Coherent Diffraction Imaging with Nano- and Microbeams

Why does lensless imaging need lenses?

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Outline

- Coherent diffraction imaging and why it will never work for x-rays.
- Coherent diffraction imaging - how it works.
- Can you really use a lens for that?
- Why should I use phasing algorithms when I have a lens?
- Putting it all together.

Some thoughts by Sayre

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 $X = 0, \pm 1/a, \pm 2/a, \ldots$. 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 $X = 0, \pm 1/a, \pm 2/a, \ldots$, 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

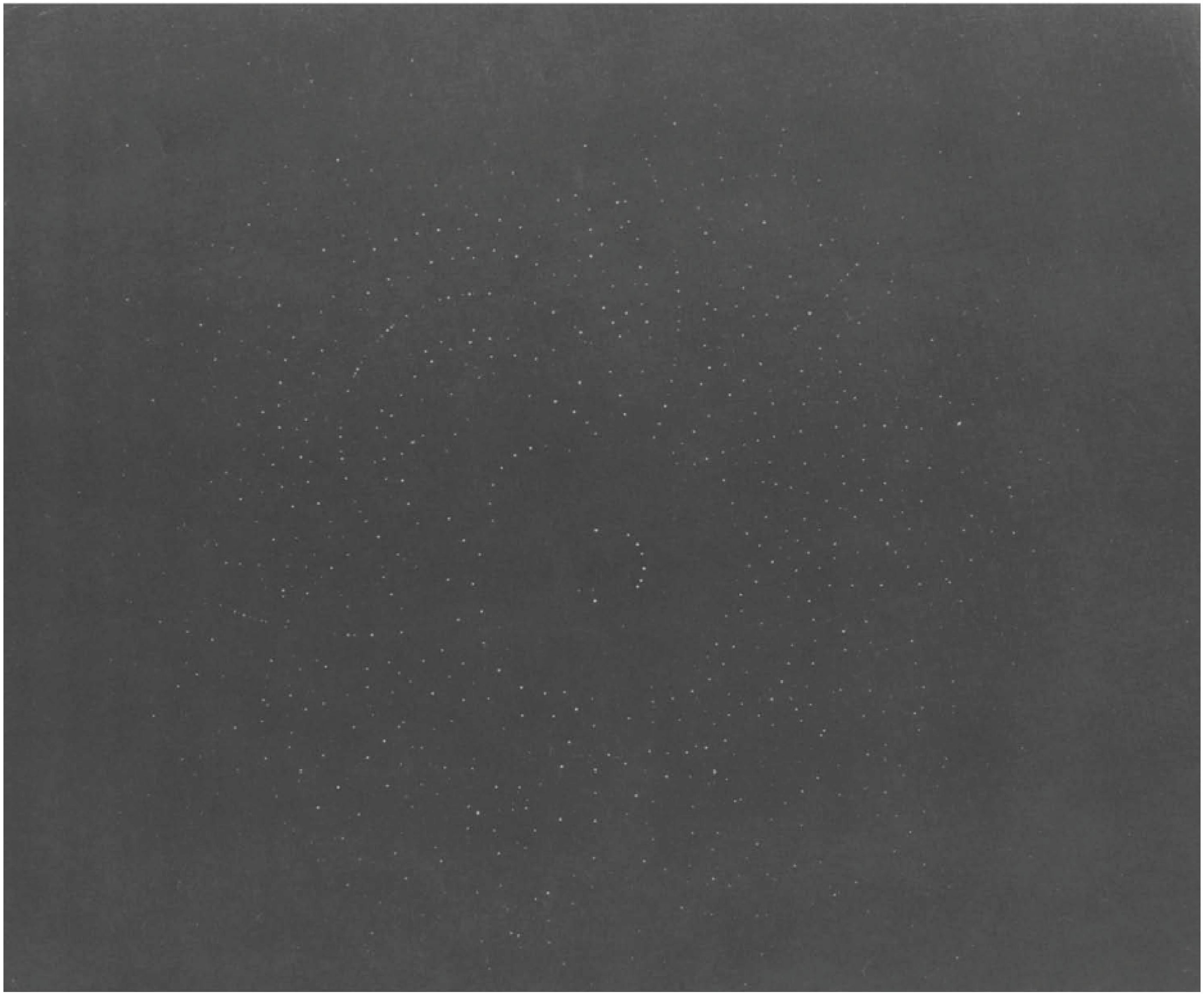
Boyes-Watson, J., Davidson, E. & Perutz, M. F. (1947). *Proc. Roy. Soc.* A, **191**, 83.

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.

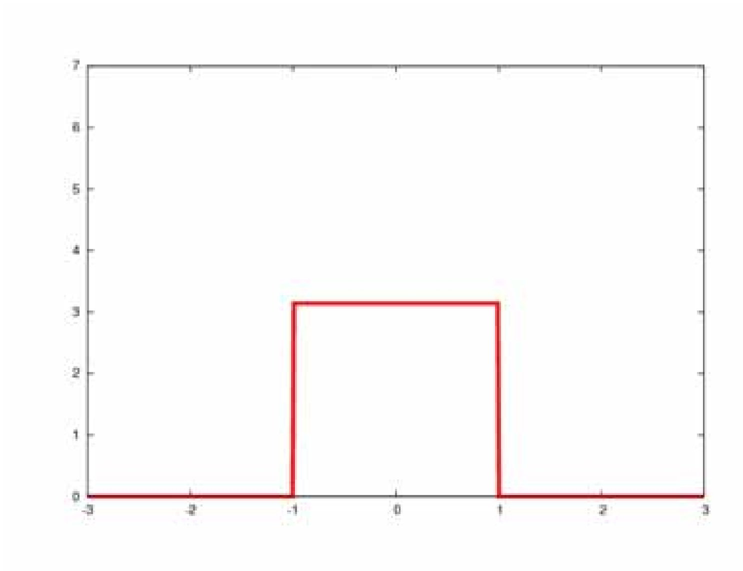
Some implications of a theorem due to Shannon (Nyquist frequency)

Some thoughts by Sayre

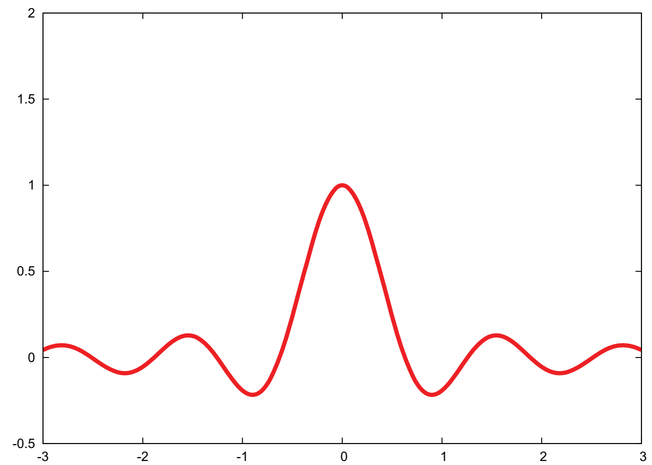


Fourier intensity measurements and the autocorrelation

density



amplitude



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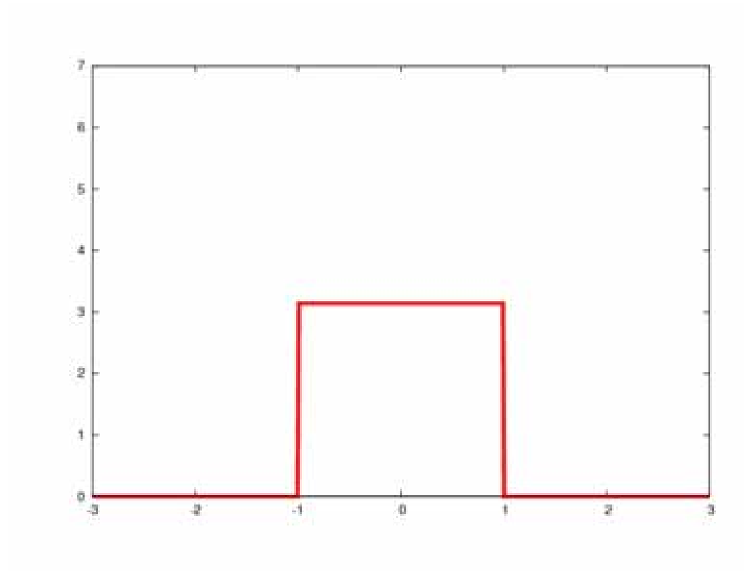
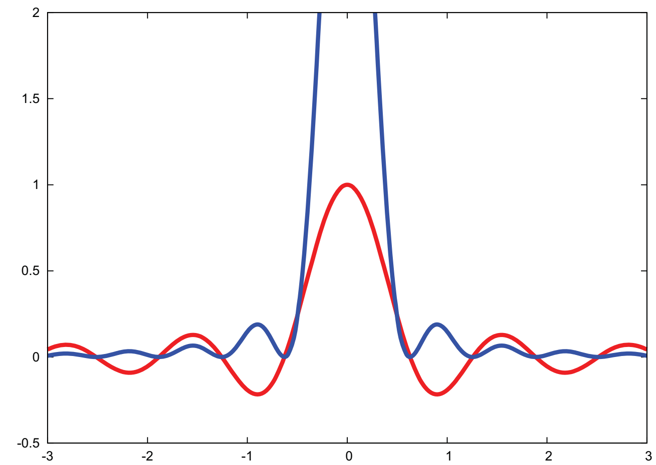
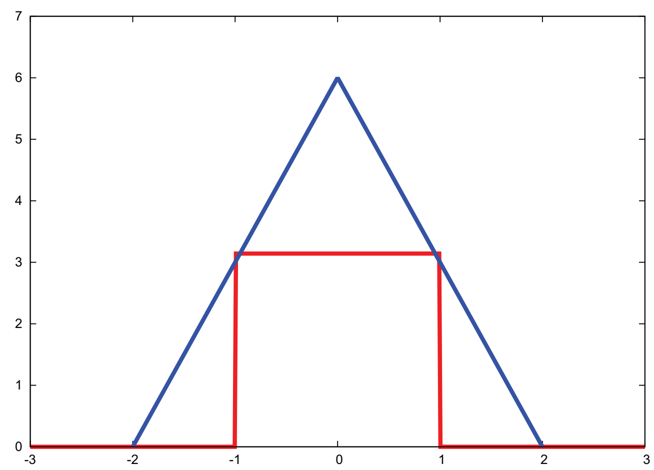


intensity

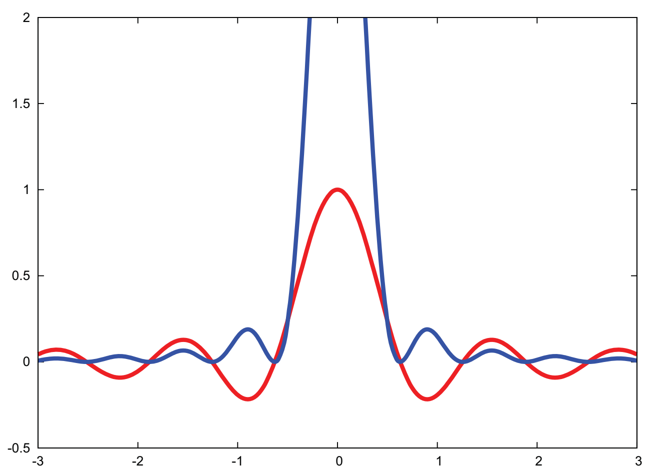


Fourier intensity measurements and the autocorrelation

autocorrelation



intensity



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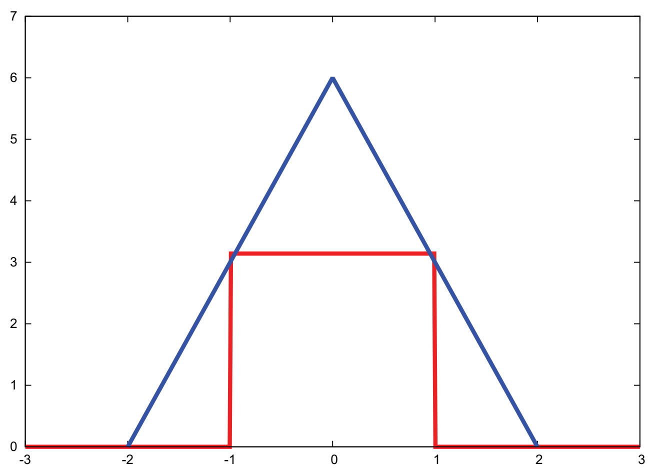
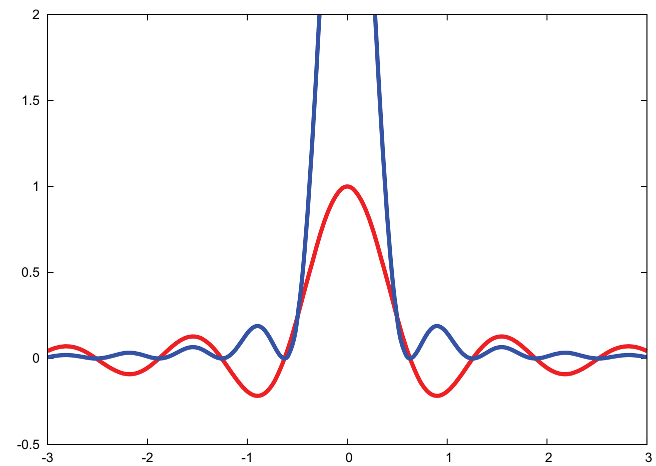


intensity



- If only intensity measured, sampling requirement doubled.
- In greater than one dimension, autocorrelation *uniquely* determines original function.

Wavefront reconstruction

- e^-: Gerchberg and Saxton - *Optik* 1971, 1972
  - intensity measurements in exit plane and far field
  - alternately enforced known intensities, kept phase estimates, propagated with FFT
  - algorithm equivalent to steepest descents
- visible light: Fienup
  - finite source size, positivity, and measured far-field
  - correct for atmospheric disturbances
  - diagnose aberration in Hubble's main mirror
  - explored range of algorithms with degrees of feedback

Born and Wolf

Born and Wolf, *Principles of Optics*:
"In the method of wave-front reconstruction, a background is artificially added. There are no conditions to be satisfied regarding symmetry or even periodicity. On the other hand this method is not suitable for X-ray analysis owing to the practical impossibility of producing a strong coherent background."

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Coherence

Rotating anode

- $L_T = \sim \frac{\lambda d}{2s} = \frac{0.14nm*2m}{2*1mm} = 70nm$
- fractional coherence $\sim 2^{-14}$

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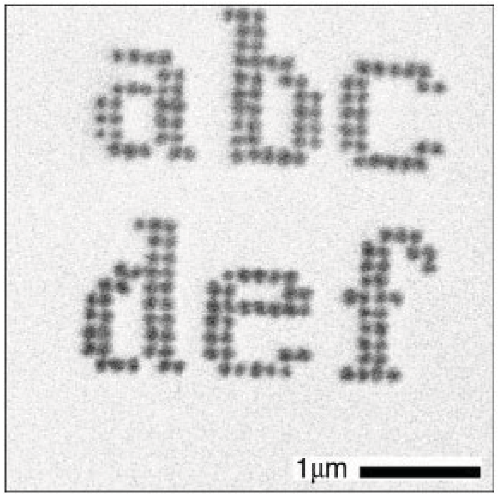
ERL helical mode delta

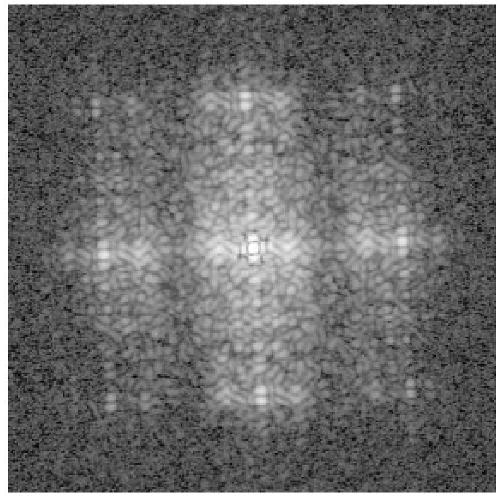
- fractional coherence$\sim 2^{-1}$
- 4.8^{14}ph/s/0.1%

First X-ray demonstration

Miao *JOSA* 1998.

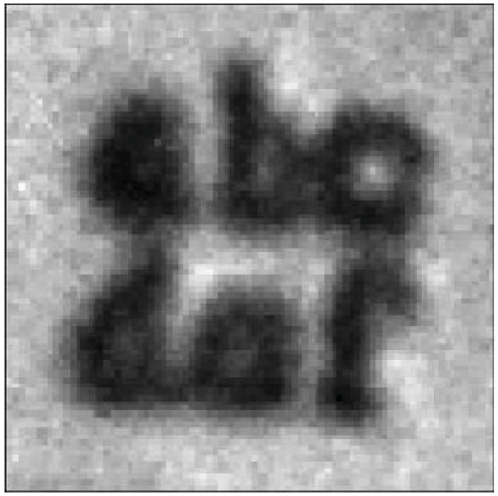
SEM





Diffraction

VLM



CDI

CDI moves into 3D and biology

Au decorated Si3N4 pyramids
Chapman, *JOSA* 2006.

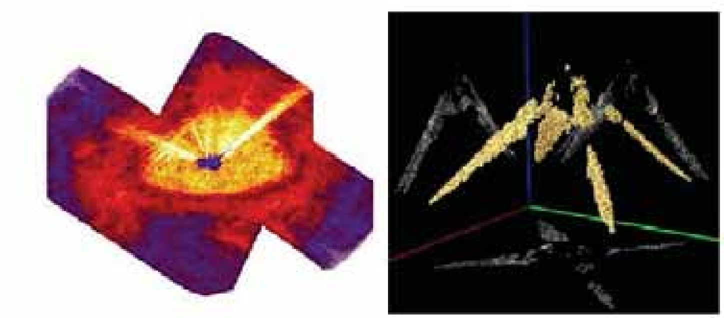
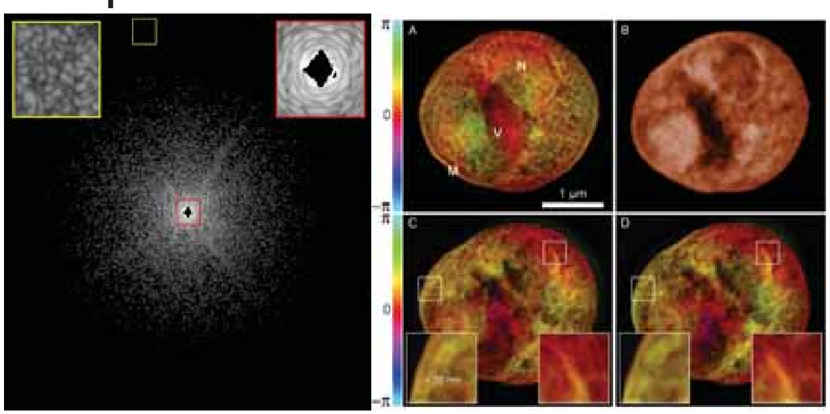
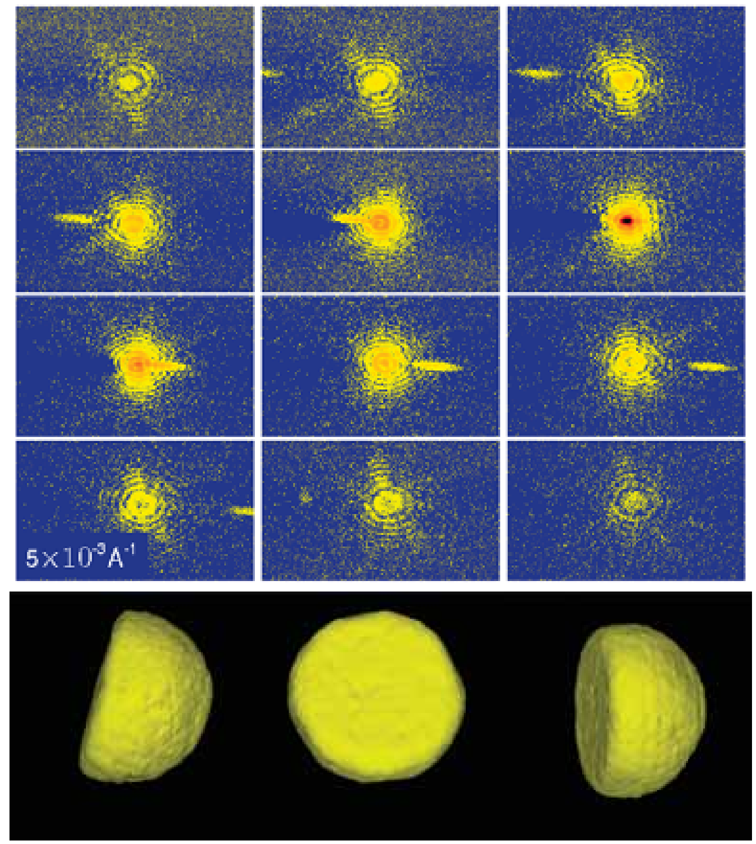


Fig. 4. Three dimensional diffraction pattern (left) (with a quadrant removed for visualization) and reconstructed 3D images [19] (right) showing the isosurface as well as the projection images of the sample.

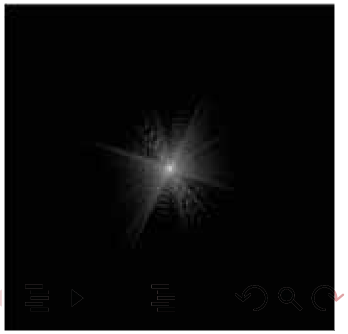
Yeast cells
Shapiro *PNAS* 2005.



Pb crystals - strain mapping
Pfeifer, *Nature* 2006.



A nice flow chart showing how CDI works



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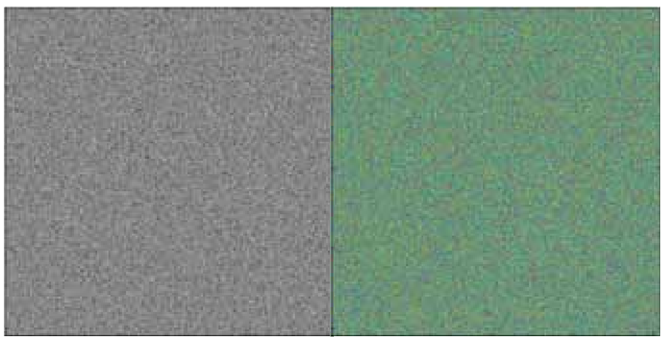

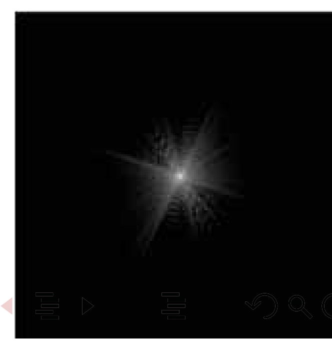

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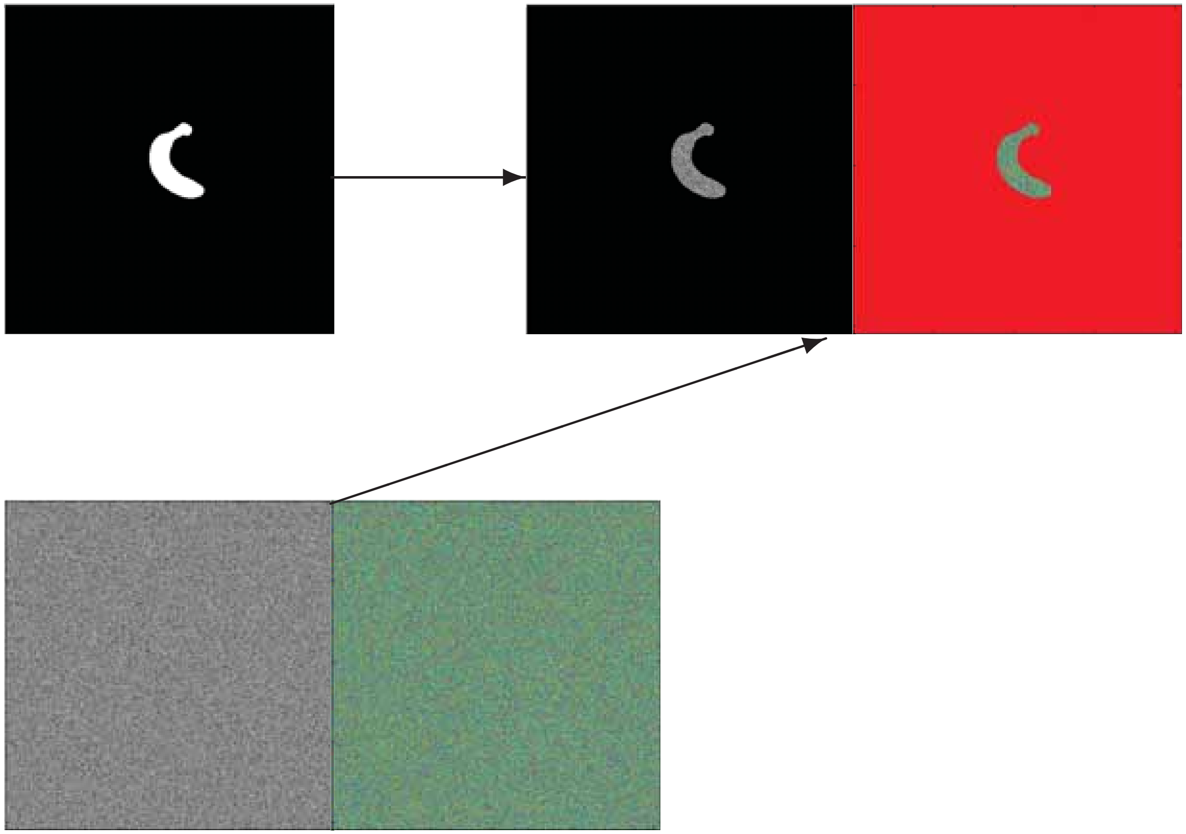
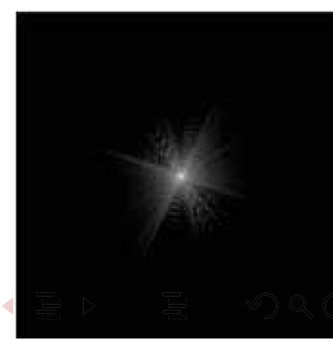
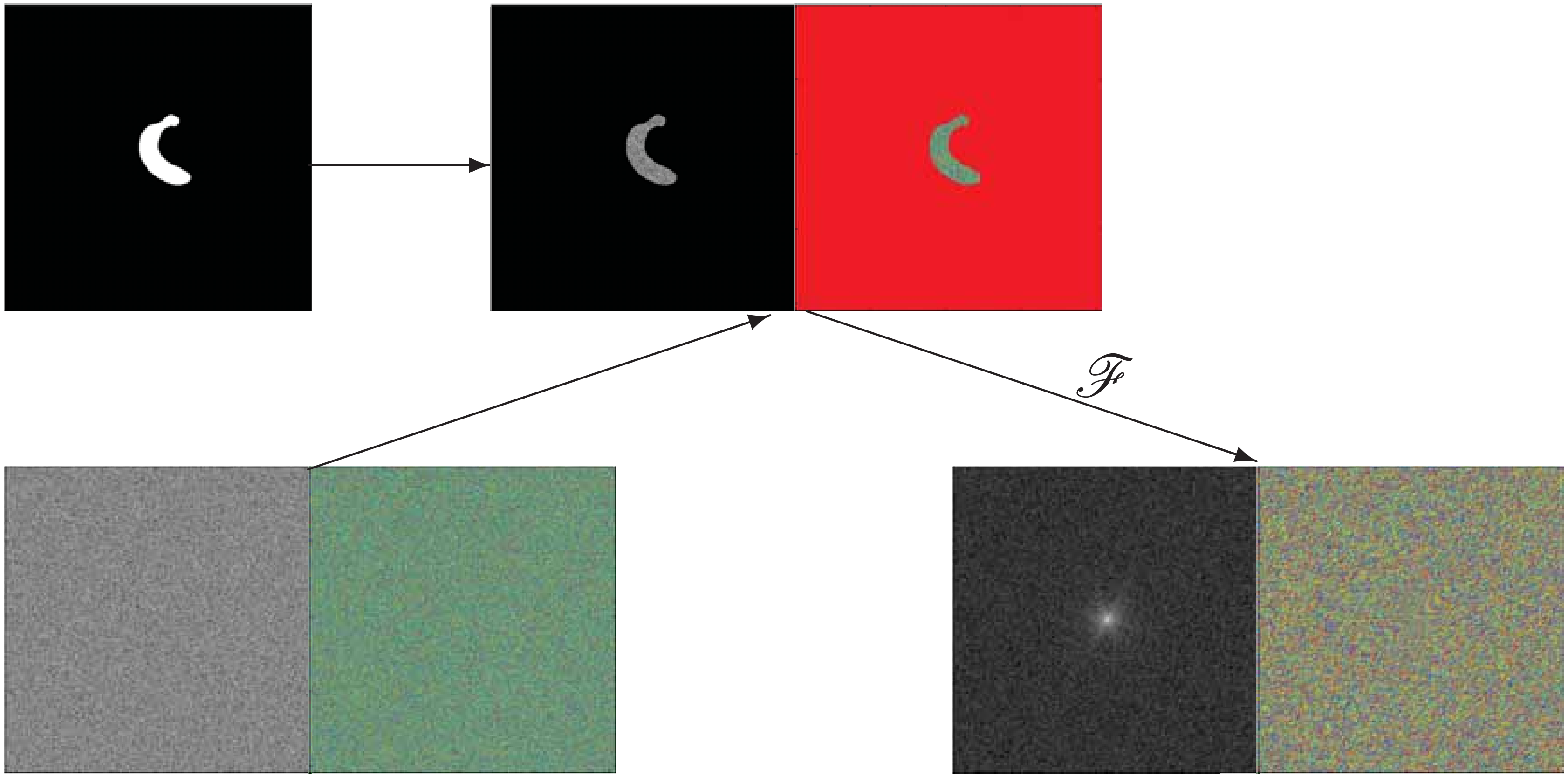


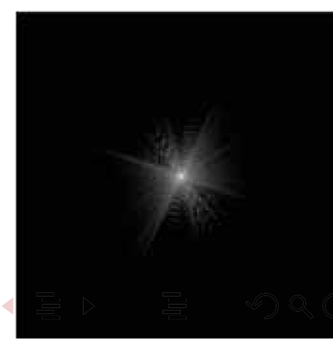


A nice flow chart showing how CDI works

Lensless imaging with lenses

M. Pfeifer





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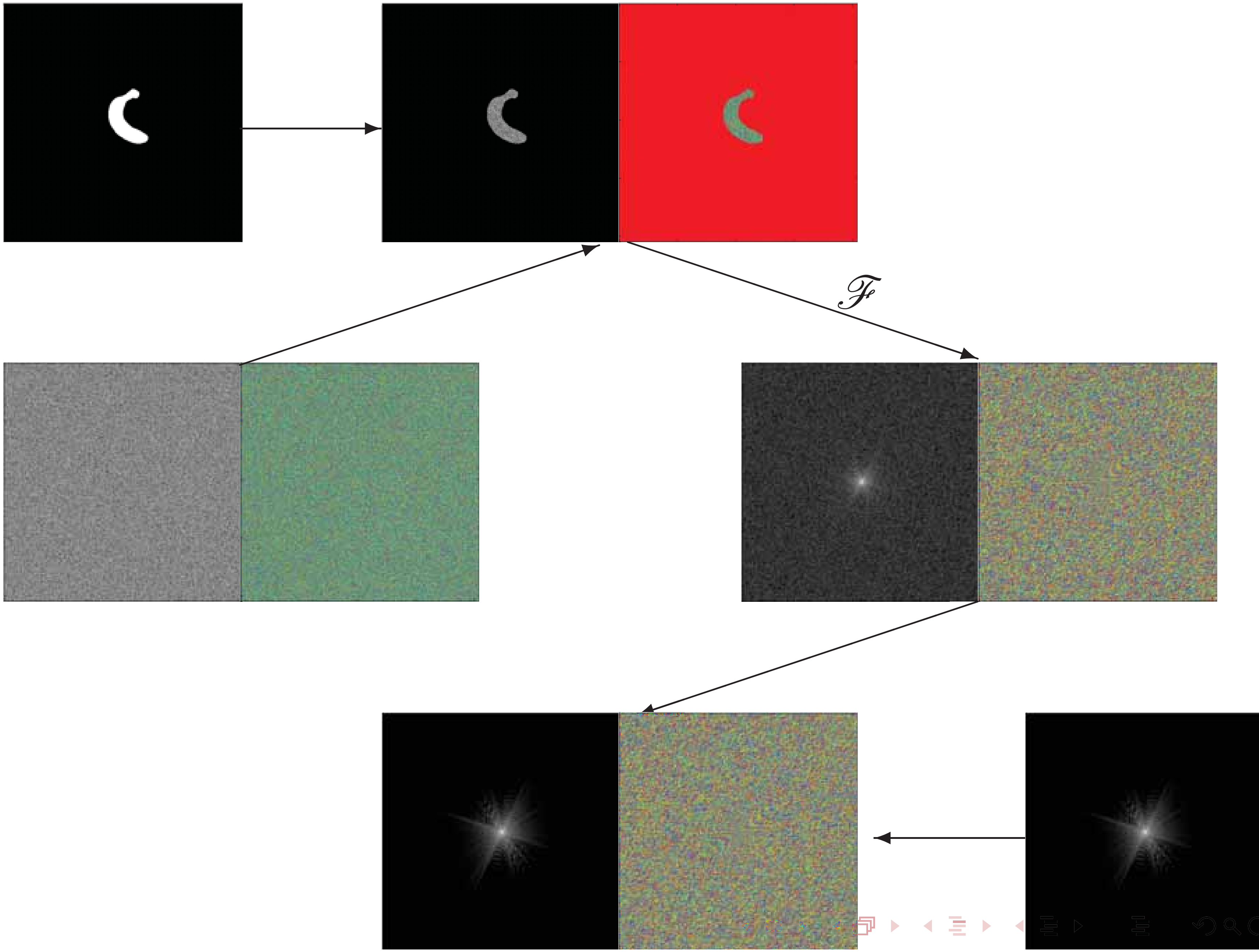

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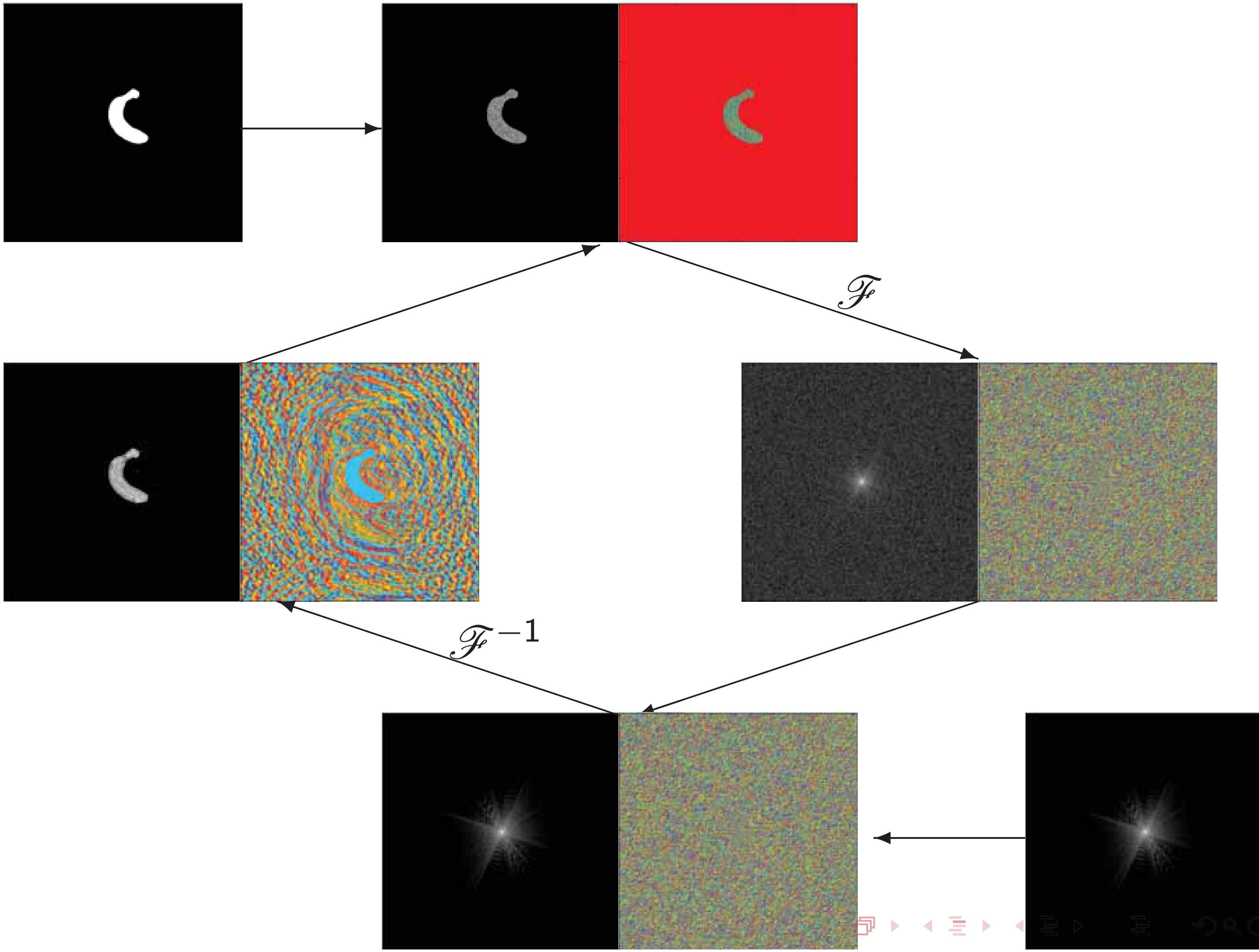

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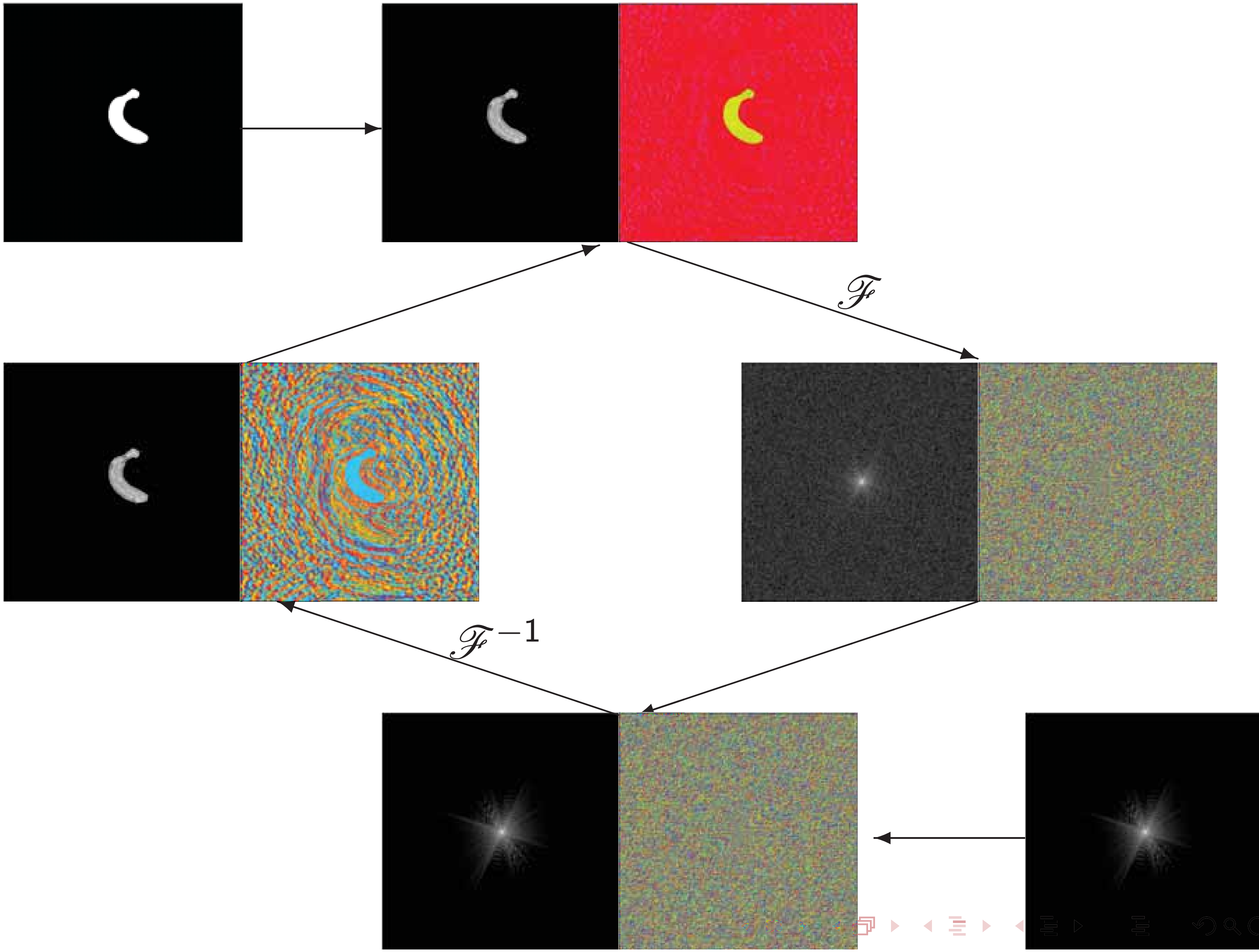

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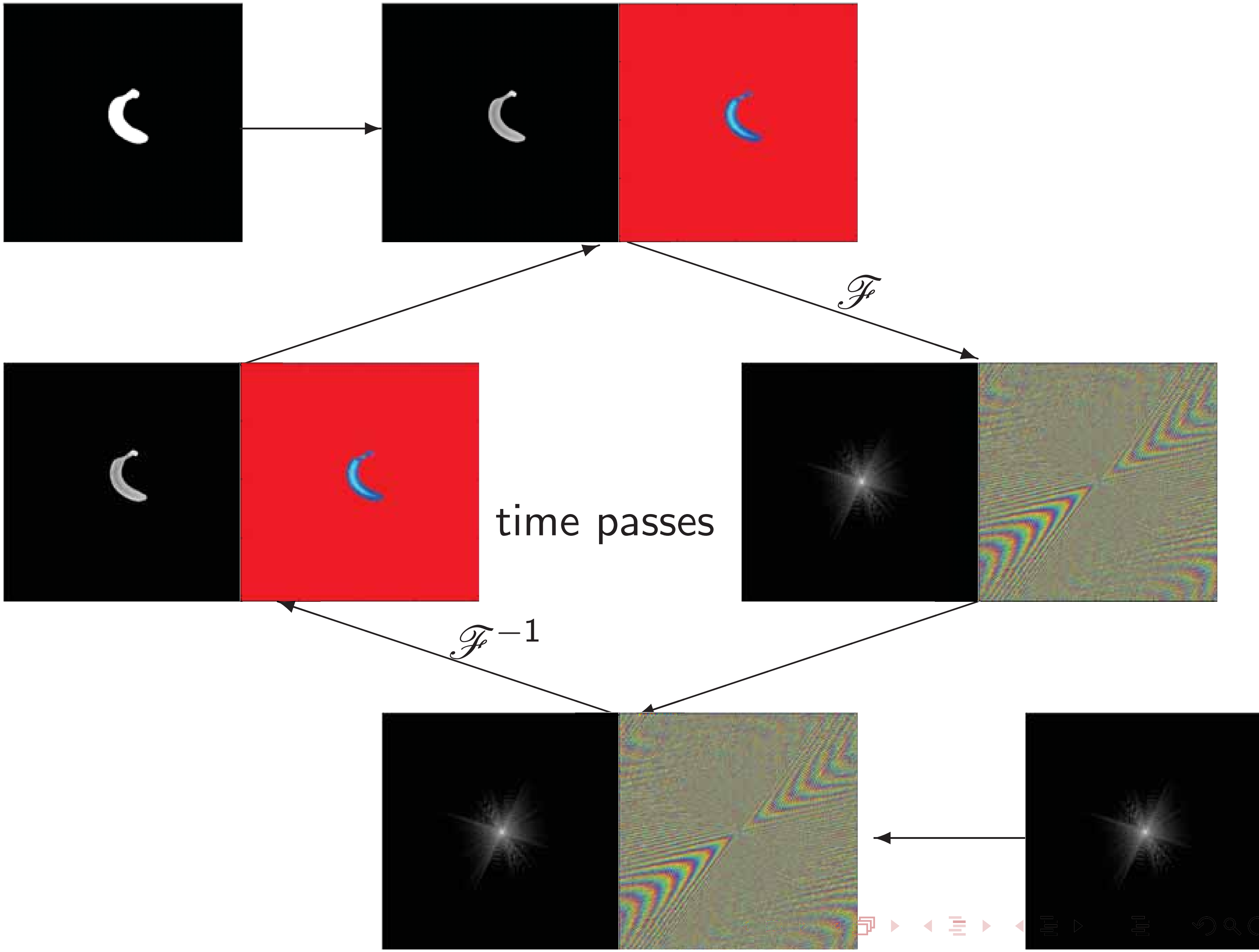
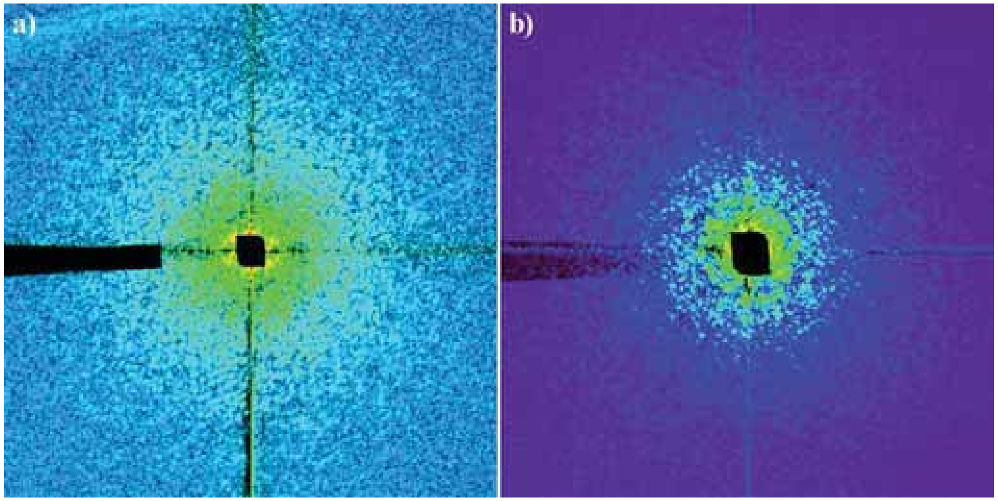
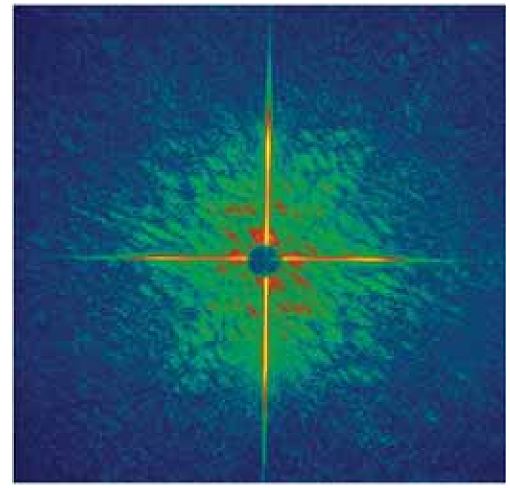
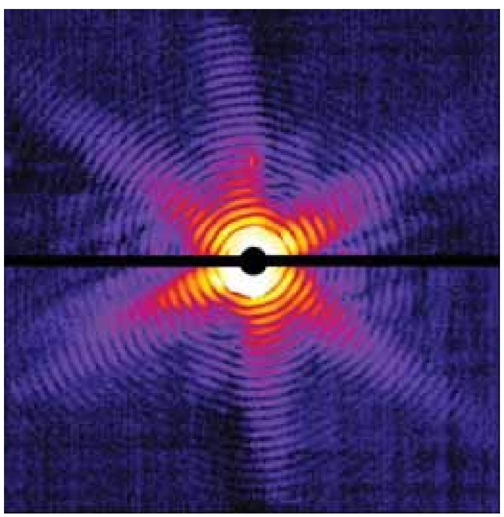
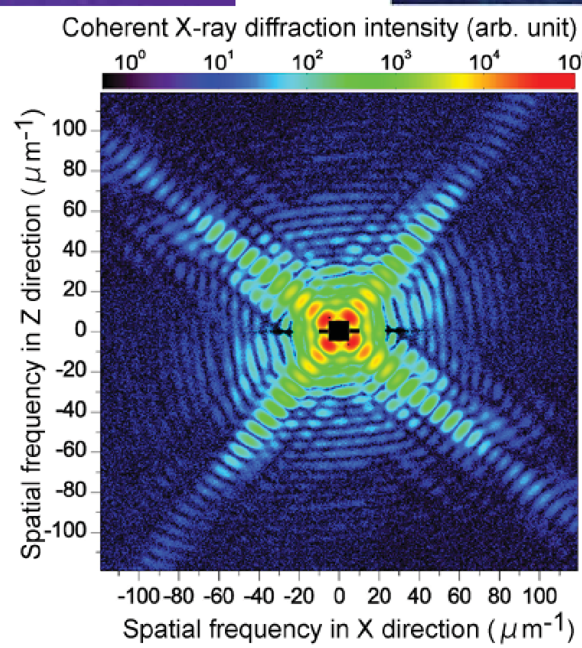


Missing information

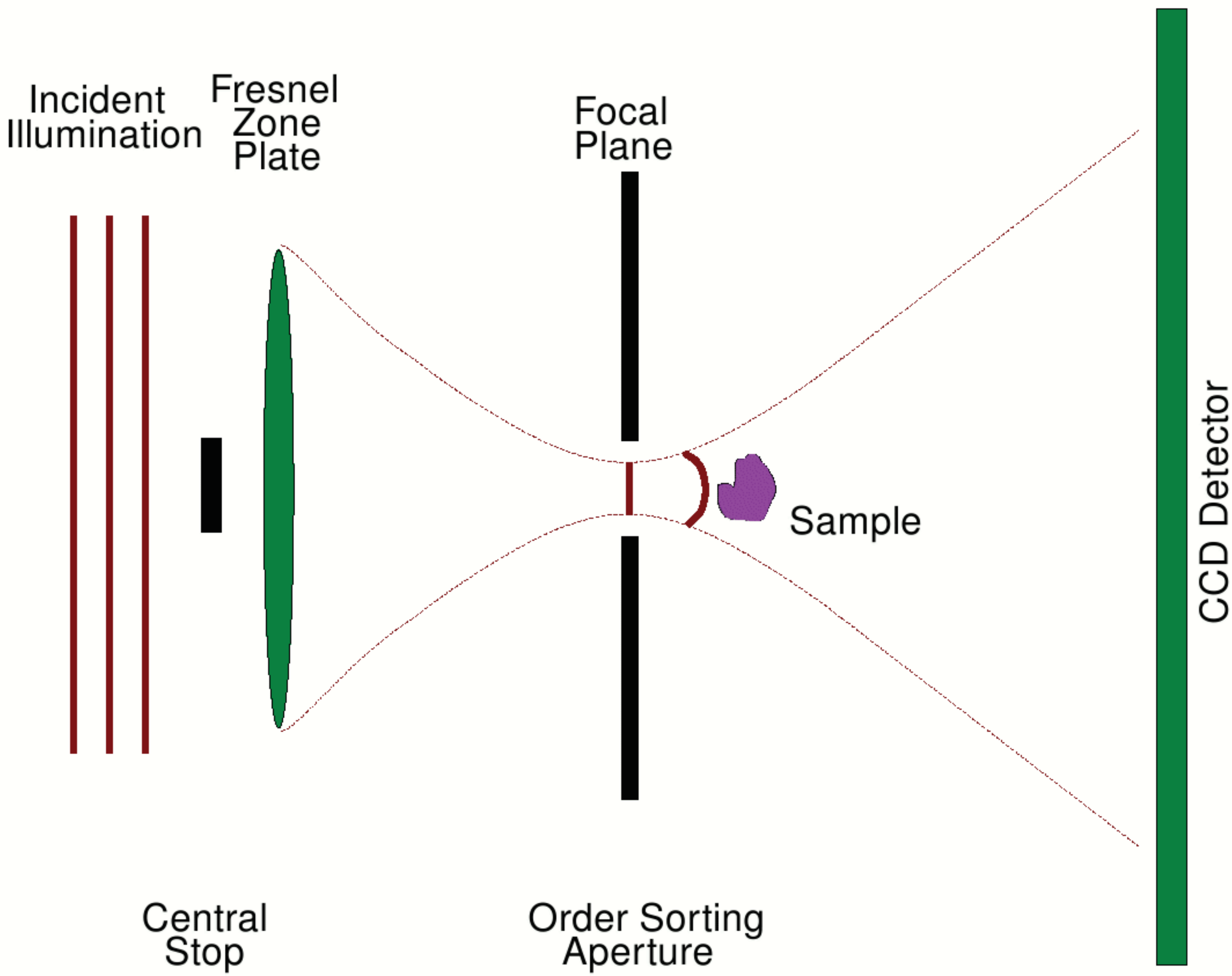




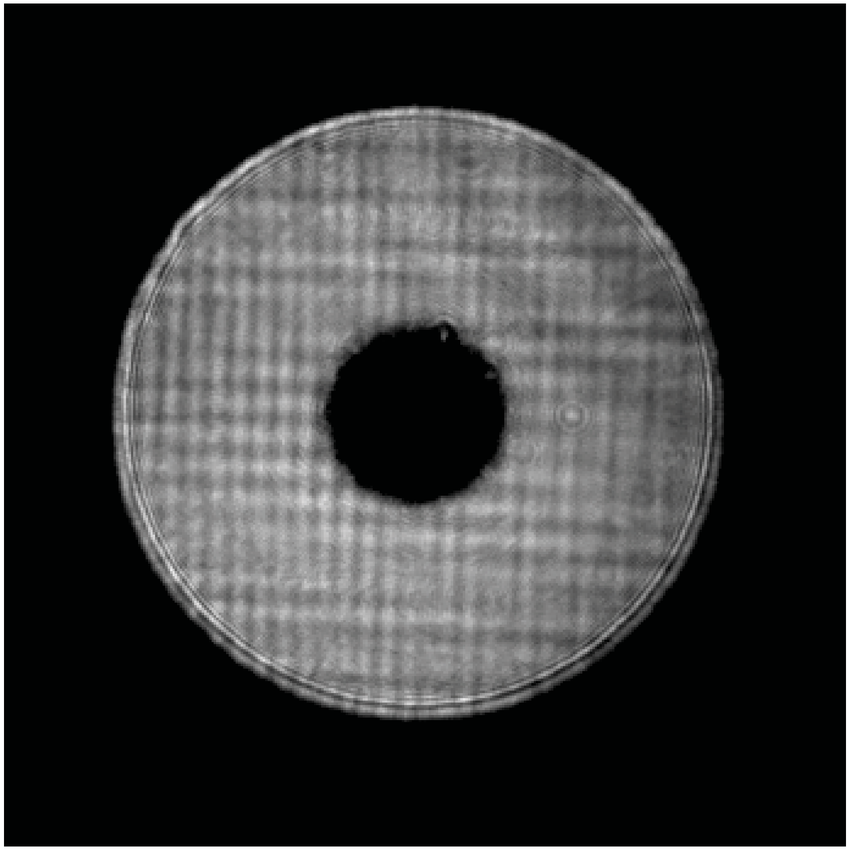




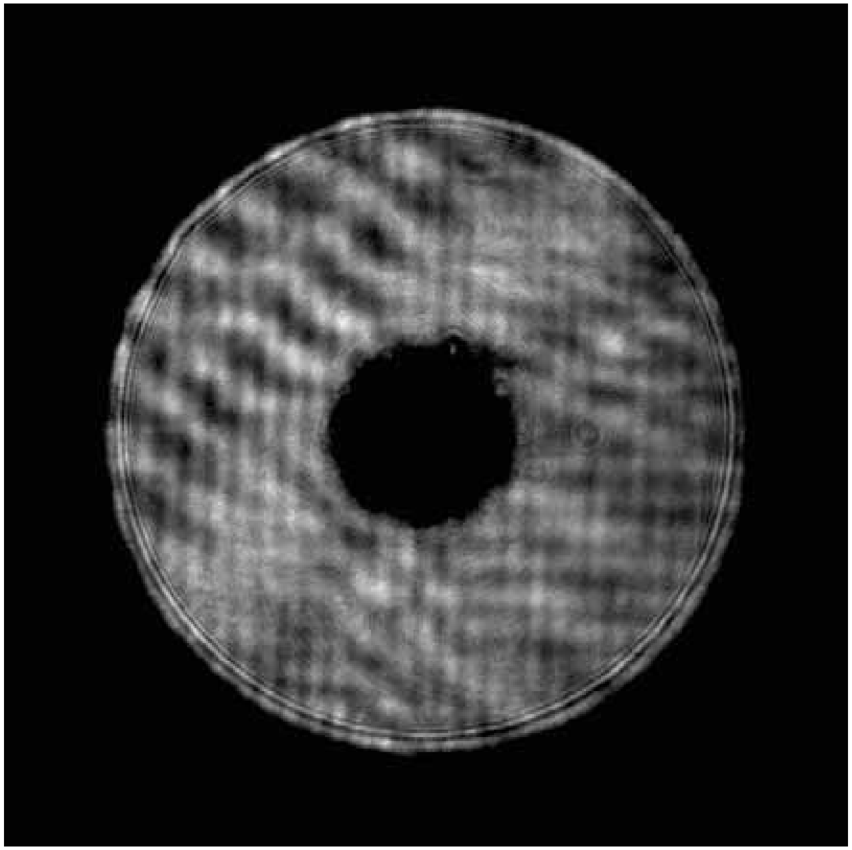
Fresnel CDI – Geometry



Fresnel CDI – Illumination

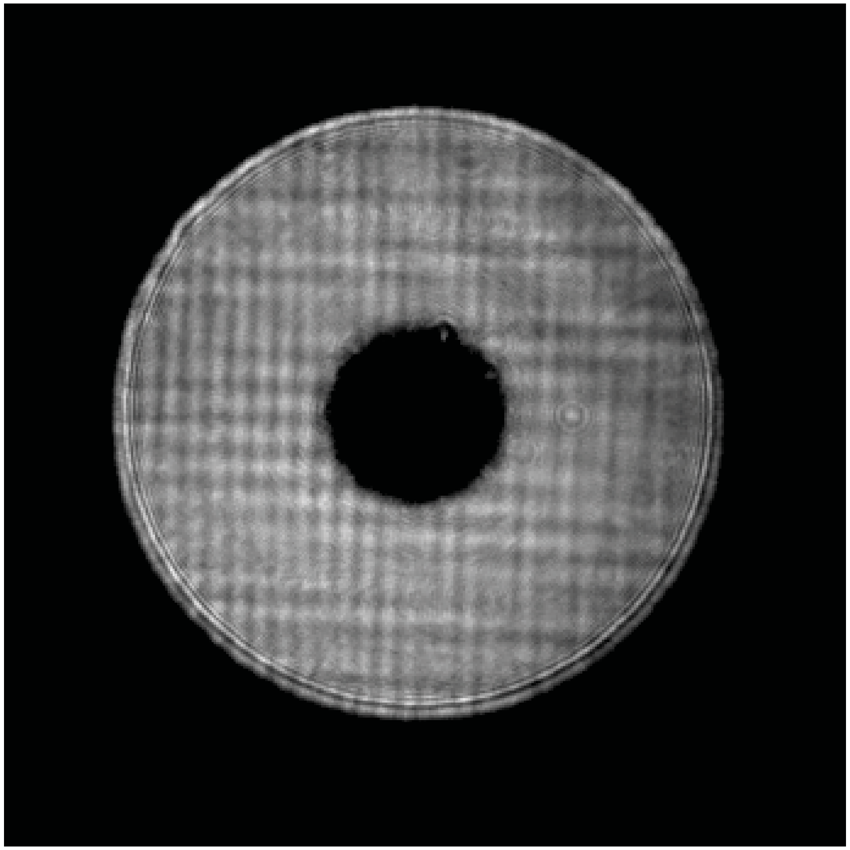


far field from Fresnel zone plate



diffraction from Au test pattern

Fresnel CDI – Illumination



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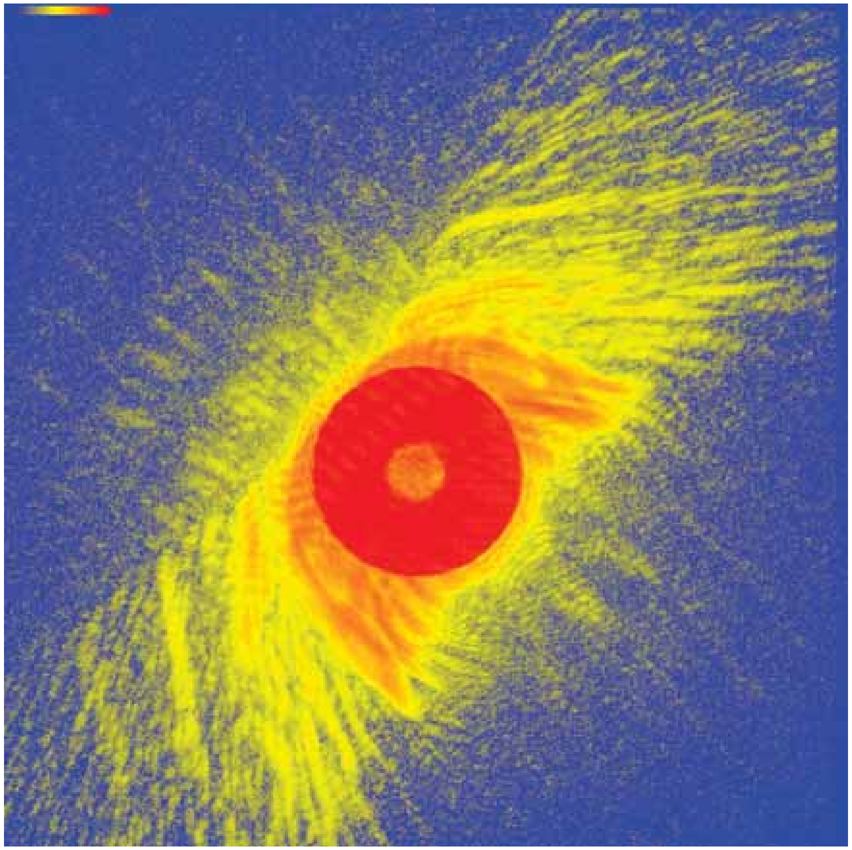
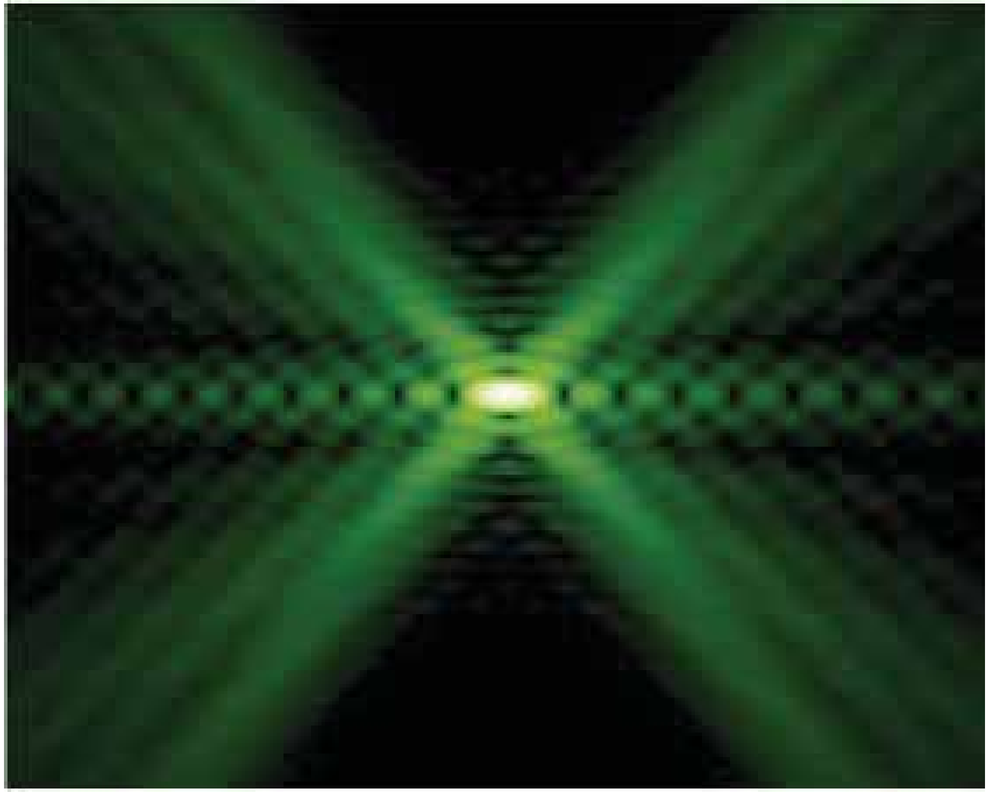


diffraction from Au test pattern

Fresnel CDI – Illumination

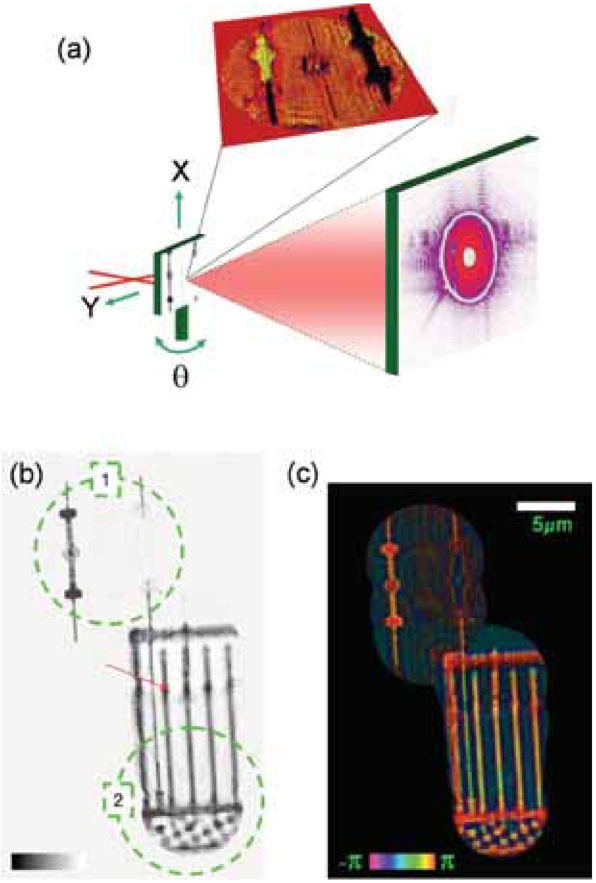
Harry Quiney, *Nature Physics* 2006.



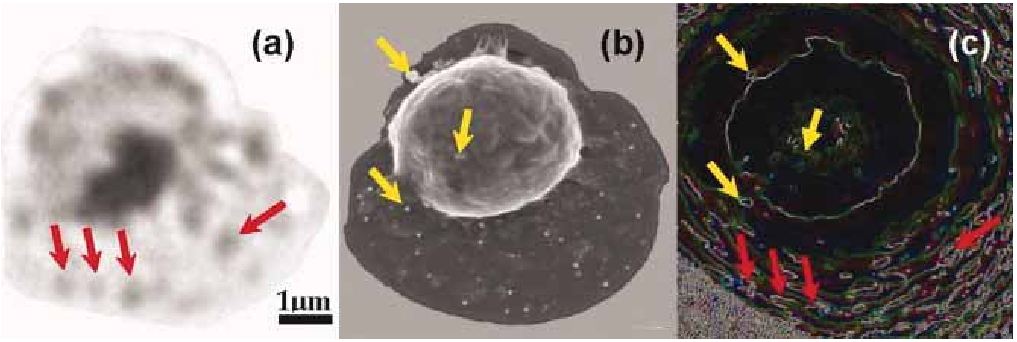
Complex wave field reconstructed in region of focus.
Only need far-field intensity pattern and knowledge of focal length.

Fresnel CDI – Sample Results

Brian Abbey *APL* 2008.
Interconnect from circuit board

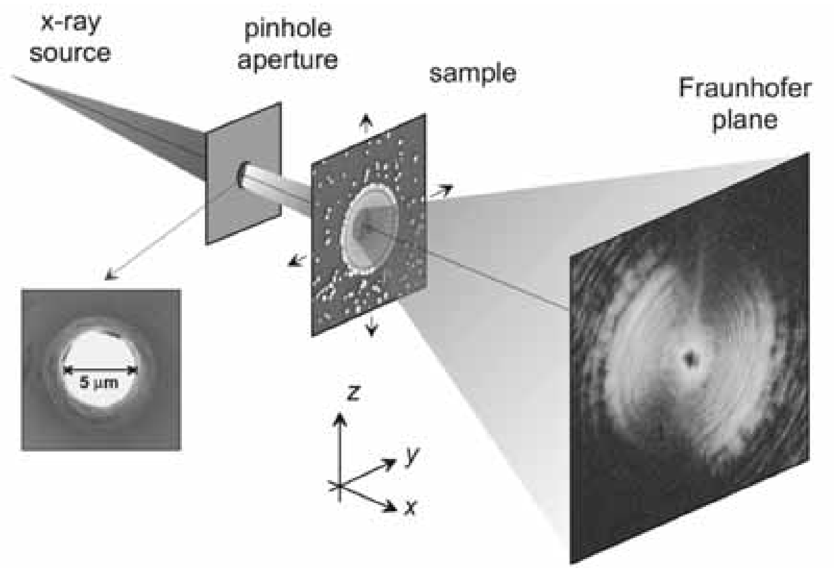


Garth Williams *Cytometry* 2008.
Malaria infected red blood Cell



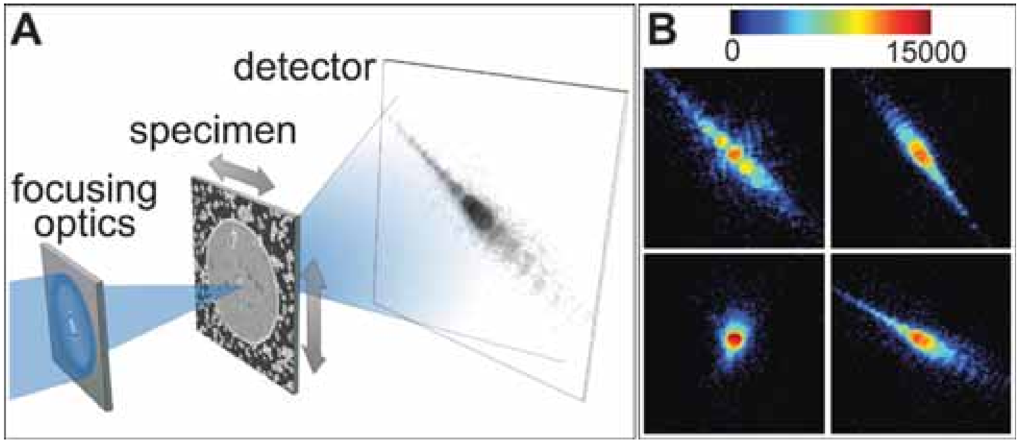
comparison of light microscopy, SEM and FCDI

Ptychography



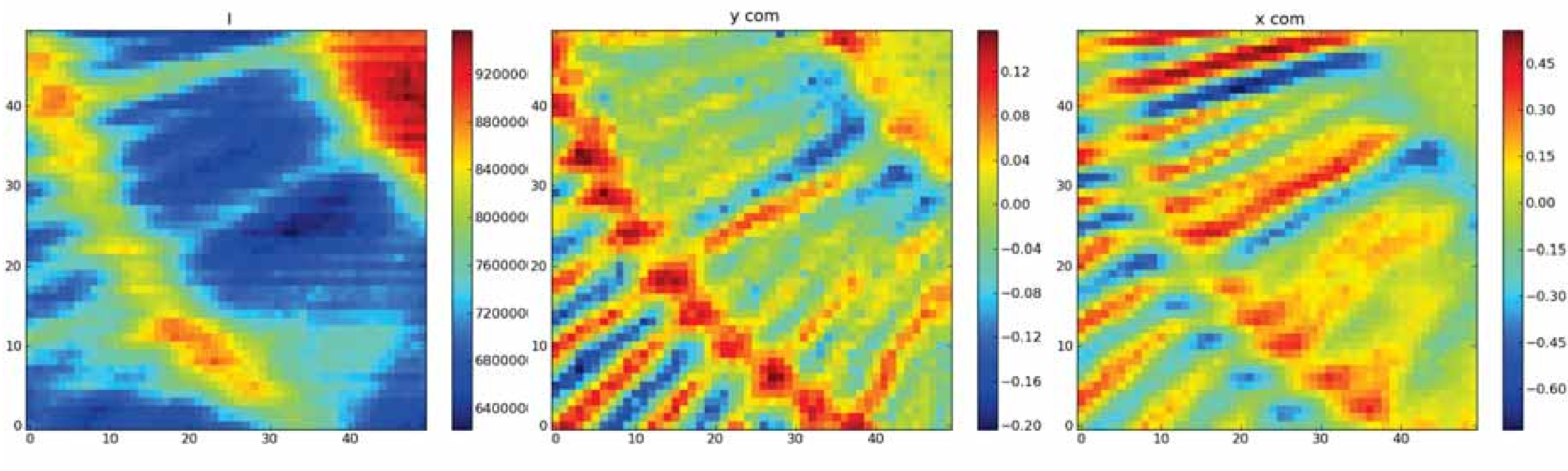
Rodenburg *PRL* 2007.
Collect diffraction patterns from overlapping regions

Thibault *Science* 2008.
Focused illumination
Beam recovered



Ptychography

Au star test pattern measured at APS 2-ID-B with MMPAD



Lensless imaging with lenses

M. Pfeifer

Coherent diffraction – theory

Coherent diffraction – theory

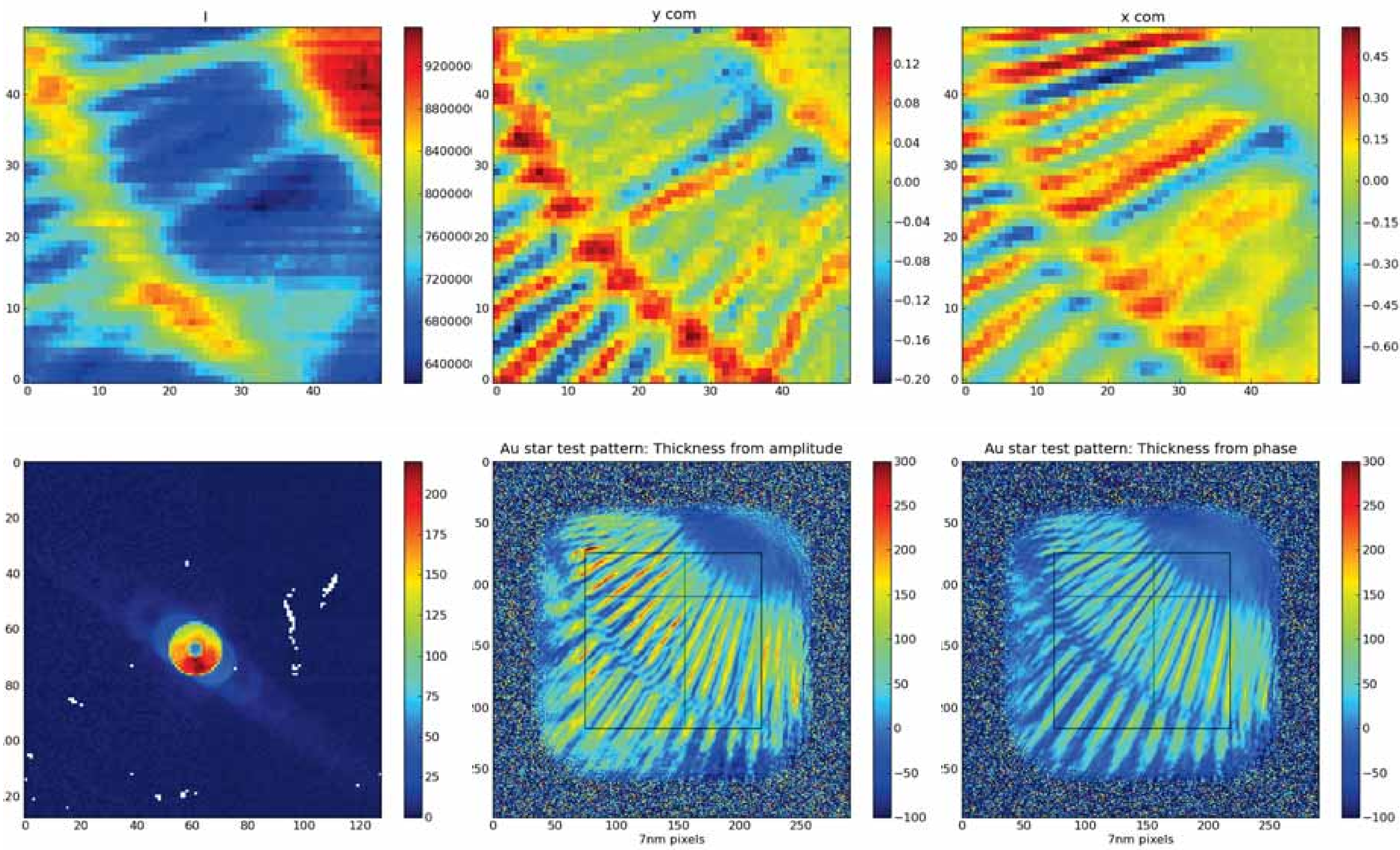
Coherent diffraction – practice

Structured illumination

Comparison of imaging methods

A few (crazy) ideas

Au star test pattern measured at APS 2-ID-B with MMPAD



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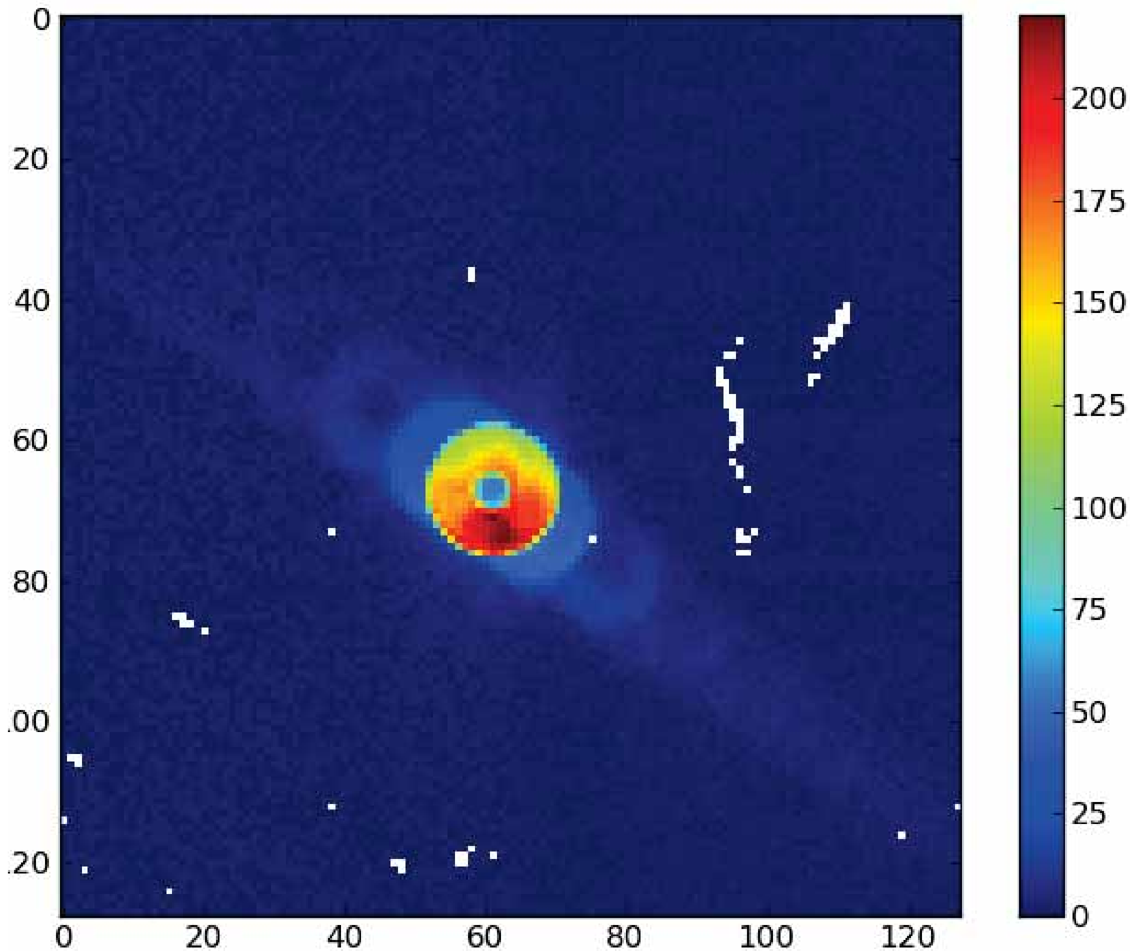

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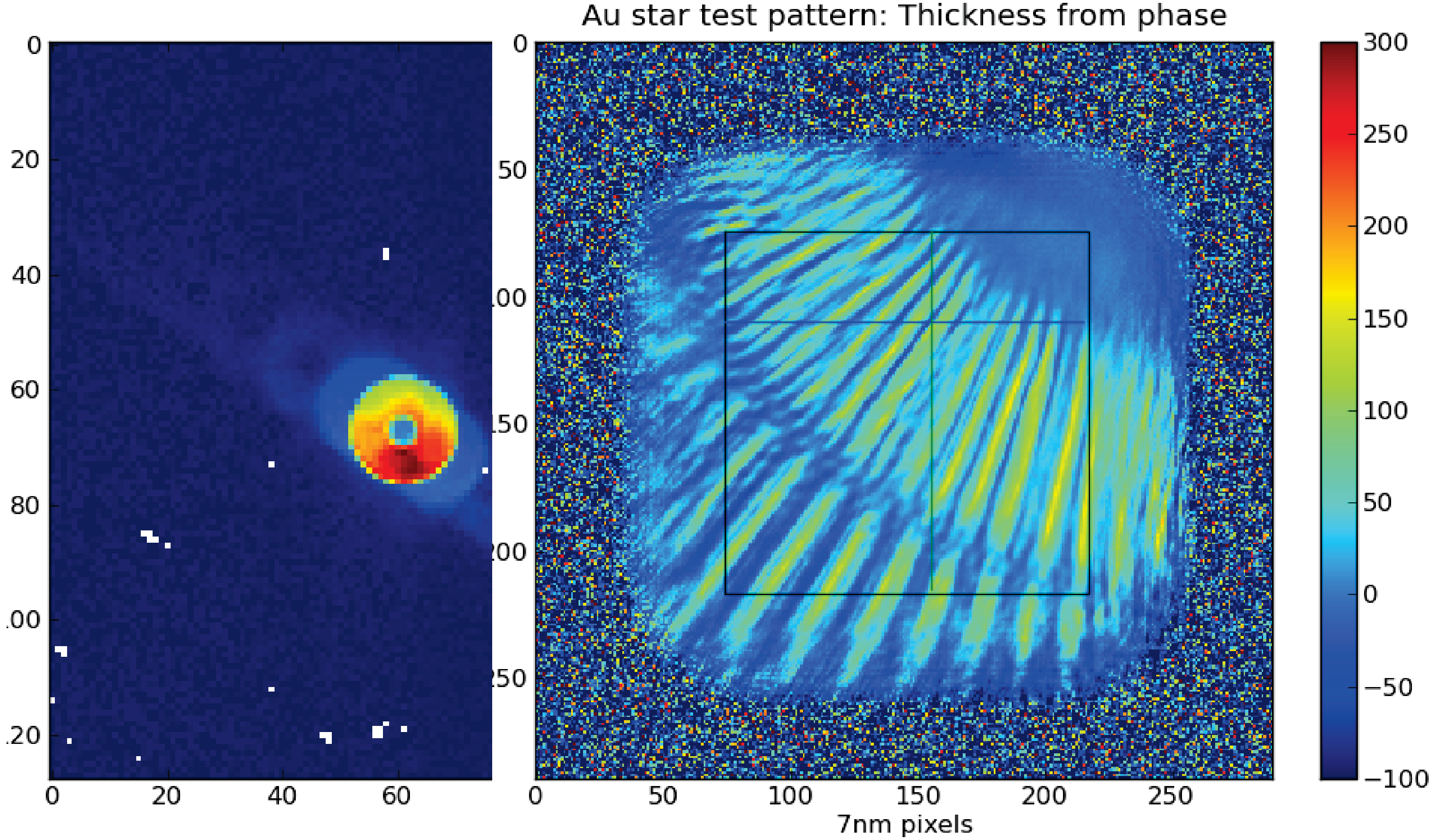
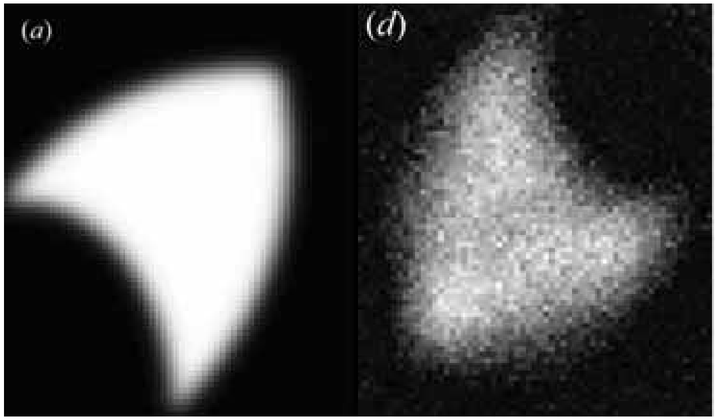


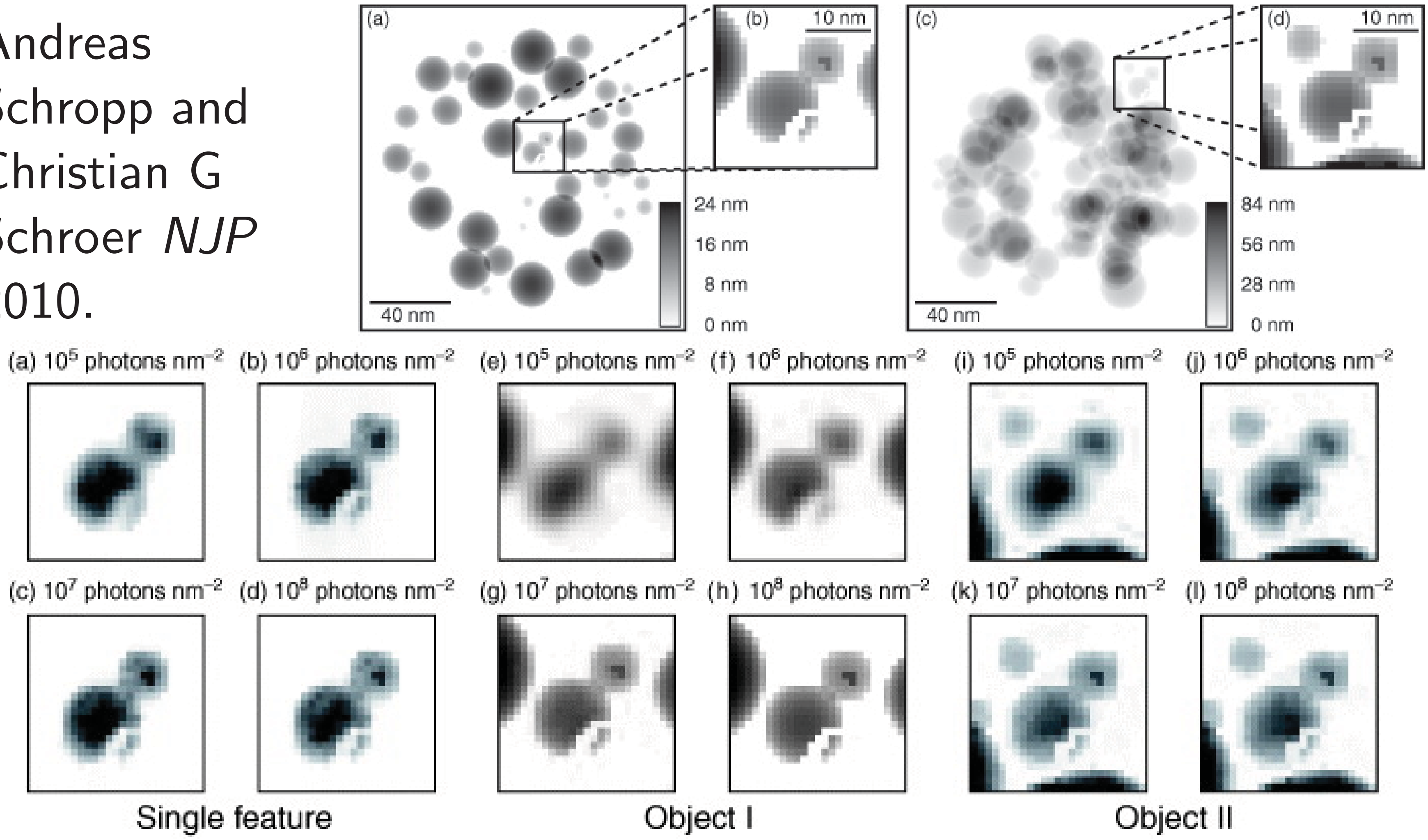
Signal to noise



Garth Williams *Acta Crys A* 2006.
Effect of Poisson noise in diffraction pattern similar to Poisson noise in image.

Signal to noise

Andreas Schropp and Christian G Schroer *NJP* 2010.



resolution for isolated feature same (or better) than same feature as part of larger sample

X-ray microscopy comparison

	NA	efficiency	mode	contrast
TXM	$\frac{\lambda}{2\Delta r}$	$e_{lens} \times e_{det}$	full field	absorption, phase
FCDI	$\sin\left(\frac{N\lambda}{4a}\right)$	e_{det}	full-field	absorption, phase
ptycho-graphy	$\sin\left(\frac{N\lambda}{4a}\right)$	e_{det}	scanning	abs., phase, fluorescence, photoelec-trons

X-ray microscopy comparison

	NA	efficiency	mode	contrast
TXM	$\frac{\lambda}{2\Delta r} = 0.01$	$e_{lens} \times e_{det}$	full field	absorption, phase
FCDI	$\sin\left(\frac{N\lambda}{4a}\right) = 0.5$	e_{det}	full-field	absorption, phase
ptycho-graphy	$\sin\left(\frac{N\lambda}{4a}\right) = 0.5$	e_{det}	scanning	abs., phase, fluorescence, photoelec-trons

assuming

- $\lambda = 0.1nm$ wavelength
- $\Delta r = 5nm$ finest zone width in zone plate
- $N = 1000$ number of rows/columns in area detector
- $a = 50nm$ illumination size

Multi-modal diffraction imaging

Fresnel CDI

- Full field imaging with variable zoom
- No fast scanning
- Dosing more even – take multiple exposures of same illuminated area and cross correlate – no partially overlapping illumination

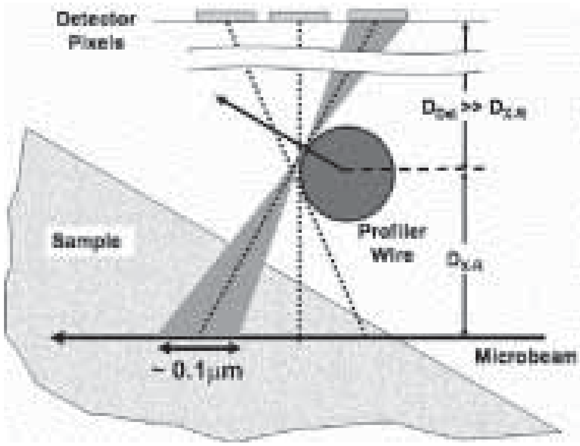
Ptychography

- X-ray fluorescence
- Photoelectrons

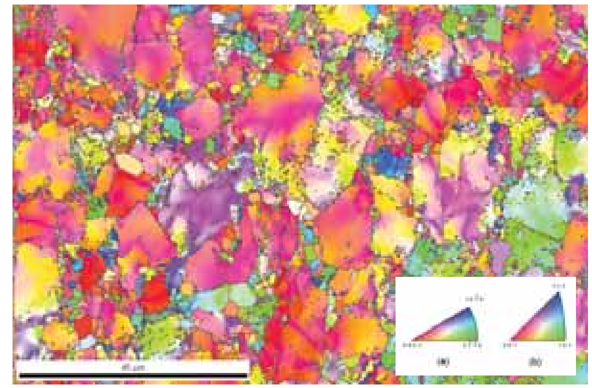
Potential for z-scanning instead of tomography (poorer resolution)

Strain mapping within polycrystalline film

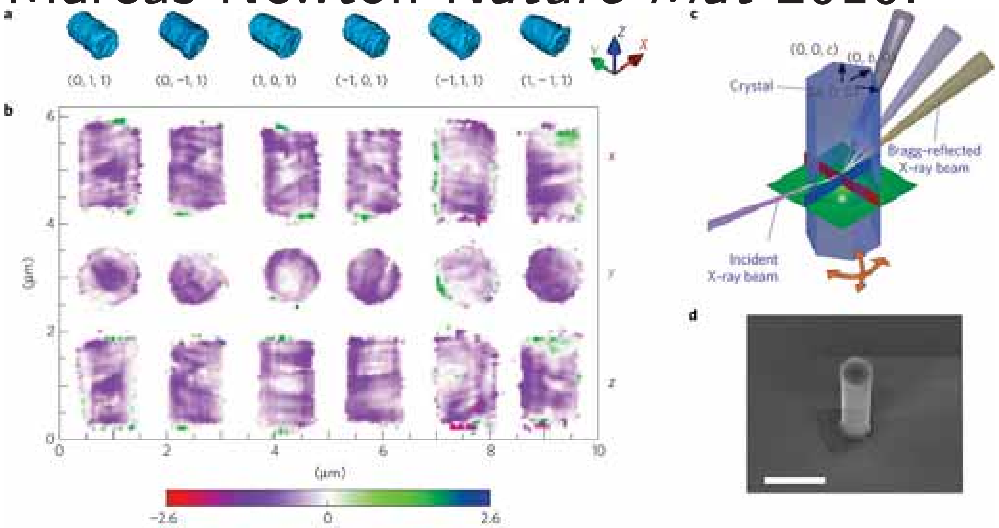
Diff. aperture diffraction imaging.
Wang, *Micron* 2004.

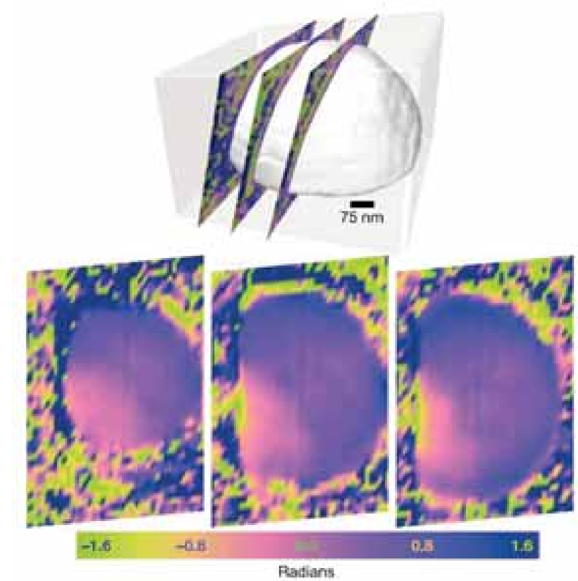


Matt Miller Group

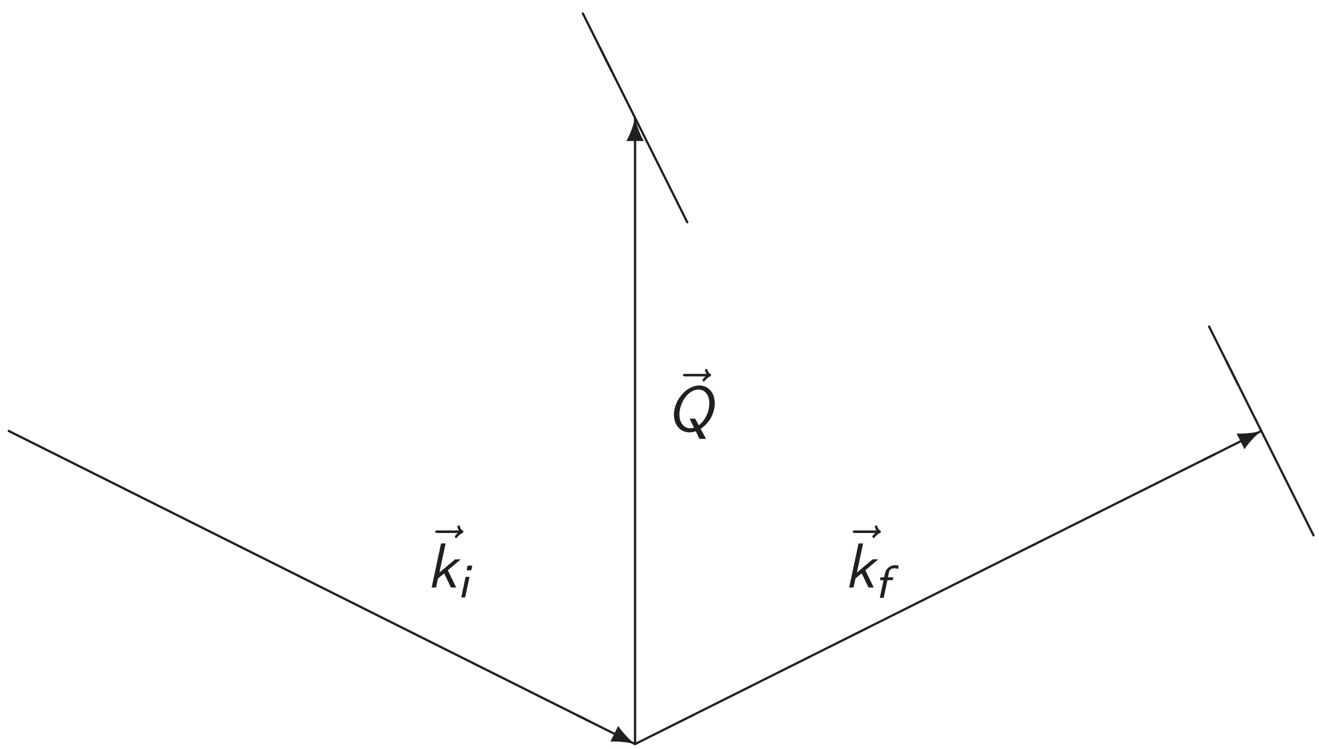


Marcus Newton *Nature Mat* 2010.

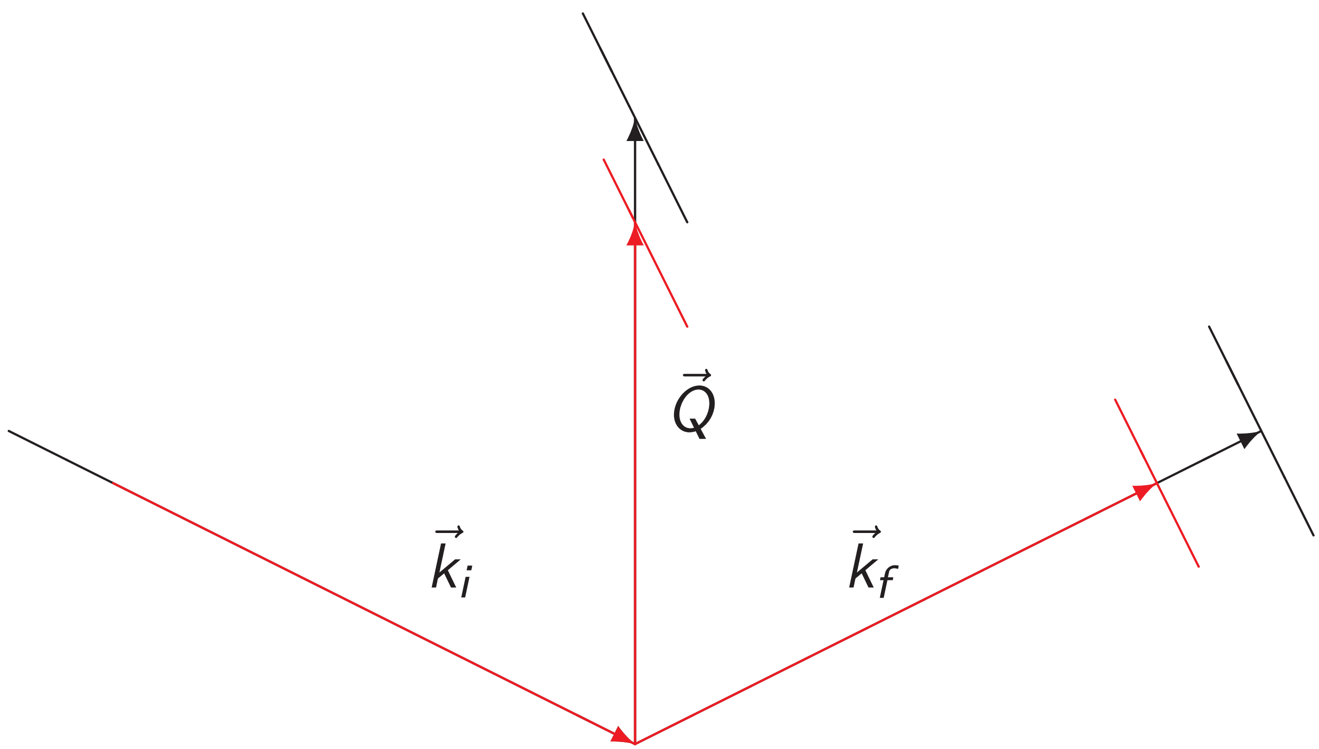




Multi-energy Bragg CDI



Multi-energy Bragg CDI



Single shot three dimensional imaging of 3D strain

Consider a detector at a distance l from a sample, centered about a Bragg peak, G, at an energy E.

Measurements made over values p_x, p_y, and $\frac{\delta E}{E}$.

$\vec{q} = \frac{k_o}{l} p_x \hat{q}_x + \left(\frac{k_o}{l} p_y - \frac{\delta E}{E} G \cos\theta\right) \hat{q}_y + \frac{\delta E}{E} G \sin\theta \hat{q}_z$

For 5nm resolution imaging of 500nm particle at detector distance l =2m, and energy E =6keV, require:

- 200^2 pixels of $(100\mu\text{m})^2$
- 480eV range at 2.4keV resolution

If an appropriate energy discriminating detector were possible, then a full three dimensional mapping of the strain a nanocrystal could be made *in situ* in a single measurement, with no scanning.

If three detectors could be located at three Bragg peaks (*i.e.* three $\{200\}$ peaks when the incident beam is co-axial with the $\{111\}$, then a three dimensional mapping of three different strain projections could be made in real time.

Summary

- STXM without phase retrieval is throwing away information.
- Coherent diffraction will be able to stay ahead of purely lens based imaging - but *high efficiency* lenses help.
- Fresnel CDI and ptychography have same basic geometry and optics, and can recover your focal spot complex wave field.
- Efficiency of optic (or optical system) and detector as important as source properties.