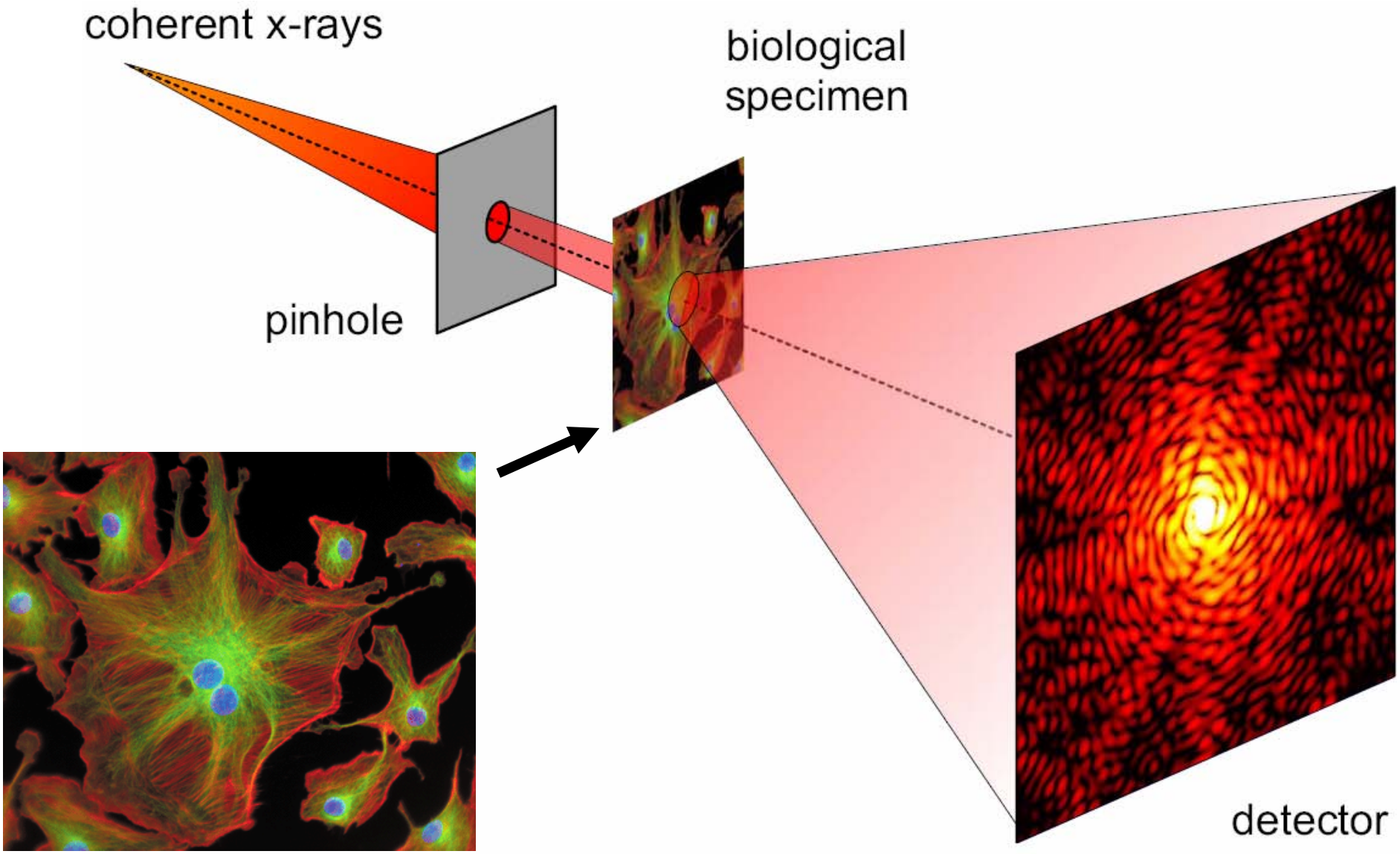




reconstruction as a function of propagation distances of the pinhole wave front

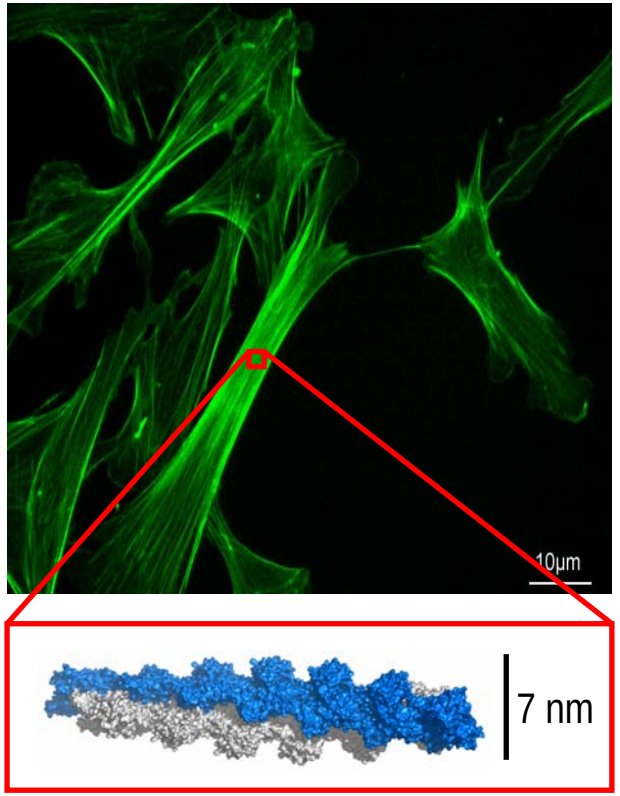
Future: High-resolution diffractive x-ray imaging of cells ?

Future: High-resolution diffractive x-ray imaging of cells ?

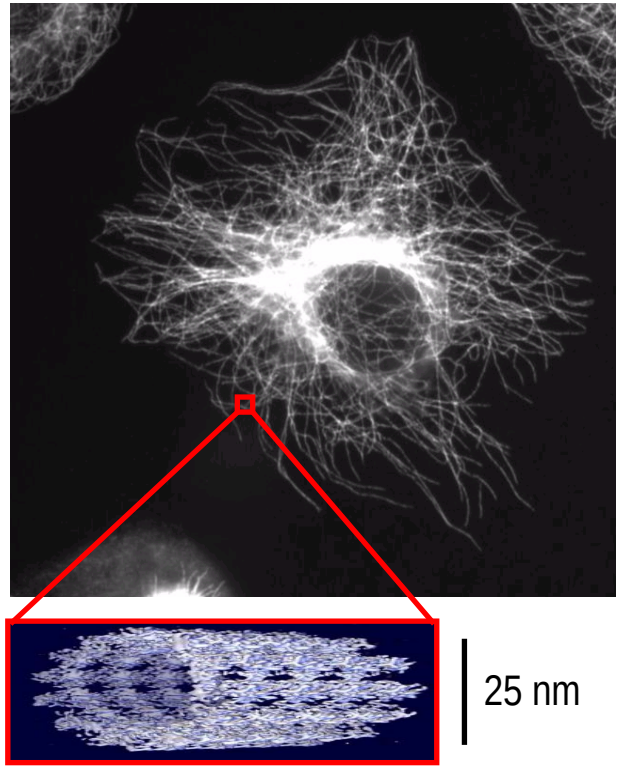


High resolution x-ray imaging of the cell cytoskeleton ?

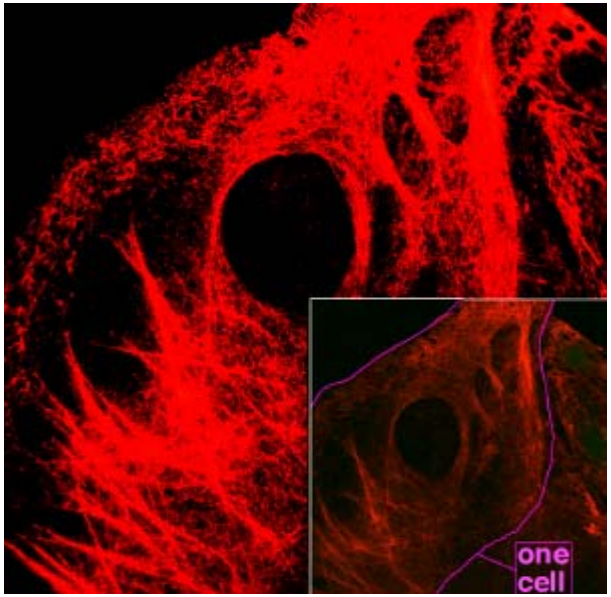
Actin cytoskeleton



Microtubules



Intermediate filaments
e.g., Keratin, 8-11 nm diameter

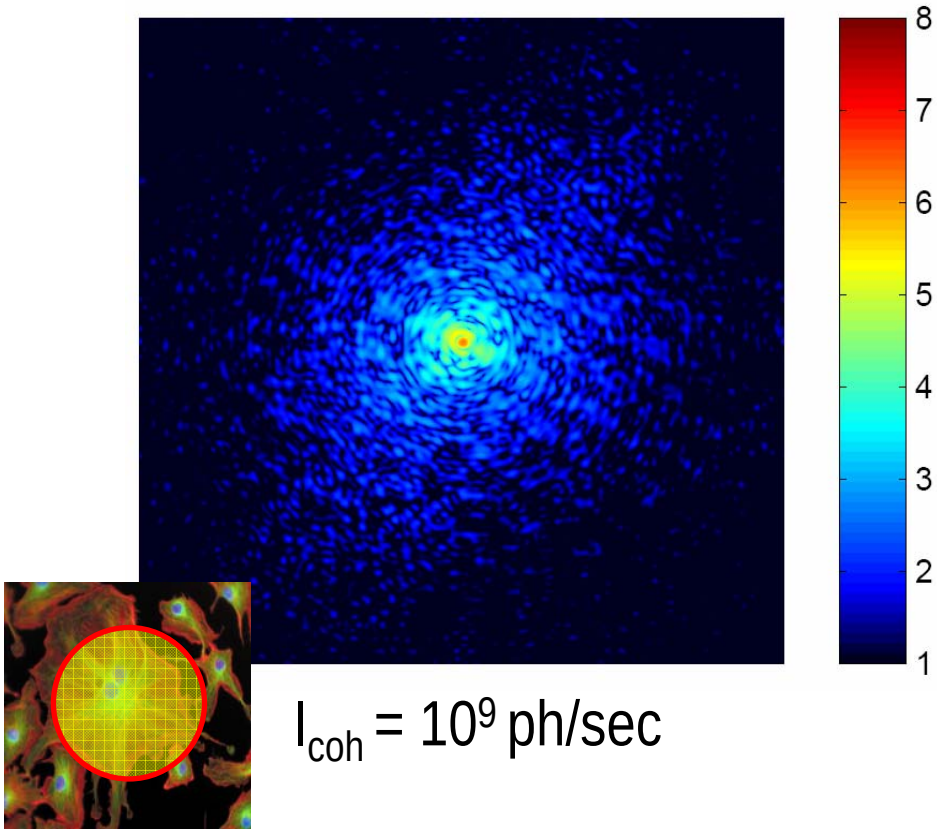


Present limitations…

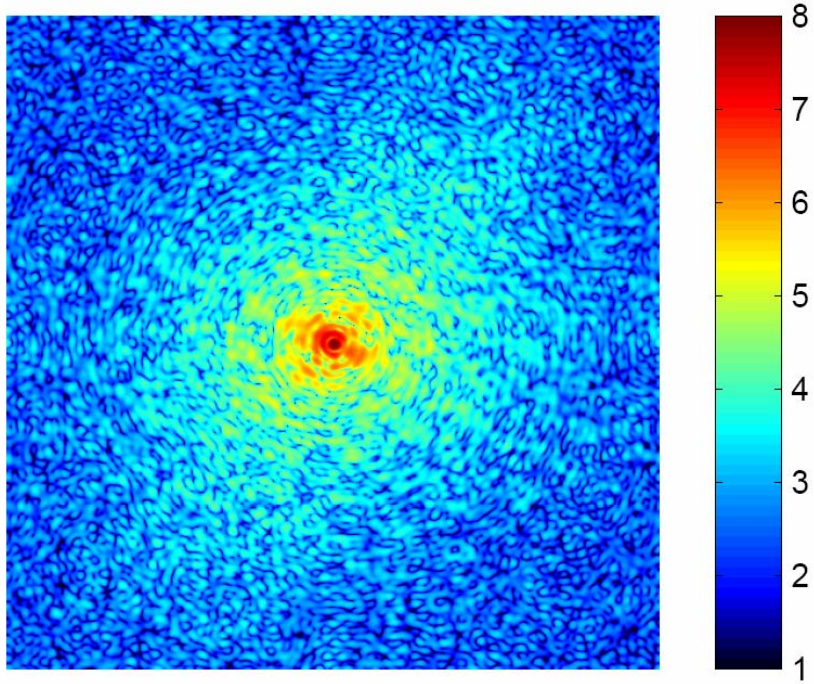
Present limitations (1)

- coherent flux available at synchrotron sources

ERL !



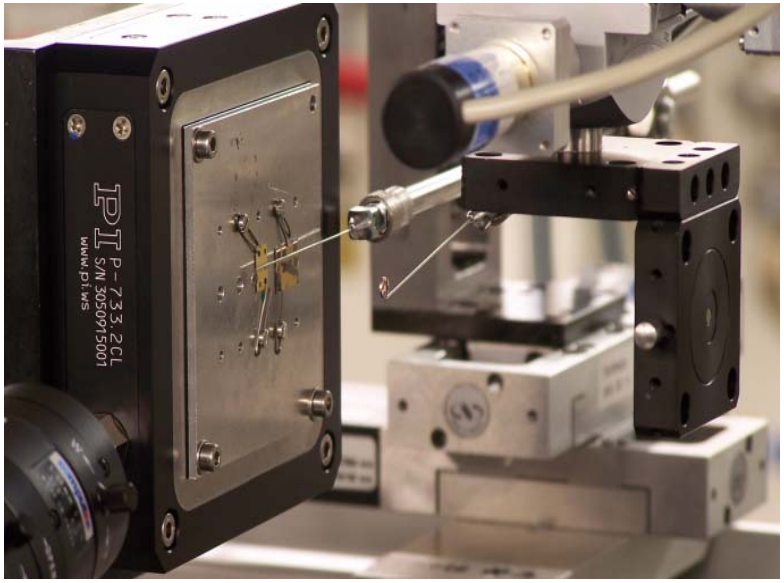
$I_{coh} = 10^9$ ph/sec

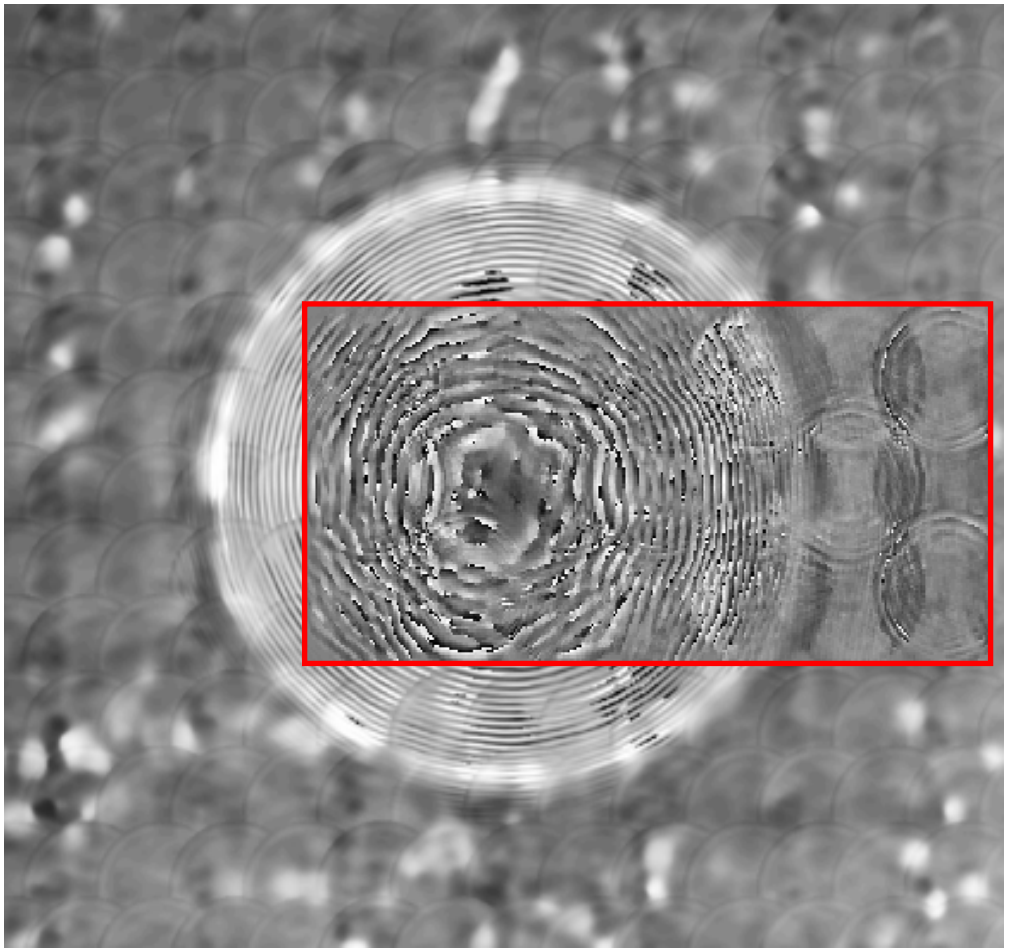


$I_{coh} = 10^{11}$ ph/sec

Present limitations (2)

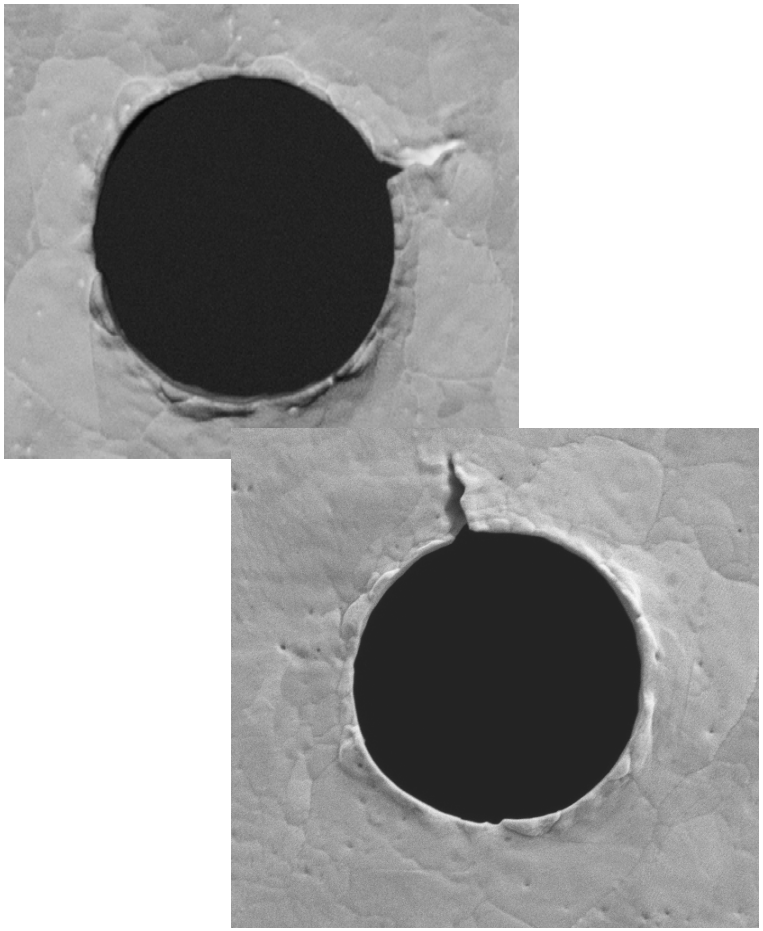
- stability and positioning accuracy

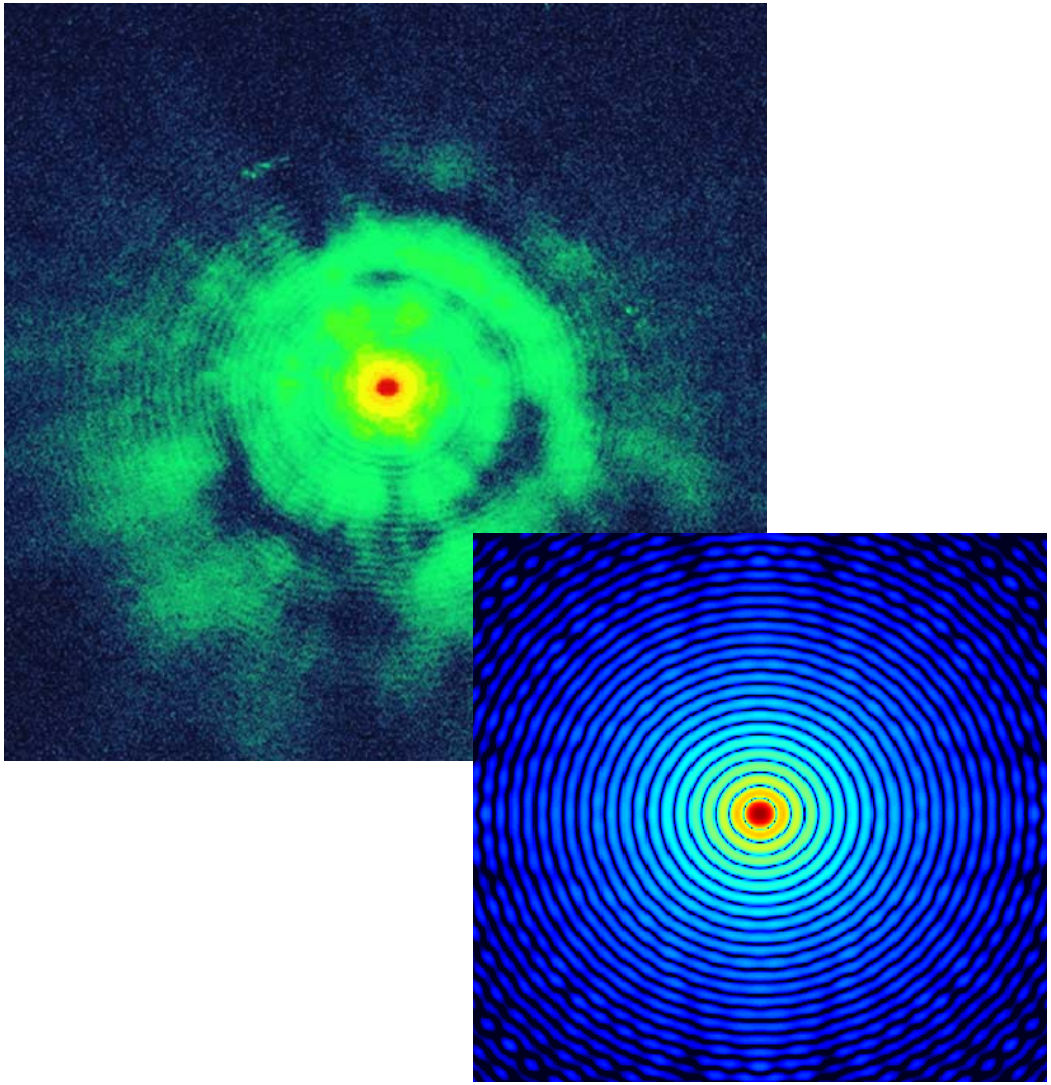




Present limitations (3)

- high quality apertures ?

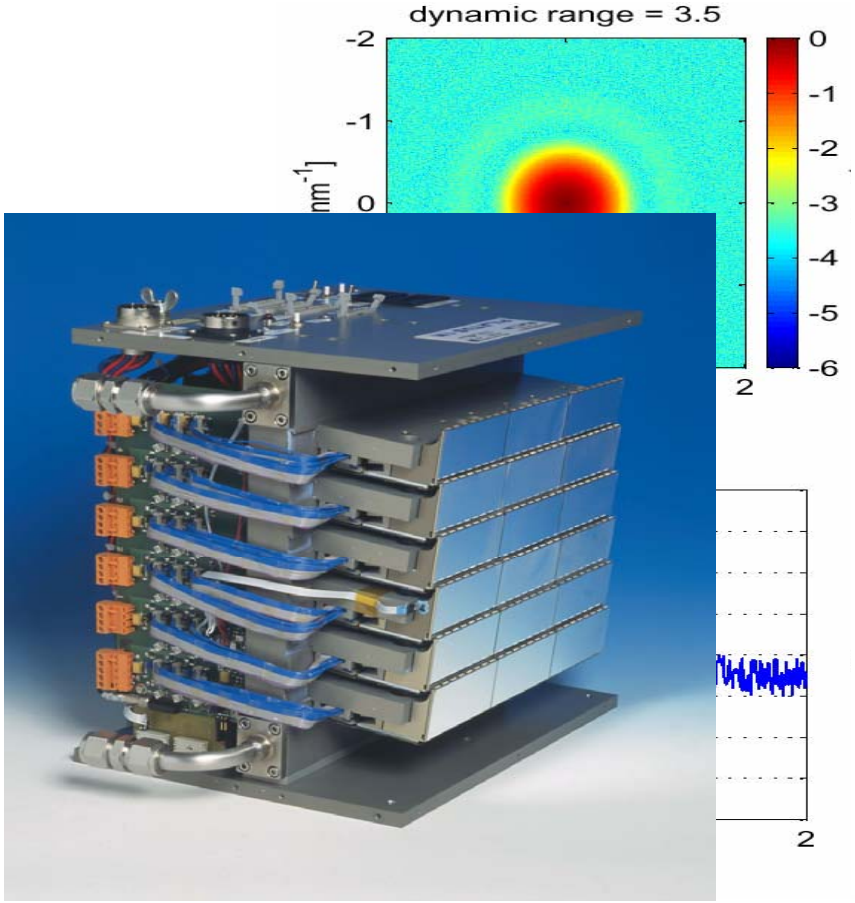




Present limitations (4)

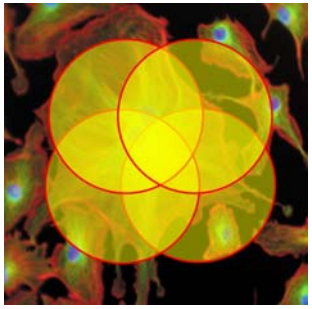
- detectors

CCD

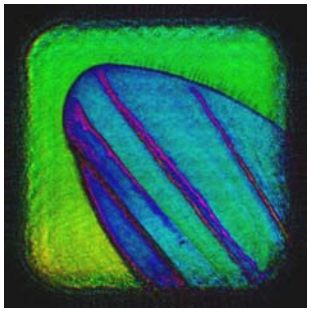


simulated diffraction pattern, colloids radius r = 50 nm, x-ray wavelength λ = 0.1 nm

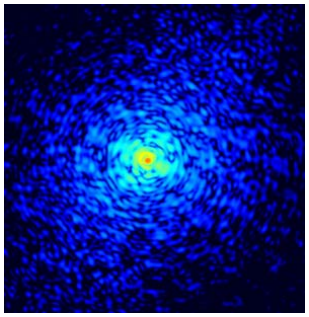
Conclusions and Summary



- PIE overcomes the restriction of a finite support and allows diffractive imaging of extended objects



- PIE converges rapidly and reliably for any given complex object



- PIE could solve some of the problems associated with the detection of coherent diffraction patterns
  (dynamic range, beam stop problem, oversampling)

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