

Coherent Diffraction Imaging

Ross Harder aka “The Imposter”

34-ID-C

Advanced Photon Source

<https://tinyurl.com/y2qtrz7e>

Acknowledgments:

Prof. Ian Robinson (BNL)

Dr. Xiaojing Huang (BNL)

Dr. Jesse Clark (~~PULSE institute, SLAG Amazon~~)

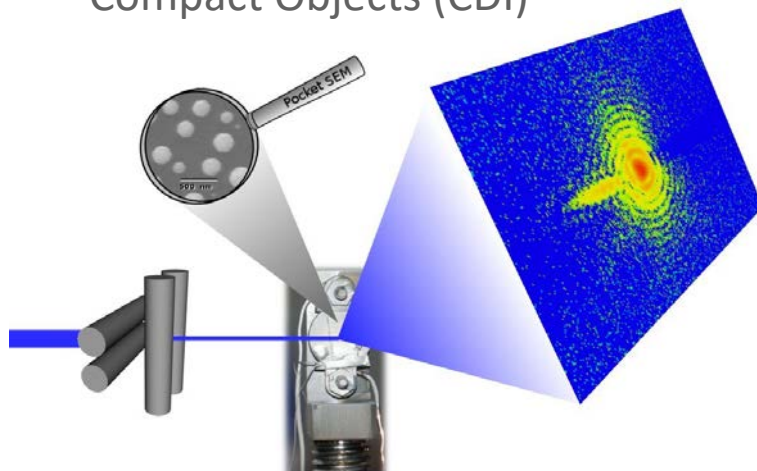
Prof. Oleg Shpyrko (UCSD)

Dr. Andrew Ulvestad (~~ANL—MSD Tesla~~)

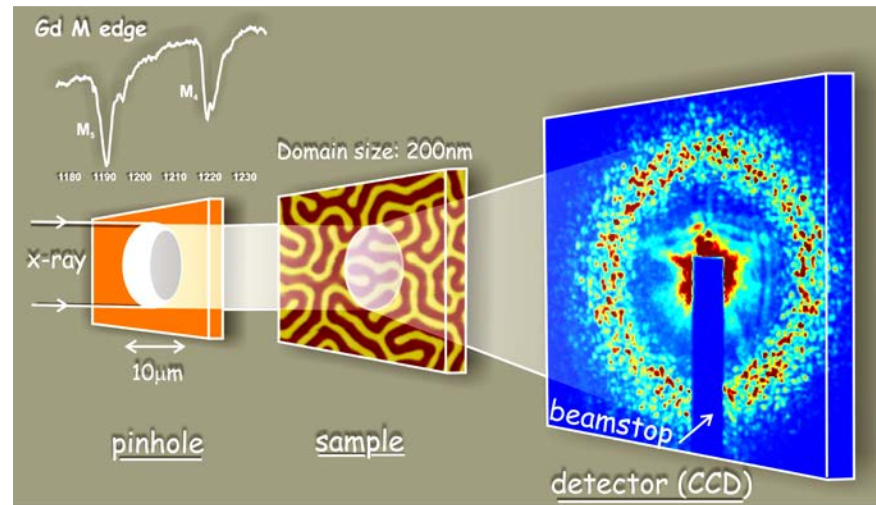
Dr. Ian McNulty (~~ANL—CNM MaxIV~~)

Dr. Junjing Deng (ANL – APS)

Compact Objects (CDI)

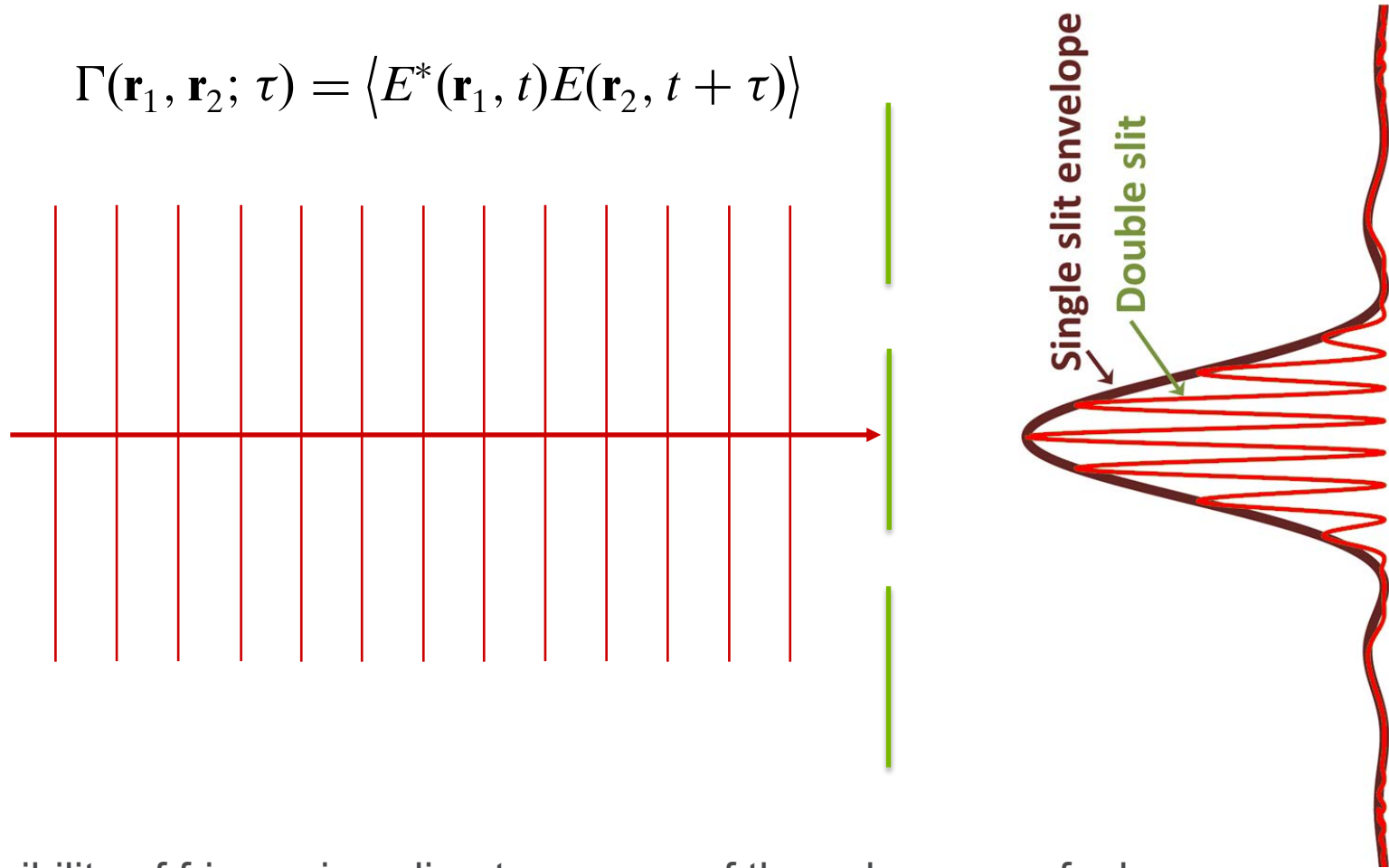


Non-compact samples (Ptychography)



COHERENCE

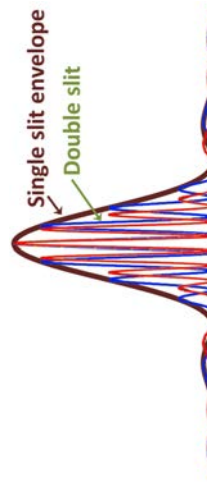
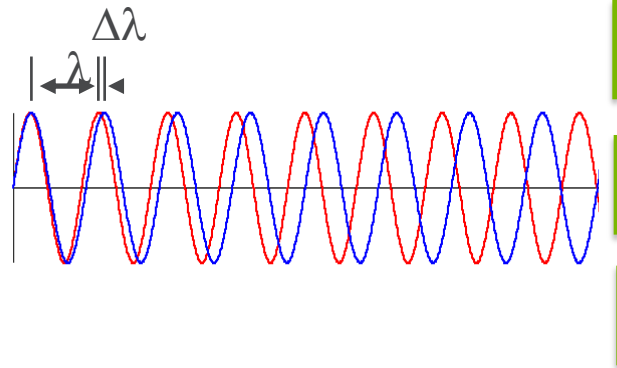
$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau) = \langle E^*(\mathbf{r}_1, t)E(\mathbf{r}_2, t + \tau) \rangle$$



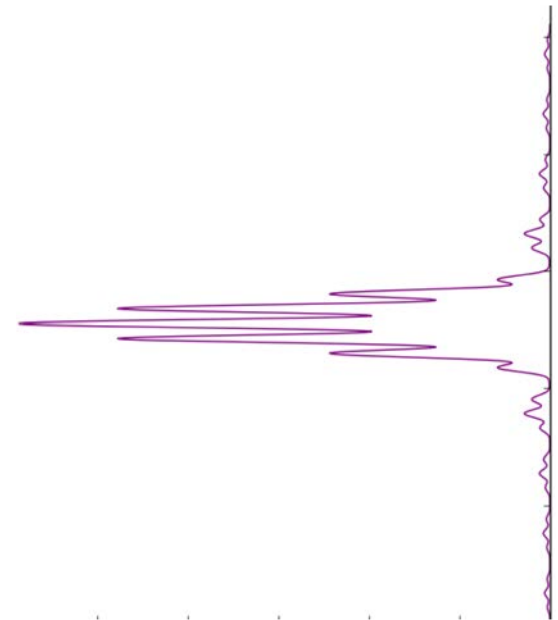
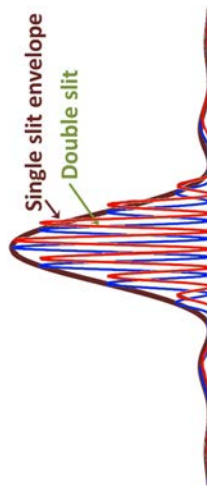
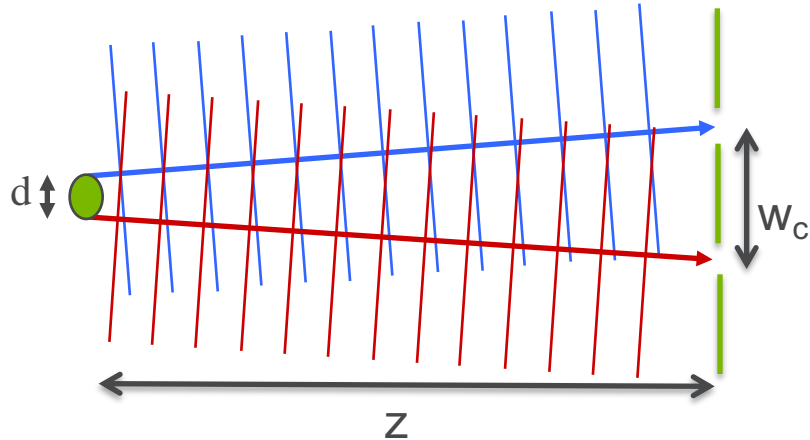
Visibility of fringes is a direct measure of the coherence of a beam. If beam is coherent across the spacing of the slits a Fourier Transform of the slit structure is observed downstream.

COHERENCE

longitudinal coherence

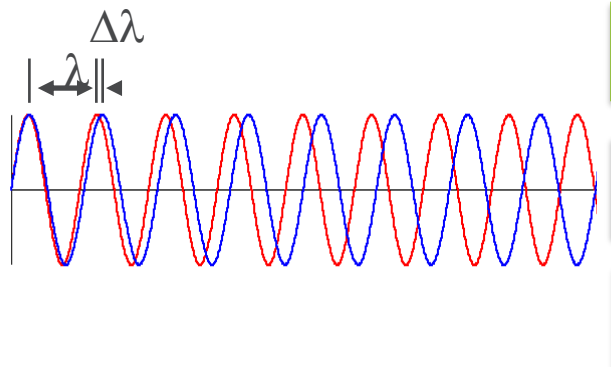


transverse coherence



COHERENCE

longitudinal coherence

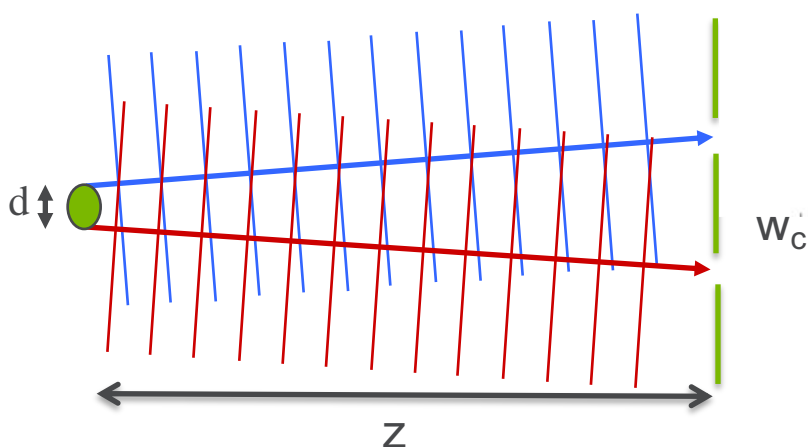


$$l_c \sim \frac{\lambda^2}{\Delta\lambda}$$

$$\tau_c \sim \frac{\lambda^2}{c\Delta\lambda}$$

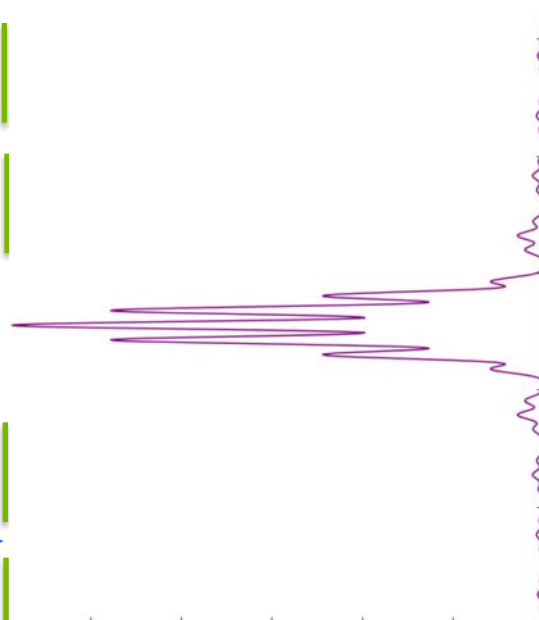
Si (111)
0.5 μm or 1.5 fs

transverse coherence

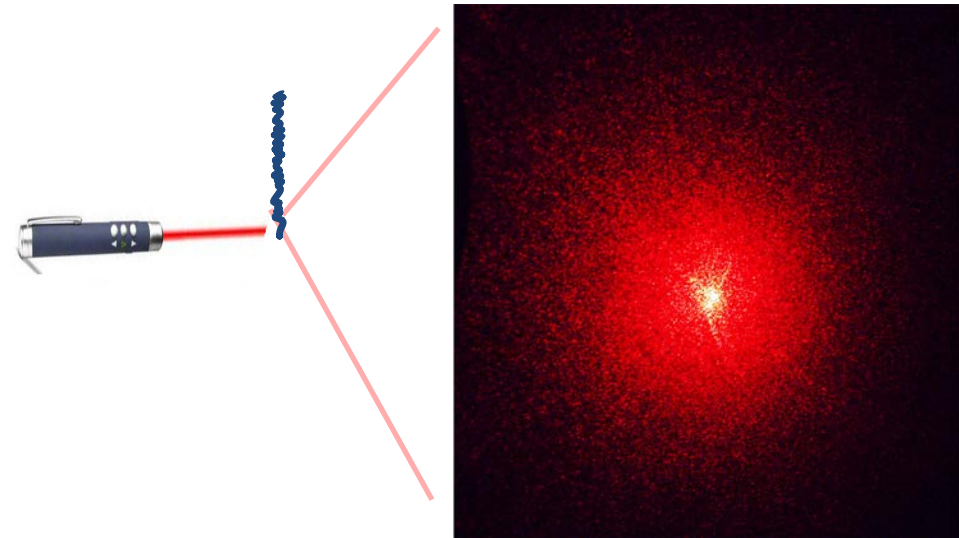
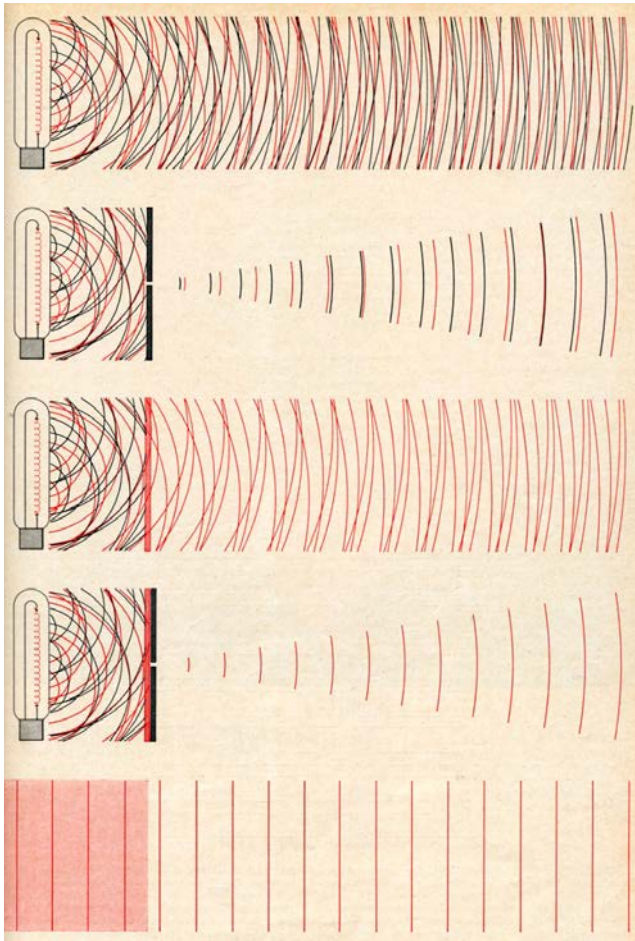


$$w_c \sim \frac{\lambda z}{d}$$

34-ID-C 50m
25x70 μm @ 9 keV



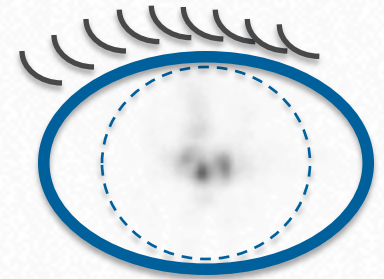
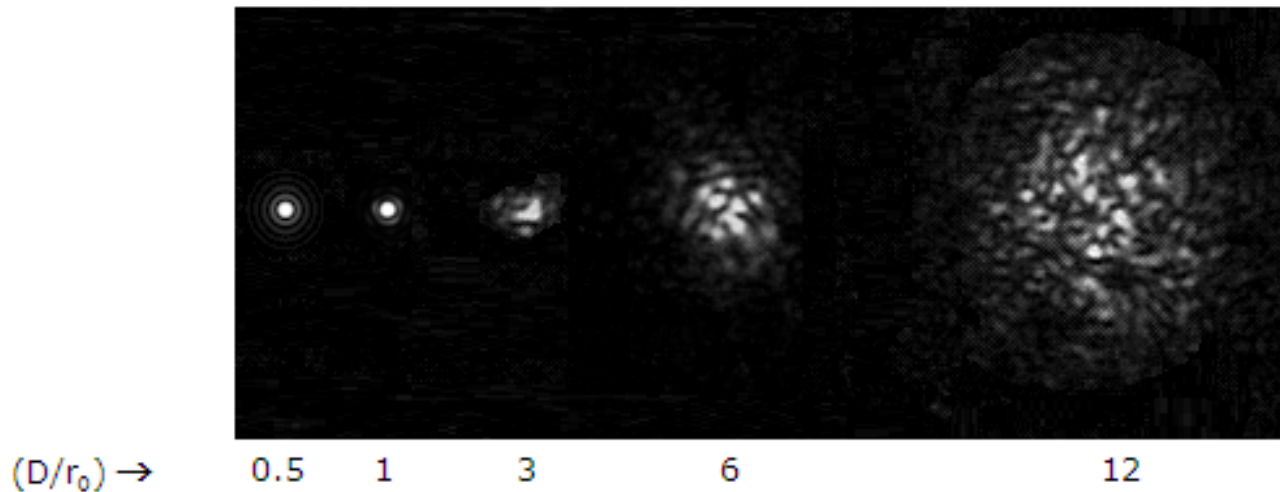
Coherence: Laser Speckle



A. L. Schawlow "Laser Light"
 Scientific American, 219 (3), p. 120, (1968)

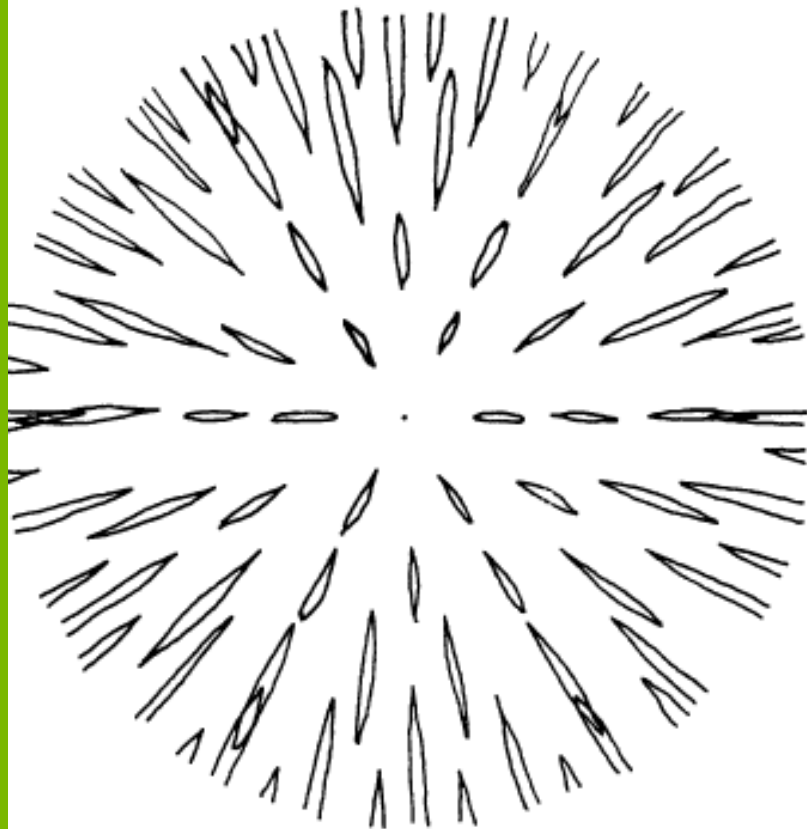
Laser Speckle: Interference pattern arising from randomly distributed scatterers

SIMPLEST SPECKLE EXPERIMENT: TWINKLE, TWINKLE LITTLE STAR



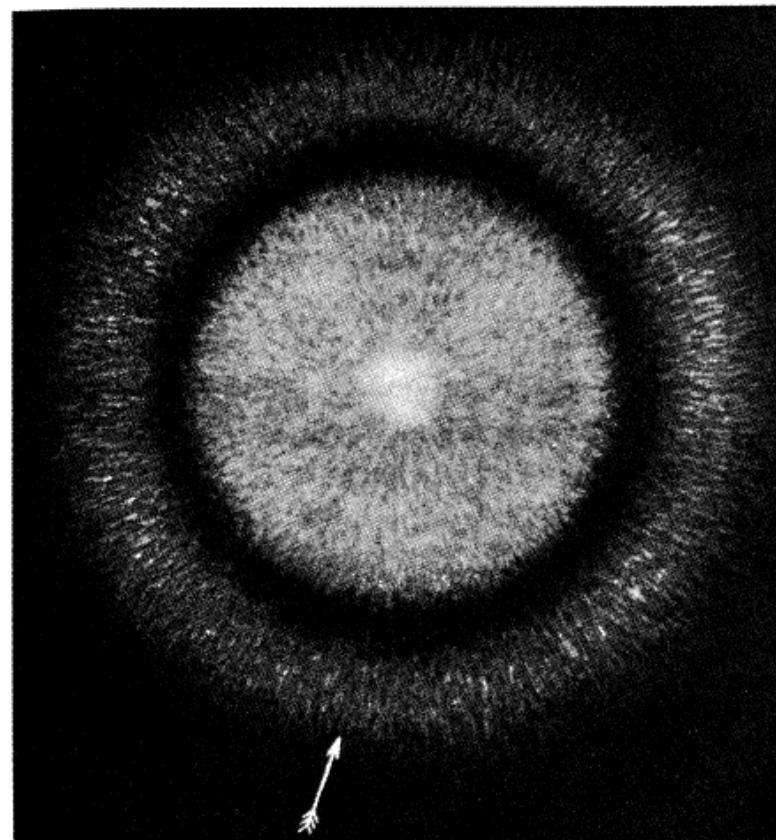
Stars are big, but very far away. As a result, their light has a high transverse coherence. As the light propagates through the atmosphere our eye detects a portion of the coherent diffraction

First Speckle: Exner, 1877 (using candle light)



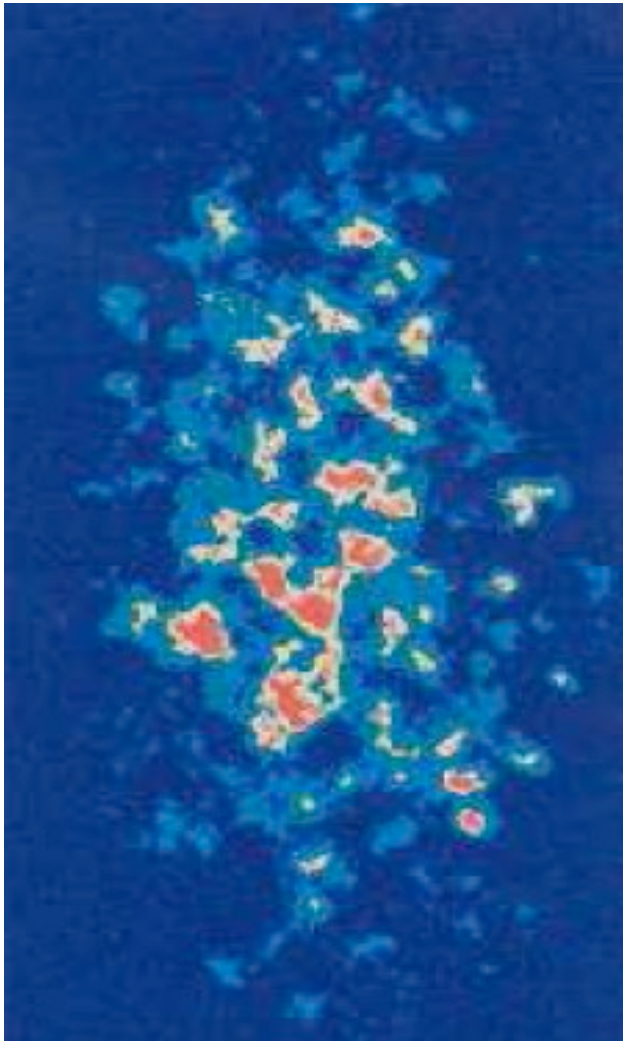
K. Exner: Sitzungsber. Kaiserl.
Akad. Wiss. (Wien) 76, 522 (1877)

First Speckle Photo: von Laue, 1914 (using arc discharge lamp)



M. von Laue: Sitzungsber. Akad.
Wiss. (Berlin) 44, 1144 (1914)

First X-ray Speckle:

M. Sutton et al., *Nature* **352**, 608-610 (1991)

$$I \propto |F(q)|^2$$

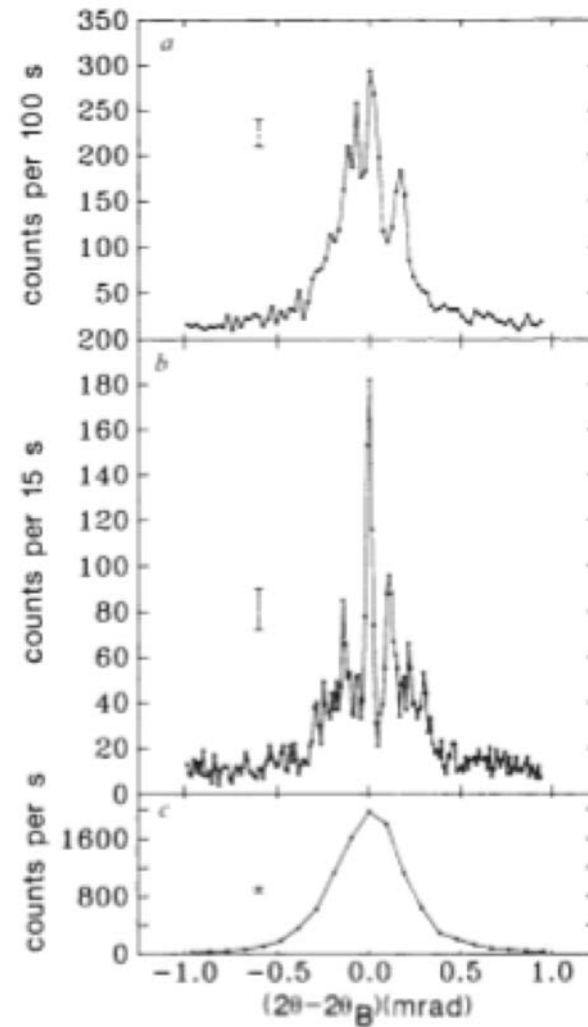


FIG. 4 Speckle patterns measured using a 2.5- μm , b, 5- μm and c, 50- μm collimating pinholes. The analysing pinholes used were 50, 25 and 100 μm , respectively. Representative error bars are indicated, and the solid lines simply connect the data points. The (001) Bragg angle, $2\theta_0$, is $\sim 23.9^\circ$.

WHY USE SYNCHROTRON RADIATION?

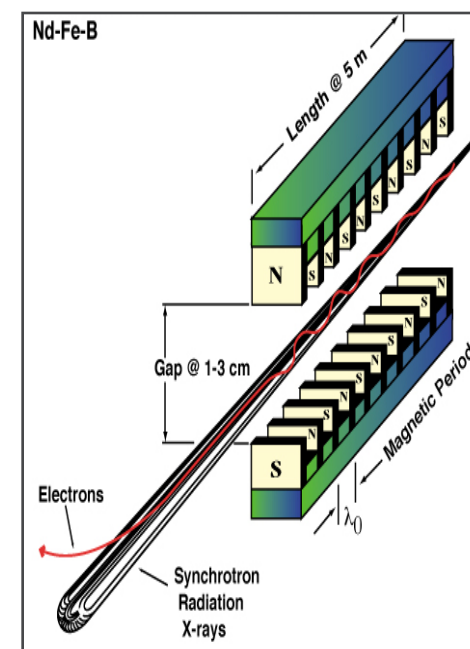
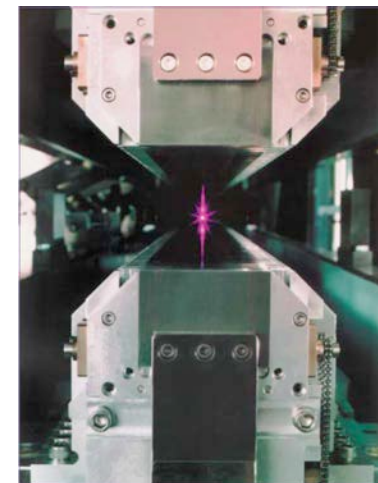
Synchrotron sources offer:

- Brightness (small source, collimated)
- Tunability (IR to hard x-rays)
- Polarization (linear, circular)
- Time structure (short pulses)

Source brightness is the key figure of merit for coherent imaging

$B = \text{photons/source area, divergence, bandwidth}$

$$F_c \sim \lambda^2 B$$



COHERENT X-RAY REFERENCES

- Vartanyants, I A, and A Singer. 2010 “Coherence Properties of Hard X-Ray Synchrotron Sources and X-Ray Free-Electron Lasers.” *New Journal of Physics* 12 (3): 035004.
- Singer, Andrej, and Ivan A Vartanyants. 2014. “Coherence Properties of Focused X-Ray Beams at High-Brilliance Synchrotron Sources.” *Journal of Synchrotron Radiation* 21 (1). International Union of Crystallography: 5–15. doi:10.1038/nnano.2008.246.
- Nugent, Keith. 2009. “Coherent Methods in the X-Ray Sciences.” *Advances in Physics* 59 (1): 1–99. doi:doi: 10.1080/00018730903270926.

X-RAYS, TWO EXTREMES FOR STRUCTURAL STUDY:

X-ray Imaging (Shadowgraphs)

- Inhomogeneous, non-periodic materials
- Limited spatial resolution (~0.001 mm)



Roentgen, Nobel 1900

X-ray Diffraction (Scattering)

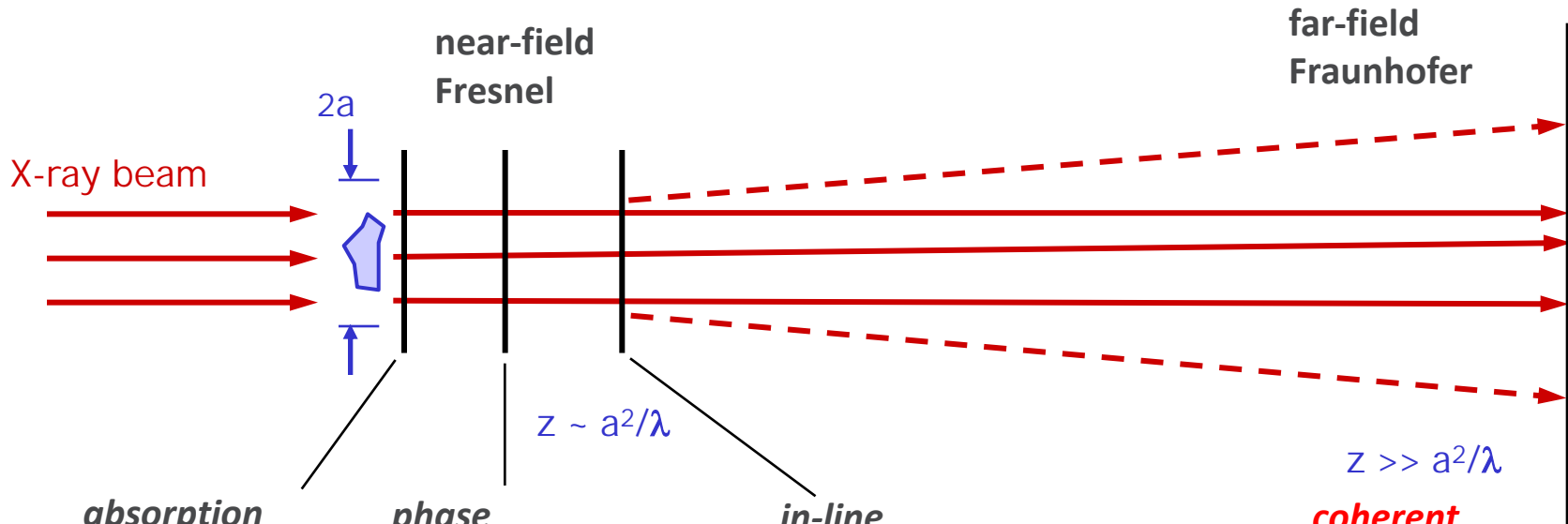
Coherent Imaging
is scattering

- Is particularly sensitive to periodicity in the sample (Crystals)
- Atomic resolution (unit cell)



Von Laue, Nobel 1914
Bragg & Bragg, Nobel 1915

IMAGING REGIMES WITH COHERENT X-RAYS



absorption radiograph

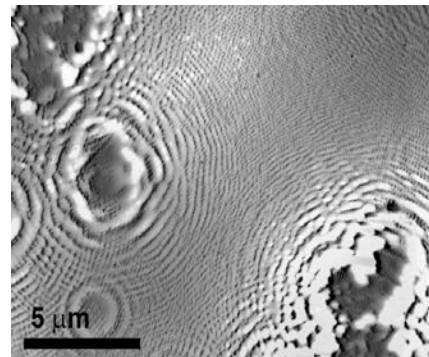


phase contrast



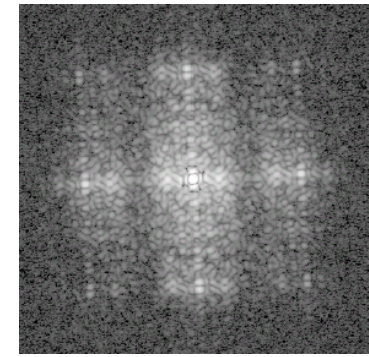
Kagoshima (1999)

in-line holography



Jacobsen (1990)

coherent diffraction



Miao (1999)

REFRACTIVE INDEX AND CONTRAST IN THE X-RAY REGION

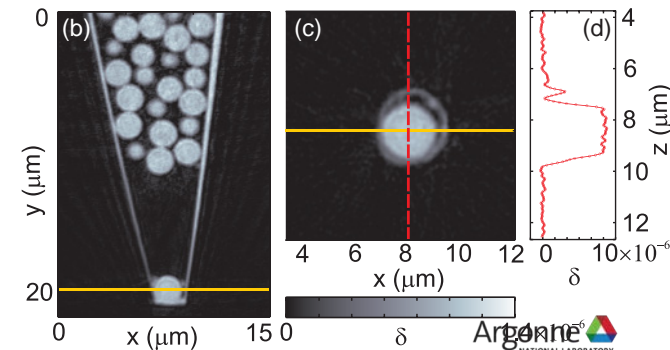
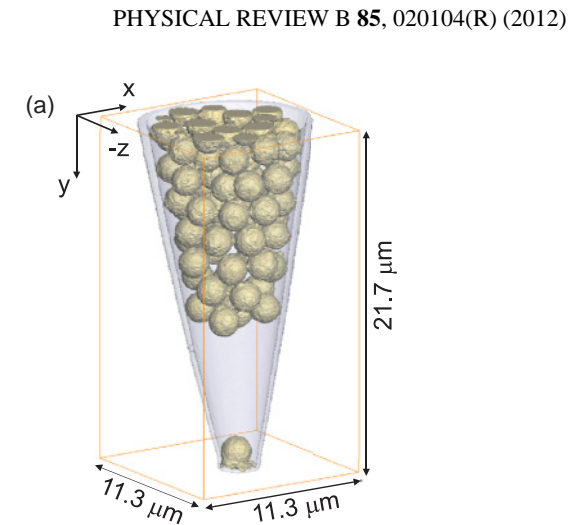
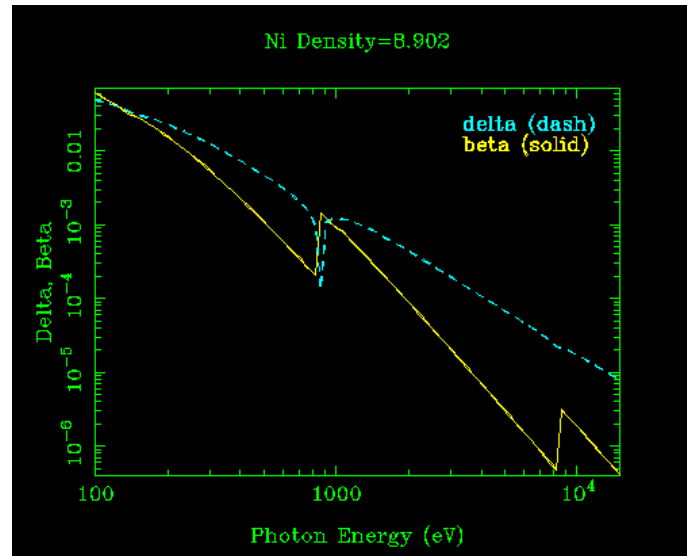
$$n = 1 - \delta - i\beta = 1 - \frac{r_e}{2\pi} \lambda^2 \sum_i n_i f_i(0)$$

$$A = A_0 \exp(-inkt)$$

$$k = 2\pi / \lambda$$

- Absorption contrast:
sensitive to $Im(n)$
 $\sim 4\pi\beta(x,y)t/\lambda$

- Phase contrast:
sensitive to $Re(n)$
 $\sim 2\pi\delta(x,y)t/\lambda$



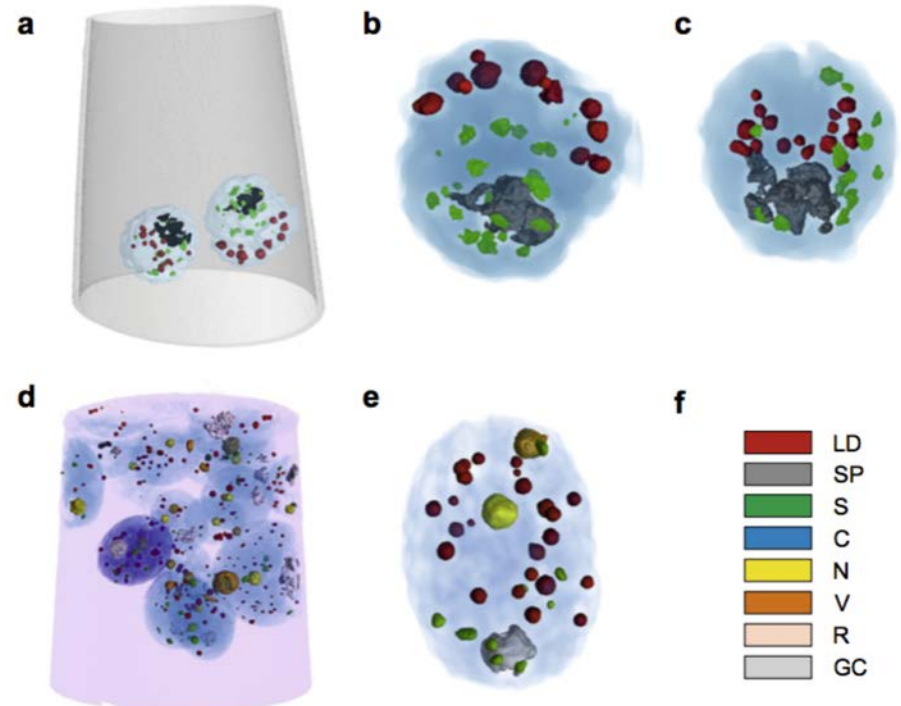
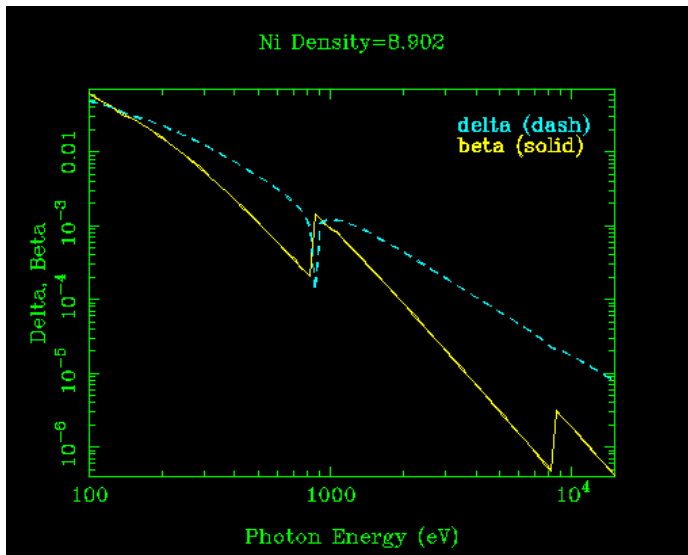
Diaz, Ana, et al, 2012. "Quantitative X-Ray Phase Nanotomography." *Physical Review B* 85.

REFRACTIVE INDEX AND CONTRAST IN THE X-RAY REGION

$$n = 1 - \delta - i\beta = 1 - \frac{r_e}{2\pi} \lambda^2 \sum_i n_i f_i(0)$$

$$A = A_0 \exp(-inkt)$$

$$k = 2\pi / \lambda$$



A. Diaz, et al., Journal of Structural Biology, vol. 192, no. 3, pp. 461–469, Oct. 2015.

Absorption contrast:

sensitive to $Im(n)$

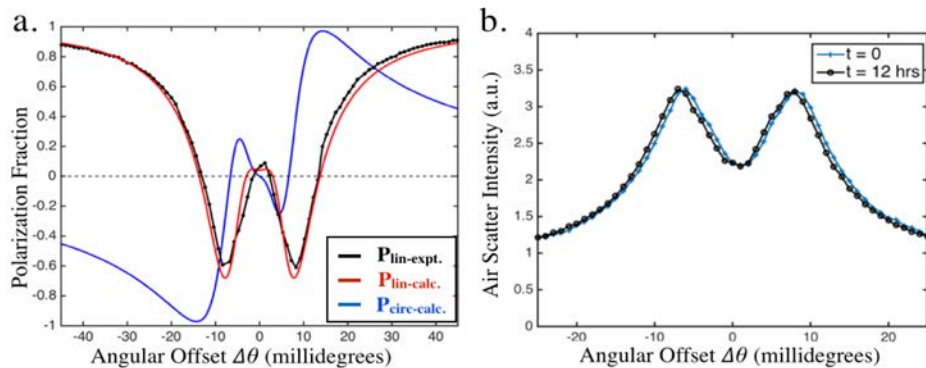
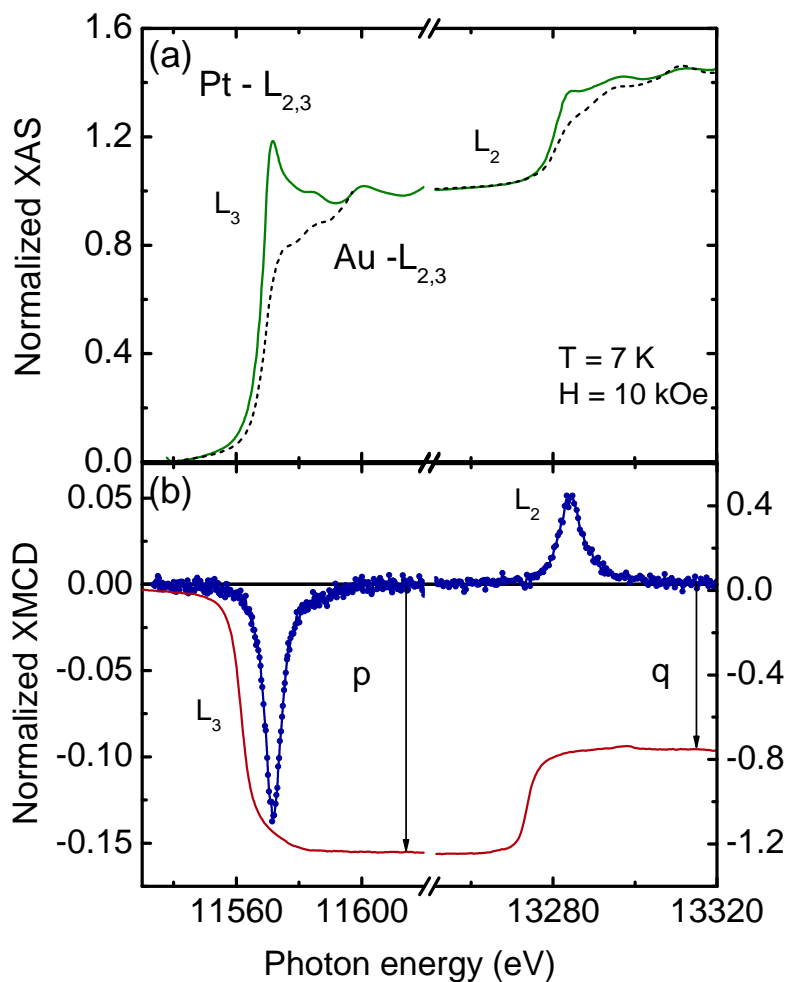
$$\sim 4\pi\beta(x, y)t / \lambda$$

Phase contrast:

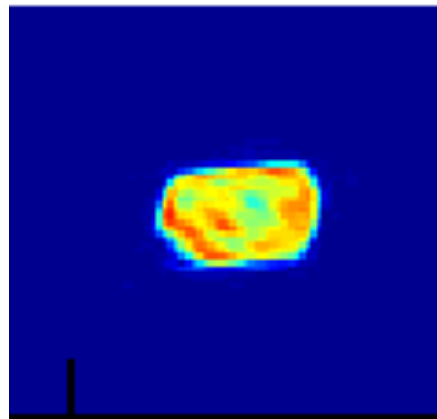
sensitive to $Re(n)$

$$\sim 2\pi\delta(x, y)t / \lambda$$

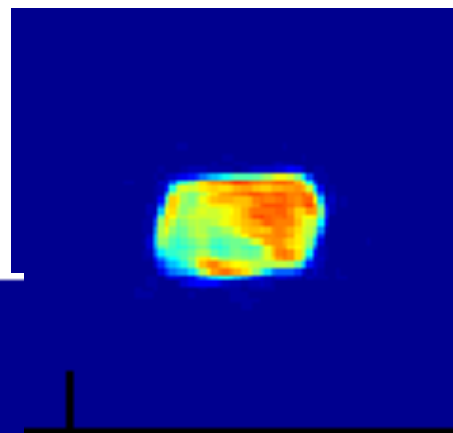
POLARIZED X-RAYS GIVE SENSITIVITY TO ELECTRON SPIN in PtCo



LCP @ 11.565keV



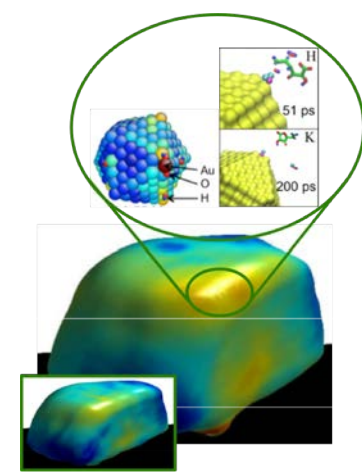
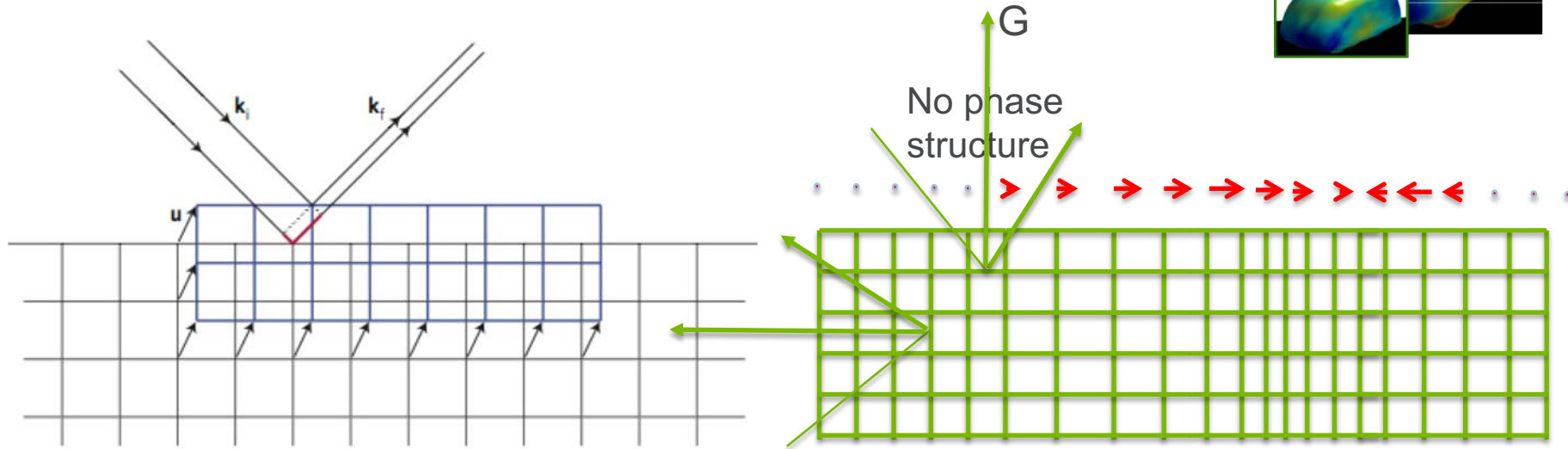
RCP @ 11.565keV



Figuroa, A. I., et al. (2014). *Physical Review B*, 90(17), 174421

CDI IN BRAGG GEOMETRY: IMAGING DISPLACEMENT FIELD (STRAIN)

Displacement field $u(\mathbf{r})$:

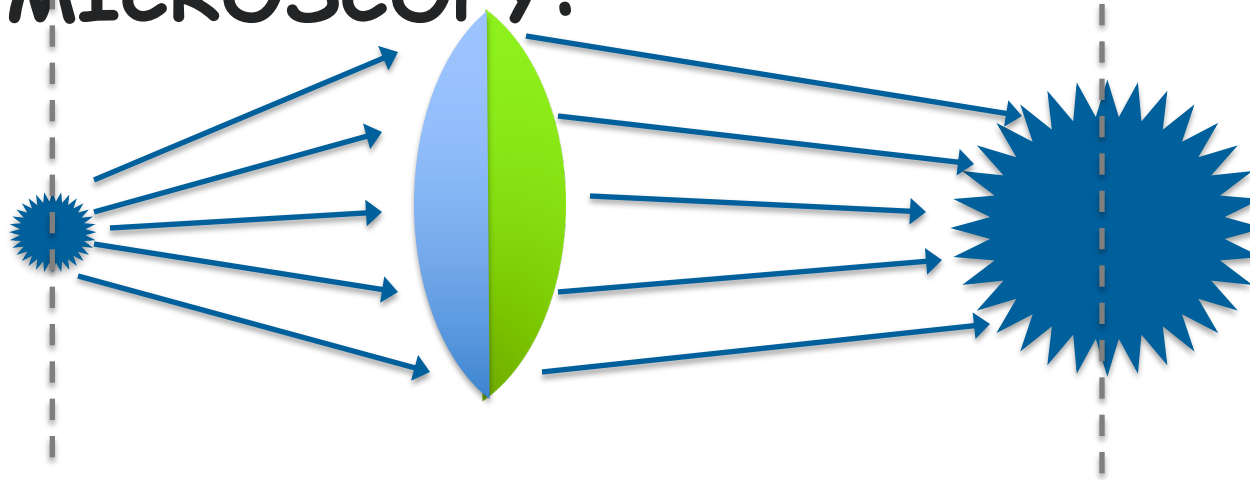


Coherent X-ray Diffraction measures:

$$\tilde{\rho}(\mathbf{r}) = \rho_{G_{hkl}}(\mathbf{r}) \exp[-i\mathbf{G}_{hkl} \cdot \mathbf{u}(\mathbf{r})]$$

Strain is a gradient of $u(\mathbf{r})$, the phase component of the complex-valued density

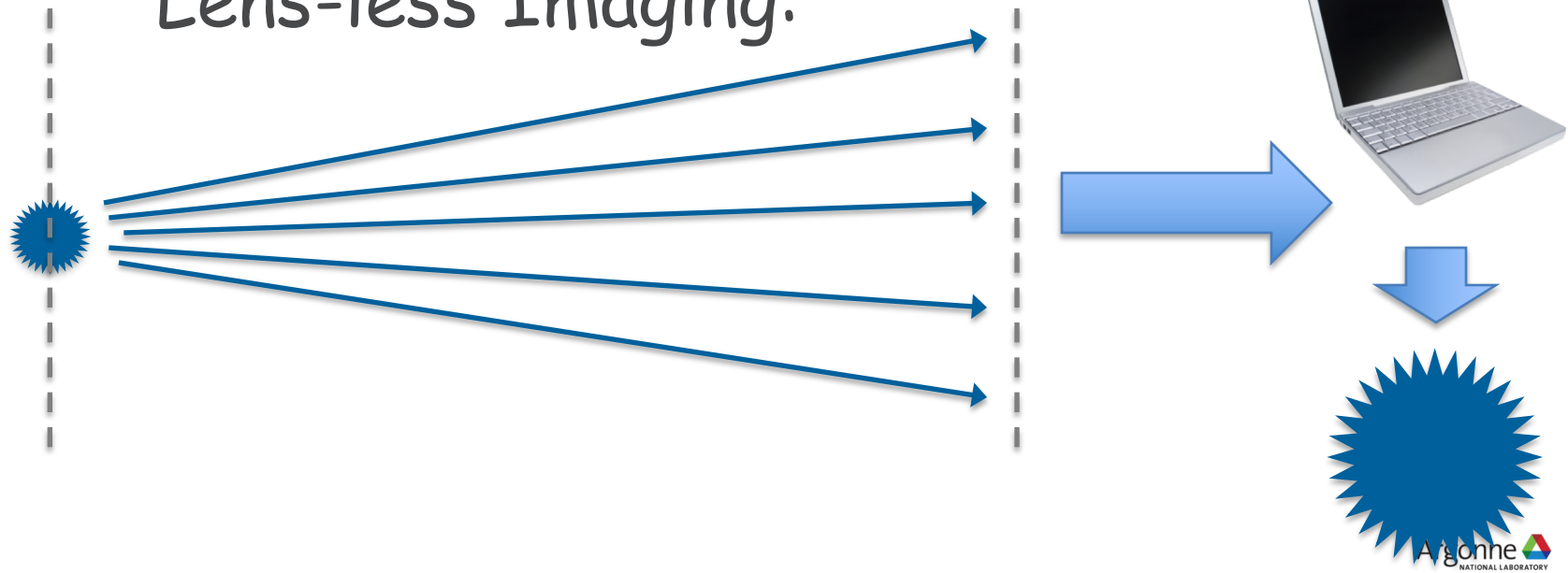
TRADITIONAL MICROSCOPY:



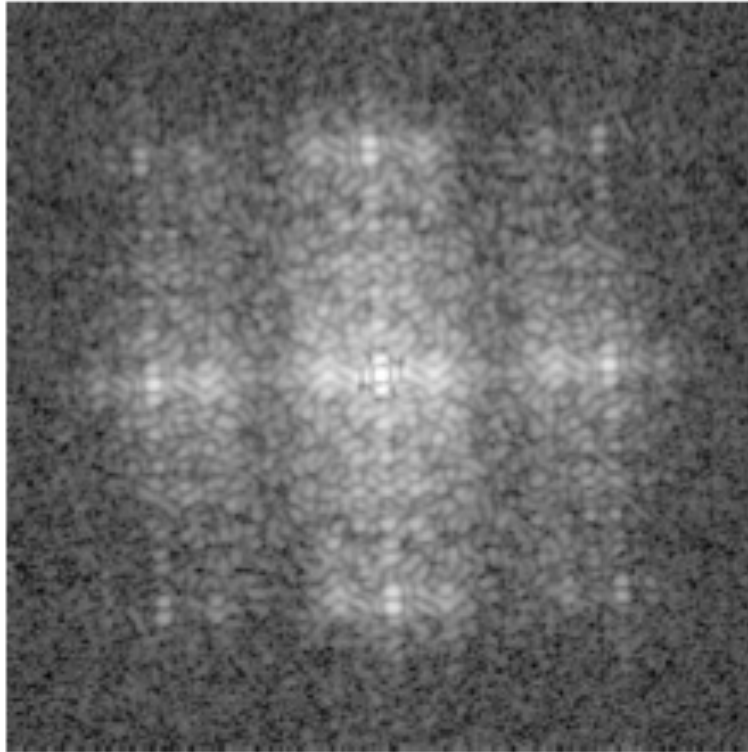
Object Plane

Detector Plane

Lens-less Imaging:



FIRST DEMONSTRATION OF CDI WITH X-RAYS



diffraction pattern

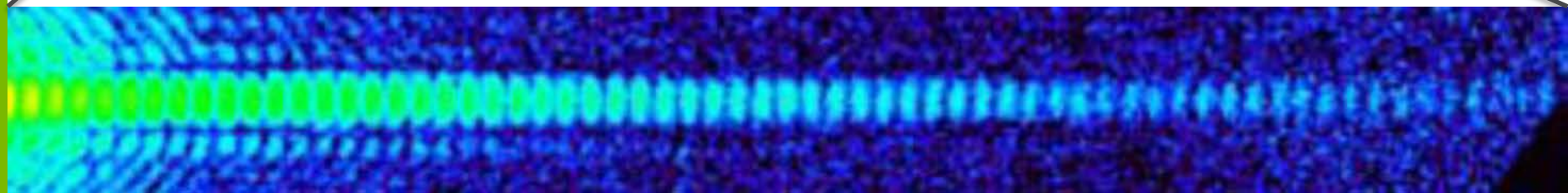
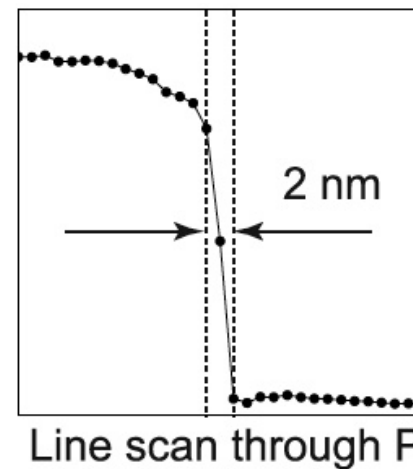
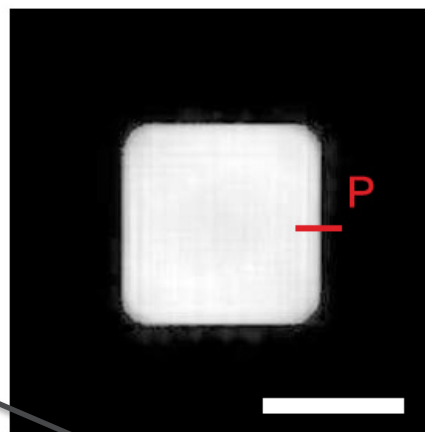
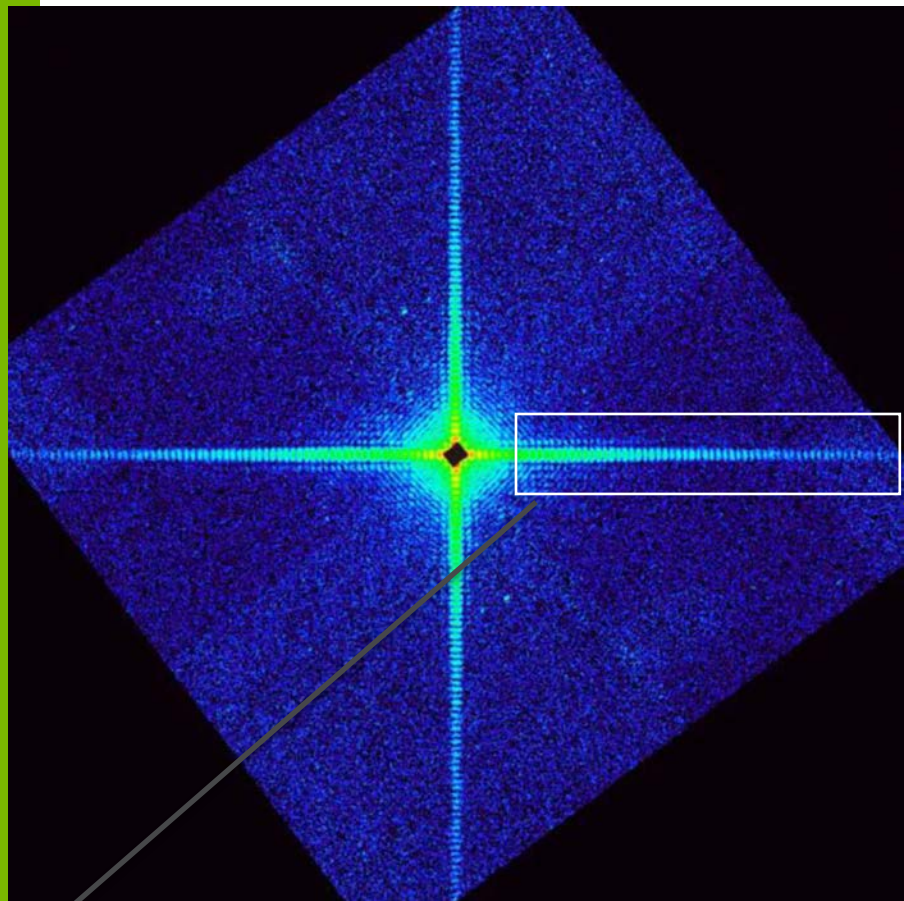


reconstruction

J. Miao, *Nature* 400, 342
(1999)

COHERENT DIFFRACTIVE IMAGING:

Y. Takahashi et al.,
Phys. Rev. B 82, 214102 (2010)



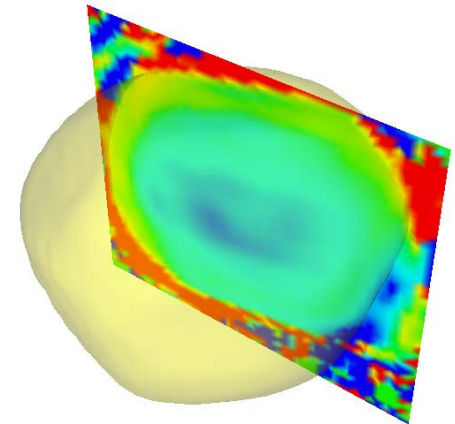
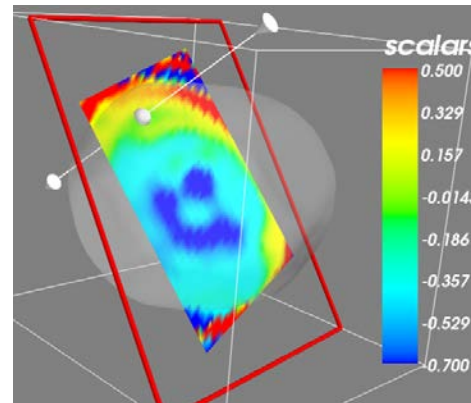
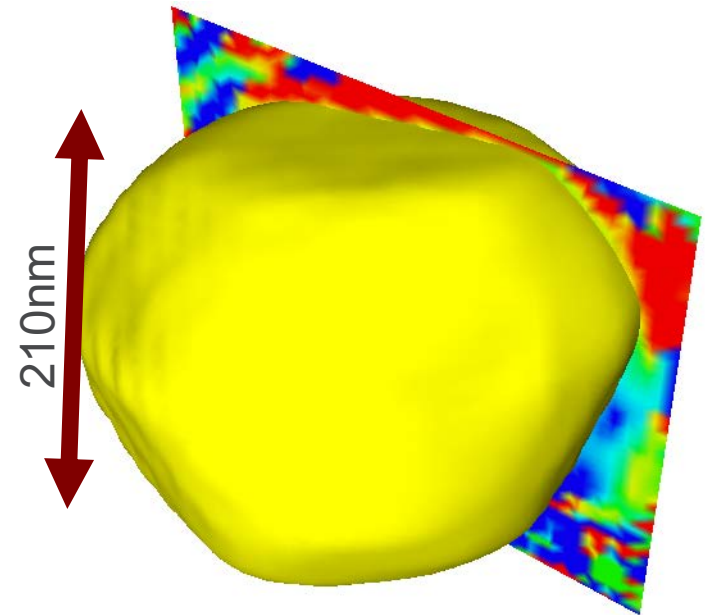
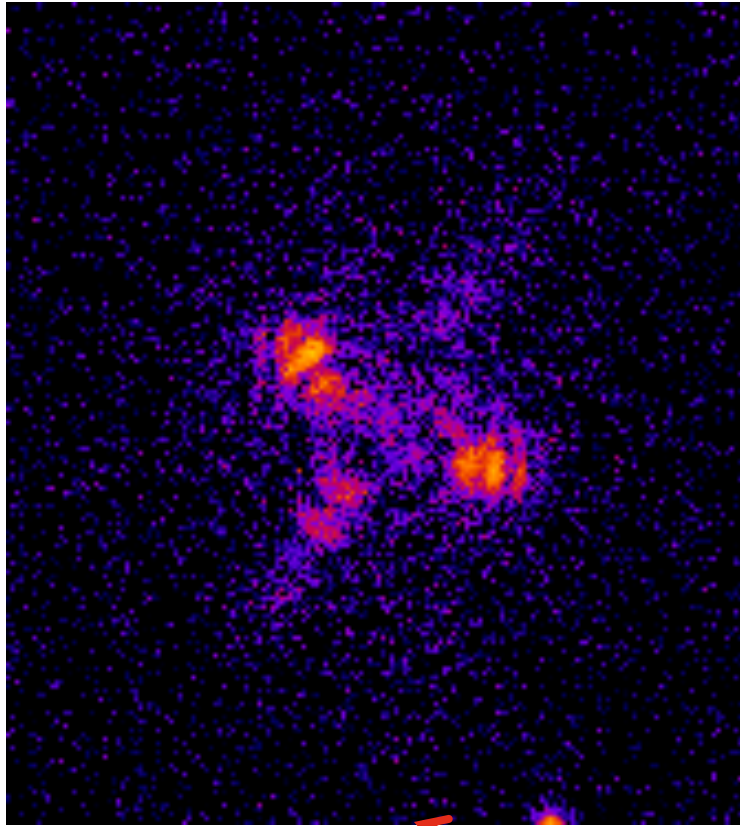
LARGE-FORMAT, SINGLE-PHOTON SENSITIVE X-RAY CCD CAMERAS OPENED THE DOOR TO COHERENT X-RAY IMAGING

Fairchild Peregrine 486 CCD Camera

- 4K x 4K pixel array (61.4 mm square area)
- 15 μm pixels, 100% fill factor
- Back-illuminated for up to 80% QE
- Readout noise $< 5 e^-$ at 50 Kpixels/s
- Dynamic range > 86 dB in MPP
- 6 s readout with four on-chip amplifiers
- Pixel binning for more rapid readout
- Peltier-cooled to -50 C for low dark current



Hi Resolution Imaging (CCD)?

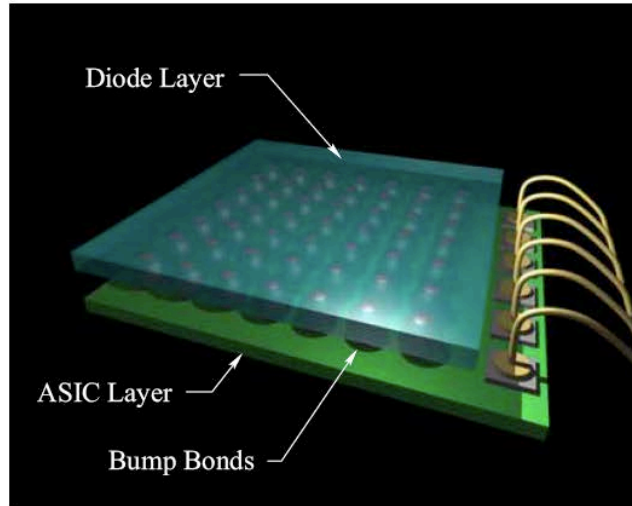


At APS 34-ID-C:
9.25 hours of scanning
38 minutes of x-ray exposure

~7nm data

Rainbow color map (still) considered harmful
<http://ieeexplore.ieee.org/document/4118486/>

PIXEL ARRAY DETECTORS: REVOLUTIONIZING COHERENT IMAGING



D. Schuette, S. Gruner (Cornell)

A Three Layer Hybrid Device

- Diode layer → converts x-rays to photocurrent.
- ASIC layer → custom signal processing electronics.
- A layer of metallic interconnects (bump bonds) between corresponding pixels on the diode and ASIC layers.

Pilatus 6M detector
(PSI/Dectris)



**PADs can be read out in ~1 ms
(CCDs take seconds!)**

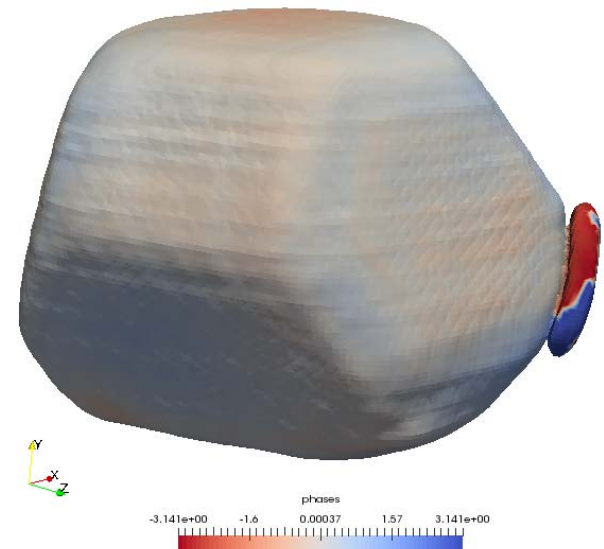
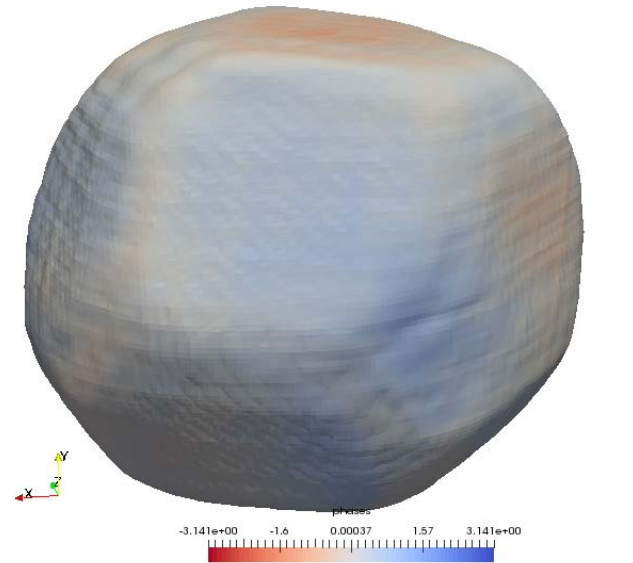
**PAD pixels are 55-150 μm .
(CCDs are 12-24 μm)**

Hi Resolution Imaging (PAD)?

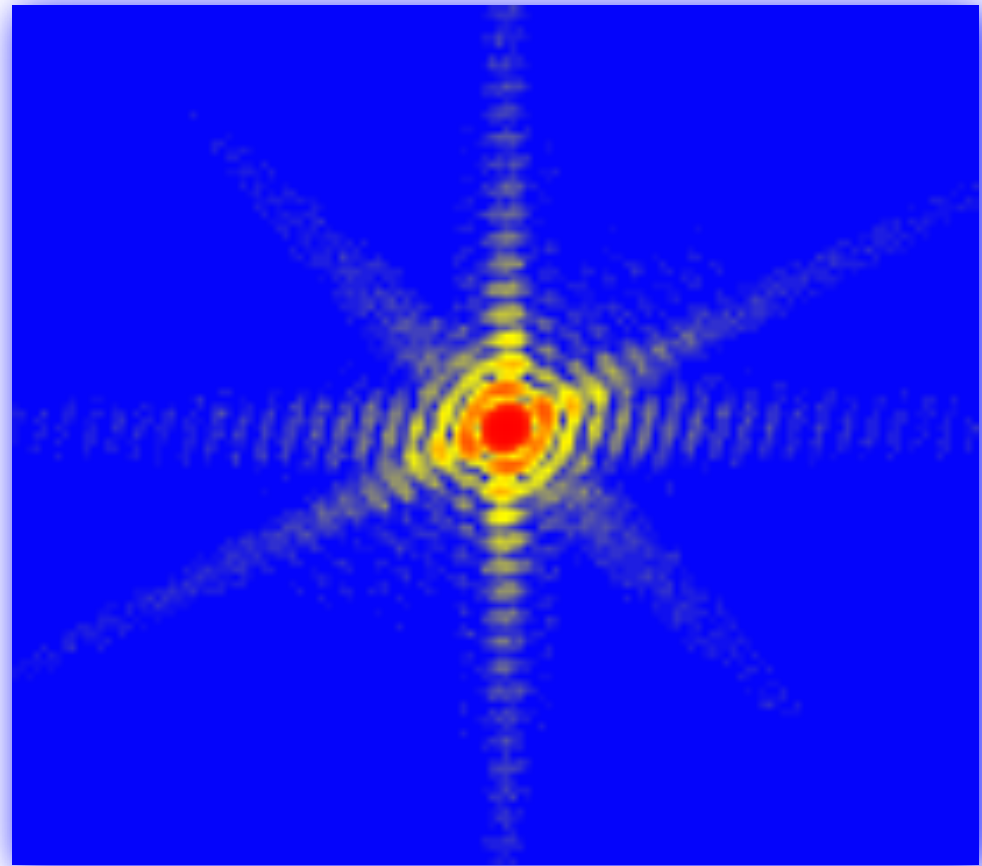
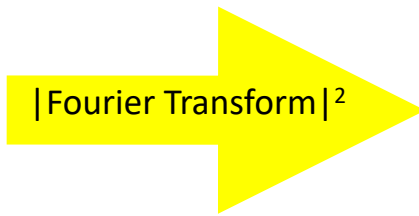
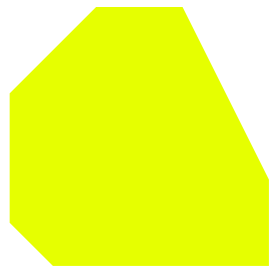


Quad Timepix GaAs sensor

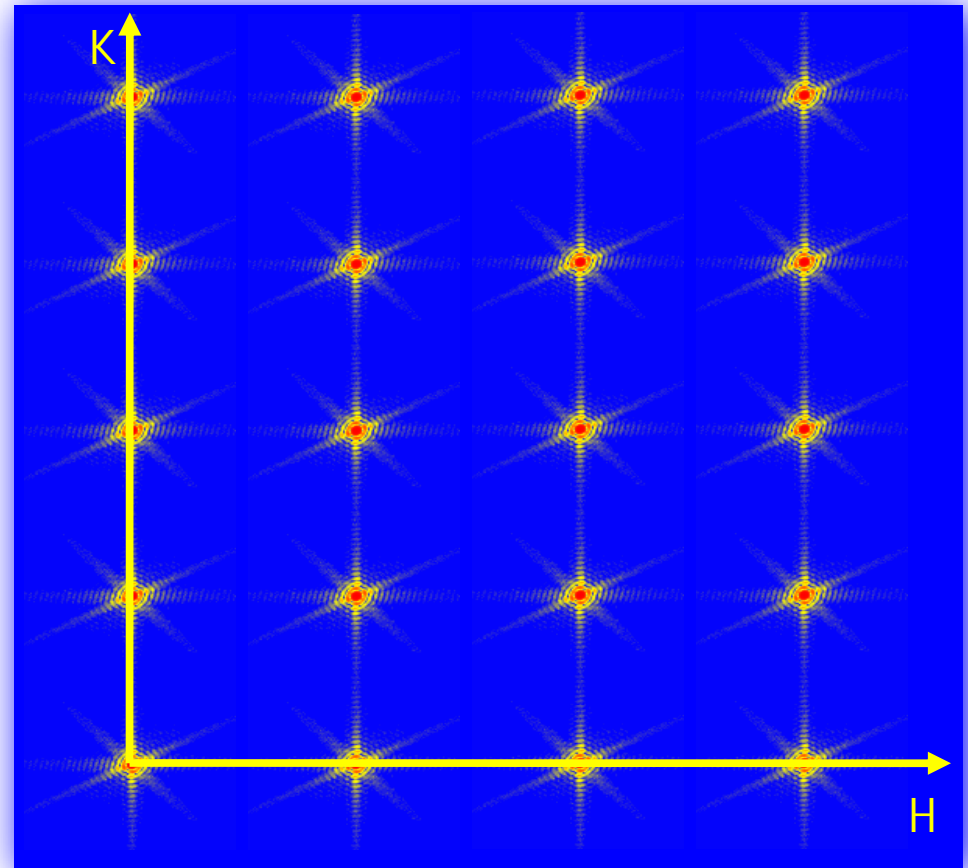
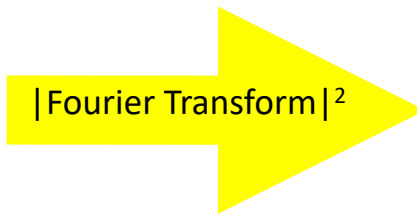
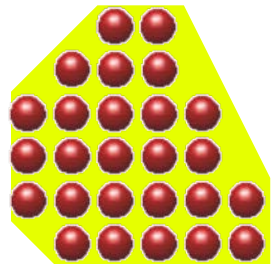
700nm gold crystal
3 degree rocking curve
25 minute measurement
15 sec movie (1X APS-U measurement)



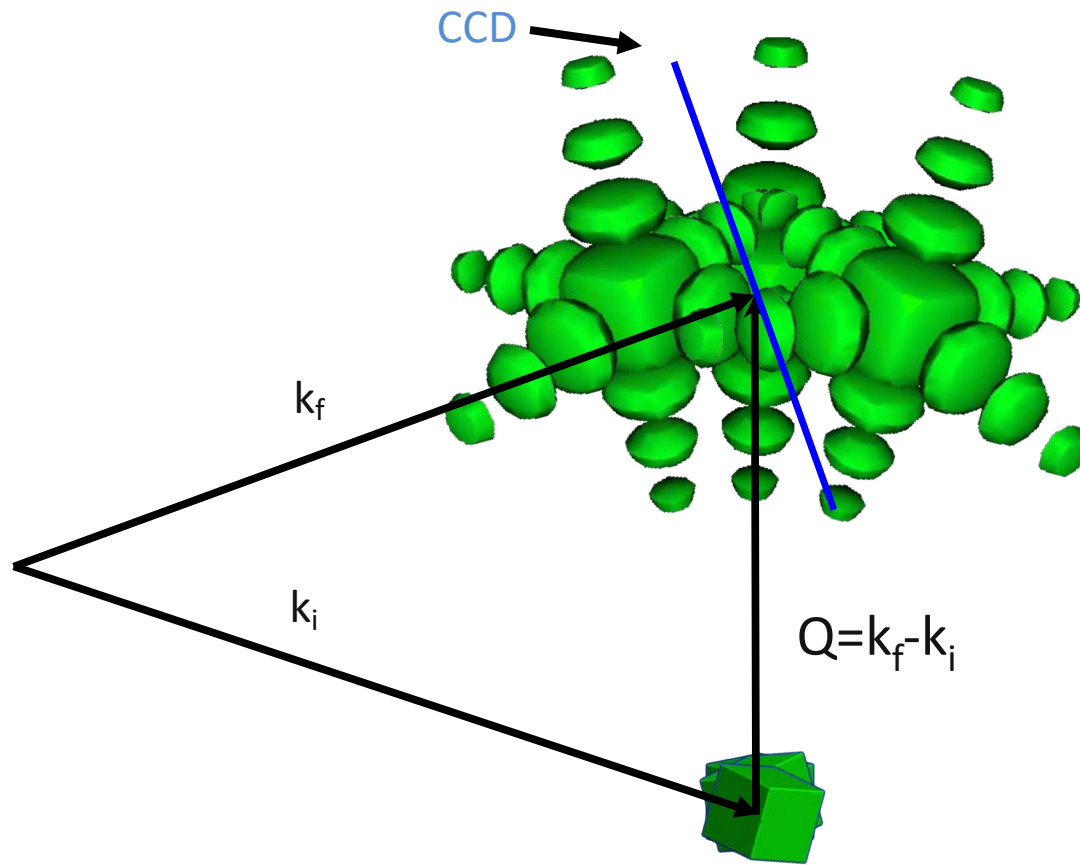
Coherent Diffraction from Crystals



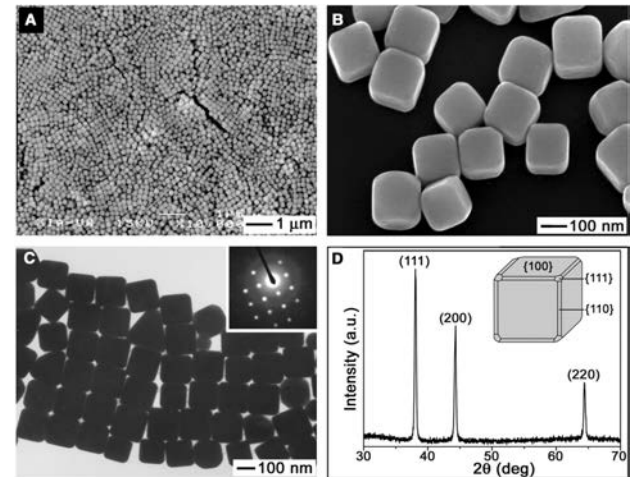
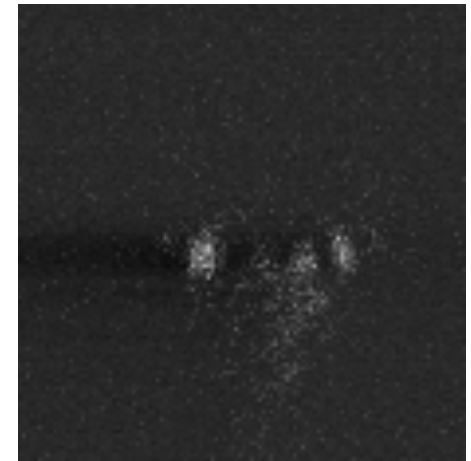
Coherent Diffraction from Crystals



Measuring 3D CXD

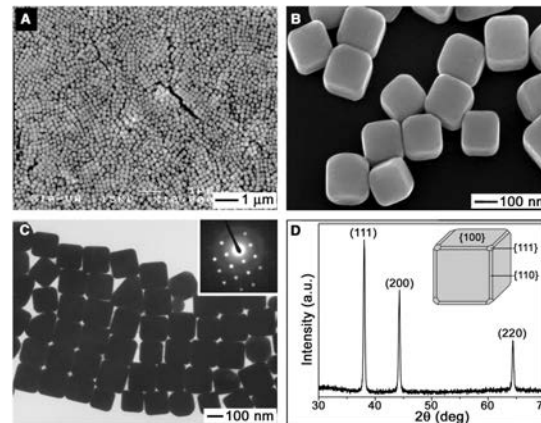
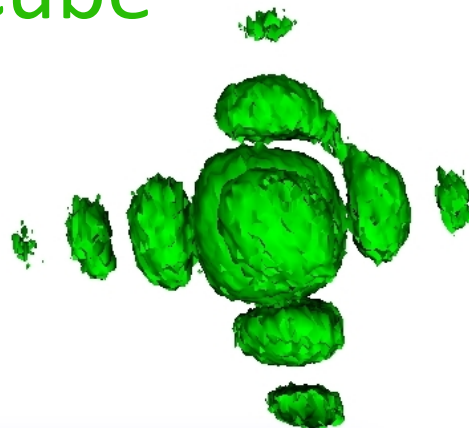
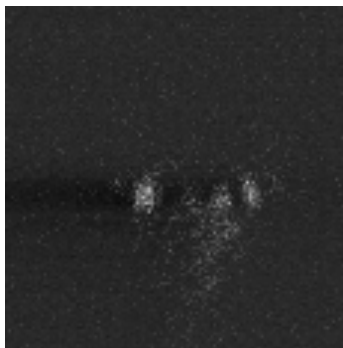


Silver Nano Cube (111)

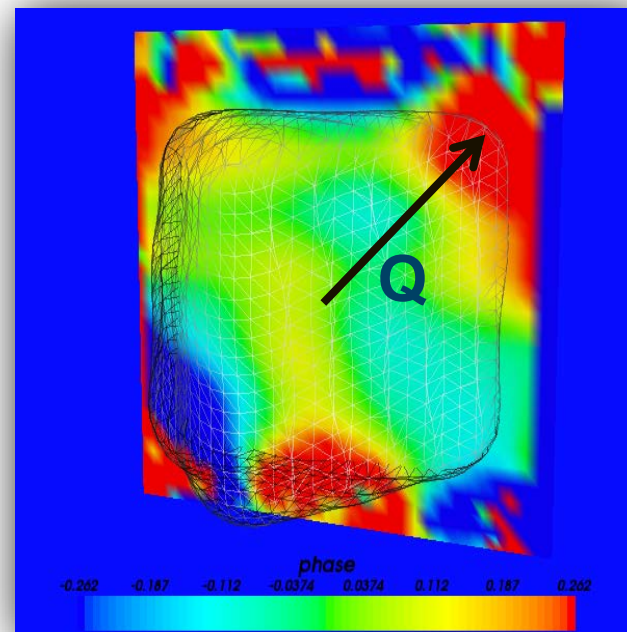
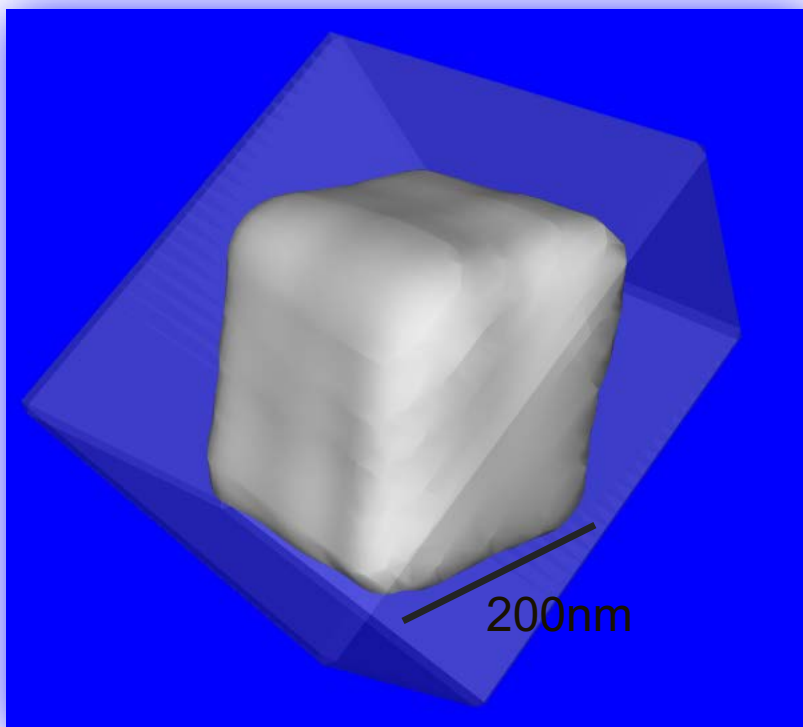


Yugang Sun and Younan Xia,
Science 298 2177 (2003)

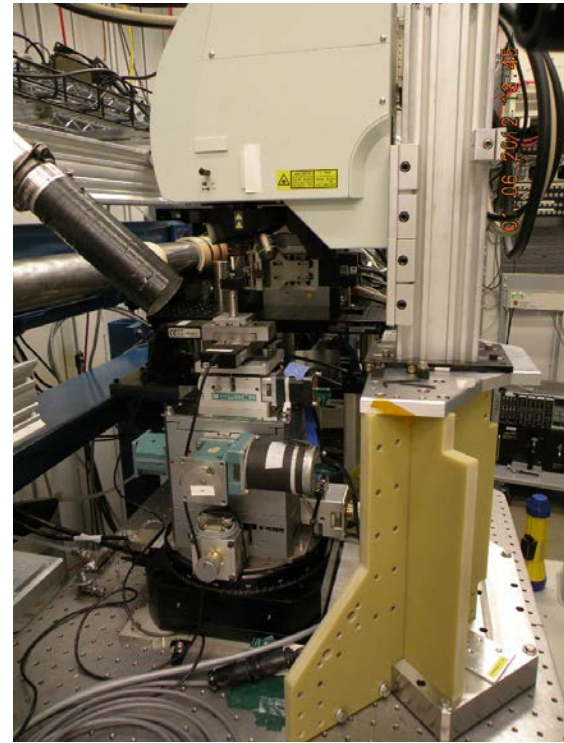
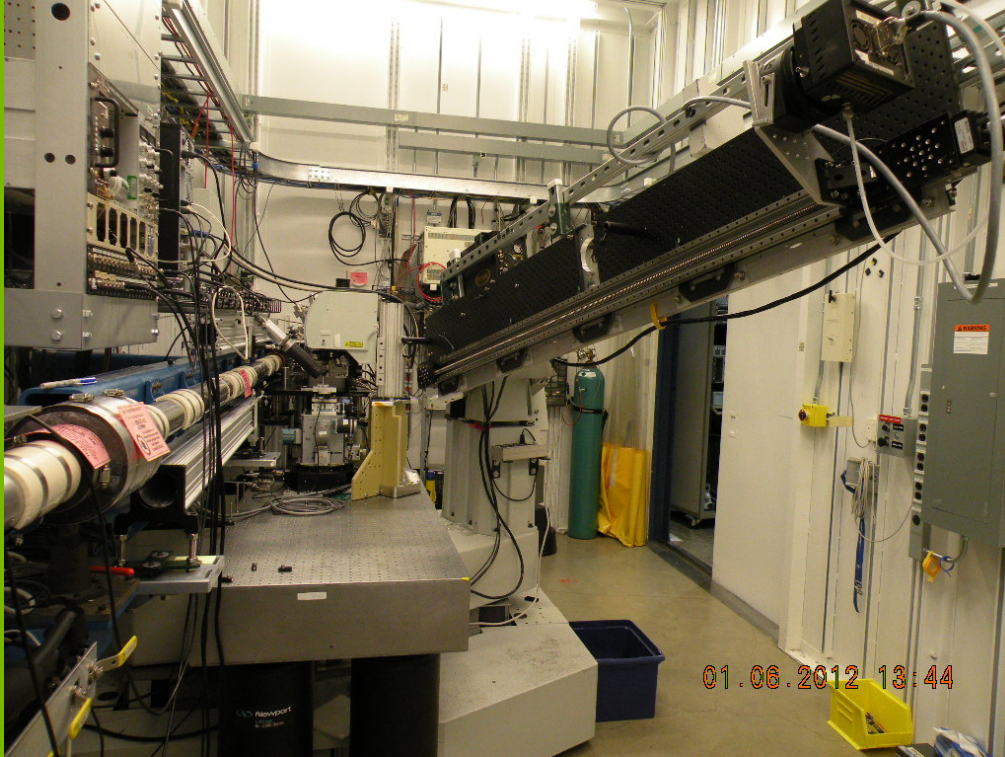
3D Ag Nano Cube



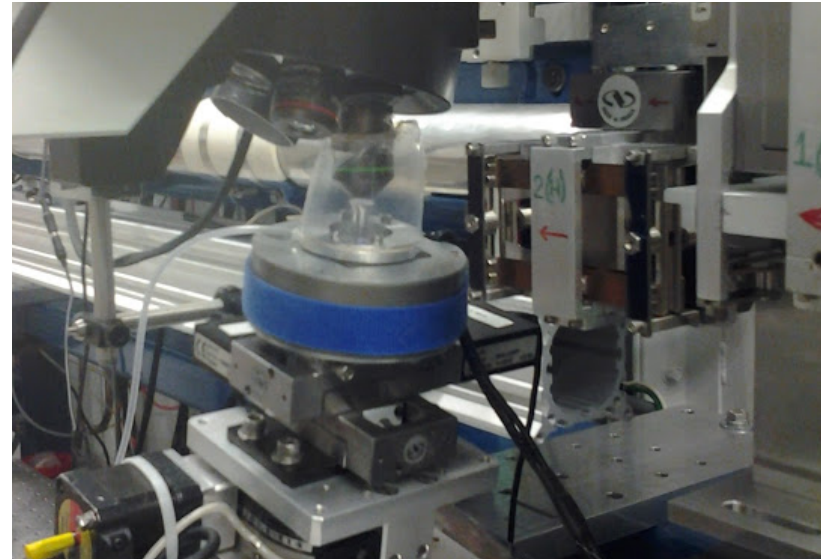
Yugang Sun and Younan Xia,
Science 298 2177 (2003)



APS 34-ID-C



Precision scanning stage



ORIGINAL PHASE RETRIEVAL PAPER (BY D. SAYRE):

Acta Cryst. (1952). 5, 843

NOT $\rho=\rho^2$ *Acta Cryst.* (1952). 5, 60

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 .

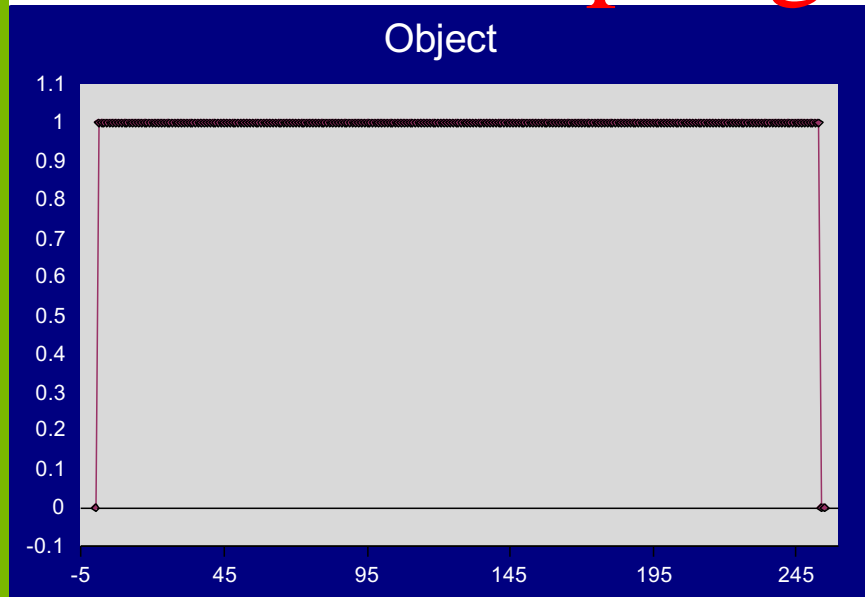
2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where $|F|^2$ was observed at non-integral h , it would suffice to have only the values at half-integral h .

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.

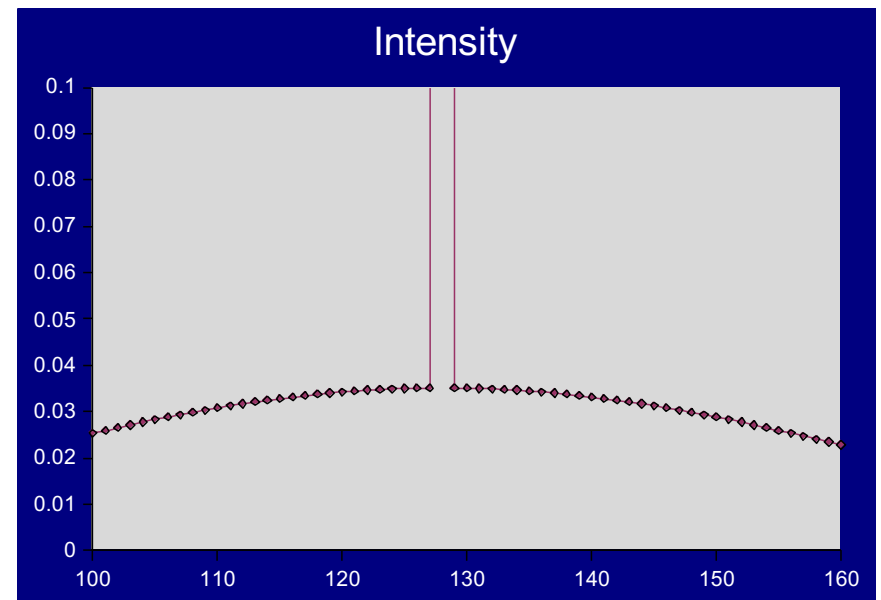
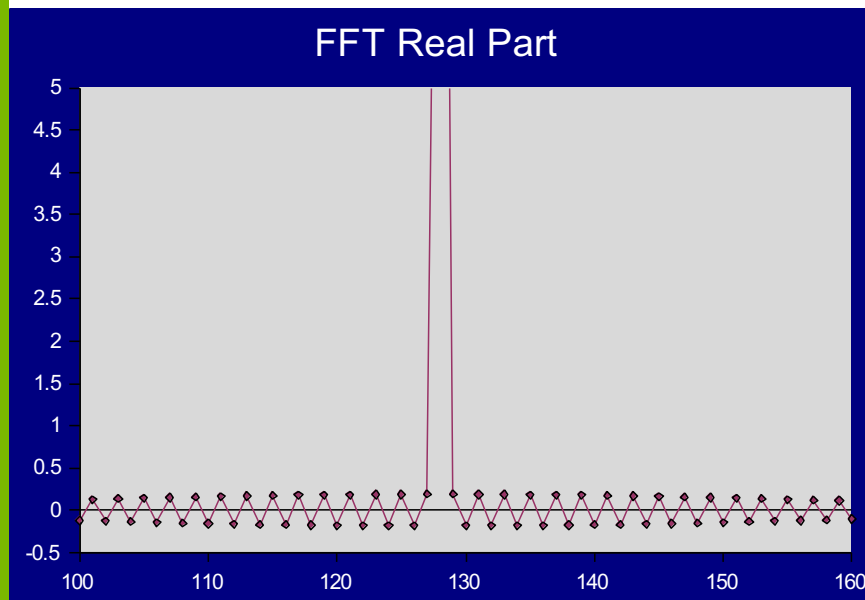
Critical sampling



N unknown densities
N/2 equations

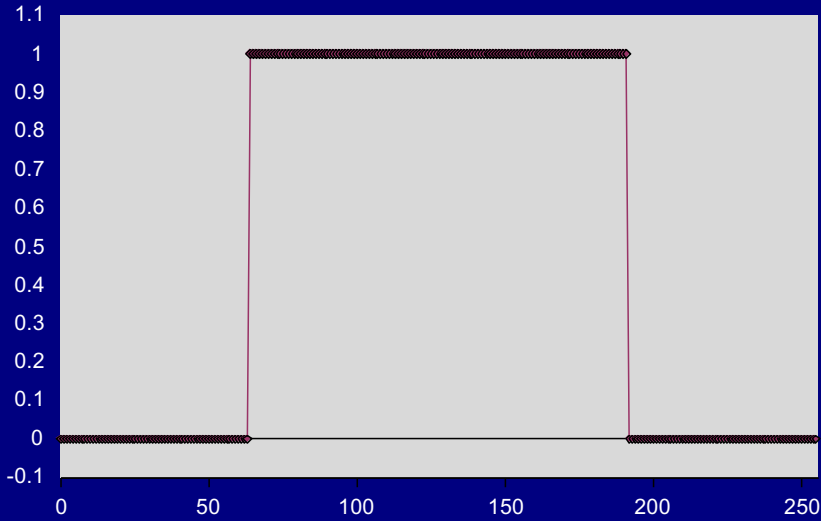
$$|A_q| = \left| \sum_0^N \rho_n e^{-iqr_n} \right|$$

Nyquist Freq = 1/(2*bandwidth)
Intensity is under sampled



Oversampling 2x

Object



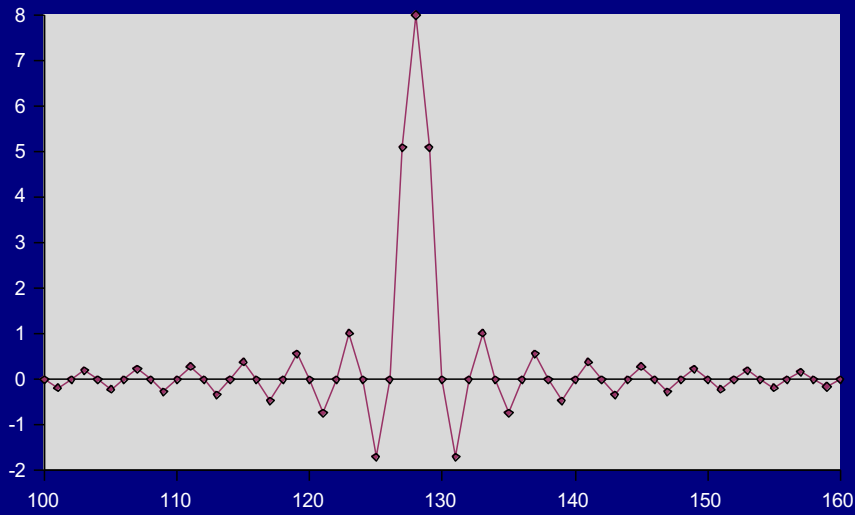
$N/2$ equations

$N/2$ Unknown densities

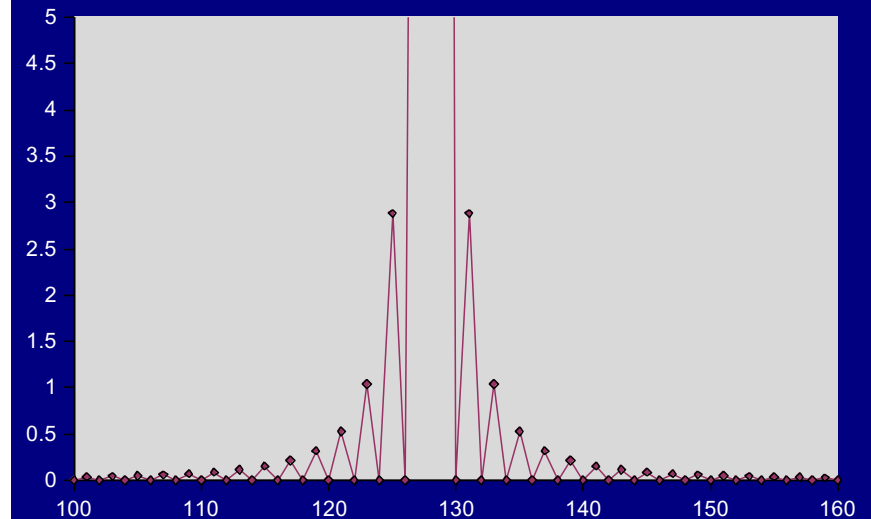
$N/2$ Known Densities(zero)

$$|A_q| = \left| \sum_0^N \rho_n e^{-iqr_n} \right|$$

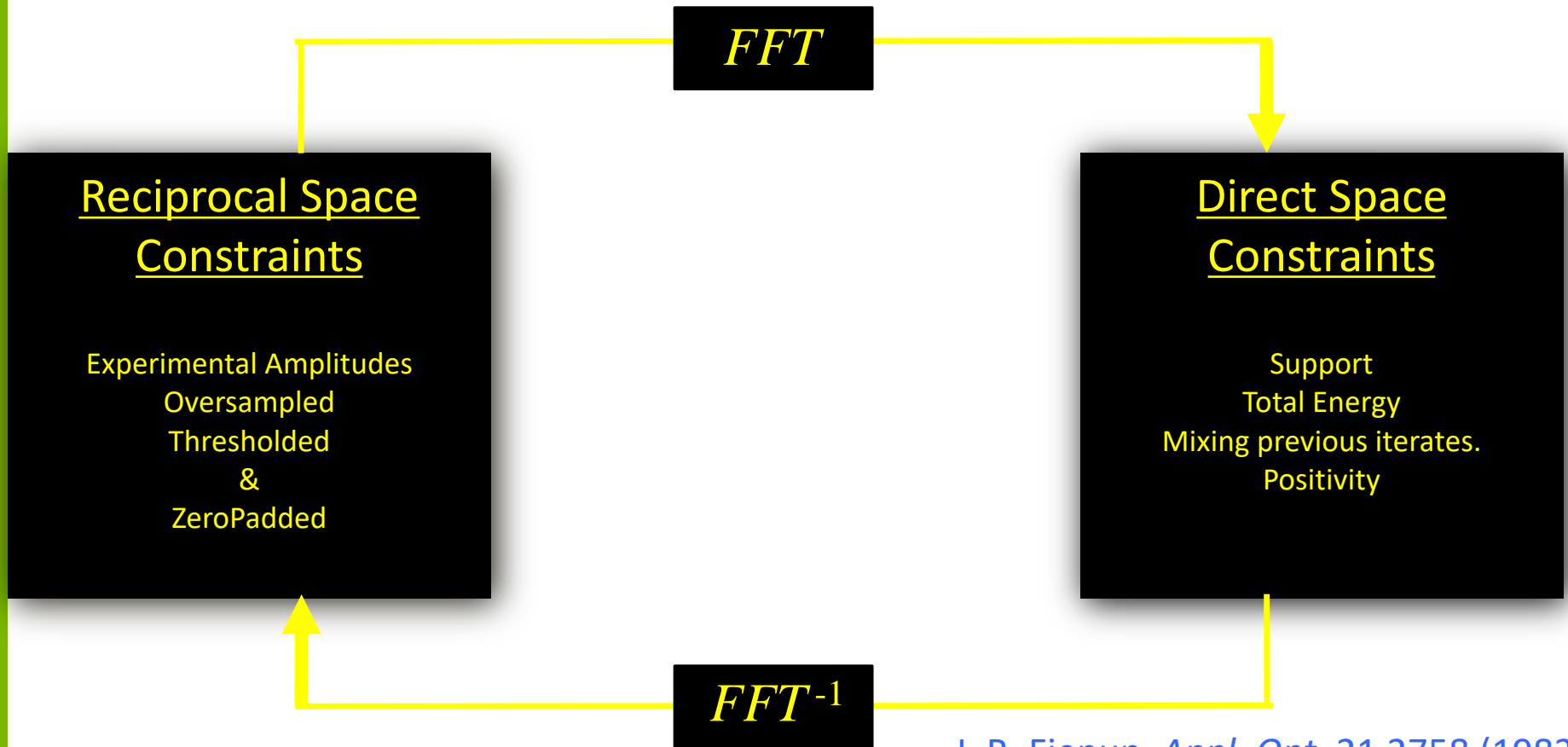
Oversampled FFT



Intensity



Input Output Algorithms

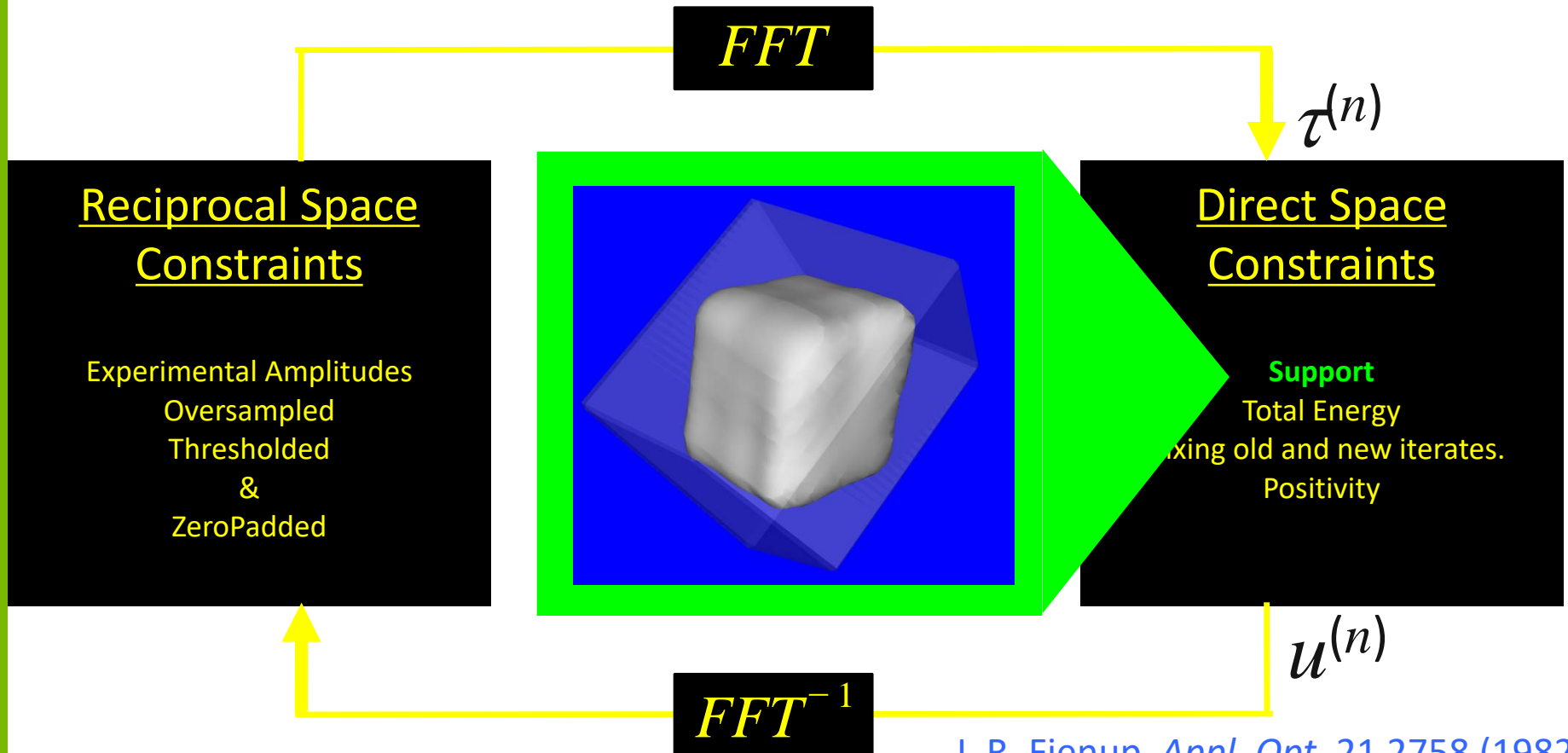


J. R. Fienup *Appl. Opt.* 21 2758 (1982)
Collins *Nature* 298, 49 (1982)

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

Fienup, James R. 2013. "Phase Retrieval Algorithms: a Personal Tour." *Applied Optics* 52 (1): 45–56.

Input Output Algorithms

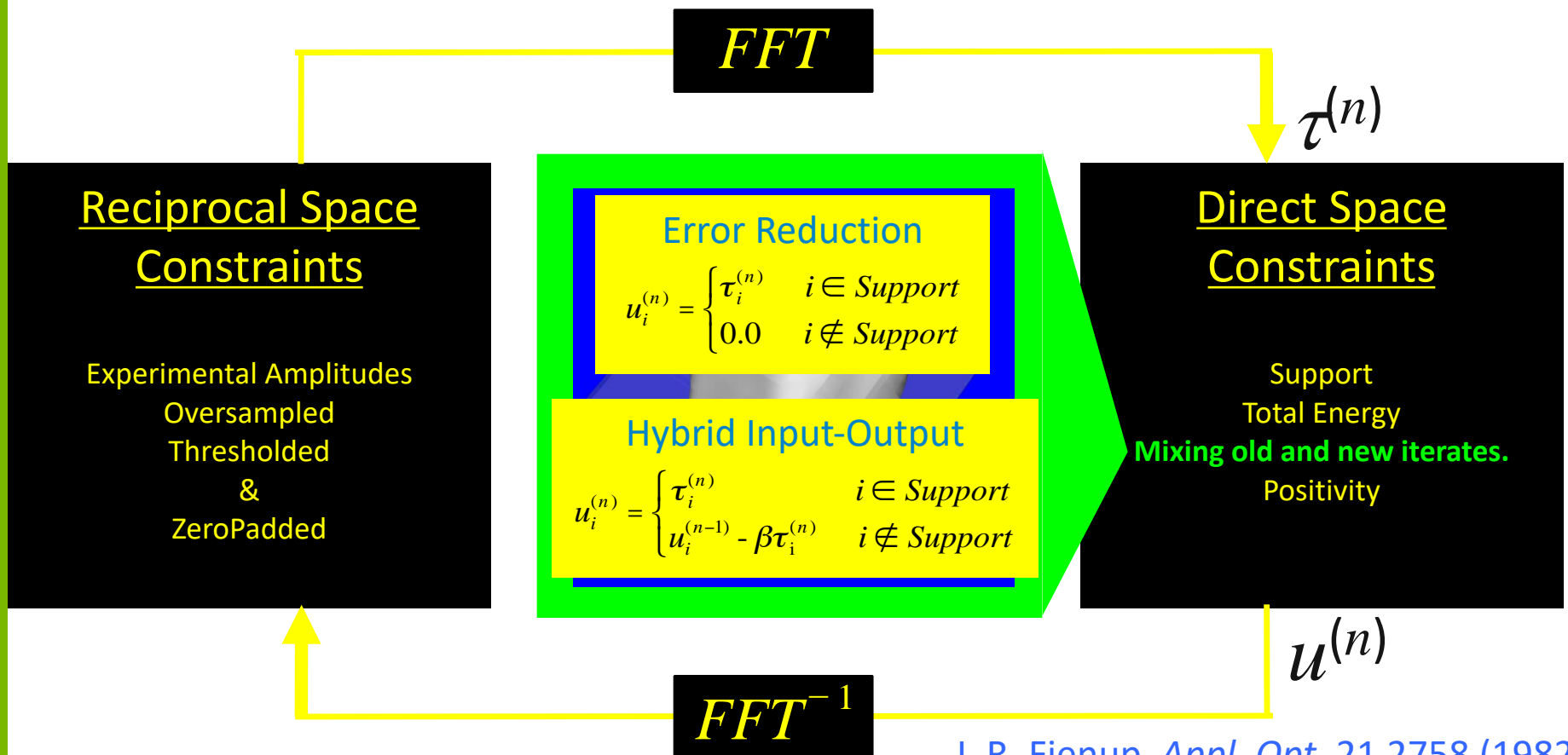


J. R. Fienup *Appl. Opt.* 21 2758 (1982)
Collins *Nature* 298, 49 (1982)

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

Fienup, James R. 2013. "Phase Retrieval Algorithms: a Personal Tour." *Applied Optics* 52 (1): 45-56.

Input Output Algorithms

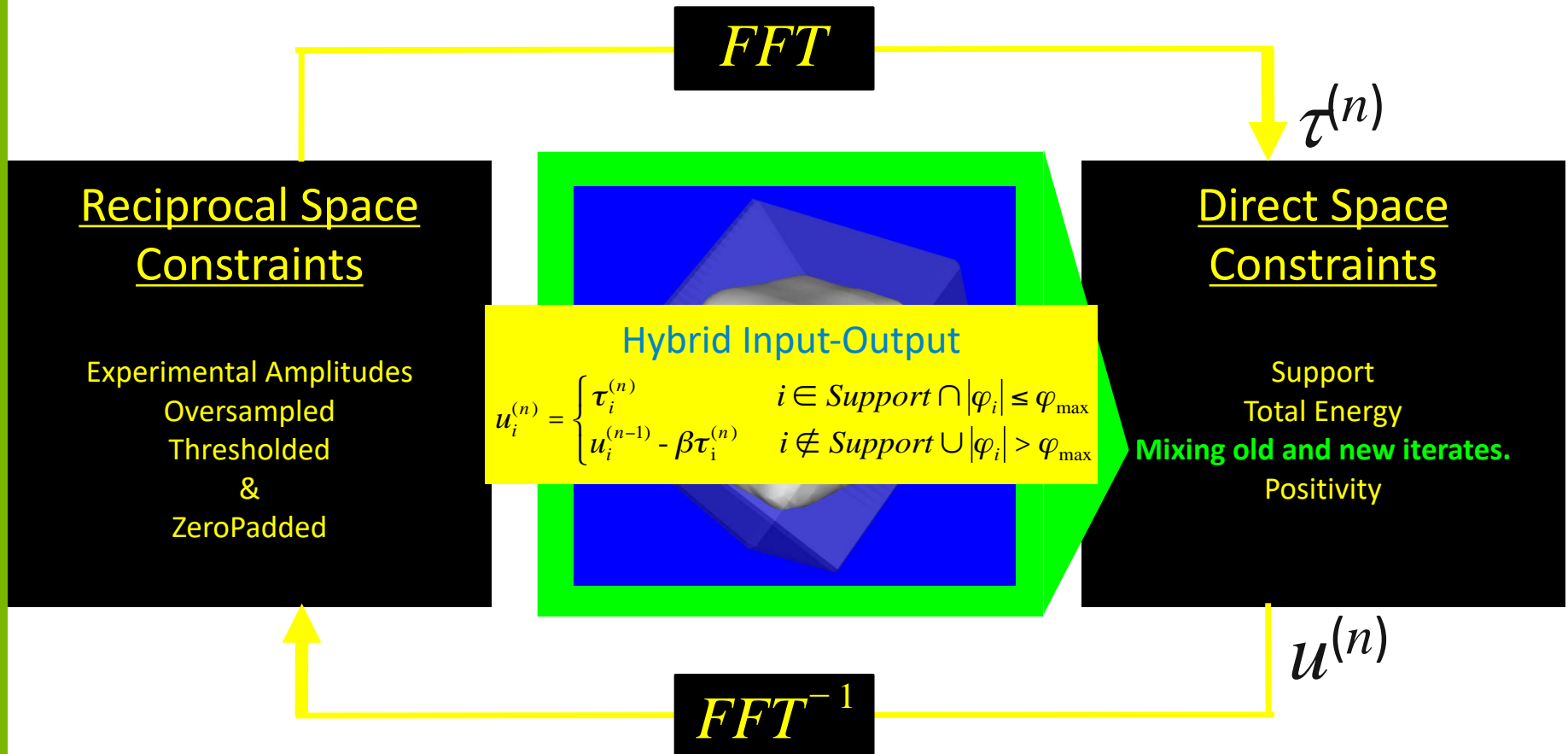


J. R. Fienup *Appl. Opt.* 21 2758 (1982)
Collins *Nature* 298, 49 (1982)

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

Fienup, James R. 2013. "Phase Retrieval Algorithms: a Personal Tour." *Applied Optics* 52 (1): 45-56.

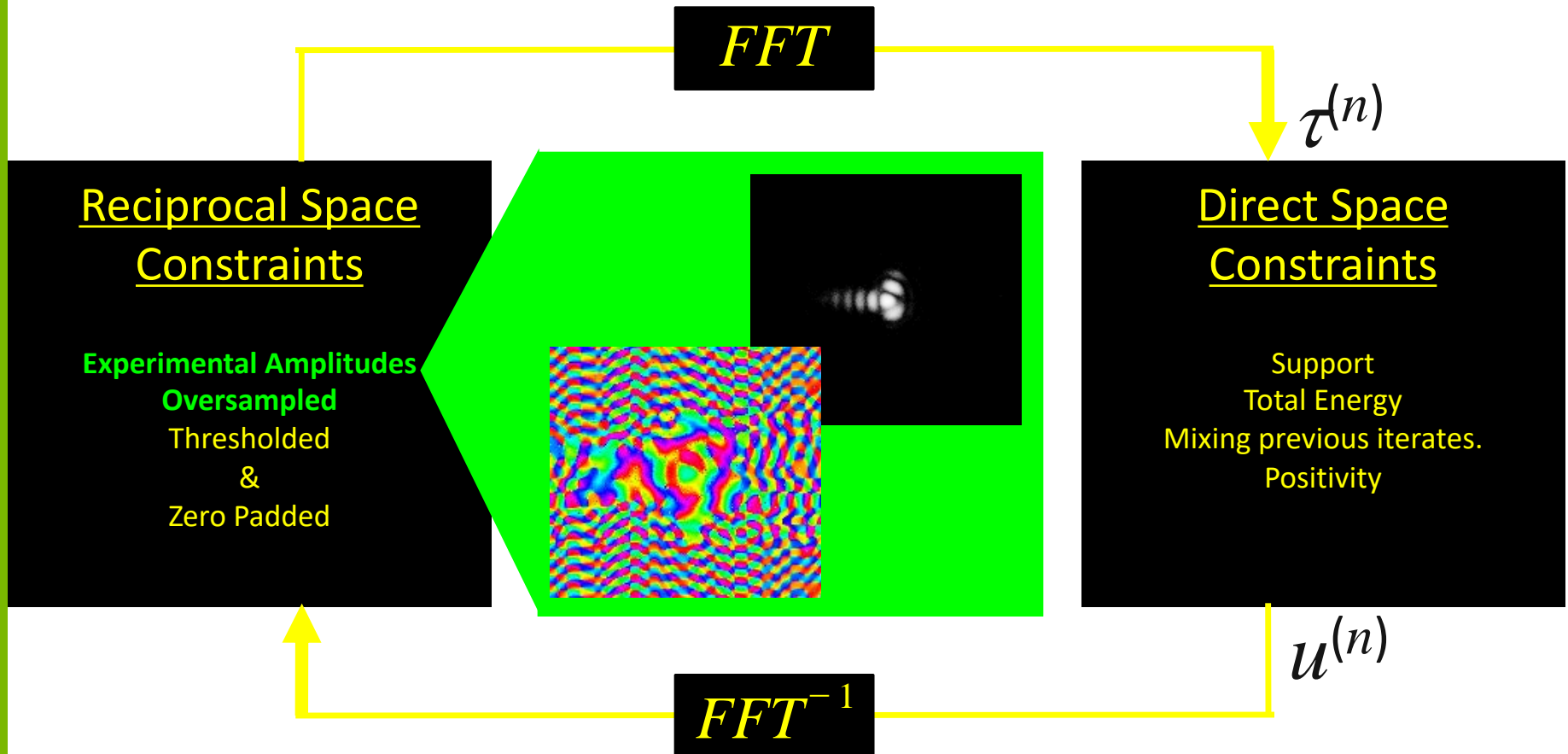
Input Output Algorithms



Harder, R., Liang, M., Sun, Y., Xia, Y., & Robinson, I. K. (2010). Imaging of complex density in silver nanocubes by coherent x-ray diffraction. *New Journal of Physics*, 12(3), 035019.

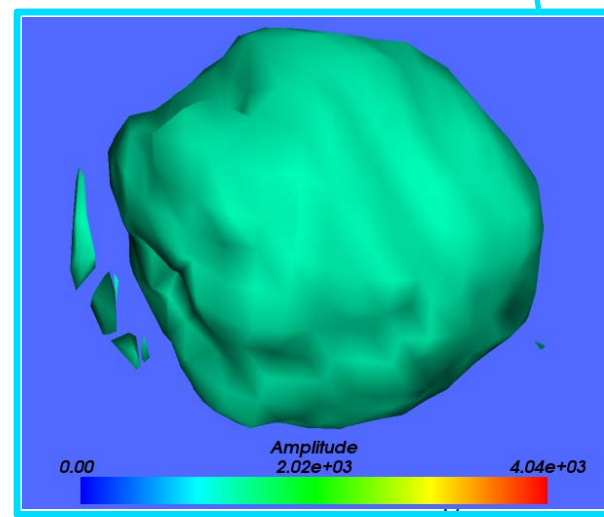
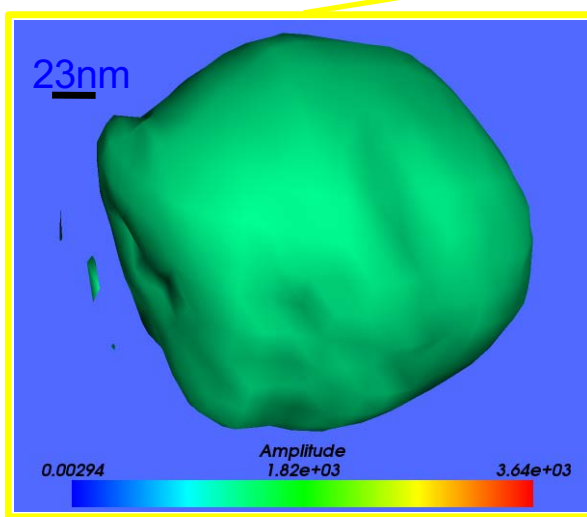
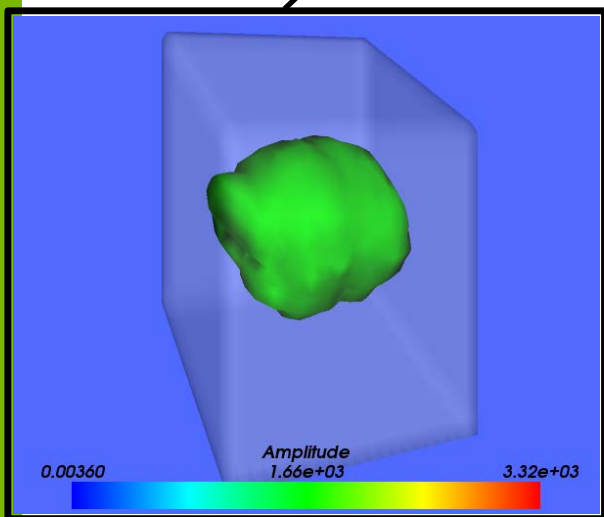
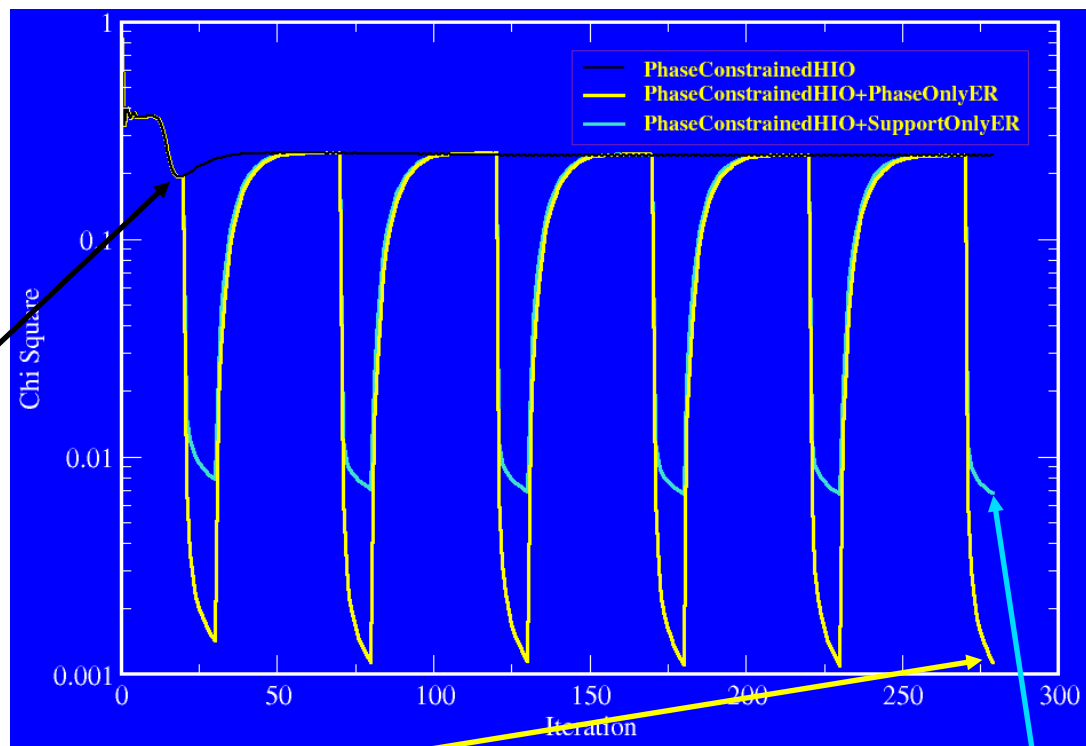
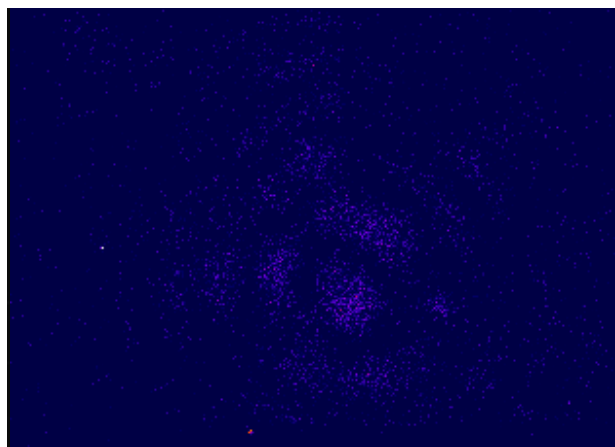
Huang, X., Harder, R., Xiong, G., Shi, X., & Robinson, I. (2011). Propagation uniqueness in three-dimensional coherent diffractive imaging. *Physical Review B*, 83(22), 224109.

Input Output Algorithms

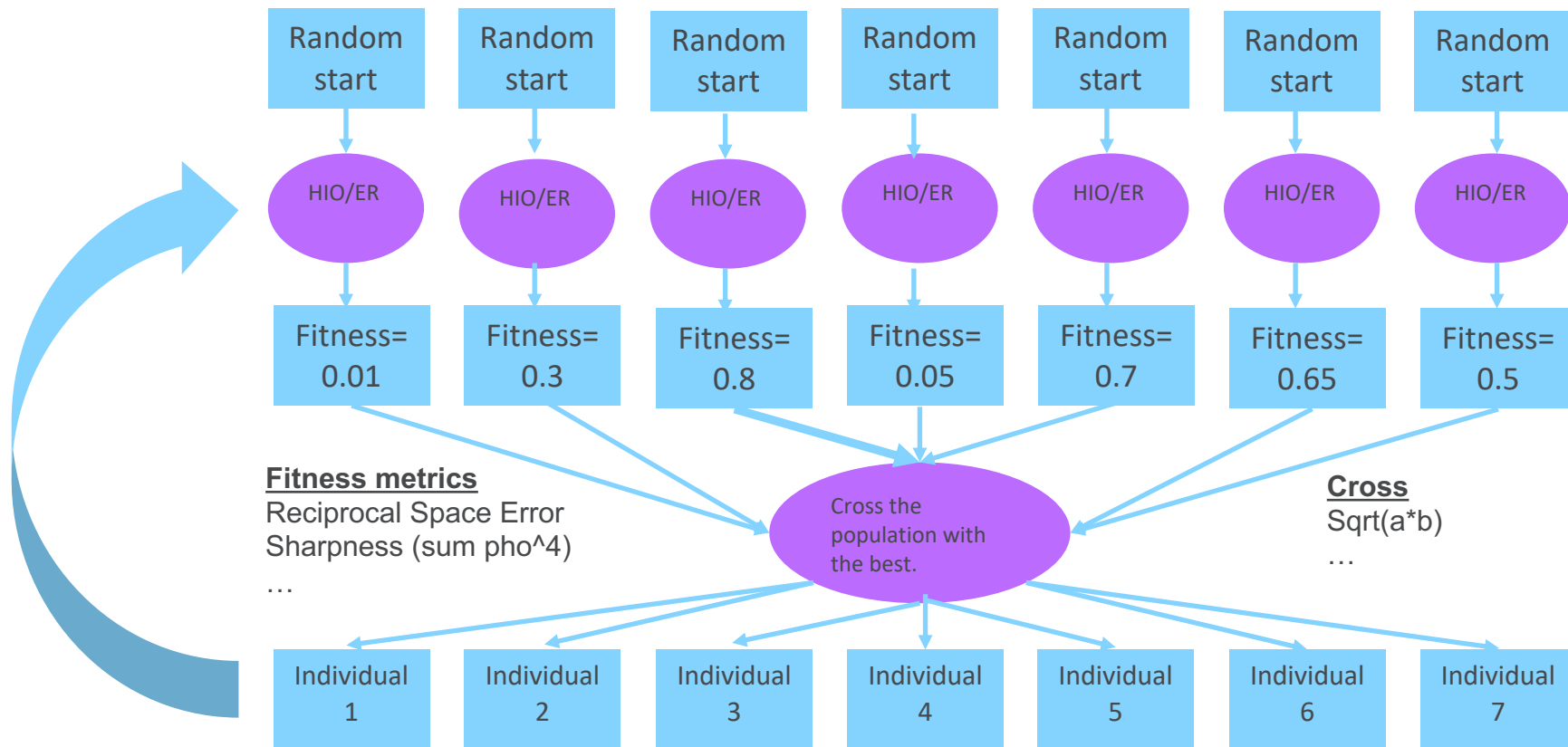


- Harder, R., Liang, M., Sun, Y., Xia, Y., & Robinson, I. K. (2010). Imaging of complex density in silver nanocubes by coherent x-ray diffraction. *New Journal of Physics*, 12(3), 035019.
- Huang, X., Harder, R., Xiong, G., Shi, X., & Robinson, I. (2011). Propagation uniqueness in three-dimensional coherent diffractive imaging. *Physical Review B*, 83(22), 224109.

Monitor Reciprocal Space Error



GENETIC/GUIDED ALGORITHM



Clark, J. N., Ihli, J., Schenk, A. S., Kim, Y.-Y., Kulak, A. N., Campbell, J. M., et al. (2015). Three-dimensional imaging of dislocation propagation during crystal growth and dissolution. *Nature Materials*, 14(8), 780–784. <http://doi.org/10.1038/nmat4320>

Clark, J. N., Huang, X., Harder, R., & Robinson, I. K. (2012). High-resolution three-dimensional partially coherent diffraction imaging. *Nature Communications*, 3, 993–. <http://doi.org/10.1038/ncomms1994>

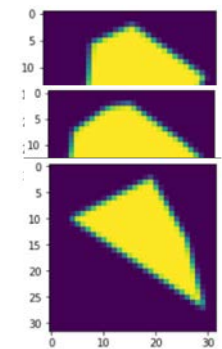
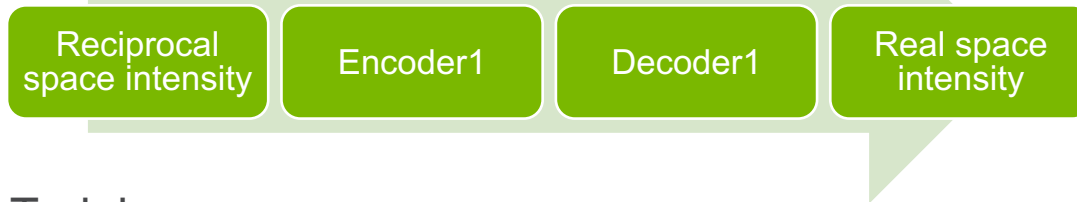
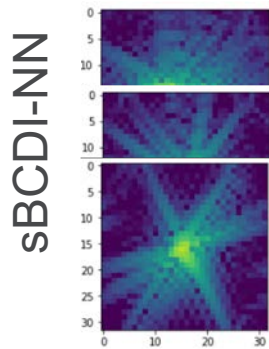
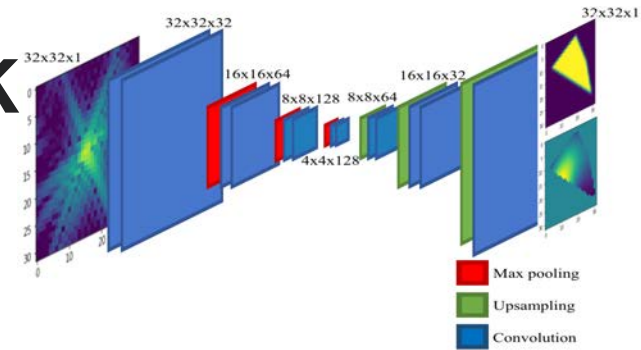


A.I. CDI

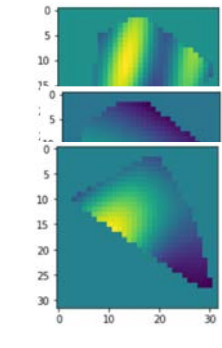
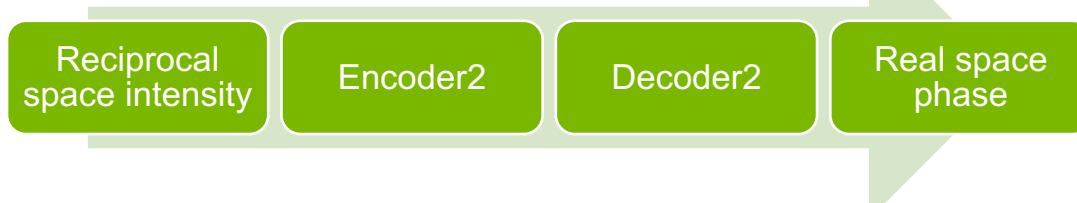
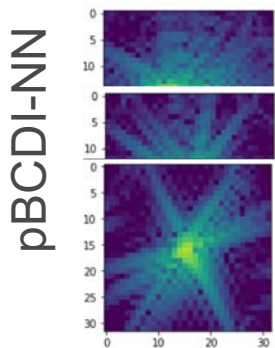
Atomistically Informed Coherent Diffraction Imaging

- ROSS J. HARDER (XSD)
- MATHEW J. CHERUKARA (XSD)
- YOUSSEF NASHED (MCS)
- TOM PETERKA (MCS)
- PRASANNA BALAPRAKASH (MCS)
- S. SANKARANARAYANAN (CNM)
- BADRI NARAYANAN (MSD)

TRAINING THE NEURAL NETWORK

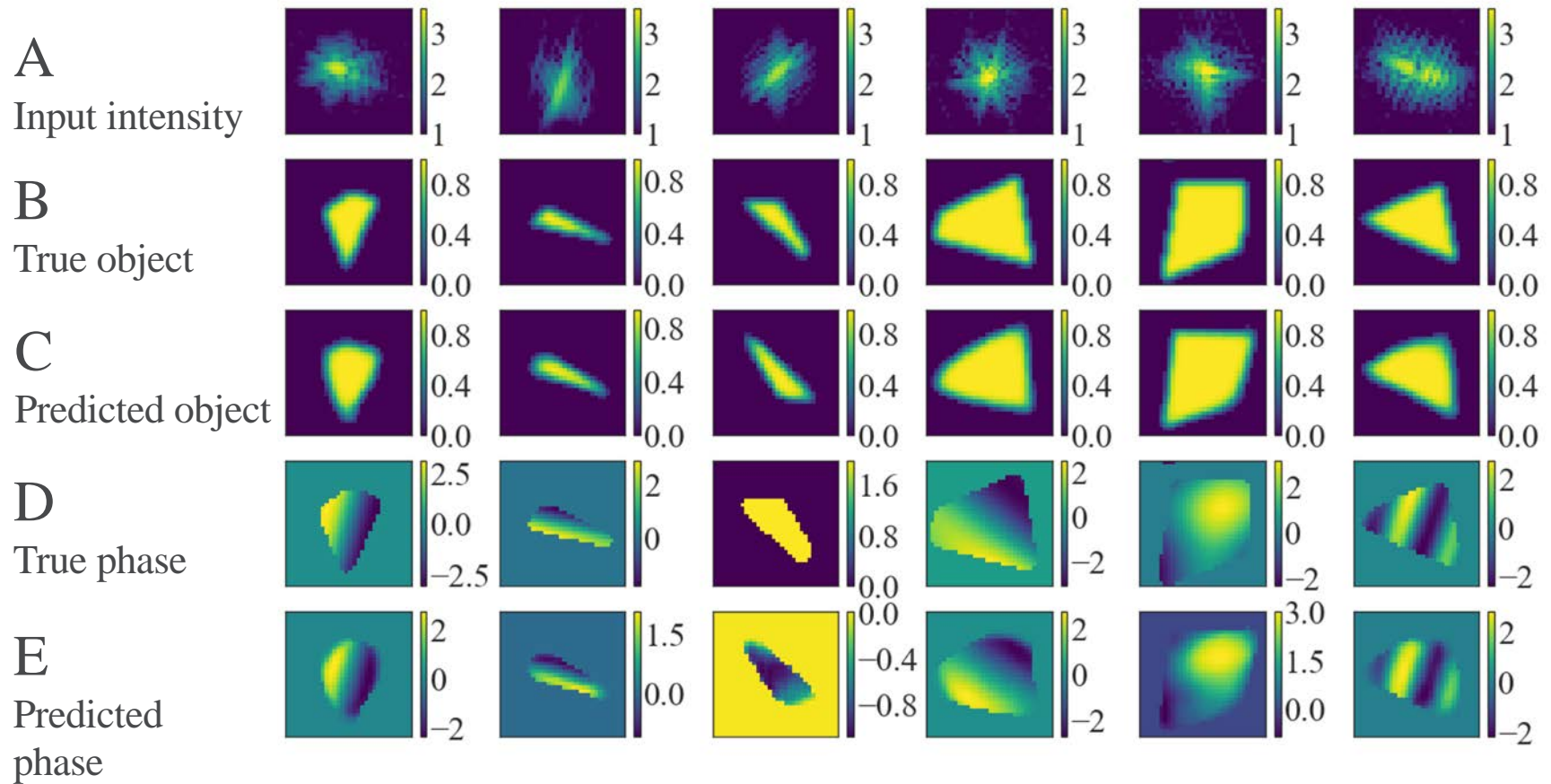


Training:
 180,000 examples generated
 20,000 held back for validation
 1,000 used for testing

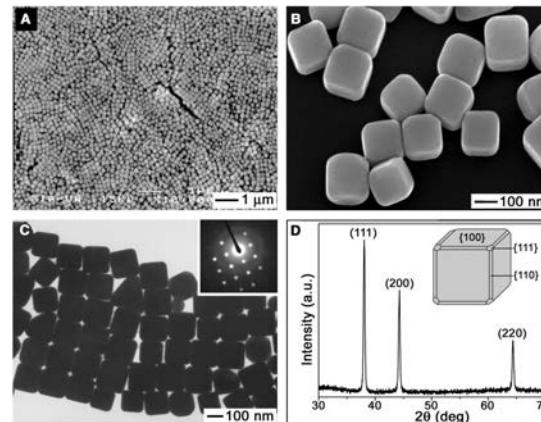
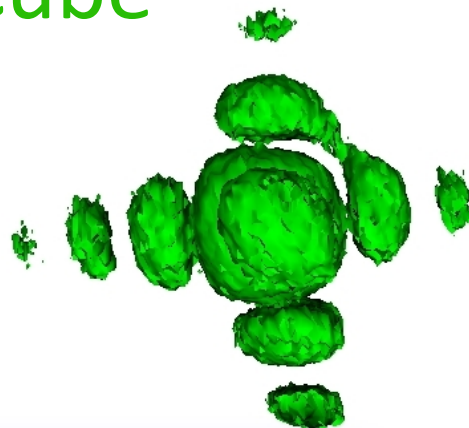
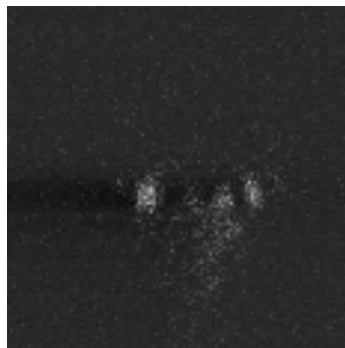


Cherukara, M. J., Nashed, Y. S. G., & Harder, R. J. (2018). *Scientific Reports*, 8(1), 16520. <http://doi.org/10.1038/s41598-018-34525-1>

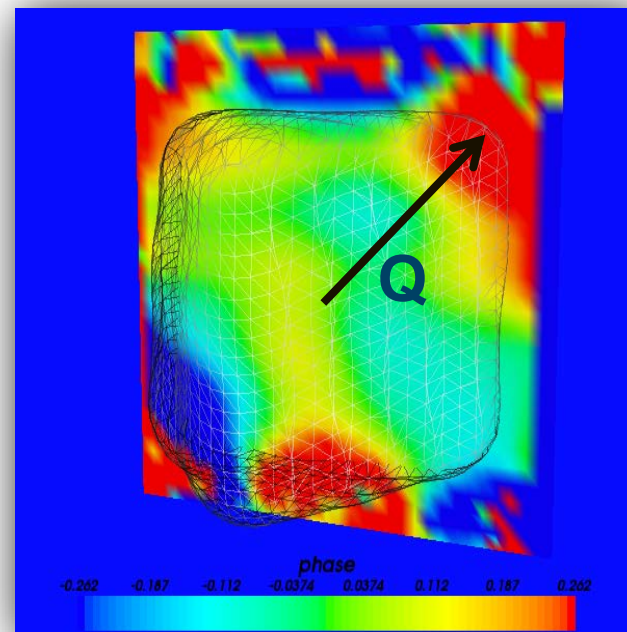
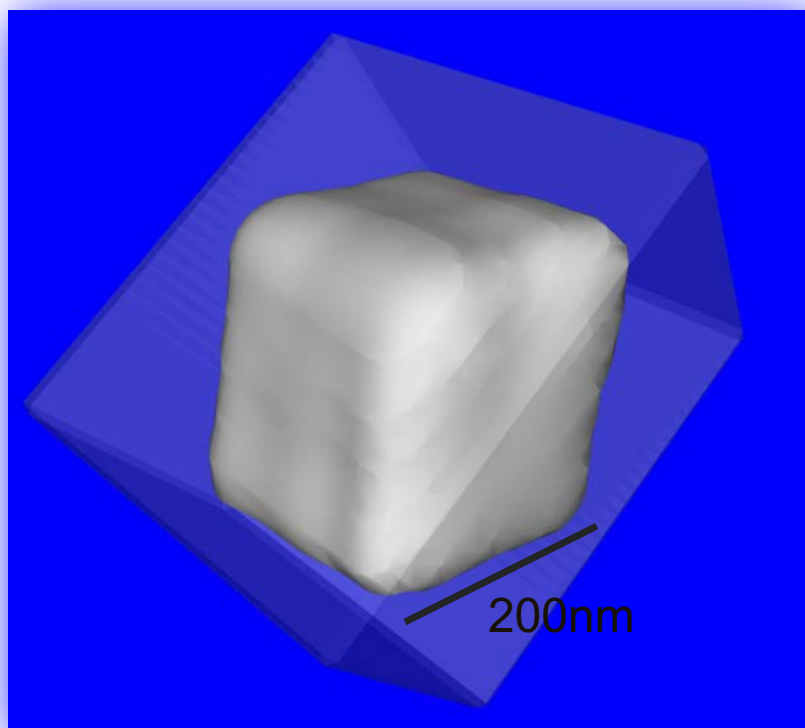
NEURAL NETWORK THAT **LEARNS** IMAGE RECONSTRUCTION



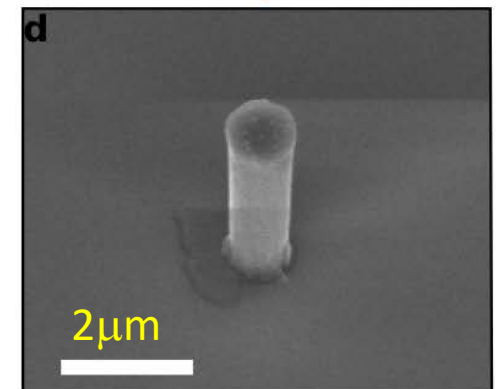
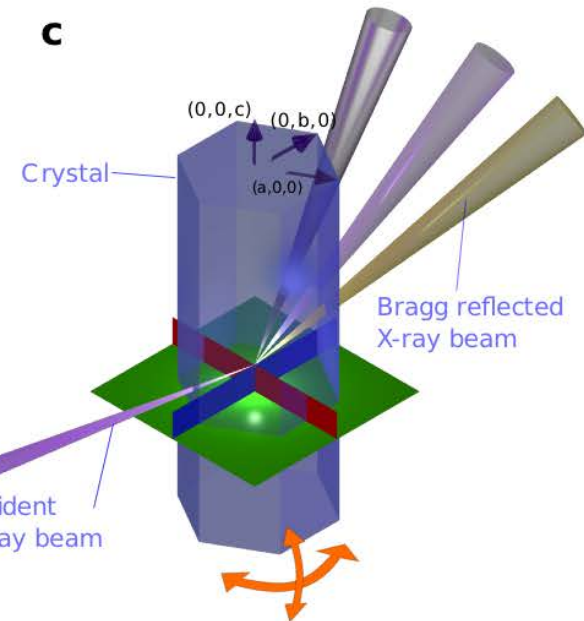
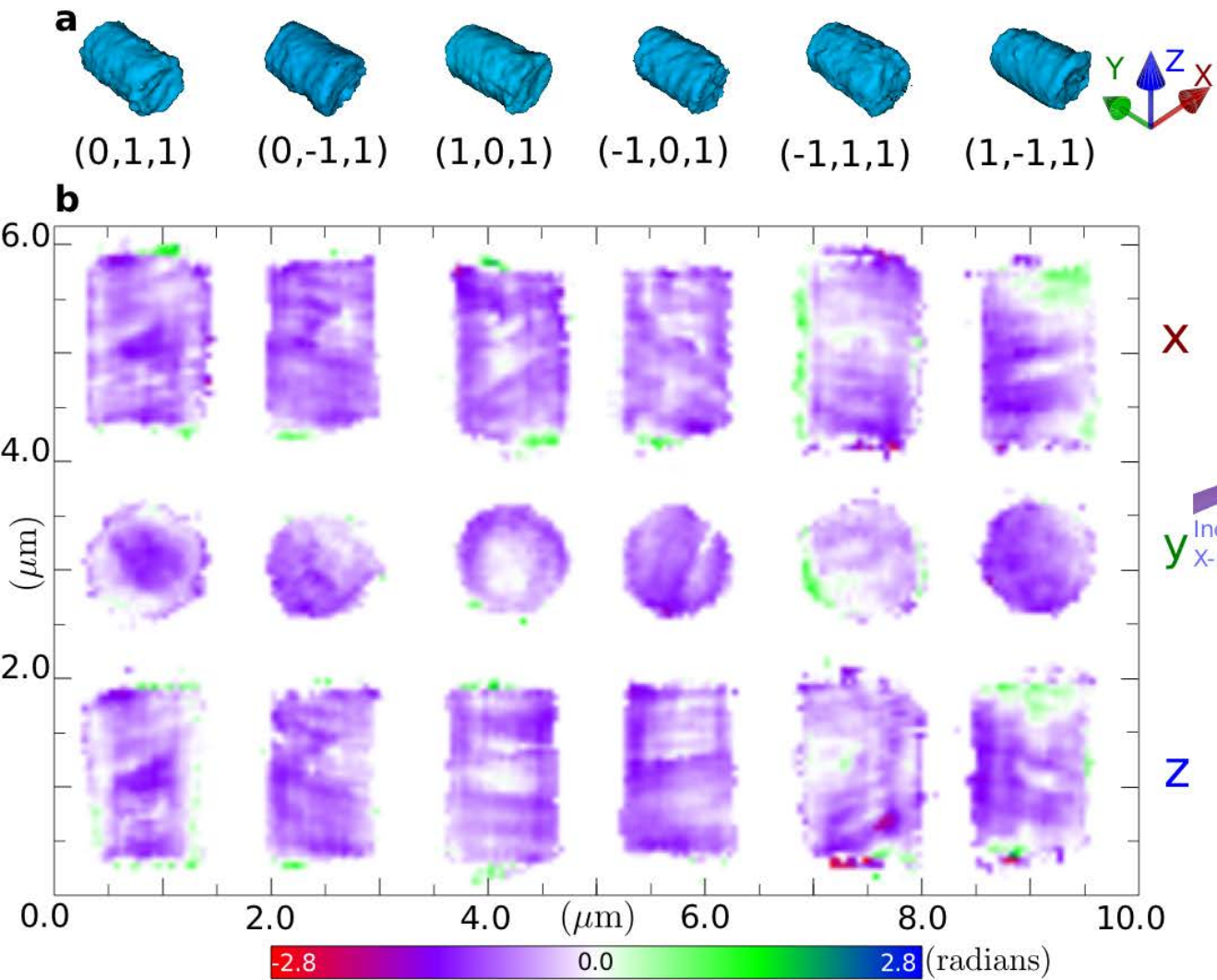
3D Ag Nano Cube



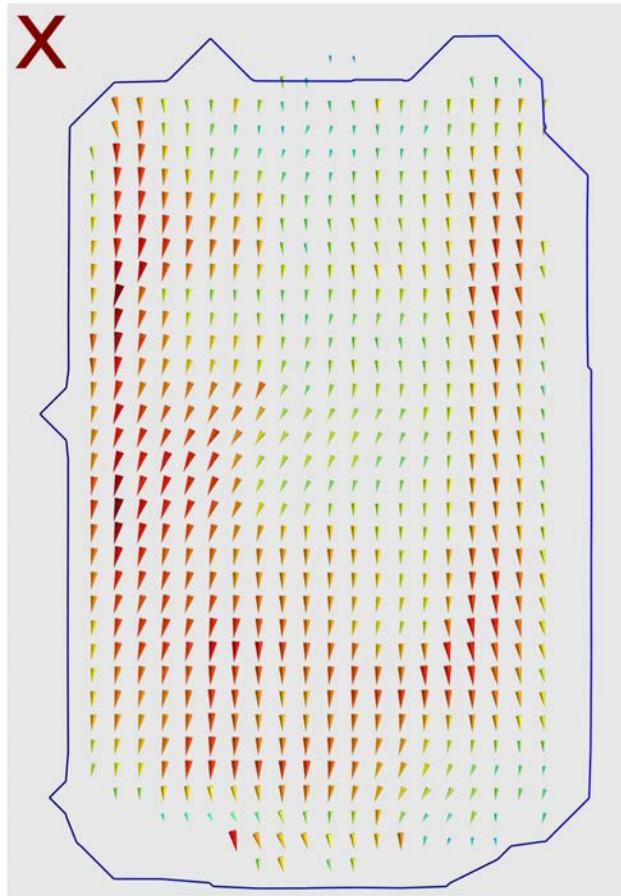
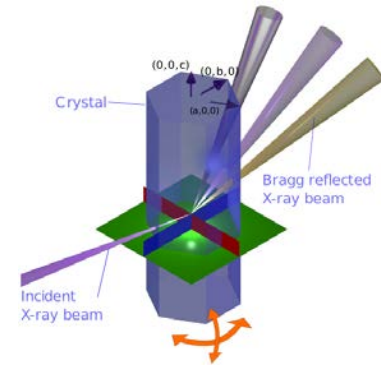
Yugang Sun and Younan Xia,
Science 298 2177 (2003)



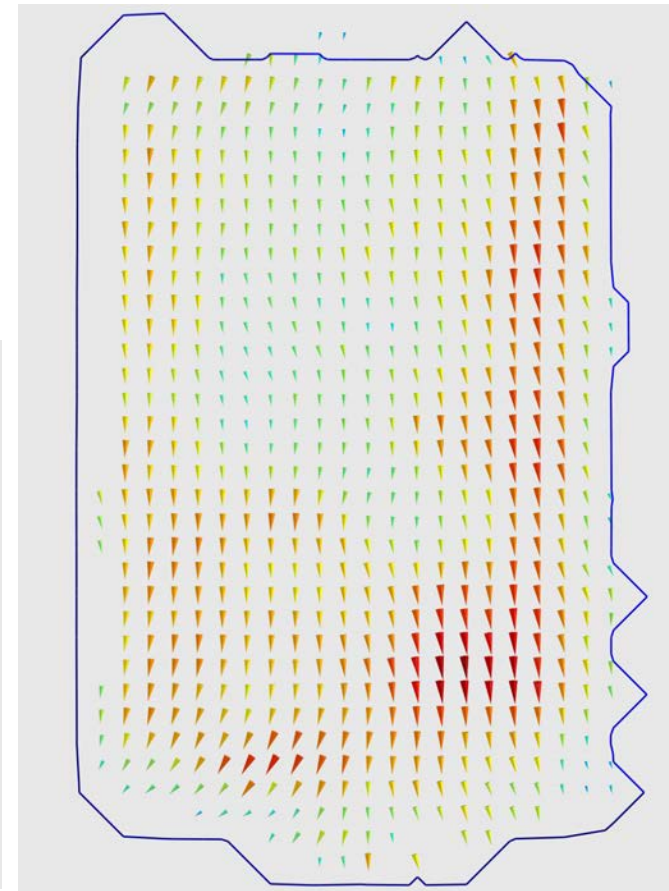
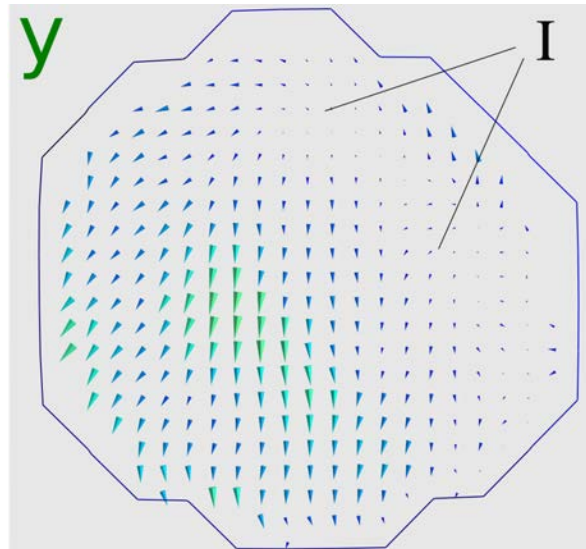
3D Strain Map in ZnO



3D Strain Map in ZnO



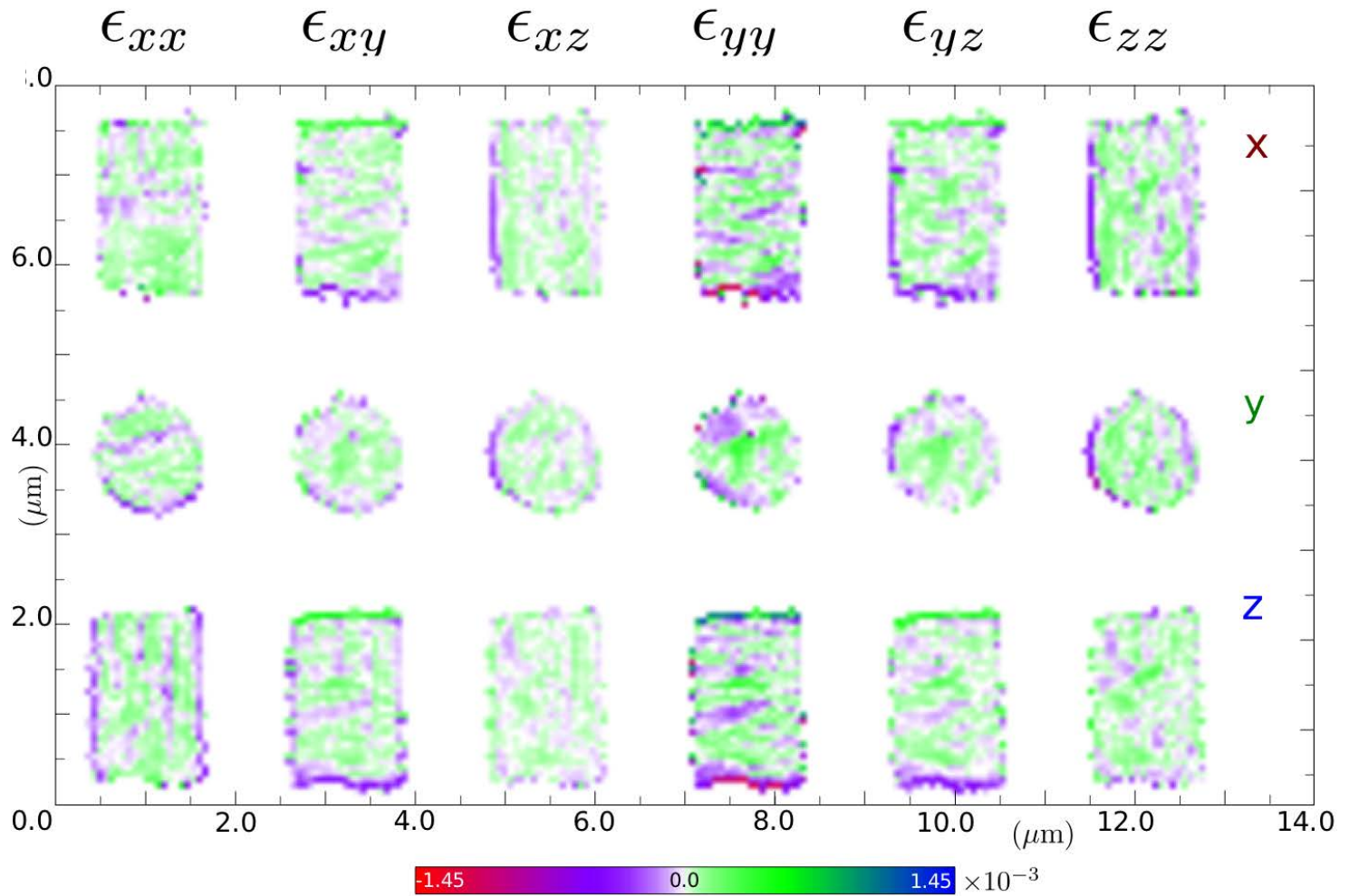
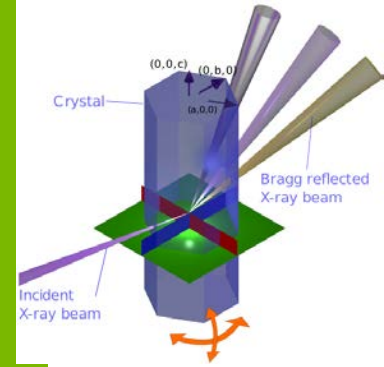
$$u_j = \xi_{ji} q_{ki} \phi_k; \quad \xi_{ji} = (q_{kj} q_{ki})^{-1}$$



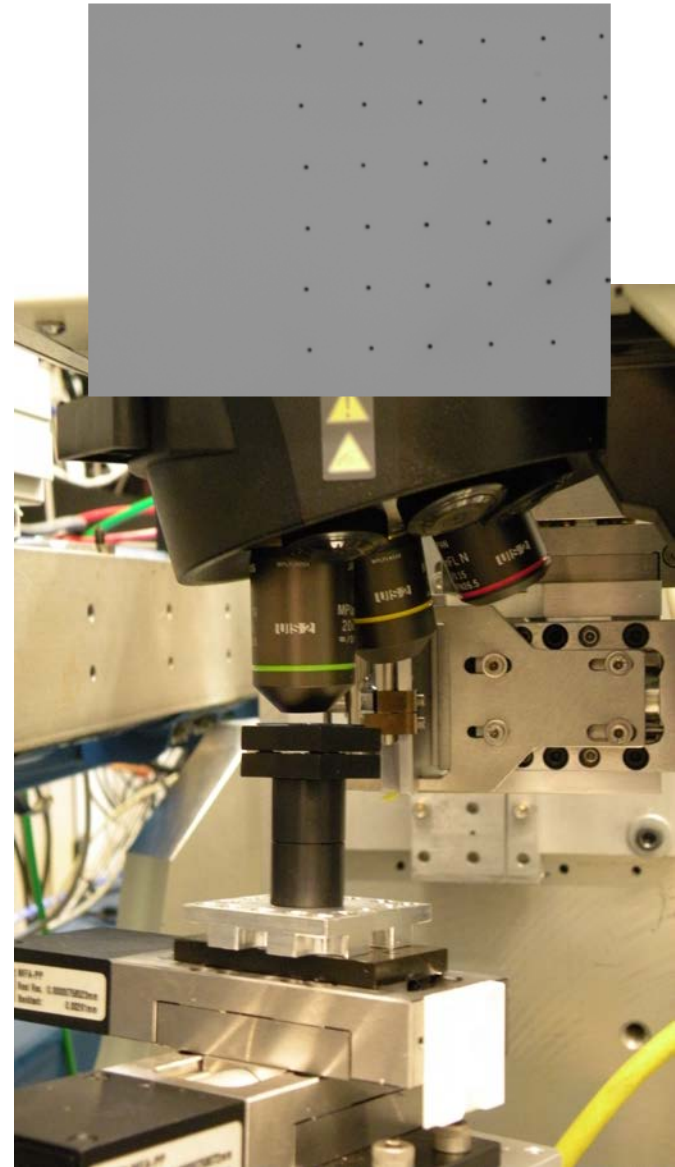
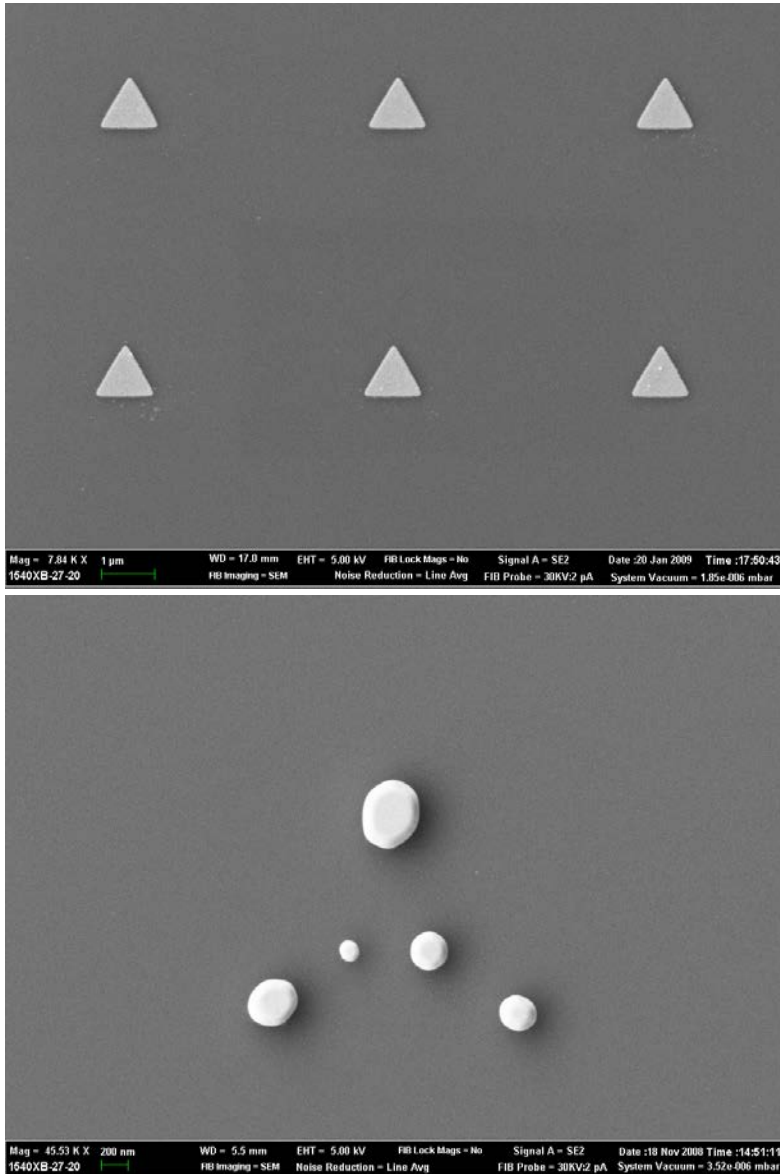
0.0 0.09 nm

3D Strain Map in ZnO

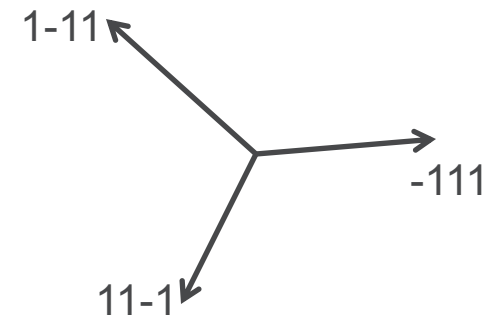
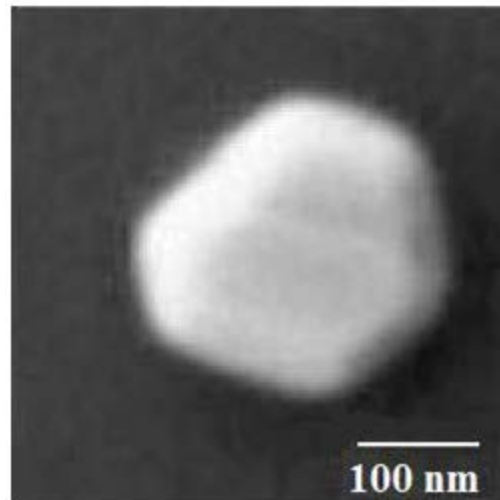
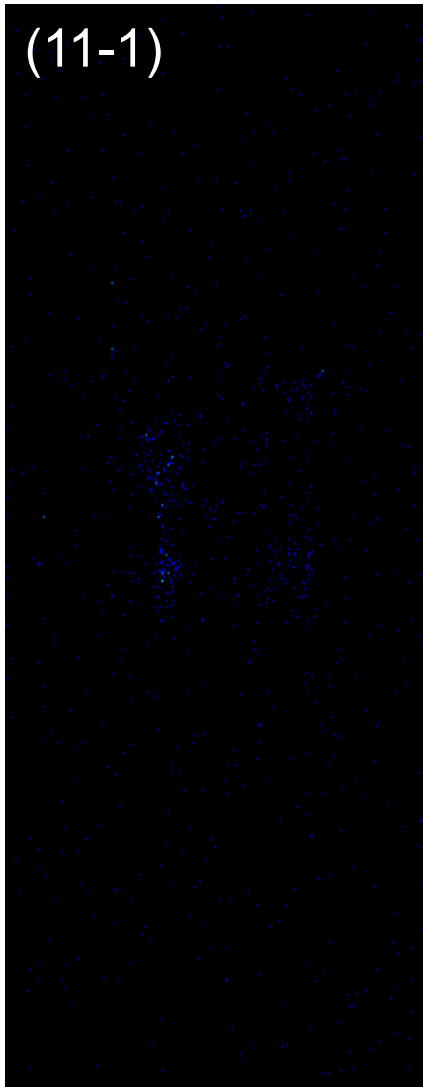
$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right), \quad \tau_{ij} = \left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right)$$



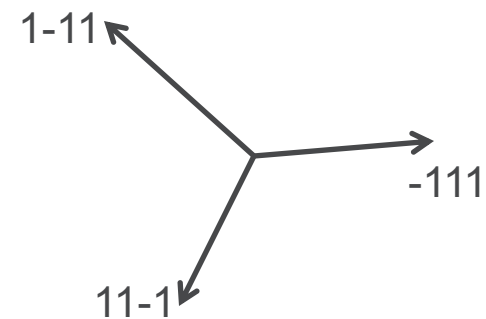
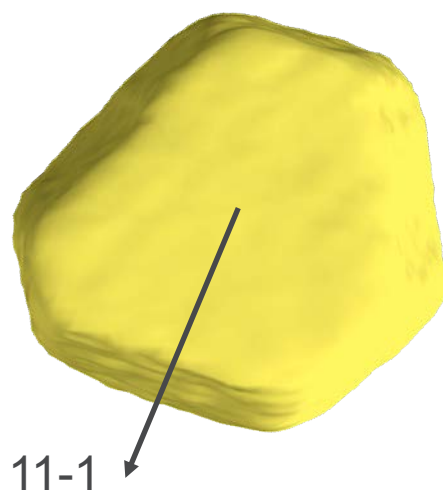
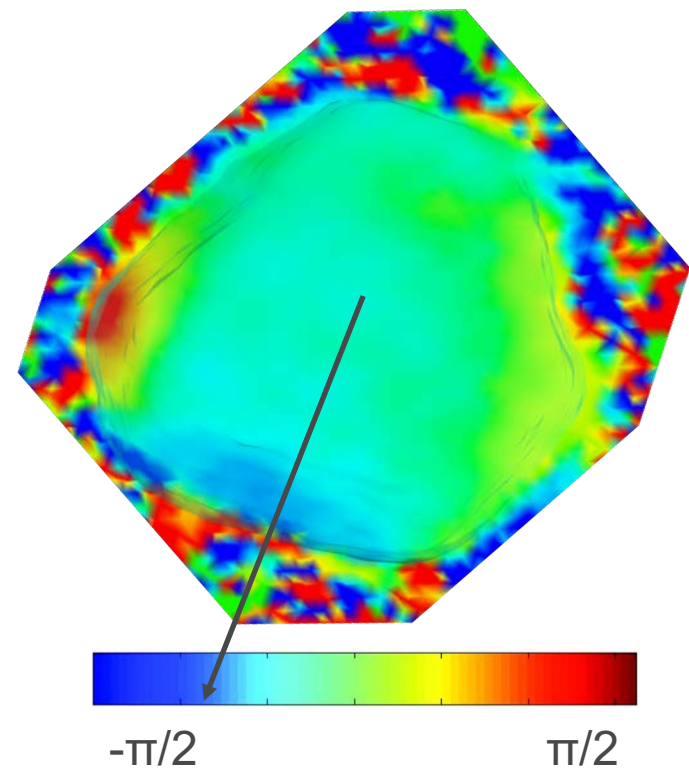
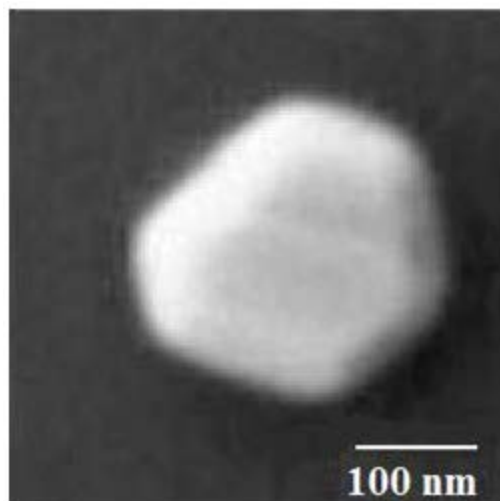
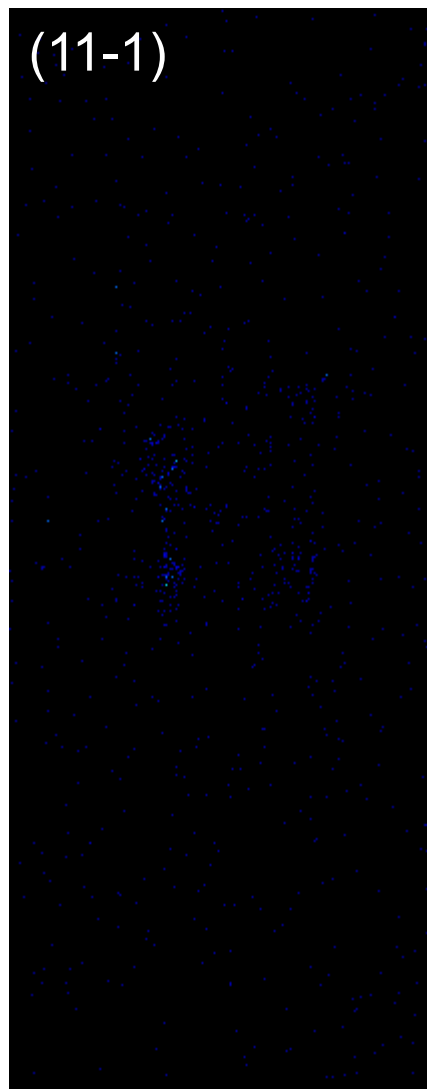
Patterned Gold Nanocrystal Samples



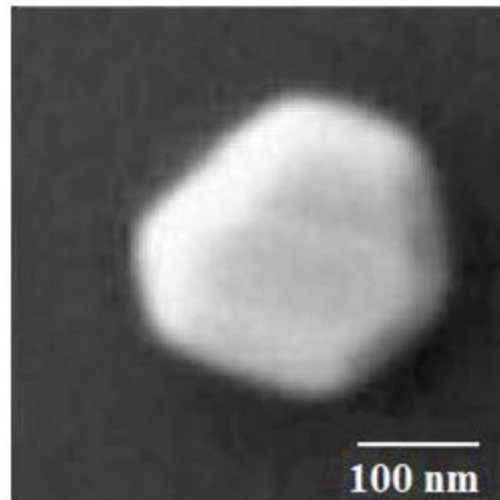
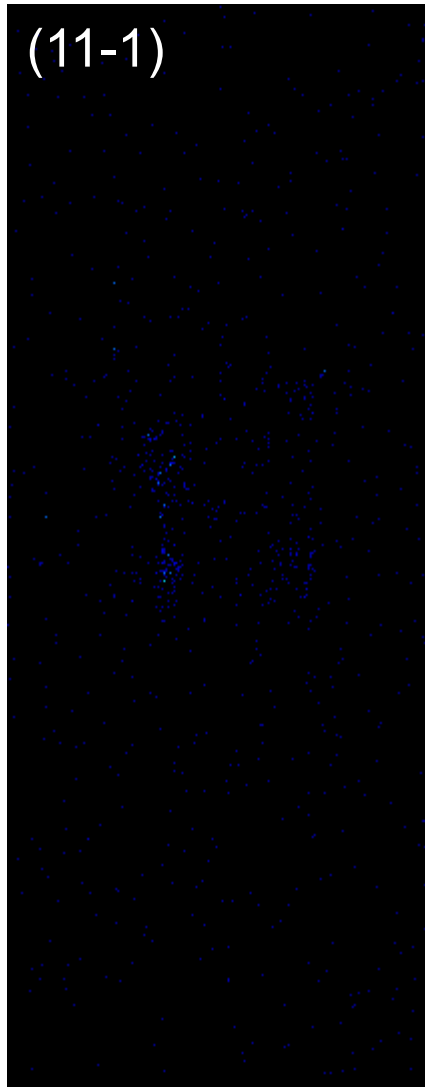
Multiple reflection reconstructions



Multiple reflection reconstructions



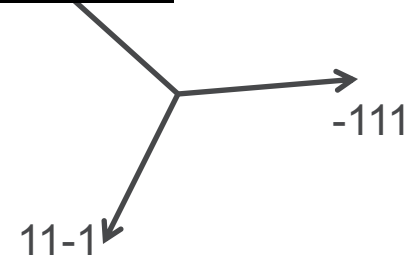
Multiple reflection reconstructions



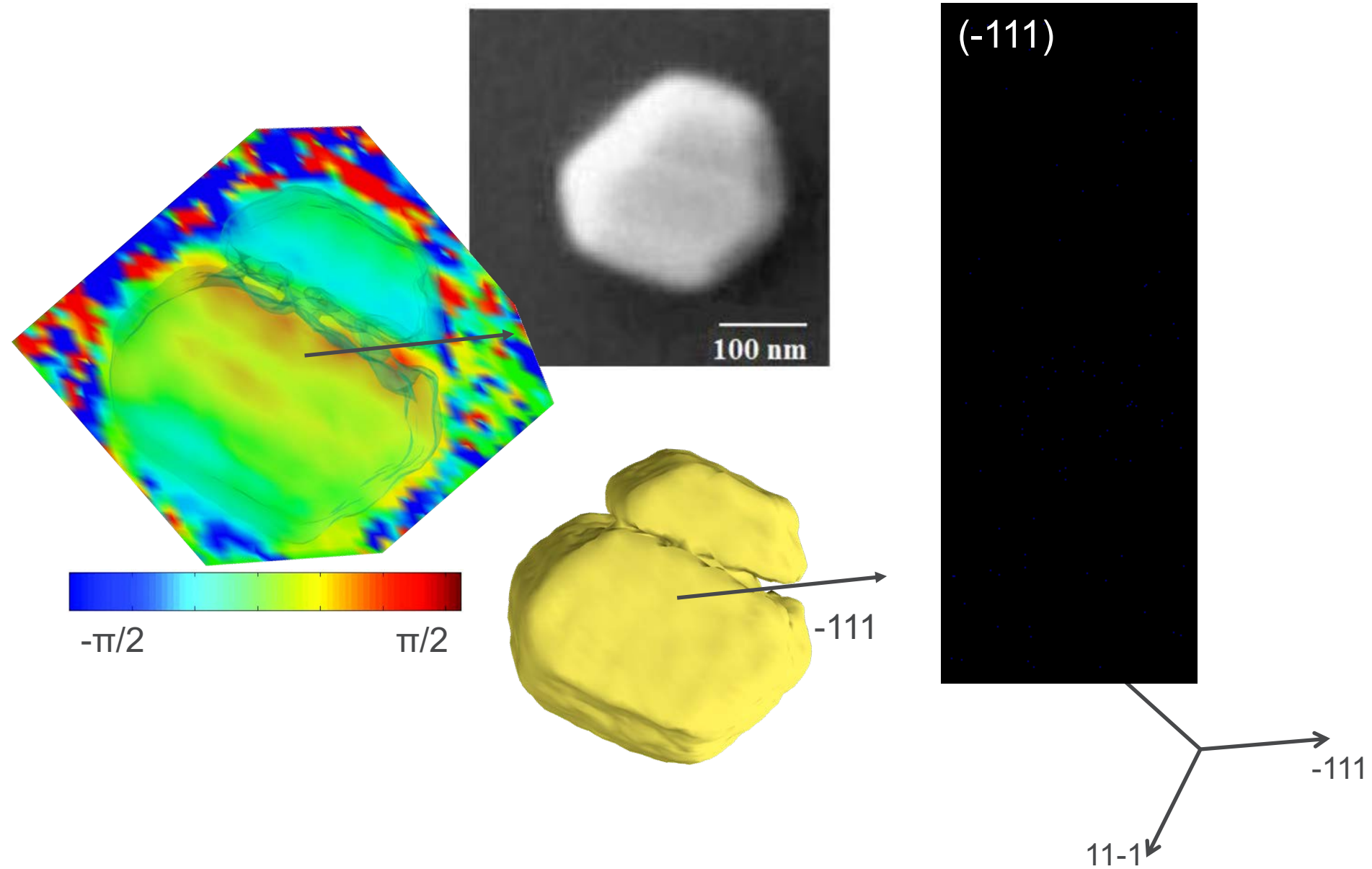
1-11

-111

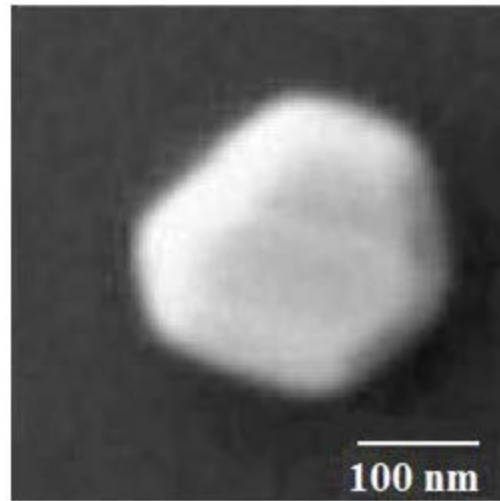
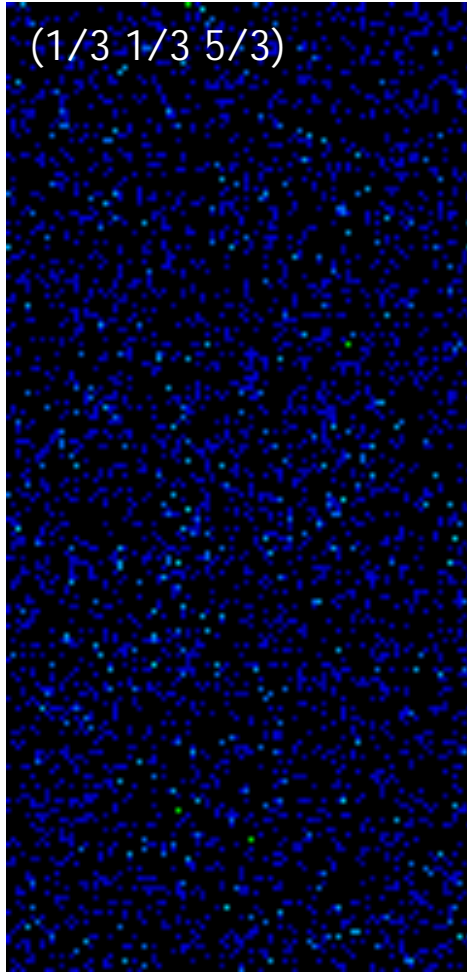
11-1



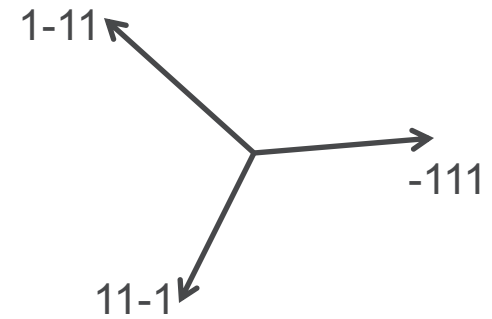
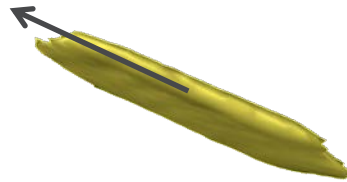
Multiple reflection reconstructions



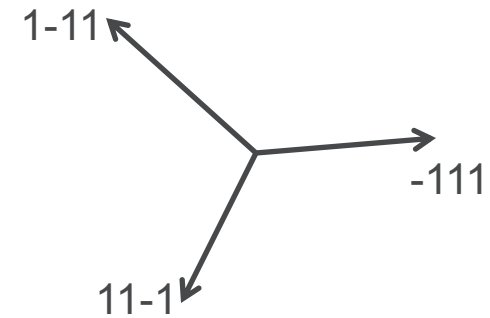
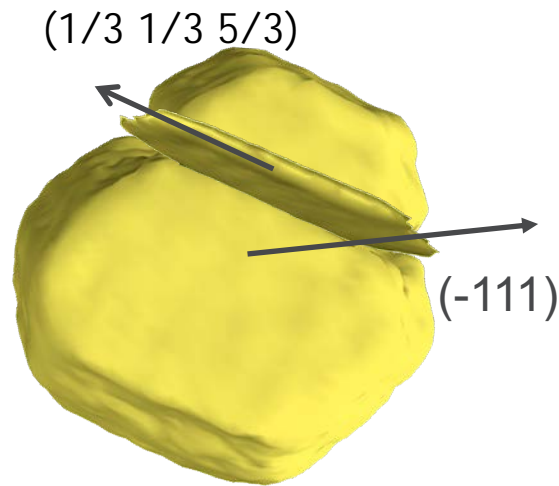
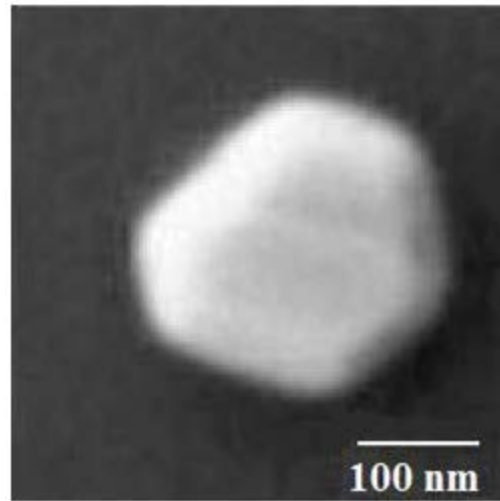
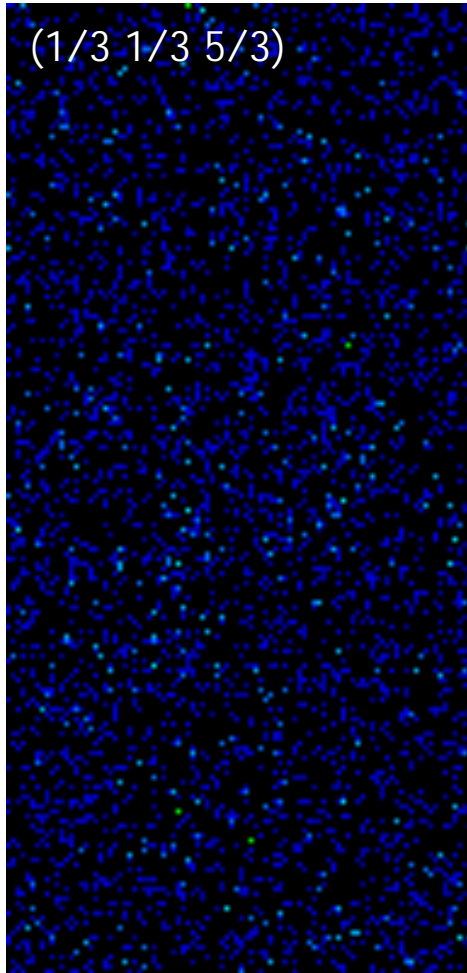
Multiple reflection reconstructions



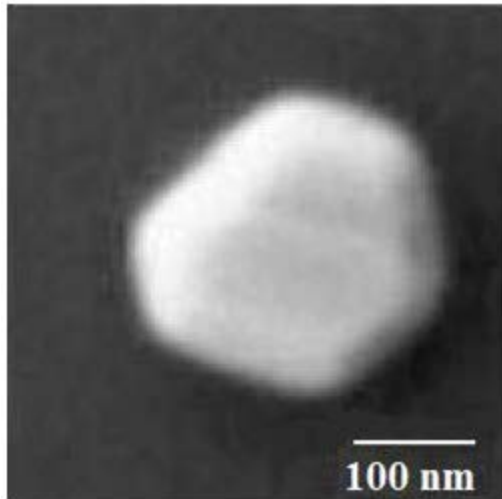
$(1/3 \ 1/3 \ 5/3)$



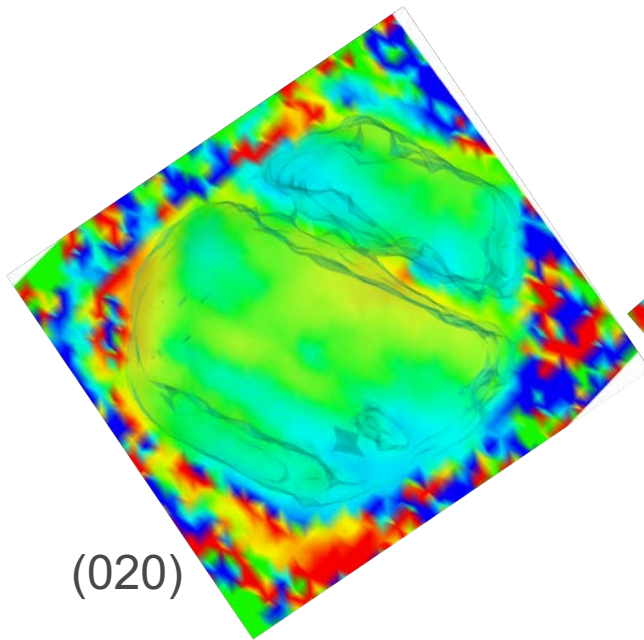
Multiple reflection reconstructions



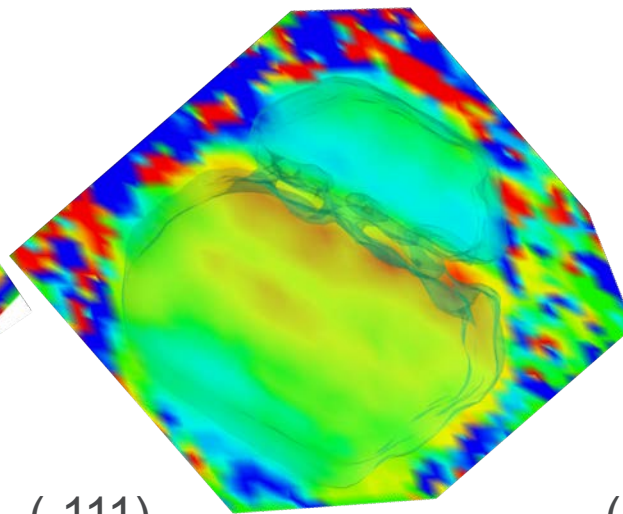
Multiple reflection reconstructions



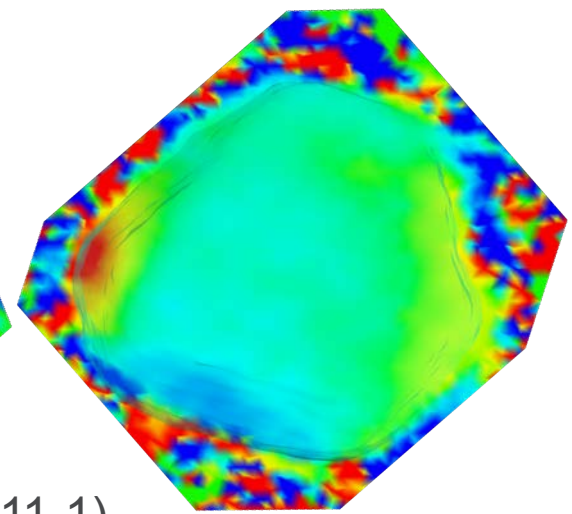
$$\varphi = q \cdot u(r)$$



(020)

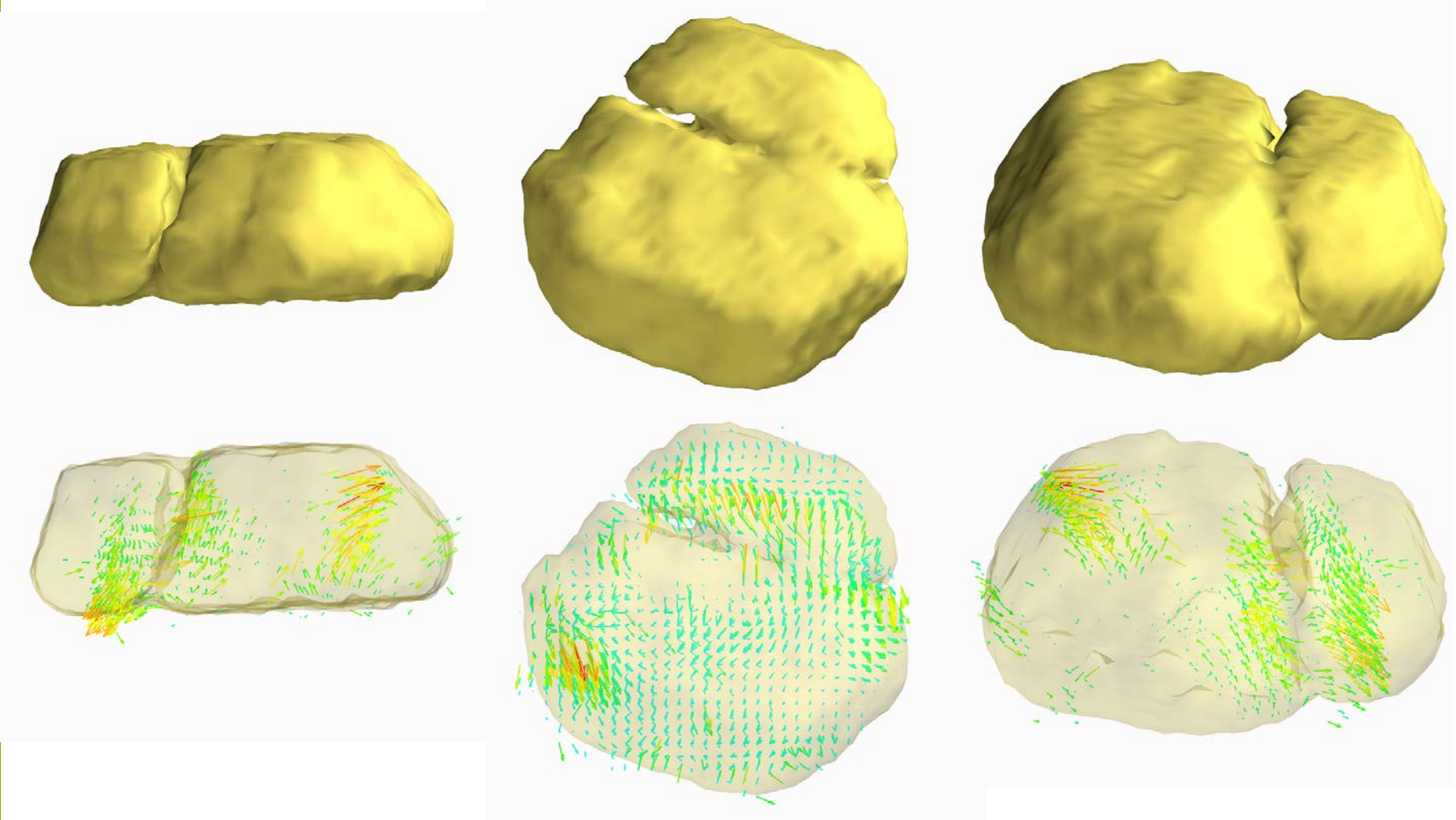


(-111)



(11-1)

Vector Displacement Field of Gold lattice

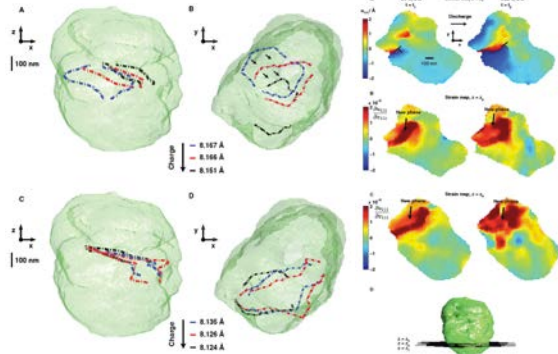


Produced by combining reconstructions from (11-1) (020) (-111)

BCDI TODAY

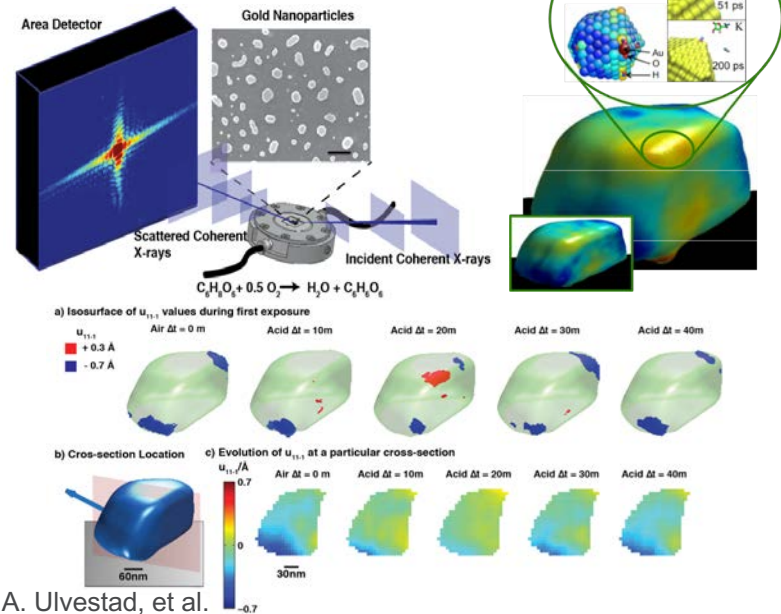
Operando Nanoscale Imaging

Dislocation dynamics in Li-Ion battery



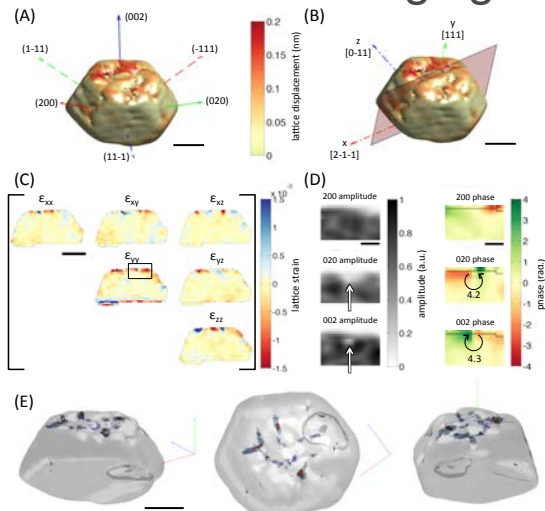
Ulvestad, A., et al. (2015).
Science, 348(6241), 1344–1347

Liquid Catalysis



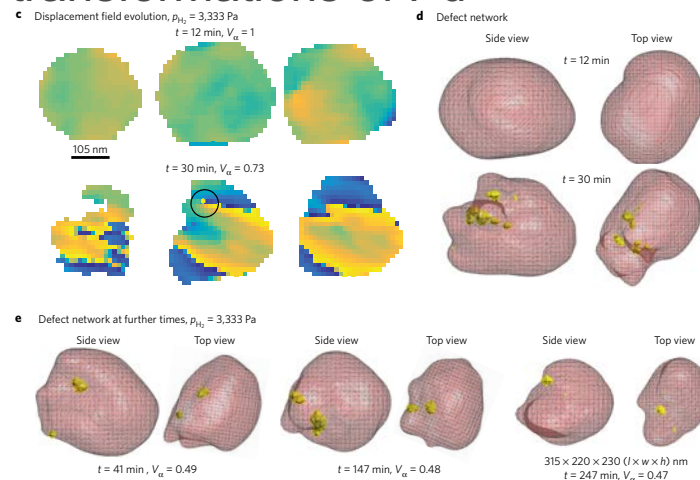
A. Ulvestad, et al.
J. Phys. Chem. Lett., vol. 7, no. 15, pp. 3008, Aug. 2016.

Strain Tensor Imaging



F. Hofmann, et al.
Sci Rep, vol. 7, p. 45993, Apr. 2017.

Dislocation dynamics in the hydriding phase transformations of Pd



Ulvestad, et al.
Nature Materials, vol. 16, no. 5, pp. 565–571, Jan. 2017.

Imaging Lattice Dynamics Laser Pump - CXD Probe@LCLS

$$S(\tau) = \sum_{n=1}^N A_n \exp\left[-\frac{\tau}{\tau_{d,n}}\right] \cos\left[\frac{2\pi}{T_n}(\tau + \tau_{0,n})\right] + C_n.$$

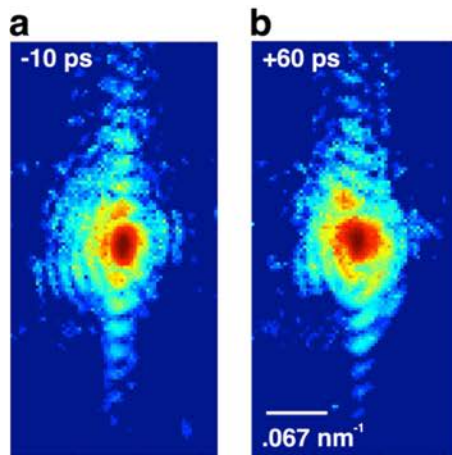
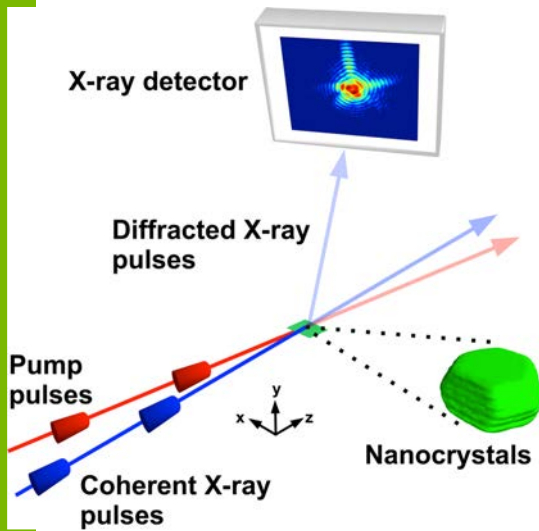
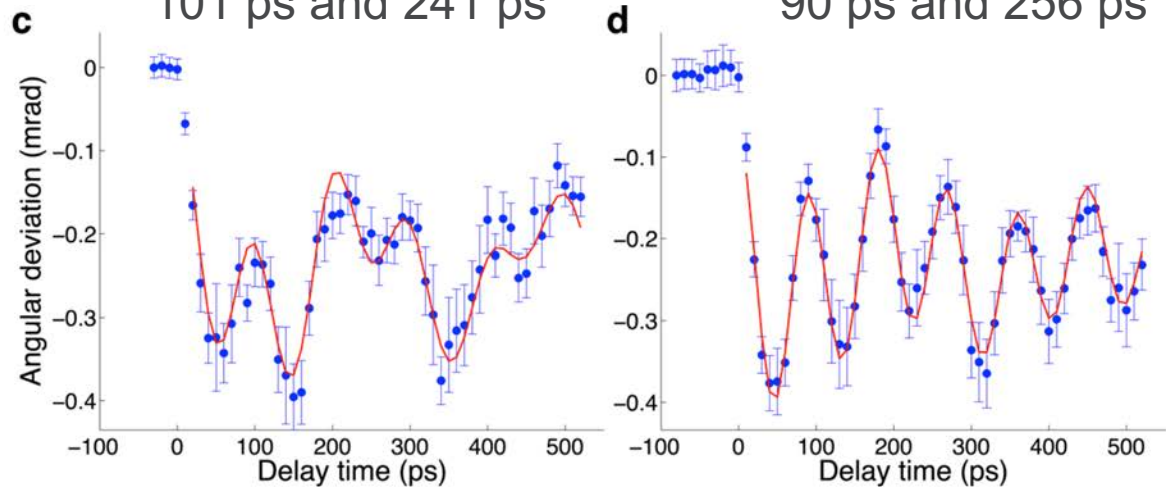
600 pm “breathing modes”

Crystal A

101 ps and 241 ps

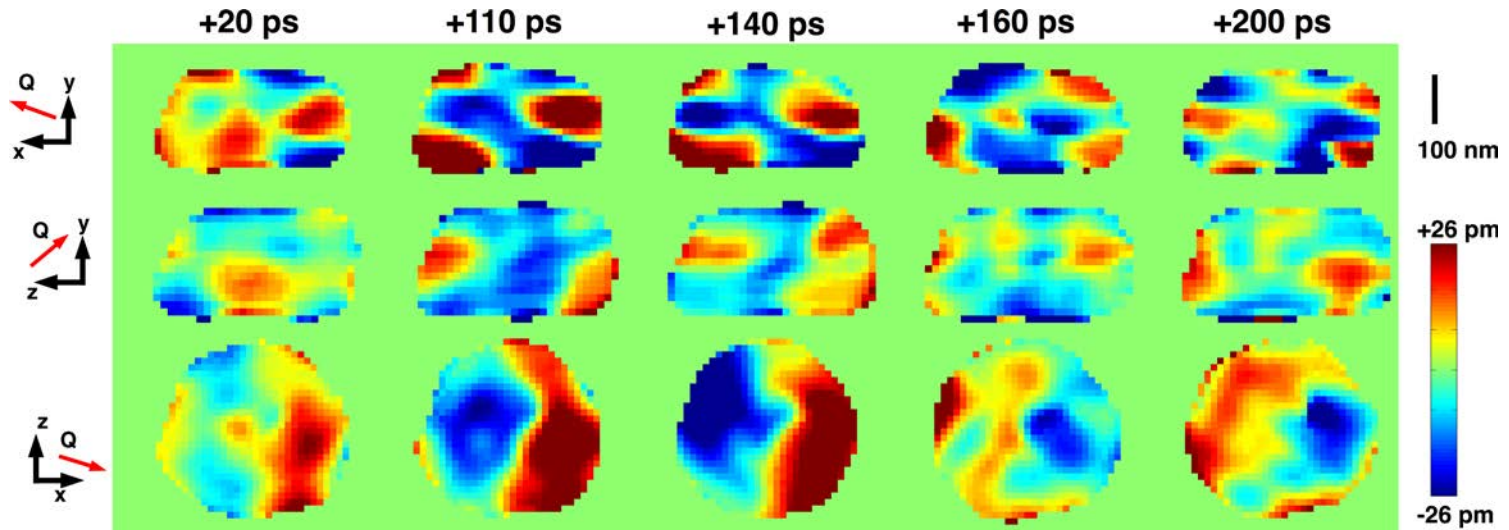
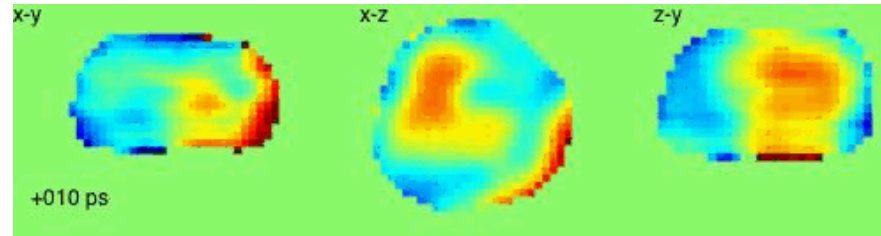
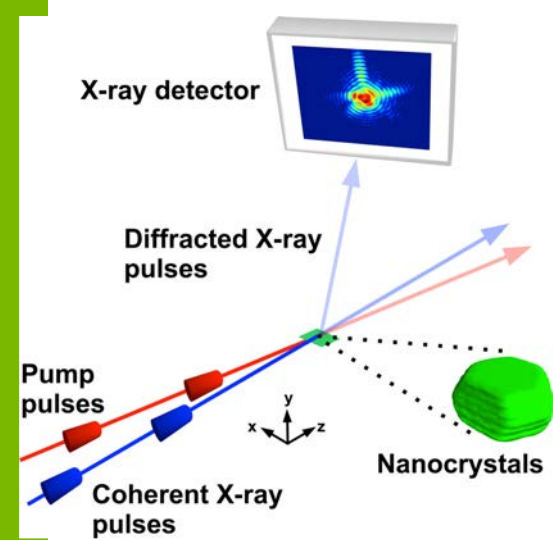
Crystal B

90 ps and 256 ps



Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals
J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu,
M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder,
A. M. Korsunsky, J. S. Wark & I. K. Robinson. (2013). *Science*, 341(6141), 56–59

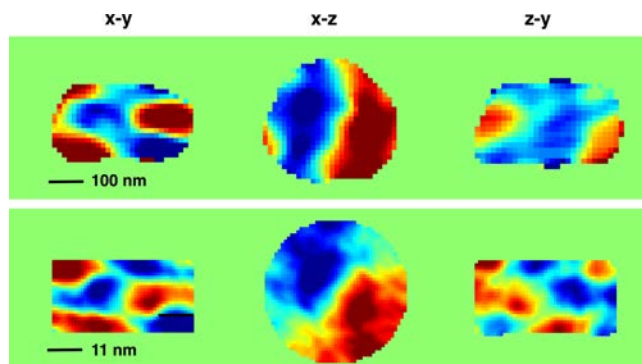
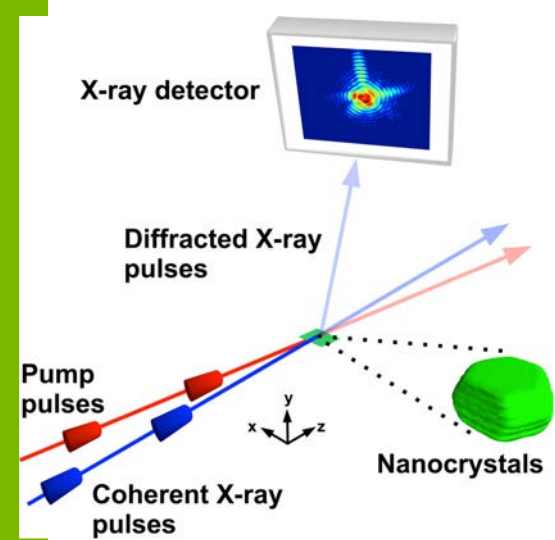
Imaging Lattice Dynamics Laser Pump - CXD Probe@LCLS



Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals
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M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder,
A. M. Korsunsky, J. S. Wark & I. K. Robinson. (2013). *Science*, 341(6141), 56–59

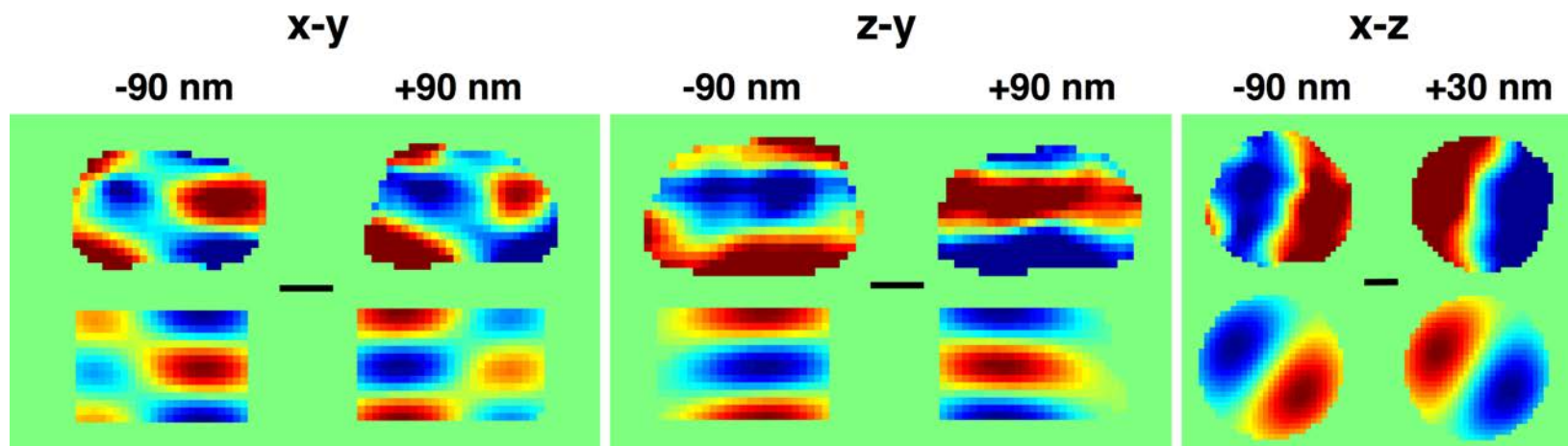
Imaging Lattice Dynamics

Laser Pump - CXD Probe@LCLS



Orthogonal slices
Through crystal density

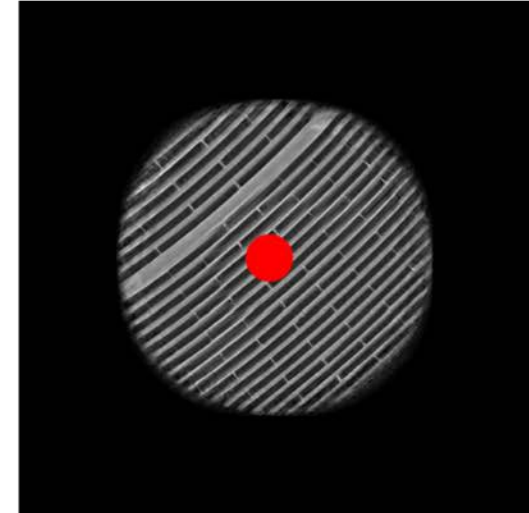
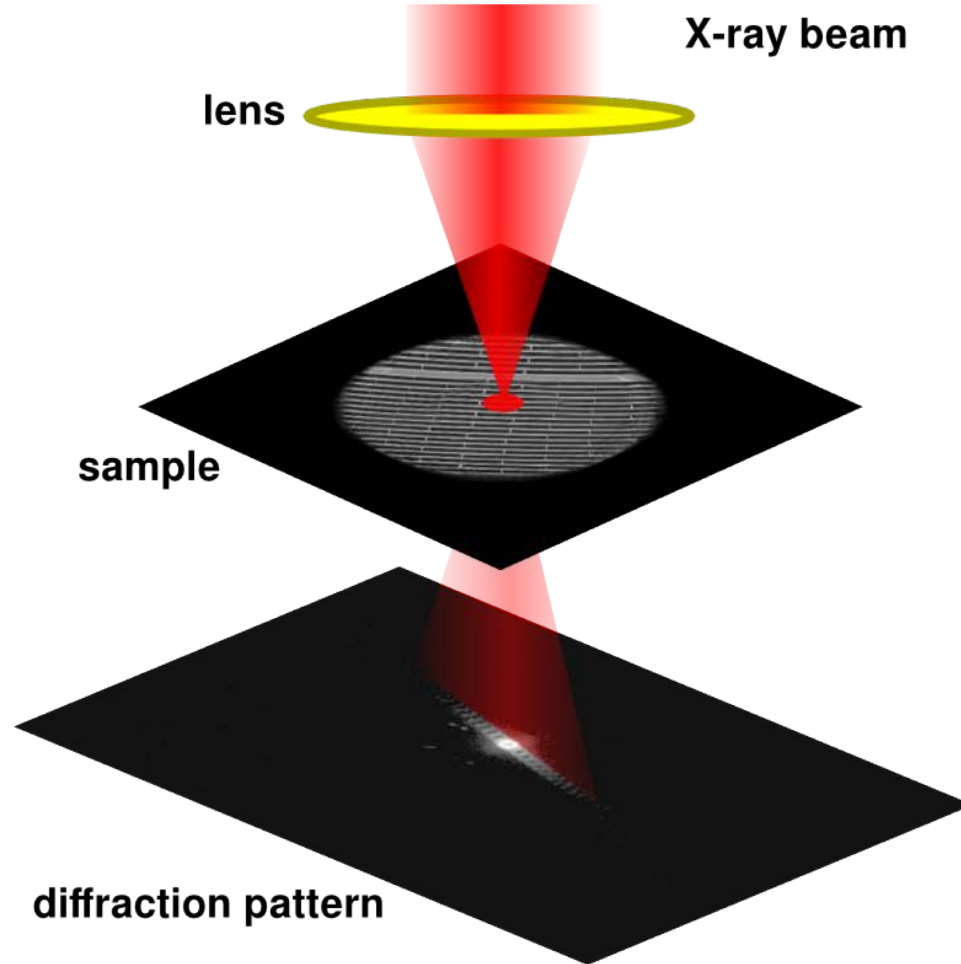
MD simulation
at +110ps



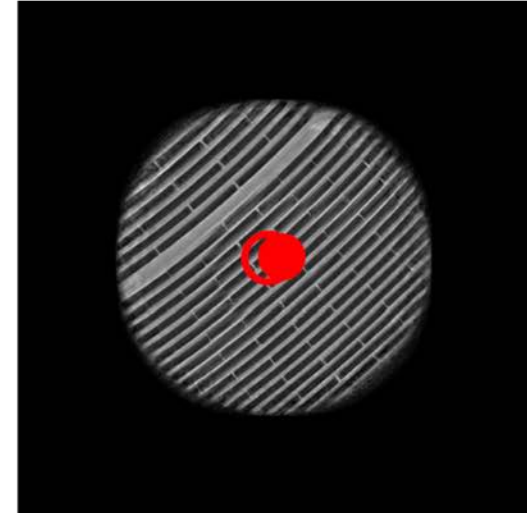
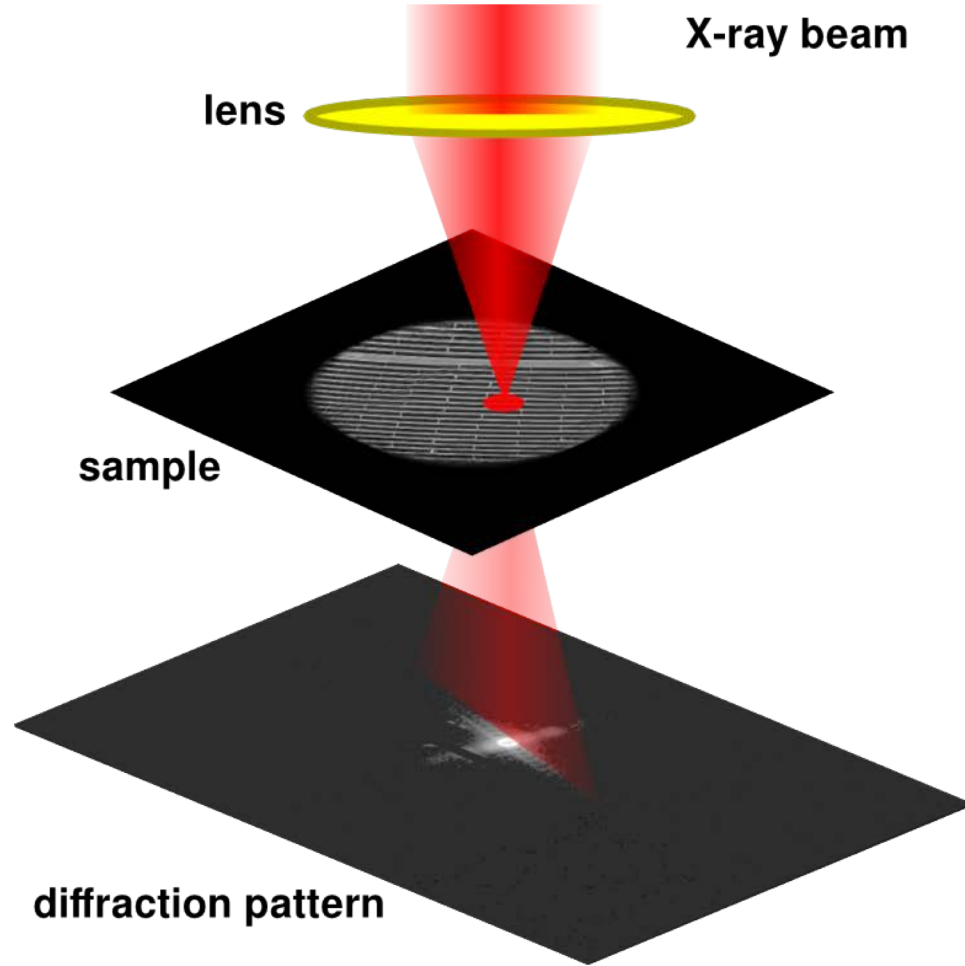
Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals

J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu, M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder, A. M. Korsunsky, J. S. Wark & I. K. Robinson. (2013). *Science*, 341(6141), 56–59

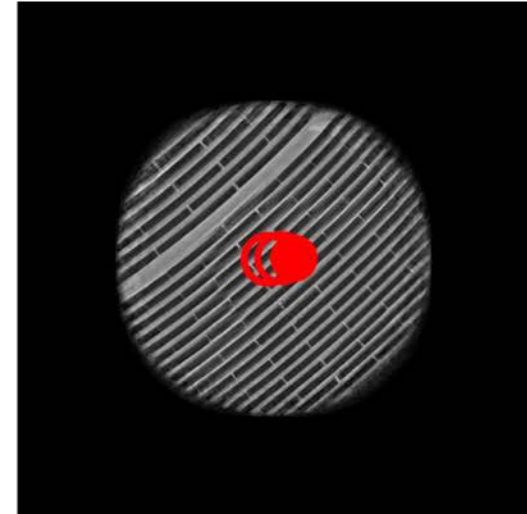
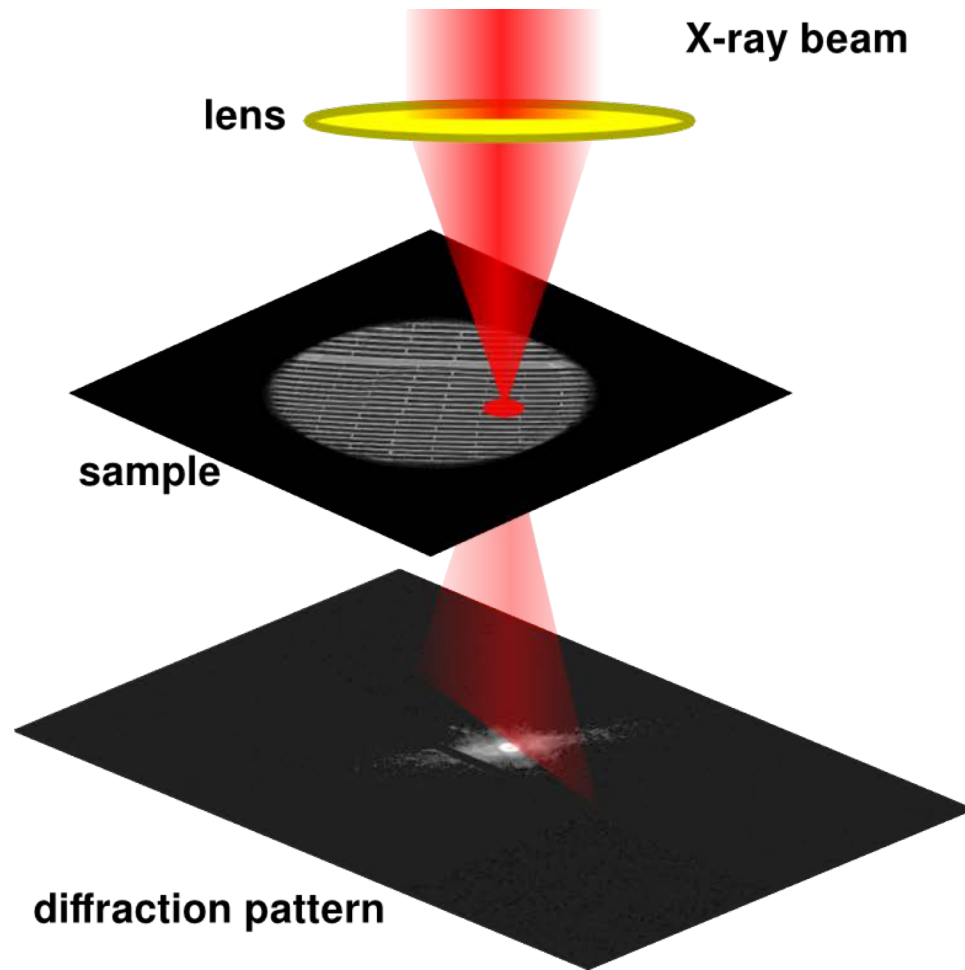
Ptychography (to fold) - Scanning CDI for extended object



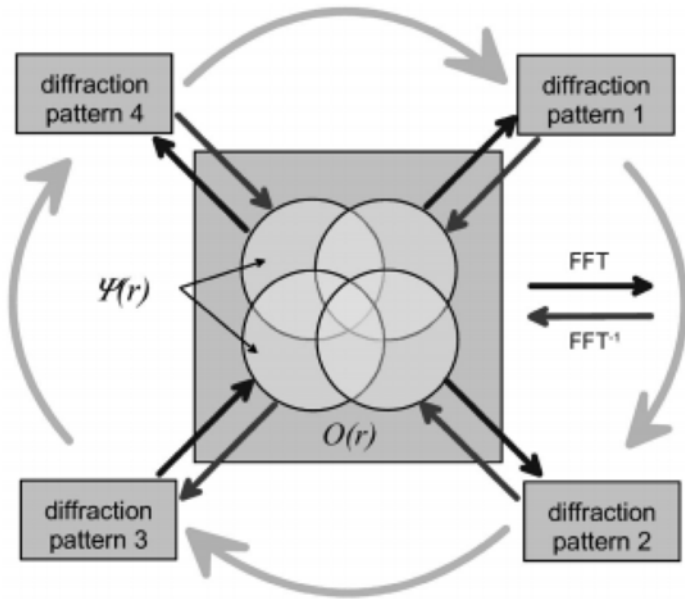
Ptychography (to fold) - Scanning CDI for extended object



Ptychography (to fold) - Scanning CDI for extended object



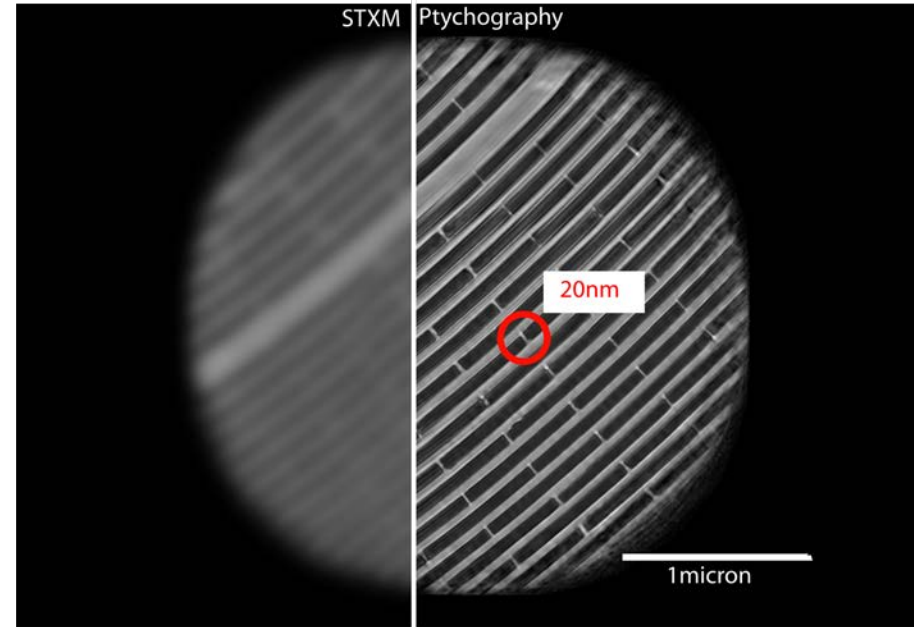
Ptychography



Ptychographic iterative engine (PIE)

J. Rodenburg *et al.*, *PRL* **98**, 034801 (2007)

Platinum nanostructure

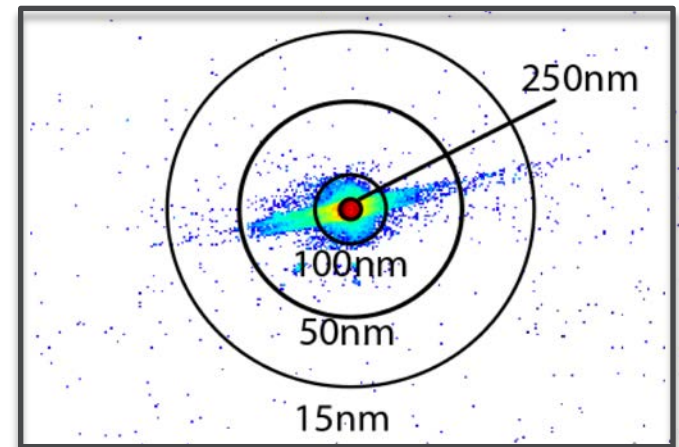


Spatial resolution: $\delta = \frac{\lambda}{\theta} = \frac{\lambda z}{N\Delta}$

Exit surface wave field: $\psi(\mathbf{r}) = P(\mathbf{r})O(\mathbf{r})$

$$O(\mathbf{r}) = \frac{\sum_j P^*(\mathbf{r} - \mathbf{r}_j)\psi_j(\mathbf{r})}{\sum_j |P(\mathbf{r} - \mathbf{r}_j)|^2} \quad P(\mathbf{r}) = \frac{\sum_j O^*(\mathbf{r} + \mathbf{r}_j)\psi_j(\mathbf{r} + \mathbf{r}_j)}{\sum_j |O(\mathbf{r} + \mathbf{r}_j)|^2}$$

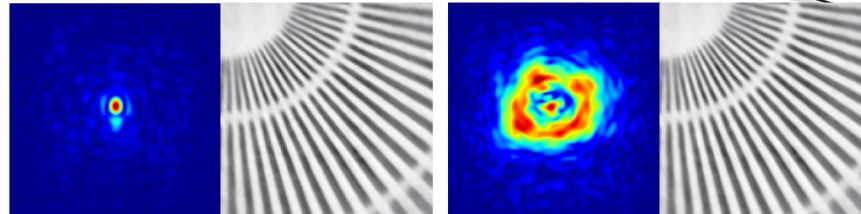
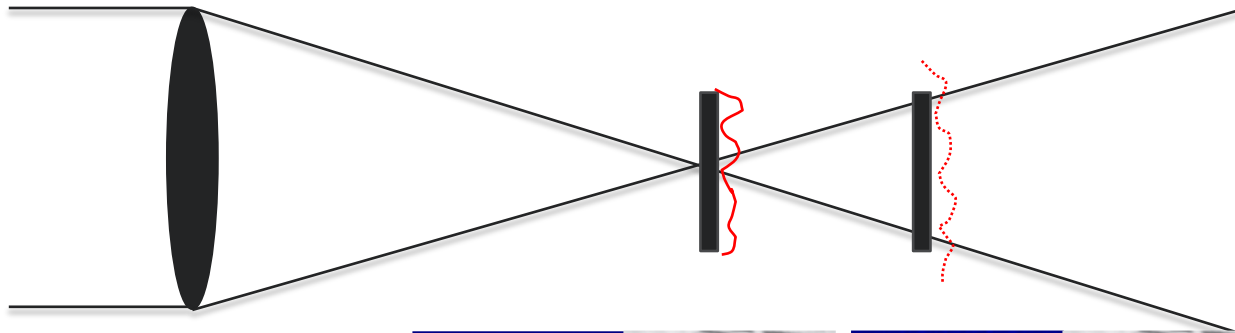
P. Thibault *et al.*, *Science* **321**, 379 (2008)



At which plane ptychographic images are reconstructed

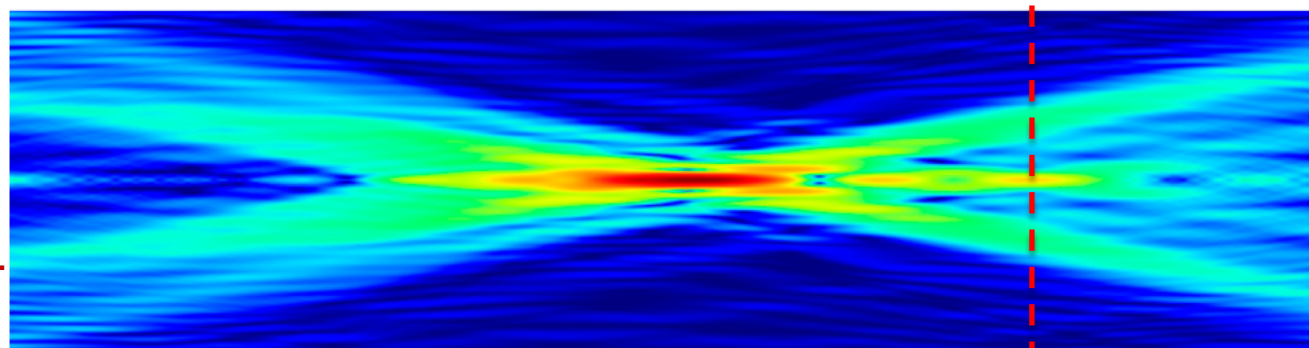
$$\psi(r) = P(r)O(r)$$

Ptychography always produces images at the sample plane.



The resolution is not limited by the beam size.

Characterization of focusing optics.

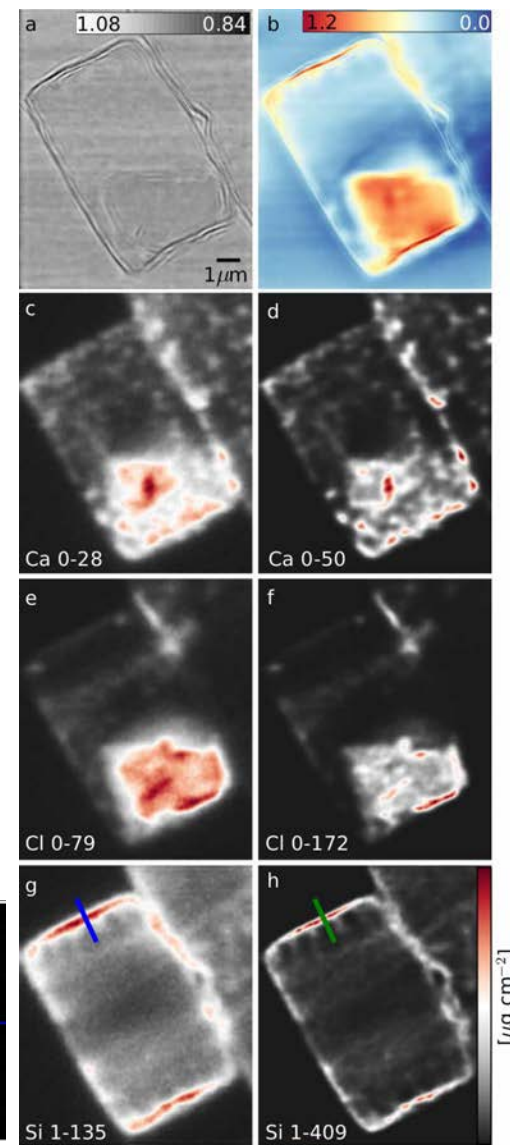
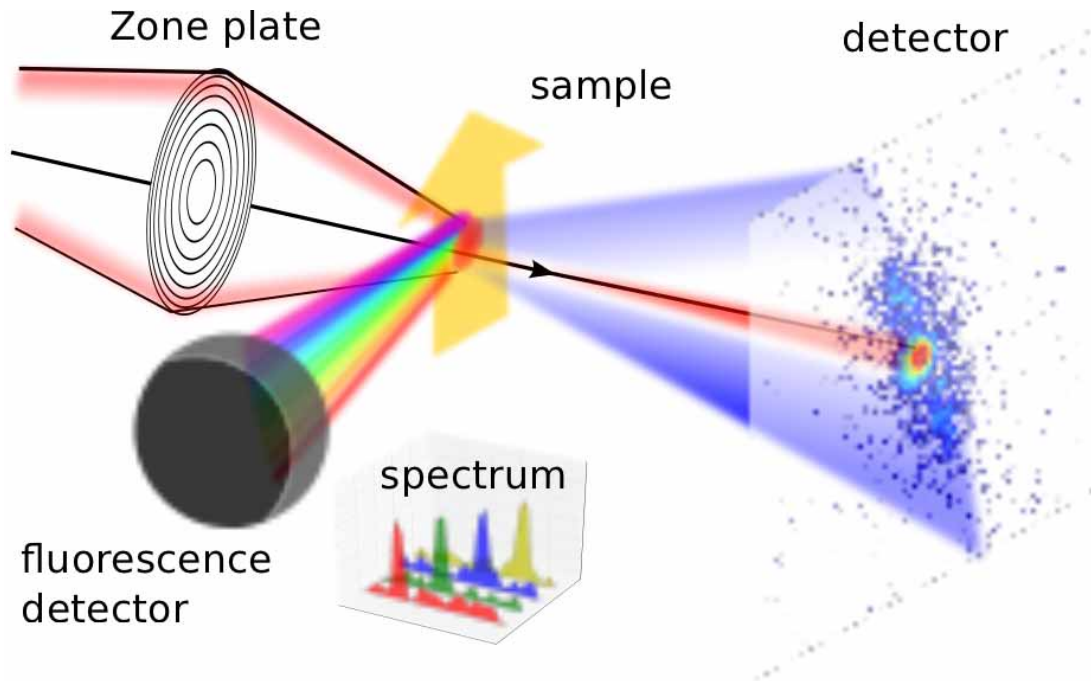


Propagation

63

Sample plane

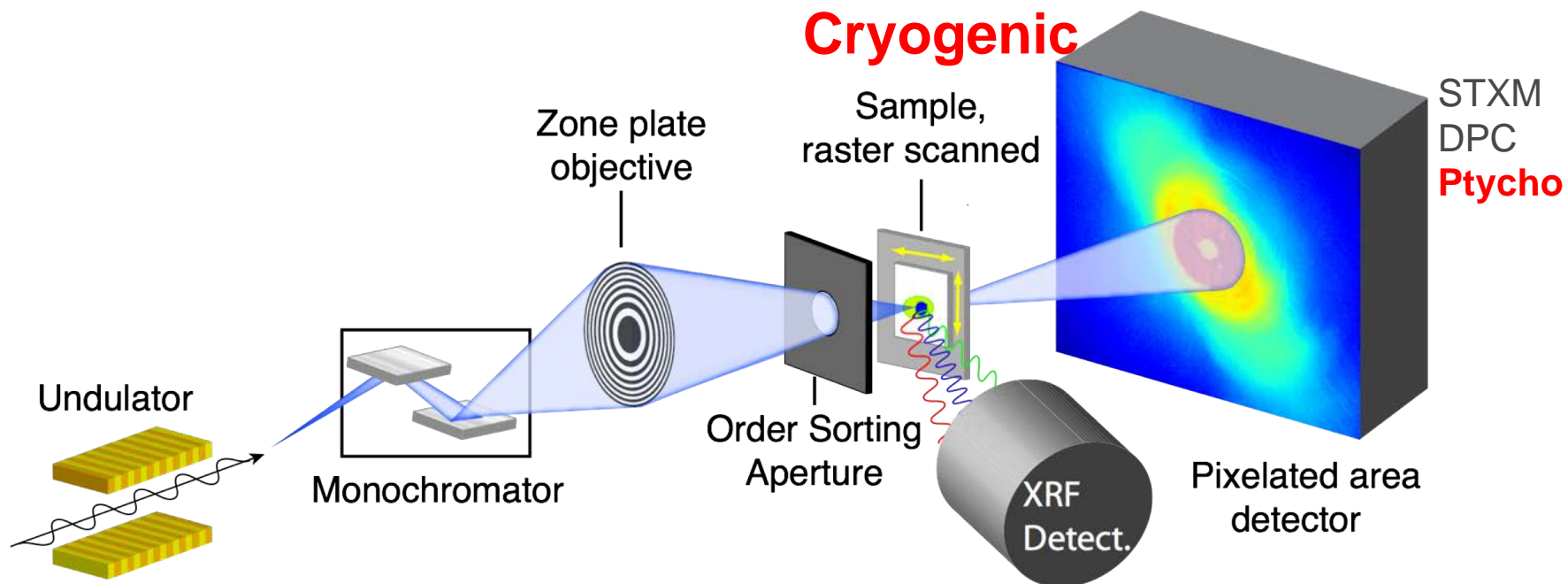
PTYCHOGRAPHY MICROPROBES -> COHERENT IMAGING INSTRUMENT



Vine, et al. (2012). *Opt. Express*, 20(16), 18287–18296.

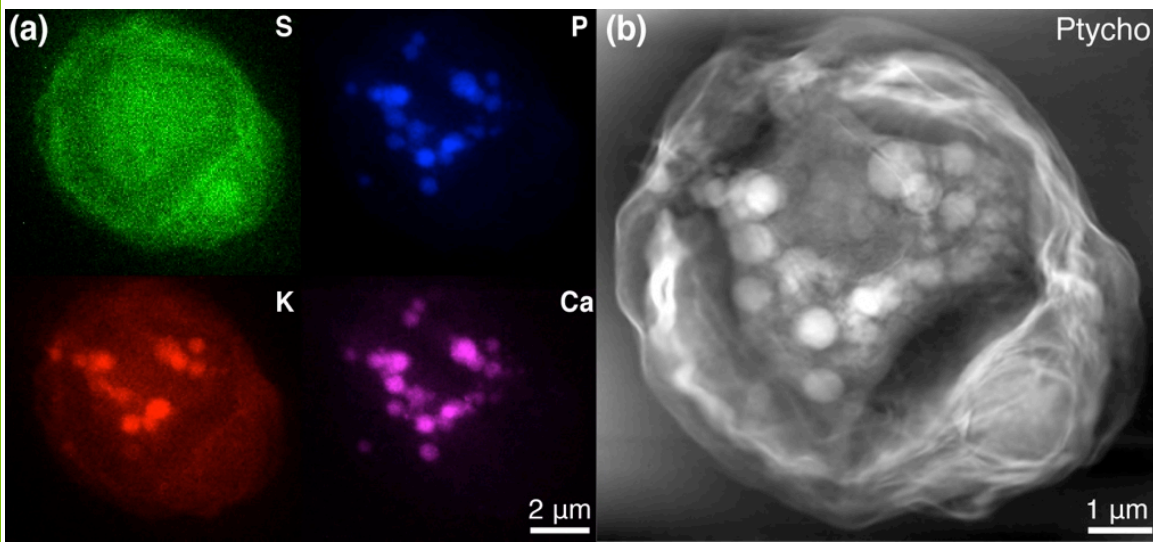
Making ptychography colorful

❖ Combination of Ptychography & Fluorescence

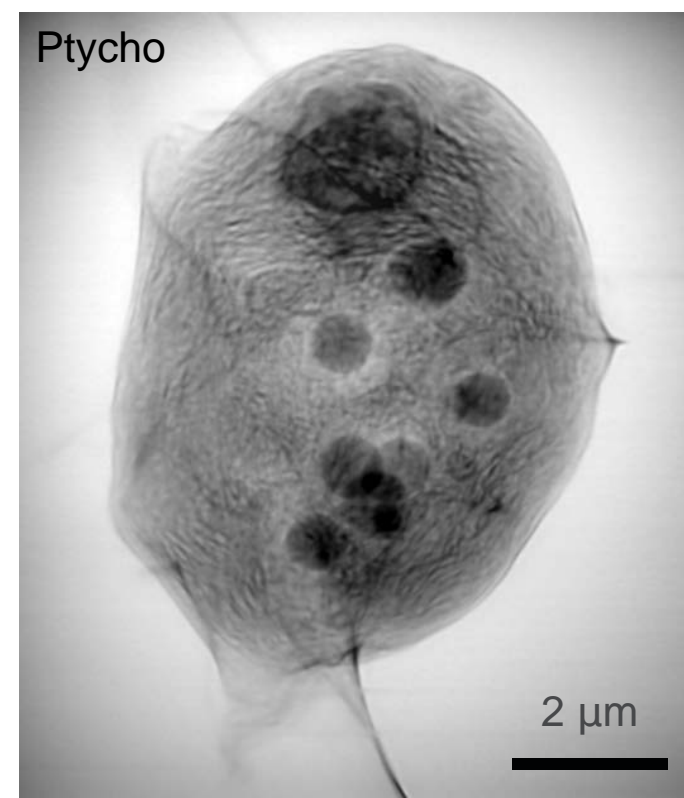


J. Deng, *et al.* PNAS 112, 2314-2319 (2015)

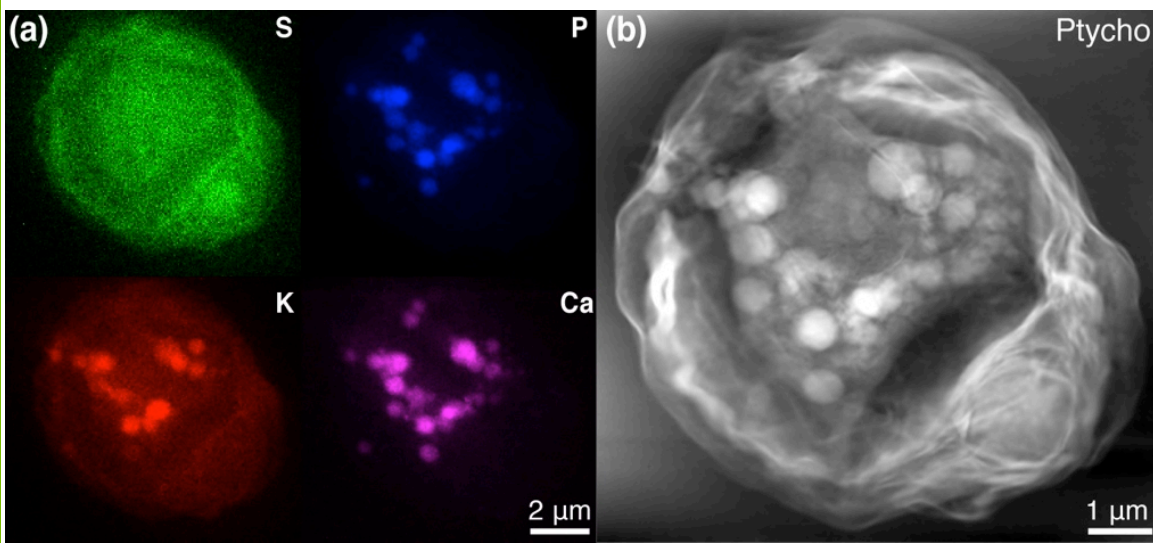
- **Frozen-hydrated samples:** closer to natural state, reduce radiation damage
- **Fluorescence:** quantitative elemental composition
- **Ptychography:** structure information with high resolution



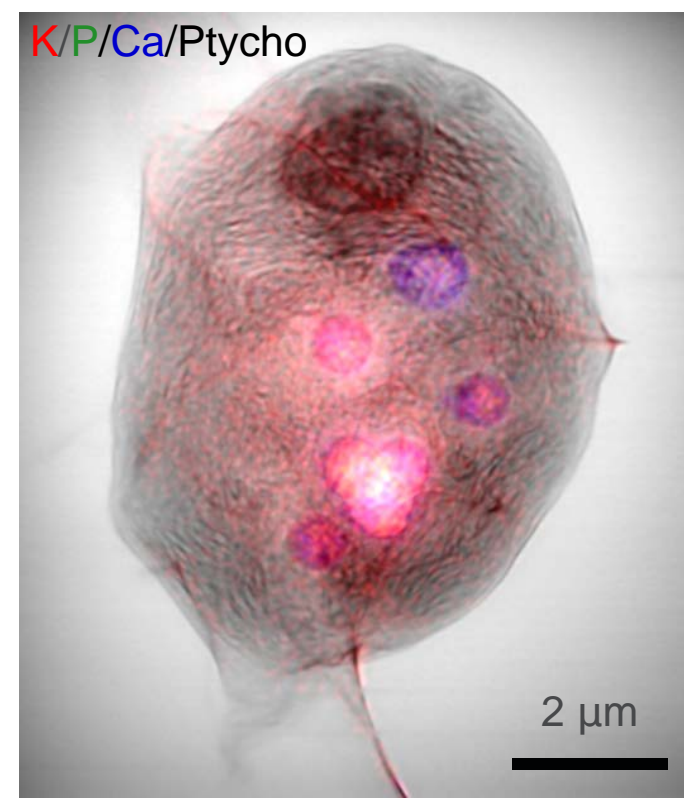
J. Deng, *et al. Sci. Rep.* (accepted)



- Frozen-hydrated *Chlamy. Alga*
- Ptychographic image resolution: ~18 nm
- Fluorescence image resolution: ~100 nm
- Complementary information helps with sample analysis

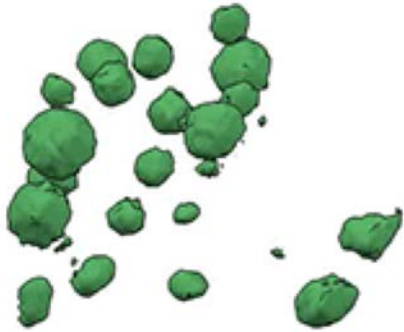


J. Deng, *et al. Sci. Rep.* (accepted)

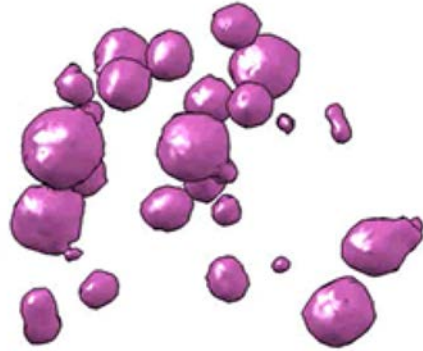


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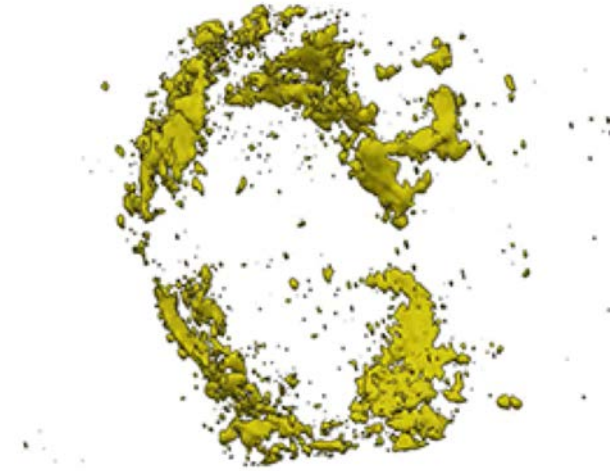
Extended to 3D



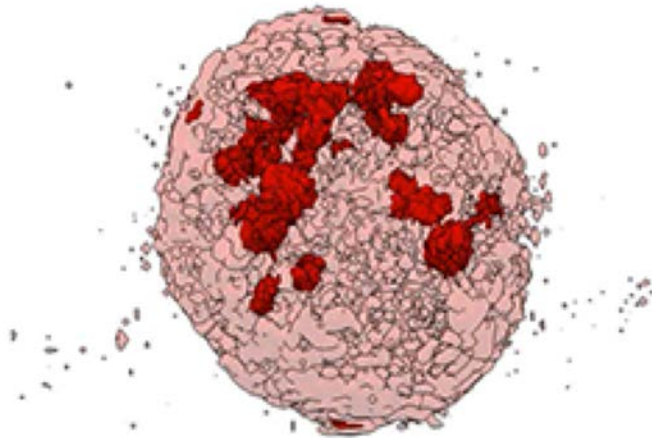
P



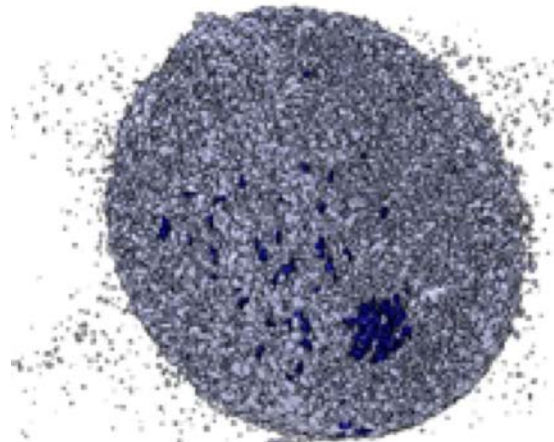
Ca



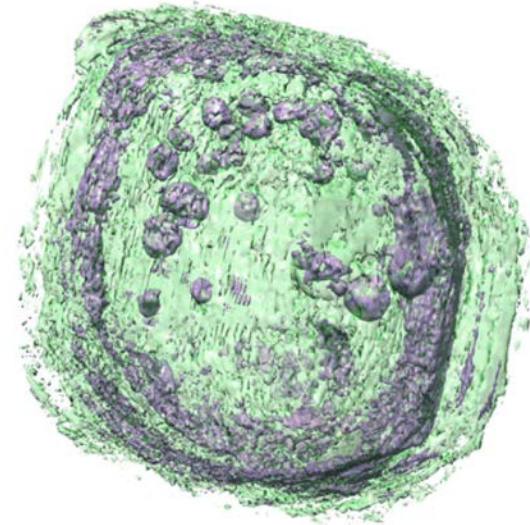
Cl



K



S

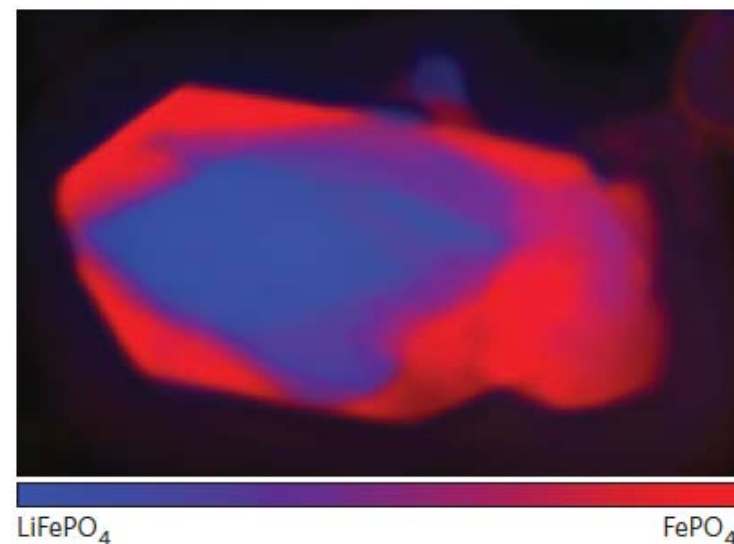
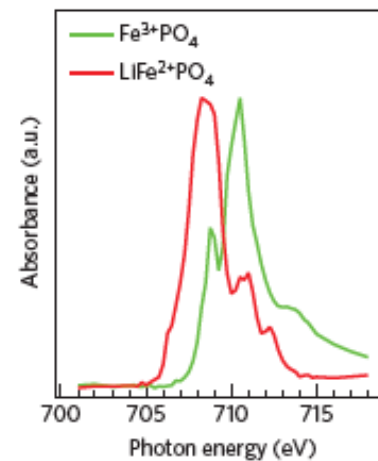
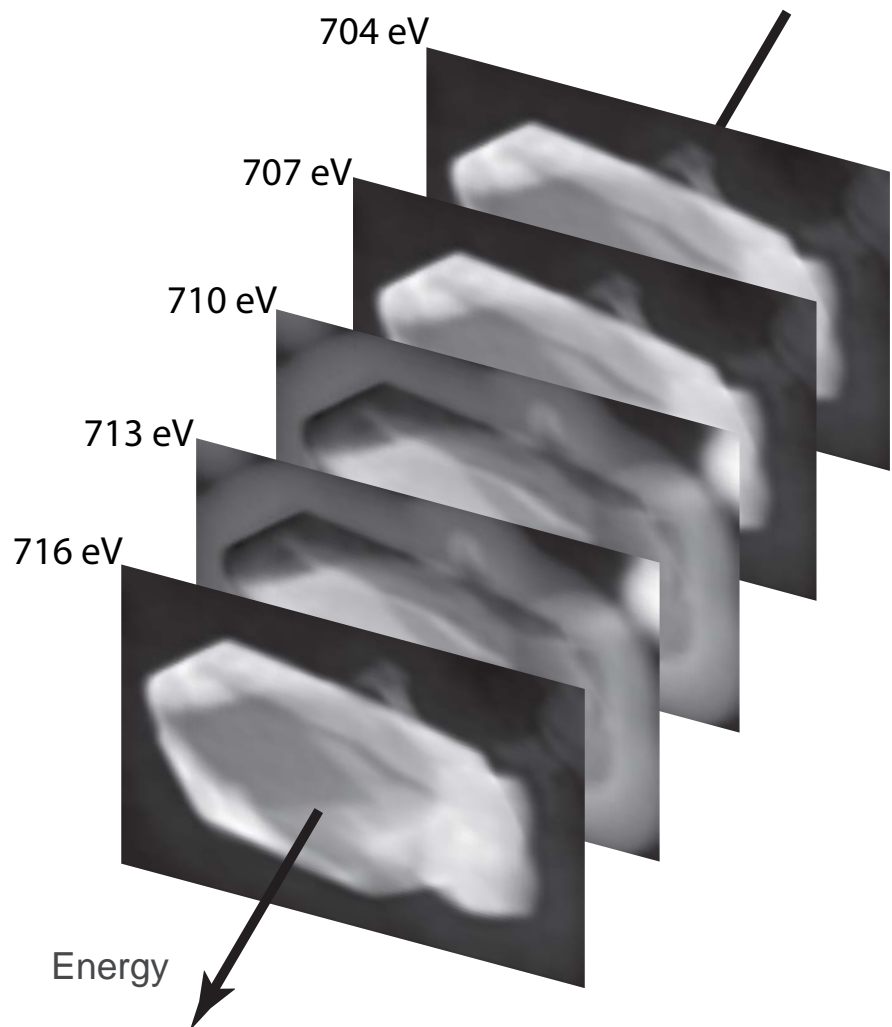


Ptycho

(In preparation)

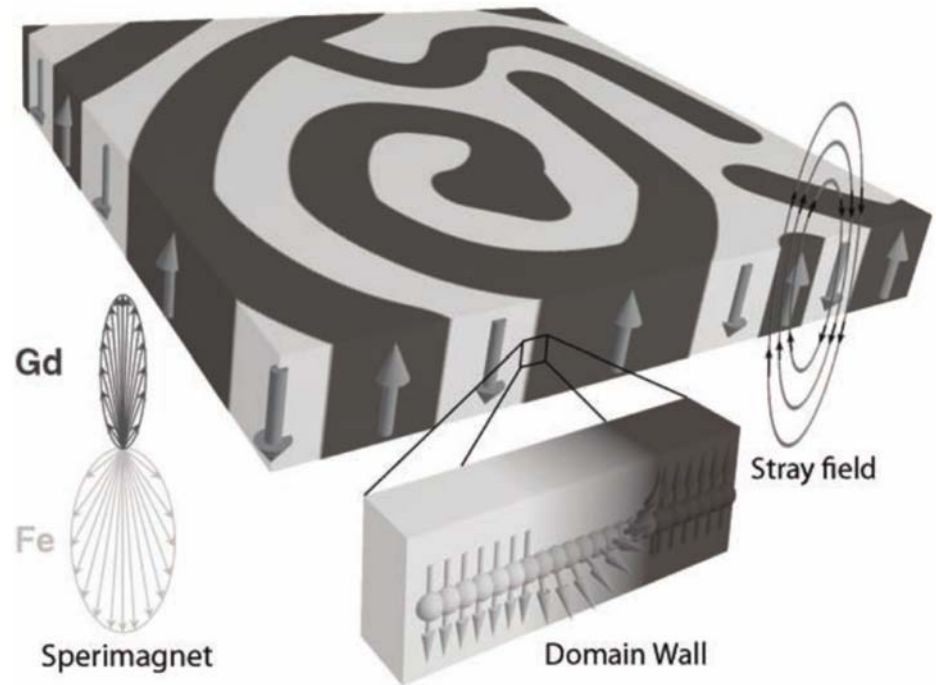
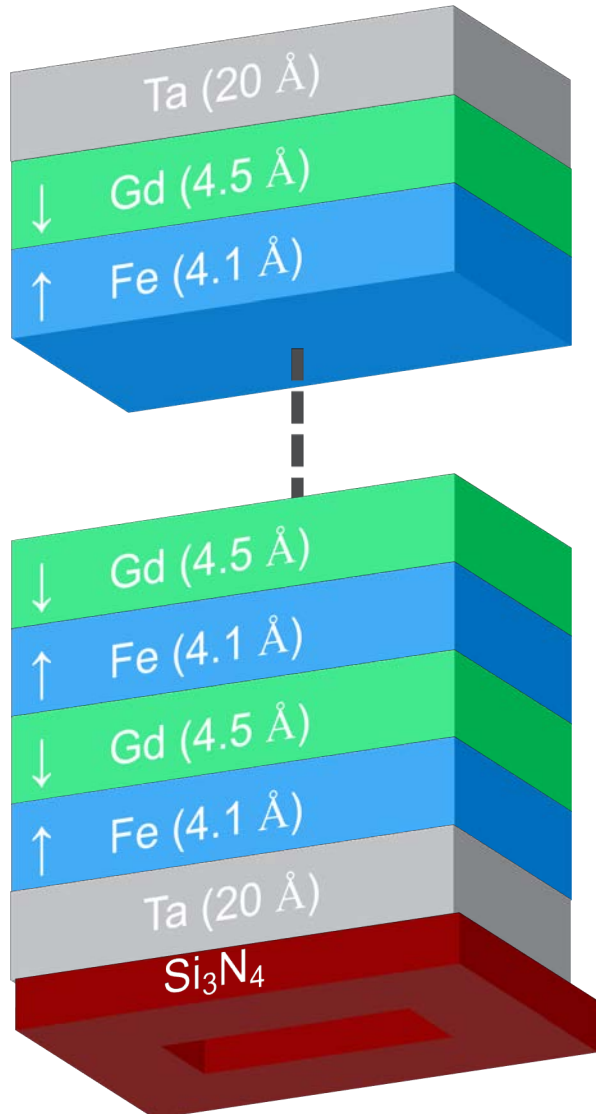
❖ Ptychographic spectroscopy

-- like STXM XNEAS analysis, but with higher resolution and more information (both absorption and phase) from refractive index



Adapted from D. Shapiro, *et al. Nat. Photon.* **8**, 765 (2014)

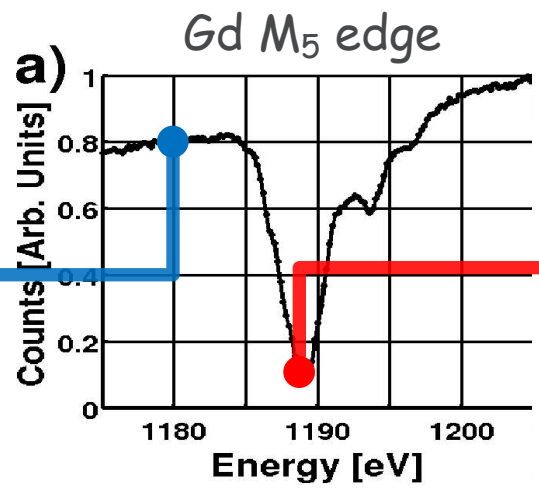
GDFE LAYERED MAGNETIC FILMS



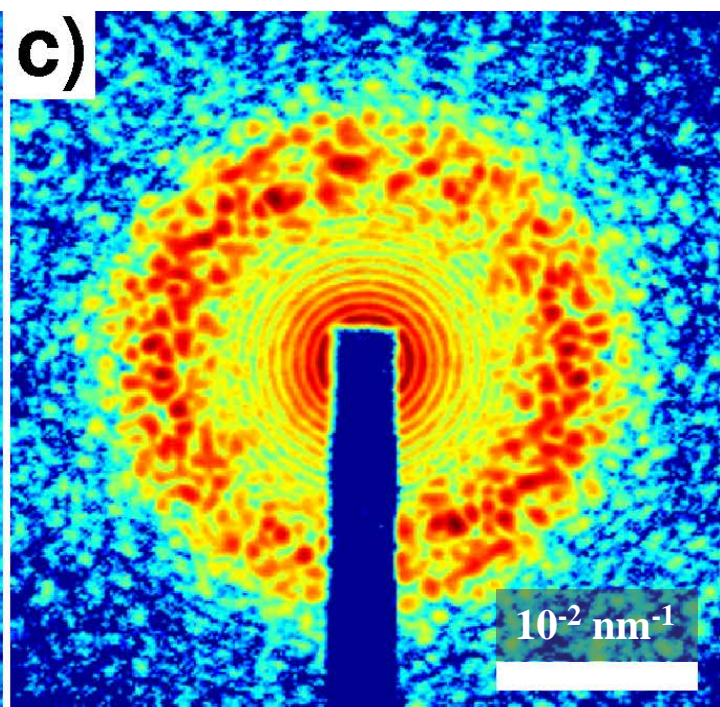
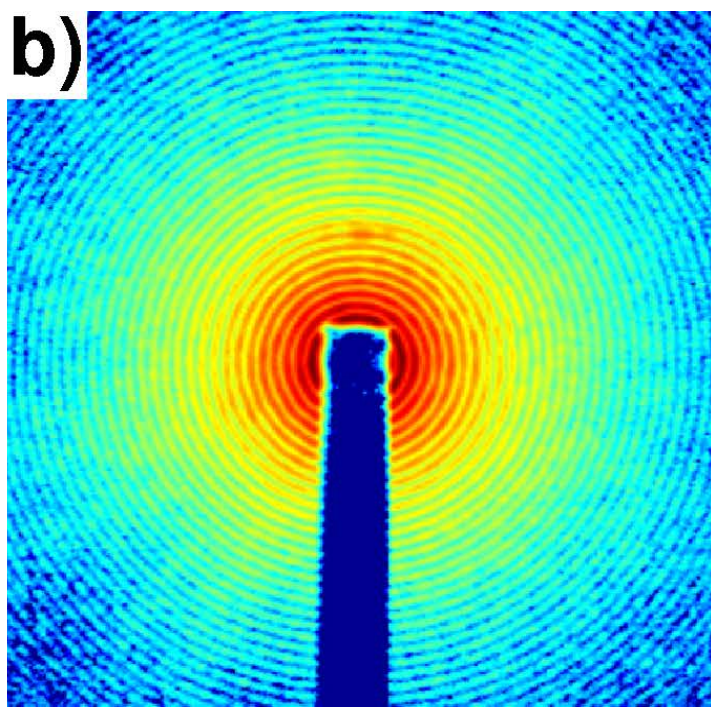
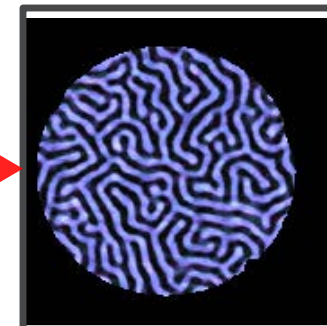
$$E_{tot} = \int \left[\underbrace{e_{ex}(\mathbf{m})}_{\text{exchange}} + \underbrace{e_{an}(\mathbf{m})}_{\text{anisotropy}} - \underbrace{\mu_0 \mathbf{H}_{ex} \cdot \mathbf{M}}_{\text{ext. field}} + \underbrace{\frac{1}{2} \mu_0 \mathbf{H}_d^2}_{\text{stray field}} \right] dV$$

MAGNETIC CONTRAST MECHANISM

Off-resonance: ●

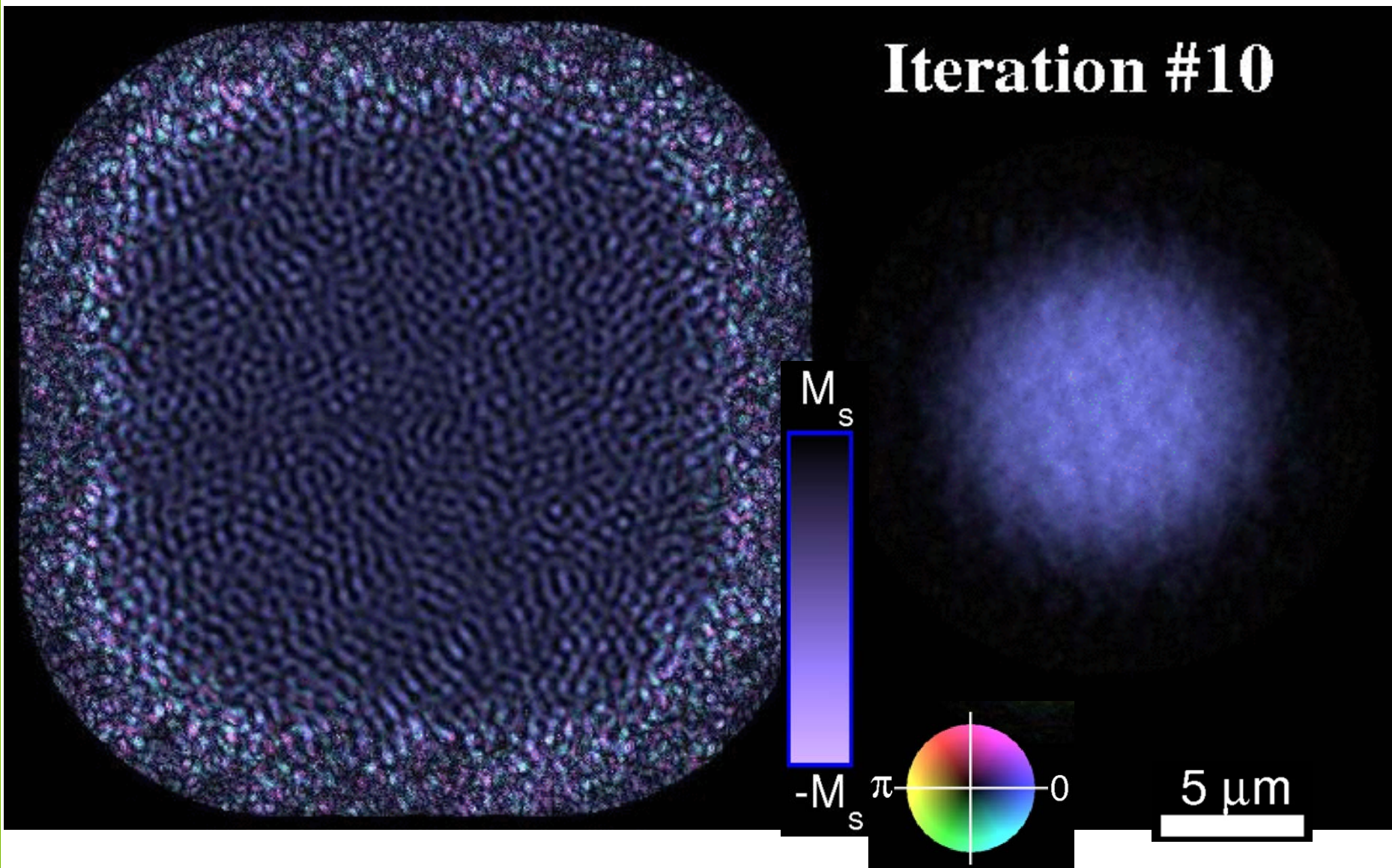


On-resonance: ●



REAL SPACE RECONSTRUCTION

Iteration #10

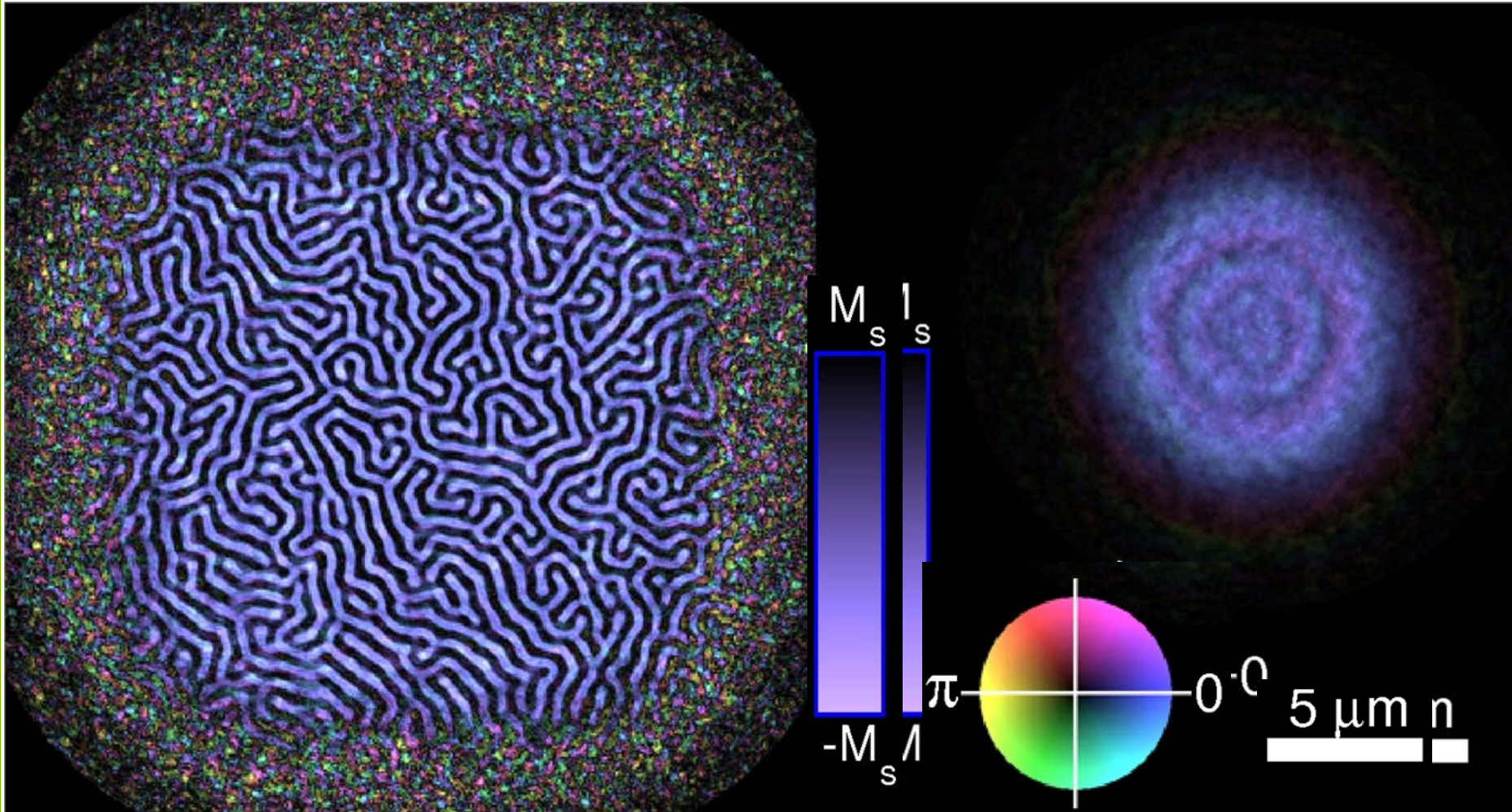


Magnetic structure

Illumination Function

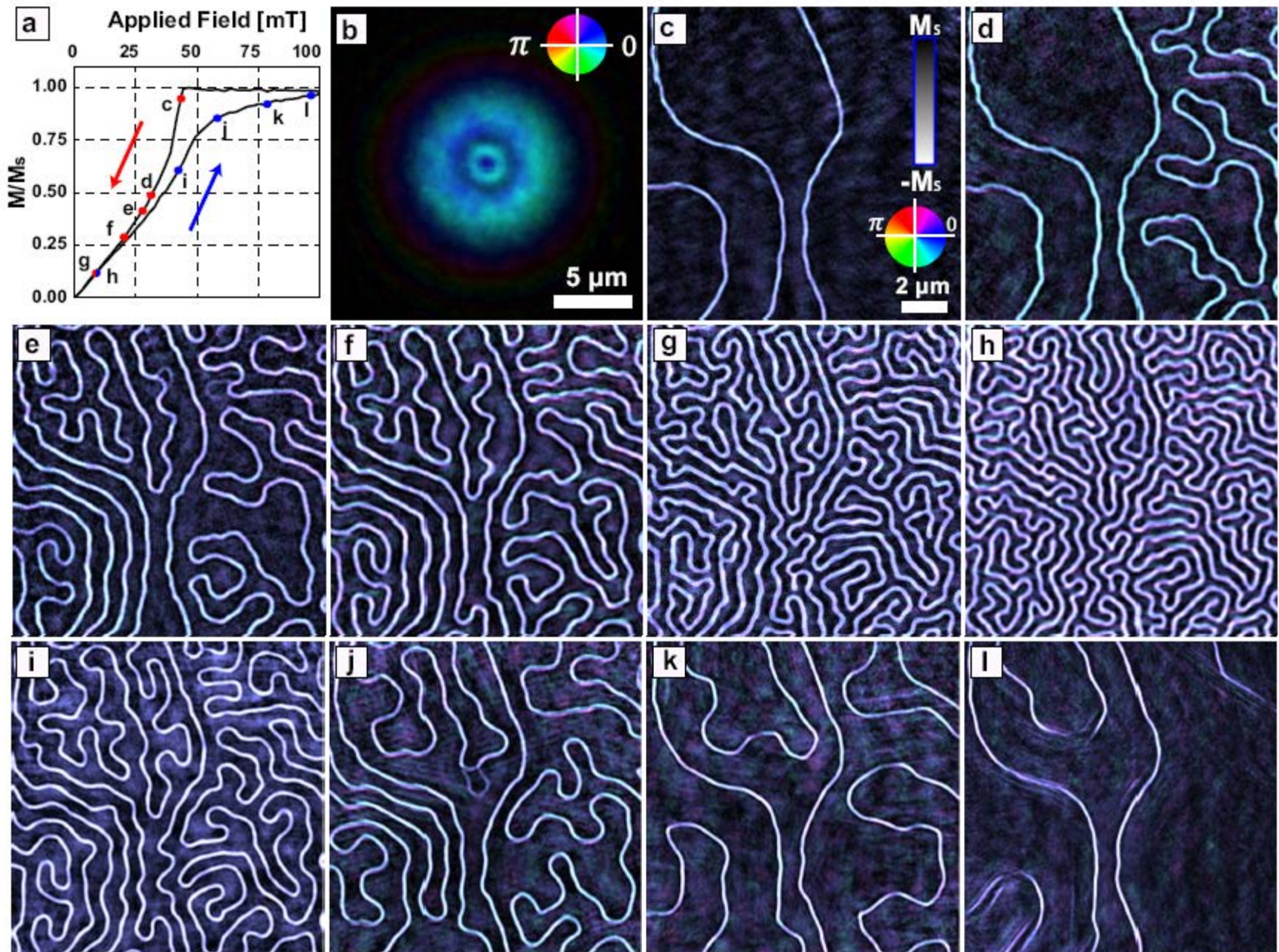
(exit wave) A. Tripathi, O.S. et al., Proc Natl Acad Sci USA 108, 13393 (2011)

REAL SPACE RECONSTRUCTION

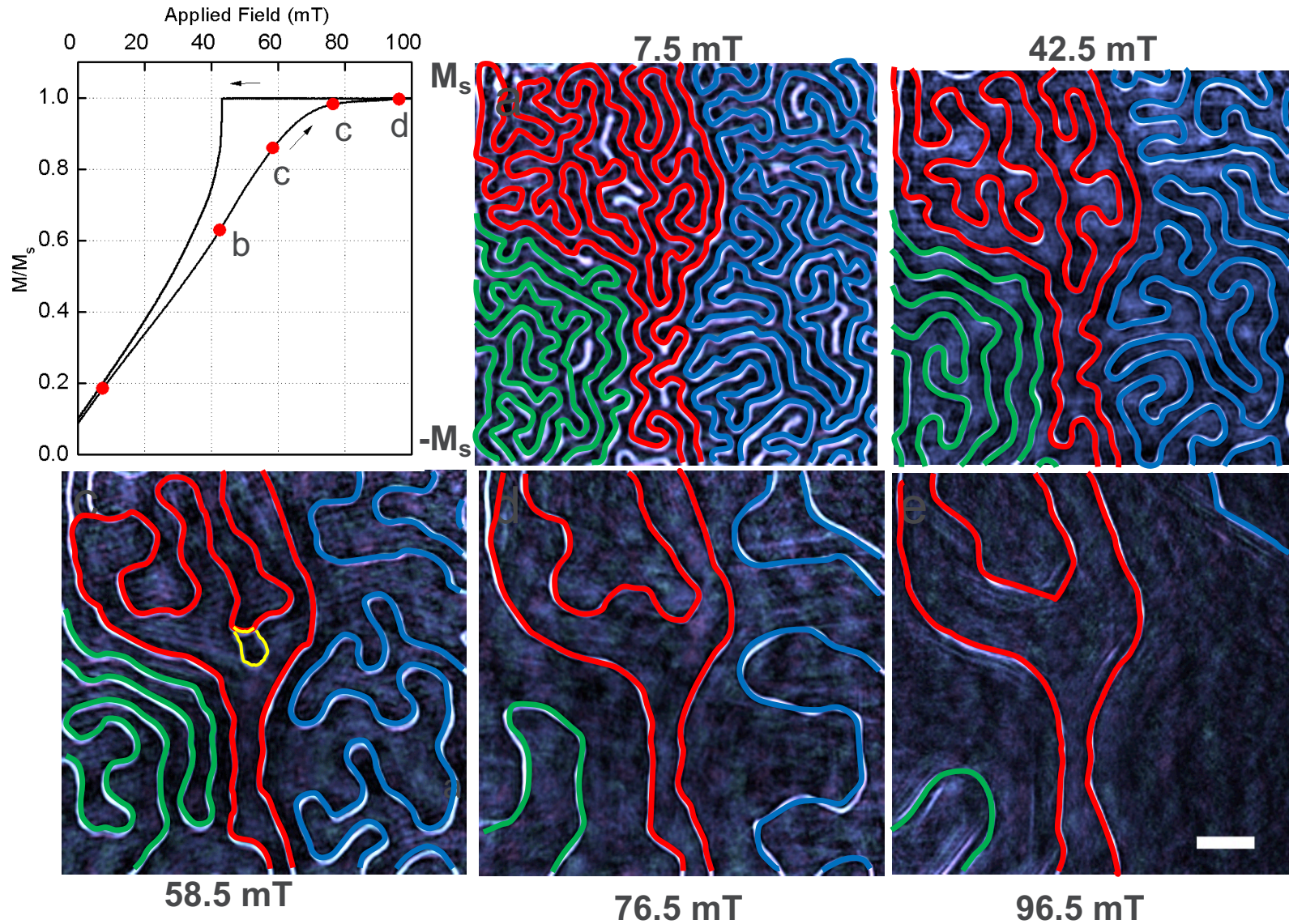


Magnetic structure
(exit wave)

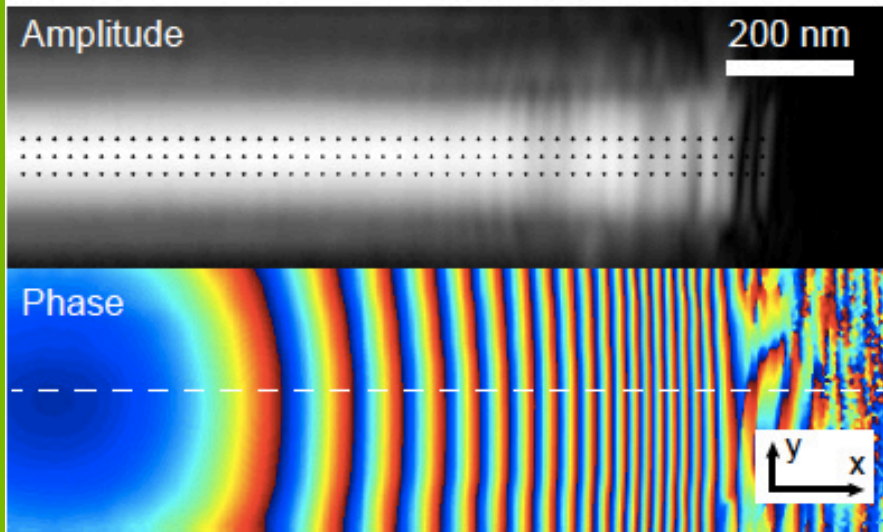
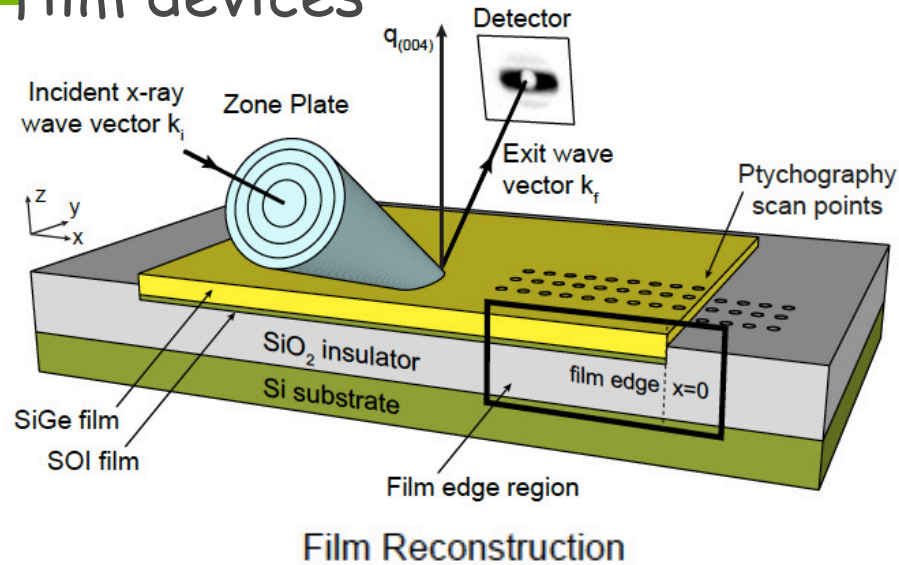
Illumination Function



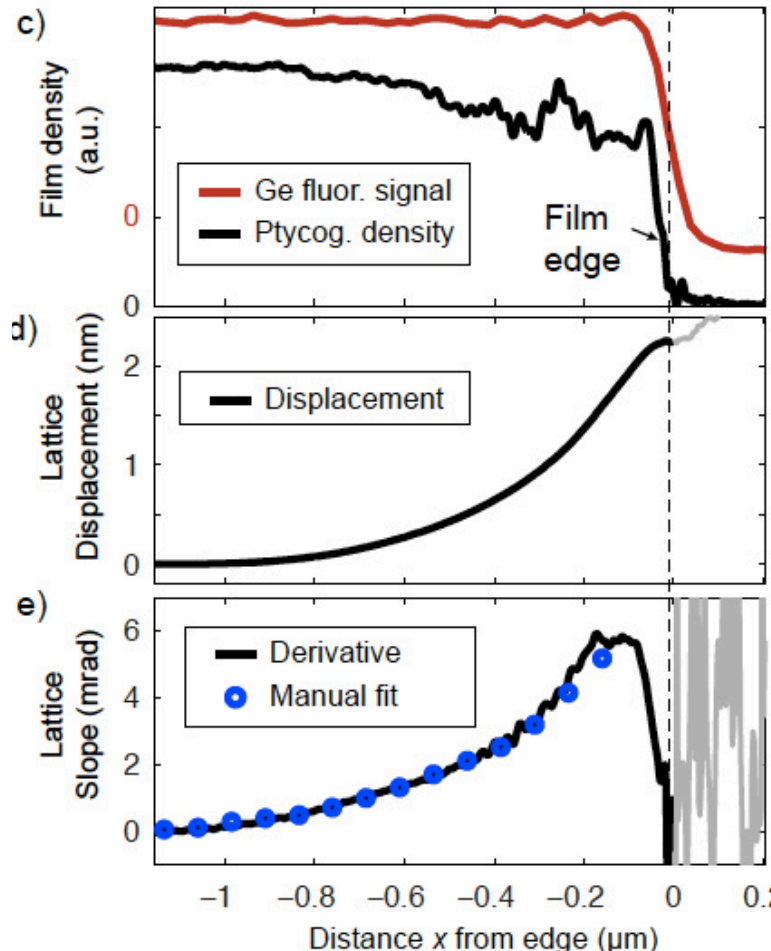
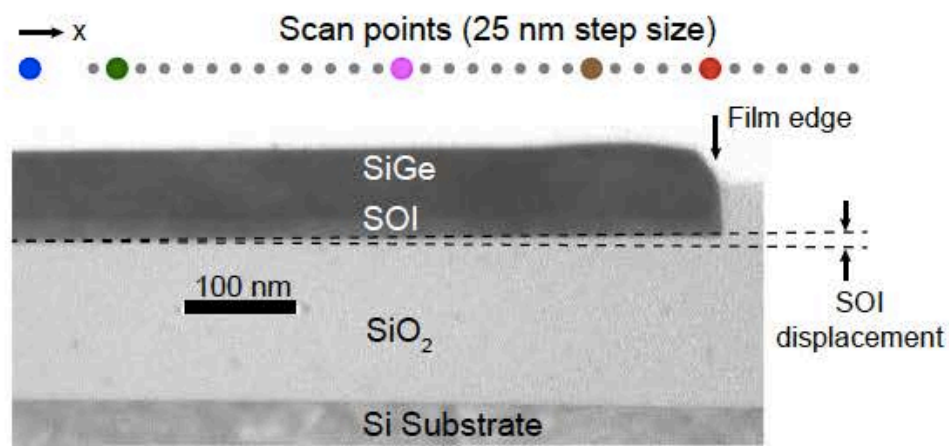
INCREASING FIELD



Nanoscale Strain in SiGe film devices

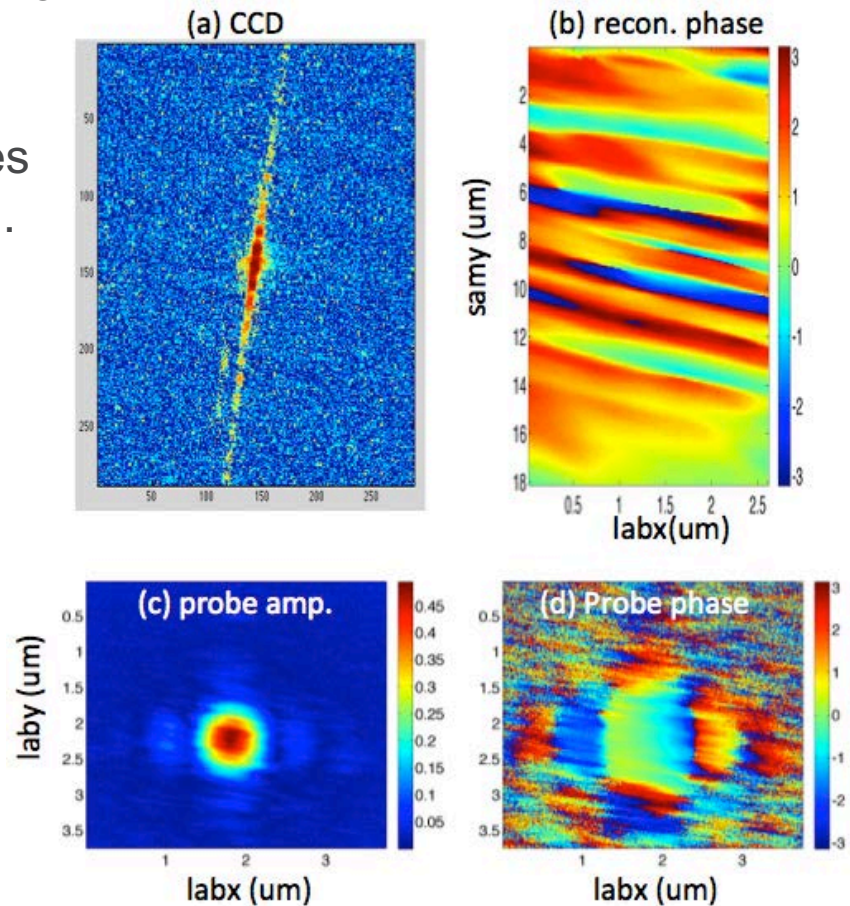
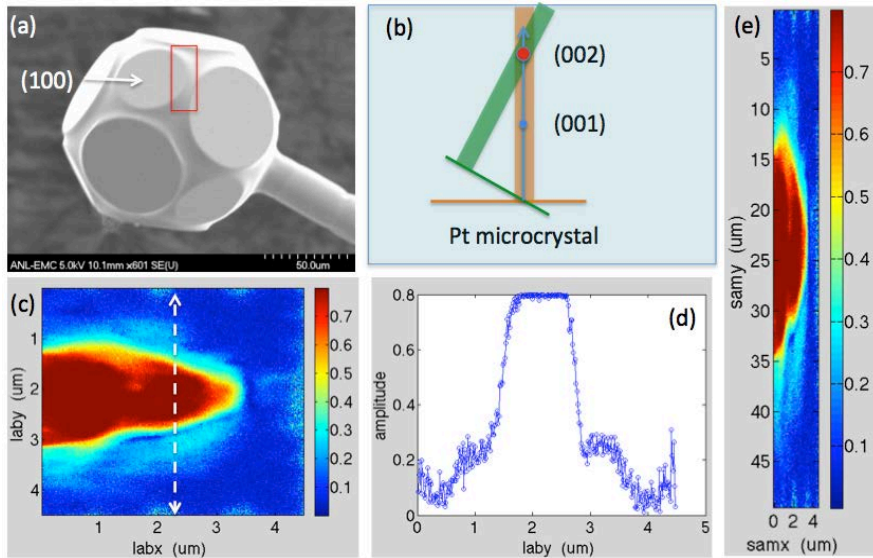


Hruszkewycz, S. O., Holt, M. V., et al. (2012). *Nano Letters*, 12(10), 5148–5154.



SURFACE DIFFRACTION COHERENT IMAGING

- Image local surface structure
- Steps and step dynamics during film growth or interfacial reactivity
- Nanoparticle nucleation
- Defect distributions, particularly at interfaces
- Combined with x-ray micro fluorescence.....

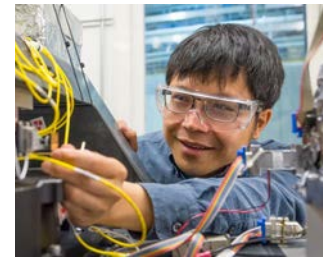
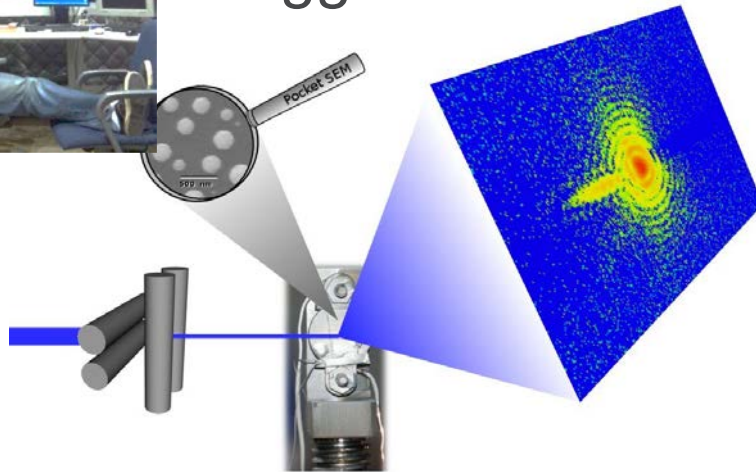


C. Zhu, et al. *Applied Physics Letters*, vol. 106, no. 10, p. 101604, Mar. 2015.

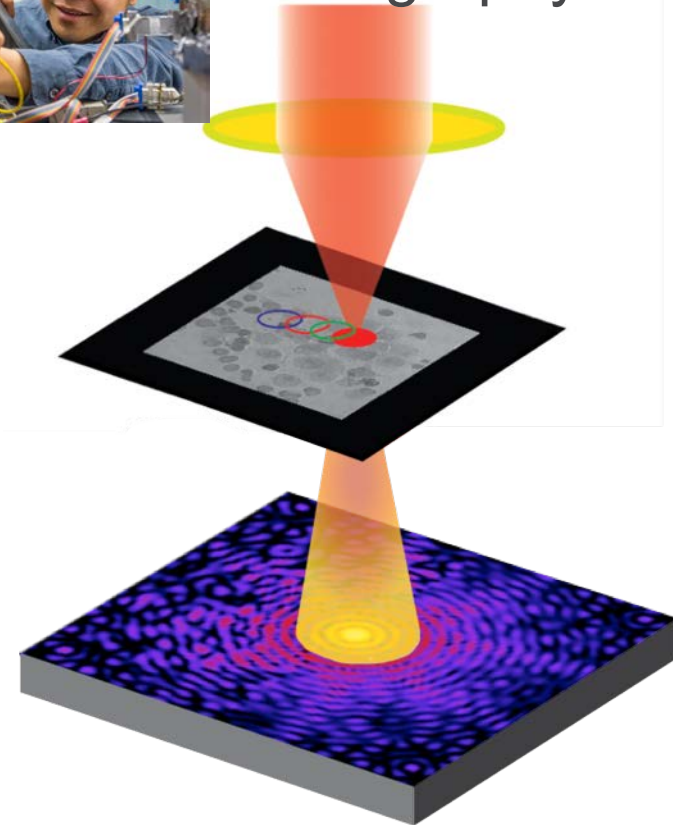
APPLY FOR COHERENT IMAGING BEAMTIME @ APS!



Bragg CDI

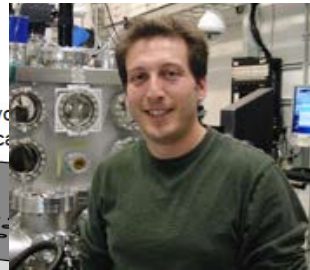
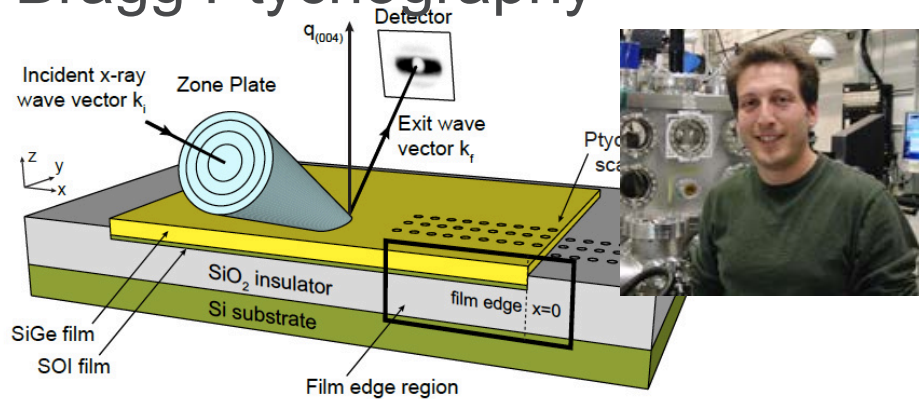


Ptychography Tomography



Email: Ross Harder rharder@aps.anl.gov
<https://wiki-ext.aps.anl.gov/s34idc/index.php/34-ID-C>

Bragg Ptychography



Email: Junjing Deng junjingdeng@aps.anl.gov

Email: Martin Holt mvholt@anl.gov
<https://wiki-ext.aps.anl.gov/s26id/index.php/26-ID>

<https://www.aps.anl.gov/Users-Information>