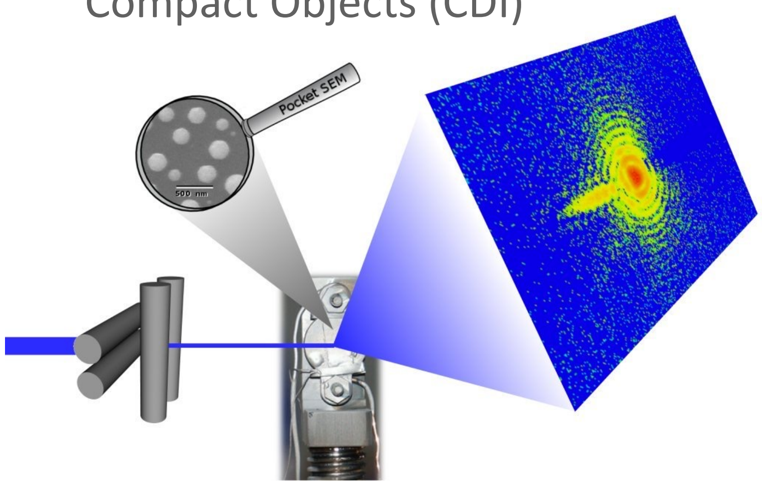
Coherent Diffraction Imaging

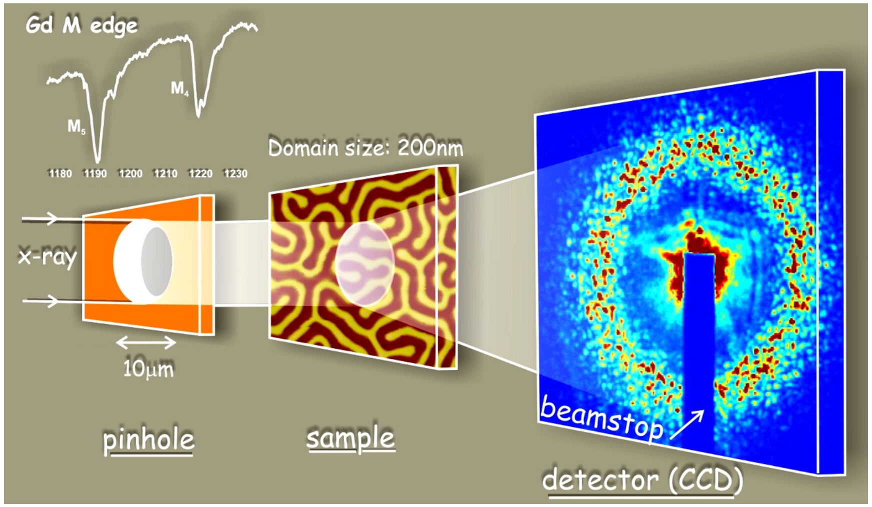
Ross Harder
34-ID-C
Advanced Photon Source

Acknowledgments:
Prof. Ian Robinson (BNL)
Dr. Xiaojing Huang (BNL)
Dr. Jesse Clark (~~PULSE institute, SLAC~~ 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)

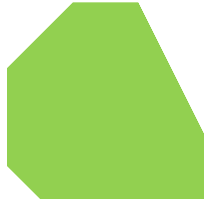


Non-compact samples (Ptychography)

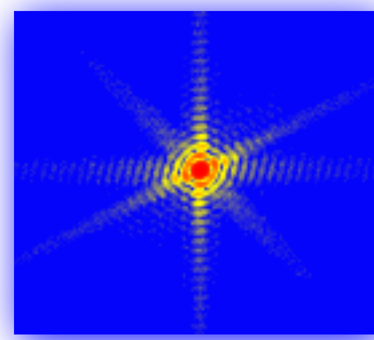


EXECUTIVE SUMMARY

Coherent X-rays



|Fourier Transform|^2



High resolution imaging of structure, beyond optics.

Coherent beam scatters from sample. (Various contrast mechanisms)

Measure modulus of Fourier Transform (Intensities).

Use computational algorithms to retrieve phases.

Recover image by Inverse Fourier Transform.

FFT

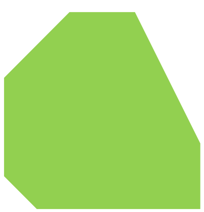
Reciprocal Space Constraints

Experimental Amplitudes
Oversampled
Thresholded
&
ZeroPadded

Direct Space Constraints

Support
Total Energy
Mixing previous iterates.
Positivity

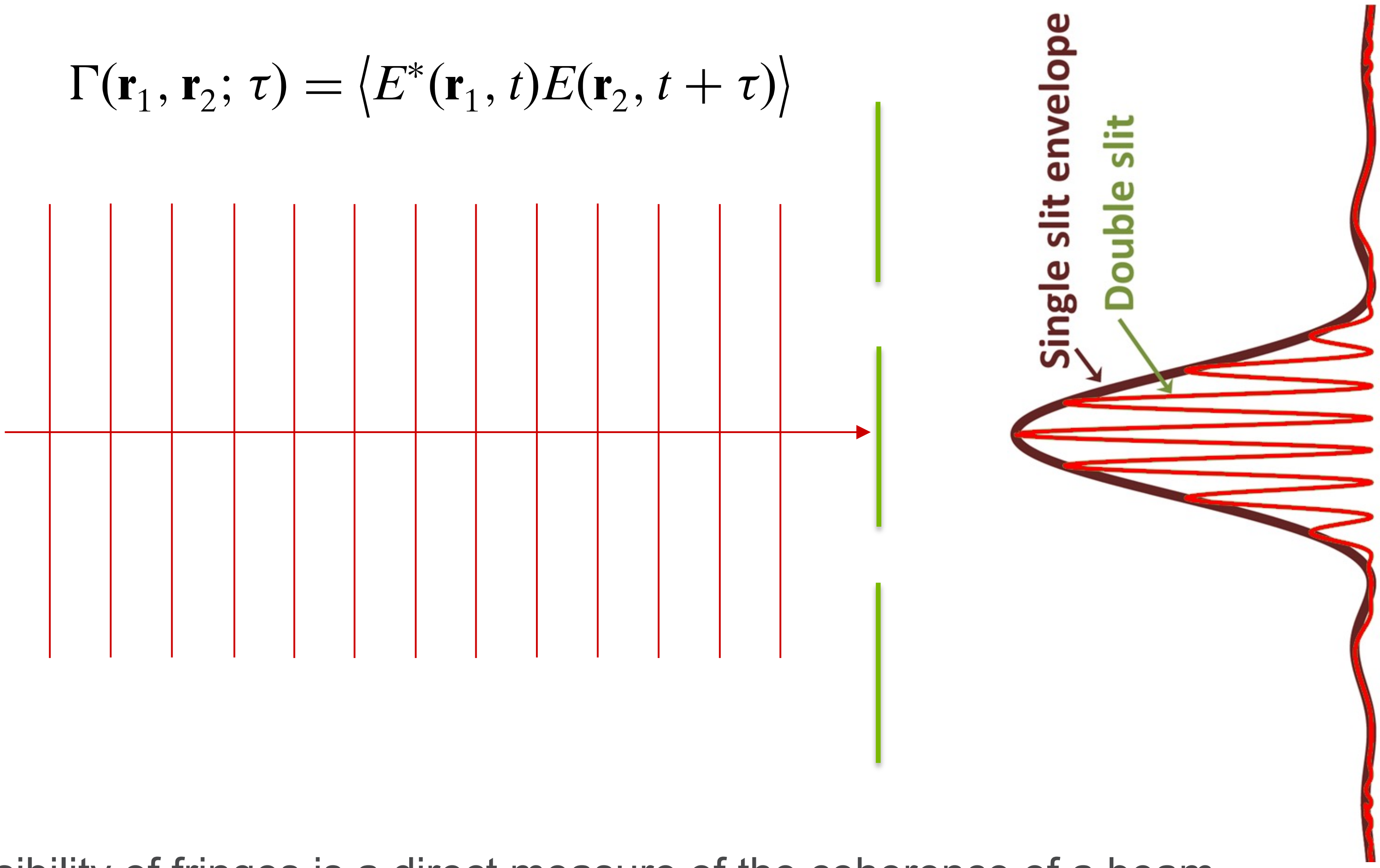
FFT^{-1}



Inverse Fourier Transform

COHERENCE

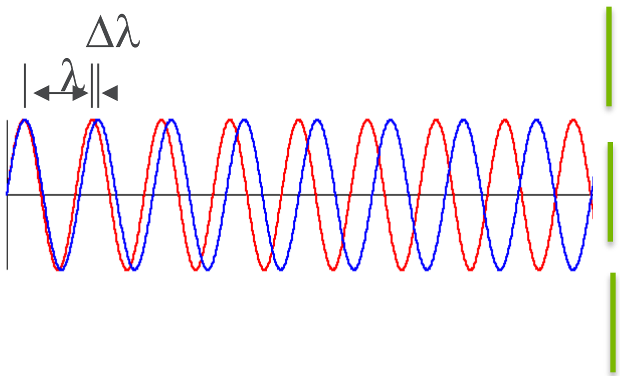
$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau) = \left\langle E^*(\mathbf{r}_1, t) E(\mathbf{r}_2, t+\tau) \right\rangle$$

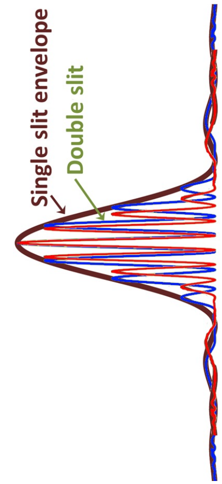


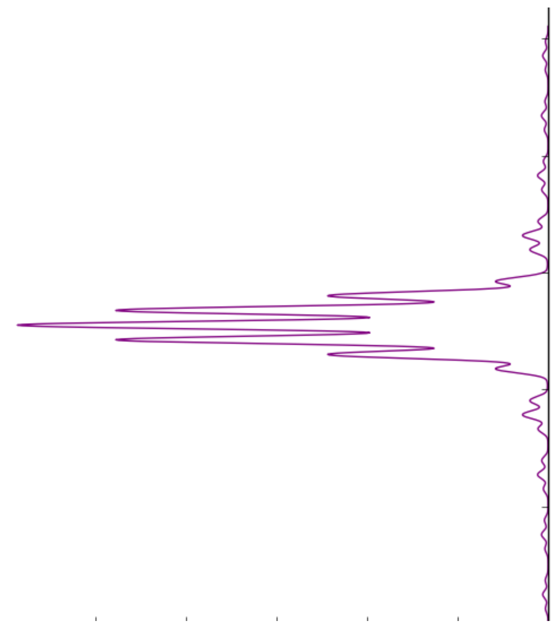
Visibility of fringes is a direct measure of the coherence of a beam.
If beam is coherent across the spacing of the slits a Fourier Transform of the slit structure is observed downstream.

COHERENCE

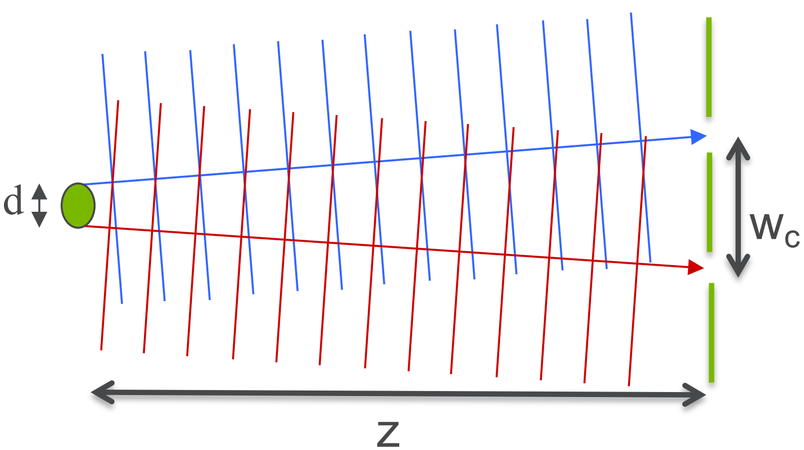
longitudinal coherence

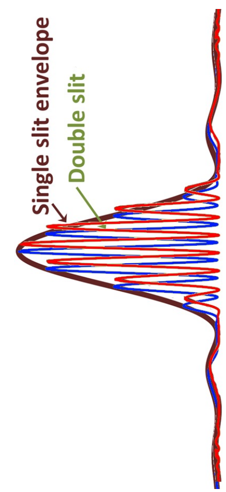






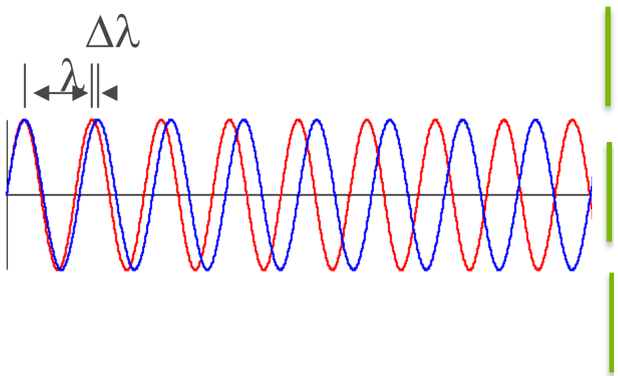
transverse coherence





COHERENCE

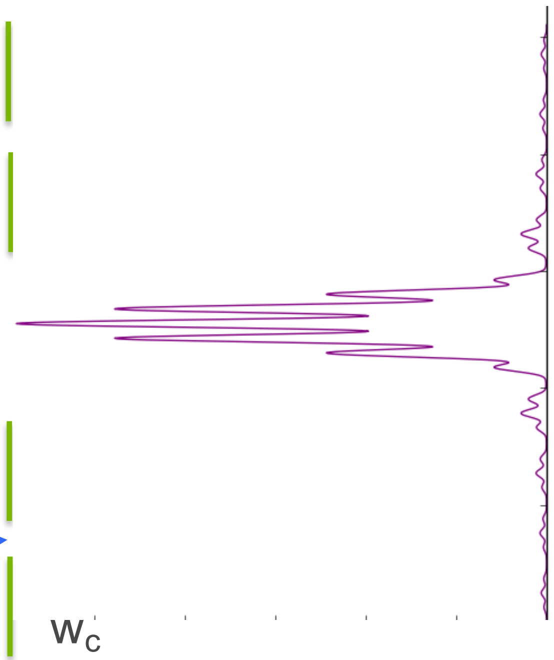
longitudinal coherence



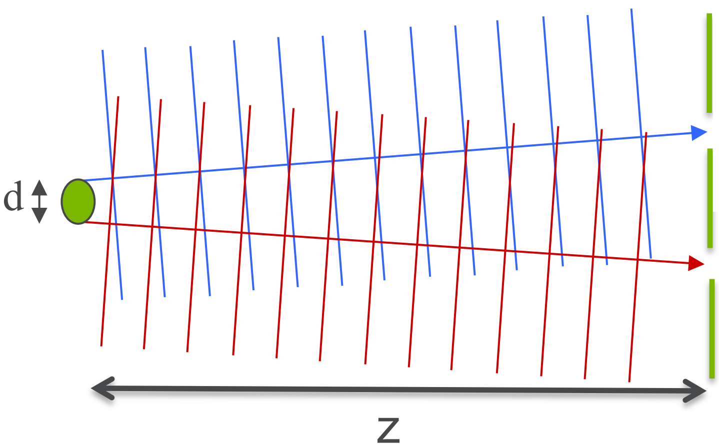
$$l_c \sim \frac{\lambda^2}{\Delta\lambda}$$

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

Si (111)
0.5 um or 1.5 fs



transverse coherence

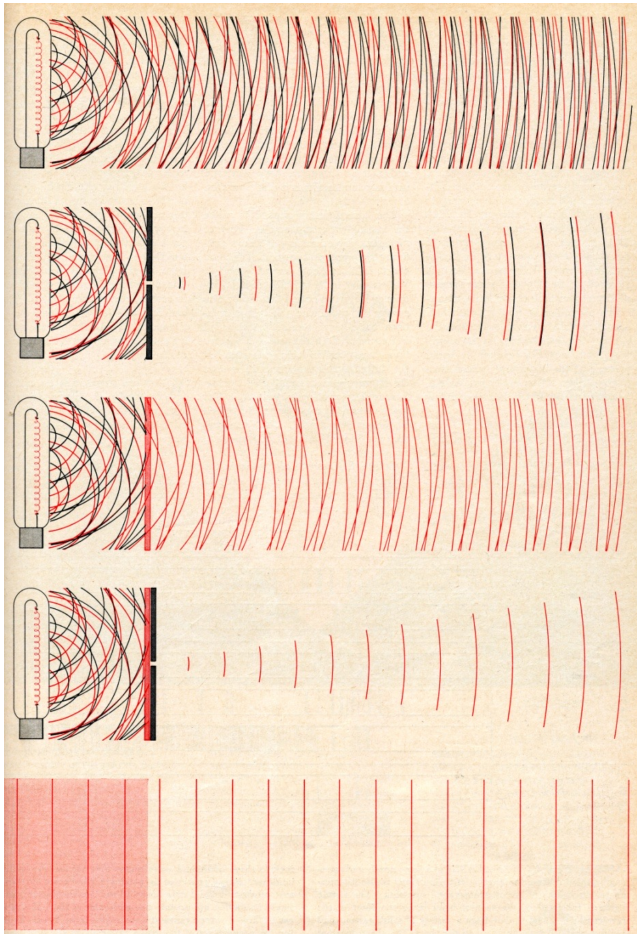


$$w_c \sim \frac{\lambda z}{d}$$

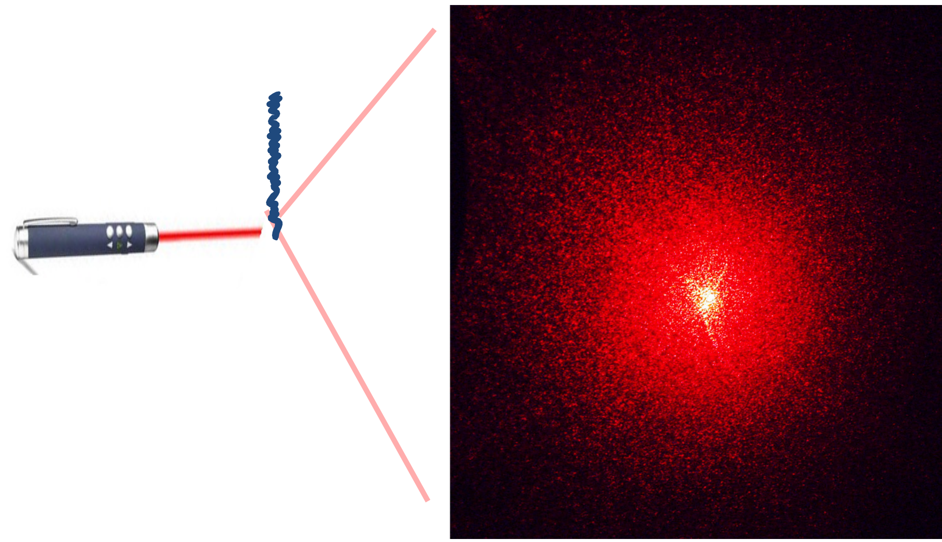
34-ID-C 50m
25x70 um @ 9 keV

Courtesy Prof. Oleg Shpyrko (UCSD)

Coherence: Laser Speckle



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



Laser Speckle: Interference pattern arising from randomly distributed scatterers

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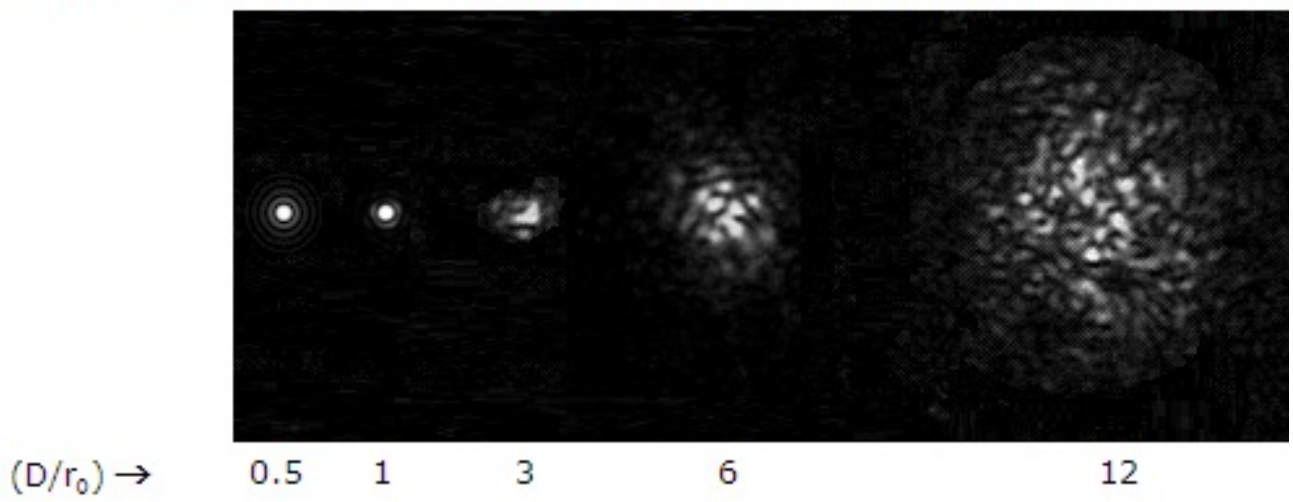
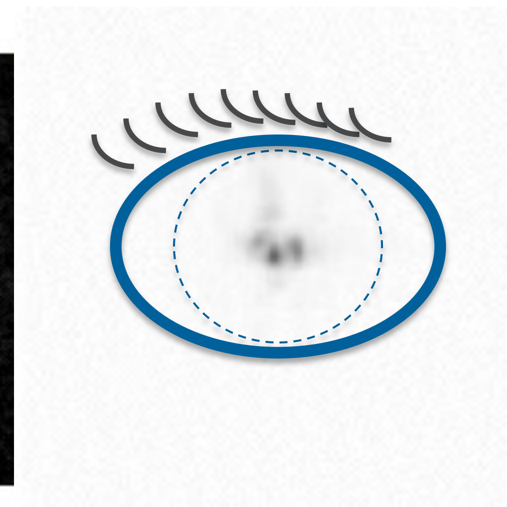
SIMPLEST SPECKLE EXPERIMENT: TWINKLE, TWINKLE LITTLE STAR



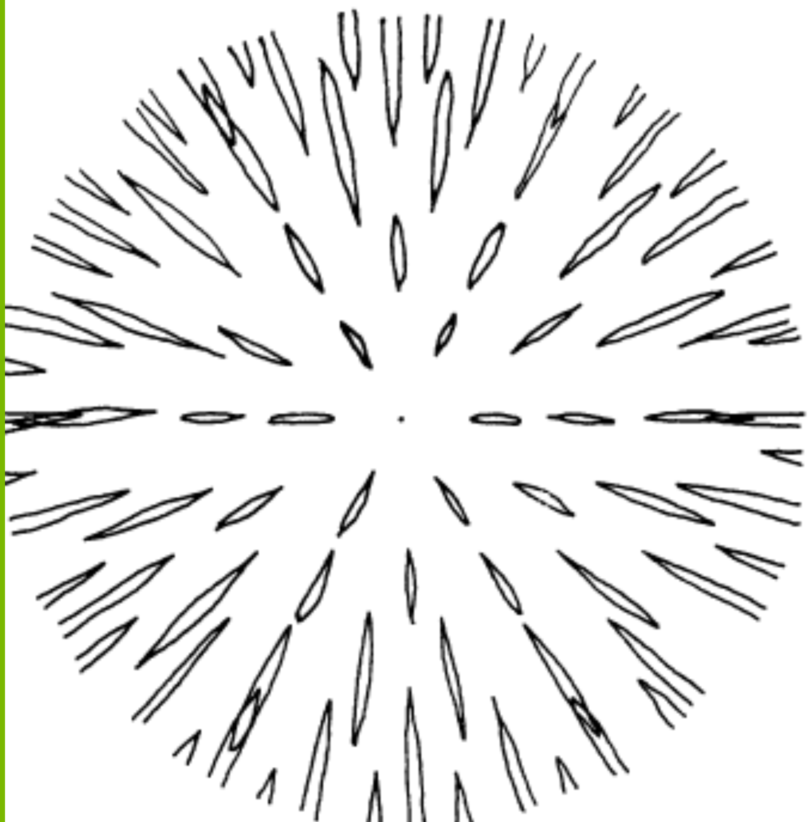


Stars are big, but very far away. As a result, their light has a high transverse coherence. As the light propagates through the atmosphere our eye detects a portion of the coherent diffraction

Courtesy Prof. Oleg Shpyrko (UCSD)

First Speckle: Exner, 1877

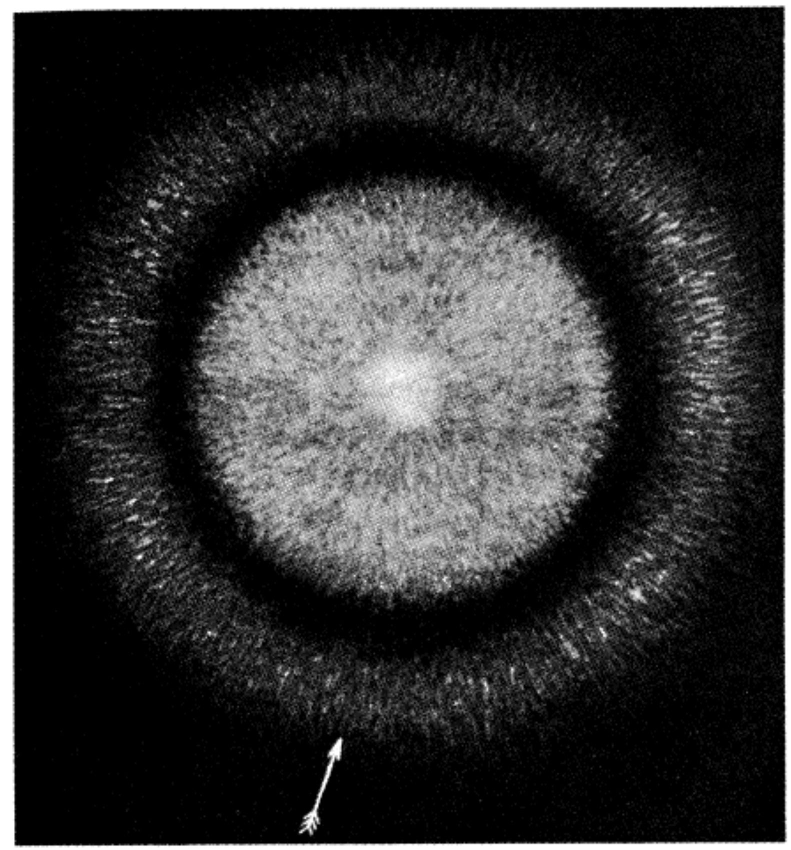
(using candle light)



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)

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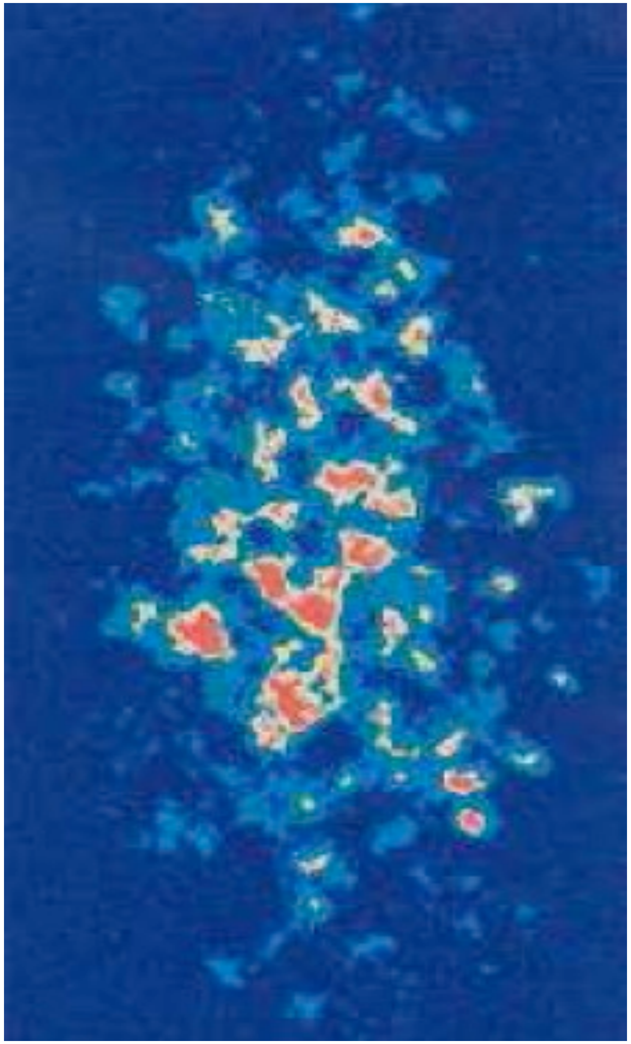
Courtesy Prof. Oleg Shpyrko (UCSD)

First X-ray Speckle:

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



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

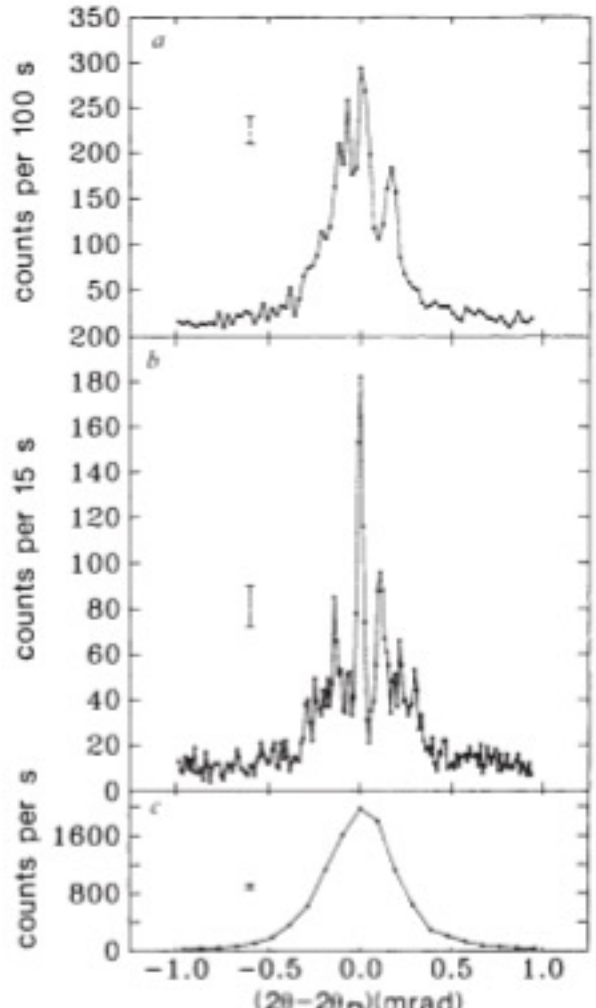


FIG. 4 Speckle patterns measured using *a*, 2.5-μm, *b*, 5 μm and *c*, 50-μm collimating pinholes. The analysing pinholes used were 50, 25 and 100 μm, respectively. Representative error bars are indicated, and the solid lines simply connect the data points. The (001) Bragg angle, $2\theta_B$, is ~23.9°.

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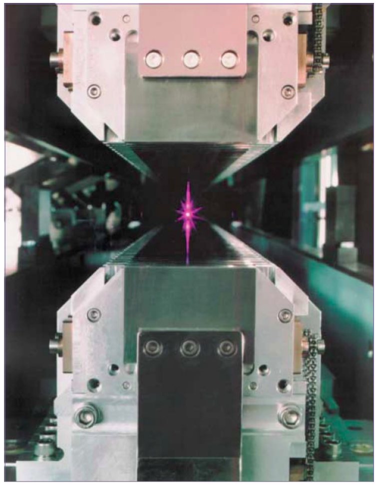
Courtesy Prof. Oleg Shpyrko (UCSD)

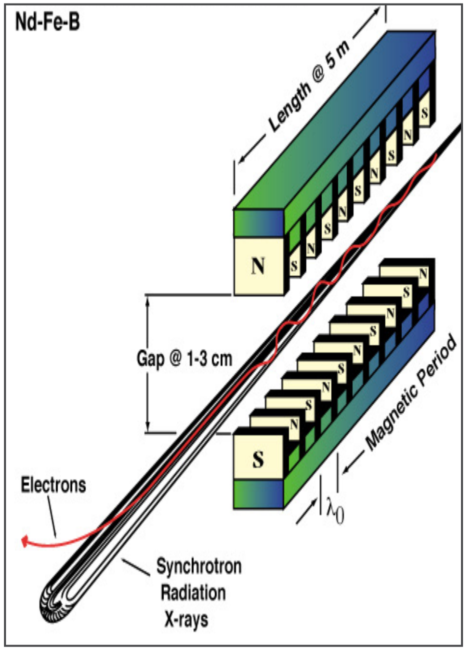
WHY USE SYNCHROTRON RADIATION?



Synchrotron sources offer:

- Brightnesss (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 = photons/source area, divergence, bandwidth

$F_c \sim \lambda^2 B$

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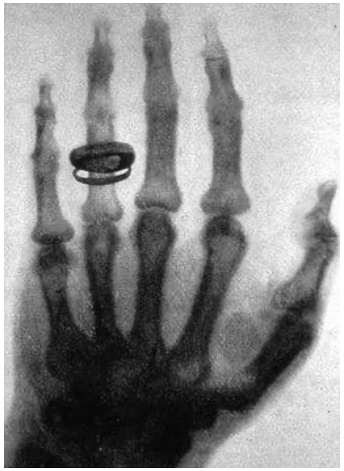
COHERENT X-RAY REFERENCES

- 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)

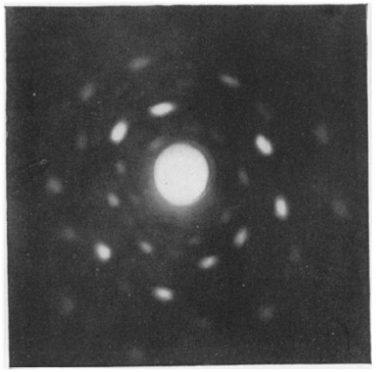


Roentgen, Nobel 1900

X-ray Diffraction (Scattering)

Coherent Imaging is scattering

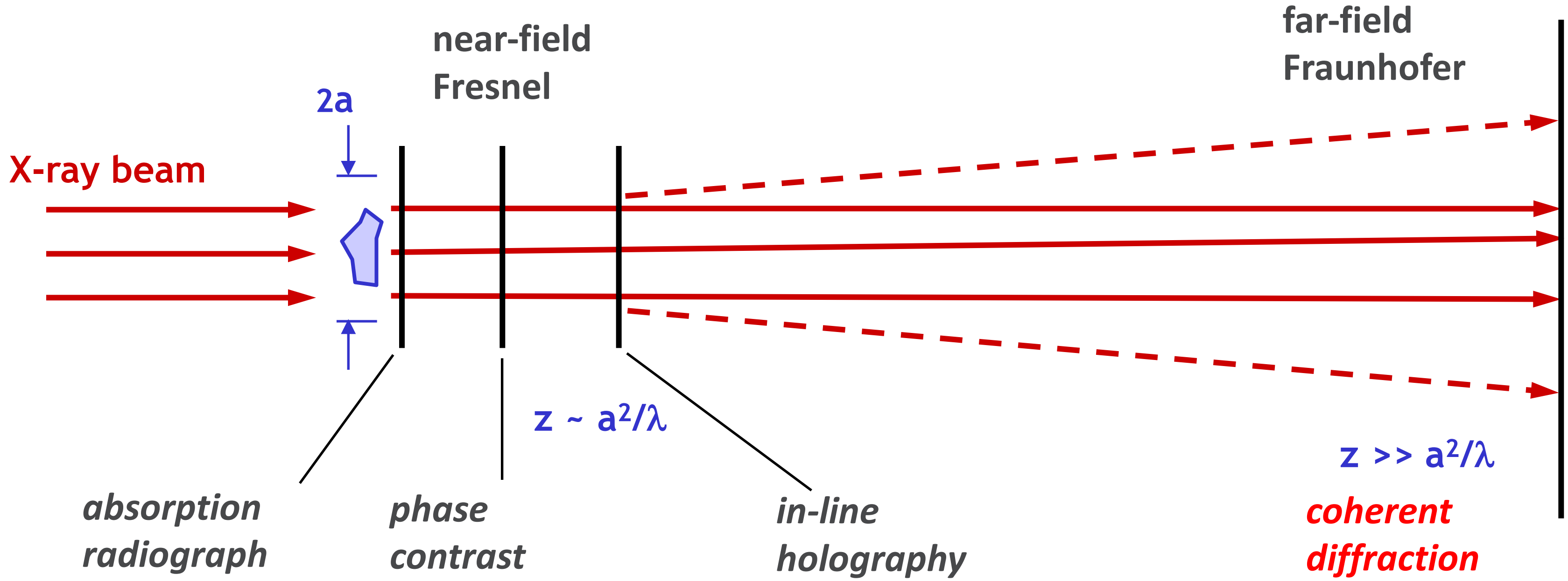
- Is particularly sensitive to periodicity in the sample (Crystals)
- Atomic resolution (unit cell)



Von Laue, Nobel 1914
Bragg & Bragg, Nobel 1915

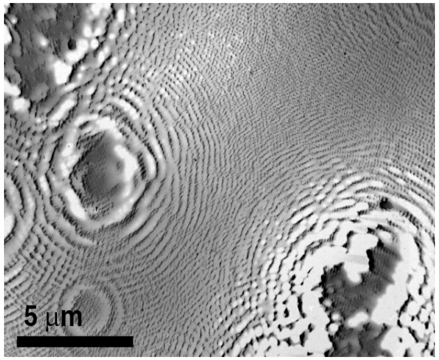
Courtesy Prof. Oleg Shpyrko (UCSD)

IMAGING REGIMES WITH COHERENT X-RAYS

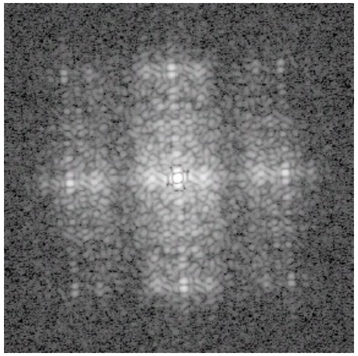


Roentgen, Nobel 1900

Kagoshima (1999)



Jacobsen (1990)

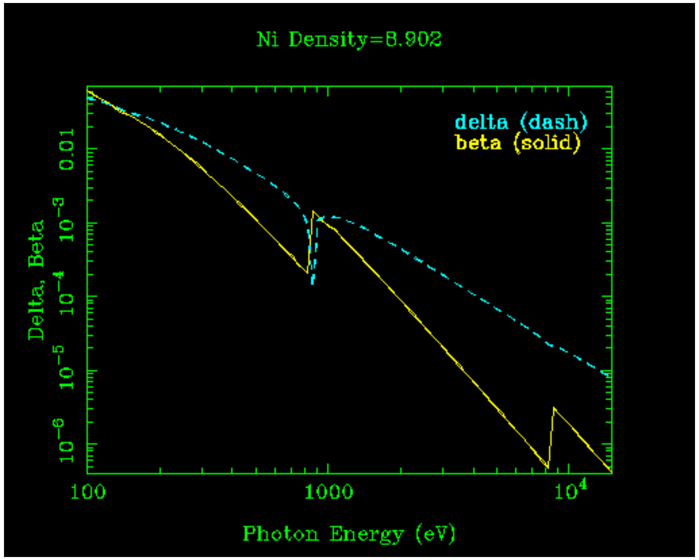


Miao (1999)

REFRACTIVE INDEX AND CONTRAST IN THE X-RAY REGION

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

$$A = A_0 \exp(-inkt)$$
$$k = 2\pi / \lambda$$



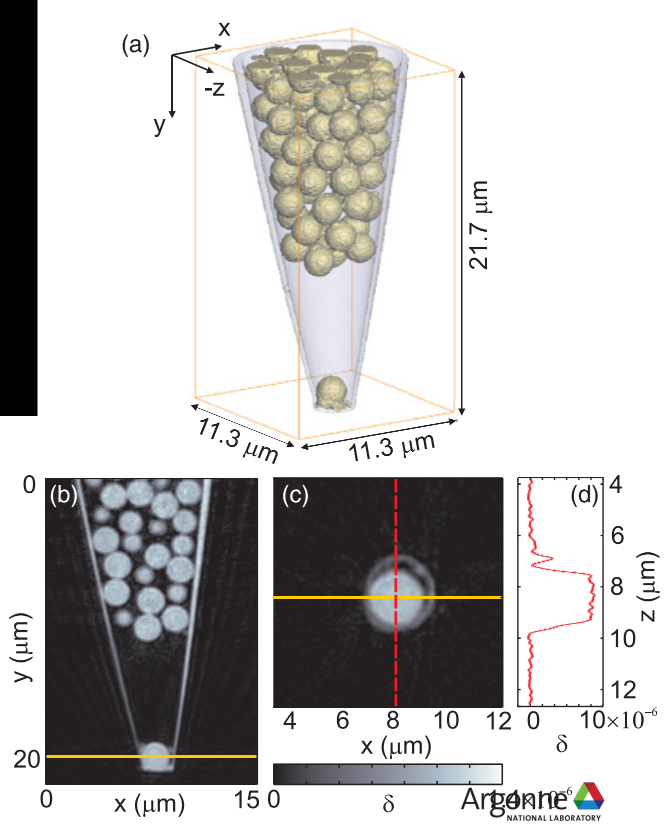
- Absorption contrast: sensitive to *Im(n)*

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

- Phase contrast: sensitive to *Re(n)*

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

PHYSICAL REVIEW B **85**, 020104(R) (2012)



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

REFRACTIVE INDEX AND CONTRAST IN THE X-RAY REGION

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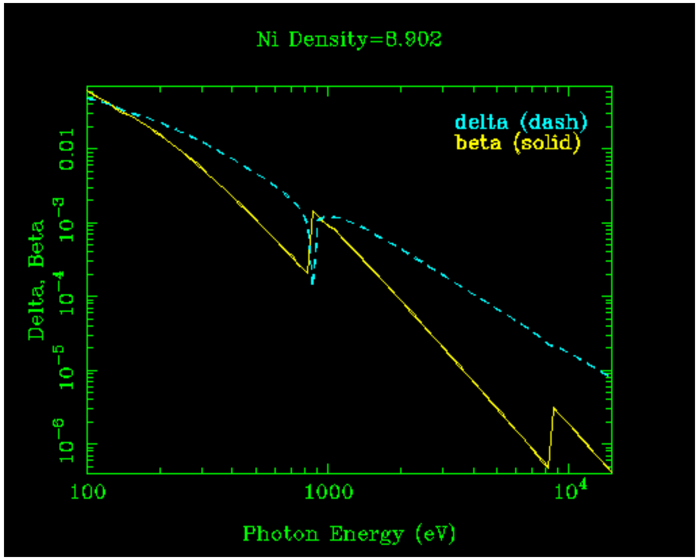

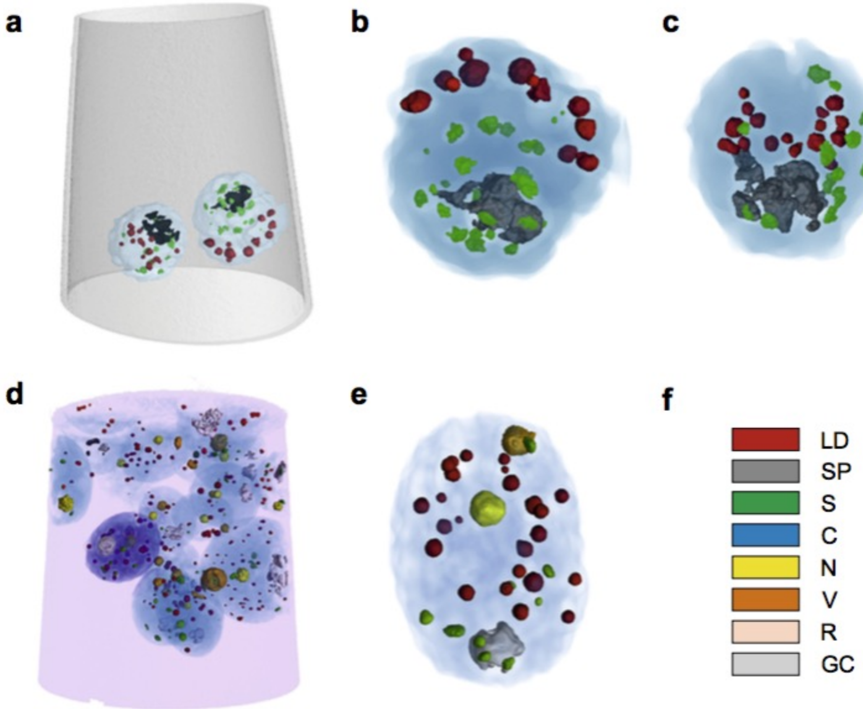

A. Diaz,et al., Journal of Structural Biology, vol. 192, no. 3, pp. 461–469, Oct. 2015.

Absorption contrast:

sensitive to *Im(n)*

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

Phase contrast:

sensitive to *Re(n)*

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

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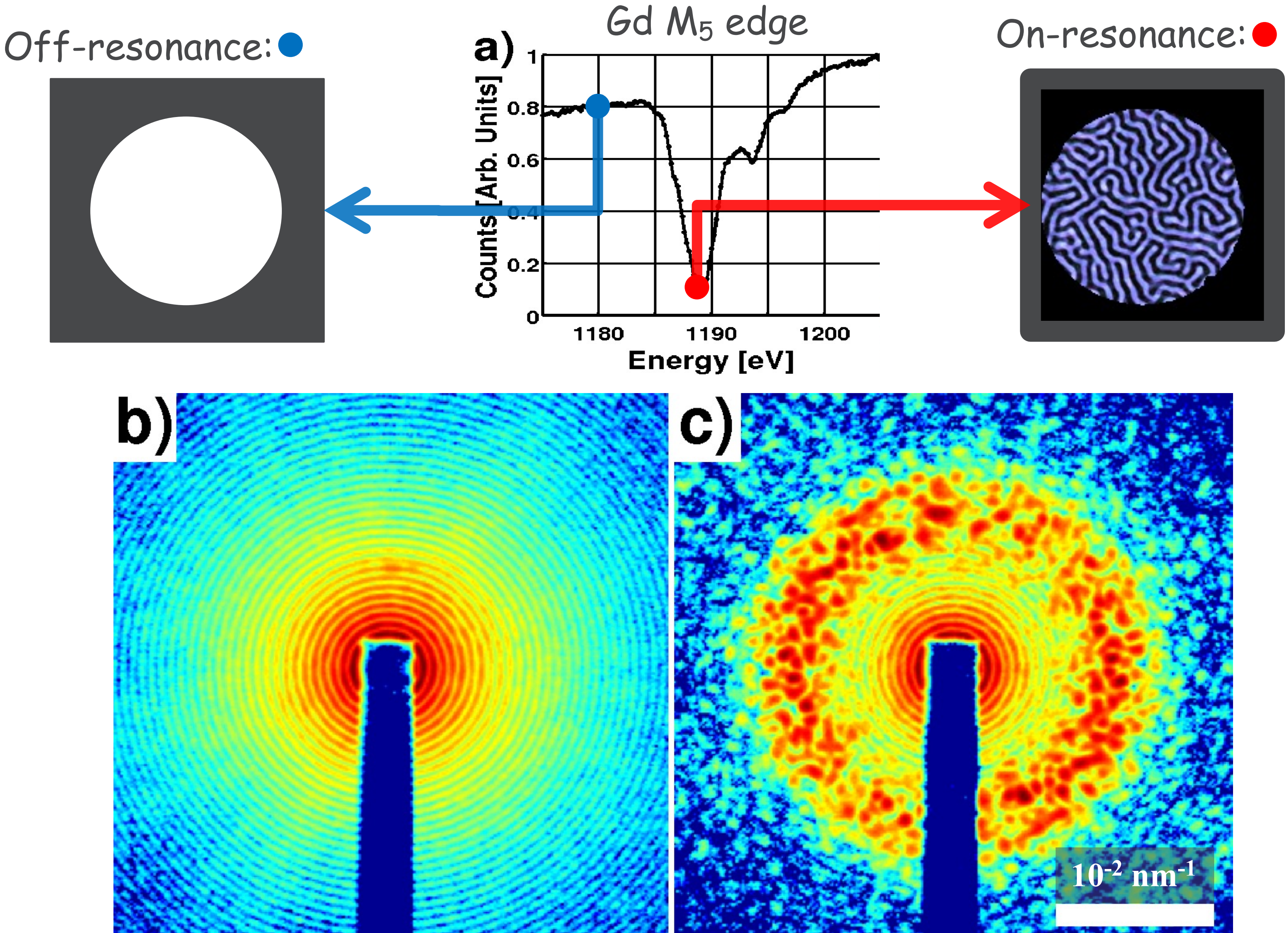
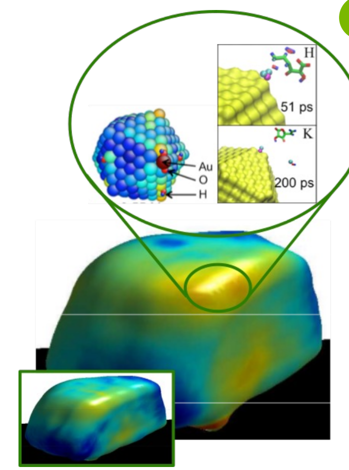
MAGNETIC CONTRAST IN FEGD

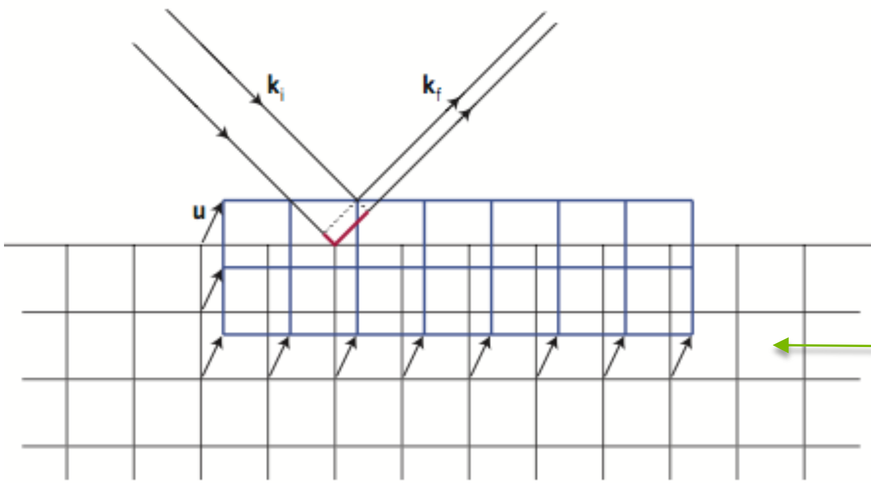


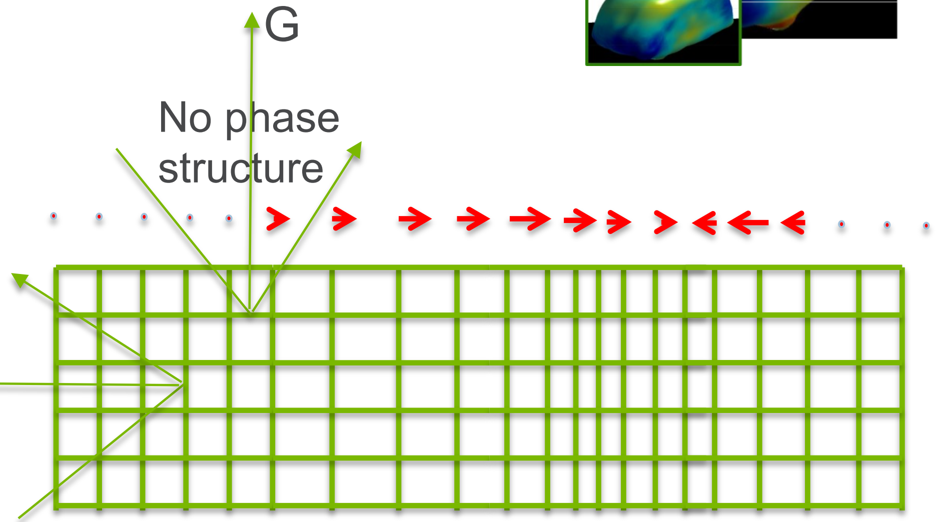
A. Tripathi, O.S. et al., Proc Natl Acad Sci USA 108, 13393 (2011)

CDI IN BRAGG GEOMETRY: IMAGING DISPLACEMENT FIELD (STRAIN)



Displacement field u(r):





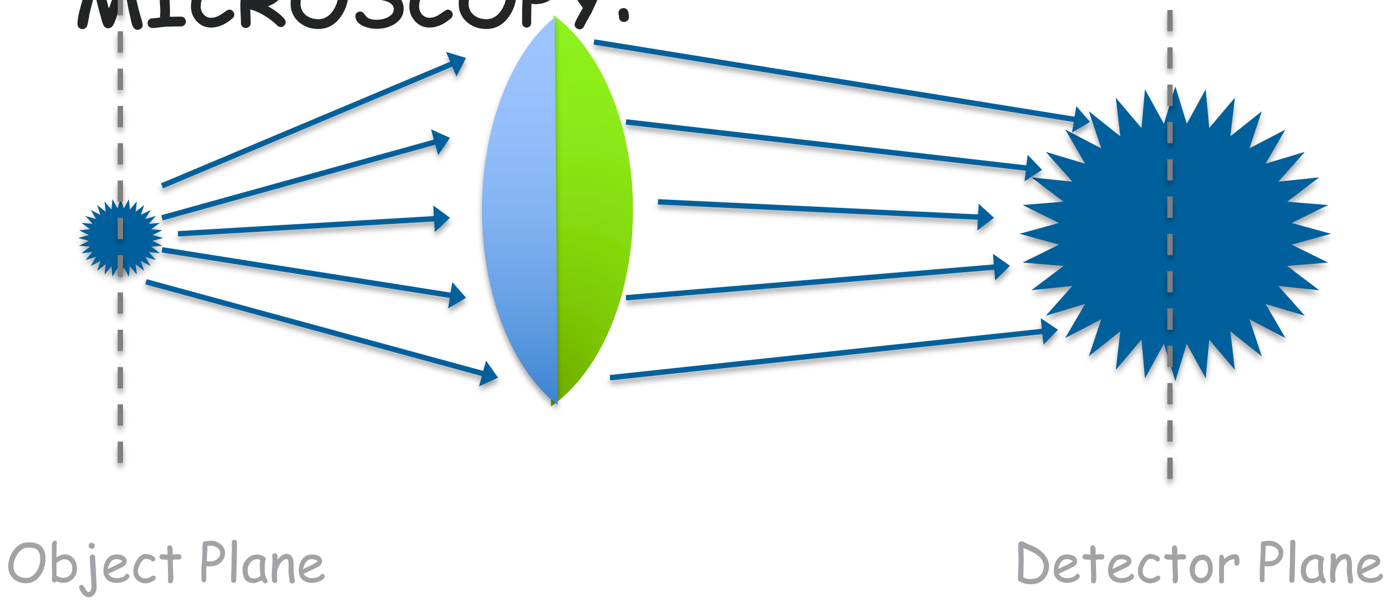
Coherent X-ray Diffraction measures:

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

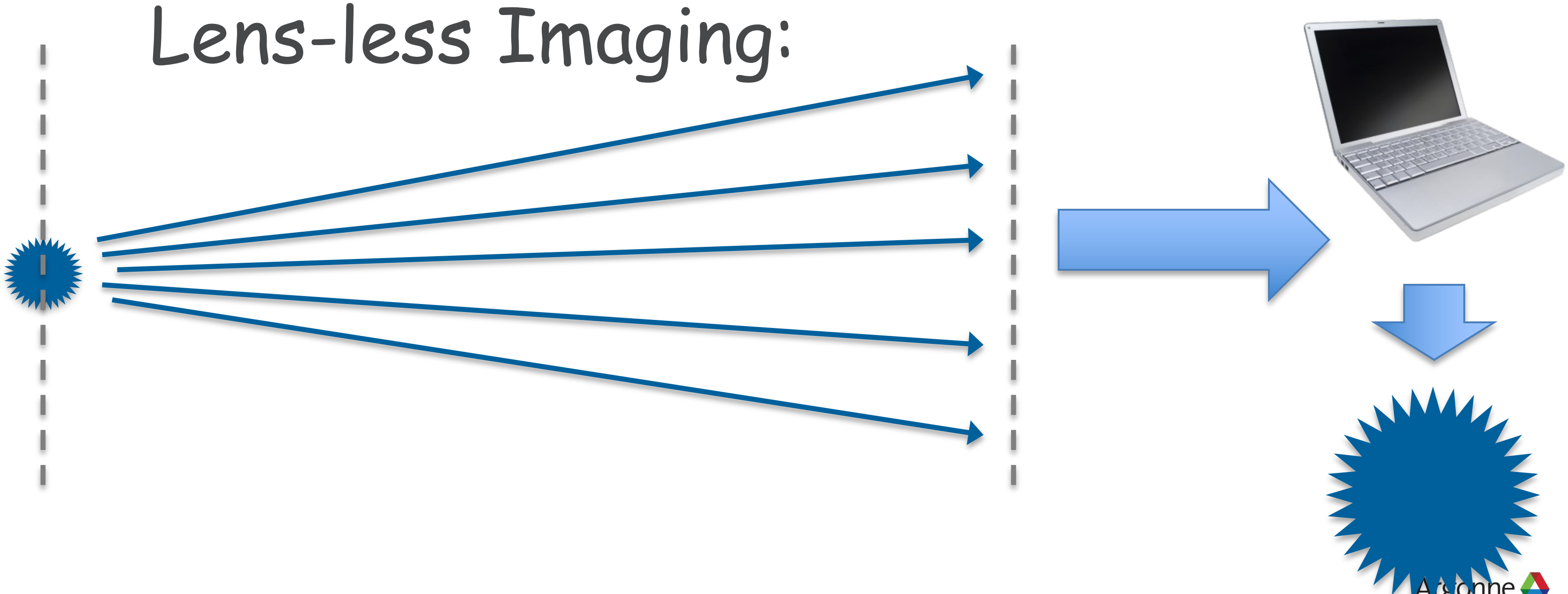
Strain is a gradient of u(r), the phase component of the complex-valued density

Courtesy Prof. Oleg Shpyrko (UCSD)

TRADITIONAL MICROSCOPY:



Lens-less Imaging:



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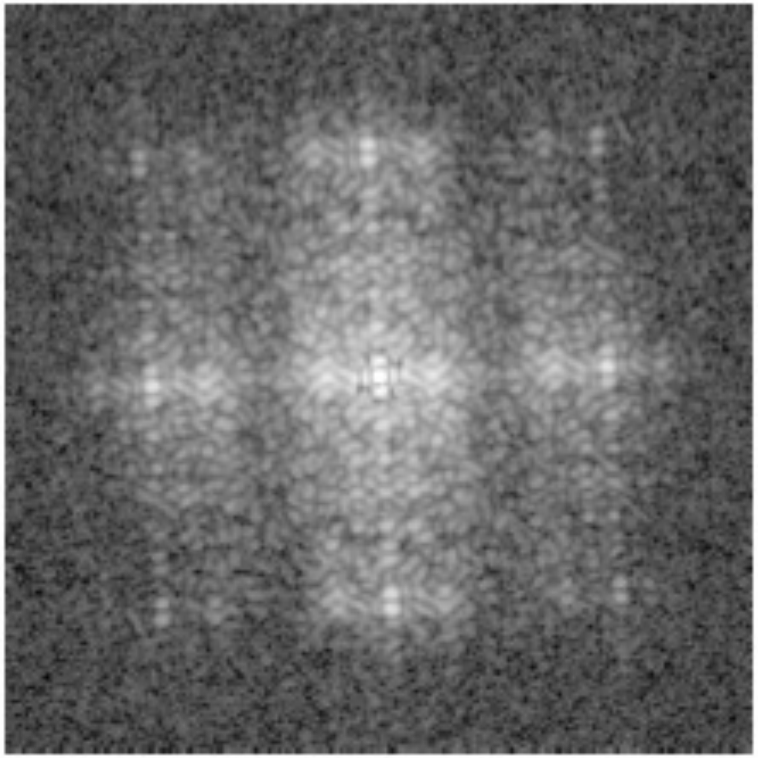
FIRST DEMONSTRATION OF CDI WITH X-RAYS



diffraction pattern

reconstruction

J. Miao, Nature 400, 342 (1999)

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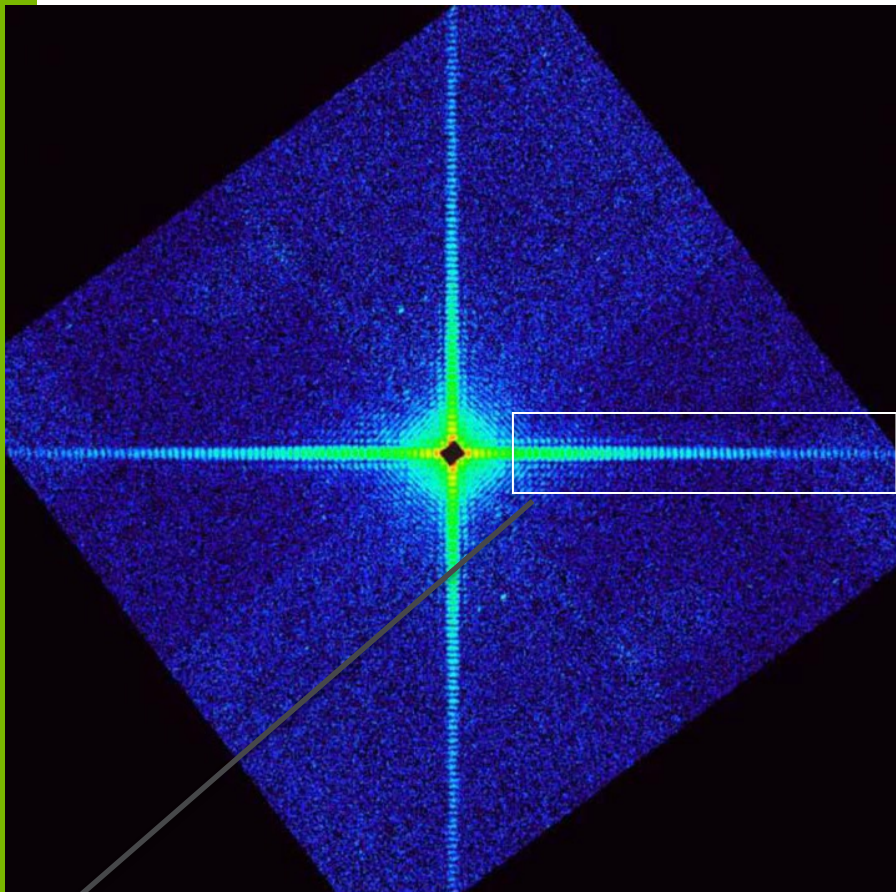
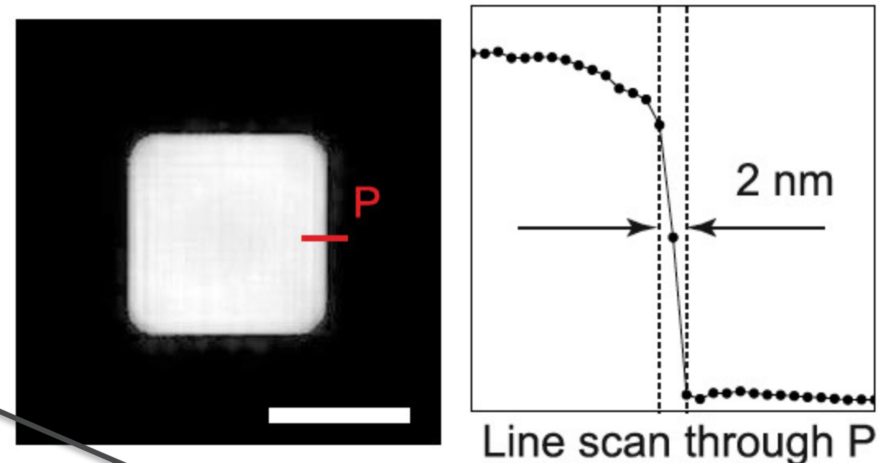
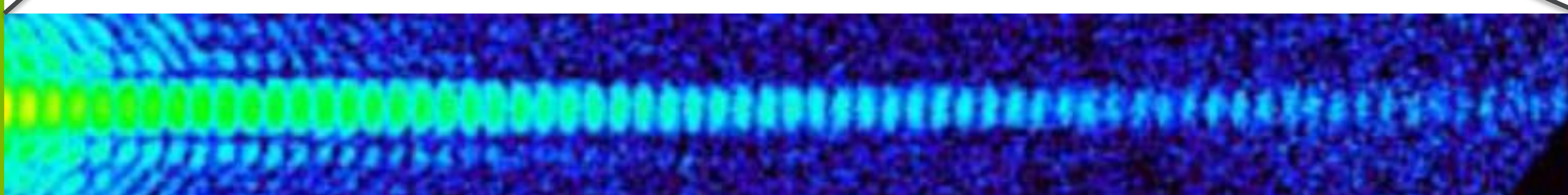
COHERENT DIFFRACTIVE IMAGING:

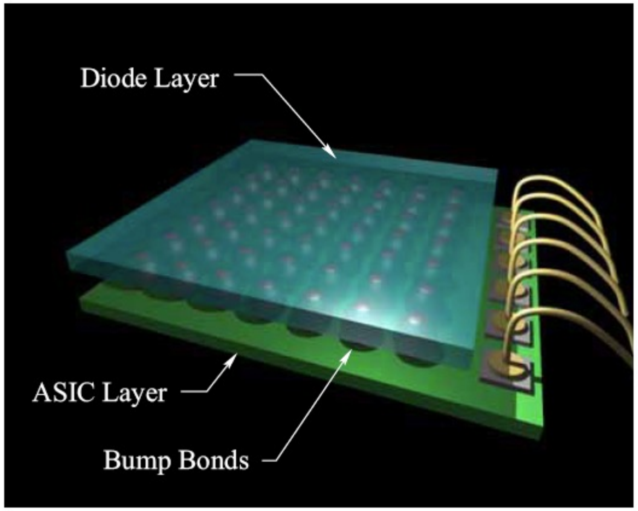


Y. Takahashi et al.,
Phys. Rev. B 82, 214102 (2010)





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)

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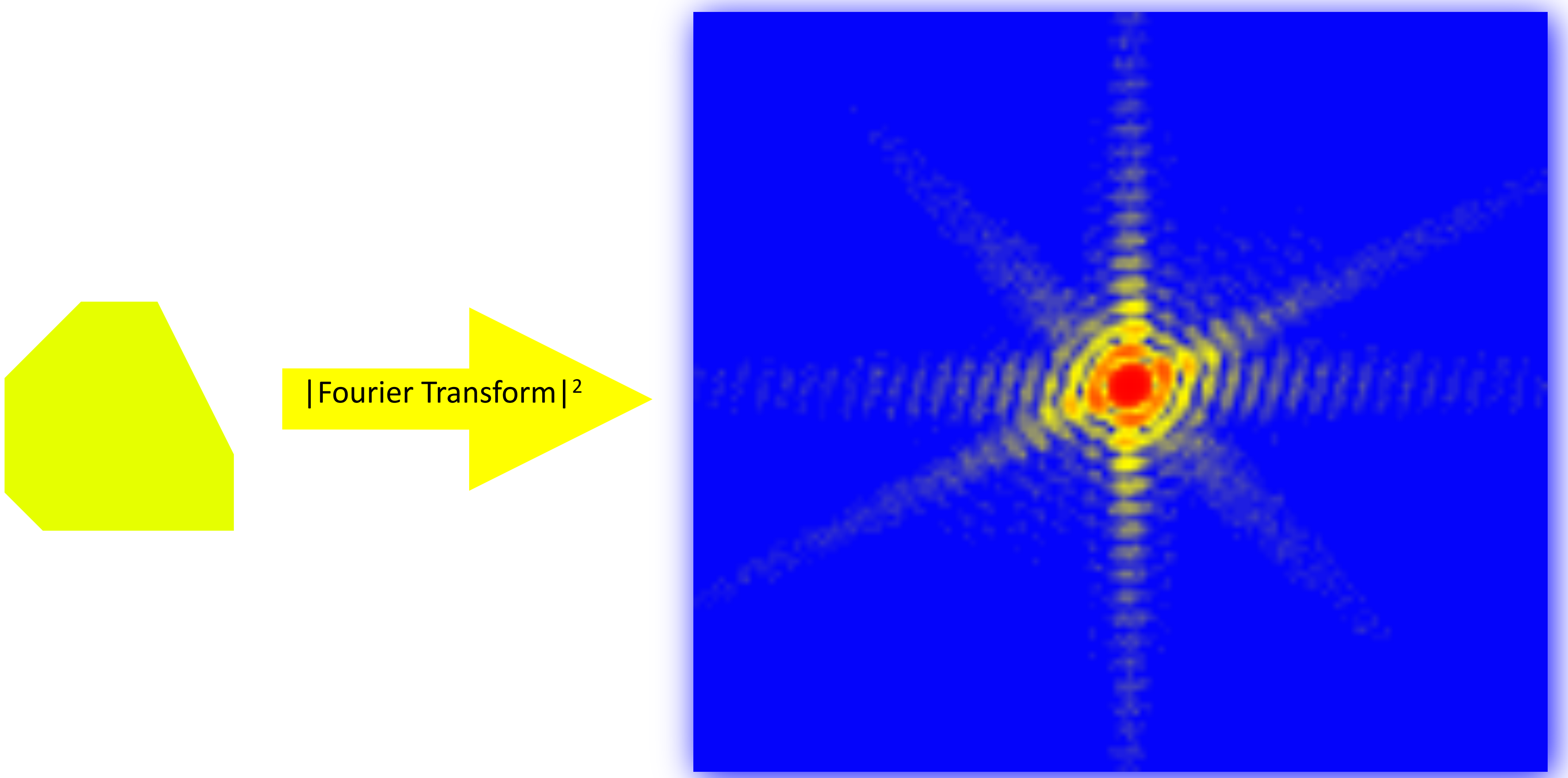
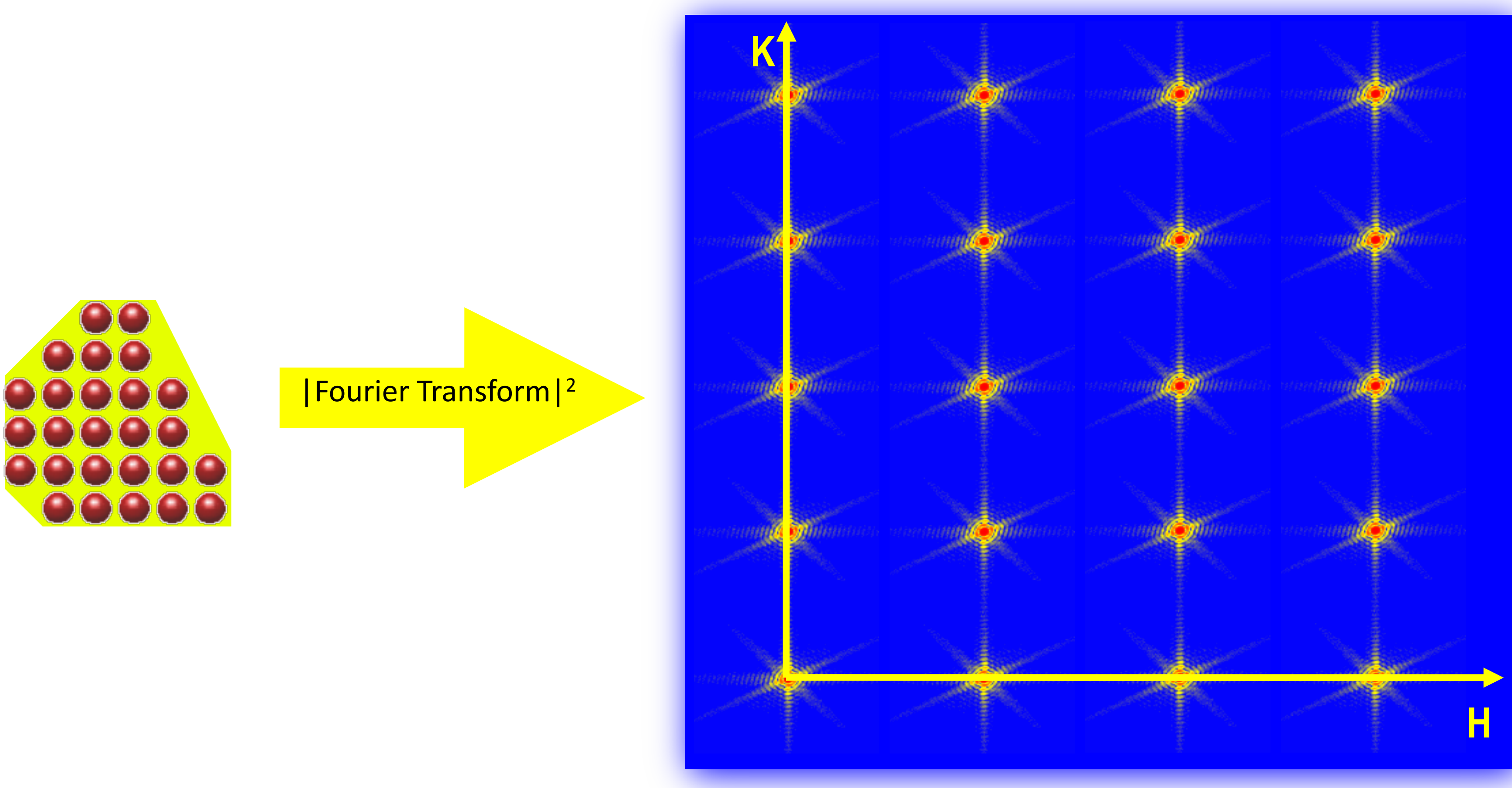
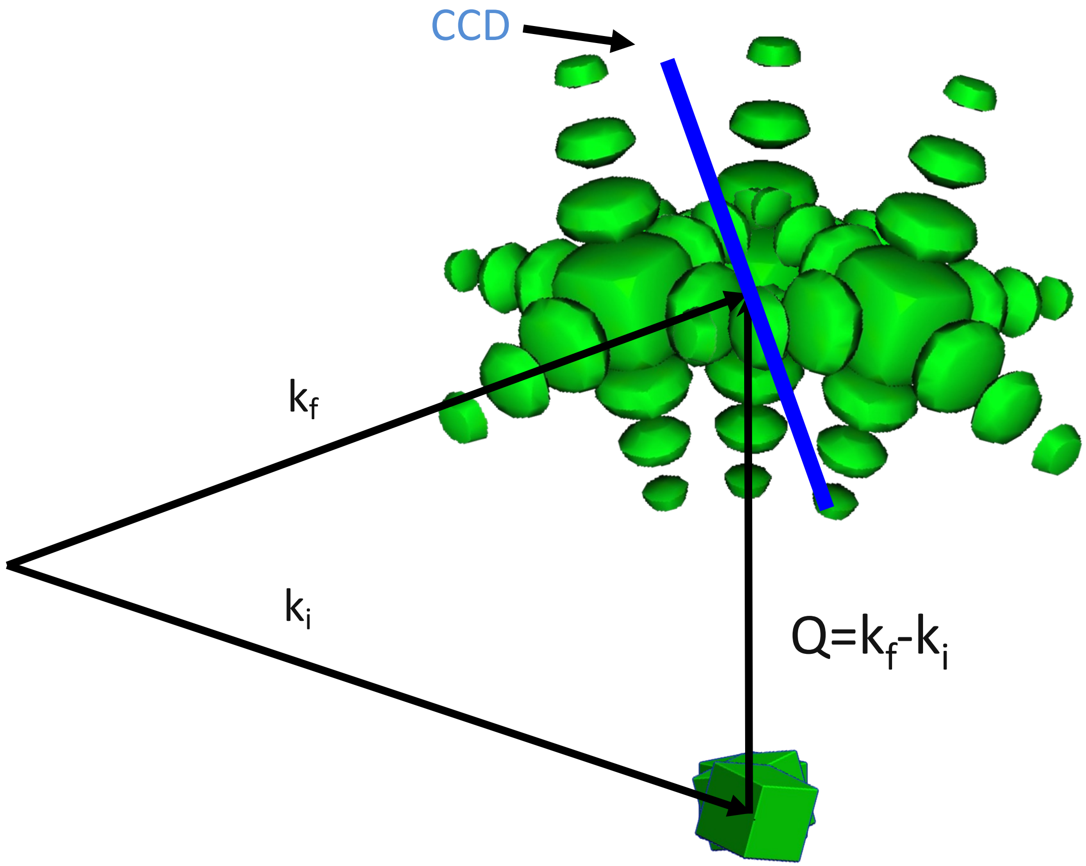
Coherent Diffraction from Crystals



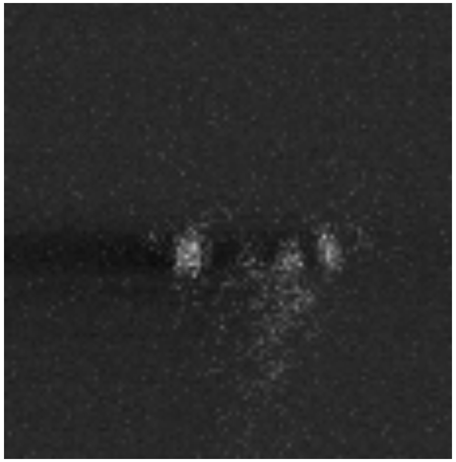
Coherent Diffraction from Crystals

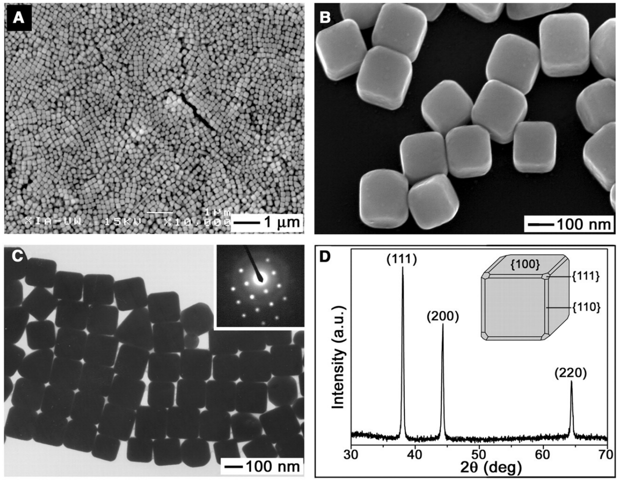


Measuring 3D CXD



Silver Nano Cube (111)





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

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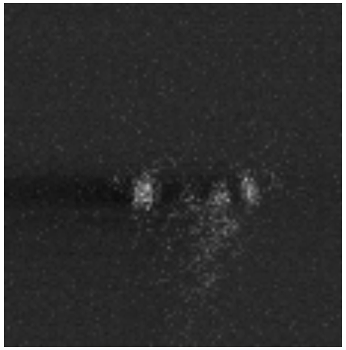
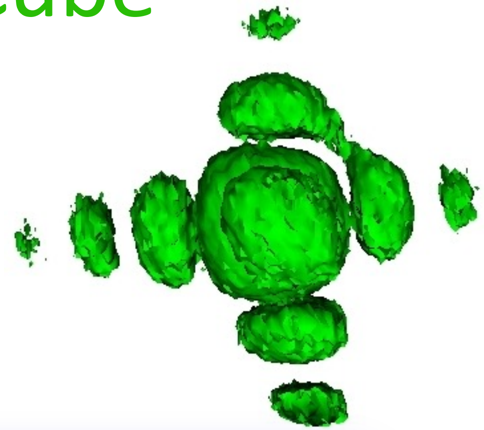
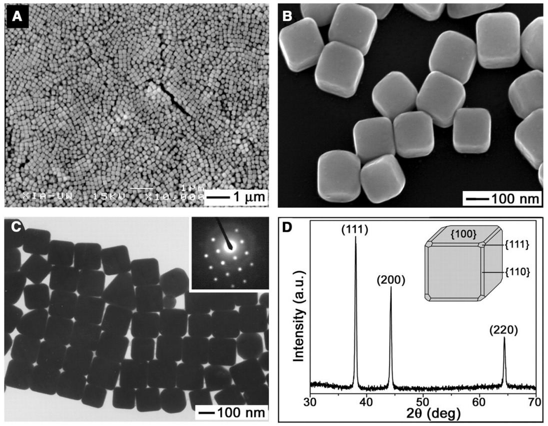
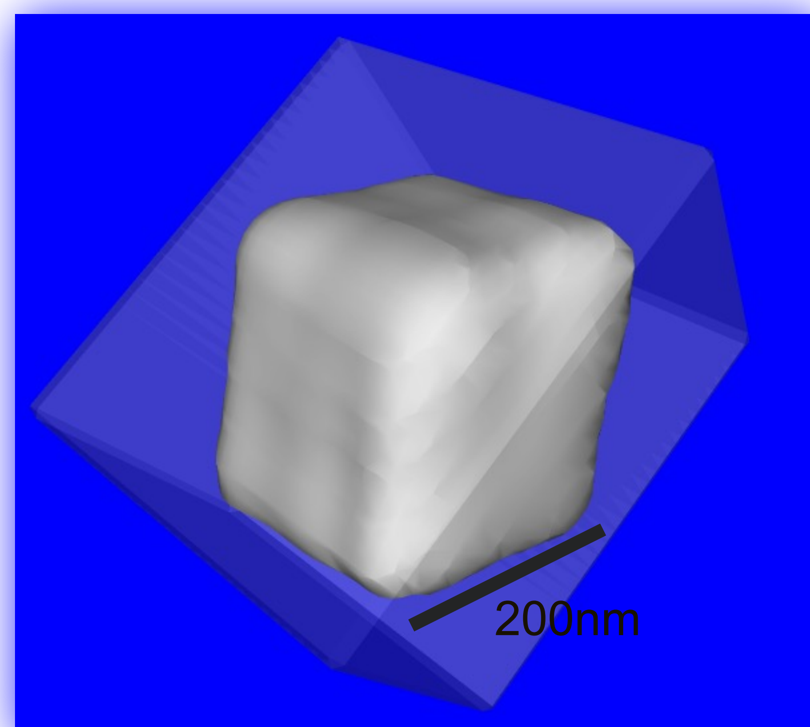
3D Ag Nano Cube

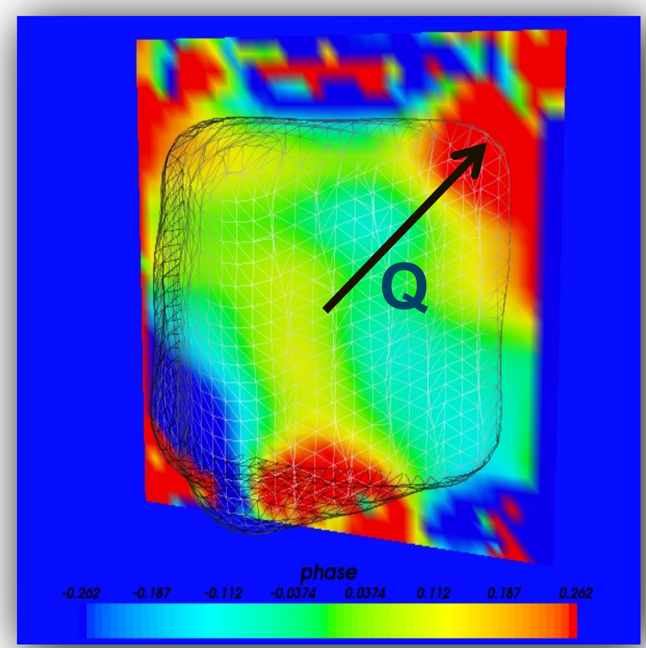




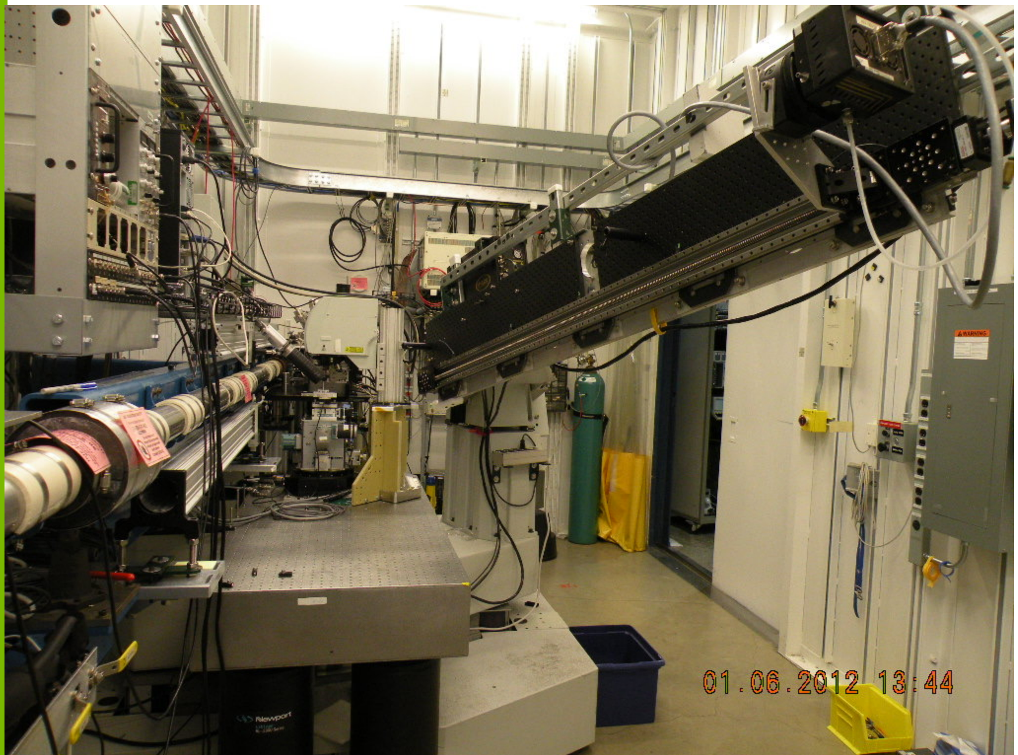


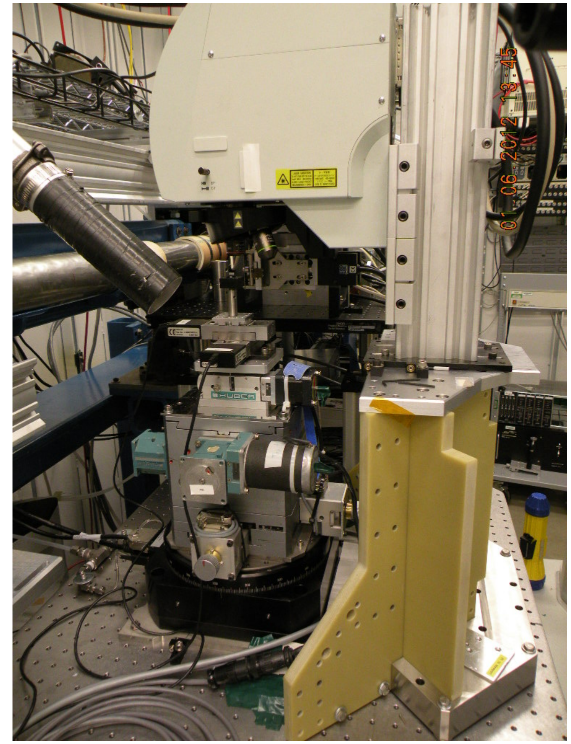
Yugang Sun and Younan Xia, Science 298 2177 (2003)





APS 34-ID-C





Precision scanning stage

ORIGINAL PHASE RETRIEVAL PAPER (BY D. SAYRE):

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

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.

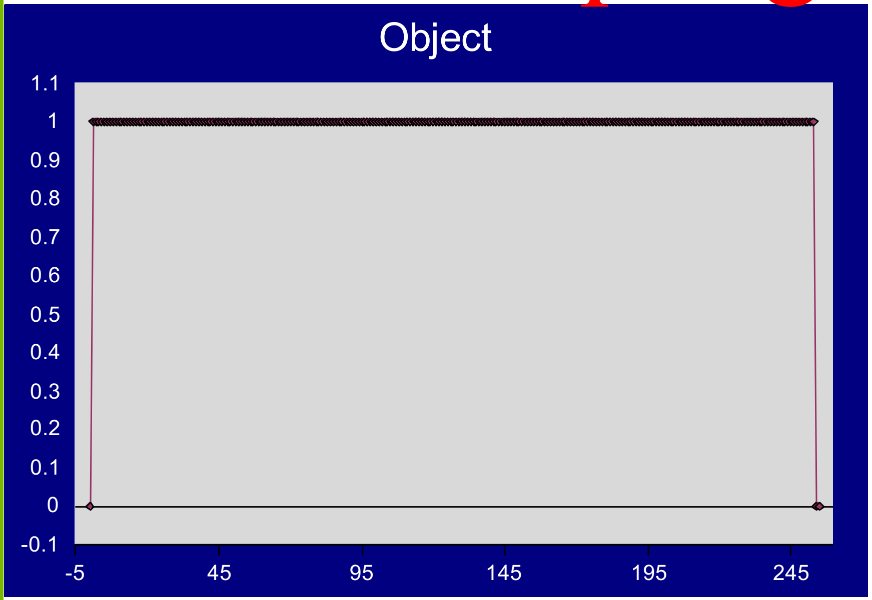
2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where $|F|^2$ was observed at non-integral h, it would suffice to have only the values at half-integral h.

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.

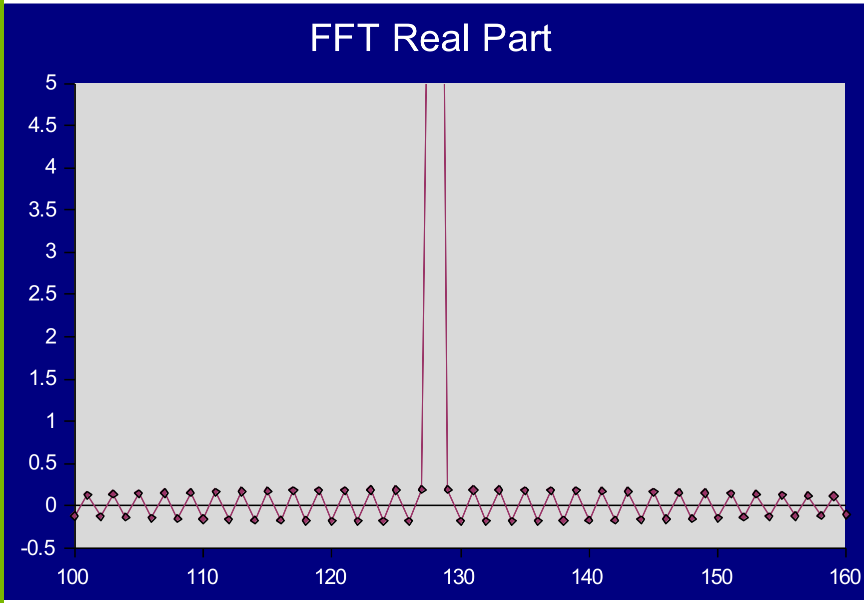
Critical sampling

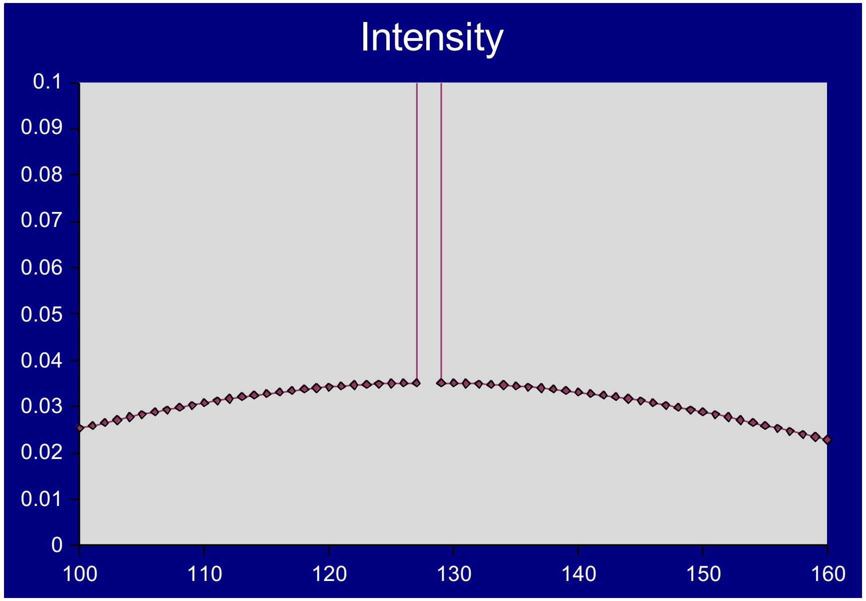


N unknown densities
N/2 equations

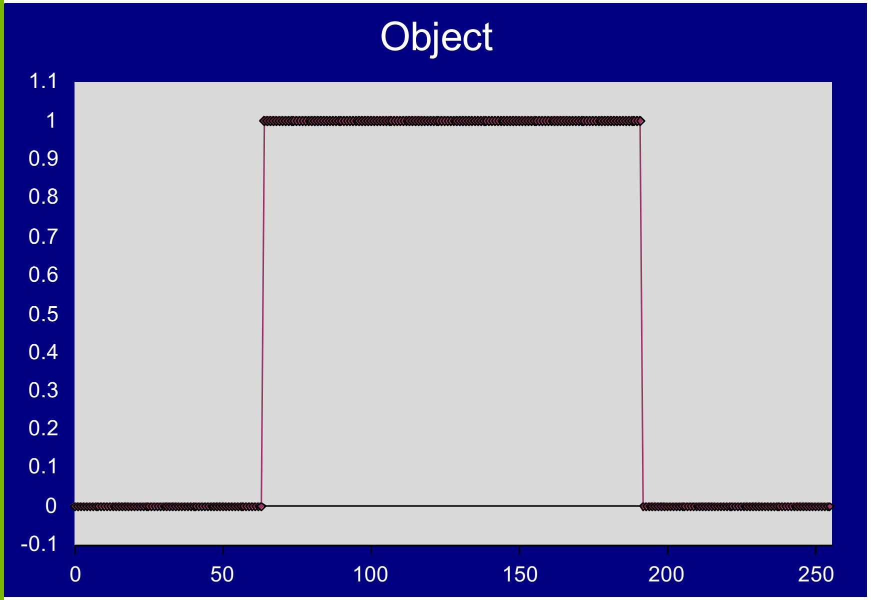
$$\left|A_q\right| = \left|\sum_{0}^{N} \rho_n e^{-iqr_n}\right|$$

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





Oversampling 2x

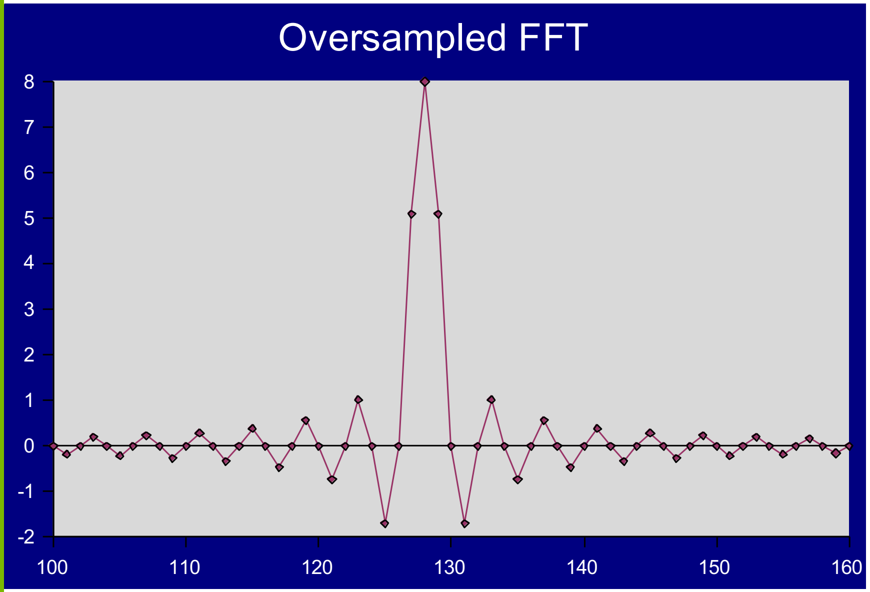


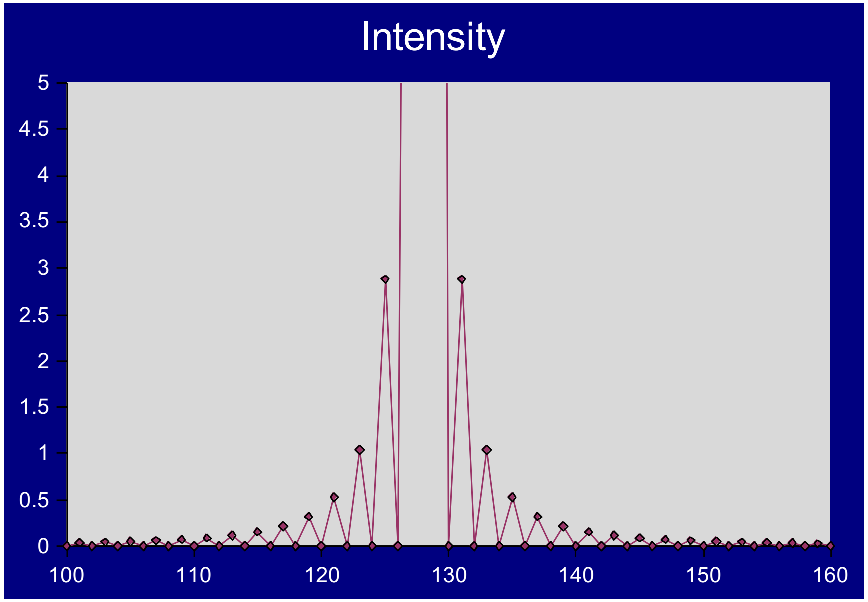
N/2 equations

N/2 Unknown densities

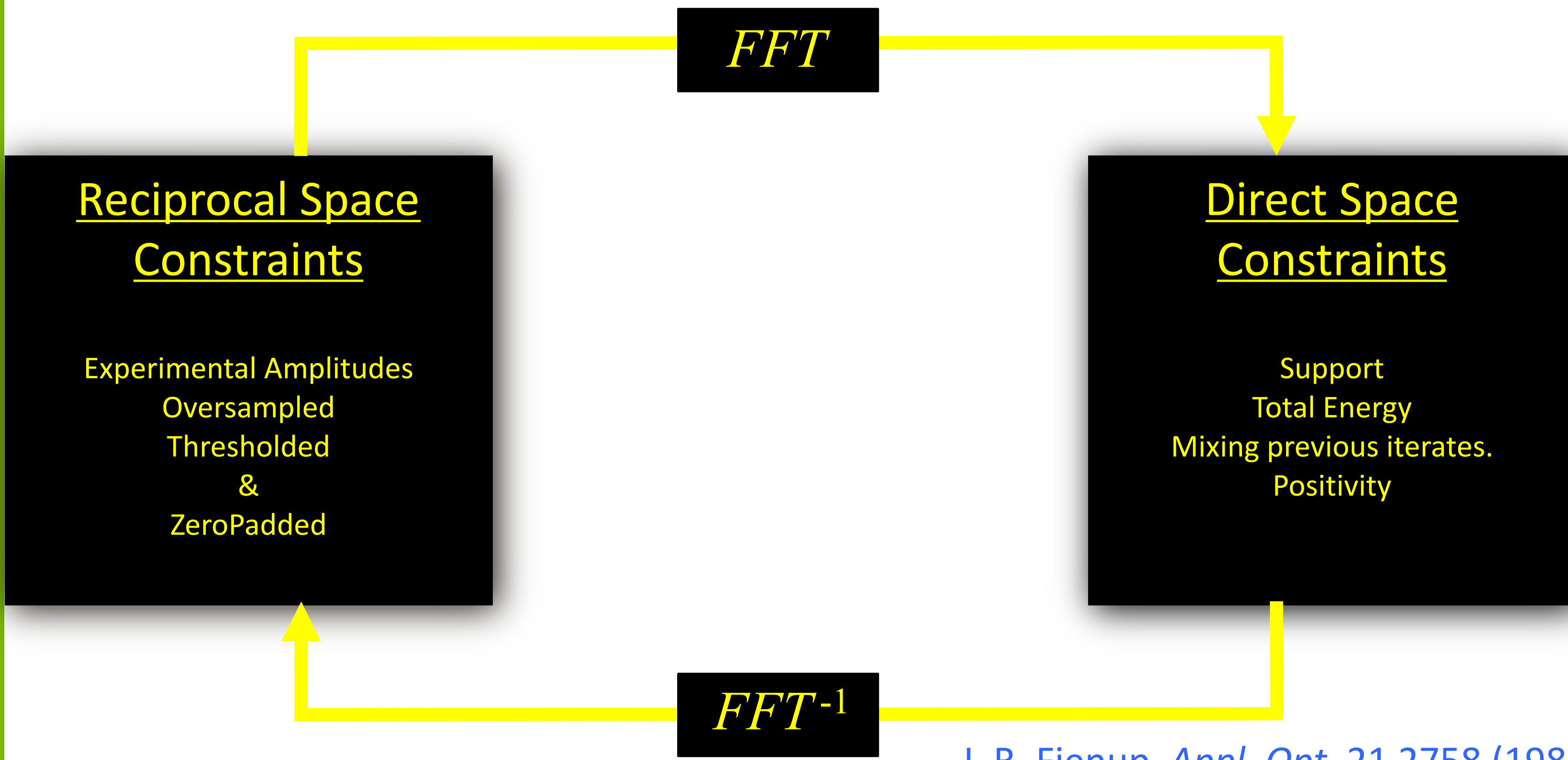
N/2 Known Densities(zero)

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



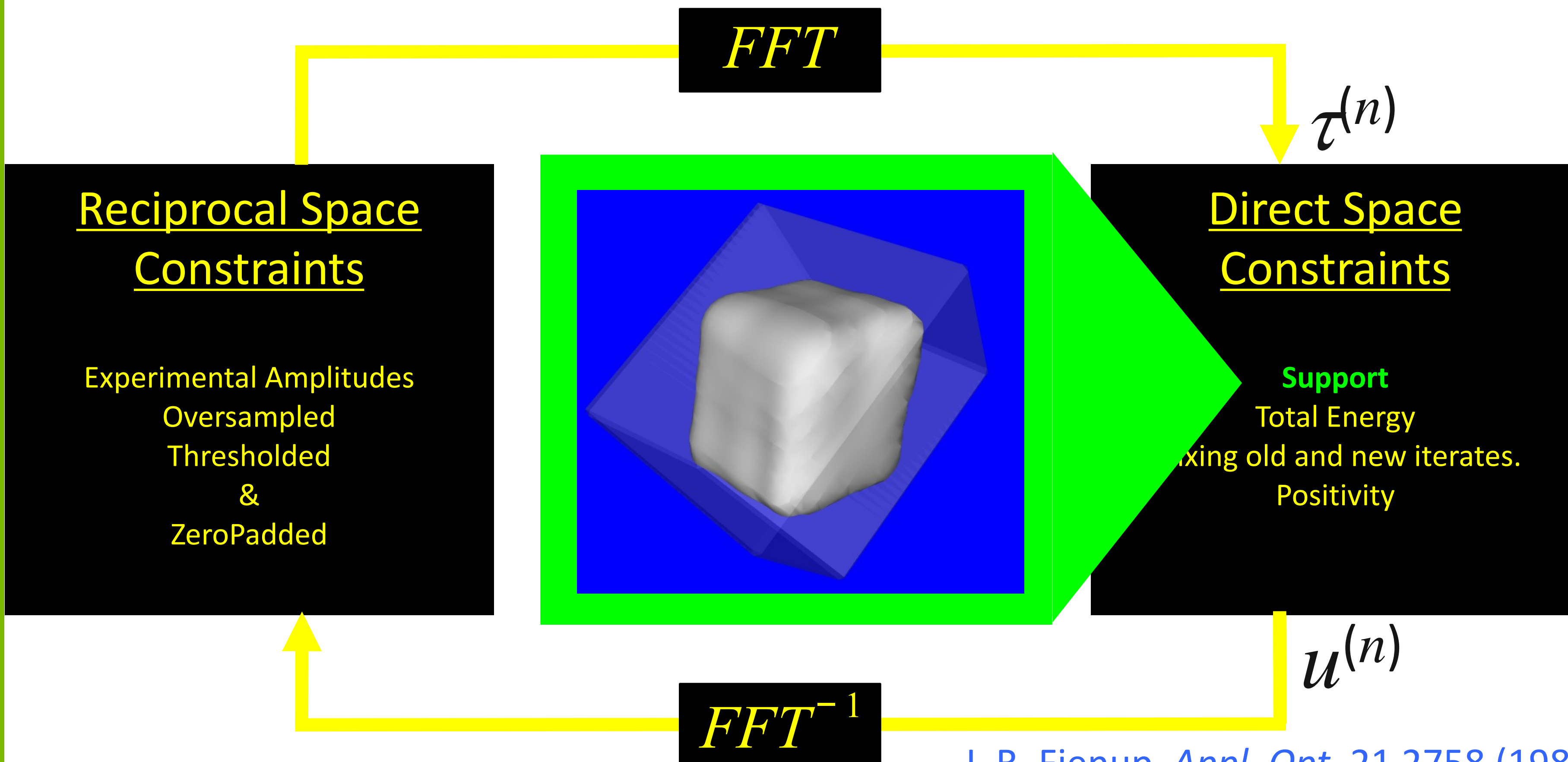


Input Output Algorithms



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



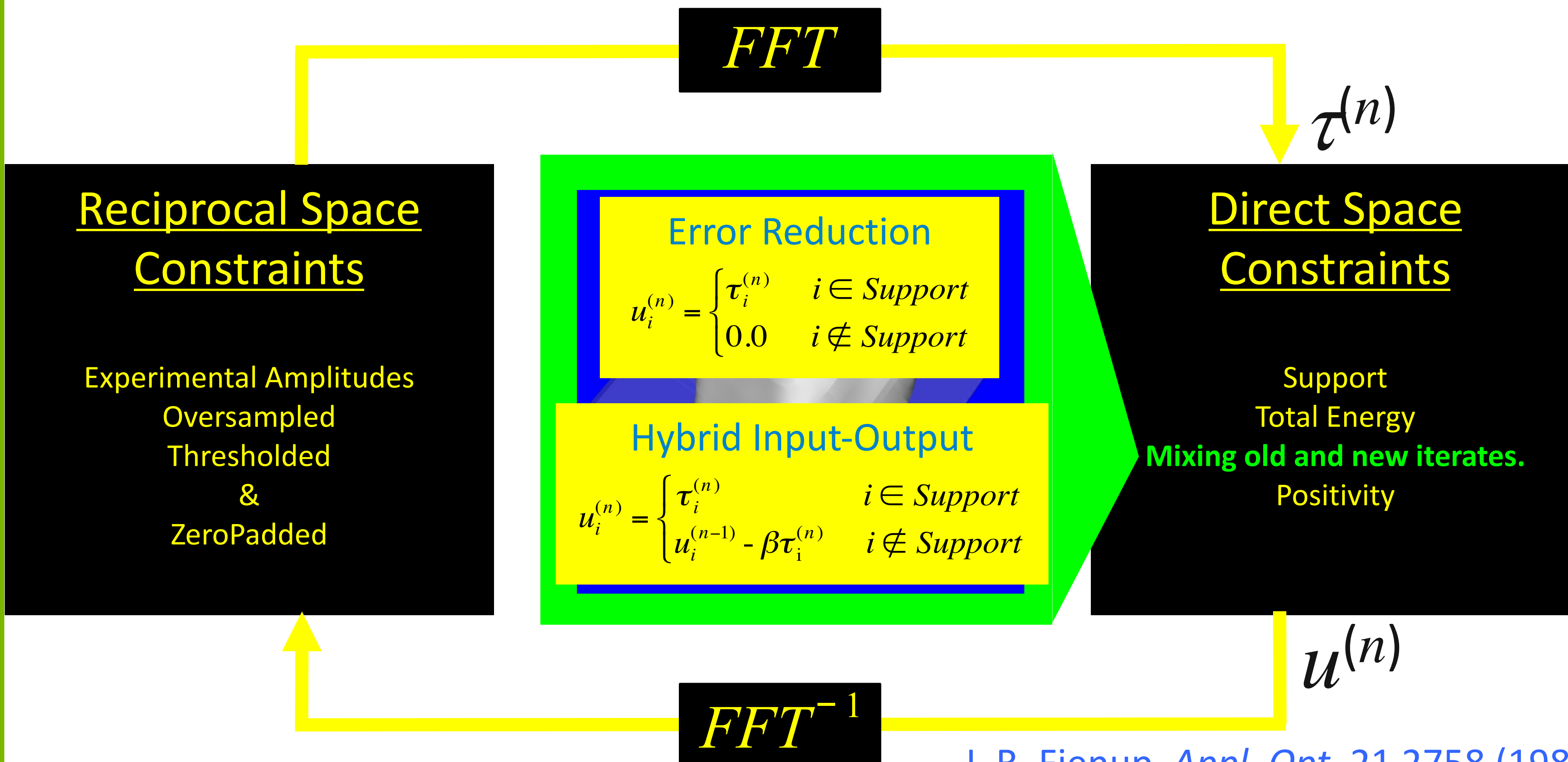
J. R. Fienup *Appl. Opt.* 21 2758 (1982)

Collins *Nature* 298, 49 (1982)

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

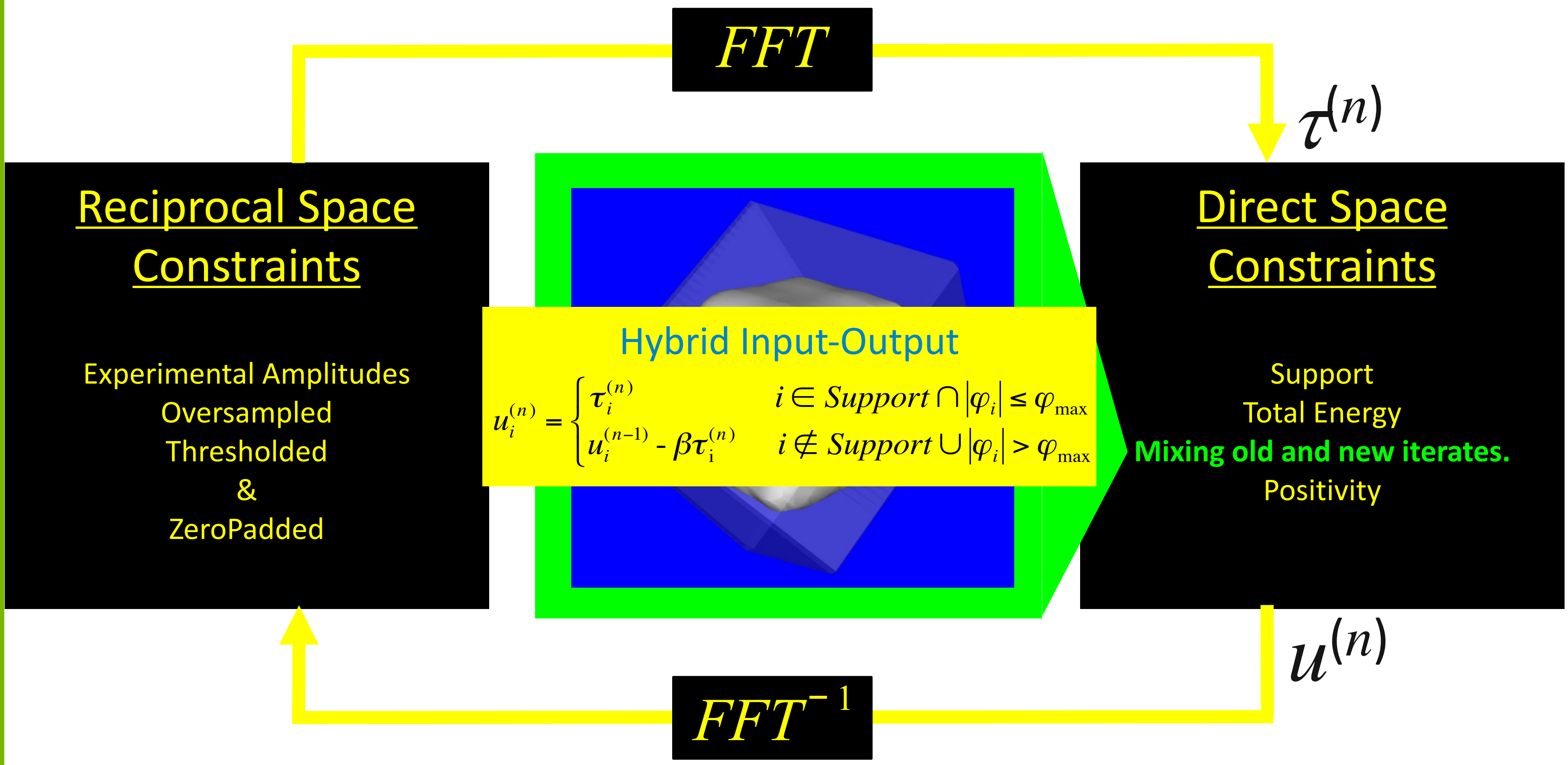
Fienup, James R. 2013. “Phase Retrieval Algorithms: a Personal Tour.” *Applied Optics* 52 (1): 45–56.

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.

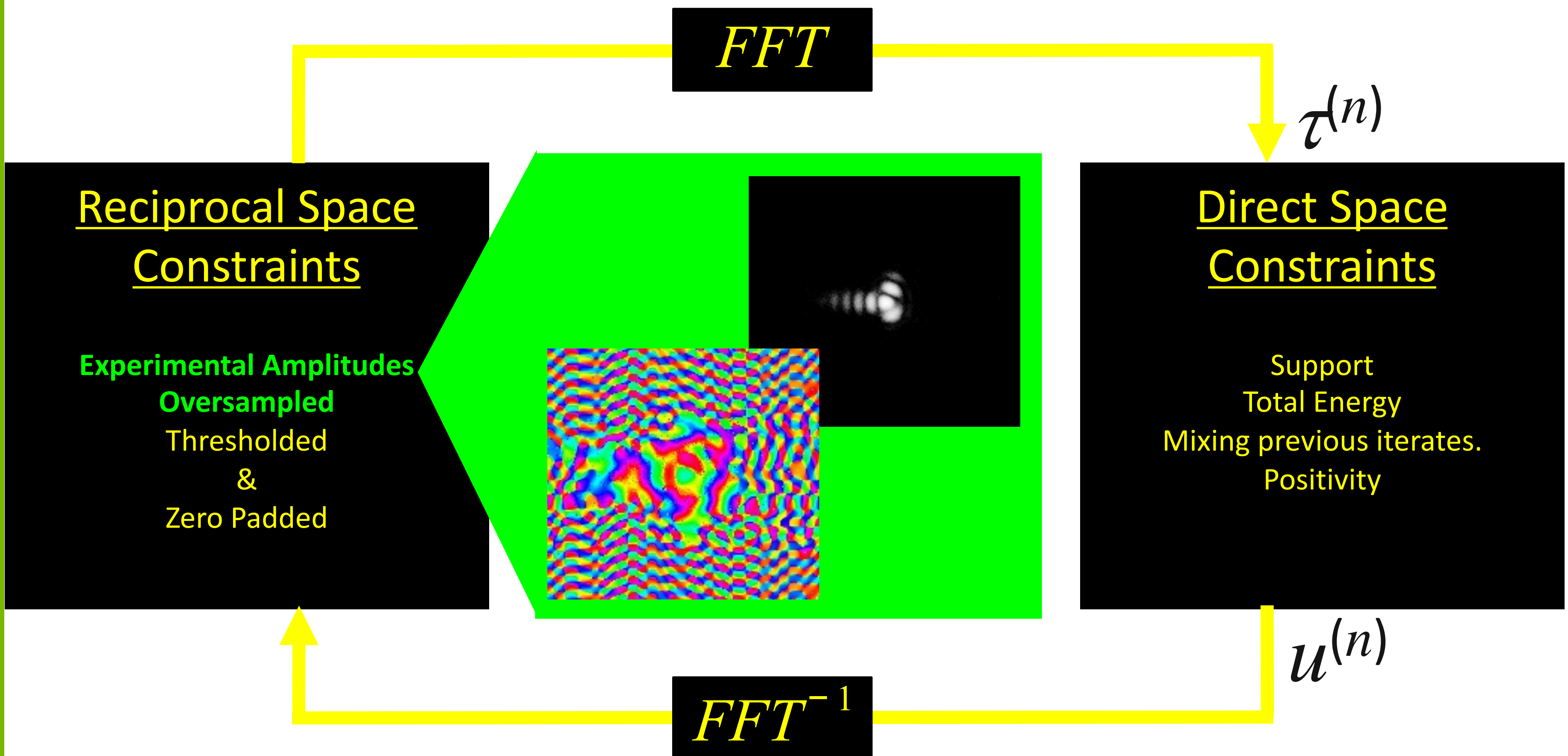
Input Output Algorithms



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.

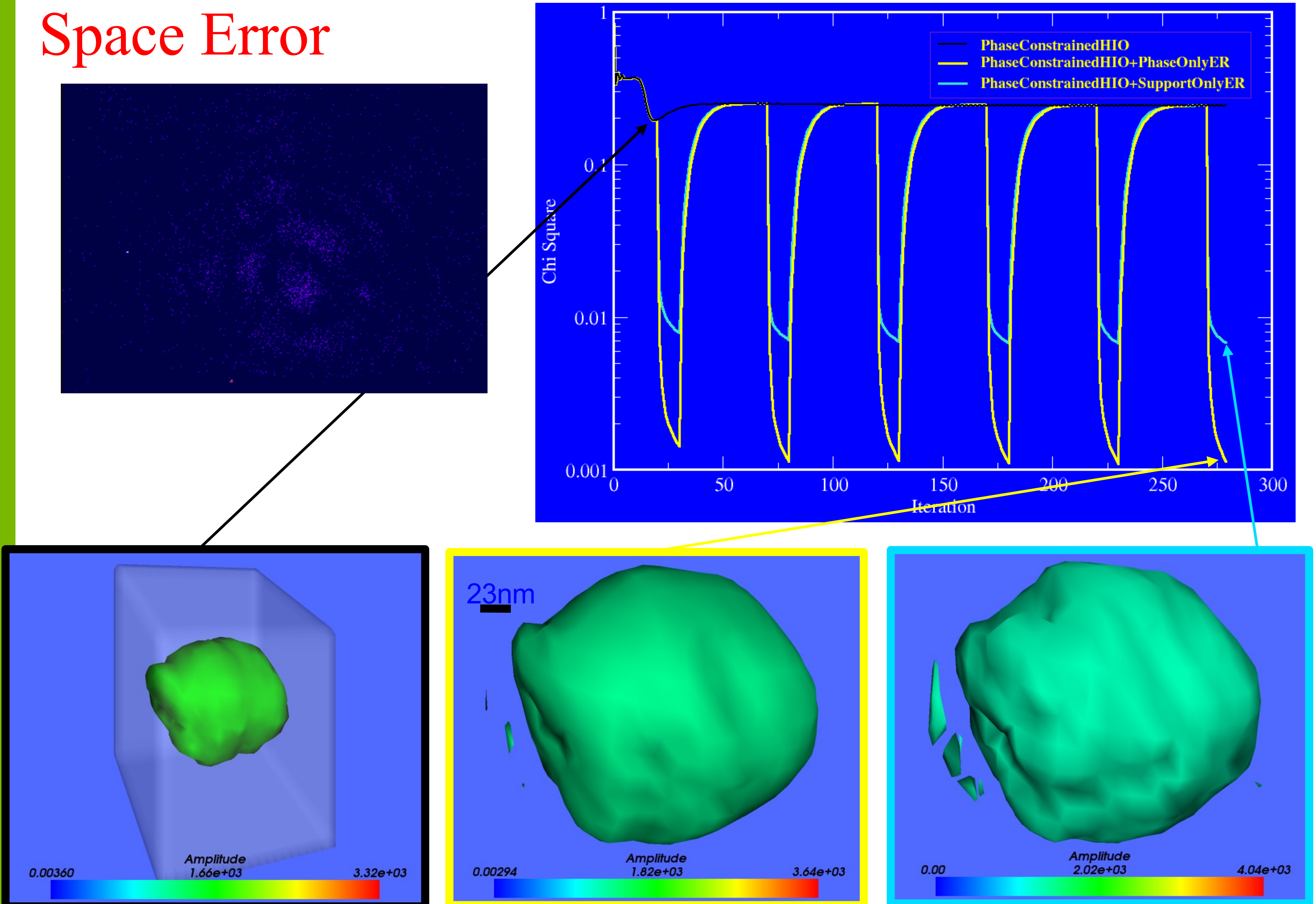
Huang, X., Harder, R., Xiong, G., Shi, X., & Robinson, I. (2011). Propagation uniqueness in three-dimensional coherent diffractive imaging. *Physical Review B*, *83*(22), 224109.

Input Output Algorithms

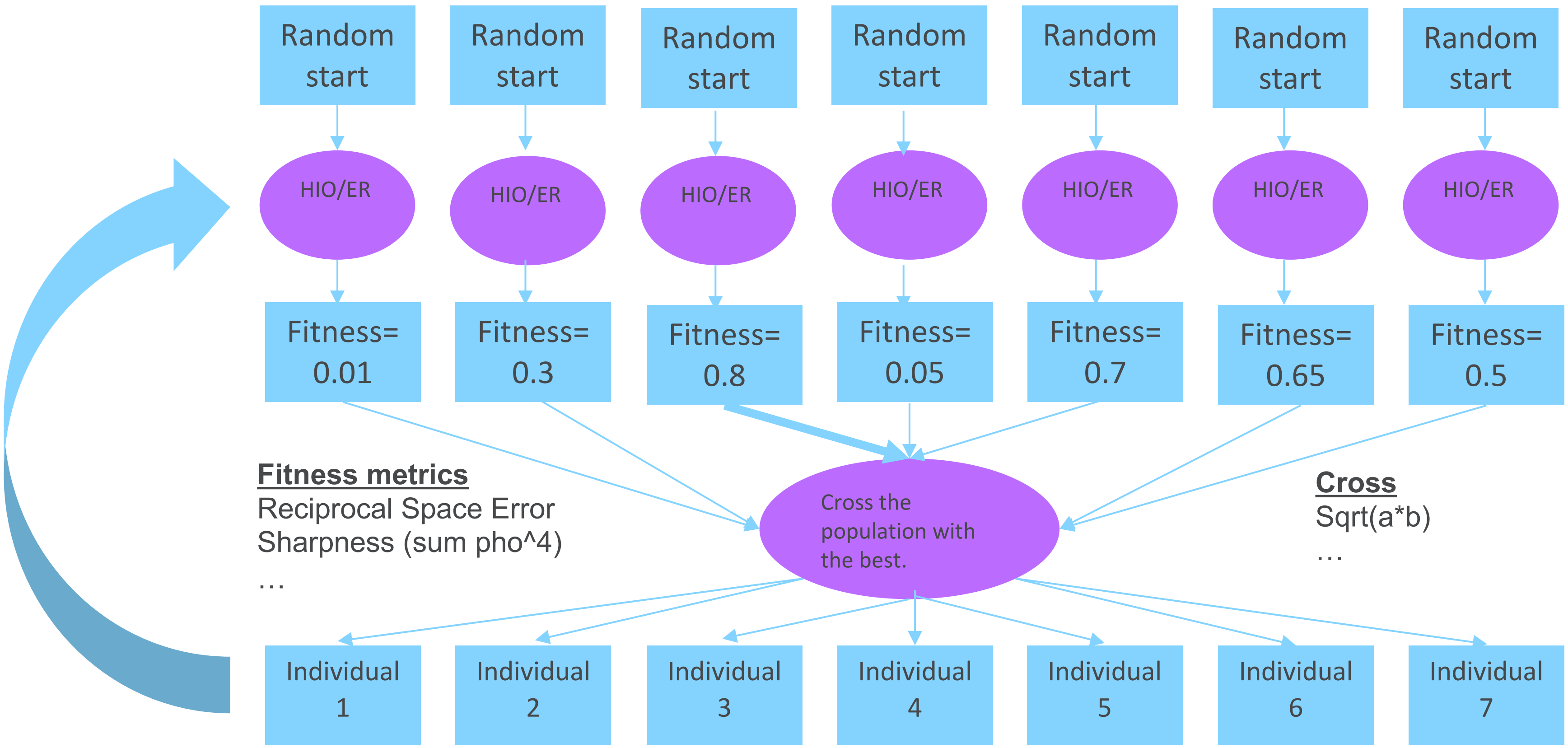


Harder, R., Liang, M., Sun, Y., Xia, Y., & Robinson, I. K. (2010). Imaging of complex density in silver nanocubes by coherent x-ray diffraction. *New Journal of Physics*, *12*(3), 035019.
Huang, X., Harder, R., Xiong, G., Shi, X., & Robinson, I. (2011). Propagation uniqueness in three-dimensional coherent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

Monitor Reciprocal Space Error



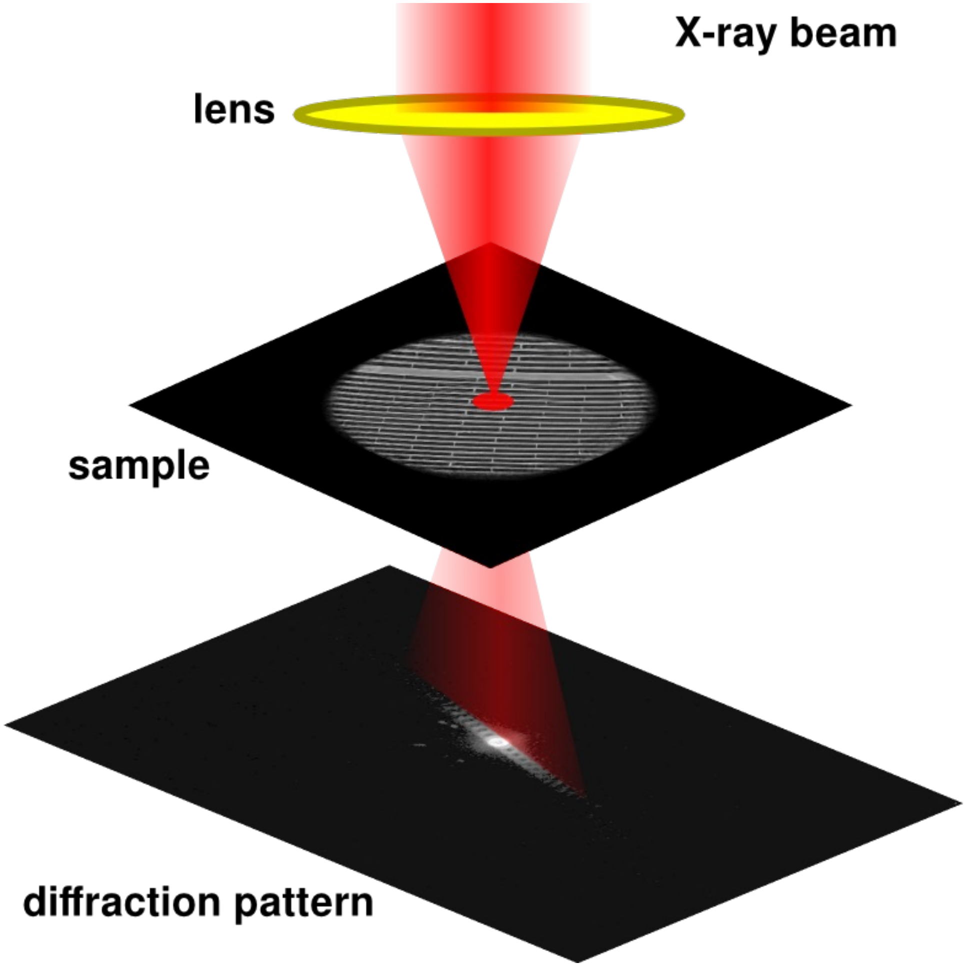
GENETIC/GUIDED ALGORITHM

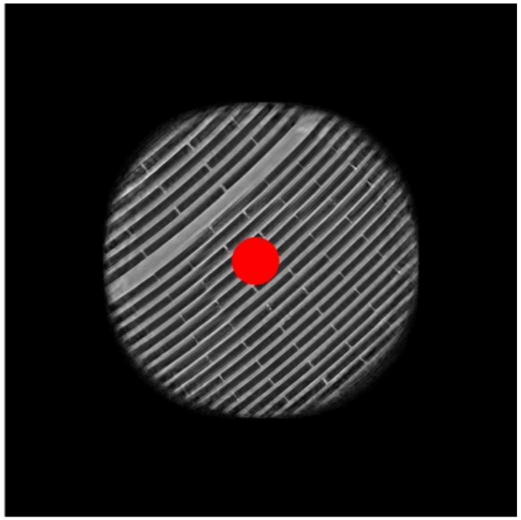


Clark, J. N., Ihli, J., Schenk, A. S., Kim, Y.-Y., Kulak, A. N., Campbell, J. M., et al. (2015). Three-dimensional imaging of dislocation propagation during crystal growth and dissolution. *Nature Materials*, *14*(8), 780–784. http://doi.org/10.1038/nmat4320

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

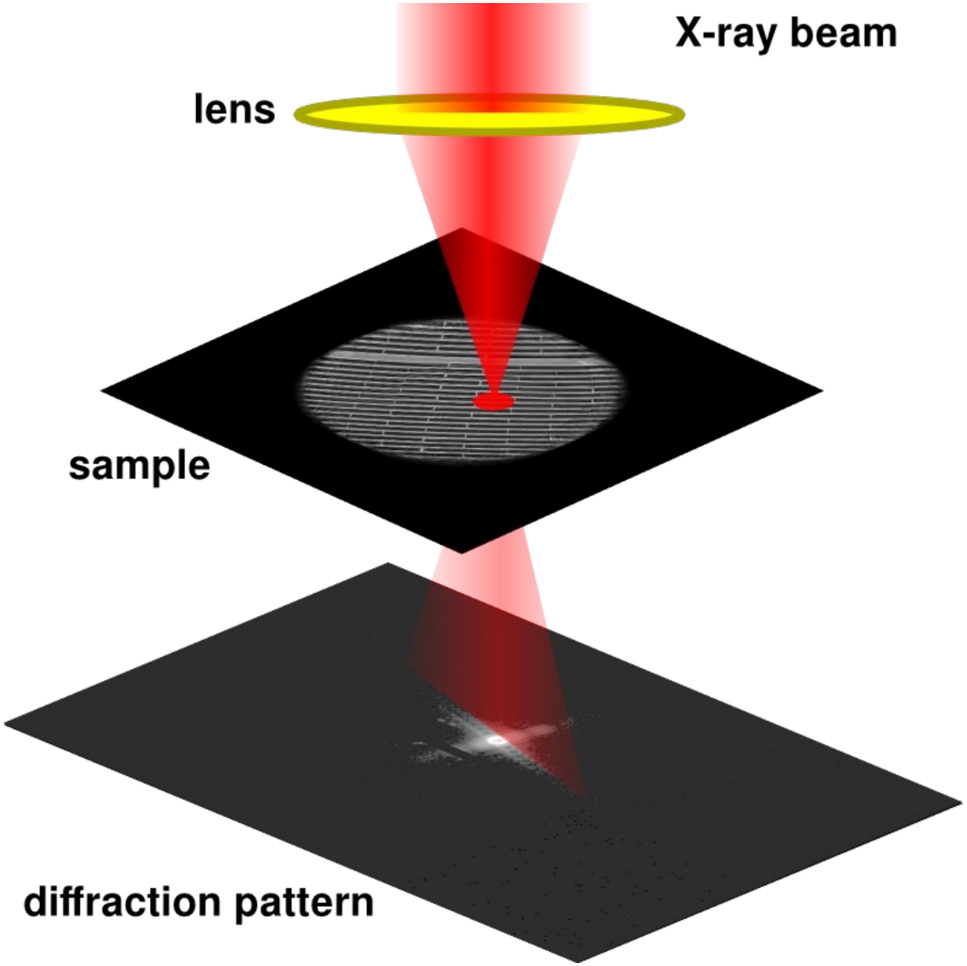
Ptychography (to fold) - Scanning CDI for extended object

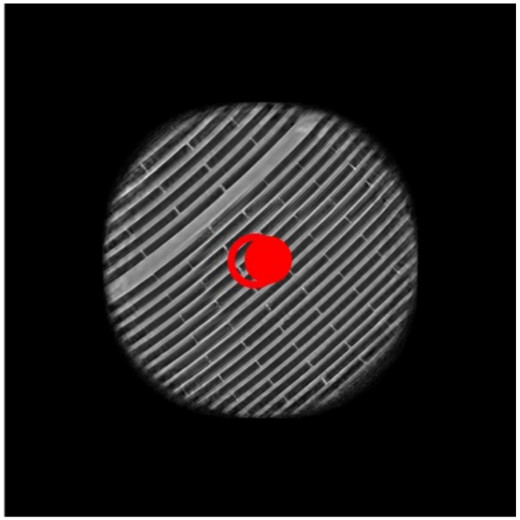




Courtesy Dr. Junjing Deng (APS)

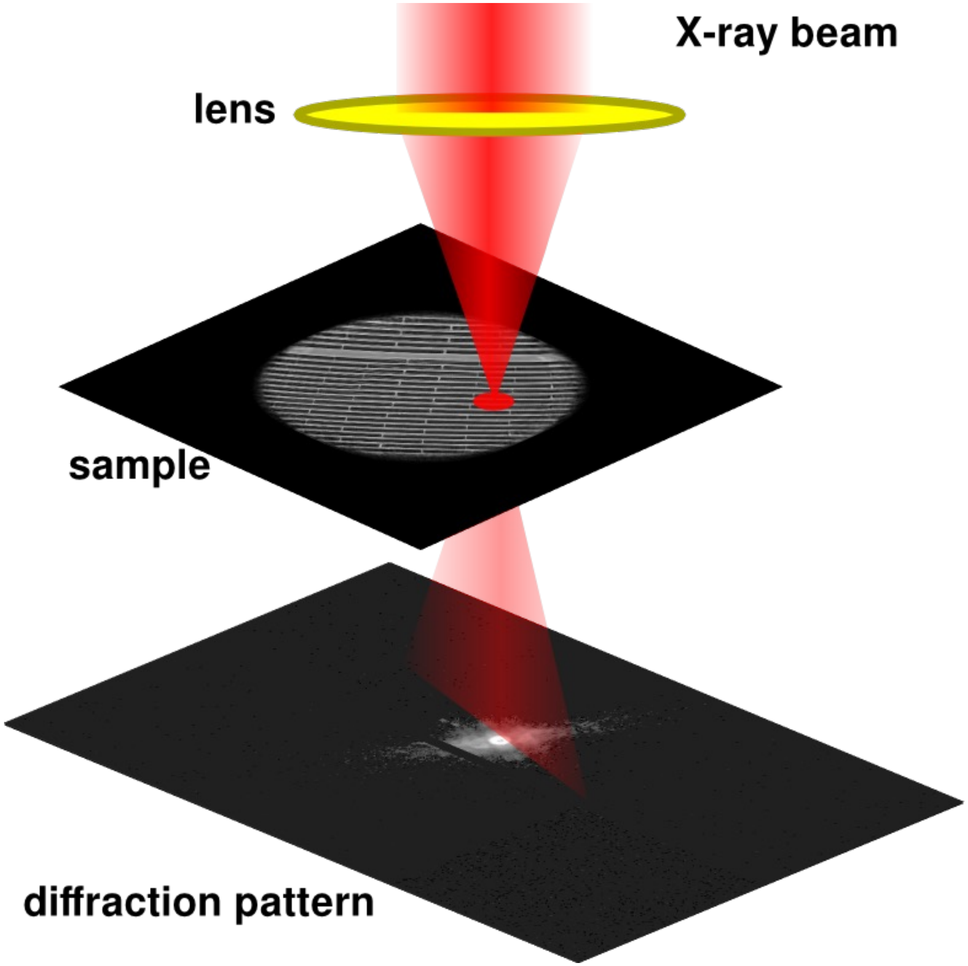
Ptychography (to fold) - Scanning CDI for extended object

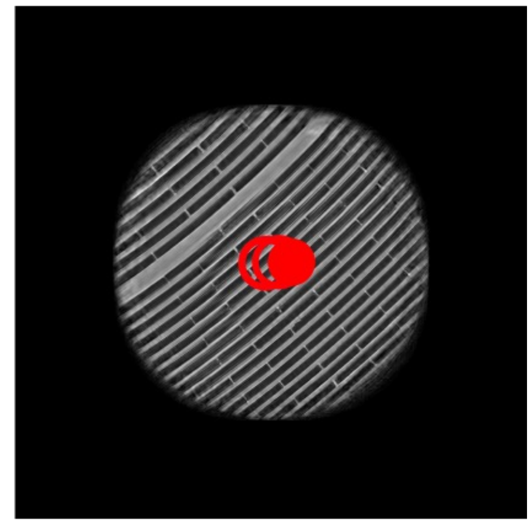




Courtesy Dr. Junjing Deng (APS)

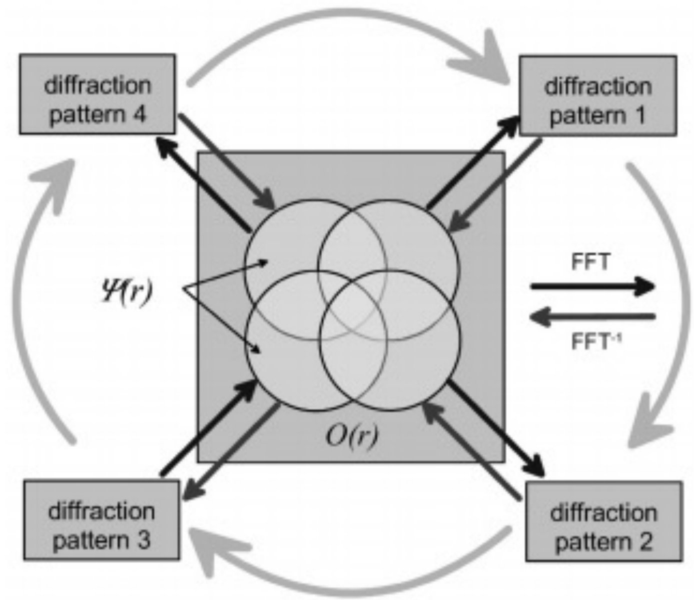
Ptychography (to fold) - Scanning CDI for extended object





Courtesy Dr. Junjing Deng (APS)

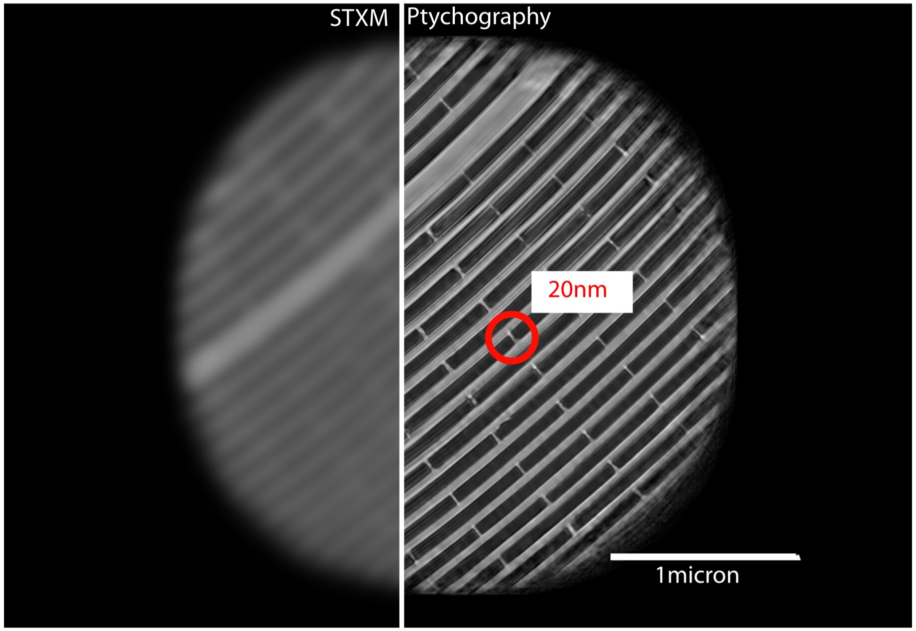
Ptychography



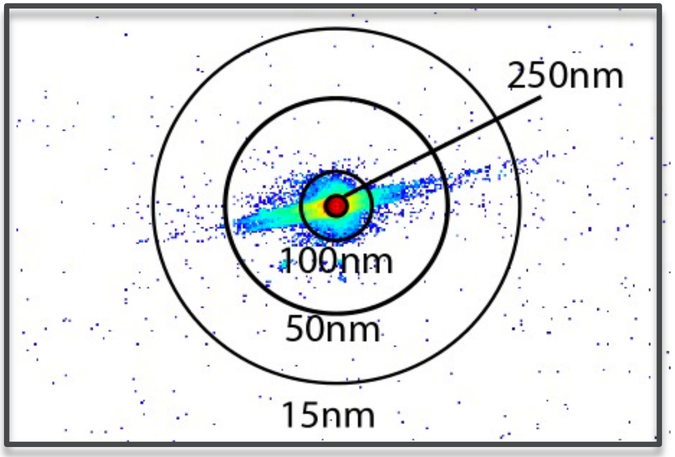
Ptychographic iterative engine (PIE)

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

Platinum nanostructure



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



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

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

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

Courtesy Dr. Junjing Deng (APS)

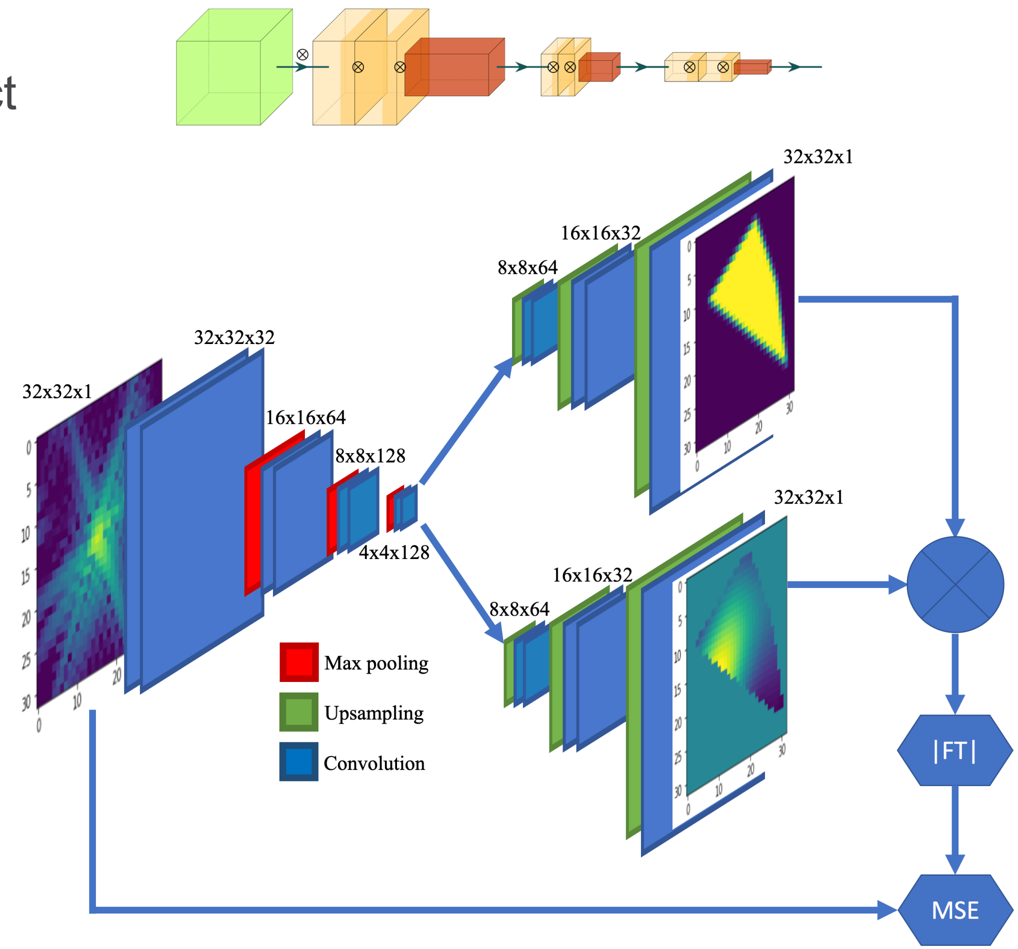
ROSS J. HARDER (XSD)
MATHEW J. CHERUKARA (XSD)
YOUSSEF NASHED (MCS)
TOM PETERKA (MCS)
PRASANNA BALAPRAKASH (MCS)
S. SANKARANARAYANAN (CNM)
BADRI NARAYANAN (MSD)

'PHYSICS-AWARE' NETWORK ARCHITECTURE

- Common encoder to a latent space, two decoders to predict structure and phase.
  - 2D or 3D convolutions

- During training goal is to minimize the prediction error.

- Prediction error has 3 terms:
  - Error in object prediction
  - Error in phase prediction
  - Error in computed diffraction.
    - This is computed from the FT of predicted shape and phase.



M. J. Cherukara, et al.,
"Real-time coherent diffraction inversion using deep generative networks,"
Sci Rep, vol. 8, no. 1, p. 16520, Nov. 2018.

Yao, Yudong, et al..
"AutoPhaseNN: Unsupervised Physics-Aware Deep Learning of 3D Nanoscale Bragg Coherent Diffraction Imaging."
Npj Computational Materials 8, no. 1 (June 3, 2022): 1–8..

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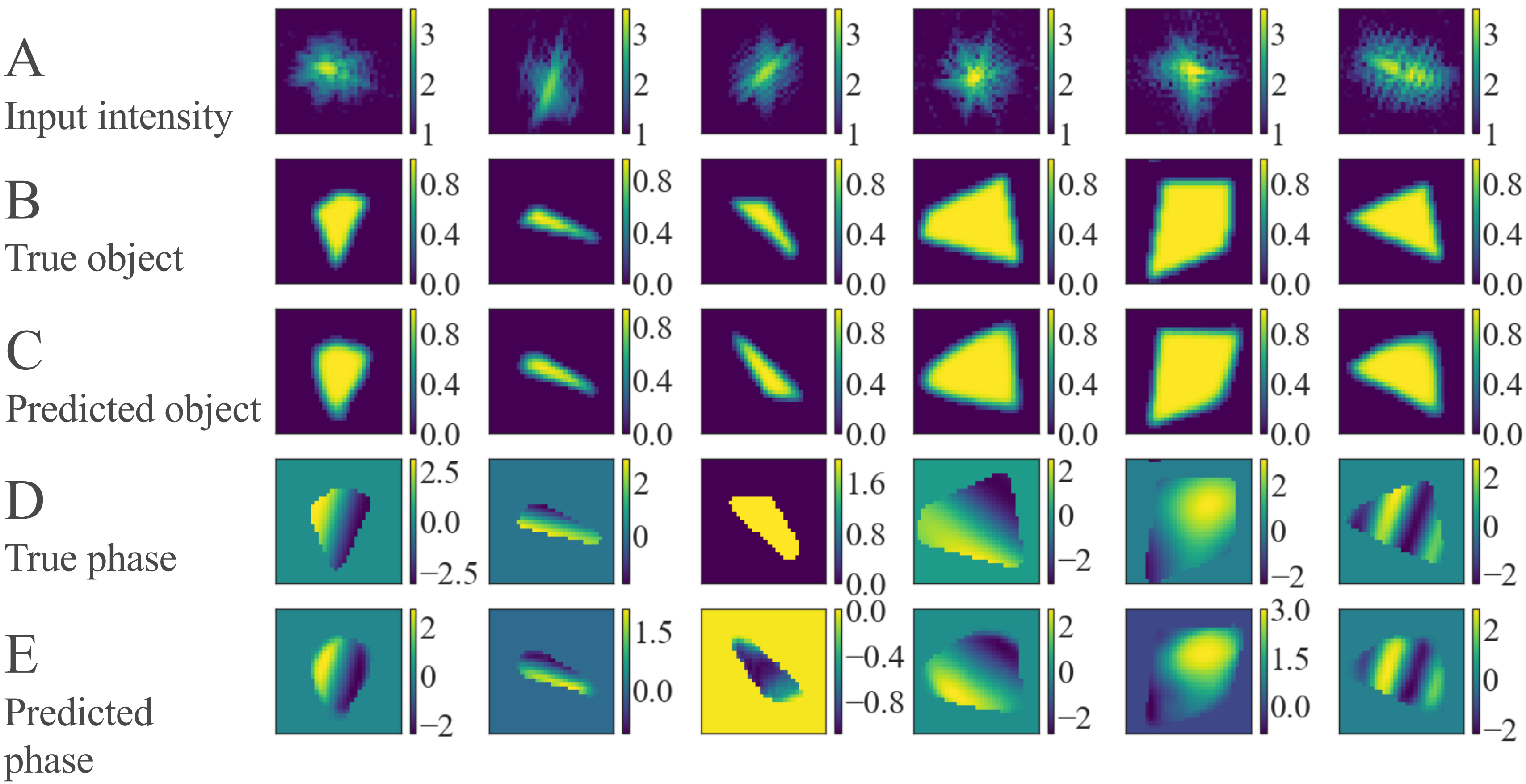
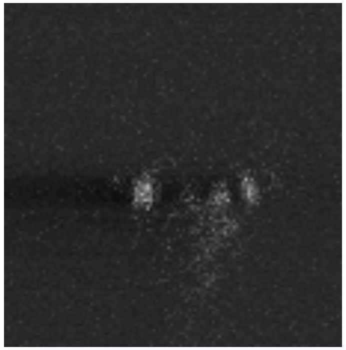
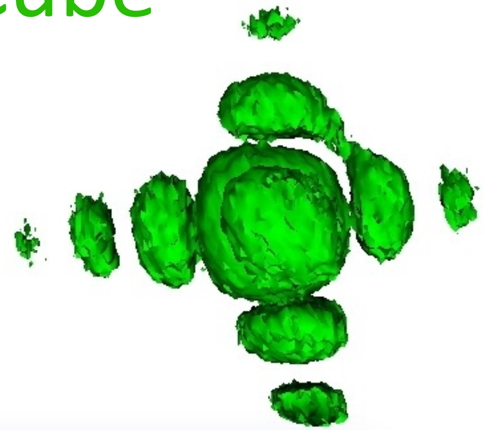
NEURAL NETWORK THAT LEARNS IMAGE RECONSTRUCTION

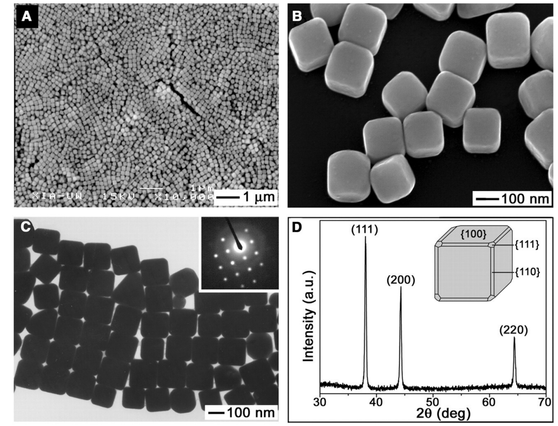


M. J. Cherukara, et al.,
“Real-time coherent diffraction inversion using deep generative networks,”
Sci Rep, vol. 8, no. 1, p. 16520, Nov. 2018.

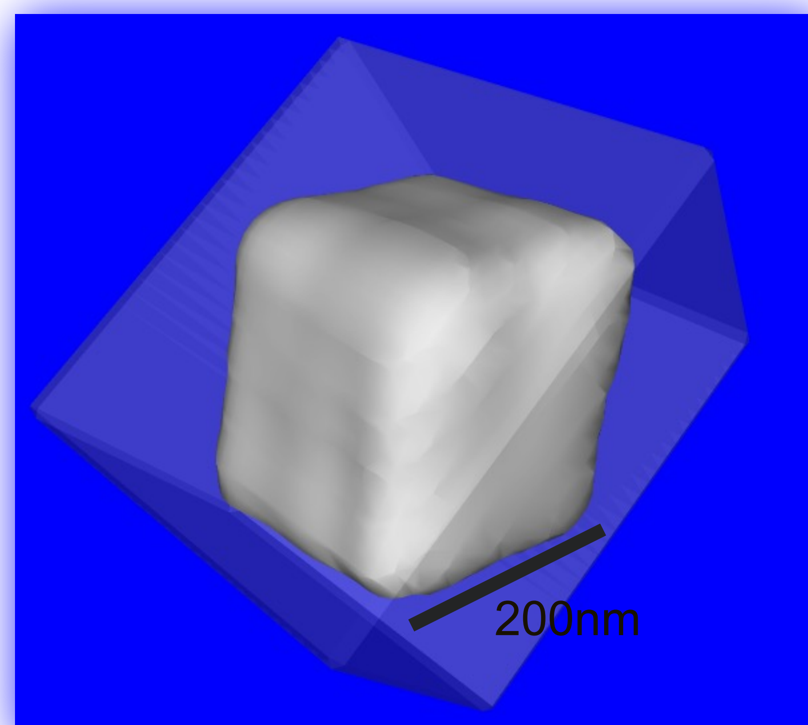
3D Ag Nano Cube

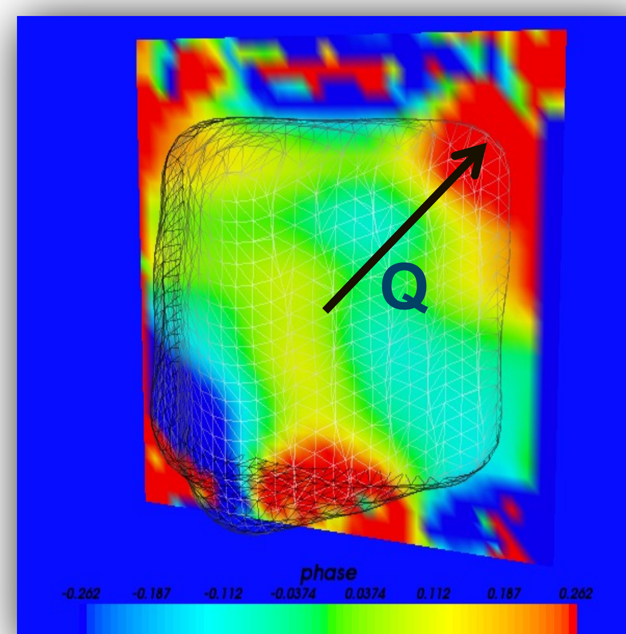




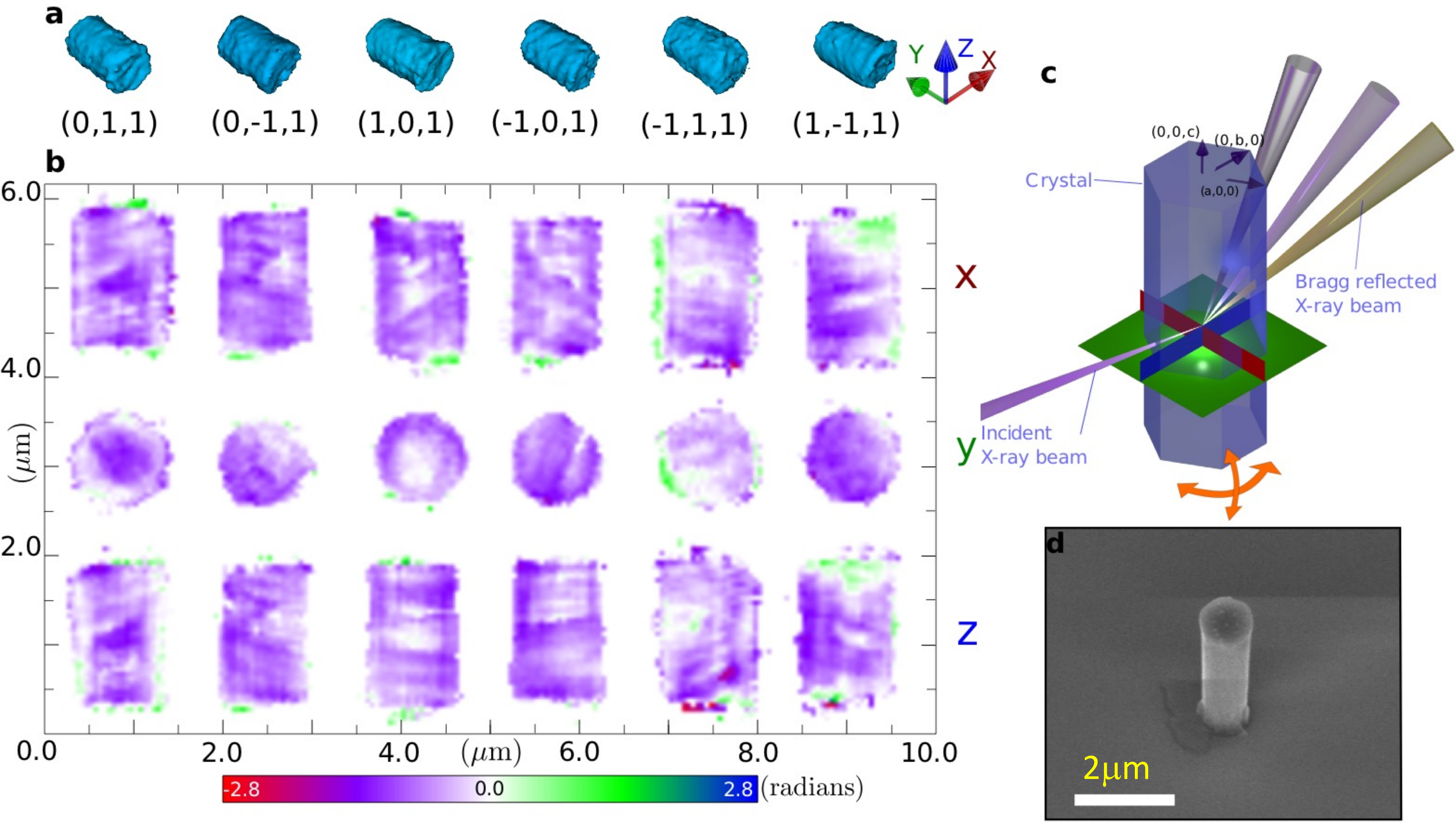


Yugang Sun and Younan Xia, Science 298 2177 (2003)



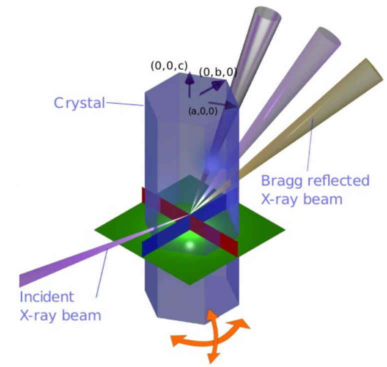


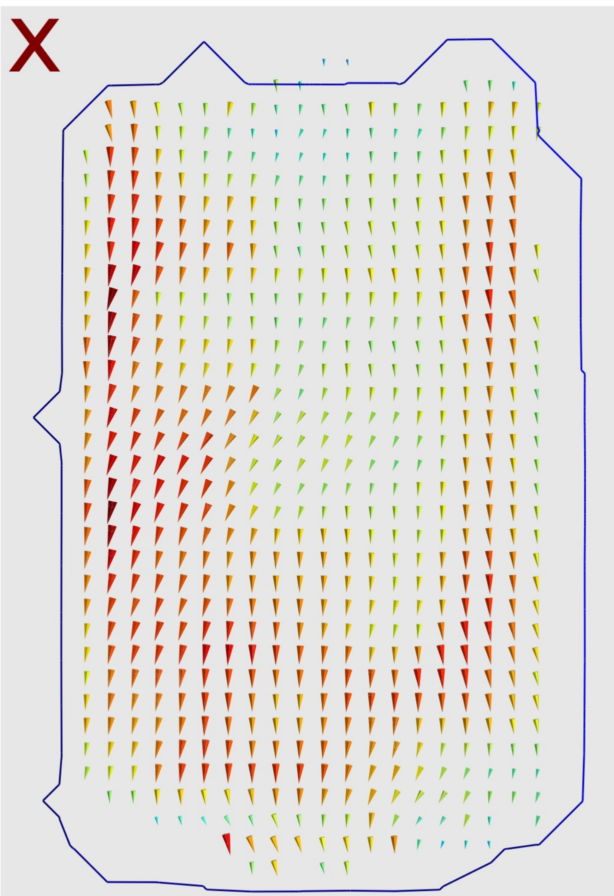
3D Strain Map in ZnO



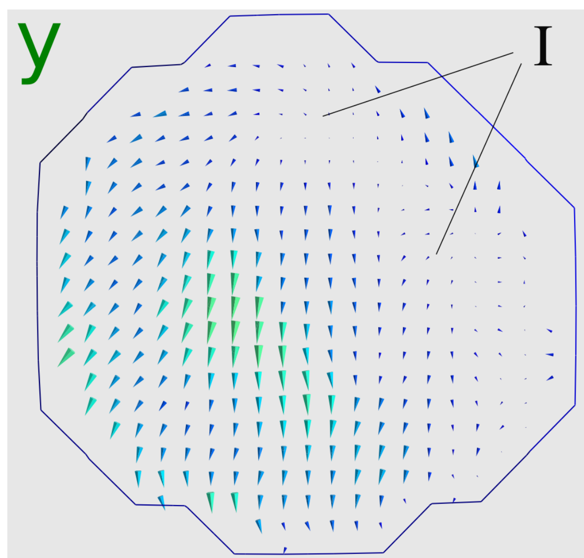
Nature Materials ***9, 120 - 124 (2010)***

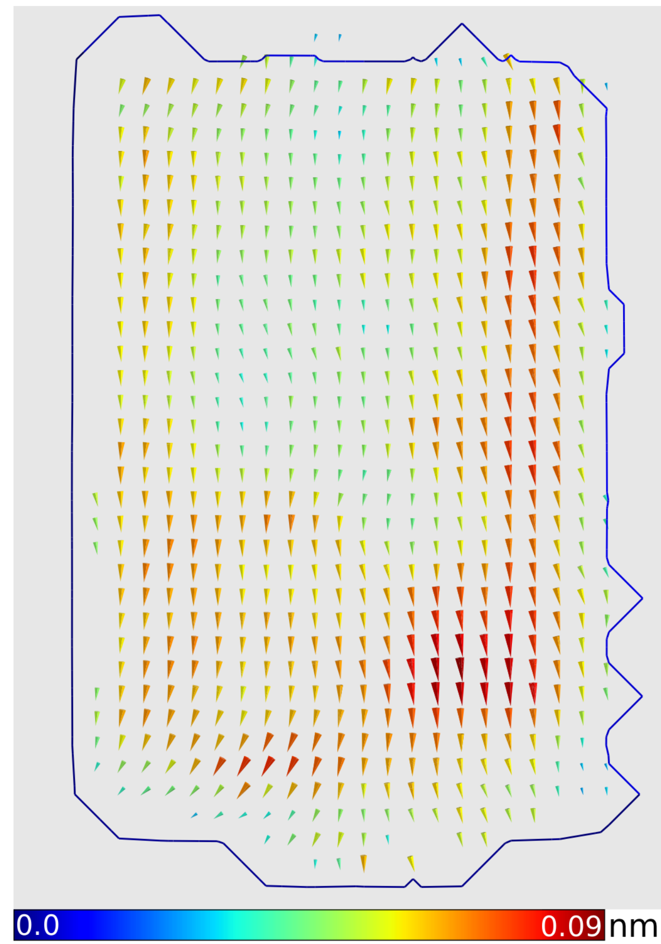
3D Strain Map in ZnO





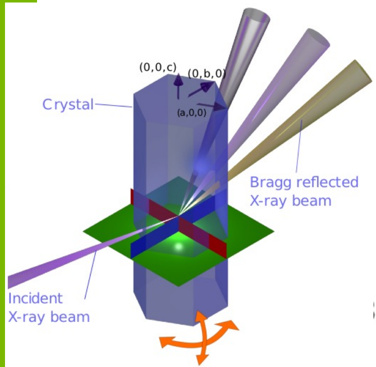
$$u_j = \xi_{ji} q_{ki} \phi_k; \qquad \xi_{ji} = (q_{kj} q_{ki})^{-1}$$



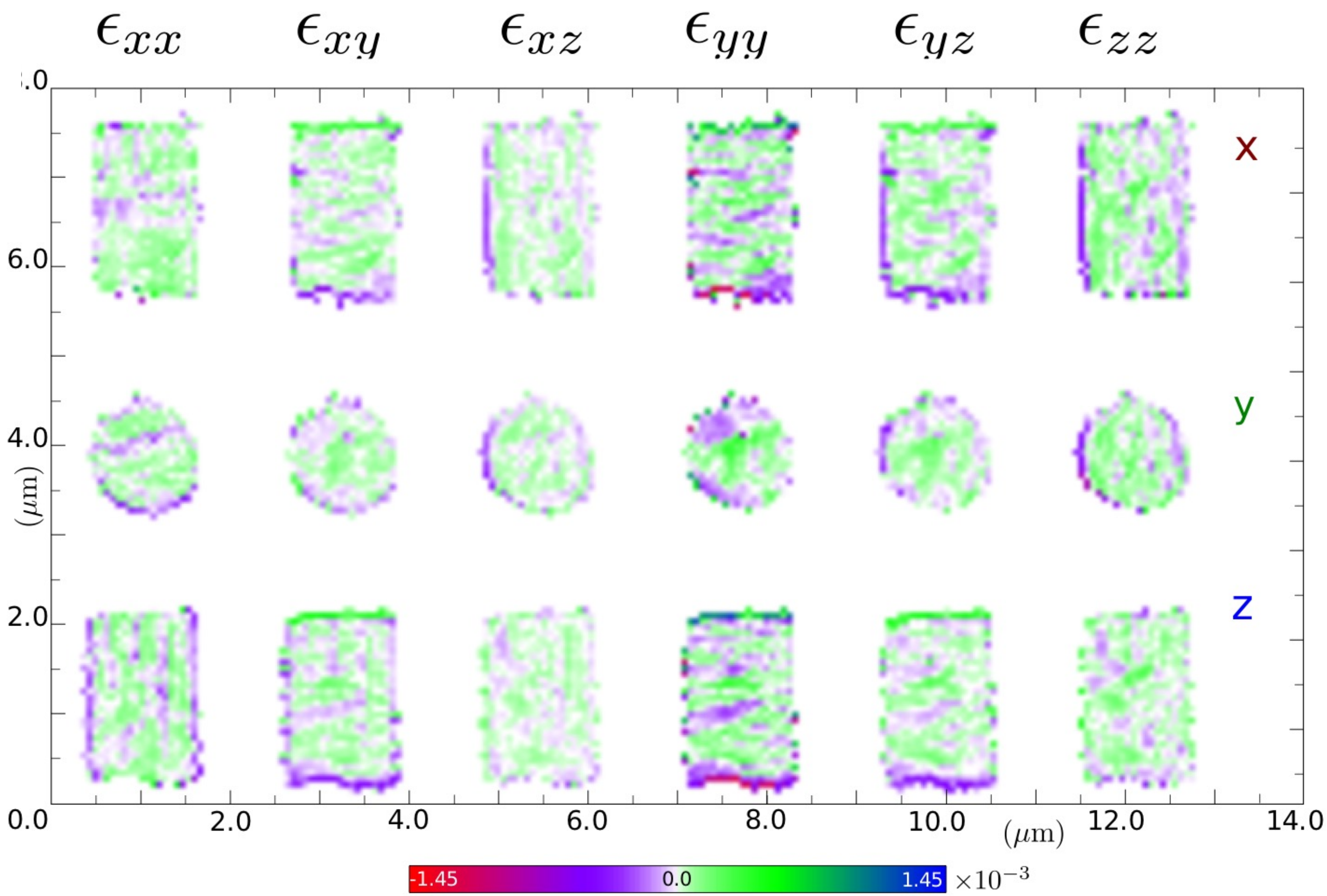


Nature Materials ***9*, *120 - 124 (2010)***

3D Strain Map in ZnO



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

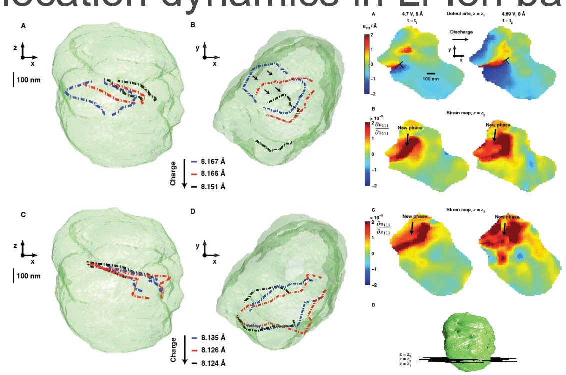


Nature Materials ***9, 120 - 124 (2010)***

BCDI TODAY

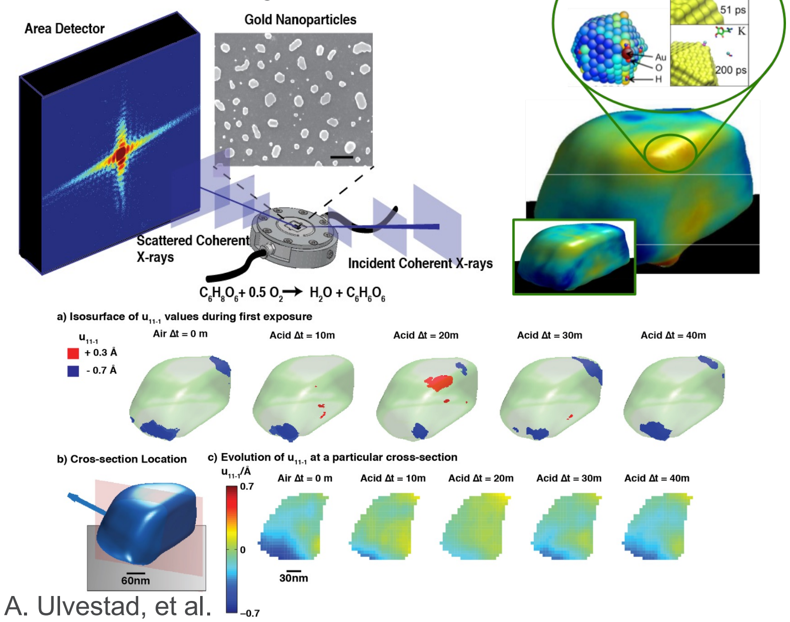
Operando Nanoscale Imaging

Dislocation dynamics in Li-Ion battery



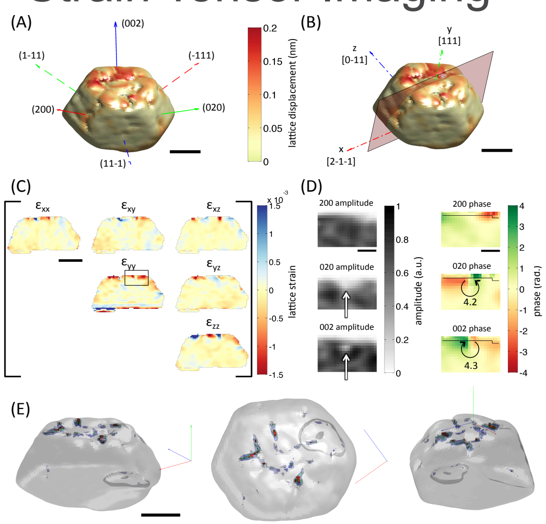
Ulvestad, A., et al. (2015). *Science*, *348*(6241), 1344–1347

Liquid Catalysis



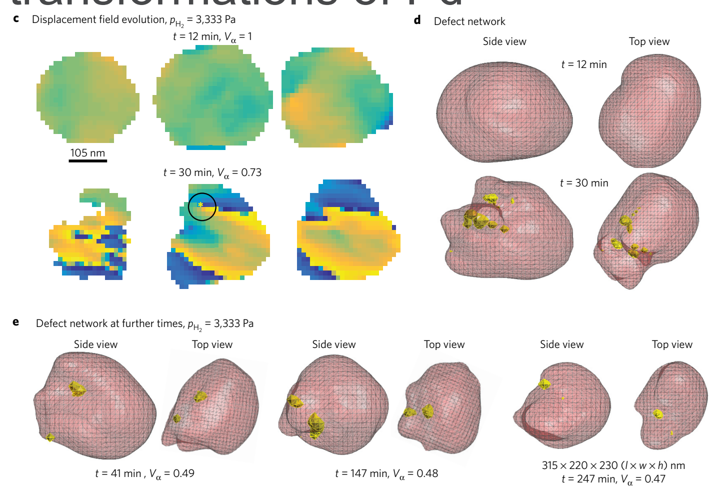
A. Ulvestad, et al. *J. Phys. Chem. Lett.*, vol. 7, no. 15, pp. 3008, Aug. 2016.

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.

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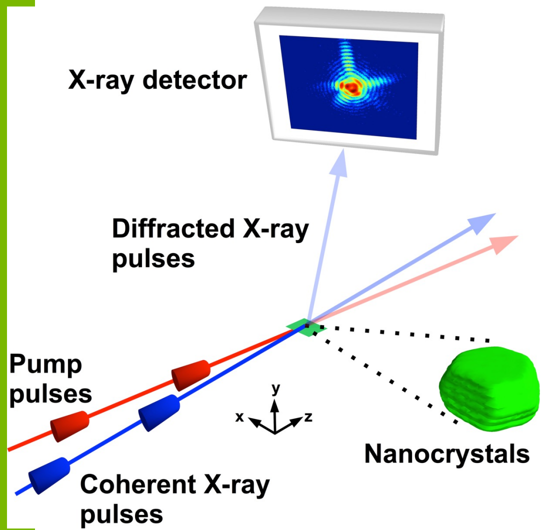
Imaging Lattice Dynamics
Laser Pump – CXD Probe@LCLS

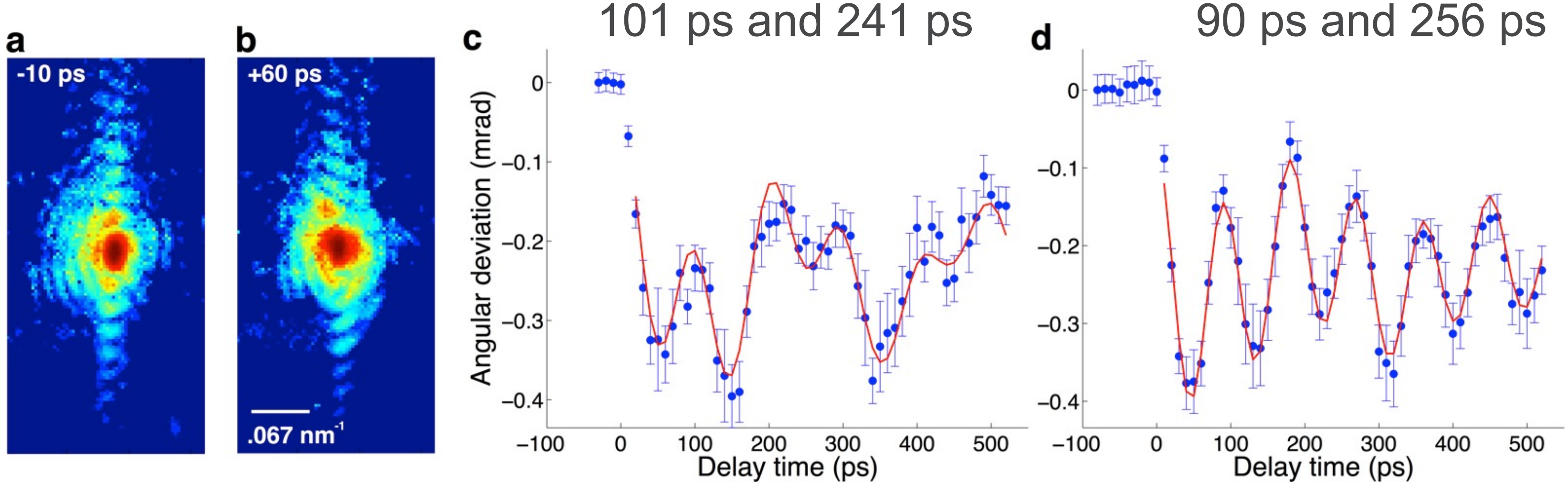


$$S(\tau) = \sum_{n=1}^{N} A_n \exp\left[-\frac{\tau}{\tau_{d,n}}\right] \cos\left[\frac{2\pi}{T_n}(\tau + \tau_{0,n})\right] + C_n.$$

600 pm "breathing modes"

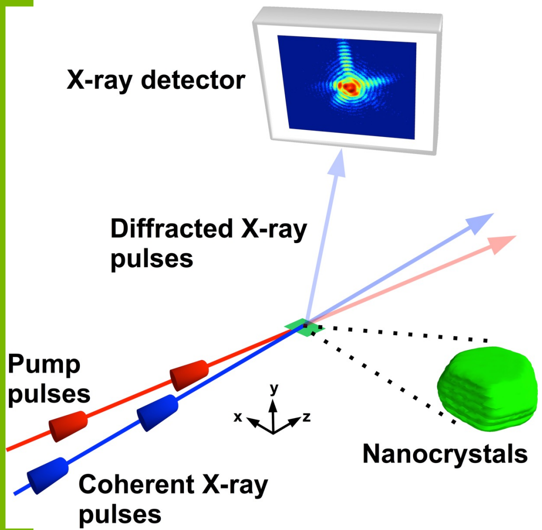
Crystal A
101 ps and 241 ps

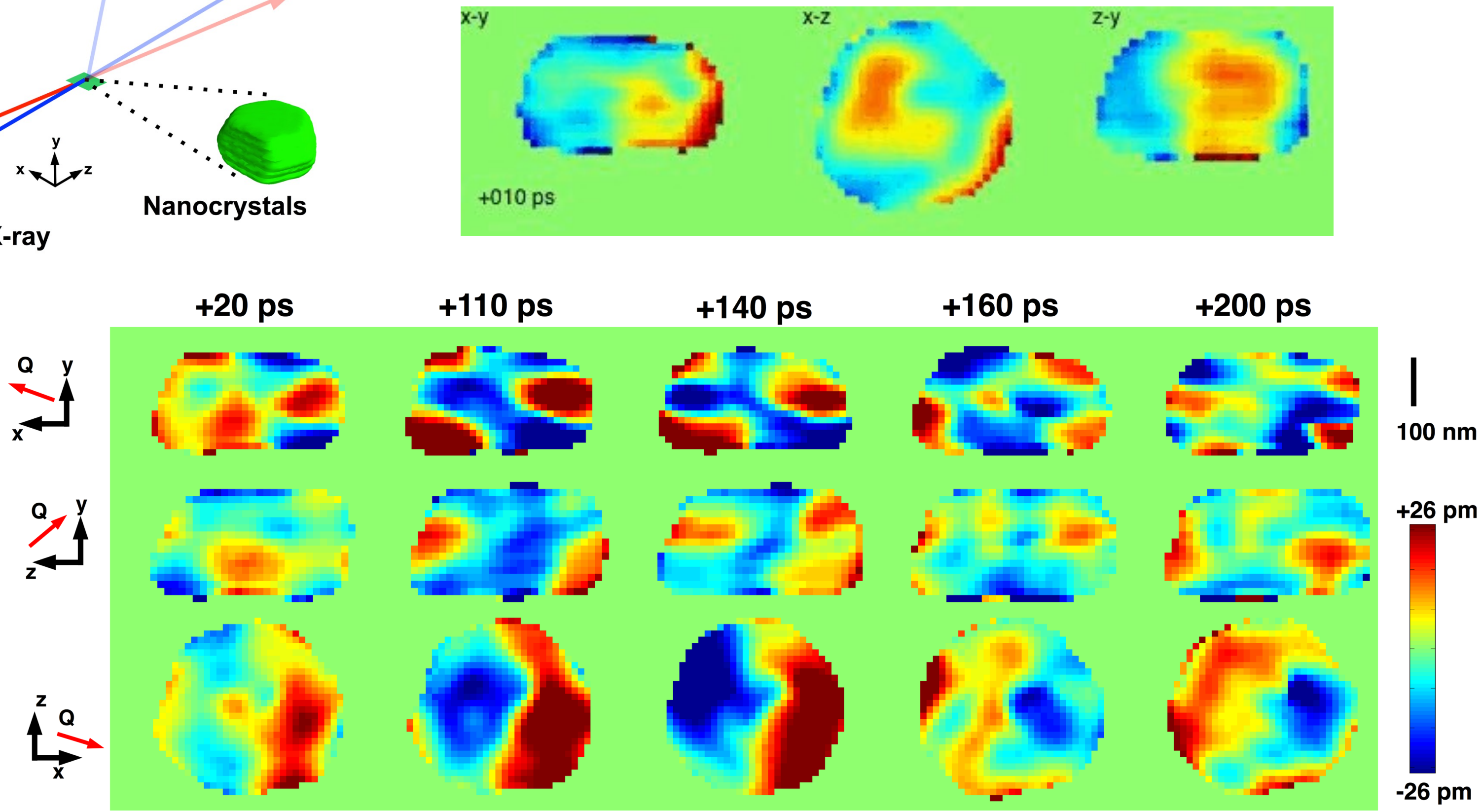
Crystal B
90 ps and 256 ps



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

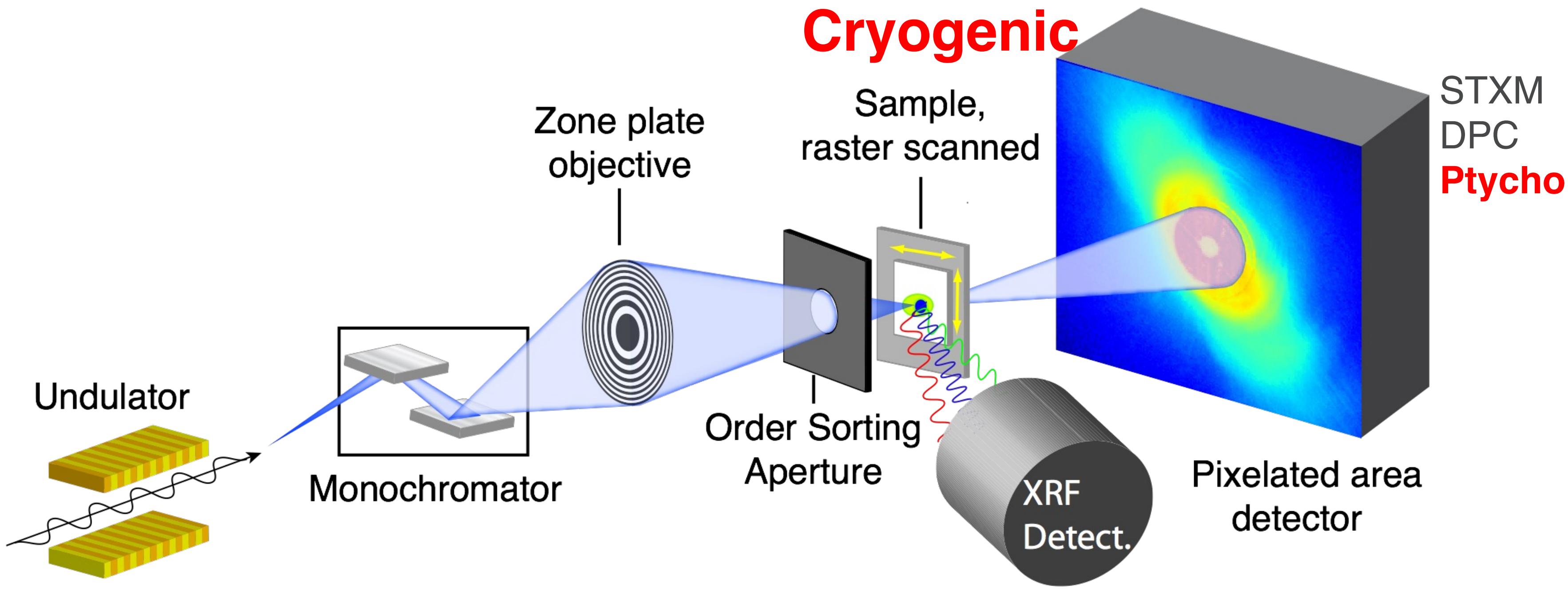




Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals
J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu, M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder, A. M. Korsunsky, J. S. Wark & I. K. Robinson. (2013). *Science*,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

Making ptychography colorful

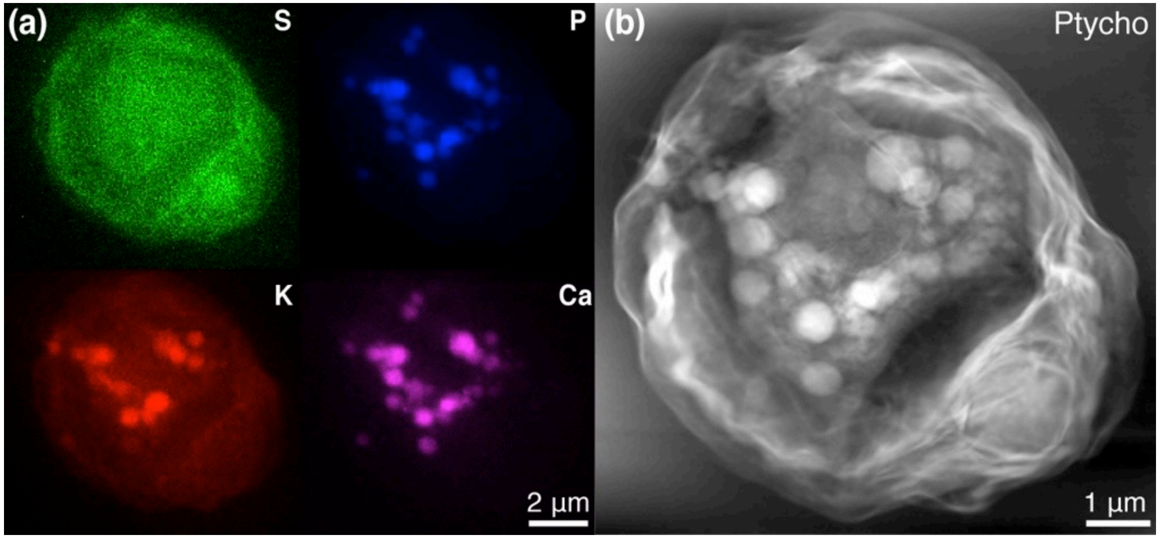
❖ **Combination of Ptychography & Fluorescence**

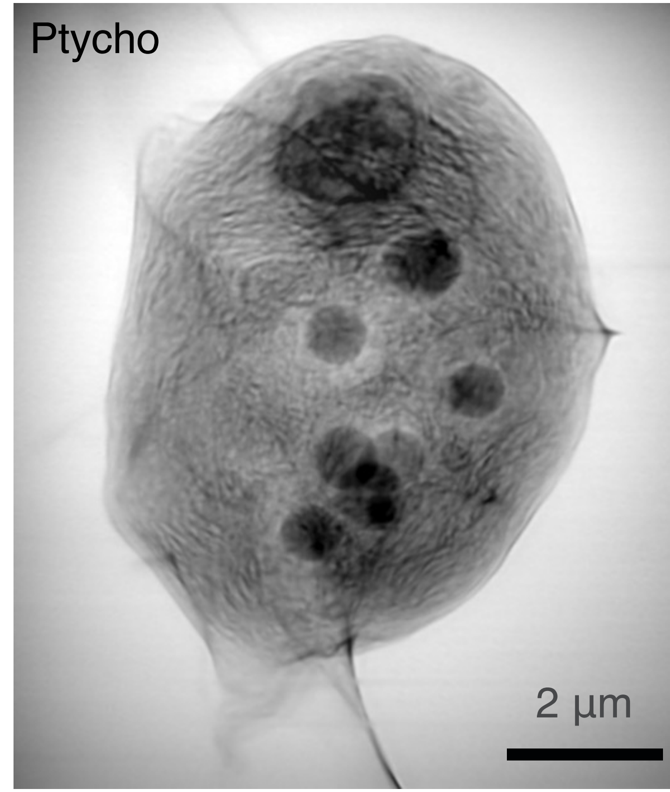


J. Deng, *et al. PNAS* **112**, 2314-2319 (2015)

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

Courtesy Dr. Junjing Deng (APS)

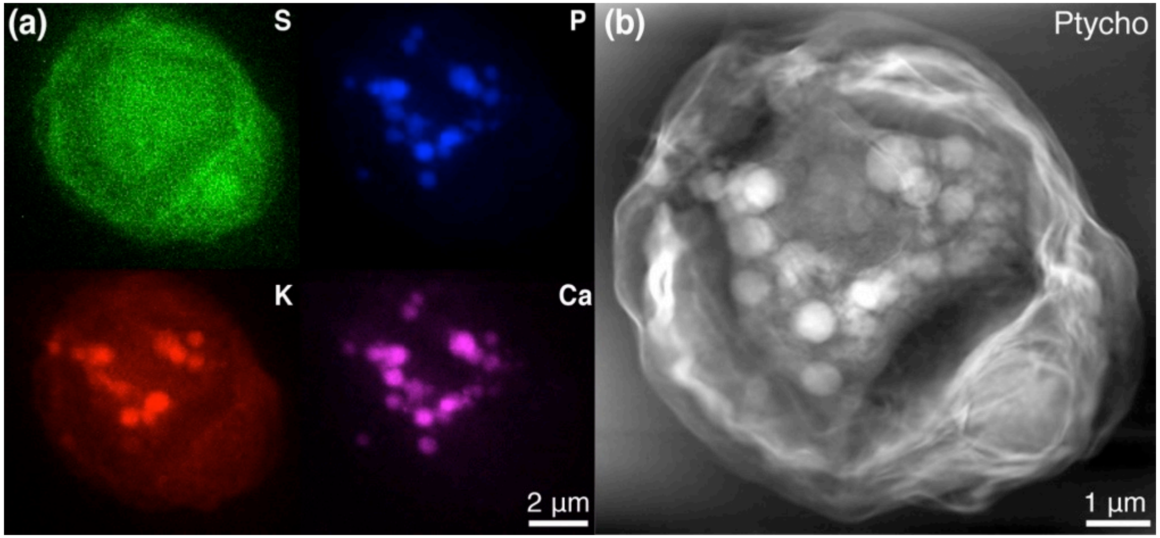


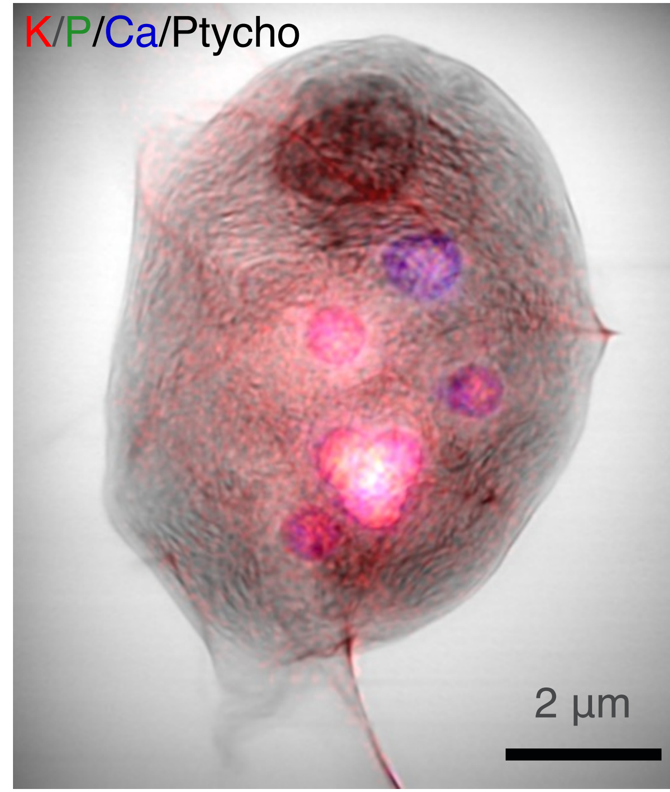


- Frozen-hydrated *Chlamy.* Alga
- Ptychographic image resolution: ~18 nm
- Fluorescence image resolution:~ 100 nm
- Complementary information helps with sample analysis

J. Deng, et al.,
"X-ray ptychographic and fluorescence microscopy of frozen-hydrated cells using continuous scanning.,"
Sci Rep, vol. 7, no. 1, p. 445, Mar. 2017.

Courtesy Dr. Junjing Deng (APS)





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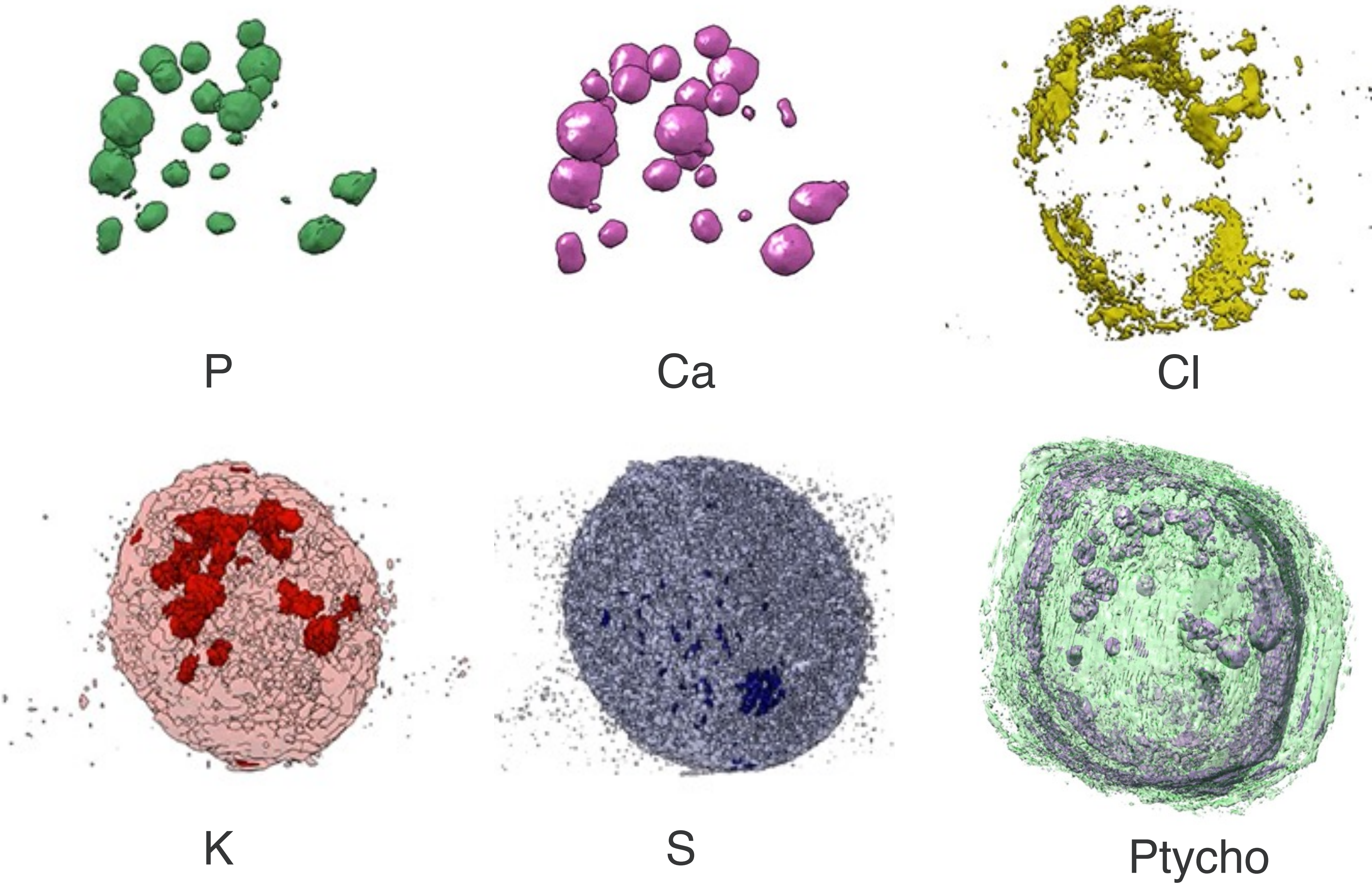
J. Deng, et al.,
"X-ray ptychographic and fluorescence microscopy of frozen-hydrated cells using continuous scanning.,"
Sci Rep, vol. 7, no. 1, p. 445, Mar. 2017.

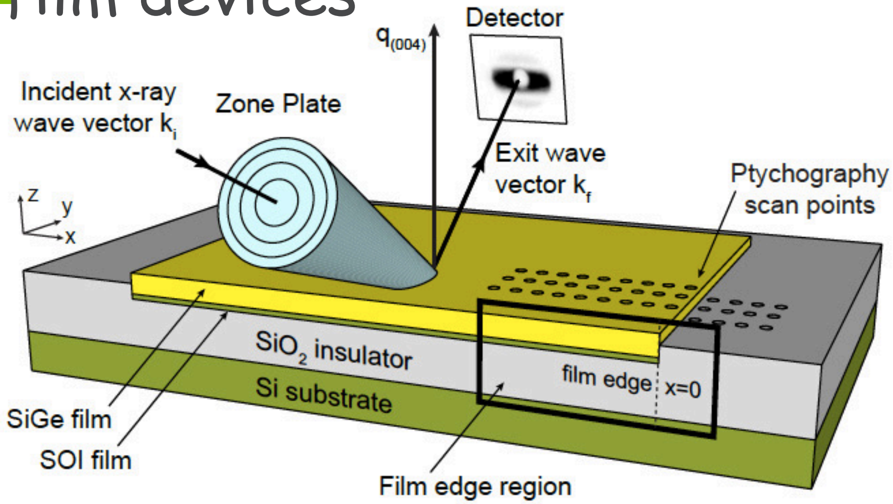
Courtesy Dr. Junjing Deng (APS)

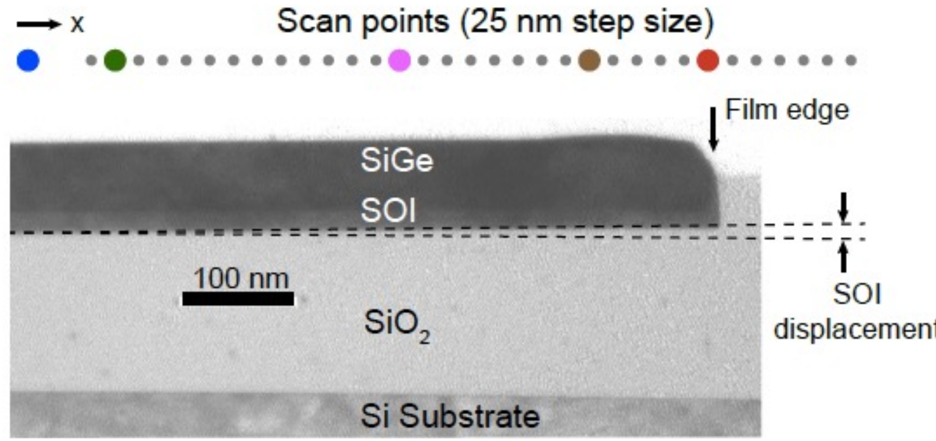
Extended to 3D

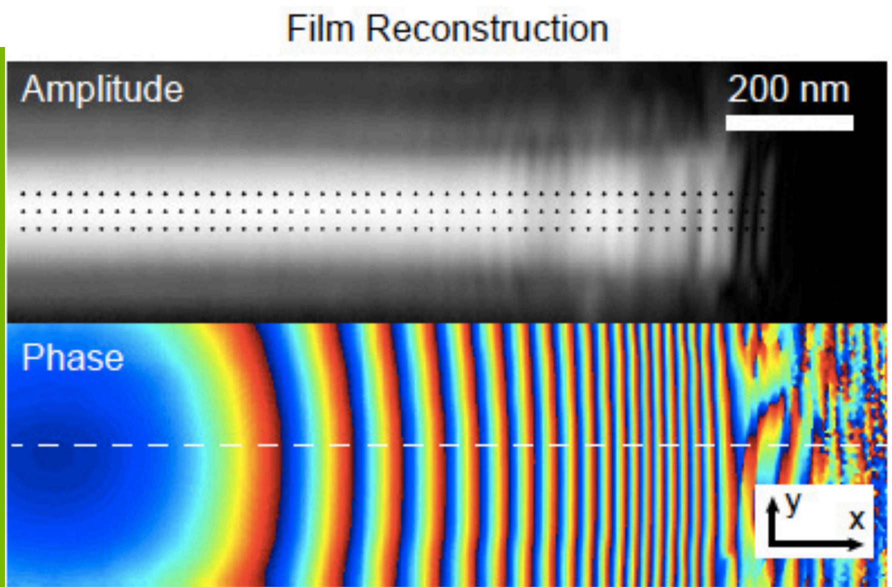


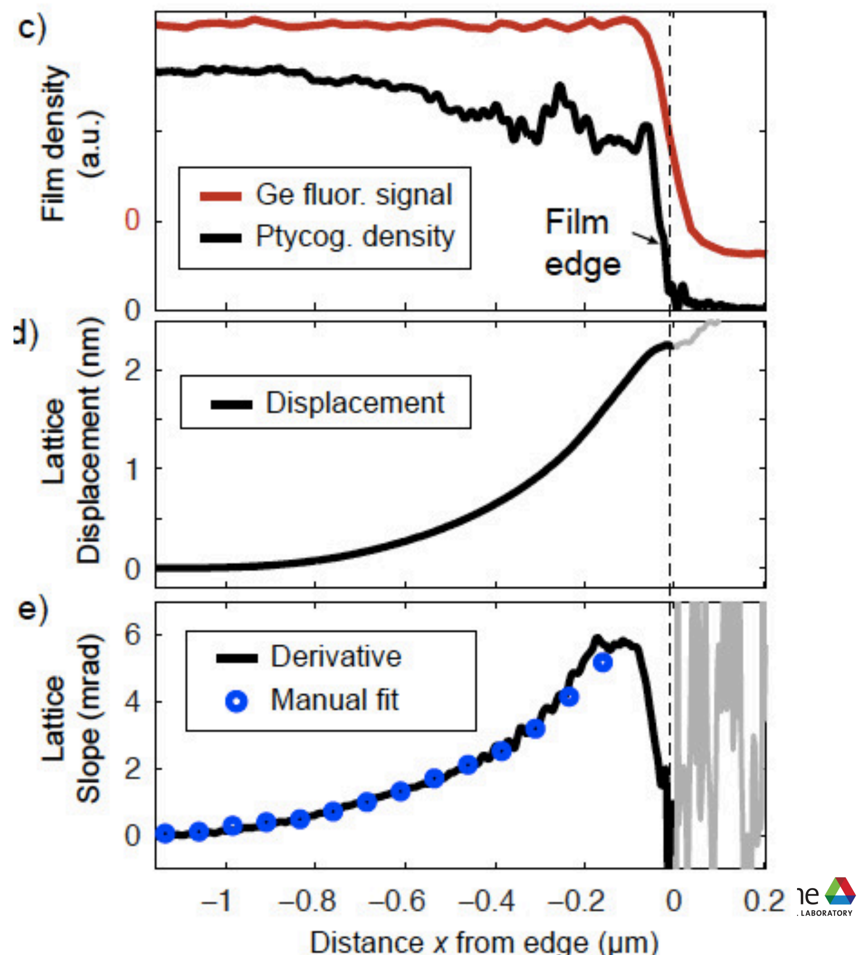
Courtesy Dr. Junjing Deng (APS)

Nanoscale Strain in SiGe film devices





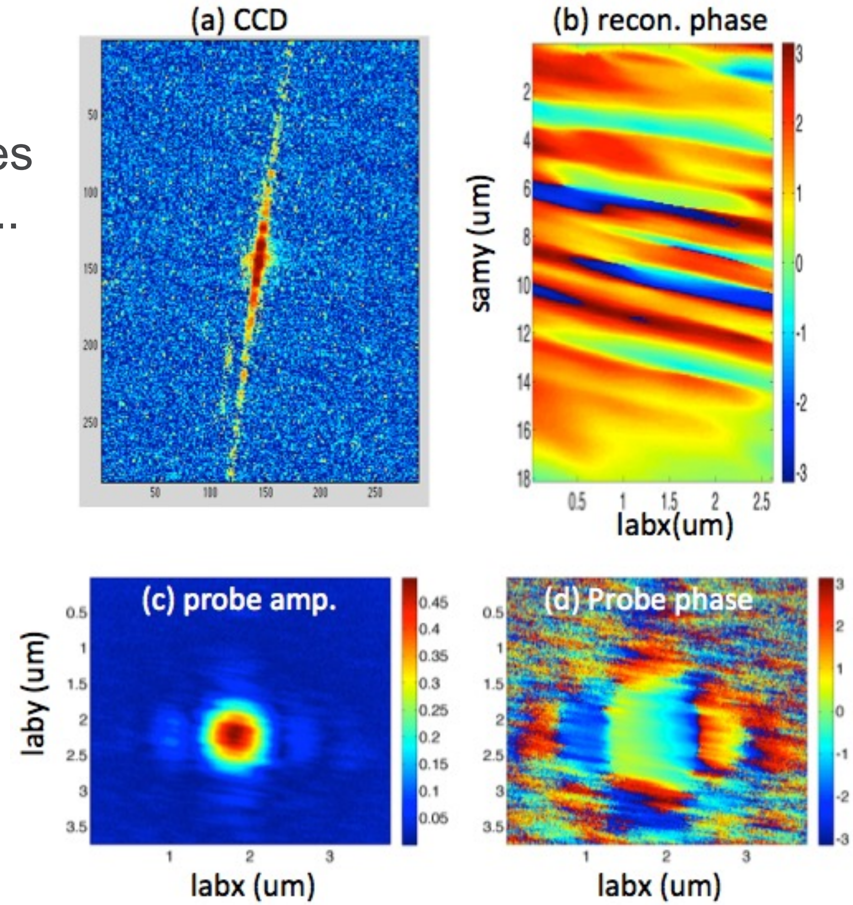


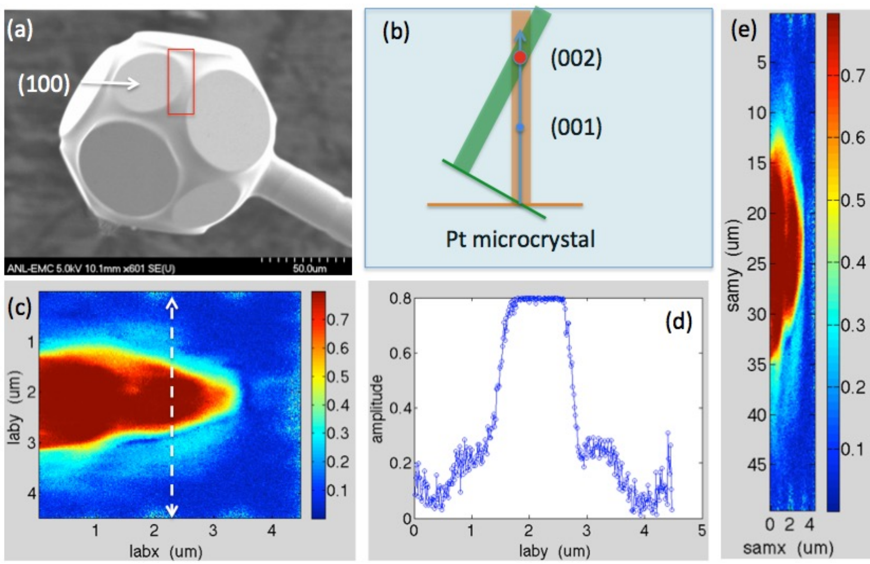


Hruszkewycz, S. O., Holt, M. V., et al. (2012). *Nano Letters*, *12*(10), 5148–5154.

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…..

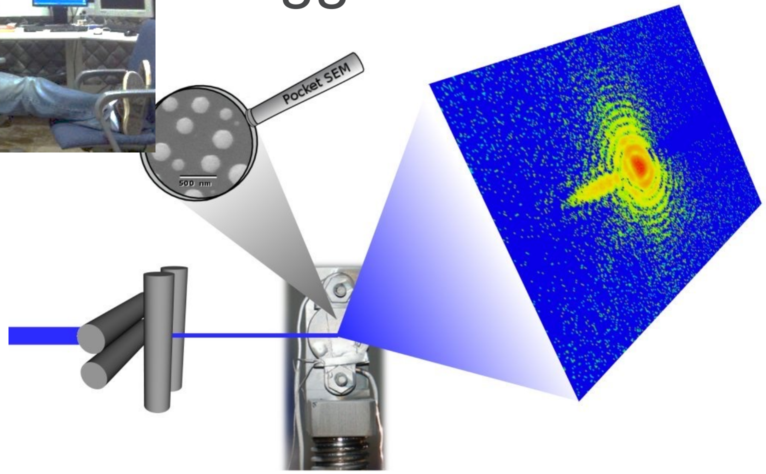




C. Zhu, et al. *Applied Physics Letters*, vol. 106, no. 10, p. 101604, Mar. 2015.

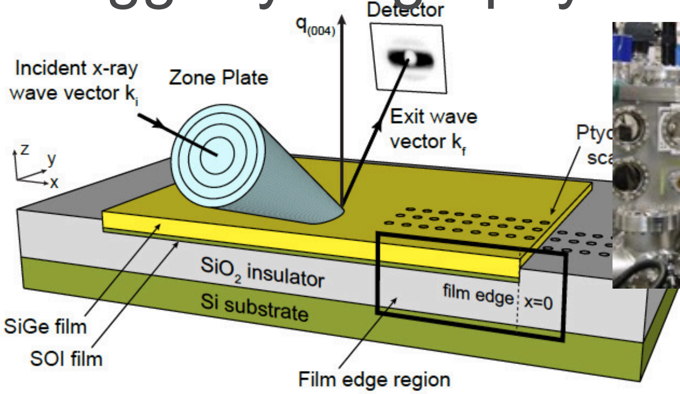
APPLY FOR COHERENT IMAGING BEAMTIME @ APS!

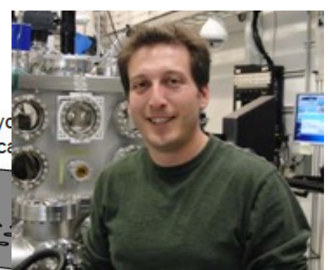
Bragg CDI



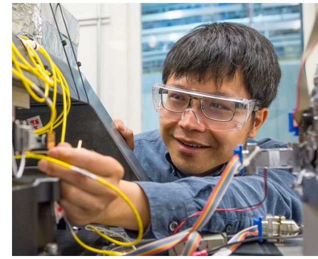
Email: Ross Harder rharder@aps.anl.gov
https://wiki-ext.aps.anl.gov/s34idc/index.php/34-ID-C

Bragg Ptychography

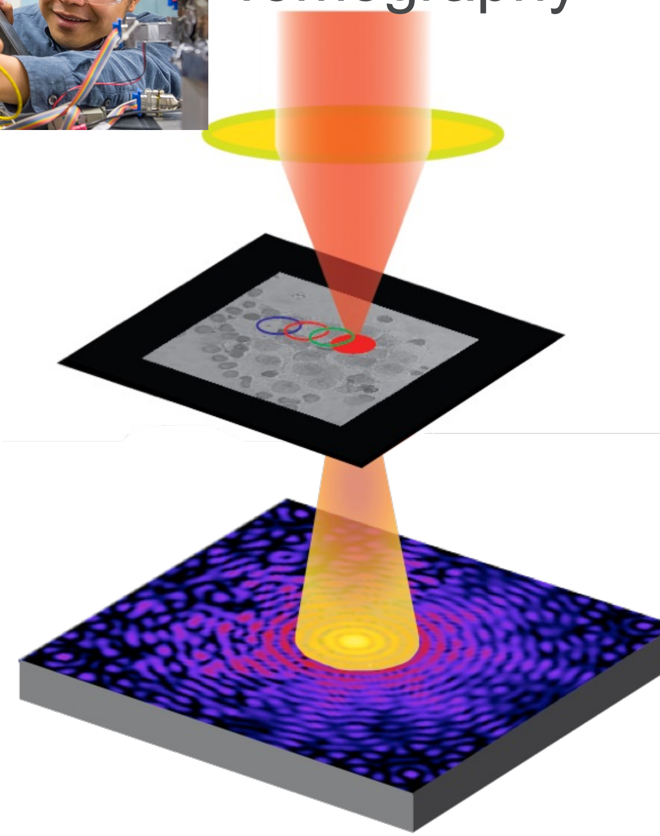




Email: Martin Holt mvholt@anl.gov
https://wiki-ext.aps.anl.gov/s26id/index.php/26-ID



Ptychography Tomography



Email: Junjing Deng junjingdeng@aps.anl.gov

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

Feedback

Lecture – 11:00 – 12:00

Coherence Based Imaging - Ross Harder

https://forms.office.com/g/52JJbFGggP

Argonne NATIONAL LABORATORY

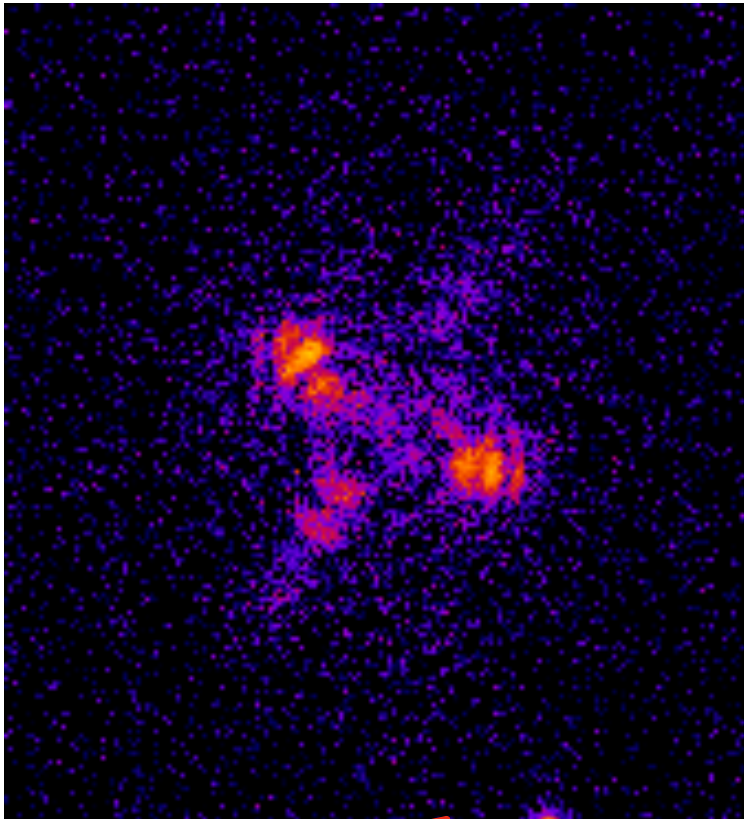
SUPPLEMENTAL SLIDES

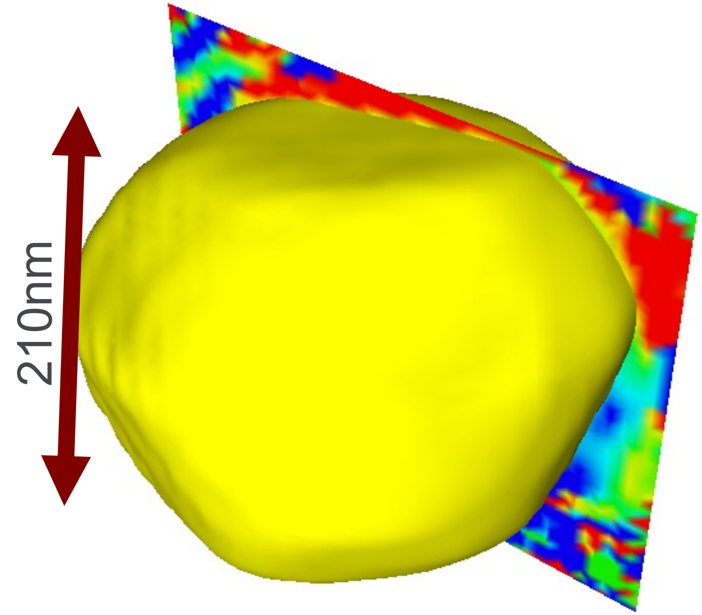
LARGE-FORMAT, SINGLE-PHOTON SENSITIVE X-RAY CCD CAMERAS OPENED THE DOOR TO COHERENT X-RAY IMAGING

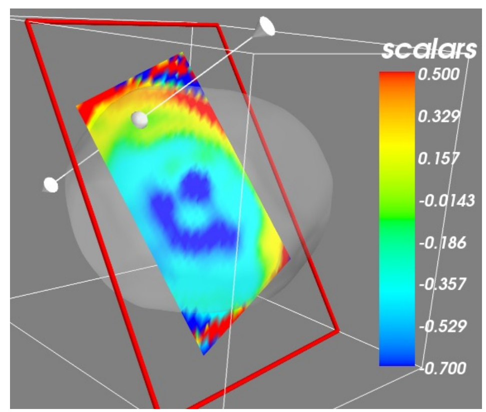
Fairchild Peregrine 486 CCD Camera

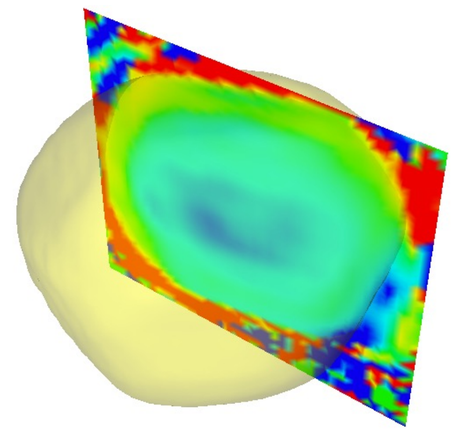
- 4K x 4K pixel array (61.4 mm square area)
- 15 μm pixels, 100% fill factor
- Back-illuminated for up to 80% QE
- Readout noise < 5 e- at 50 Kpixels/s
- Dynamic range > 86 dB in MPP
- 6 s readout with four on-chip amplifiers
- Pixel binning for more rapid readout
- Peltier-cooled to -50 C for low dark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

Hi Resolution Imaging (CCD)?







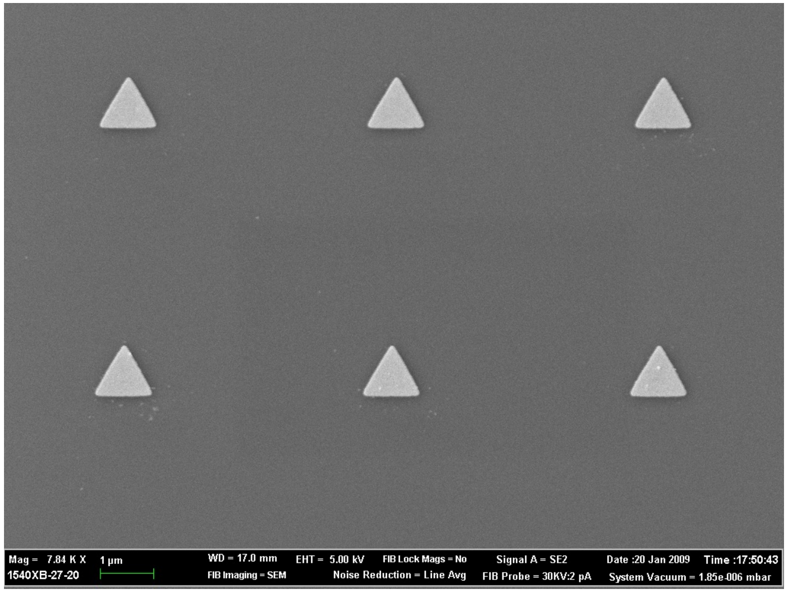


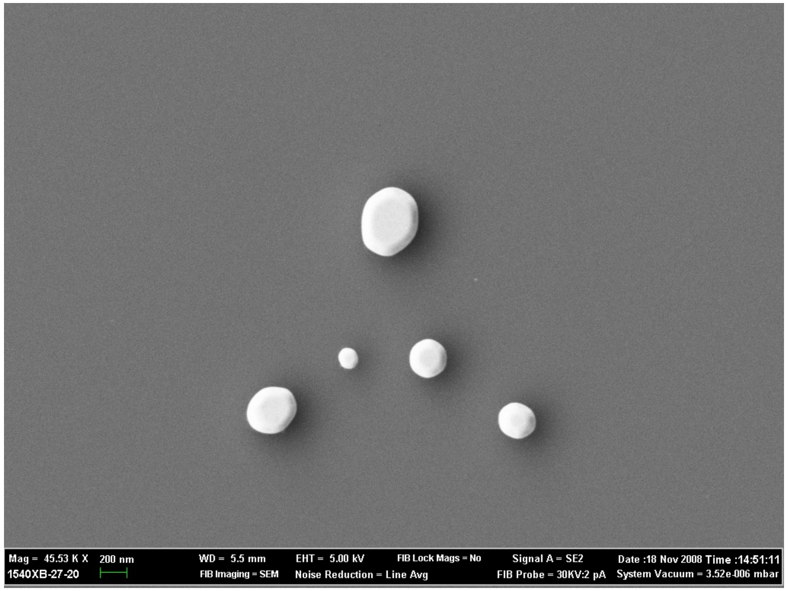
~7nm data

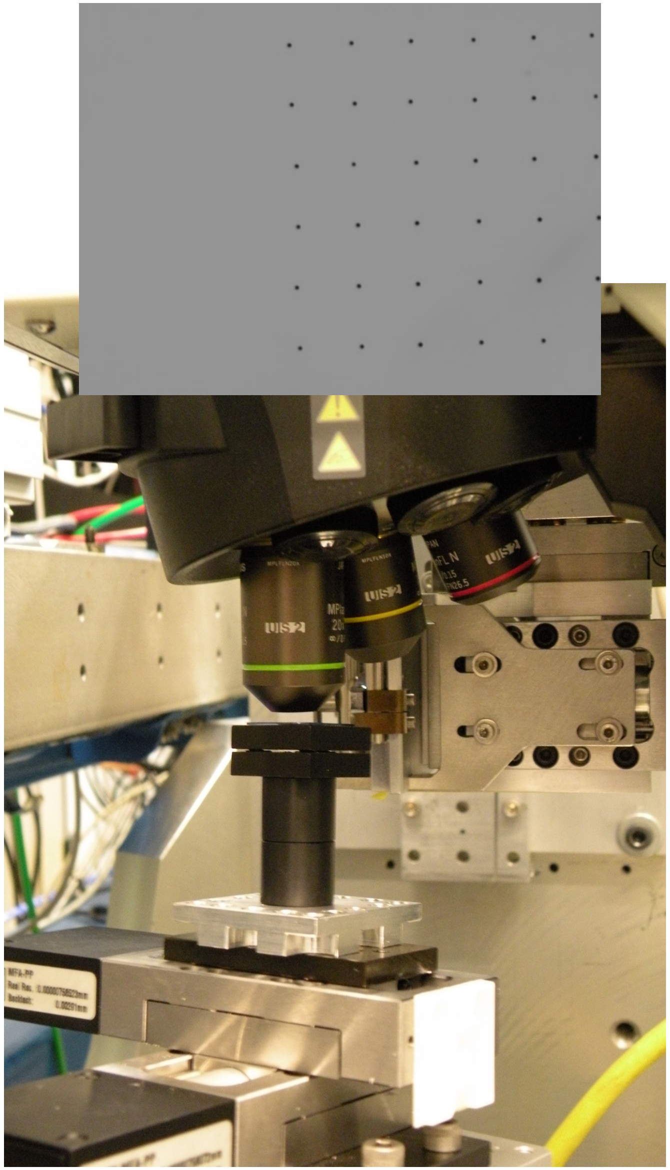
At APS 34-ID-C:
9.25 hours of scanning
38 minutes of x-ray exposure

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

Patterned Gold Nanocystal Samples

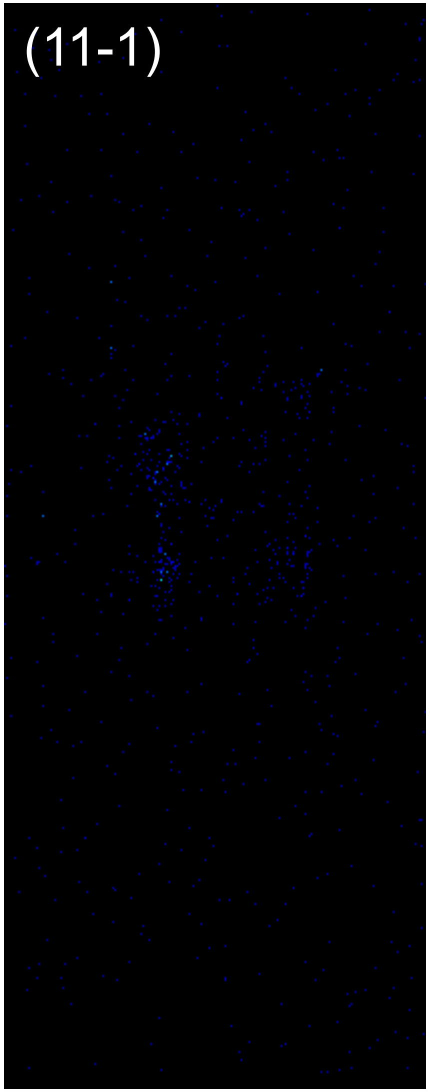


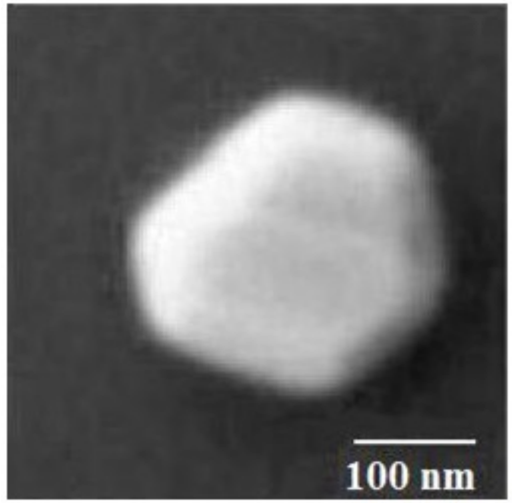


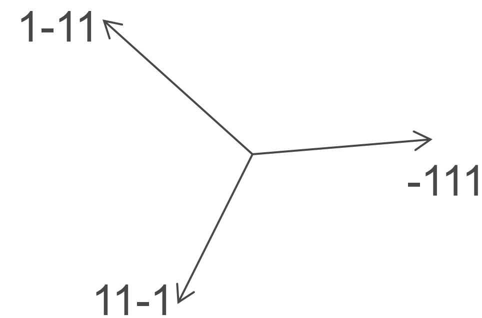


Argonne NATIONAL LABORATORY

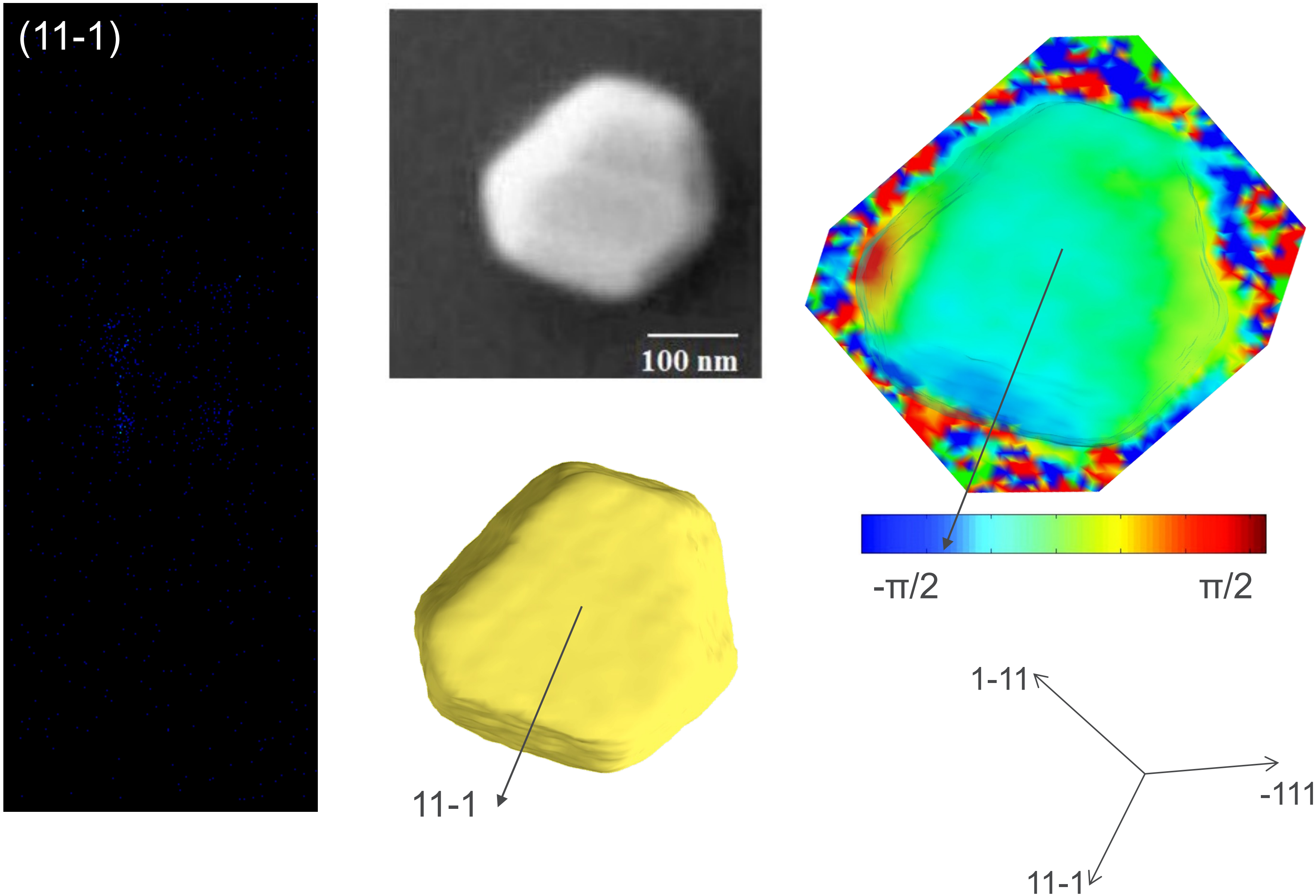
Multiple reflection reconstructions



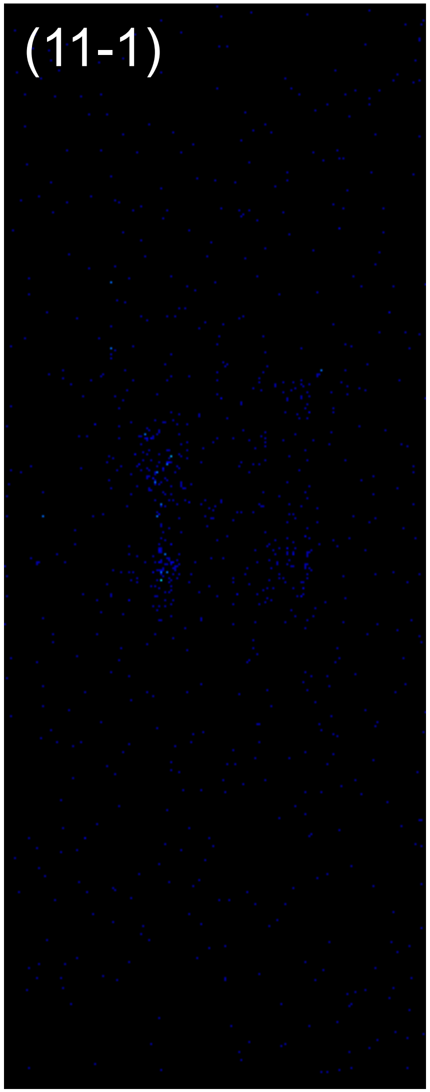


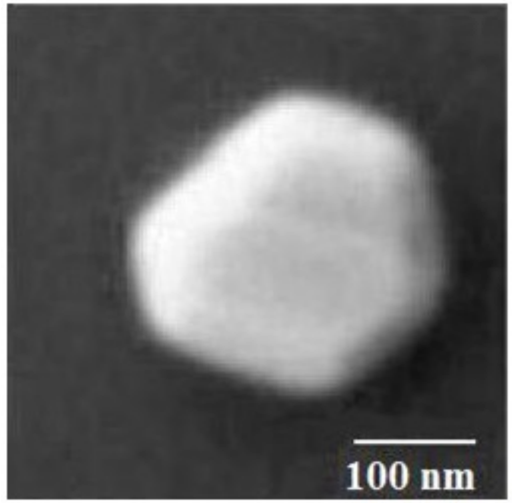


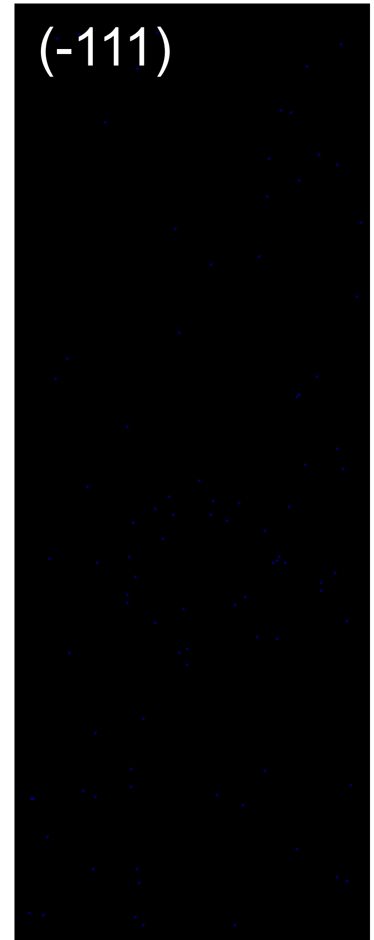
Multiple reflection reconstructions

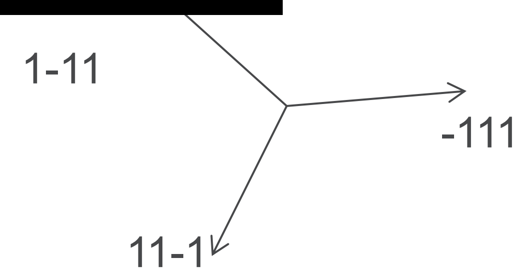


Multiple reflection reconstructions

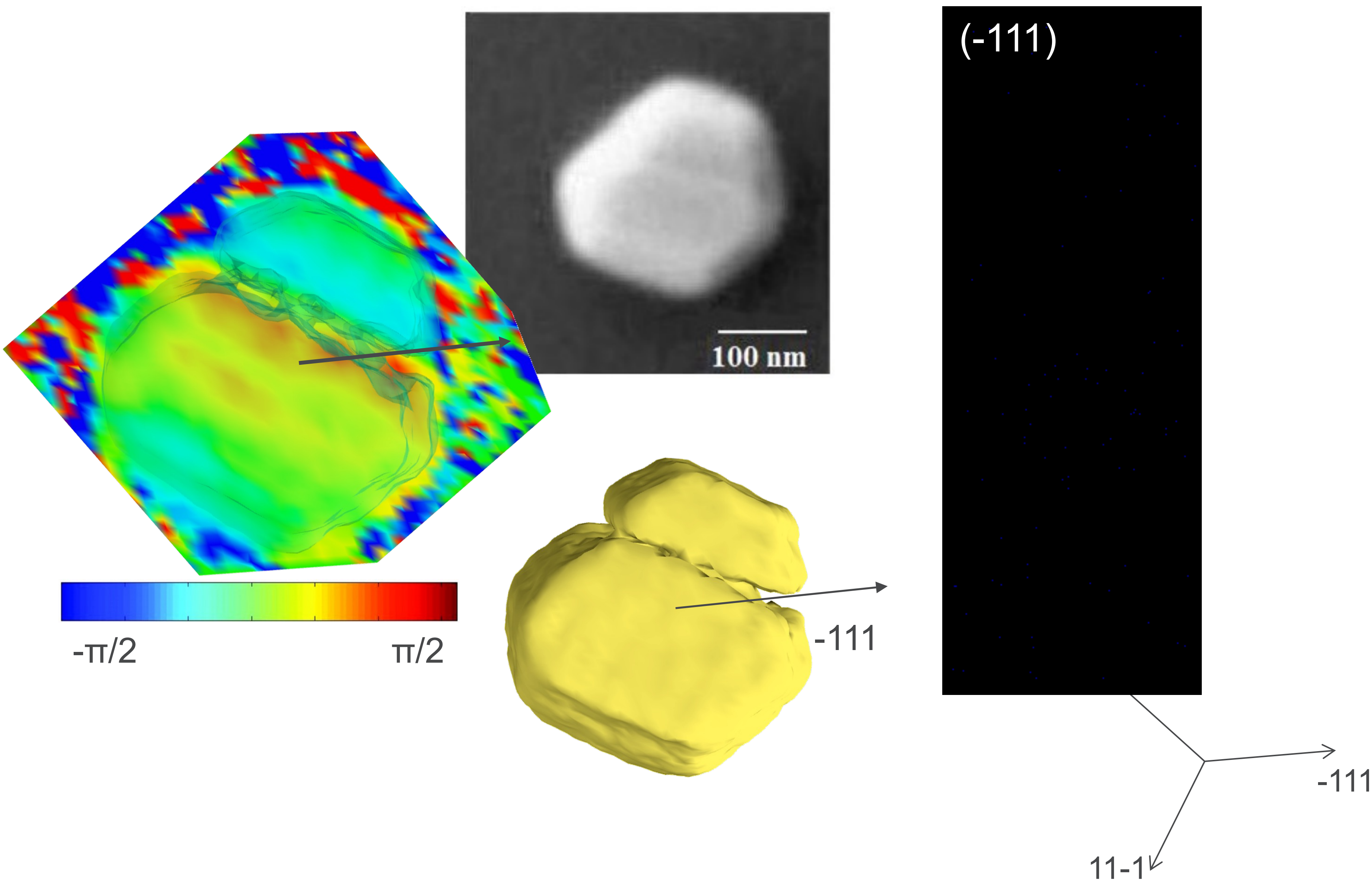




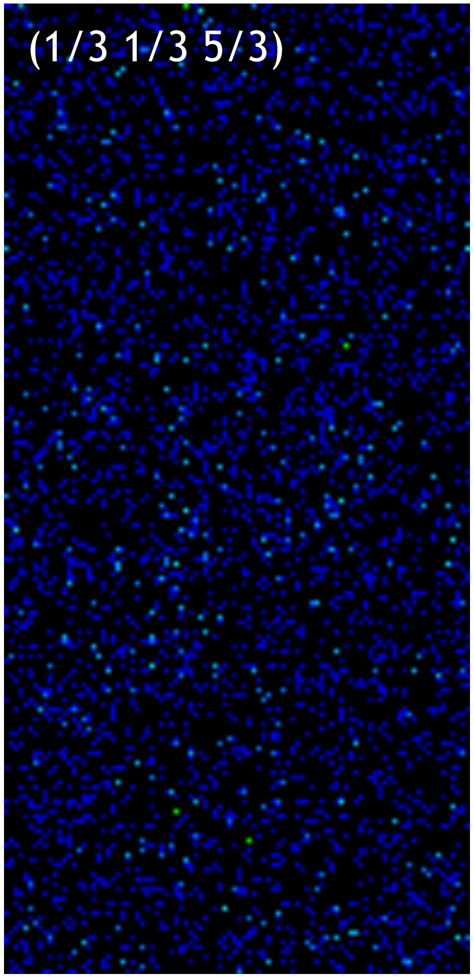


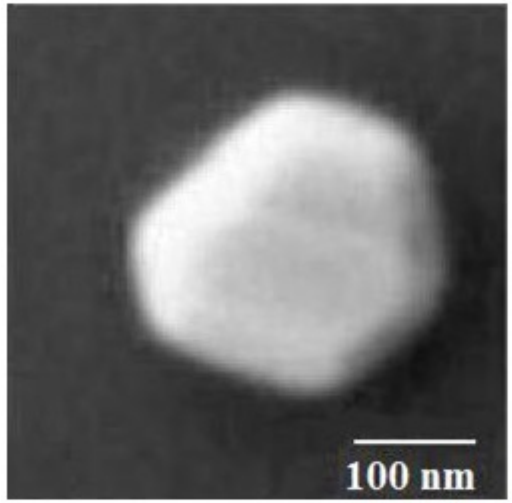


Multiple reflection reconstructions

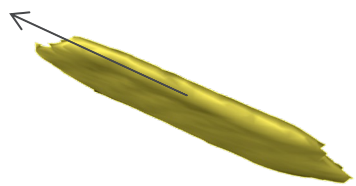


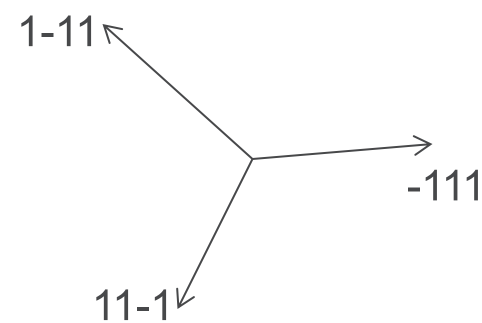
Multiple reflection reconstructions



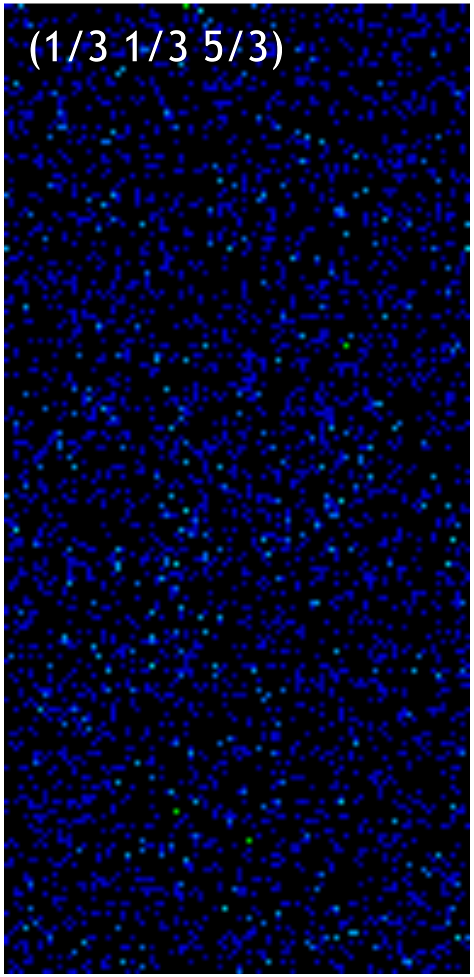


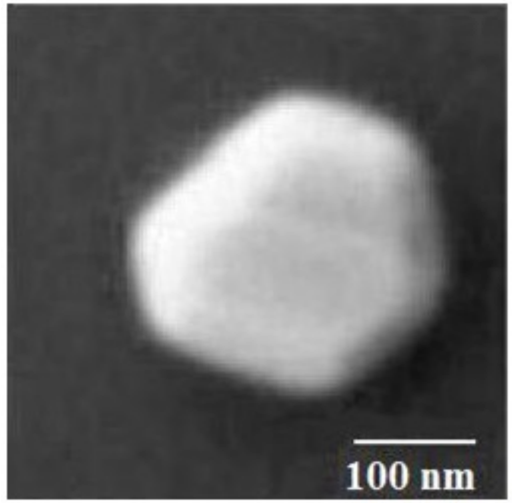
(1/3 1/3 5/3)

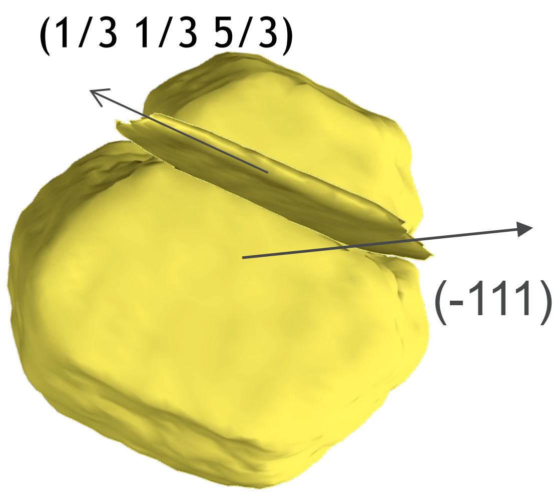


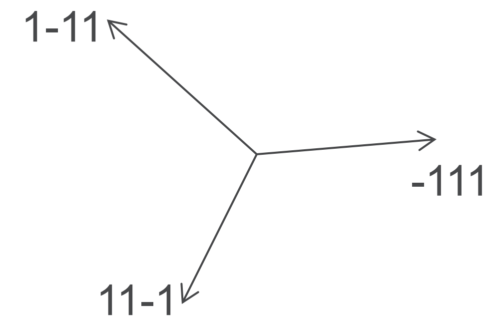


Multiple reflection reconstructions

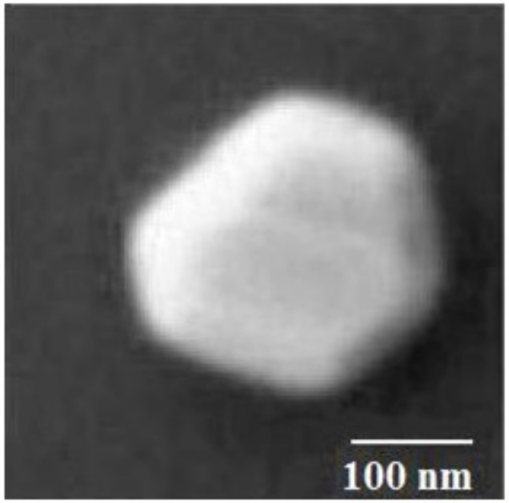




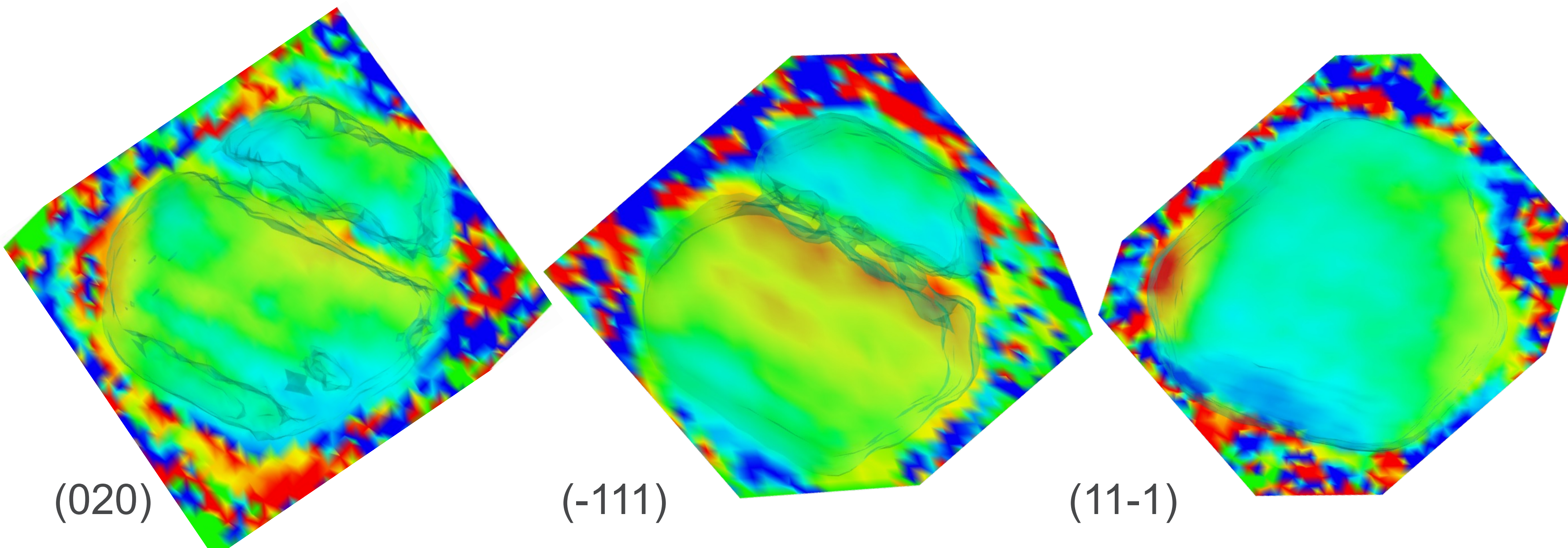




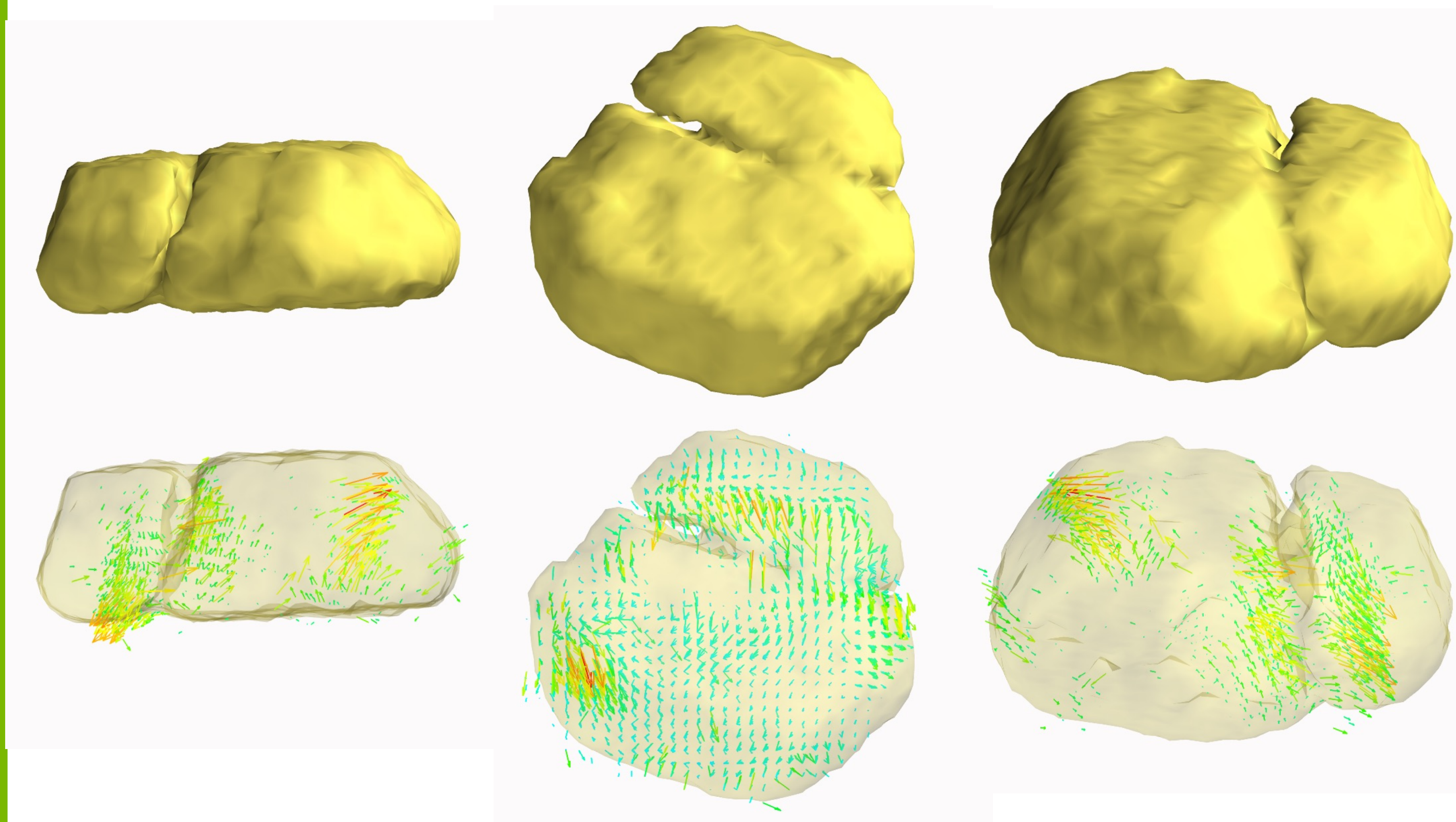
Multiple reflection reconstructions



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



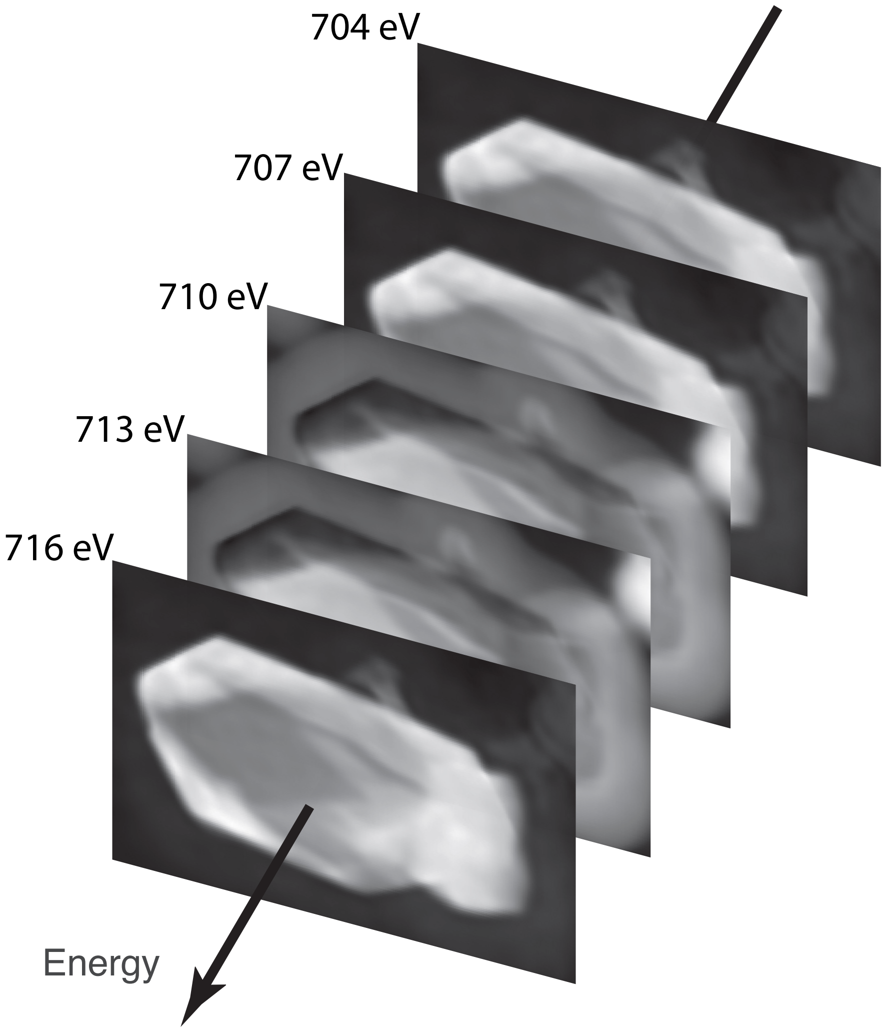
Vector Displacement Field of Gold lattice

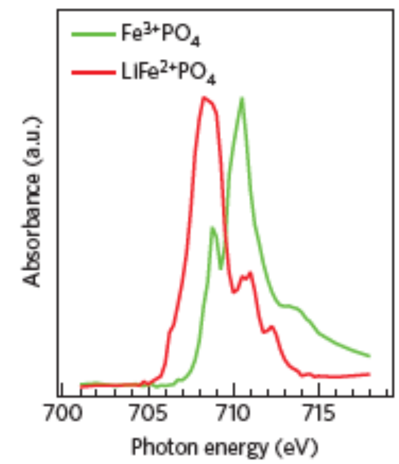


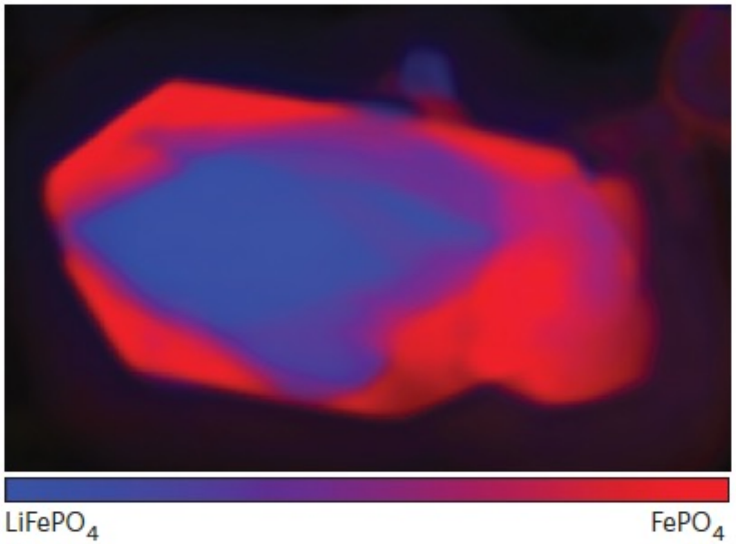
Produced by combining reconstructions from (11-1) (020) (-111)

❖ Ptychographic spectroscopy

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

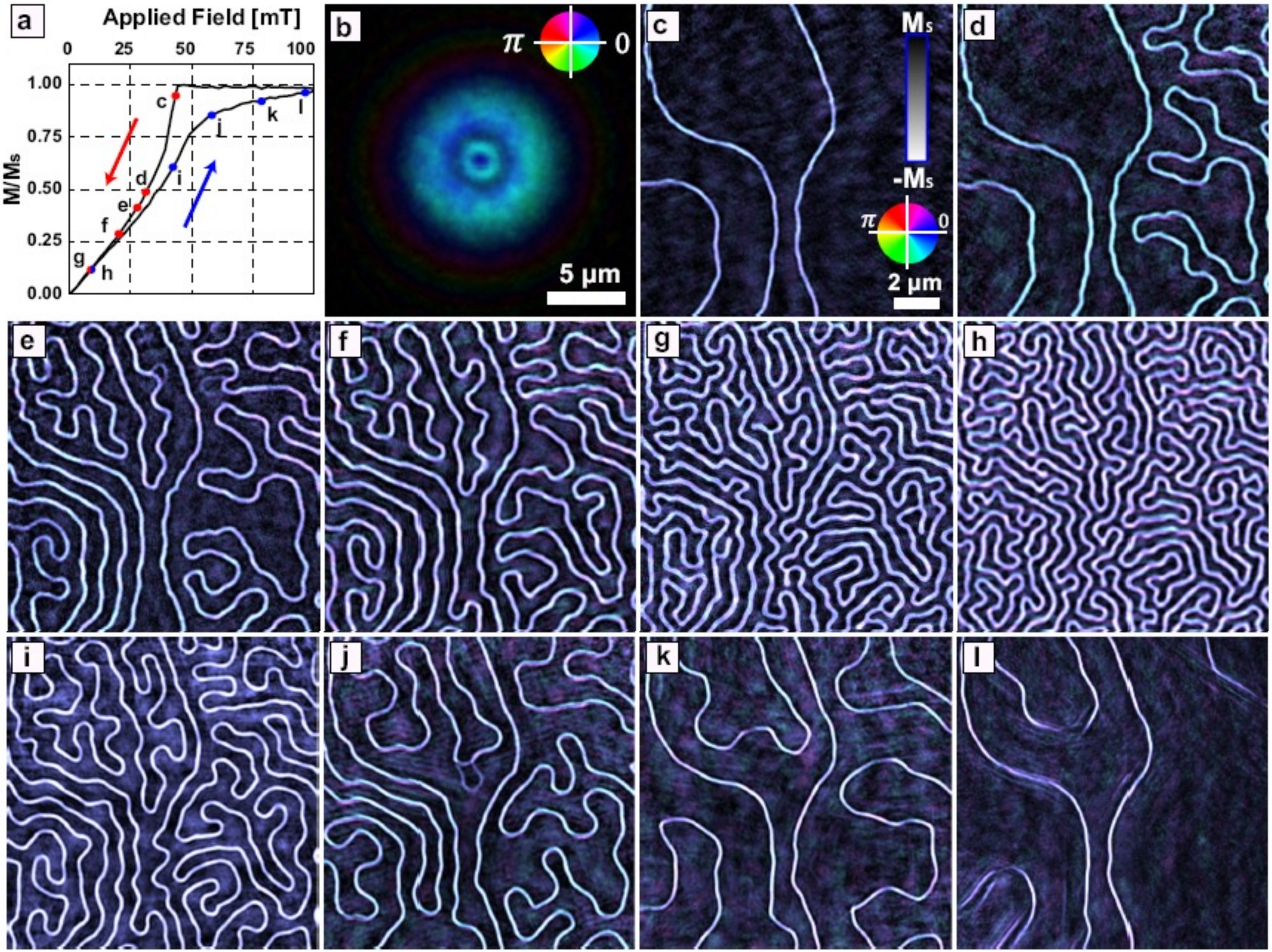






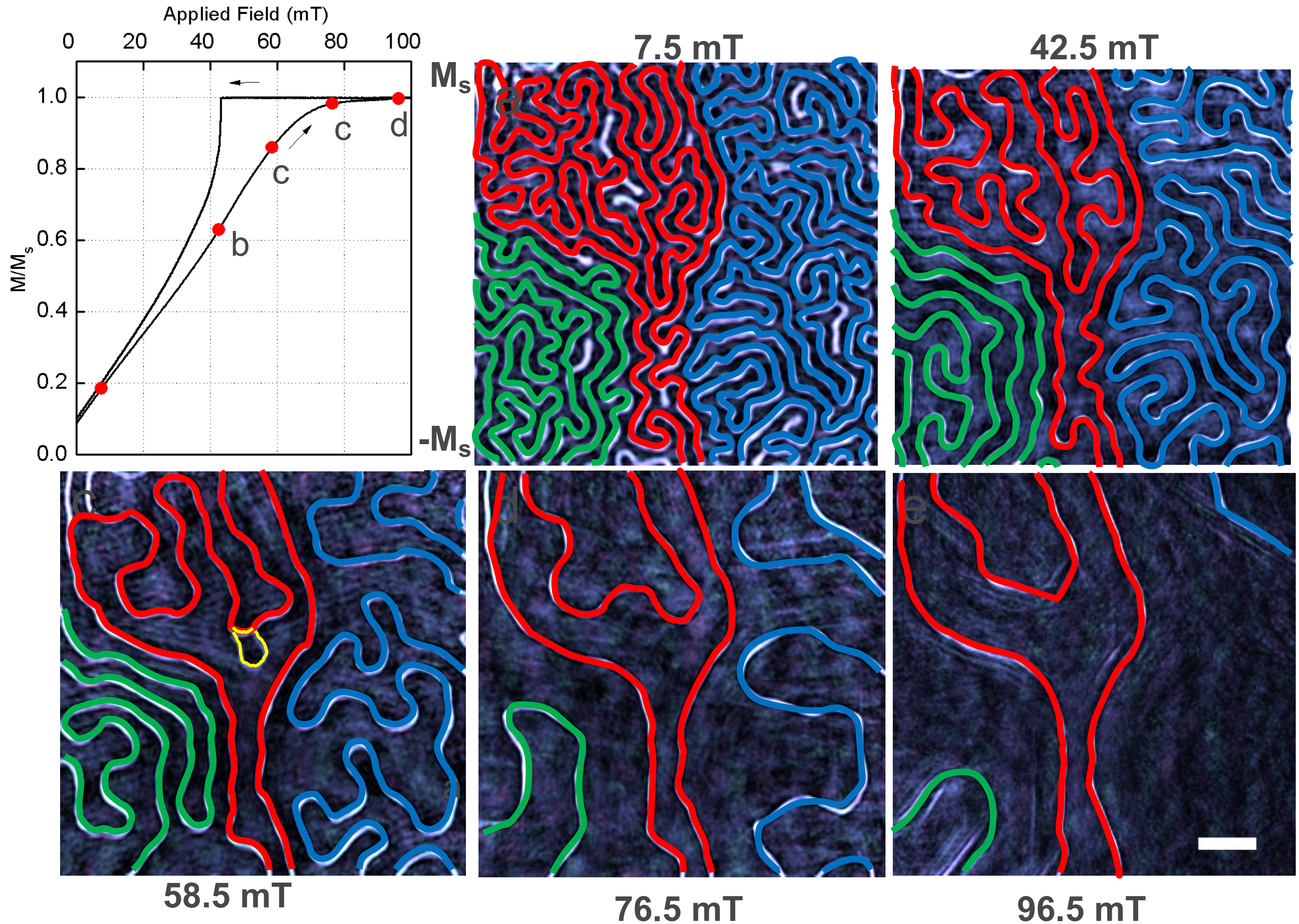
Adapted from D. Shapiro, *et al. Nat. Photon.* **8**, 765 (2014)

Courtesy Dr. Junjing Deng (APS)



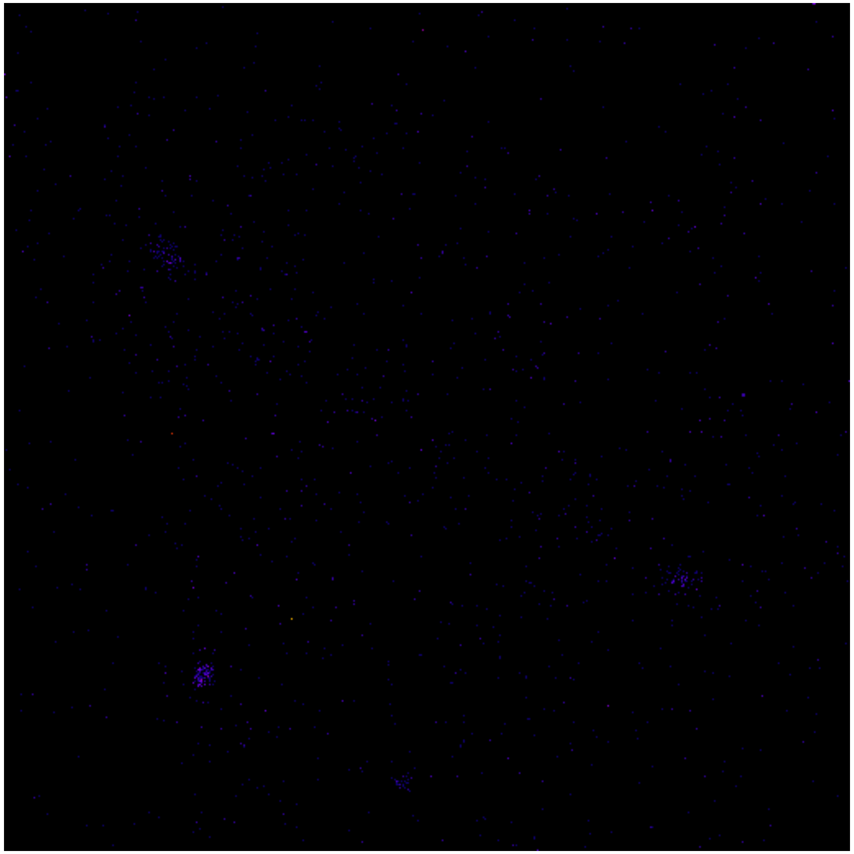
A. Tripathi, O.S. et al., Proc Natl Acad Sci USA 108, 13393 (2011)

INCREASING FIELD

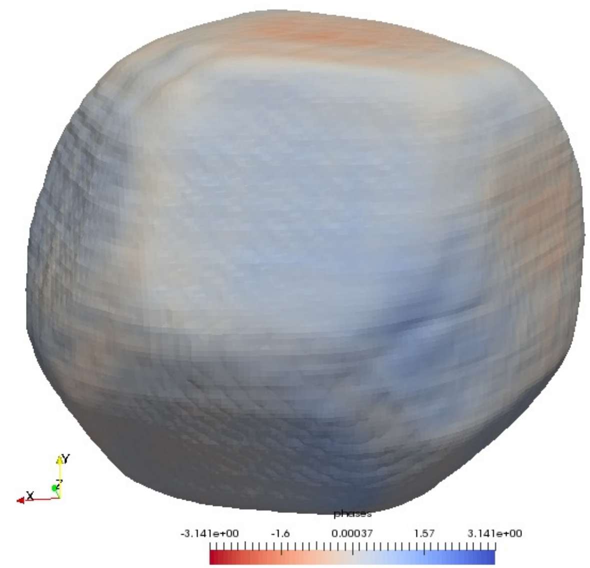


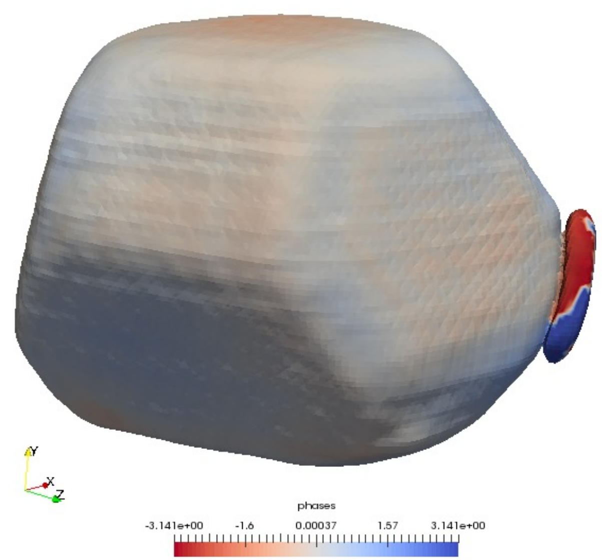
A. Tripathi, O.S. et al., Proc Natl Acad Sci USA 108, 13393 (2011)

Hi Resolution Imaging (PAD)?



Quad Timepix GaAs sensor





700nm gold crystal

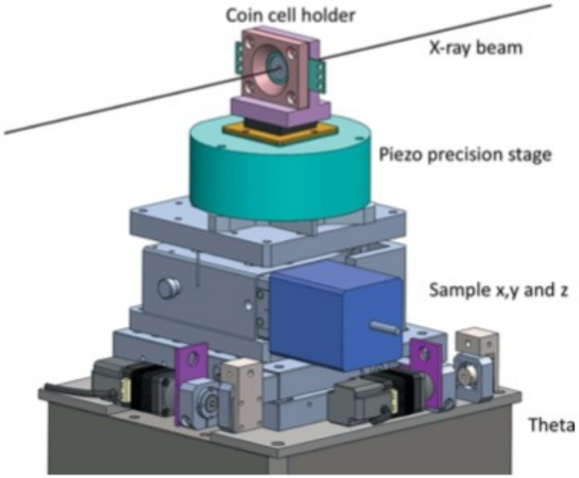
3 degree rocking curve

25 minute measurement

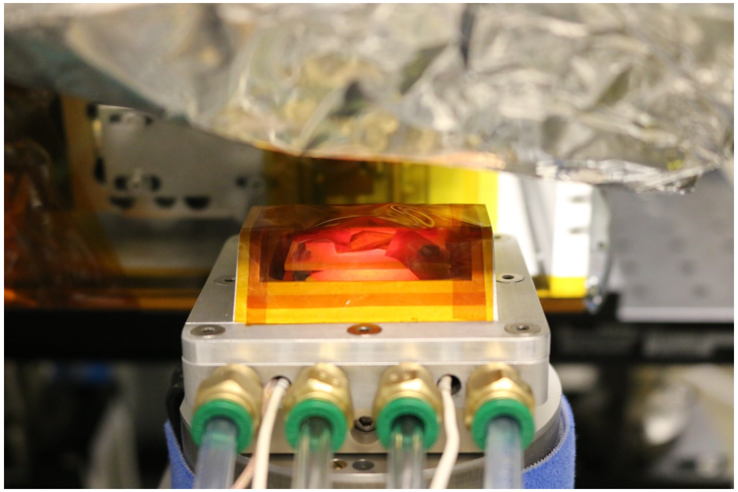
15 sec movie (1X APS-U measurement)

Equipment for In-situ BCDI at APS 34-ID-C Beamline

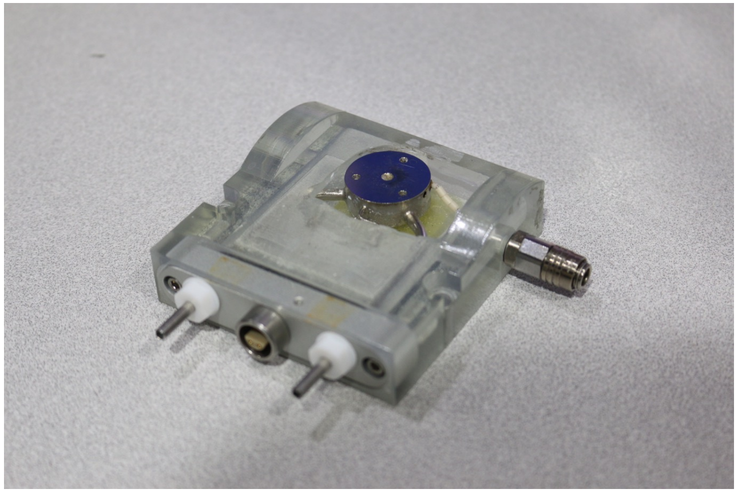
Coin Cell Holder



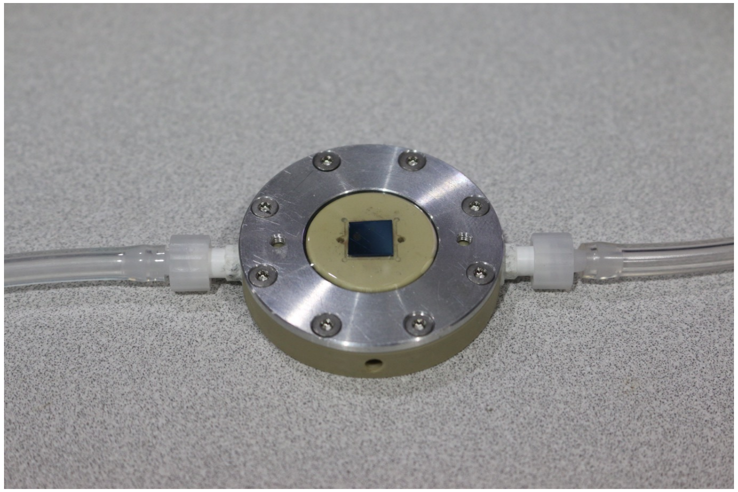
Heating Chamber 2



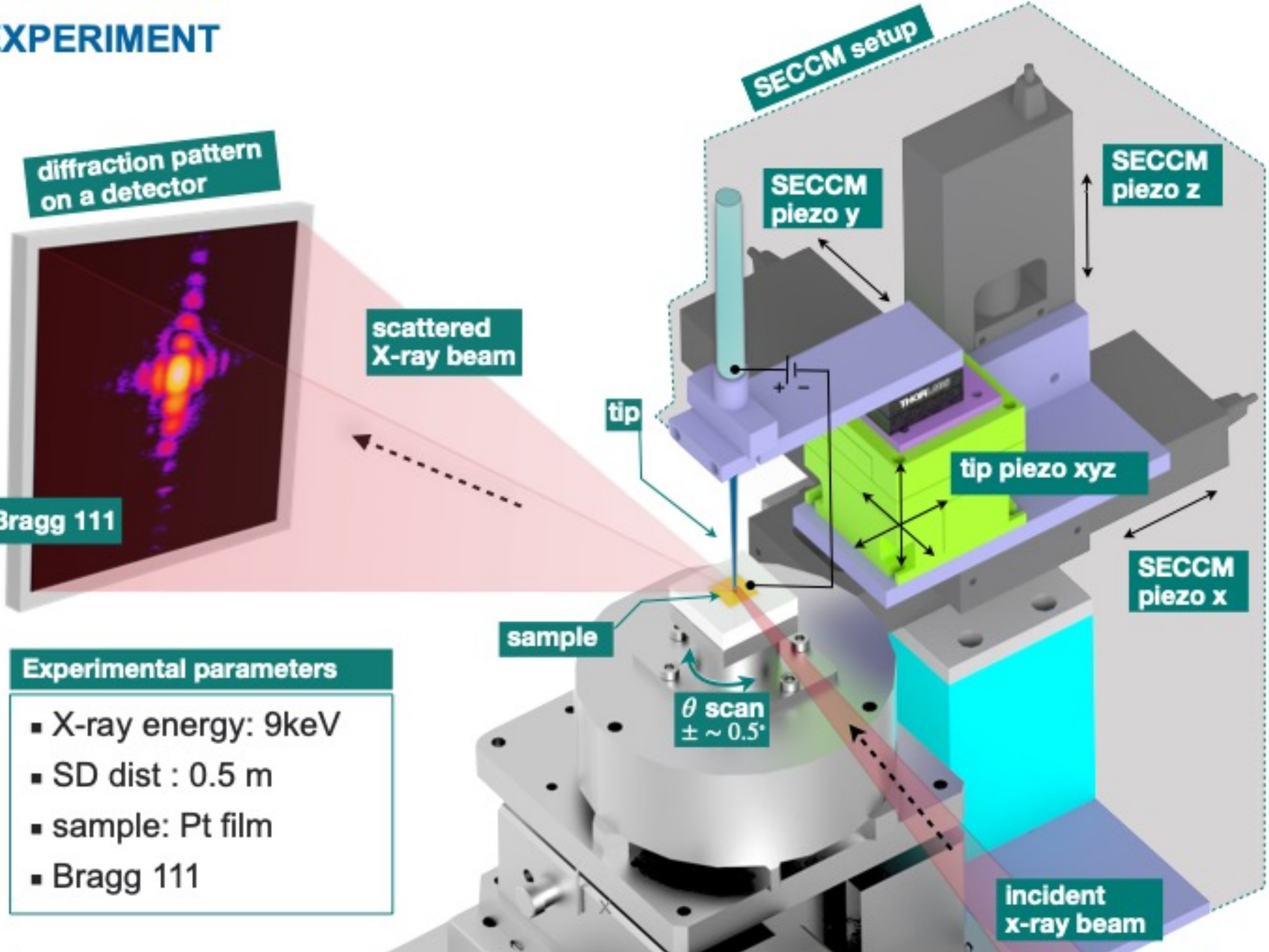
Cooling Chamber



Gas/Liquid Flow Cell



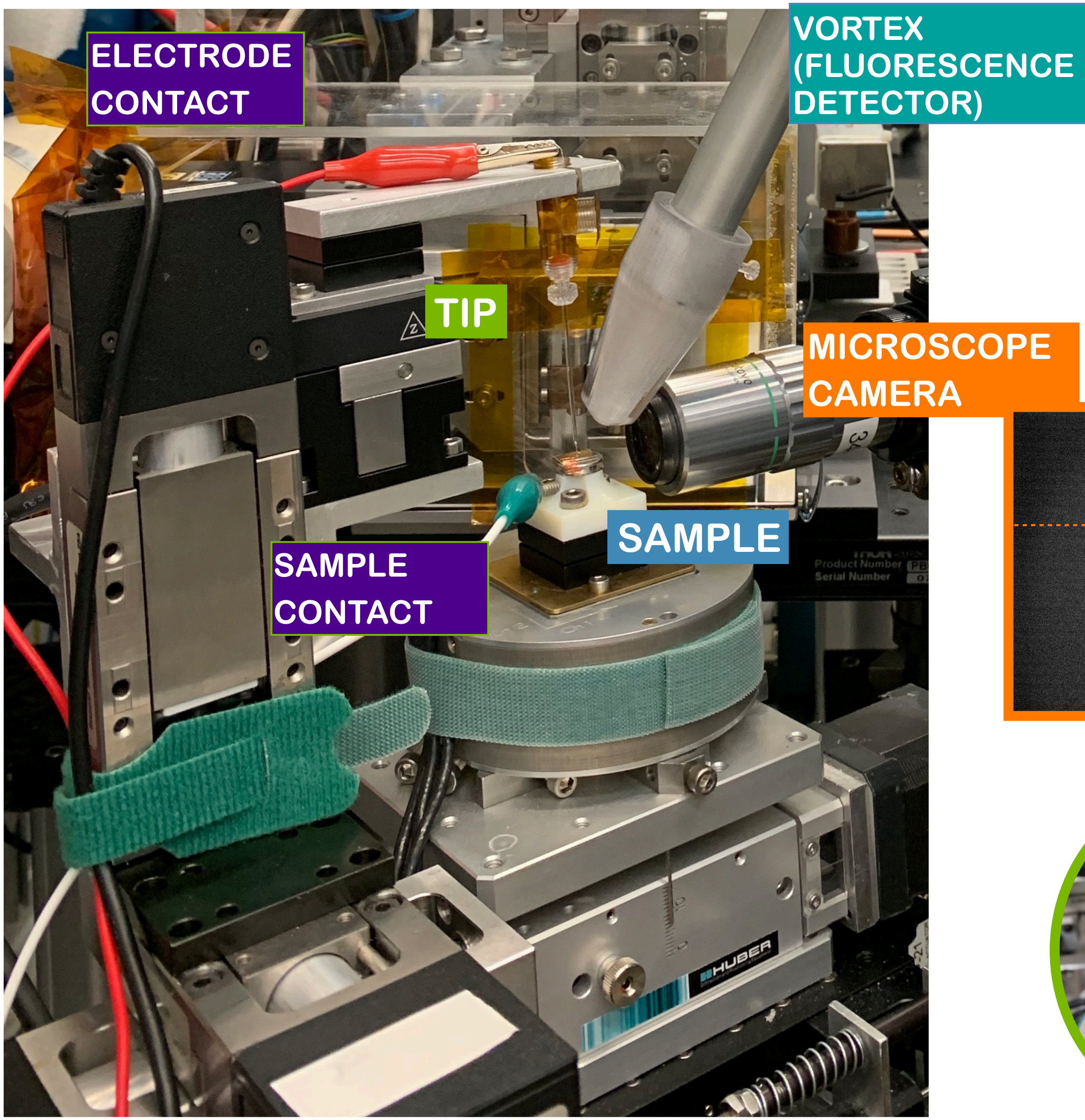
EXPERIMENT



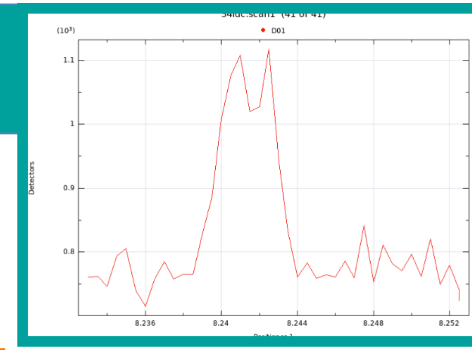
Experimental parameters

- X-ray energy: 9keV
- SD dist : 0.5 m
- sample: Pt film
- Bragg 111

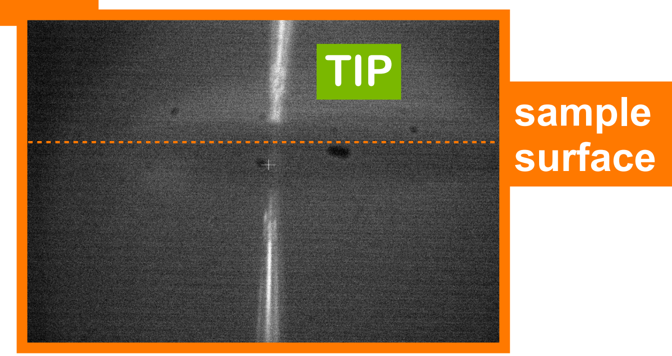
EXPERIMENT

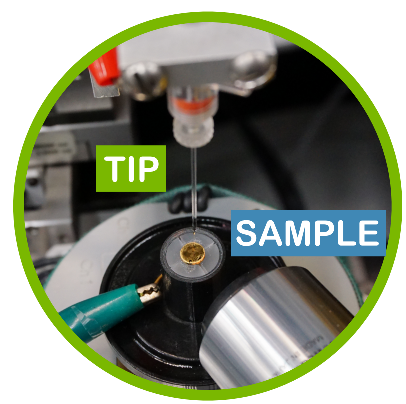


alignment of tip to X-ray



tip in contact with sample

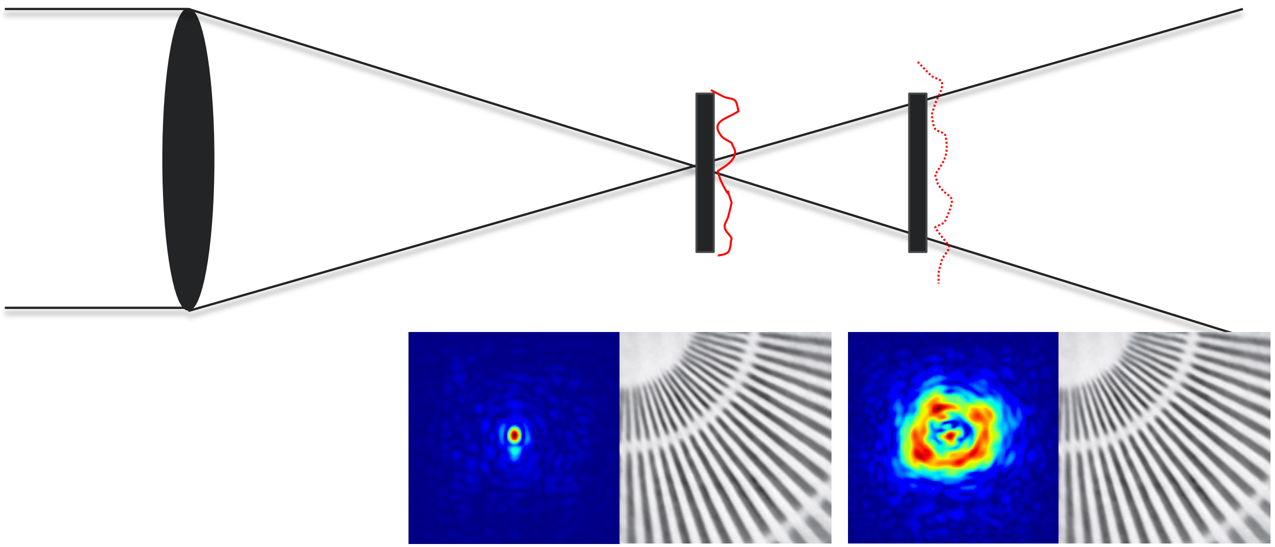




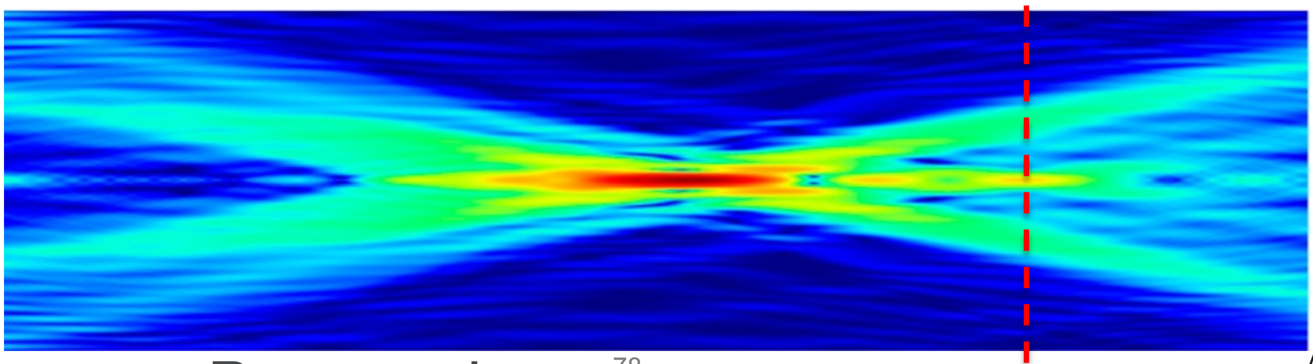
At which plane ptychographic images are reconstructed

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

Ptychography always produces images at the sample plane.



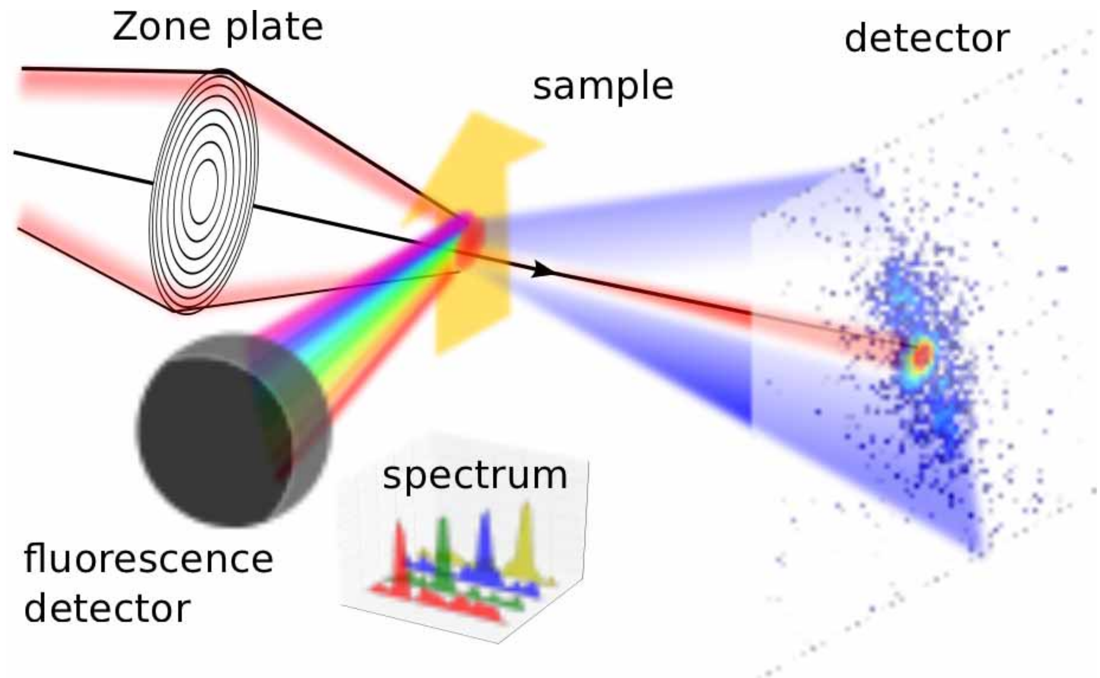
The resolution is not limited by the beam size.

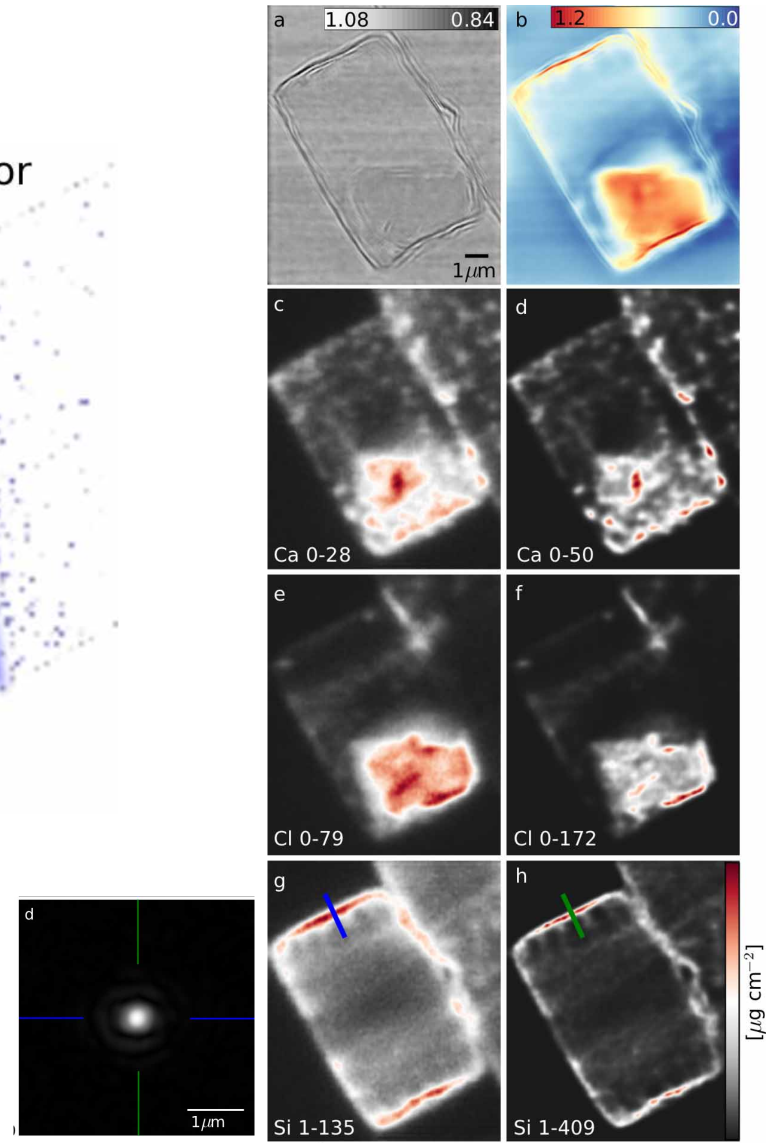


Characterization of focusing optics.

Courtesy Dr. Junjing Deng (APS)

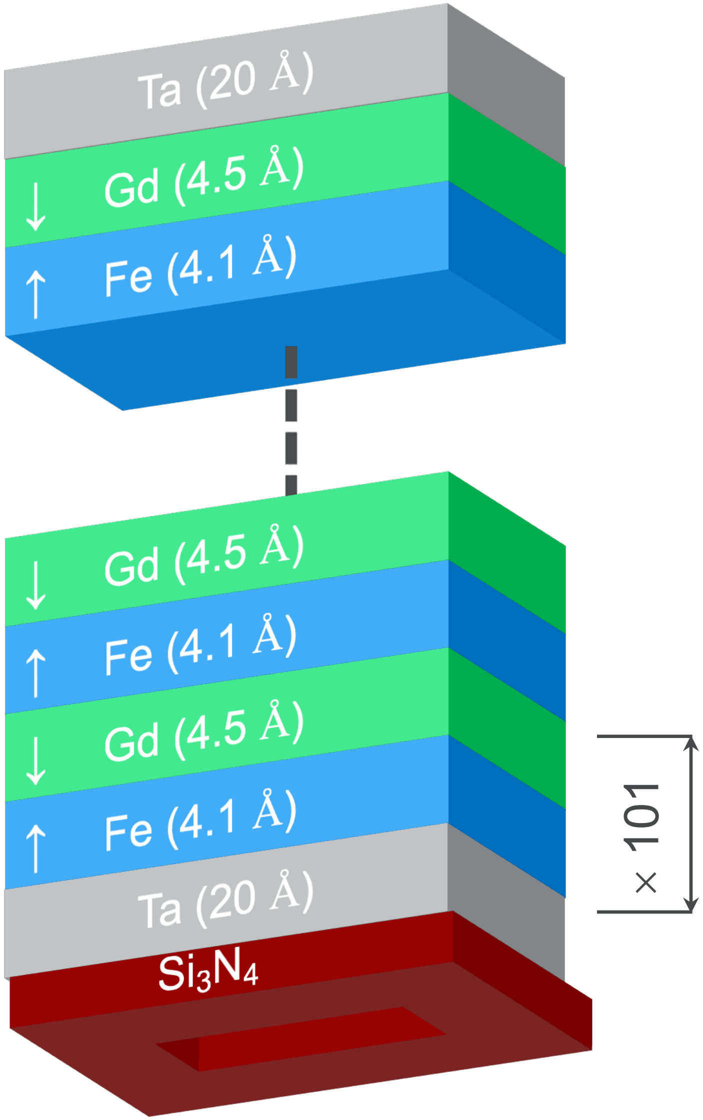
PTYCHOGRAPHY
MICROPROBES -> COHERENT IMAGING INSTRUMENT

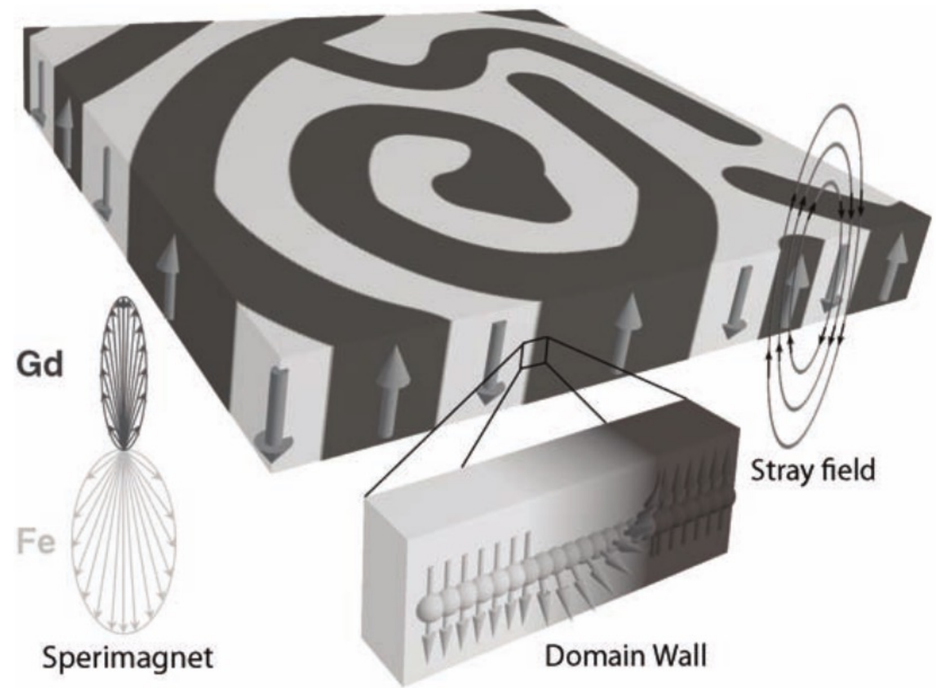




Vine, et al. (2012). *Opt. Express*, *20*(16), 18287–18296.

GDFE LAYERED MAGNETIC FILMS





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

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

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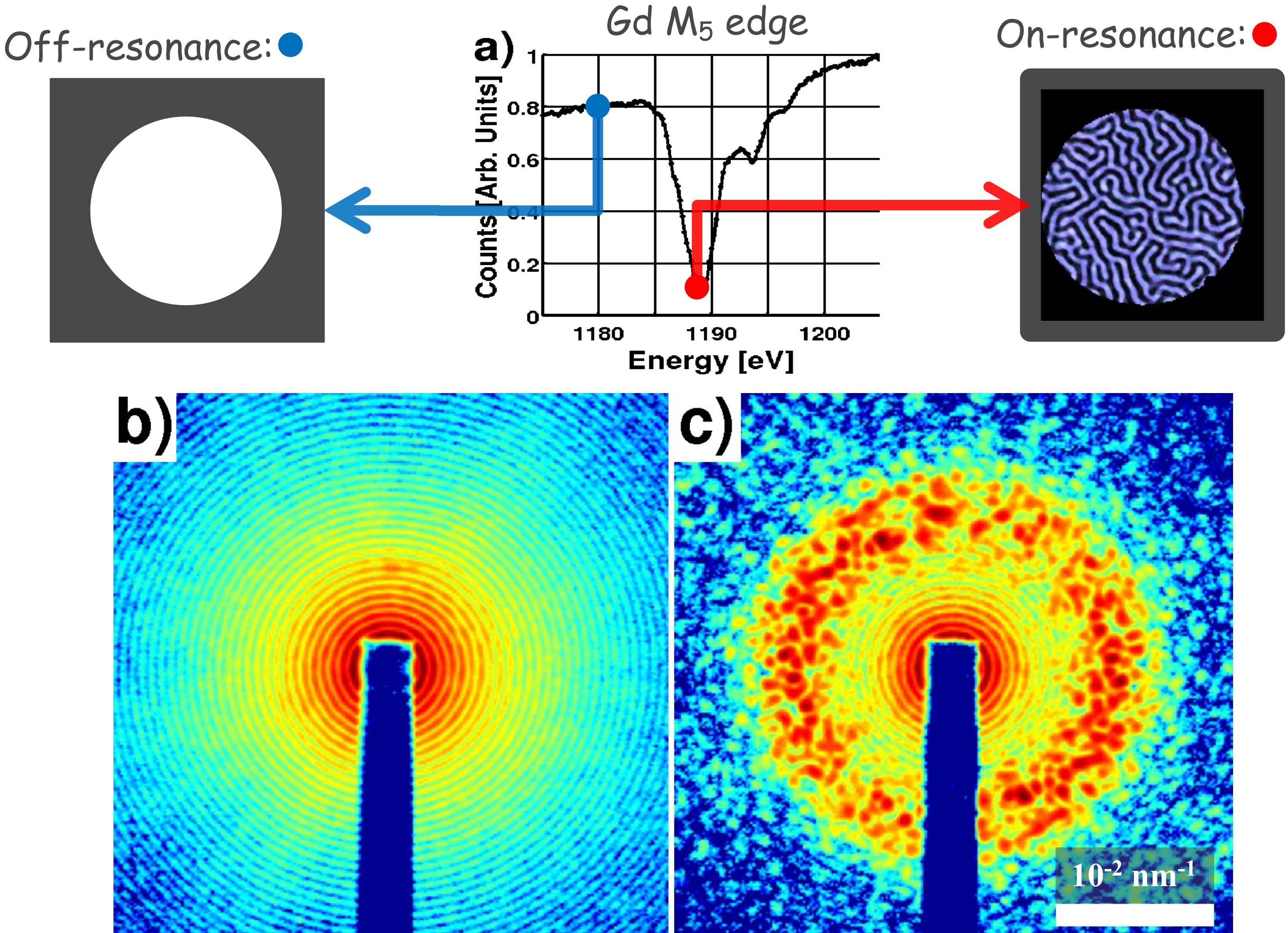
MAGNETIC CONTRAST MECHANISM



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

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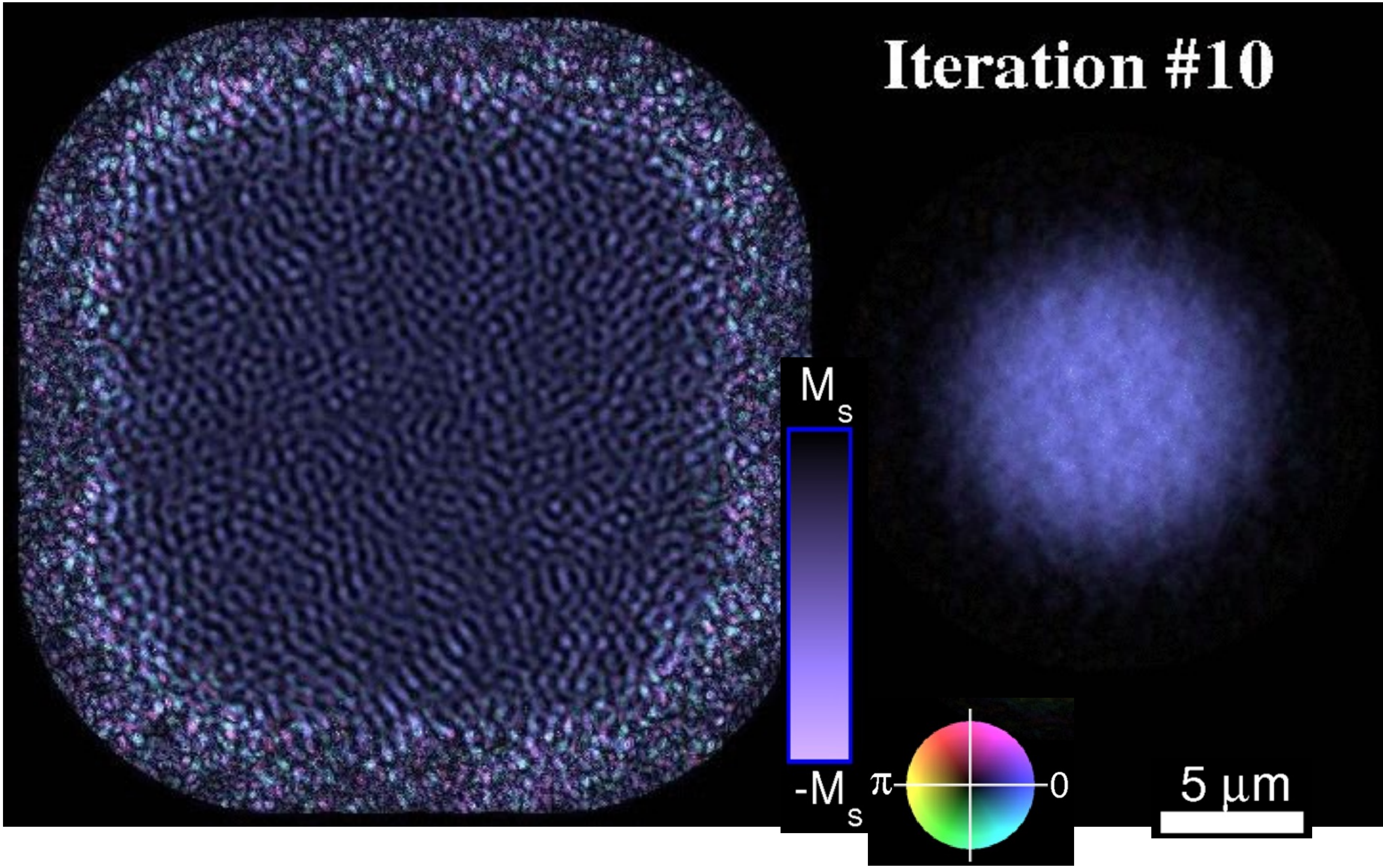
REAL SPACE RECONSTRUCTION

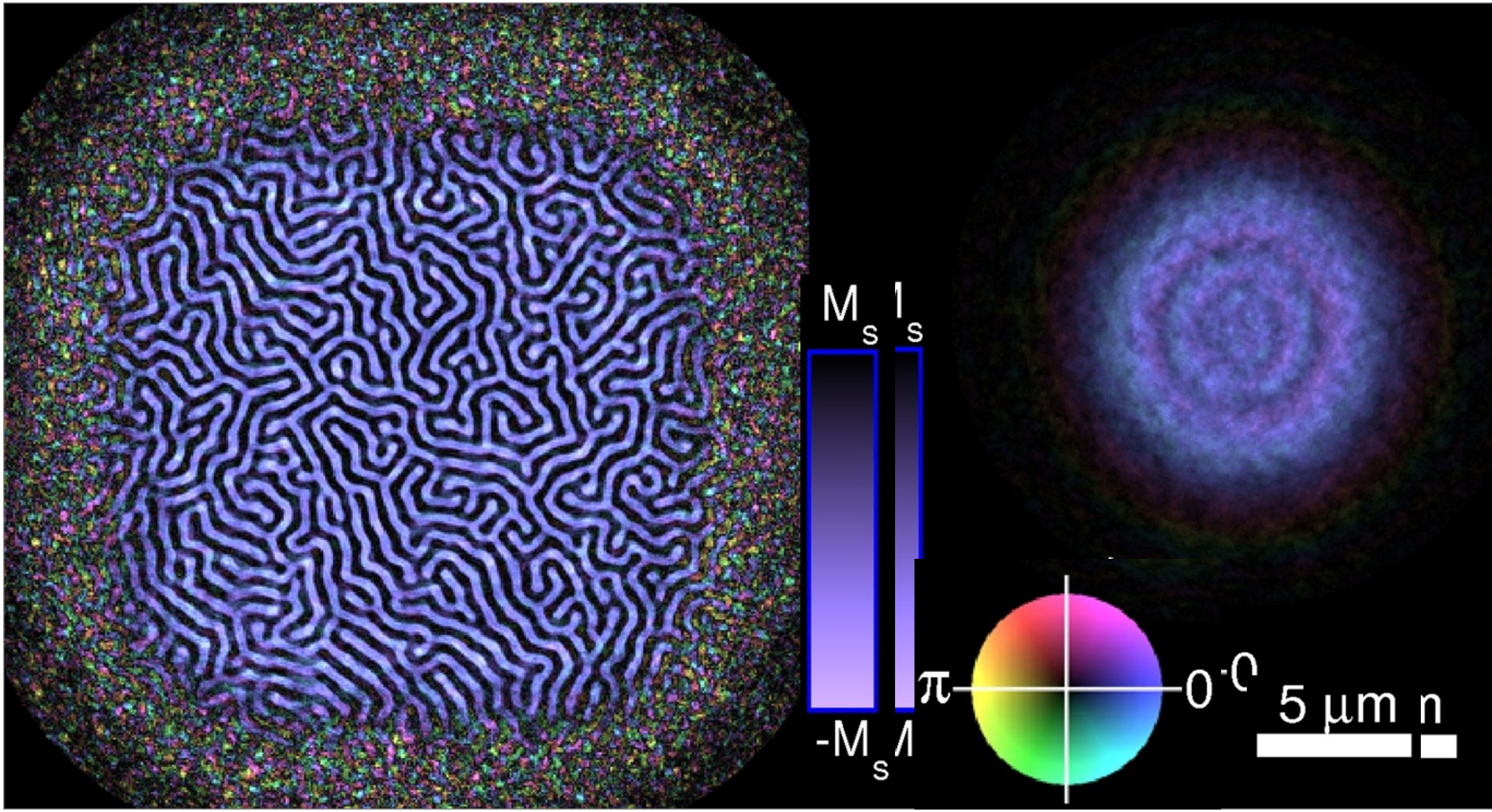


Magnetic structure
(exit wave)

Illumination Function

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

REAL SPACE RECONSTRUCTION



Magnetic structure
(exit wave)

Illumination Function

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