Argonne NATIONAL LABORATORY

X-ray Imaging at 3rd Generation Synchrotron Source

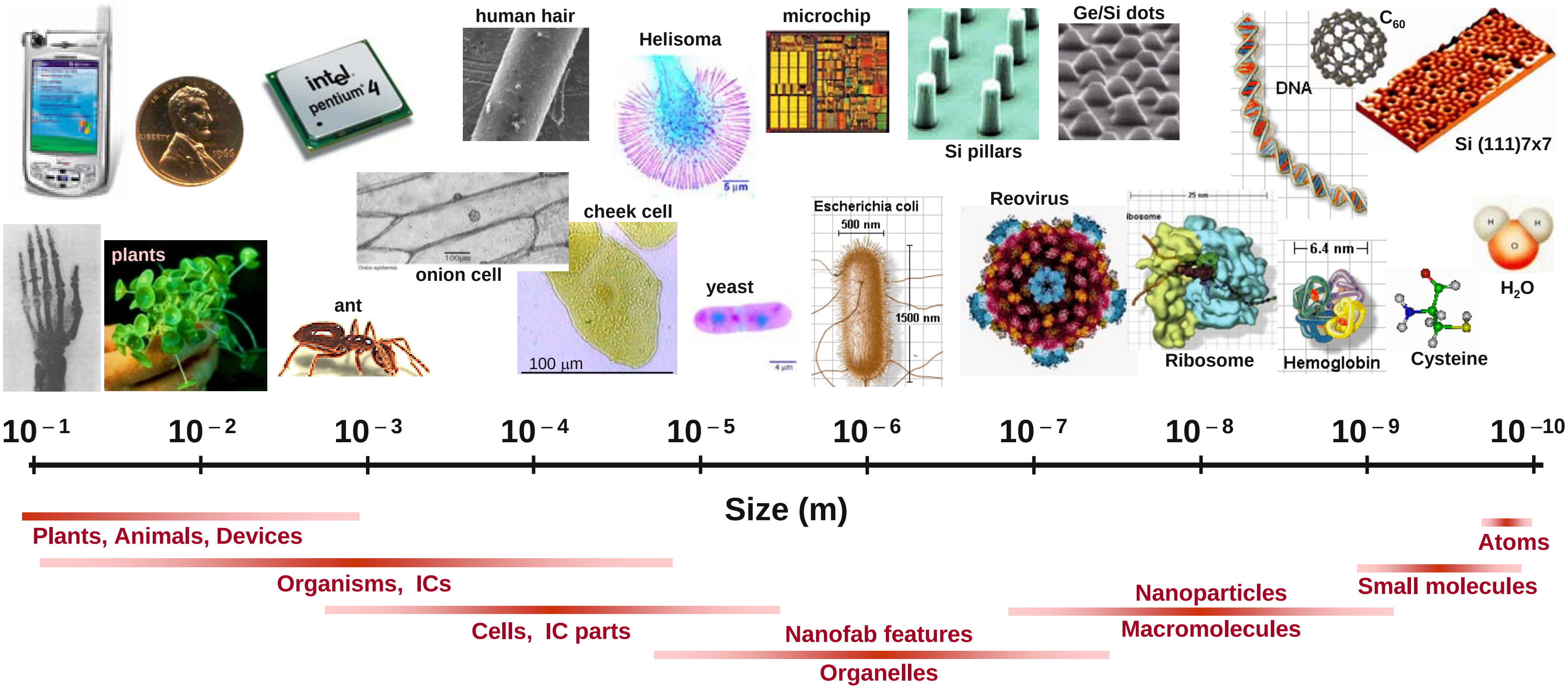
Qun Shen
X-ray Microscopy and Imaging Group
Advanced Photon Source
Argonne National Laboratory

THE UNIVERSITY OF CHICAGO

Office of Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory
managed by The University of Chicago

Imaging and X-rays



Medical Imaging

→ low contrast tissues
→ real time & flash imaging
→ high resolution

Cellular Imaging

→ subcellular organelles
→ protein location & function
→ natural state

Molecular Imaging

→ with or without crystals
→ atomic resolution ??
→ less damage

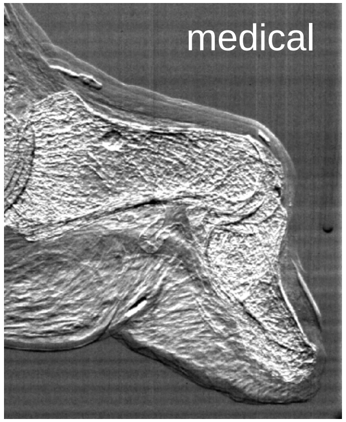
Anatomical / Device

Functional

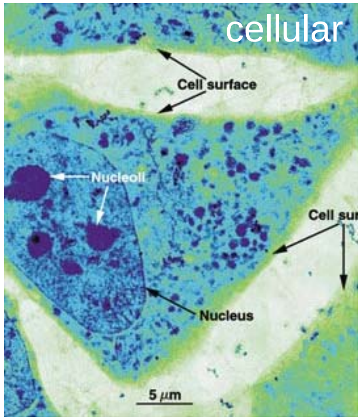
Fundamental

Advances in X-ray Imaging

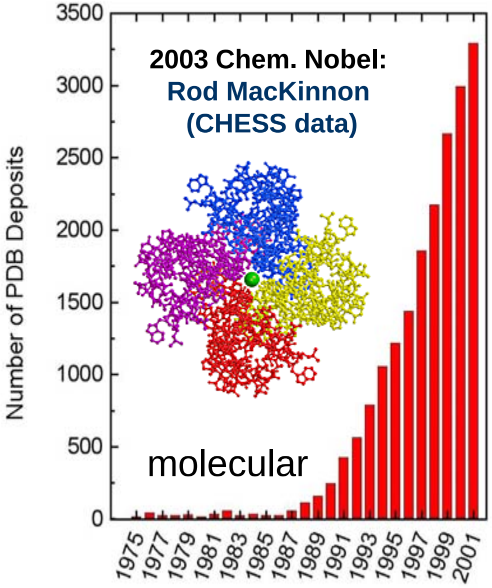
Sir Wilhelm Röntgen
1st Physics Nobel (1901)



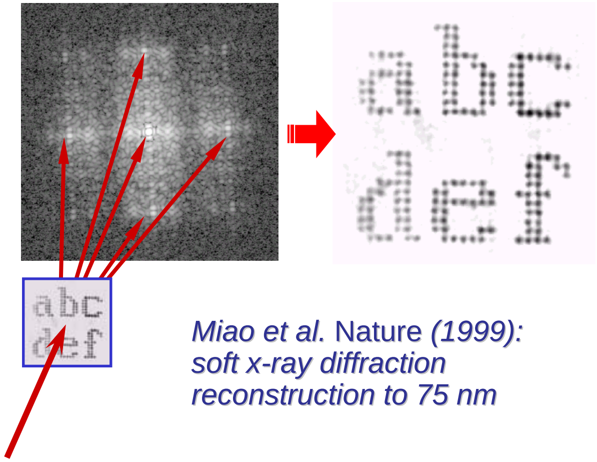
Li, Zhong, et al. (2003)



Larabell (ALS, XM-1)



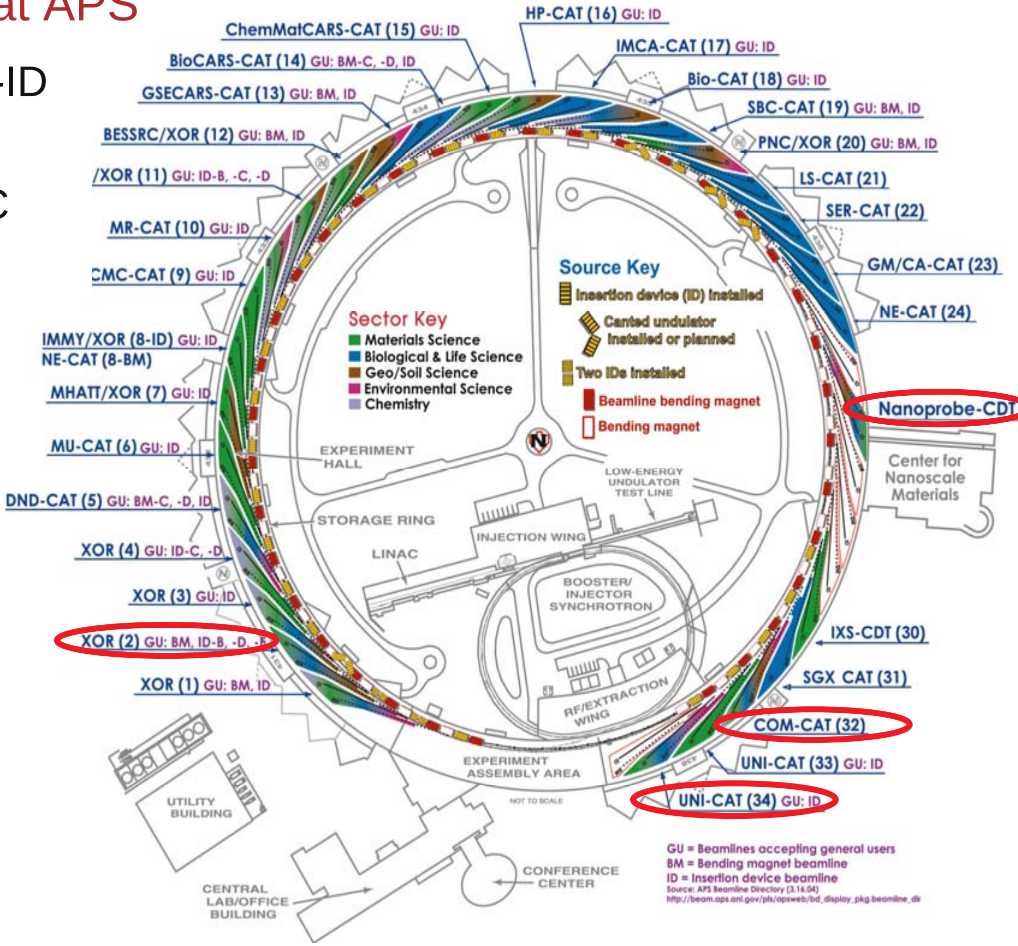
- Old & new: emerging x-ray technologies in source & optics, advances in all 3 areas: fundamental, functional, anatomical
- Phase-contrast imaging: weak-absorbing features, less dose, far more clarity than traditional radiograph
- X-ray microscopy: could have high impact on cell biology, similar to x-ray crystallography ⇔ molecular biology
- Coherent diffraction imaging: new frontier on noncrystalline structures, structural molecular biology w/o need for crystals



Miao et al. Nature (1999):
soft x-ray diffraction
reconstruction to 75 nm

Outline

- Overview: imaging & x-rays
- X-ray microscopy & imaging group at APS
  - → Scanning x-ray microscopy: 2-ID, 26-ID
  - → Full-field x-ray imaging: 2-BM, 32-ID
  - → Coherent diffraction imaging: 34-ID-C
- Dedicated x-ray imaging beamline
  - → Phase-contrast imaging
  - → Diffraction-enhanced/USAXS imaging
  - → Full-field x-ray microscope
  - → Coherent diffraction in near-field
- Future upgrade paths
  - → 200m long beamline ?
  - → Optimized machine parameters & IDs
  - → R&D activities
- Summary



Souce: APS Beamline Directory (3.16.04)
http://beam.aps.anl.gov/pls/apsweb/bd_display_pkg.beamline_dir

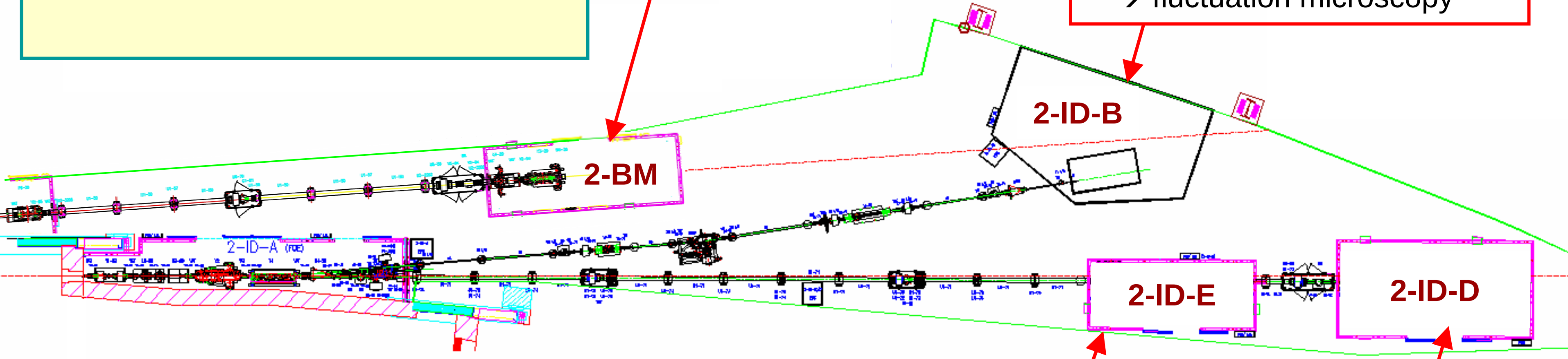
X-ray Microscopy & Imaging at APS Sector 2

APS Sector 2

- Scaning x-ray microscopy (SXM)
- 1-4 keV coherent scattering
- High throughput micro-tomography
- Diffraction topography & imaging

- Microtomography
  - → high throughput
  - → 3D reconstruction
- Diffraction imaging
  - → full field, phase-contrast
  - → microprobe with KB (1um)

- 1-4keV scanning probe
  - → double-mirror + ML grating
  - → spectromicroscopy (20nm)
- Coherent scattering
  - → imaging by phase retrieval
  - → holographic imaging
  - → fluctuation microscopy



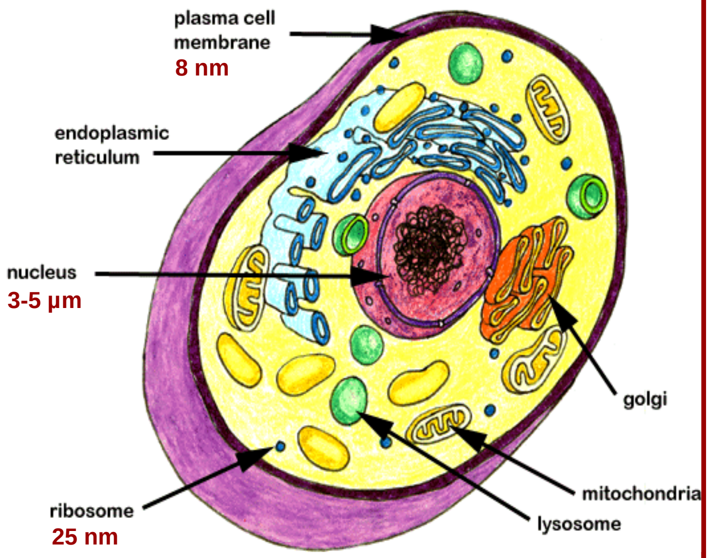
- One bend magnet
- Two undulators
  - → soft x-ray 1-4 keV
  - → undulator A

- 7-17 keV scanning probe
  - → side branch Si + FZP
  - → fluorescence (200nm)
  - → differential phase contrast
  - → 80% biological studies

- 5-30 keV scanning probe
  - → Si (111) or ML + FZP
  - → fluorescence (150nm)
  - → nanodiffraction
  - → 50% materials studies

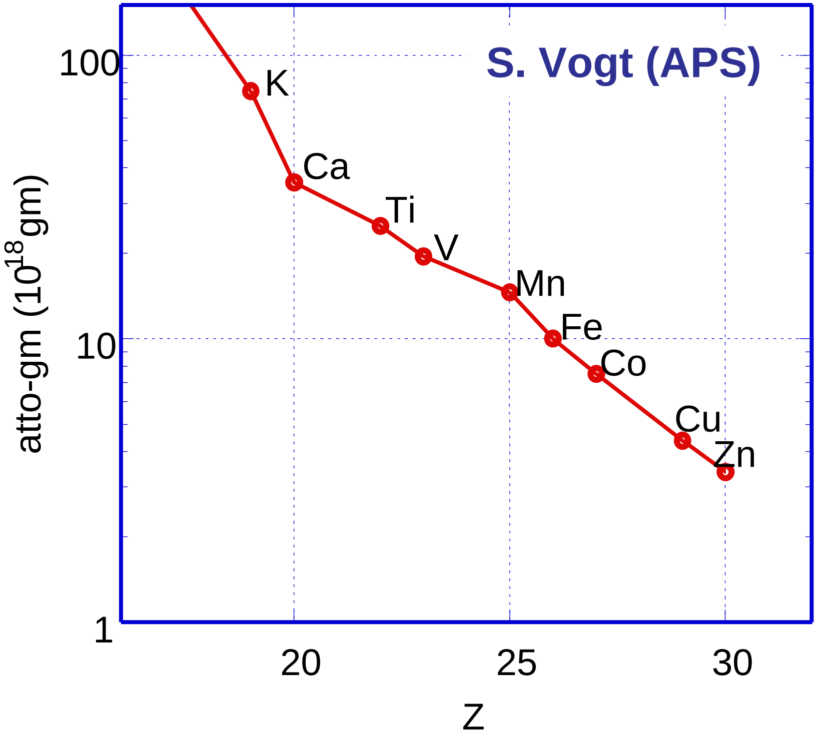
μ-XRF Studies of Trace Metals in Biological Cells

- **simultaneously map 15+ elements**
- **no dyes necessary**
- **very high sensitivity (<ppm)**
- **quantitative**
- **large penetration depth (> 100 μm)**
- **chemical state mapping & μ-XANES**



CELL: ~ 10 µm

typical size of a protein: a few nanometer

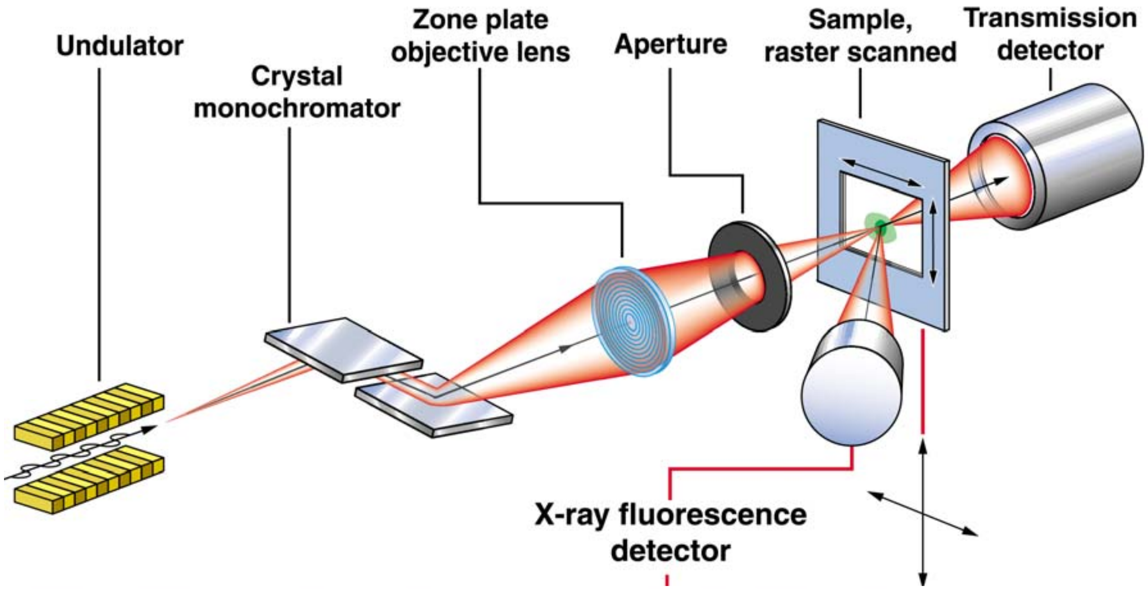


S. Vogt (APS)

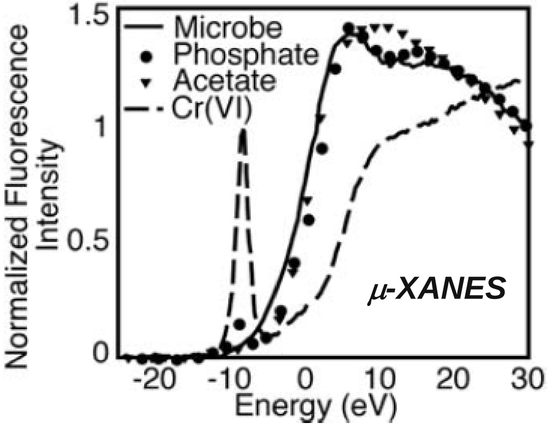
Detection limit for transition elements: for 1s acquisition time, 0.2 x 0.2 μm^2 beam size, E=10 keV

Detection limit depends on incident Energy and Z

X-Ray Fluorescence Imaging of Bacterial Cells



Kemner et al.
Science 306, 686 (2004).



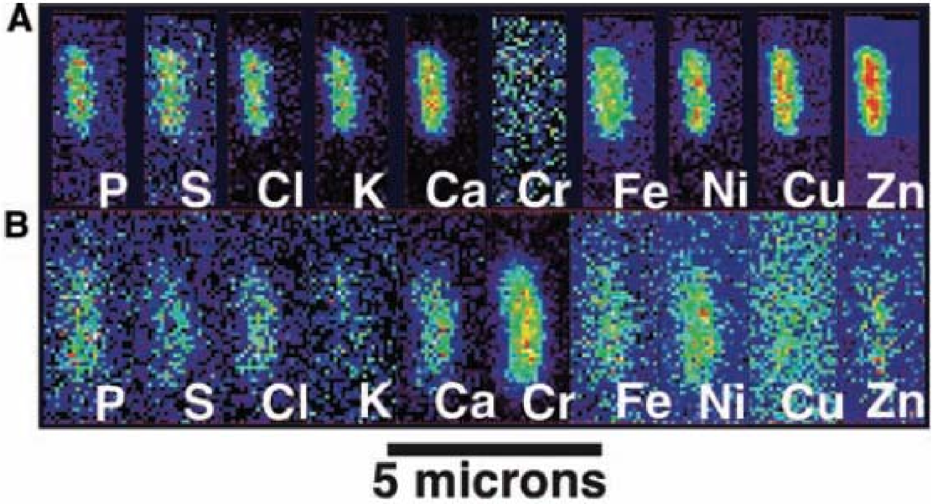


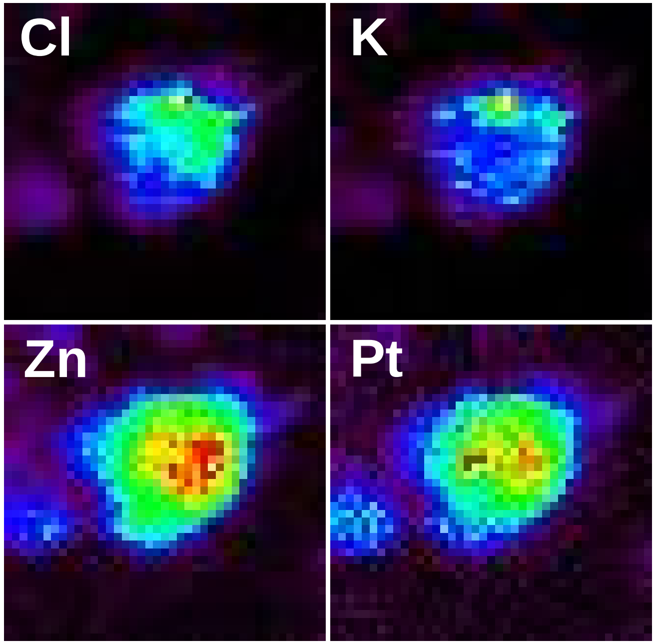
Fig. 1. False-color micro-XRF maps of qualitative spatial distributions and concentration gradients of elements in and around planktonic *P. fluorescens* microbes harvested before (**A**) and after (**B**) exposure to potassium dichromate [Cr(VI)] solution (1000 ppm) for 6 hours.

→ XRF image of single bacterial cells

→ Elemental distribution

→ Redox states Cr(III) by μ-XANES

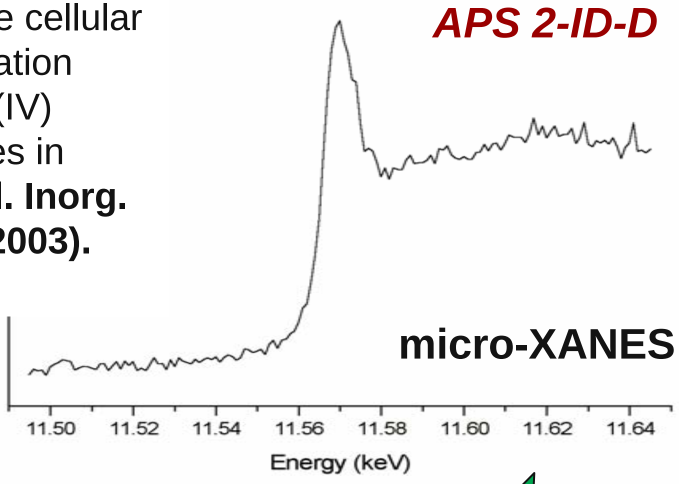
Understanding Metabolic Pathways of Drugs



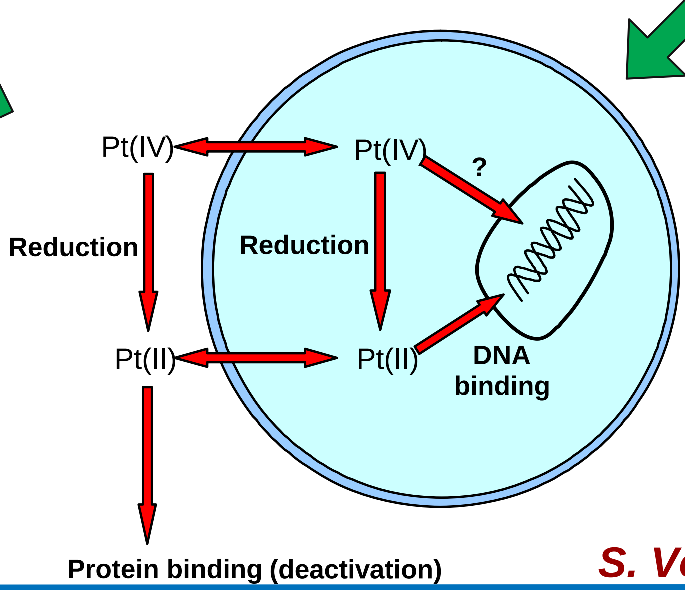
XRF microscopy

M. D. Hall, *et al,* "The cellular distribution and oxidation state of Pt(II) and Pt(IV) antitumour complexes in cancer cells," **J. Biol. Inorg. Chem. 8, 726-732 (2003).**

APS 2-ID-D



micro-XANES

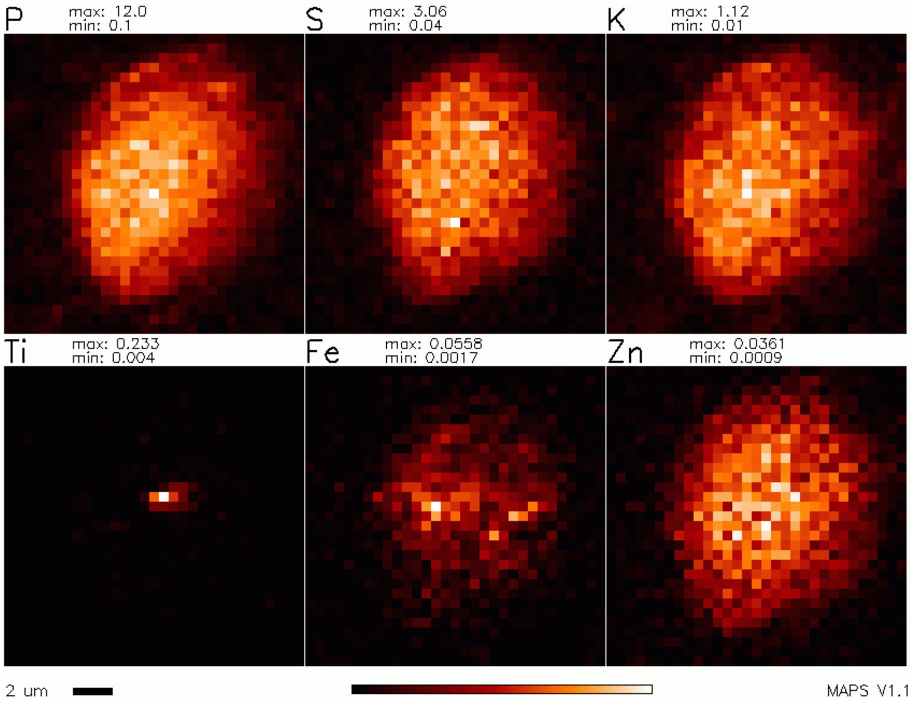


Pt(IV) complexes are more inert:

- less likelihood of deactivation
- potentially fewer side effects
- possibility of selective activation

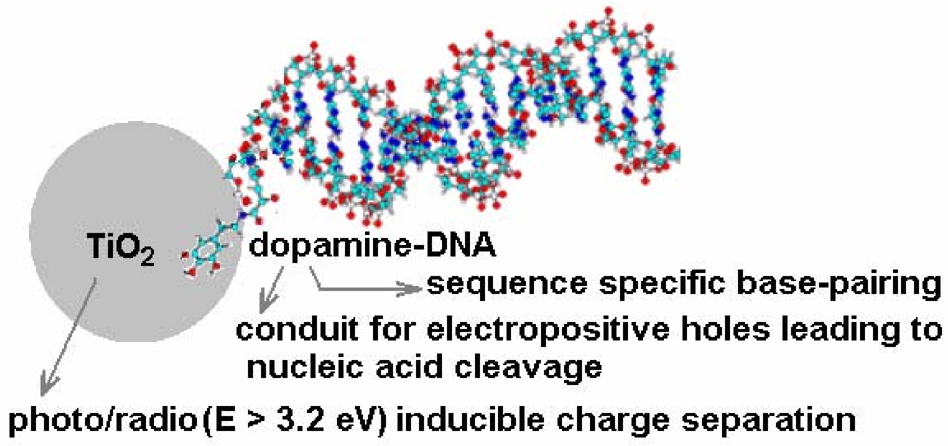
S. Vogt (APS)

Nanocomposites as Intracellular Tools



MCF-7 cell transfected with nanocomposite combining ribosomal DNA w. TiO_2.

Ti K_α fluorescence is visible in a small location of the nucleus, corresponding nucleolar localization. Nucleus of the cell is visible using P $K\alpha$ fluorescence (DNA content)



TiO_2 **dopamine-DNA**

sequence specific base-pairing

conduit for electropositive holes leading to nucleic acid cleavage

photo/radio (E > 3.2 eV) inducible charge separation

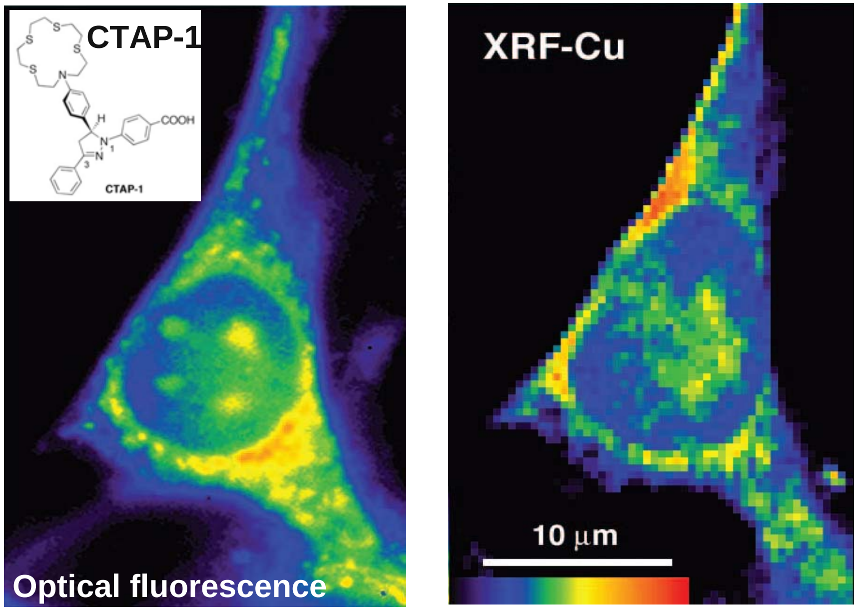
- attach TiO_2 nanoparticle (4.5 nm diameter) to DNA
- combine DNA biochemistry with semiconductor properties of TiO_2
- carrier-particle that can bind to a specific chromosomal region w/ ability to cleave it upon illumination

Gene therapy: Correct defective genes responsible for disease development

Paunesku et al, *Nature Materials 2, 343 (2003)*

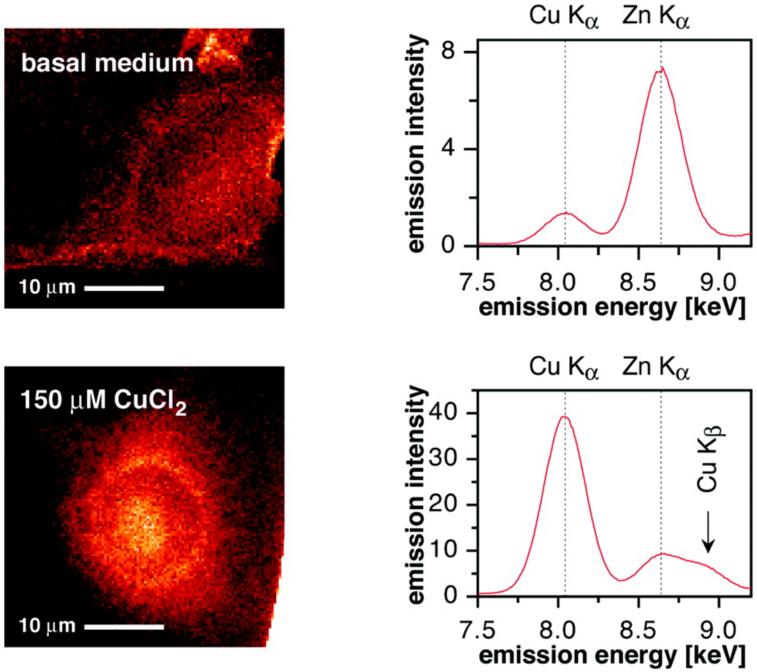
Development of Intracellular Optical Sensors

XRF: 1) Validate Cu sensor CTAP-1

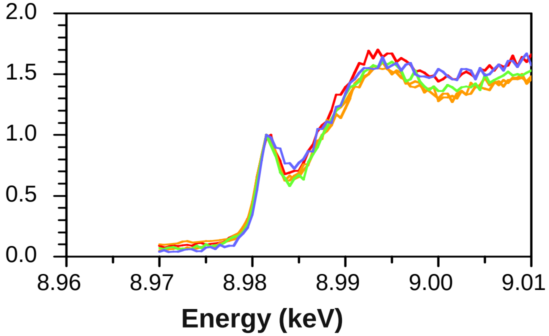


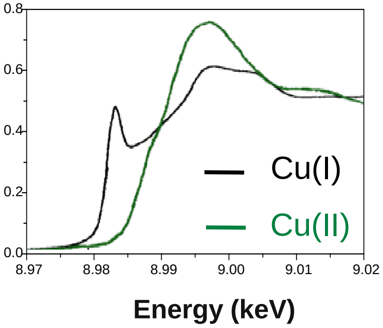
Mouse fibroblast cell + 150 μM $CuCl_2$

2) Quantify cellular Cu



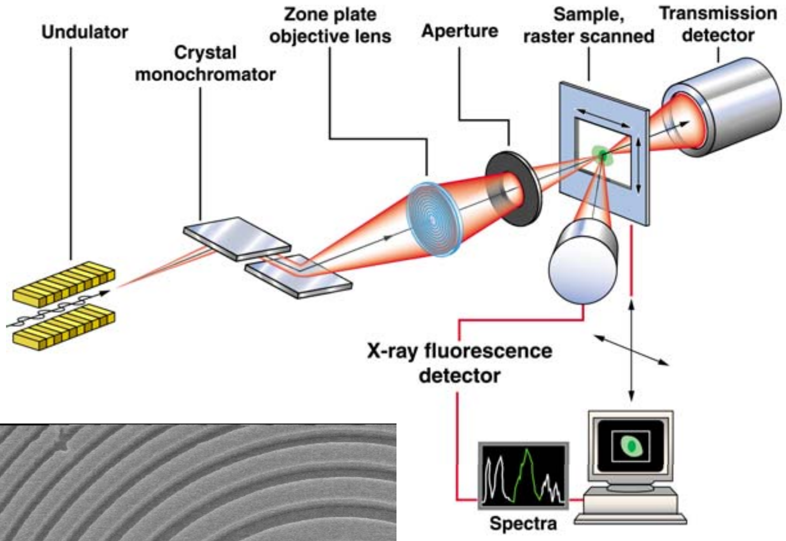
3) μ-XANES indicated Cu(I), confirming the reducing cellular environment

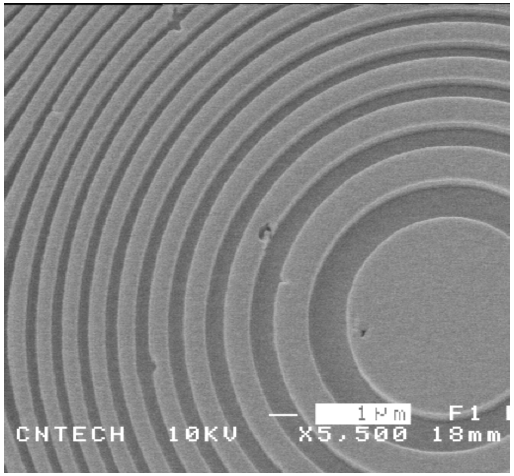




Yang, et al., PNAS 102, 11179 (2005)

APS 2-ID-D X-ray Diffraction Microprobe





- *Zone plate mounted on κ-diffractometer*
- *CCD on 2θ detector arm*

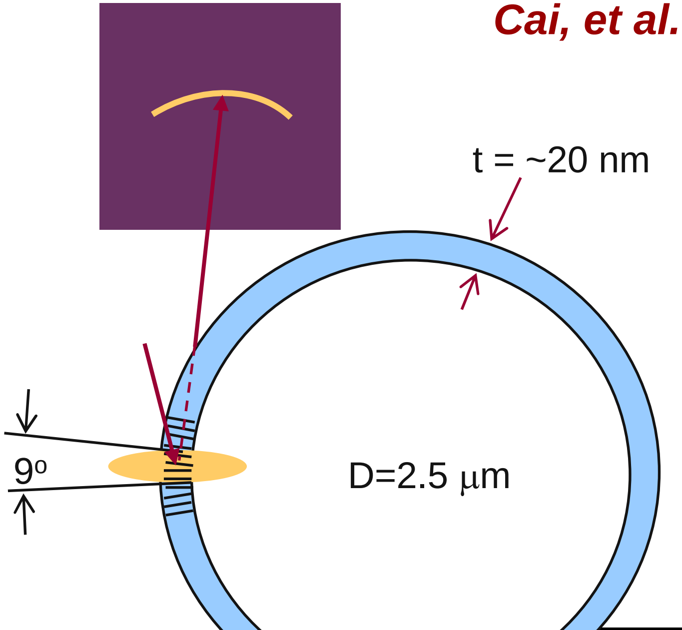
Spot size: 150 nm FWHM
Efficiency: 20-25%
Flux density:
5×10^4 phs/s/nm^2/0.01%BW

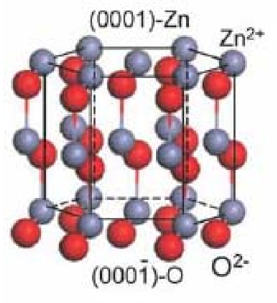
Zhonghou Cai & Barry Lai (APS)

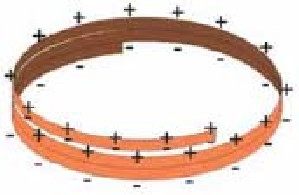

Kappa diffractometer in 2-ID-D

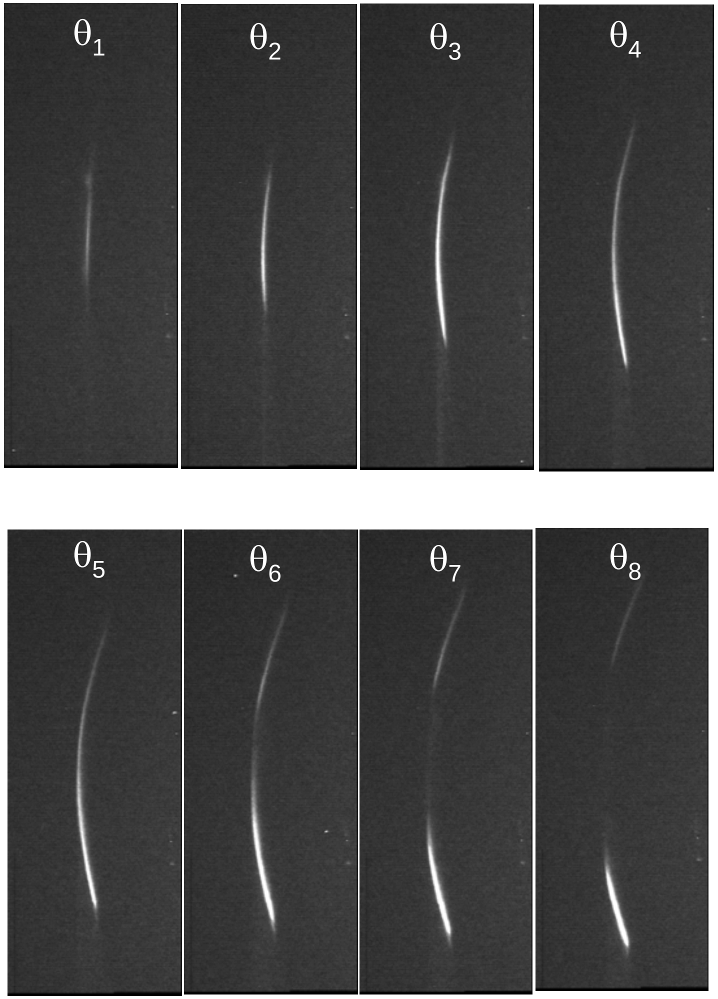
μ-Diffraction from ZnO ring (110)

Cai, et al. (2005): diffraction from 20nm metal oxide wires!!

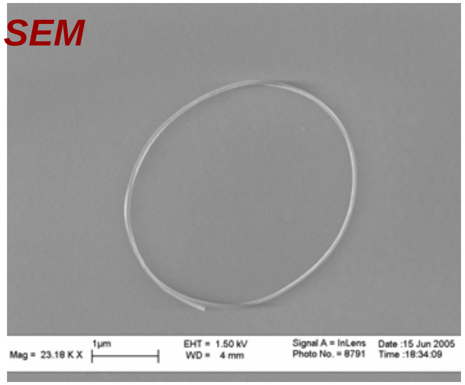


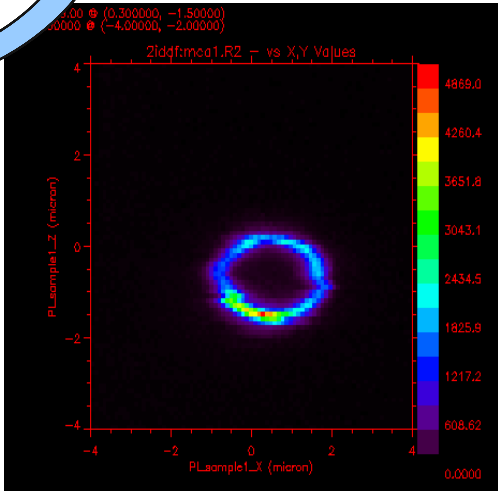




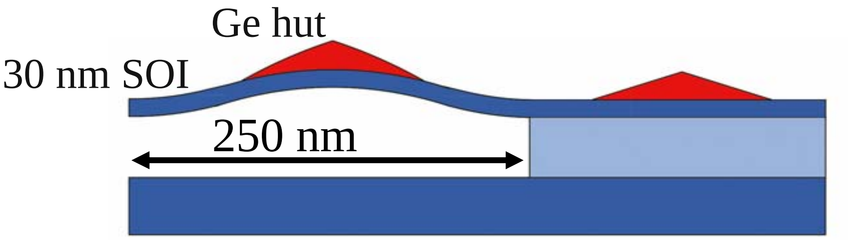


SEM



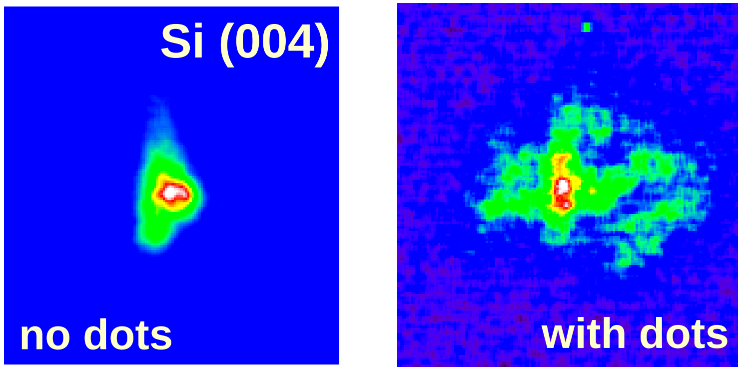


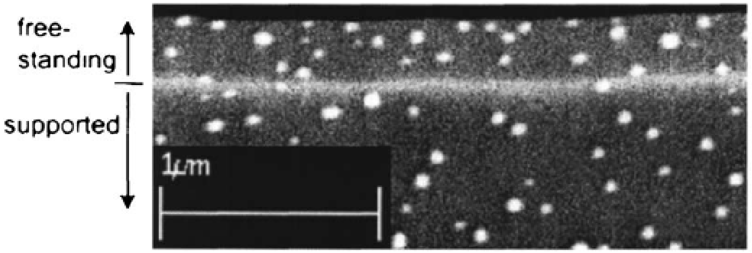
Nanostressors on Freestanding Silicon Membranes



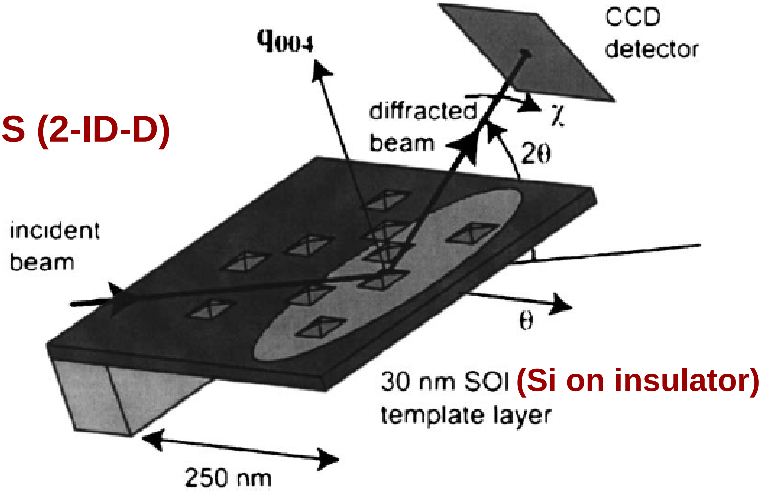
Ge-Si Lattice Mismatch ➔ Si Distorted

Evans, *et al.*, Appl. Phys. Lett. **87**, 073112 (2005)

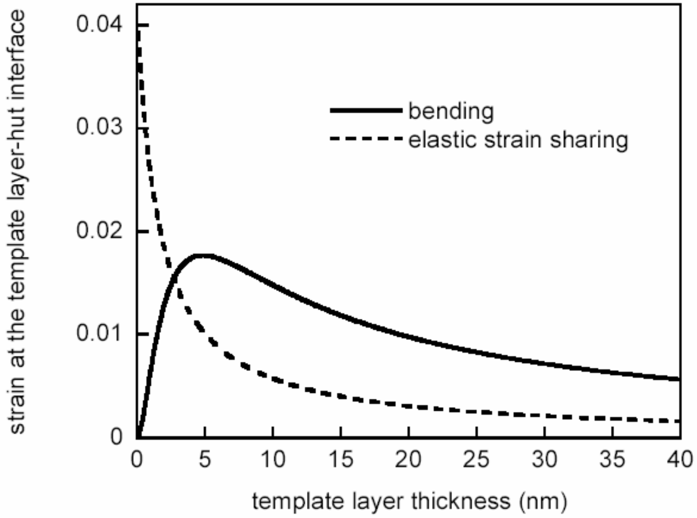




APS (2-ID-D)



30 nm SOI **(Si on insulator)** template layer



Improving Solar Cell Materials by Defect Engineering

T. Buonassisi, A. A. Istratov, M. A. Marcus, E. R. Weber (LBNL), B. Lai, Z. Cai (APS), S. M. Heald (PNNL)

High-purity Semiconductor-grade Polysilicon

- Used in 90% of photovoltaic devices which has annual growth > 25%
- In 2004, demand exceeded supply for silicon feedstock ⇒ higher price

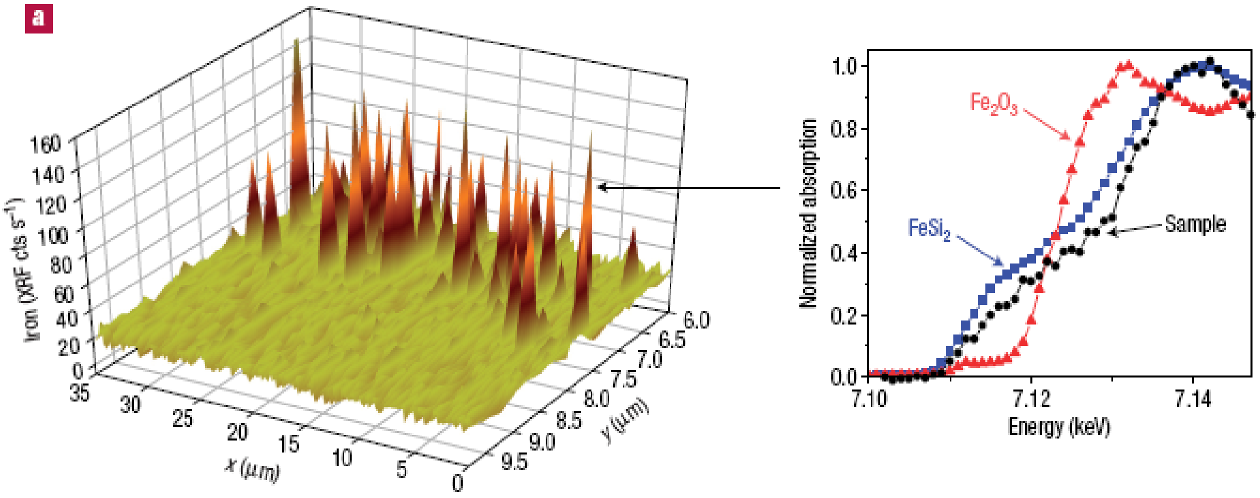
Low-cost Solar-grade Multicrystalline Silicon (mc-Si)

- High impurity (~10^{15} cm^{-3}) ⇒ short minor carrier diffusion length ⇒ low efficiency
- Removing metal impurities (gettering, passivation) is difficult and expensive
- Questions:
  1) Are all metal defects created equal?
  2) What type of defect is most detrimental to device performance?
  3) Can one live with the metal impurity by defect engineering?

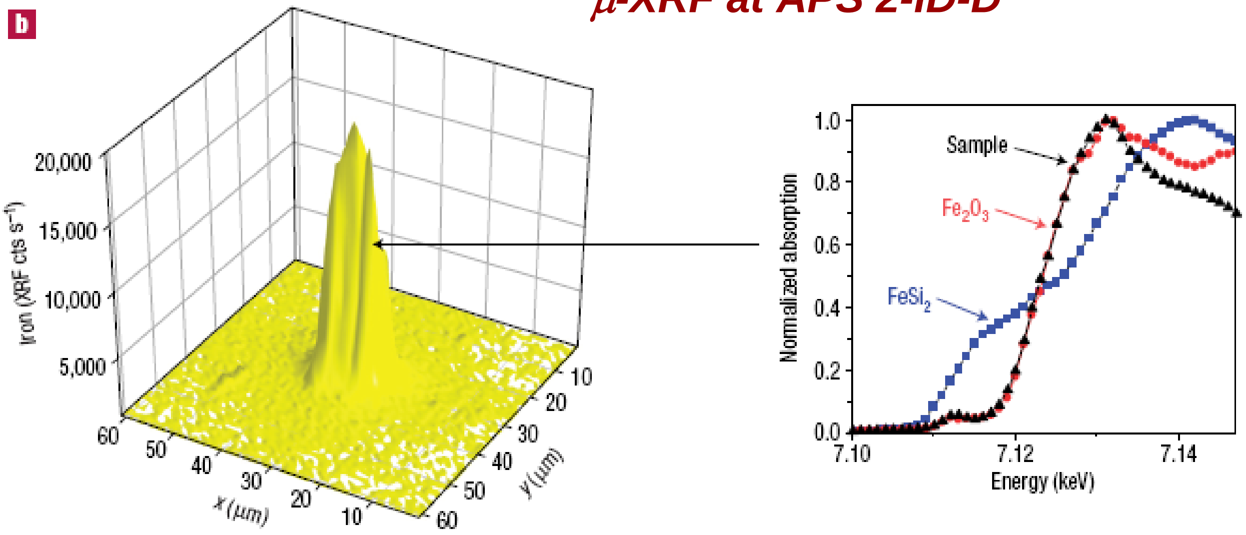
Metal Defects in Commercial Grade Solar-Cell Si

Buonassisi, et al.
Nature Materials
(August 14, 2005)

The different types of metal defect in commercial solar-cell material. a, Iron silicide nanoprecipitates, with radii 20–30 nm. **b**, Iron oxide inclusion, several micrometres in diameter. X-ray fluorescence (left) maps the iron nano- and microdefects, whereas X-ray absorption spectra (right) determine their chemical states.



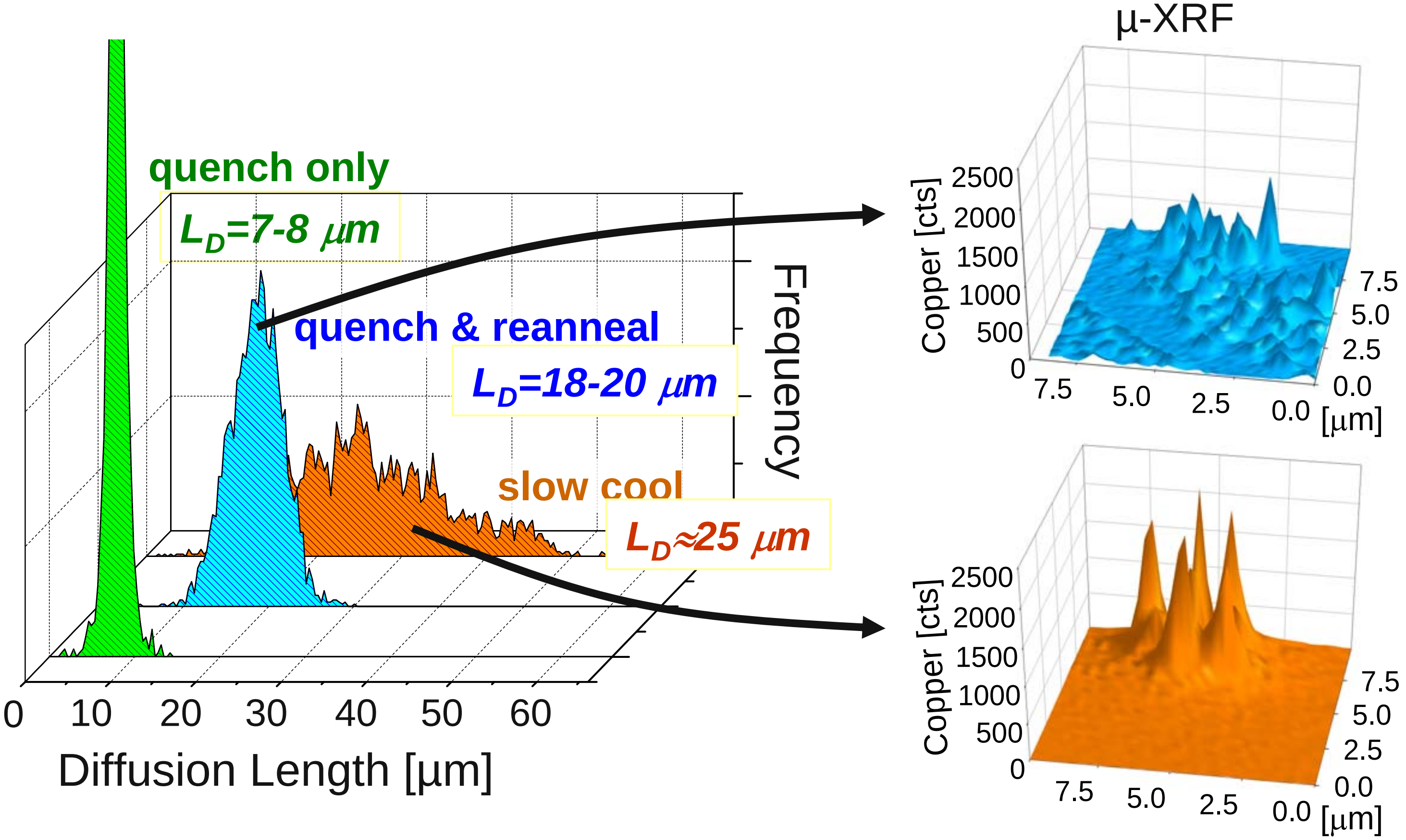
μ-XRF at APS 2-ID-D



Engineering Metal-impurity Nanodefects in Solar Cells

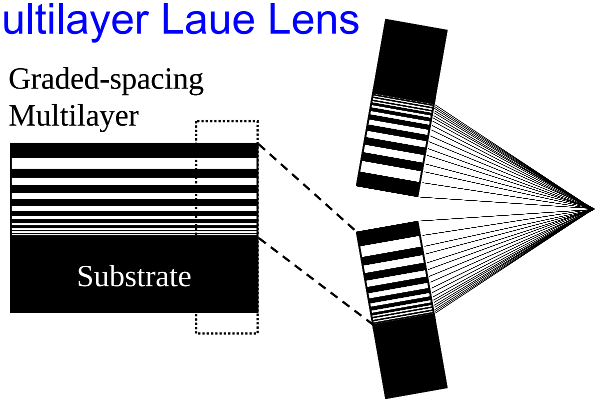
Properly chosen annealing sequence decreases spatial density of metal clusters and improves the minority carrier diffusion length L_D

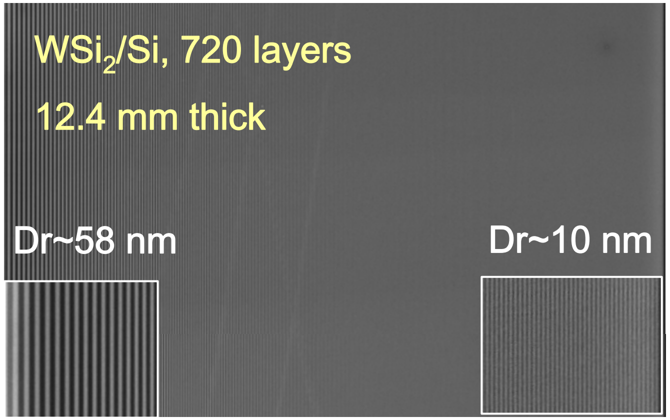
T.Buonassisi, et al., Nature Materials, online Aug. 14 (2005)



Multilayer Laue Lens: Towards 1-nm Focusing of Hard X-rays

Multilayer Laue Lens





Deposition of thick, graded multilayer at APS; sectioning and microscopy at MSD/EMC/CNM.

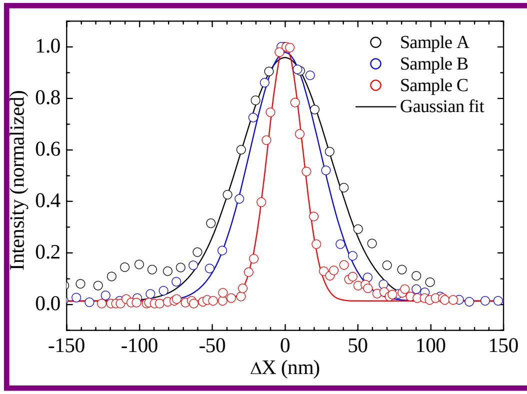
Electron microscopy shows accuracy of layer spacings

Theory

Ideal Multilayer Laue Lens should focus X-rays to 1 nm with high efficiency.

Experiments

We have fabricated partial MLLs and measured their performance. The world-record results obtained for hard x-ray focusing support the predictions of theory.



Nearly diffraction-limited performance of test structures

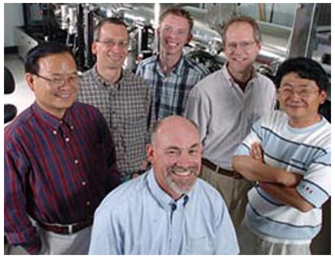
30 nm FWHM, 44% efficiency, 0.06 nm wavelength

Measurements at APS beamlines 12BM and 8ID. Kang et al. *Phys. Rev. Lett.* (2006)

H.C. Kang, G.B. Stephenson, J. Maser, C. Liu, R. Conley, S. Vogt, A.T. Macrander

The 43rd Anniversary R&D 100 Awards

2005 R&D 100 Award



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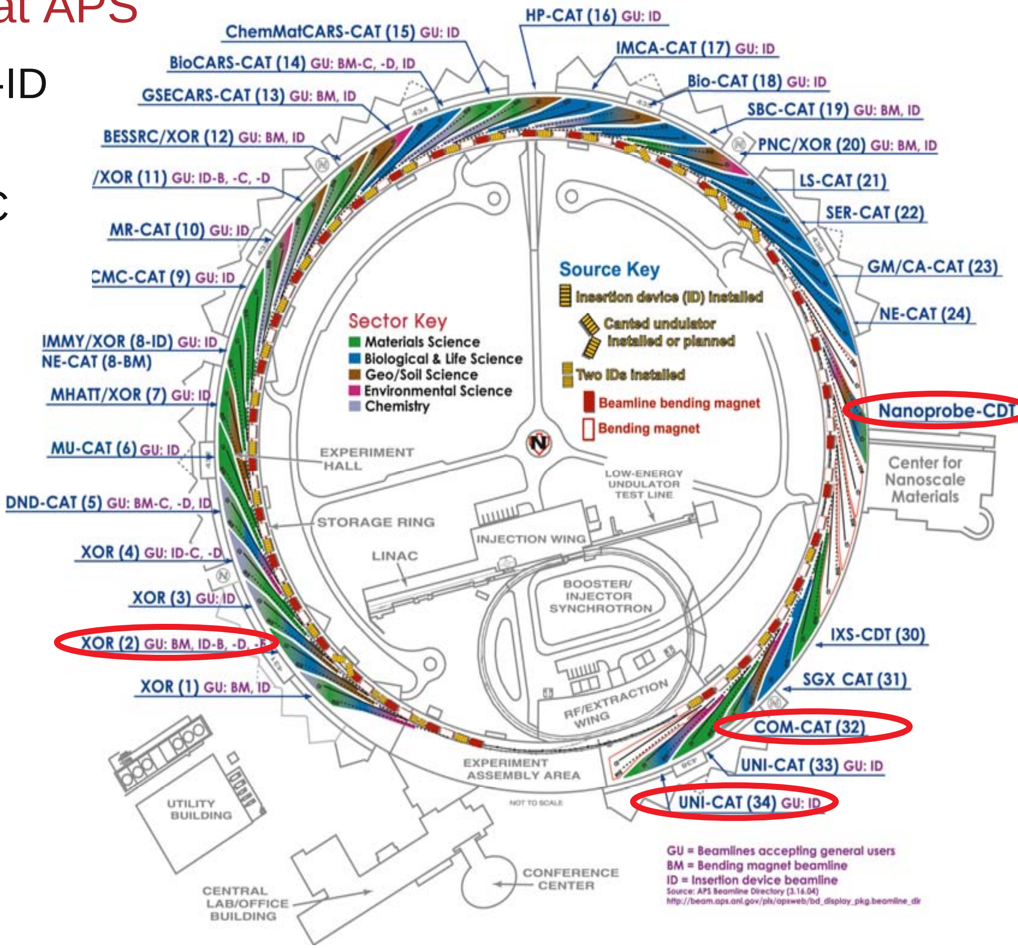
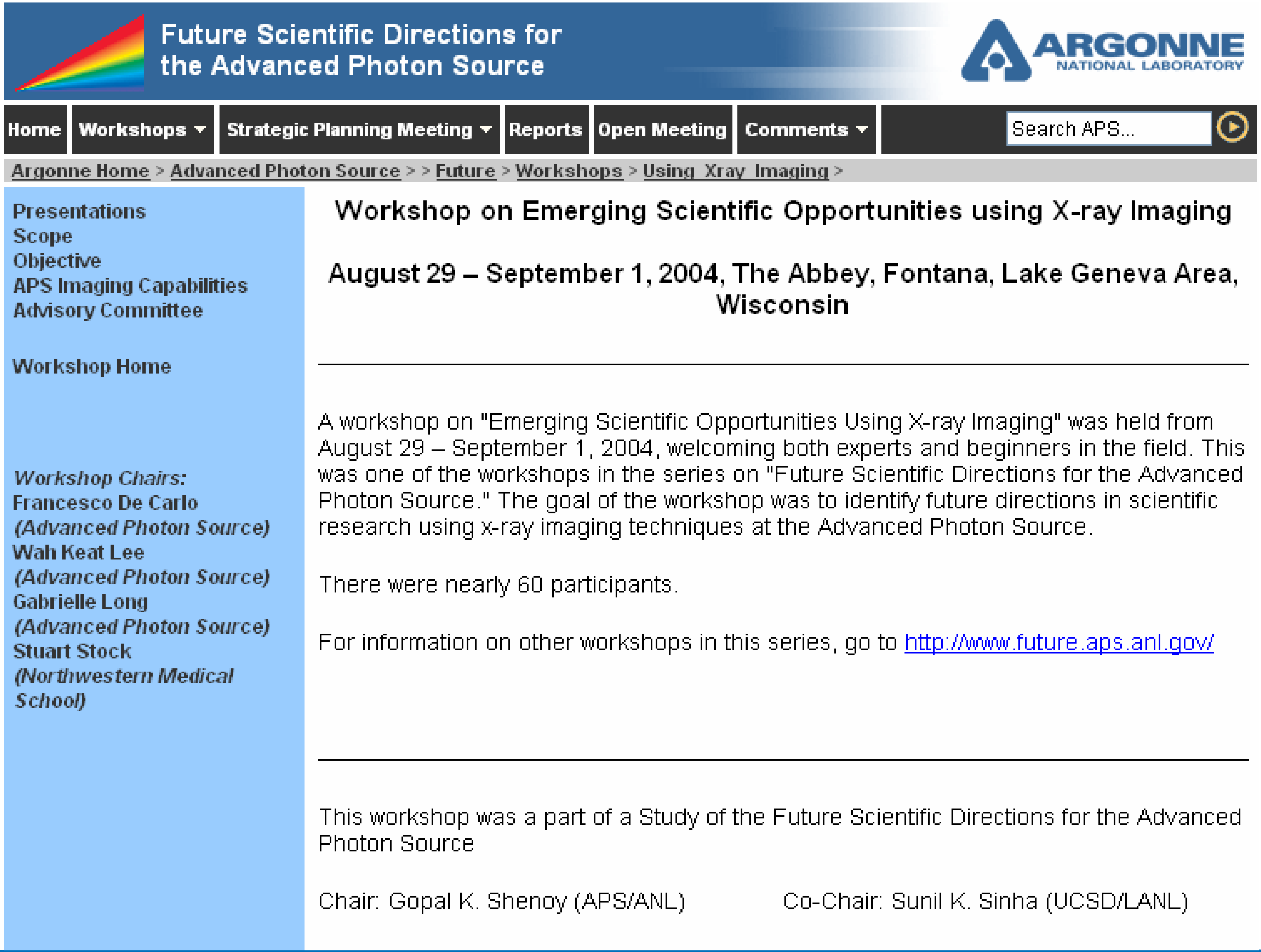


APS Strategic Planning 2004



Workshop Chairs:
Francesco De Carlo
(Advanced Photon Source)
Wah Keat Lee
(Advanced Photon Source)
Gabrielle Long
(Advanced Photon Source)
Stuart Stock
(Northwestern Medical School)

Workshop on Emerging Scientific Opportunities using X-ray Imaging

August 29 – September 1, 2004, The Abbey, Fontana, Lake Geneva Area, Wisconsin

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A workshop on "Emerging Scientific Opportunities Using X-ray Imaging" was held from August 29 – September 1, 2004, welcoming both experts and beginners in the field. This was one of the workshops in the series on "Future Scientific Directions for the Advanced Photon Source." The goal of the workshop was to identify future directions in scientific research using x-ray imaging techniques at the Advanced Photon Source.

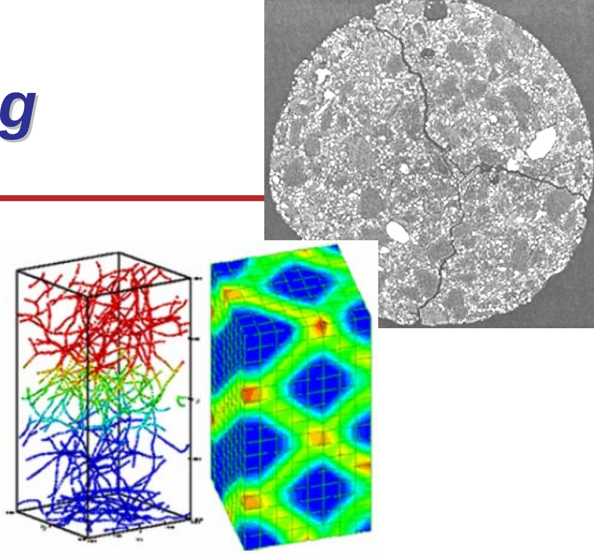
There were nearly 60 participants.

For information on other workshops in this series, go to http://www.future.aps.anl.gov/

This workshop was a part of a Study of the Future Scientific Directions for the Advanced Photon Source

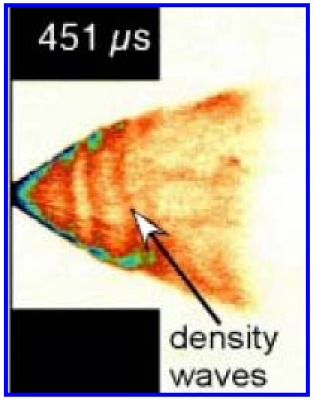
Chair: Gopal K. Shenoy (APS/ANL)   Co-Chair: Sunil K. Sinha (UCSD/LANL)

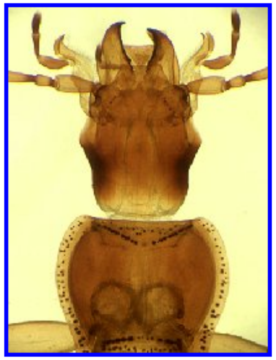
Grand Challenges in X-ray Imaging



Materials Science:

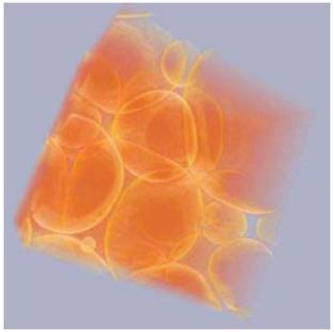
- ➔ Materials deformation, fatigue and fracture
- ➔ Failure mechanisms in engineered structures
- ➔ Dynamic processes in extreme environments
- ➔ High-resolution imaging of nonperiodic structures



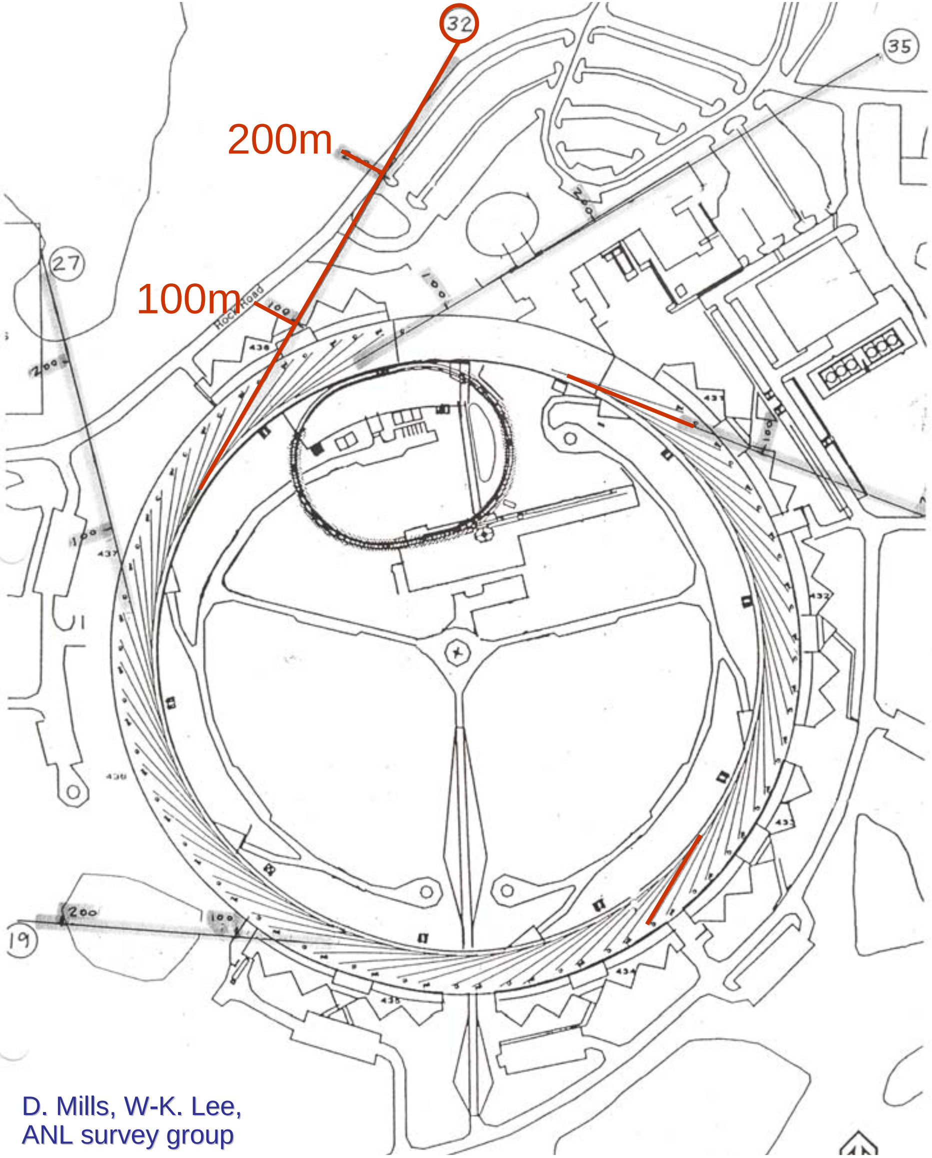


Biological Science:

- ➔ Developing a digital micromorphometry library
- ➔ Real-time imaging of physiological processes
- ➔ Comparative biology on evolutionary transitions
- ➔ Discovery & description of early life in micro-fossils



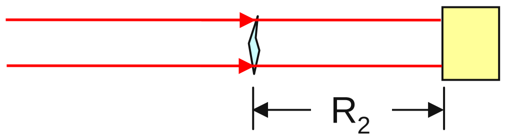
Dedicated X-ray Imaging Beamline at APS

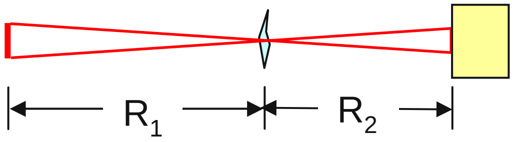


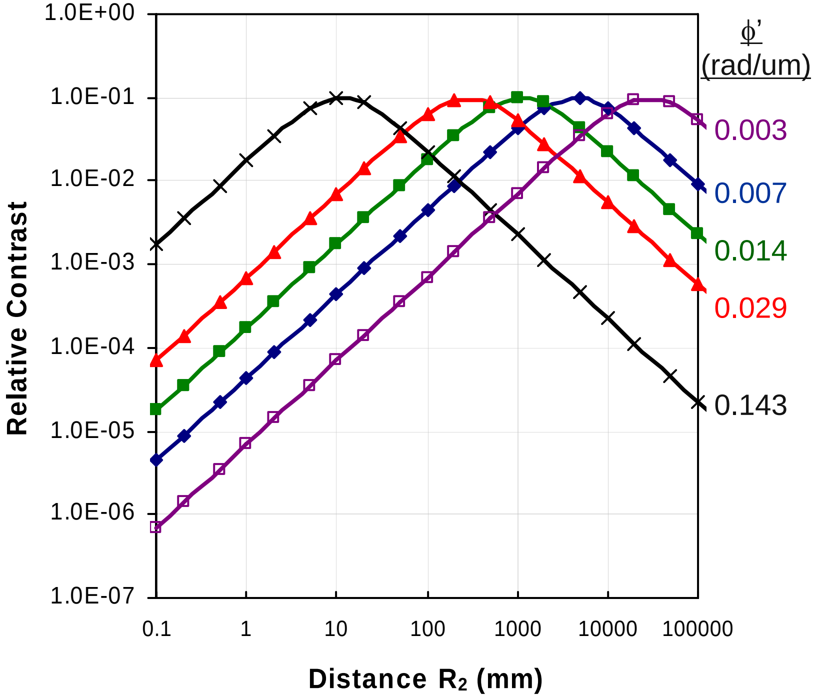
D. Mills, W-K. Lee,
ANL survey group

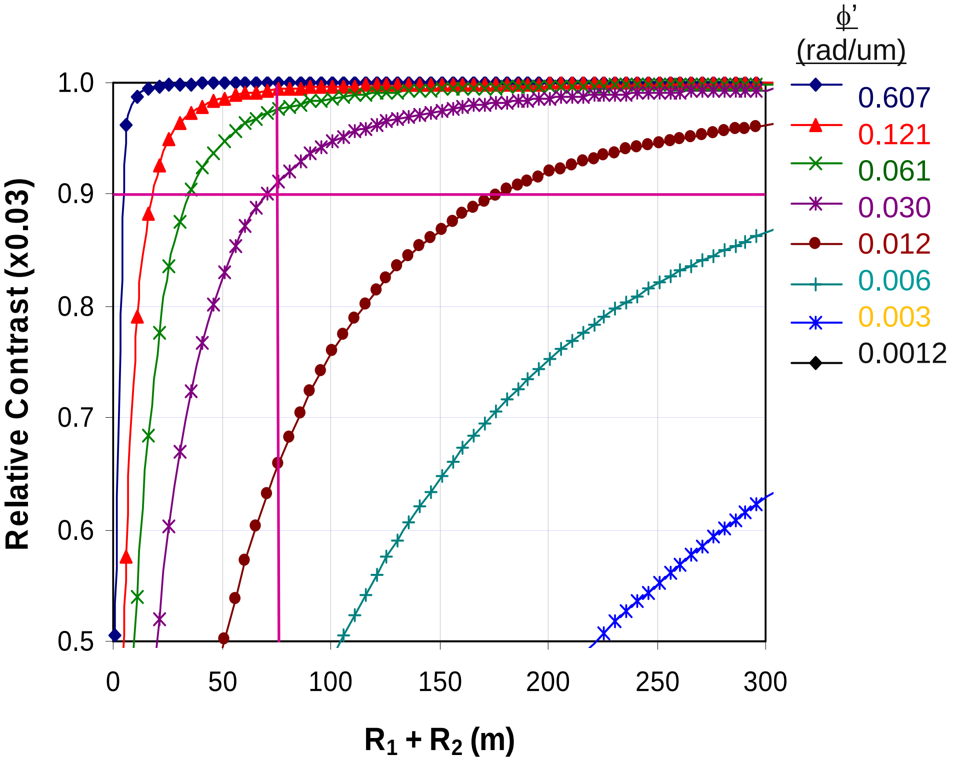
- Consideration of making Sector 32 (Com-CAT) a dedicated imaging XOR-Sector:
  - *Phase imaging / tomography*
  - *Diffraction topography*
  - *Diffraction enhanced /USAXS imaging*
  - *Coherent Fresnel diffraction*
- Many Benefits:
  - *Provides immediate home for the imaging group to satisfy users demand, to expand user base, and to test new application & ideas.*
  - *Frees up 1-ID so Sector 1 can proceed to become a dedicated high-energy sector.*
  - *Potential for future expansion perhaps into a long beam line (~200m) with optimized insertion devices.*
- X-ray Imaging: recommended by SAC as one of top three priorities at APS ➔ XOR Tactical Plan.

Phase Contrast Sensitivity vs. Distance









Note: 3um thick biomatter (ρ=1.35) in 30um thick H_2O corresponds to ~0.03 rad at λ = 1 A

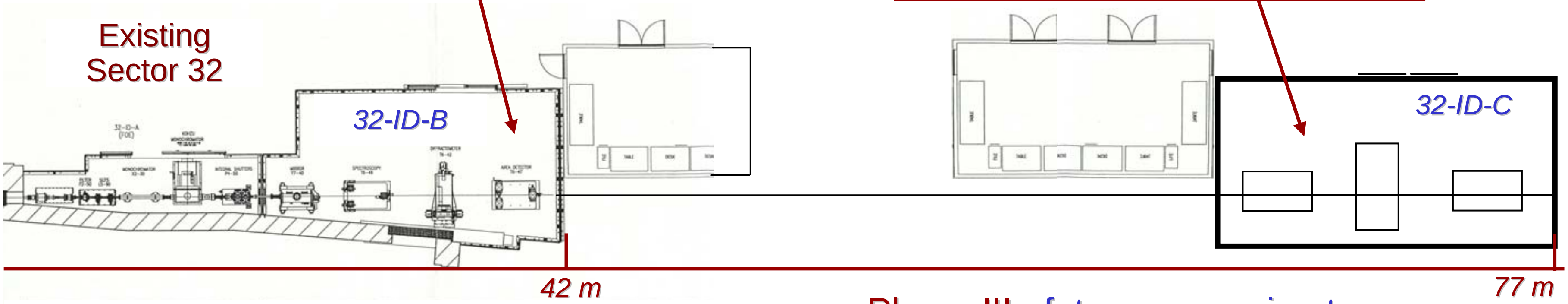
Dedicated X-ray Imaging Beamline at APS

Phase I: make use of existing hutch and equipment, with upgrades to monochromator & Be windows

- → *Phase imaging*
- → *Diffraction topography*
- → *USAXS imaging*

Phase II: expansion to ~75m by building a new white-beam capable hutch at 75m and beam transport

- → *High-sensitivity phase imaging*
- → *Coherent Fresnel diffraction*
- → *Projection microscopy*



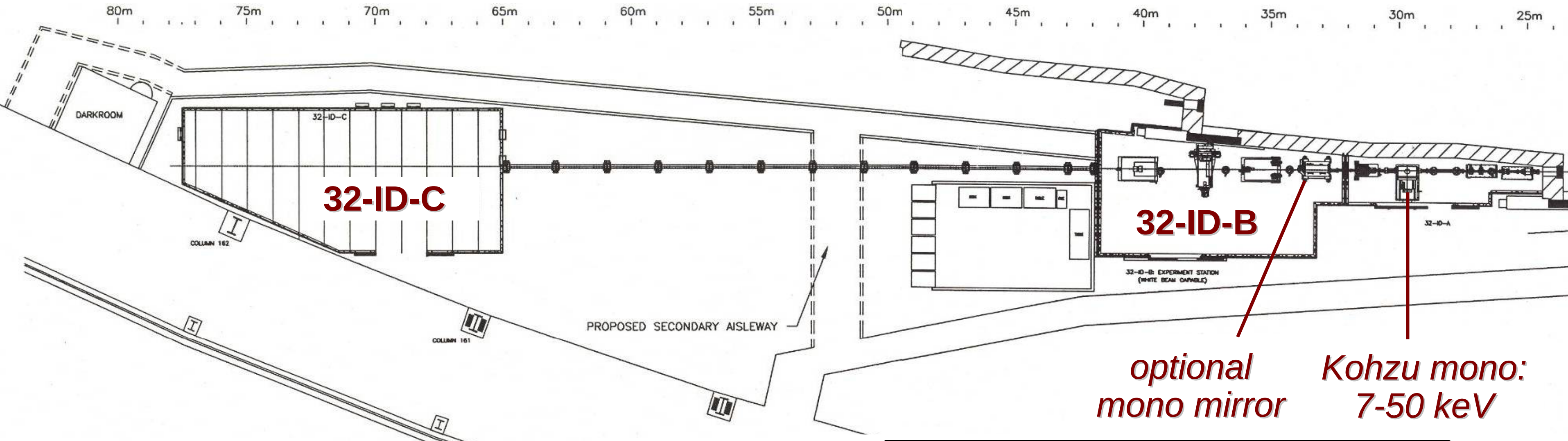
Phase III: future expansion to ~200m (ID-D) with additional outside funding, and with optimized insertion devices and optics

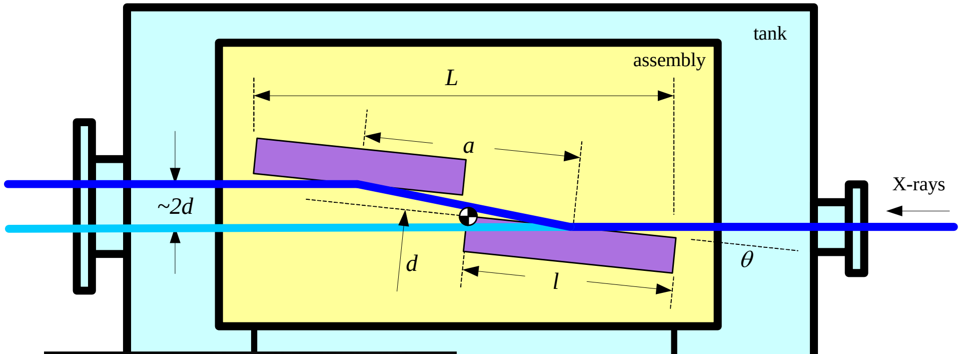
- → *Ultra-sensitivity phase imaging*
- → *Ultra-plane-wave topography*
- → *Medical imaging ?*

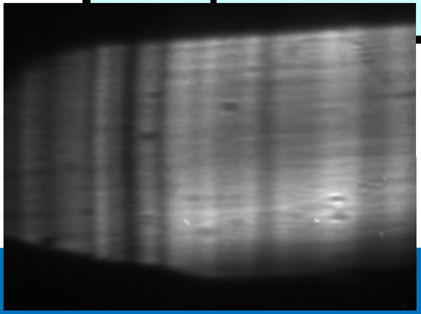
Funding Profile (Phase I & II):

- **FY'05: $760K AIP approved**
- **FY'06: additional AIP funds ?**
- **FY'07: more funds for instrumentation**
- **Phase III will require outside funding**

New Hutch 32-ID-C and Beam Transport



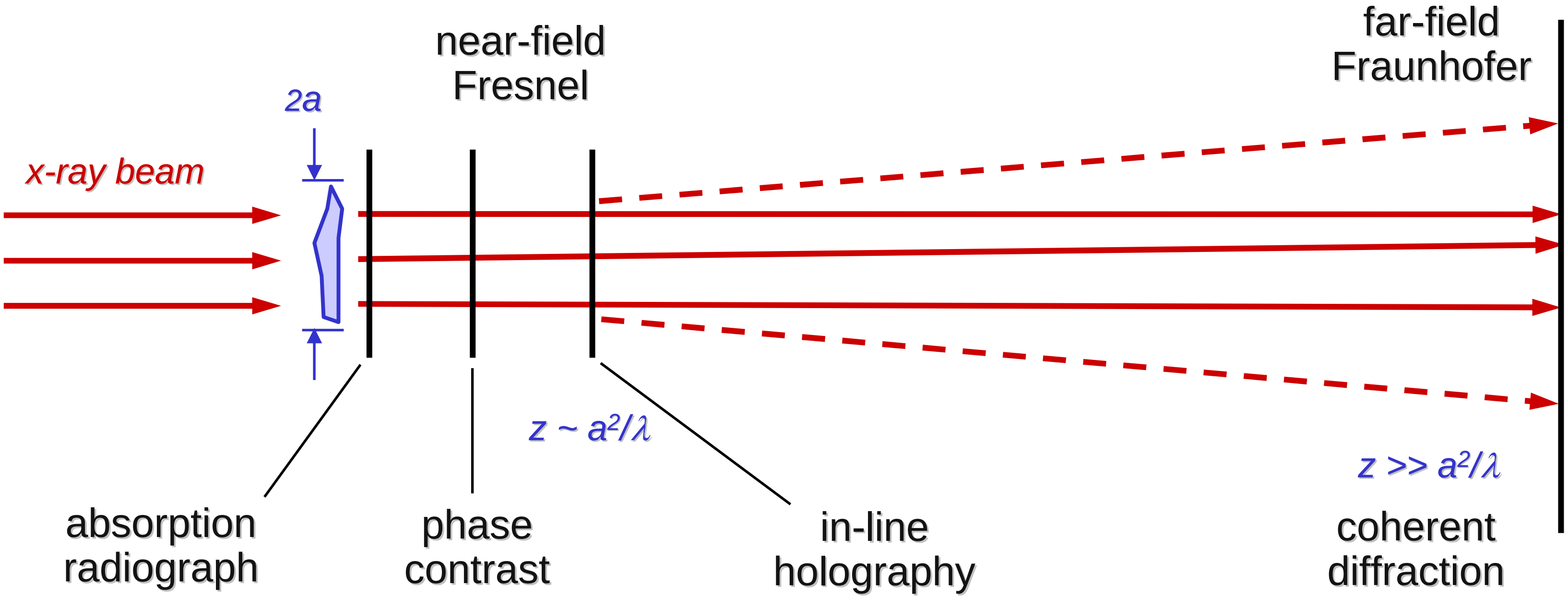




New Experiment Hutch:

- White-beam hutch for filtered pink-beam experiments
- Option of mini-hutch upstream of 32-ID-C for monochromator
- As far from source as possible without affecting 33-BM darkroom
- Rerouting of aisleway between 33 and 32

Different Regimes of X-ray Imaging



near-field
Fresnel

far-field
Fraunhofer

2a

x-ray beam

$z \sim a^2/\lambda$

$z >> a^2/\lambda$

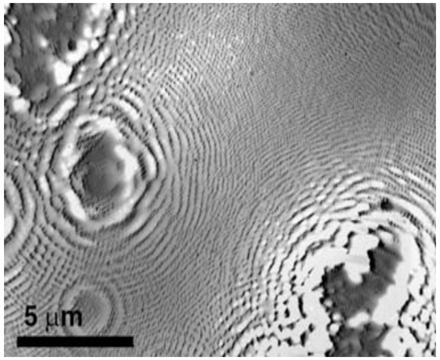
absorption
radiograph

phase
contrast

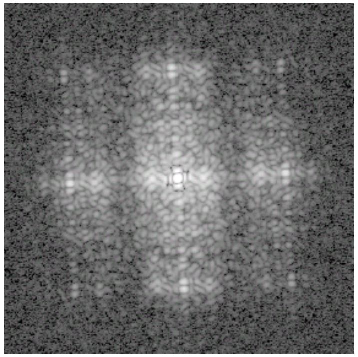
in-line
holography

coherent
diffraction

Kagoshima et al.
JJAP (1999).



Jacobsen (2003).



Miao et al.
Nature (1999).

Four Scientific Programs

Phase-Contrast Imaging

- fracture mechanics of composites and biomaterials,
- materials microstructure/properties e.g. deformation and sintering,
- bone and cartilage growth and formation,
- small animal and soft tissue research,
- vascular and pulmonary functions,
- porosity distribution in foods,
- structure and development of plant seeds,
- characterization of geological structures and microfossils,
- cement mortar research,
- structure and development of foams,
- granular packing of non-equilibrium systems,
- time-resolved studies of internal complex fluid flow and fluid sprays.

Diffraction-enhanced/USAXS imaging

- microstructures and defects in materials,
- deformation, sintering, and cracks formations,
- porosity in bones and calcification effects,
- soft tissue and vascular network detections
- diagnosis of cancerous tumors in soft tissues,
- diffraction applications with 25-50keV x-rays – unique capability @ APS.

Coherent diffraction imaging

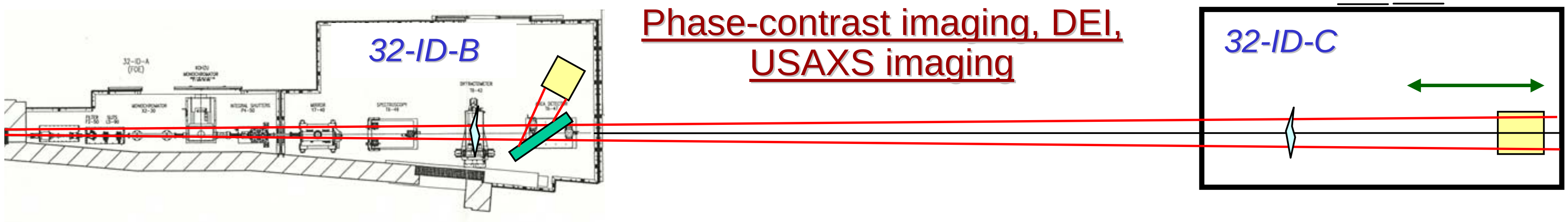
- structures of large biological functioning units e.g. tissues, myocytes, muscles, bones, cartilage, etc.
- identification of organelles and critical protein assemblies in biological cells,
- self-assembly of macromolecule arrays with nano-templates and nanogrids,
- structural imaging of multi-unit inorganic/small-molecule/biomolecule composites,
- noncrystalline nanoparticles e.g. nanoclusters and nanowires,
- structural imaging of precipitates and defects in engineering materials,
- topographic imaging of domain growths in ferroelectics.

Transmission X-ray Microscopy (??)

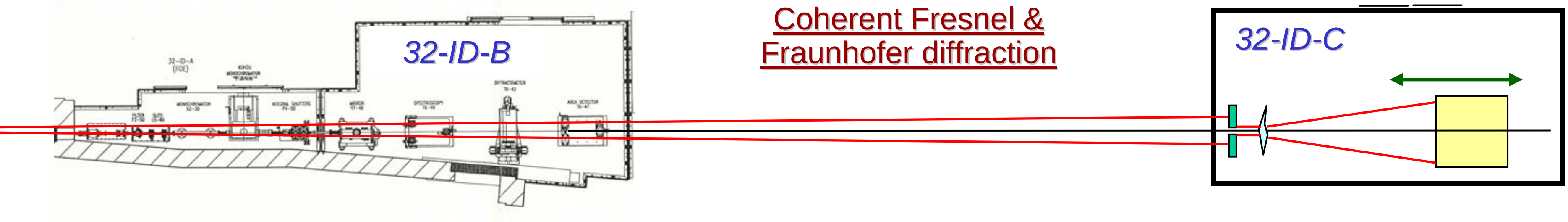
- in-situ studies of precipitates in metallic alloy formation,
- in-situ studies of crystalline domain formation in multi-phased systems,
- microscopic imaging of strain around domain boundaries,
- interfacial structures near buried interfaces,
- mesoscopic structures of soft matter that are difficult to image with EM,
- structures in frozen hydrated thick biological specimens,
- real-time imaging of fluid flow in nano-fluidics.

Several Operating Modes

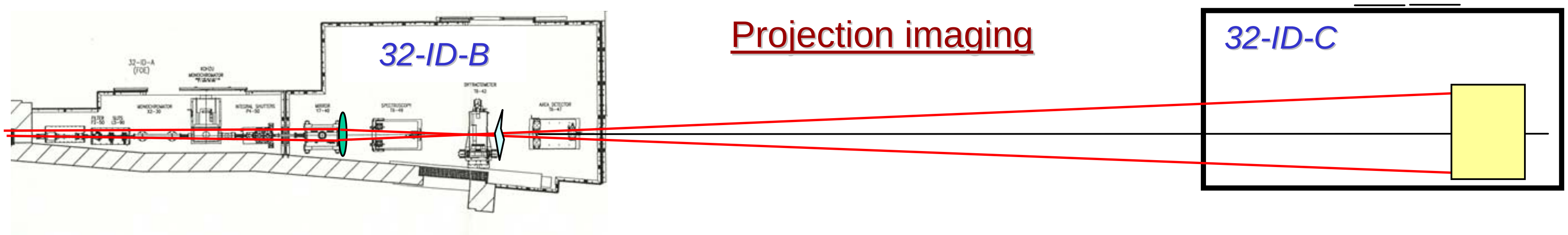
Phase-contrast imaging, DEI, USAXS imaging



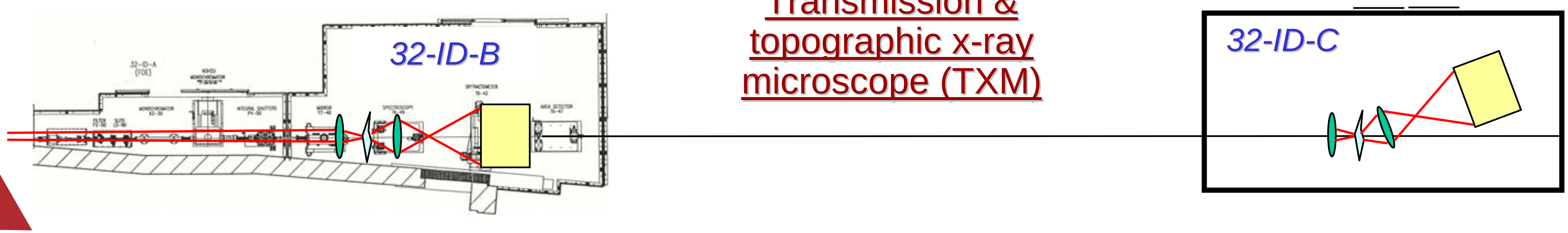
Coherent Fresnel & Fraunhofer diffraction



Projection imaging



Transmission & topographic x-ray microscope (TXM)



Phase Contrast Imaging

Fresnel propagation from 0 to D : $$E_D(y) = \frac{1}{\sqrt{i\lambda D}} \int_{-\infty}^{\infty} E_0(y_o)\exp\left[-i\frac{\pi}{\lambda D}(y-y_o)^2\right] \mathrm{d}y_o$$

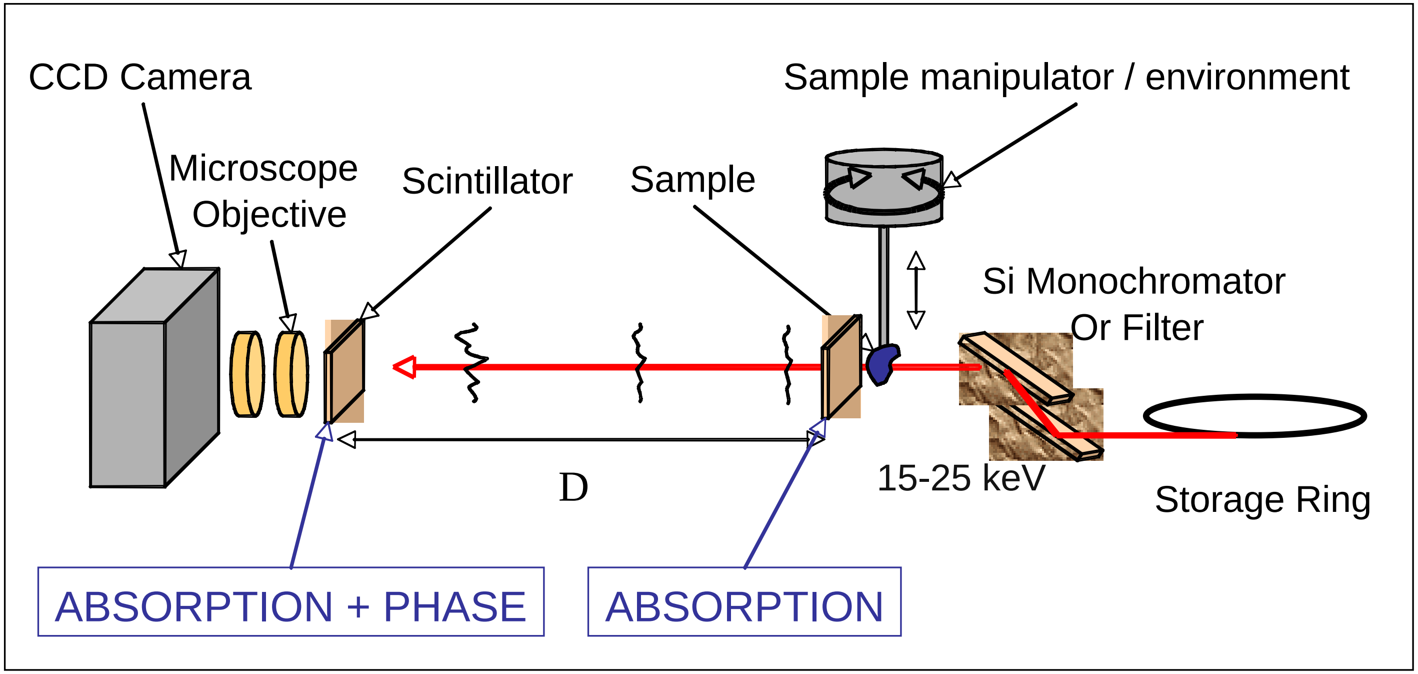


Figure 1: Sketch of the experimental setup.

Imaging Biomechanics and Animal Physiology

Tracheal Respiration in Insects Visualized with Synchrotron X-ray Imaging

Mark W. Westneat,*[1] Oliver Betz,[1,2] Richard W. Blob,[1,3]
Kamel Fezzaa,[4] W. James Cooper,[1,5] Wah-Keat Lee[4]

Field museum of Chicago & APS, Argonne National Lab.

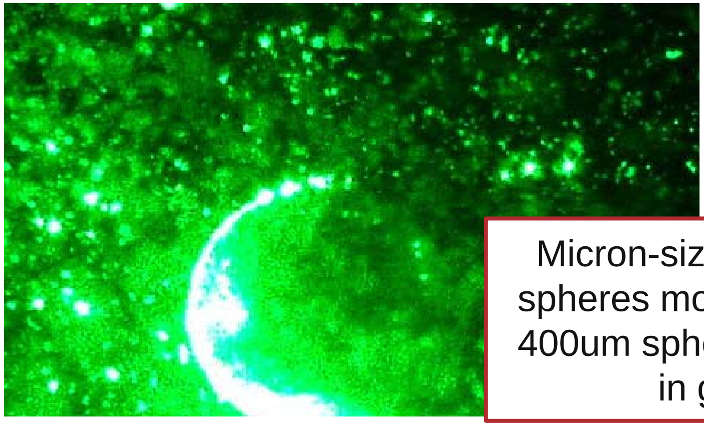
- **Animal functions**
- **Biomechanics**
- **Internal movements**
- **New findings not known before**

wood
beetle

Science (2003) 299, 598-599.

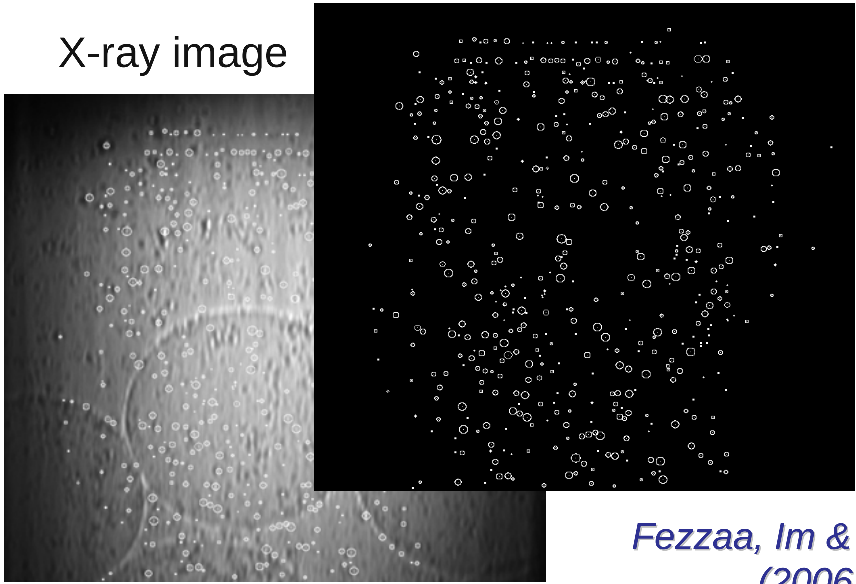
Particle Imaging Velocimetry (PIV)

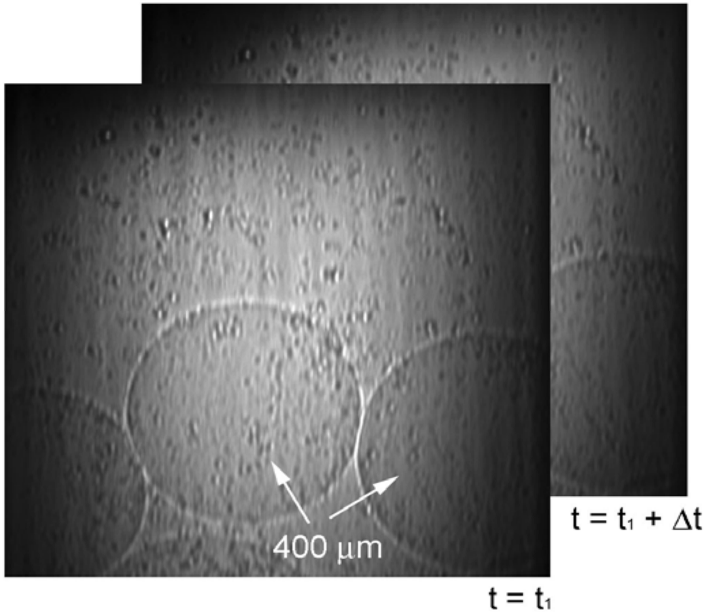
Visible light image



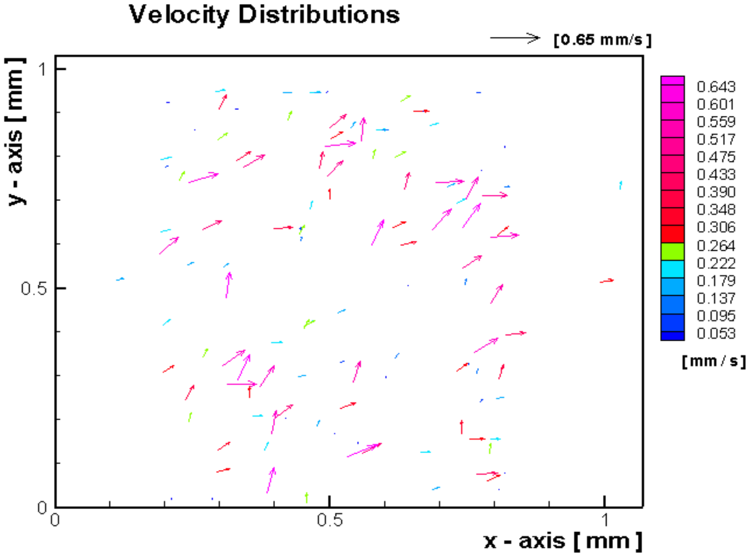
Micron-sized polystyrene spheres moving around big 400um spheres (obstacles) in glycerin

X-ray image



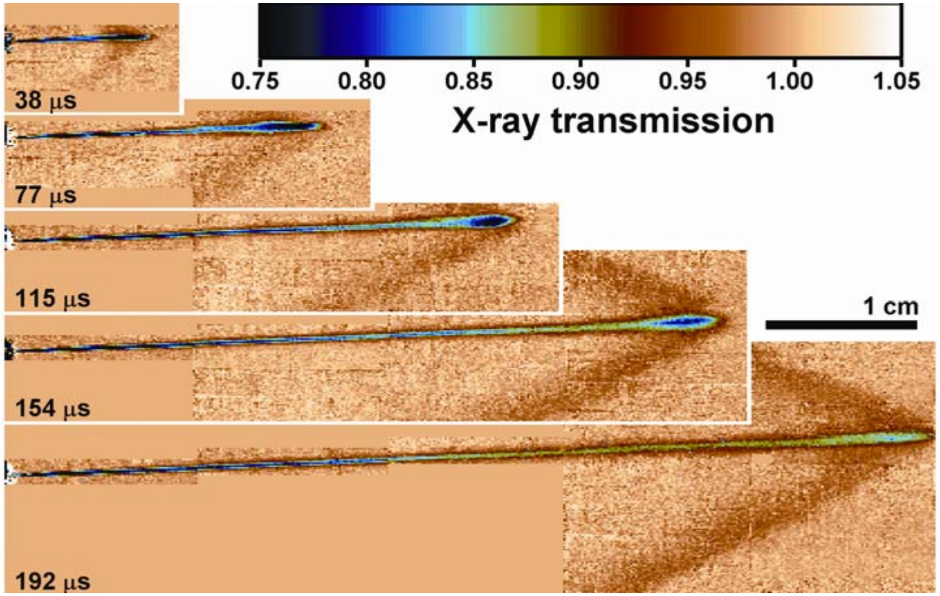


Two consecutive frames in x-ray phase contrast mode, of the polystyrene spheres in motion.

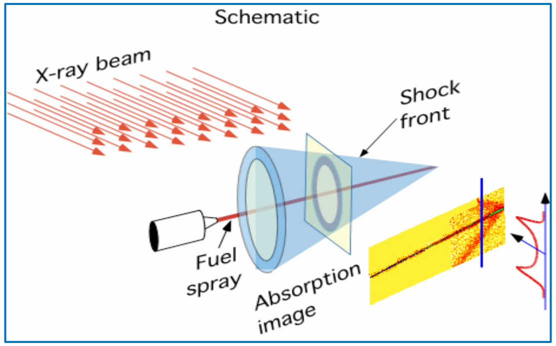


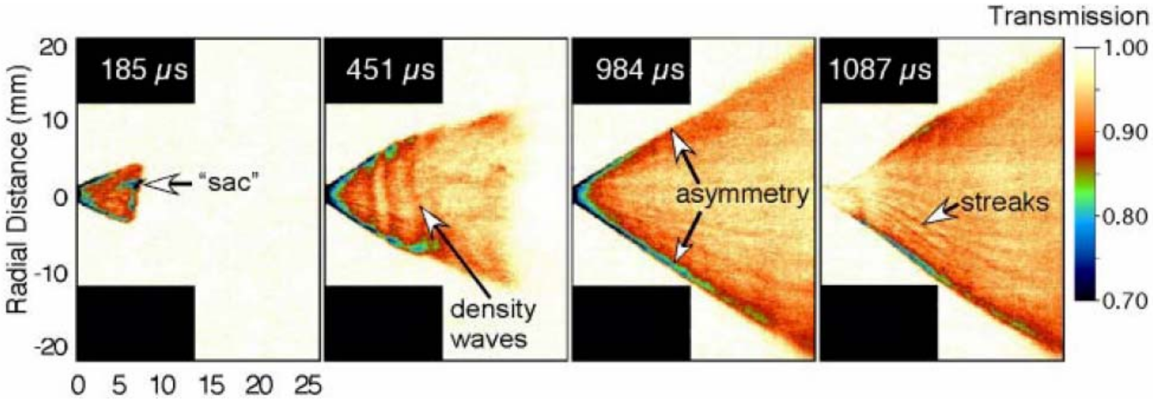
Fezzaa, Im & Cheong (2006)

Time-Resolved Imaging of Fuel Spray in Gasoline Engines



- ✓ Supersonic liquid jet can generate shock waves
- ✓ X-radiographs yield characteristics of the shock waves
- ✓ The shock waves can be quantitatively simulated





*AG MacPhee, MW Tate, CF Powell, et al., Science, **295**, 1261 (2002).*

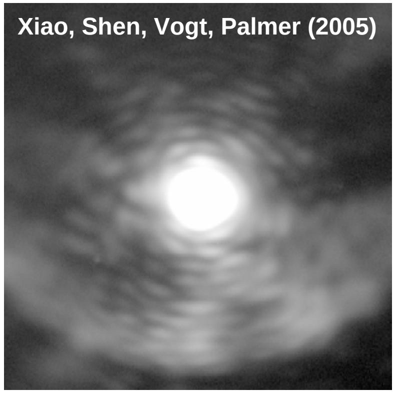
Frontier Imaging Applications that Require Undulator

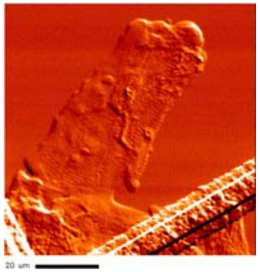
⇒ Coherent imaging
- Fresnel diffraction imaging/holography
- full density reconstruction by phase retrieval

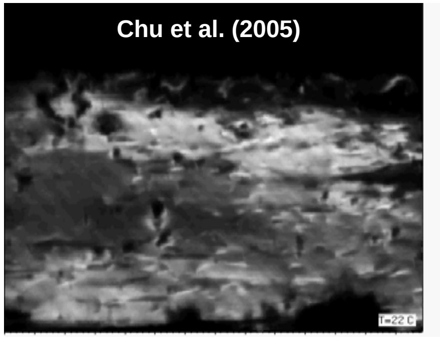
⇒ Time-resolved XRD topography
- nucleation & growth with ms resolution
- phase-contrast, nanocrystals, thin-films

⇒ Ultrafast imaging
- single pulse imaging with filtered pink beam
- 1um spatial & 150ps temporal resolution

10^9 phs/mm^2/pulse/1% ➔ 10^3 phs/pulse/pixel in pink-beam


Xiao, Shen, Vogt, Palmer (2005)




Chu et al. (2005)

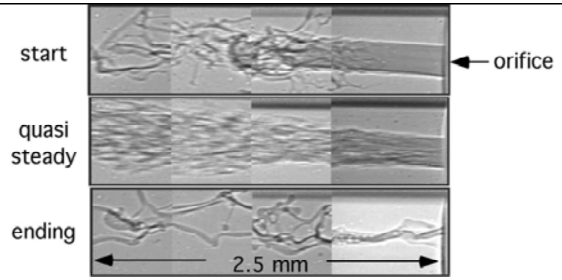


Figure 1. Phase-contrast images of a high-speed, pulsed liquid jet at different time instances of the injection with 300-ns exposure time. Fine structures are readily observable in the start and ending stages but not in the quasi-steady stage due to high jet speed.

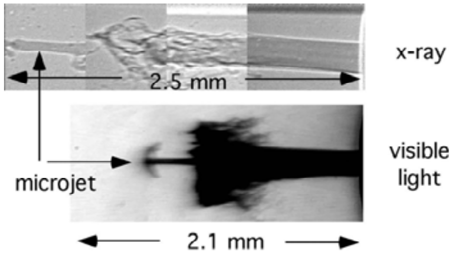
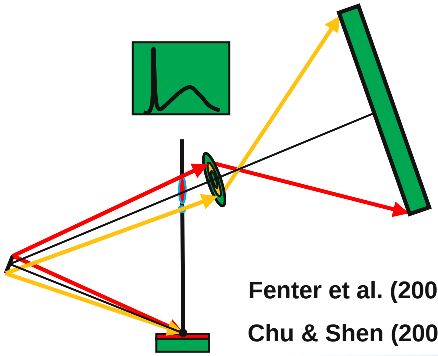


Figure 2. Microjets generated from spontaneous implosion of microcavitation captured by both x-ray phase-contrast imaging and visible light shadowgraph.

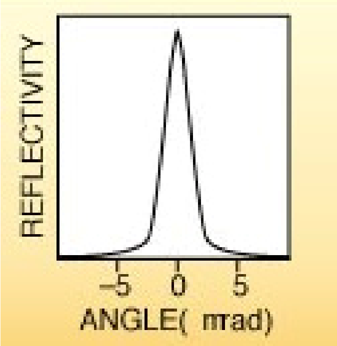
Wang, Lee, Fezzaa (2005)



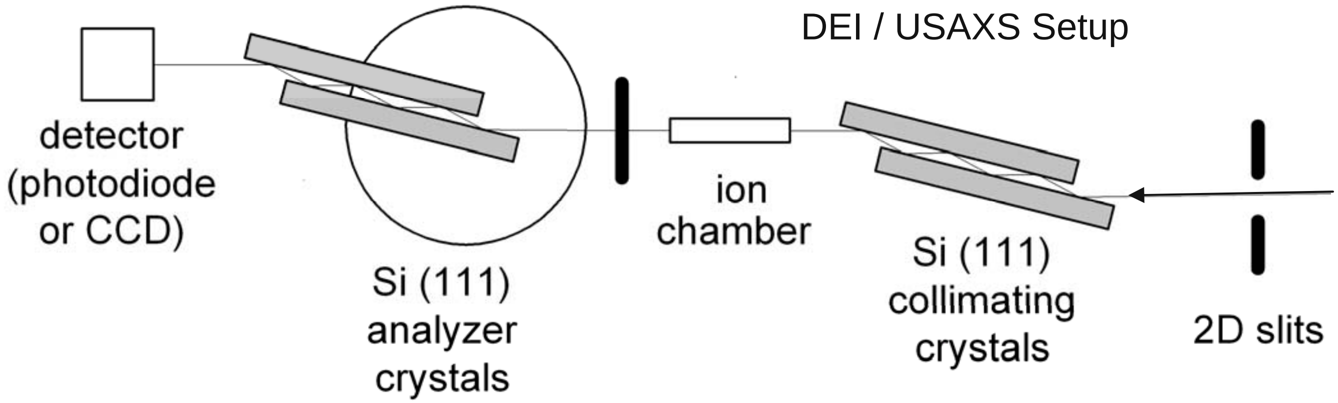
Fenter et al. (2006)

Chu & Shen (2006)

Diffraction-Enhanced & USAXS Imaging



Chapman, Zhong, *et al.* (1996)



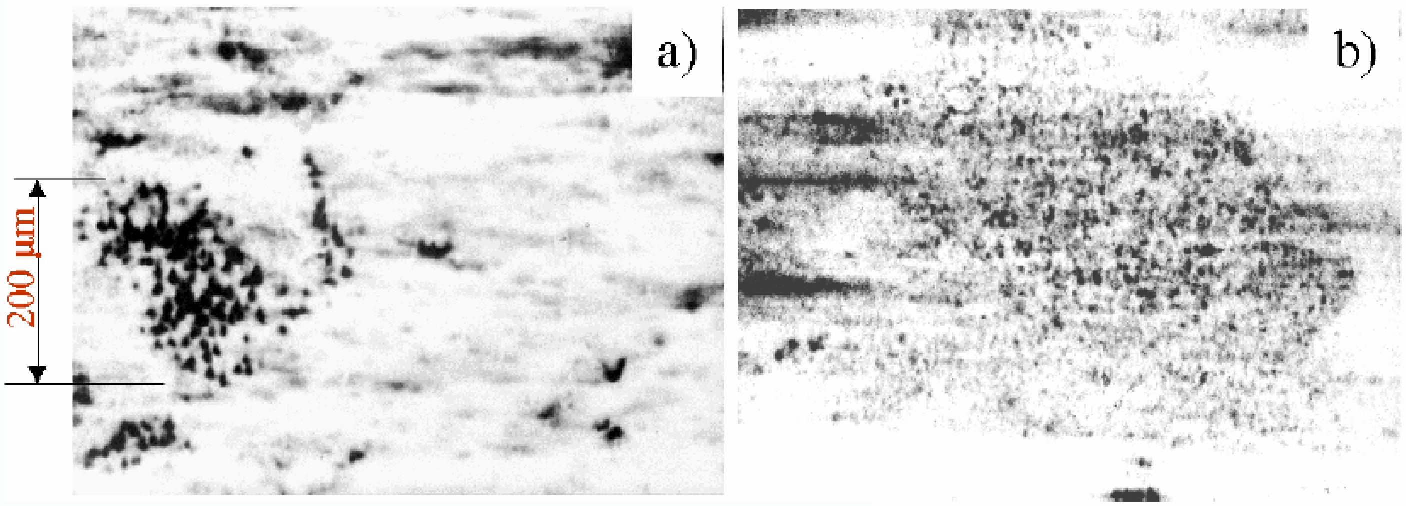
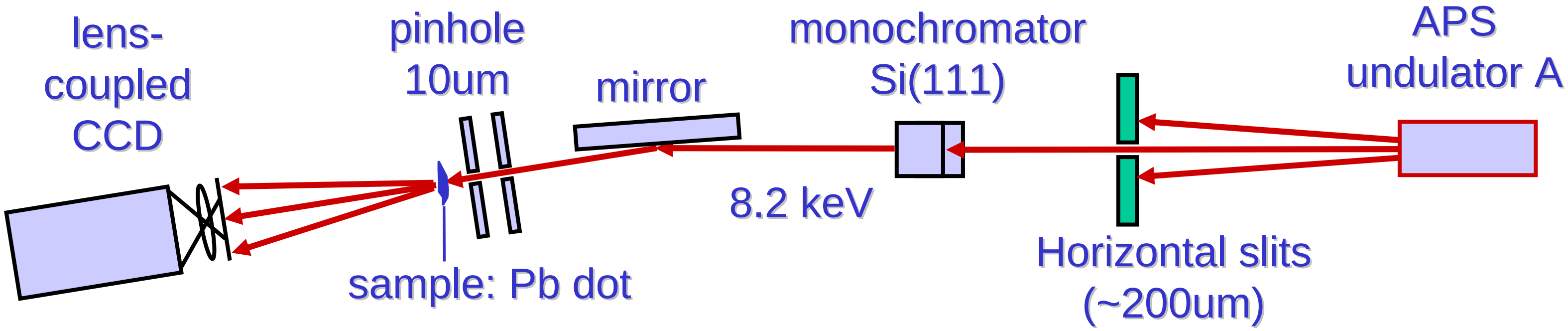
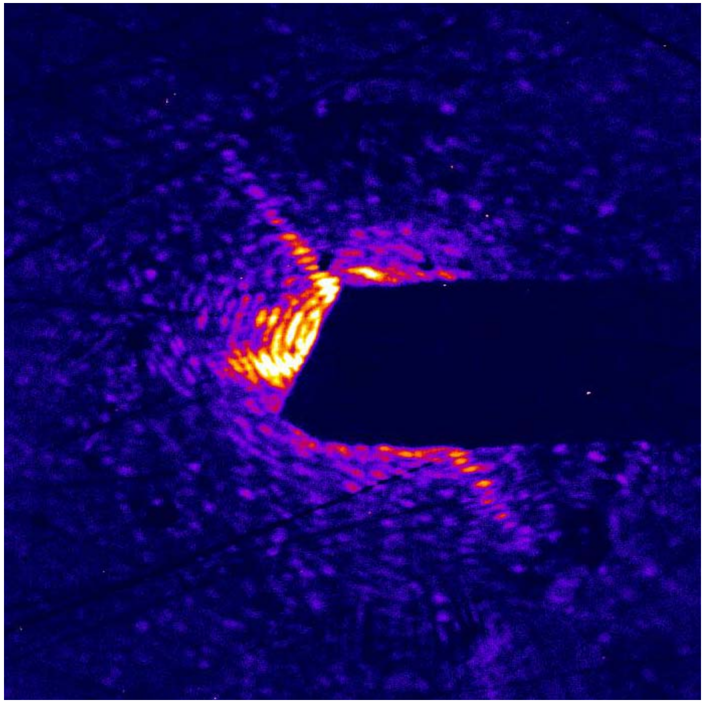


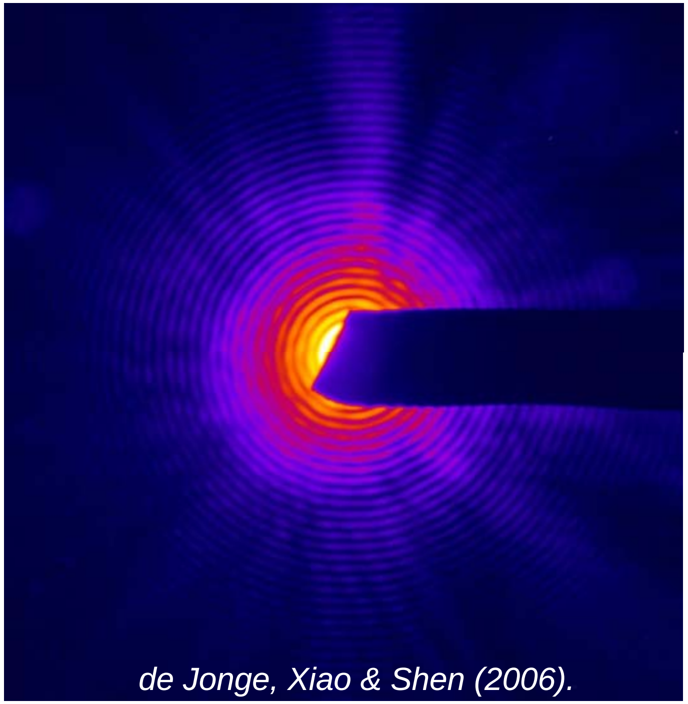
FIG. 1. USAXS images of the same region of the sample taken with a photon energy of 8.94 keV, a sample-to-detector distance of 24 cm and with (a) $q = 1.3 \times 10^{-4}$ Å^{-1} *and (b)* $q = 7.5 \times 10^{-4}$ Å^{-1}.

Levine & Long (2001)

Coherent Diffraction Imaging



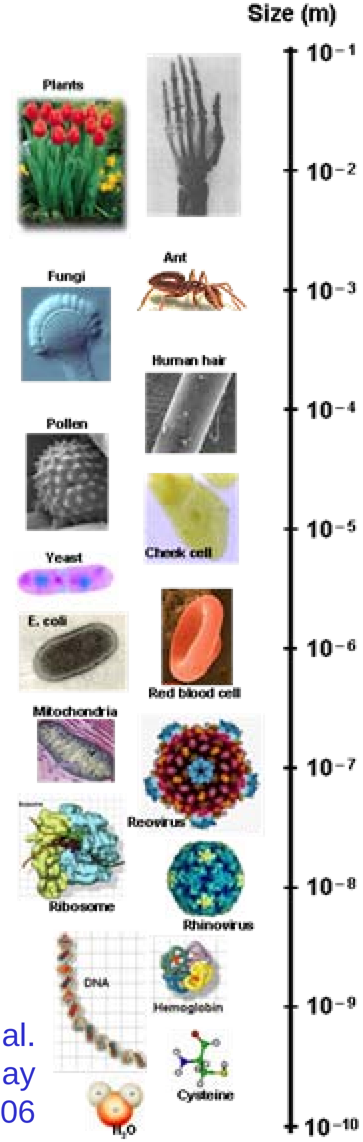


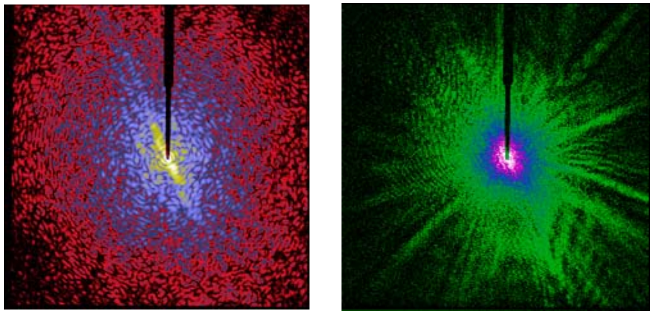


de Jonge, Xiao & Shen (2006).

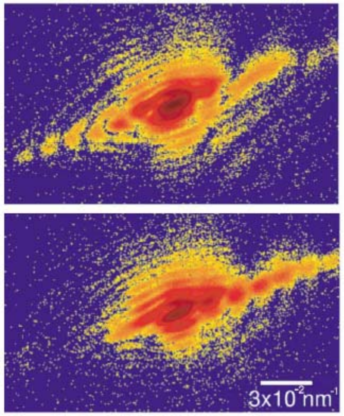
Consolidation of Coherent Diffraction Efforts

- Currently looking at possibility of consolidating coherent diffraction imaging (CDI) activities at a new dedicated undulator beamline
- CDI opens up possibility of structural biology on 2D membrane proteins and laser-oriented macromolecule droplets, without the need for 3D crystals as done today
- Allows in-situ, nondestructive, high-resolution imaging of nanoparticles and self-assembled bio-organic-inorganic hybrids
- Possibility to identify critical proteins and other macromolecules by shape or tertiary structures in biological cells to provide the missing link in structure-function relations of gene products





Miao – actin filaments, 2-ID-B



Robinson –
Au particles
34-ID-C

Shen et al.
Physics Today
March 2006

Coherent Diffraction Imaging

Diffraction by Distorted Object – a Unified Description of Coherent X-ray Diffraction and Imaging

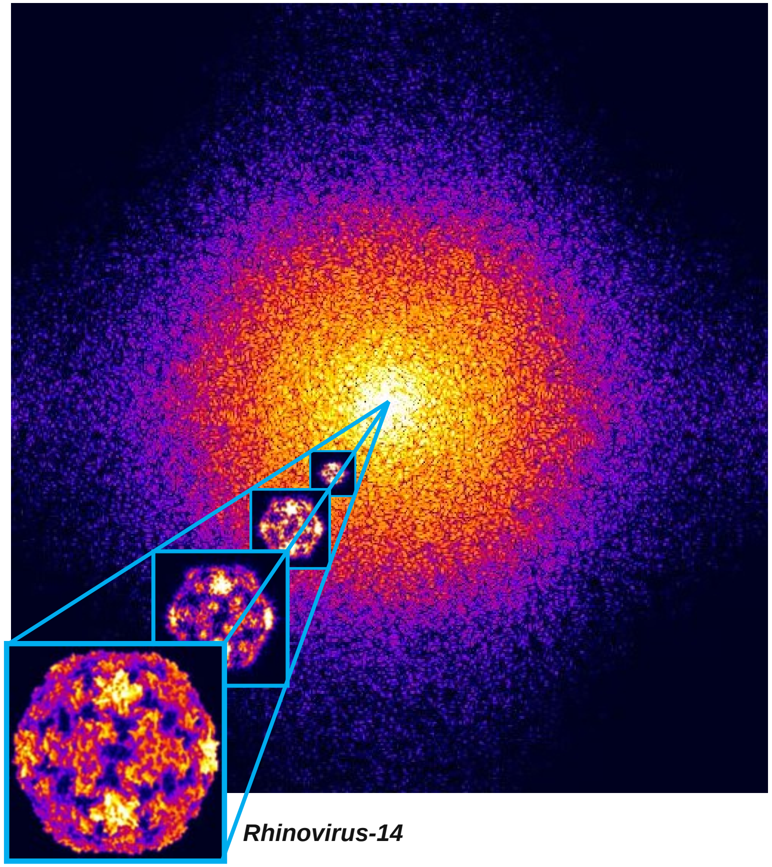
⇒ Imaging by diffraction?
- ❖ far-field Franhofer → FT { ρ(x,y) }
- ❖ near-field Fresnel → ?? or FT {??}

⇒ Distorted object approach
- ❖ Fresnel wave propagation by FT
- ❖ unified iterative phasing method

⇒ Related topics & applications
- ❖ phase-contrast topography
- ❖ coherent diffraction imaging
- ❖ diffraction limited optics

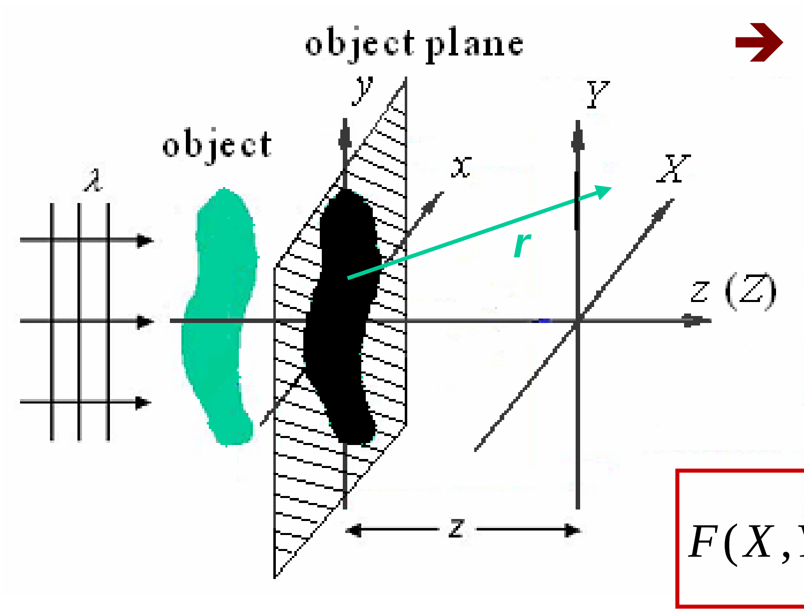
⇒ Summary

Xiao & Shen, PRB 72, 033103, July 2005.



Rhinovirus-14

Fresnel Wave Field Propagation



➔ Fresnel formula for wave propagation

$$\boxed{F(X,Y)=\frac{i}{\lambda}\iint u(x,y)\frac{e^{-ikr}}{r}dxdy}$$

$$r=[z^2+(X-x)^2+(Y-y)^2]^{1/2}$$

$$\approx\ z+[(X-x)^2+(Y-y)^2]/2z$$

$$\boxed{F(X,Y)=\frac{i\,e^{-ikR}}{\lambda R}\iint \underbrace{u(x,y)e^{-\frac{i\pi}{\lambda z}\left(x^2+y^2\right)}}\, e^{-\frac{i2\pi}{\lambda z}(Xx+Yy)}dxdy}$$

$$R=(x^2+y^2+z^2)^{1/2}$$

➔ Wave-field in the object plane

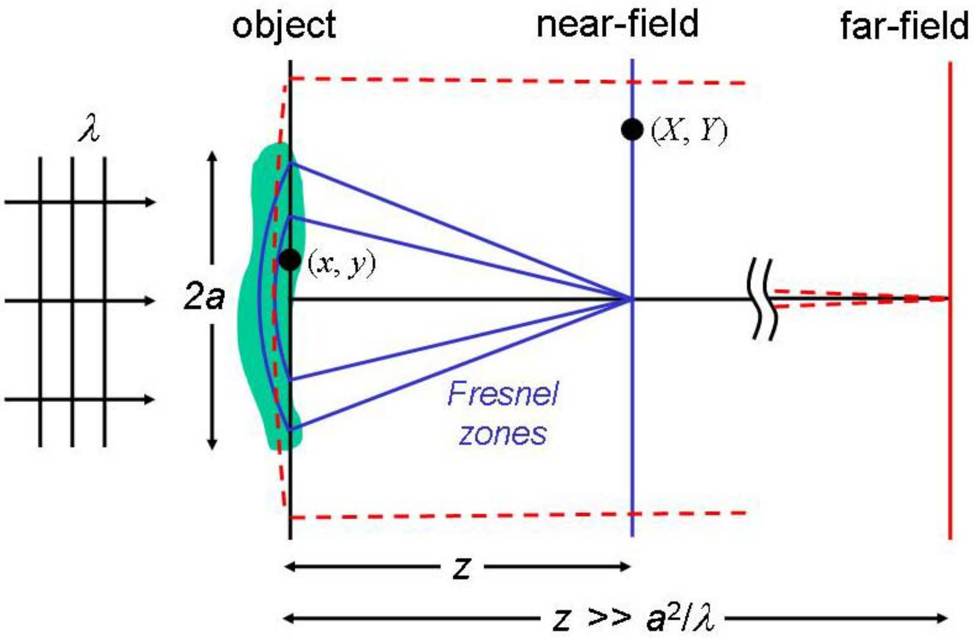
$$u(x,y,0)=\exp\left(-ik\cdot\int_{-\infty}^{0}(\delta(x,y,z)-i\beta(x,y,z))dz\right)$$

$$u(x,y,0)=A\exp(-i\phi(x,y,0))=a(x,y,0)+ib(x,y,0)$$

$$\approx\exp\left(-ik\int_{-\infty}^{0}\delta(x,y,z)dz\right)\quad\text{(pure phase object)}$$

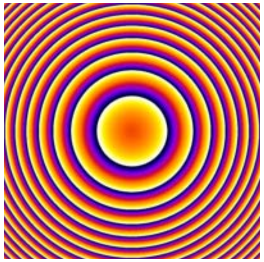
Van der Veen & Pfeiffer, *J. Phys.: Condens. Matter 16, 5003 (2004)*

Distorted Object Approach



Phase-chirped distorted object:

$$\bar{u}(x,y) \equiv u(x,y)e^{-\frac{i\pi}{\lambda z}\left(x^2+y^2\right)}$$



$$\boxed{F(X,Y) = \frac{i\,e^{-ikR}}{\lambda R} \iint \bar{u}(x,y)\,e^{-\frac{ik}{z}(Xx+Yy)}\,dxdy}$$

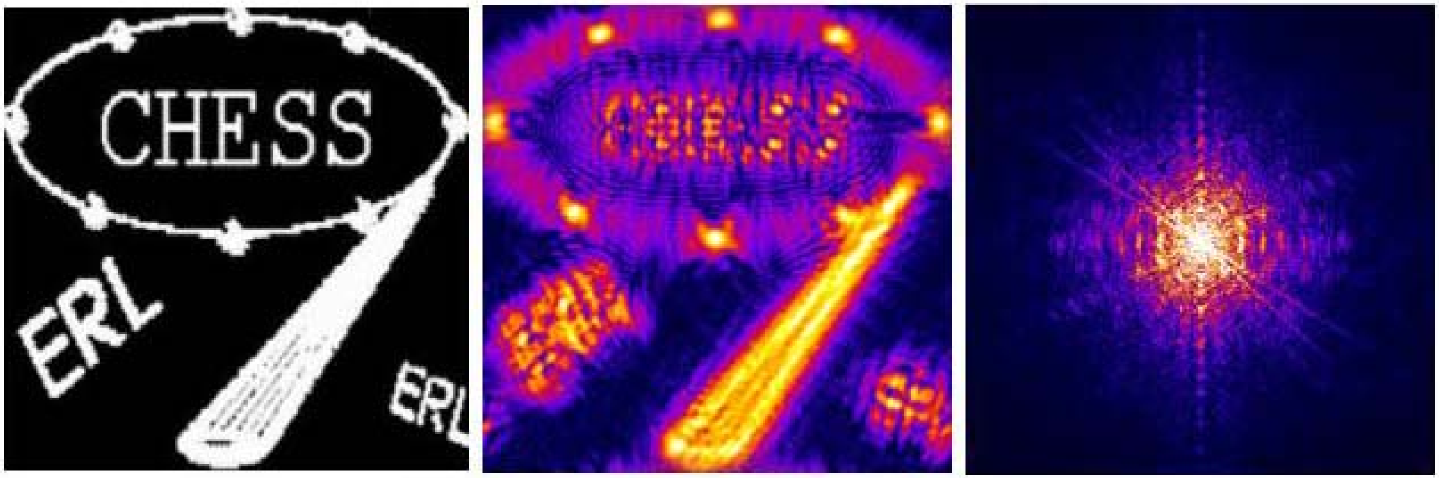
⇒ **Unified wave propagation method by Fourier transform**

Momentum transfer: $(Q_x, Q_y) = (kX/z, kY/z)$

Number of Fresnel zones: $N_z = a^2/(\lambda z)$

Xiao & Shen, PRB 72, 033103, July 2005.

Example of Distorted Object Approach



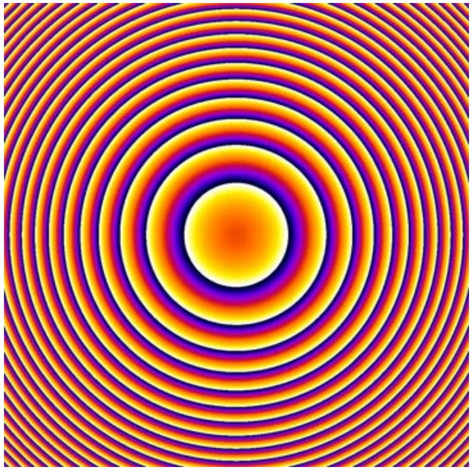


Fig.2: Simulated diffraction amplitudes $|F(X,Y)|$, of an amplitude object (a) of 10μm x 10μm, with $\lambda = 1$ Å x-rays, at image-to-object distance (b) z = 2mm and (c) z = ∞, using the unified distorted object approach (above) with $N_z = 500$ zones in (b) and $N_z = 0$ in (c). Notice that the diffraction pattern changes from noncentrosymmetric in the near-field (b) to centrosymmetric in the far-field (c).

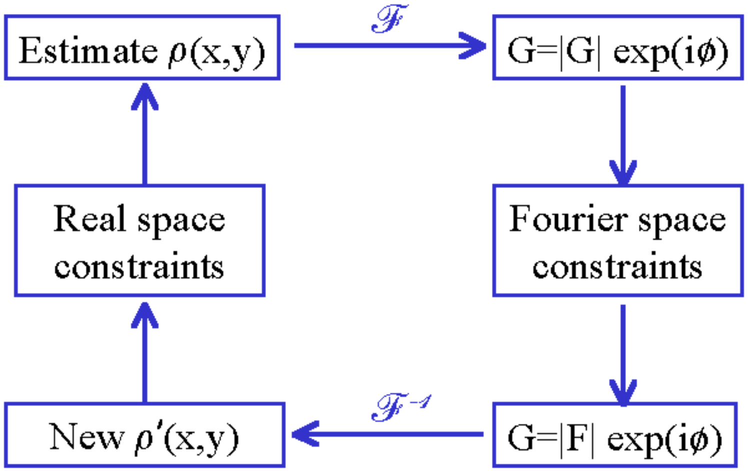
Xiao & Shen, PRB 72, 033103, July 2005.

Iterative Method in Far-field Diffraction

Gerchberg & Saxton, Optik 35, 237 (1972)

Fienup, Appl. Opt. 21, 2758 (1982)

$$\rho(x,y) \xleftrightarrow{\mathscr{F}} F(u,v) = |F(u,v)|\ \exp[i\phi(u,v)]$$



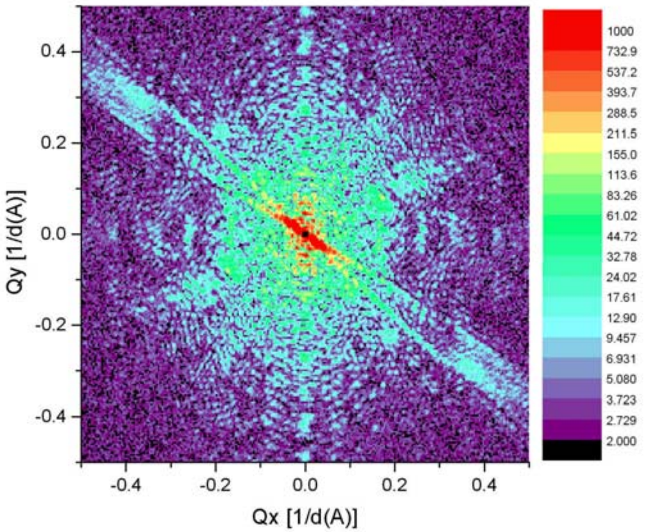
Estimate $\rho(x,y)$ $\xrightarrow{\mathscr{F}}$ $G=|G|\ \exp(i\phi)$

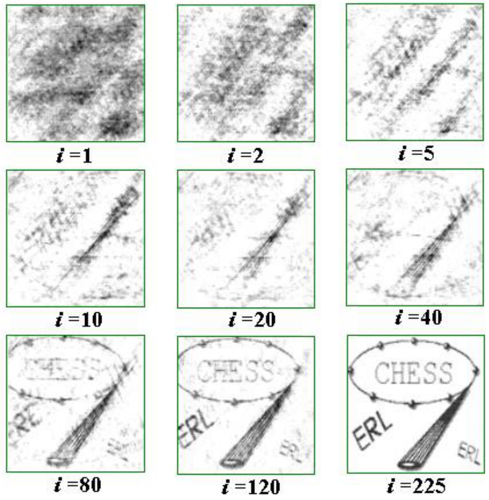
Fourier space constraints

$G=|F|\ \exp(i\phi)$ $\xrightarrow{\mathscr{F}^{-1}}$ New $\rho'(x,y)$

Real space constraints

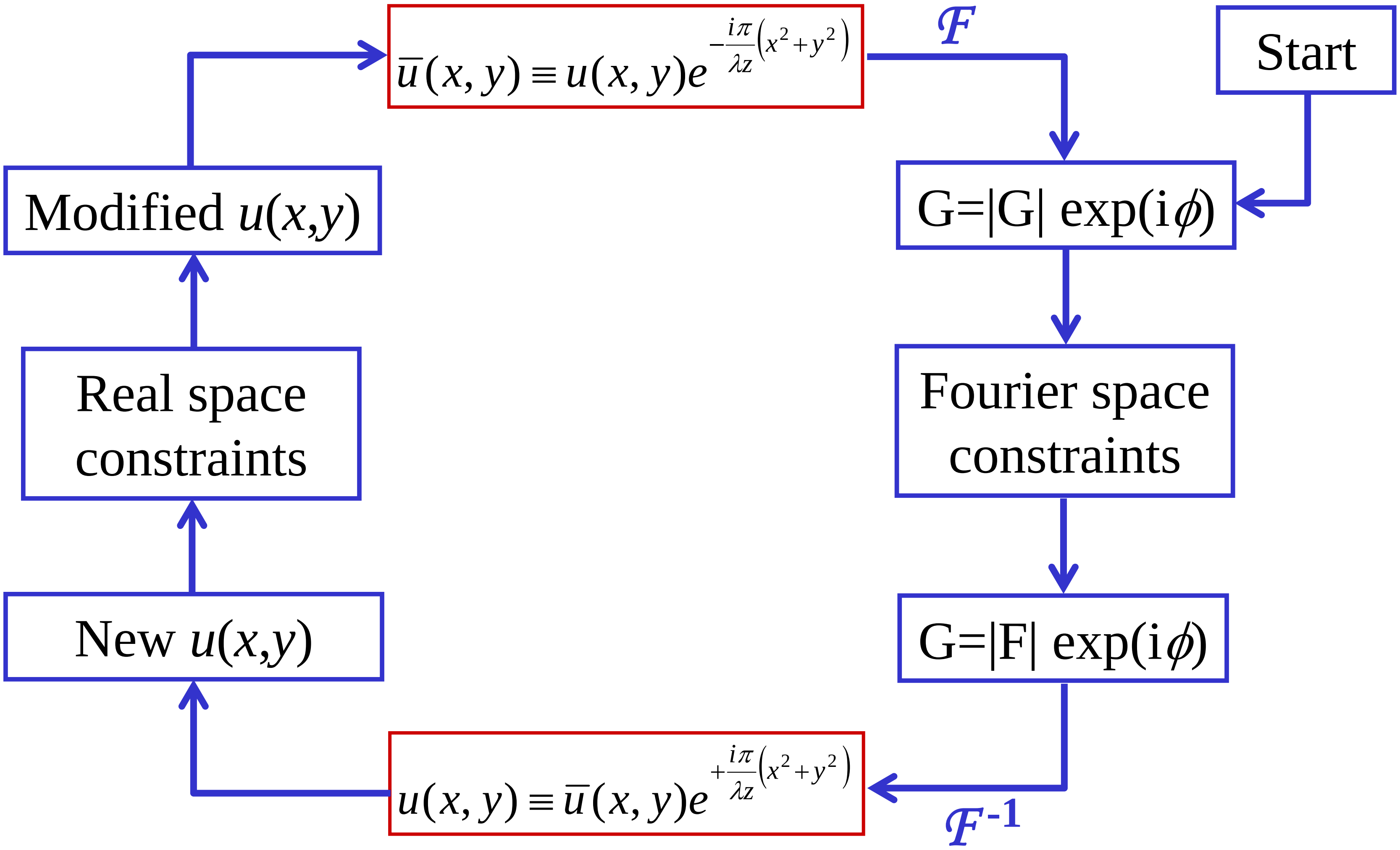
Distorted-object can extend FFT-based iterative algorithm to near-field





Shen et al, JSR 11, 432 (2004)

Unified Iterative Phasing with Distorted Object



Start

G=|G| exp(iϕ)

Fourier space constraints

G=|F| exp(iϕ)

$\mathcal{F}^{-1}$

$$u(x,y) \equiv \bar{u}(x,y)e^{+\frac{i\pi}{\lambda z}\left(x^2+y^2\right)}$$

New $u(x,y)$

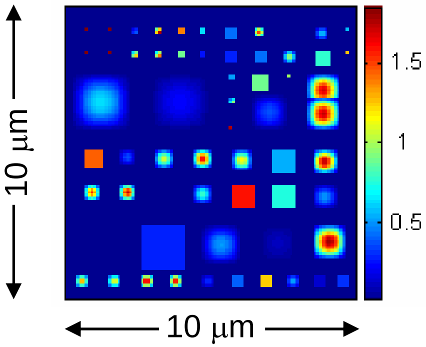
Real space constraints

Modified $u(x,y)$

$$\bar{u}(x,y) \equiv u(x,y)e^{-\frac{i\pi}{\lambda z}\left(x^2+y^2\right)}$$

$\mathcal{F}$

Numerical Simulation Example



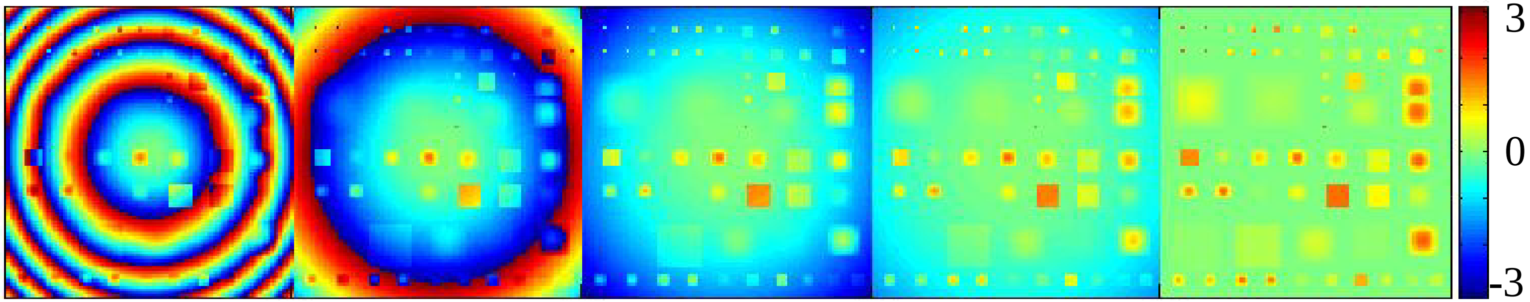
Carbon object: Maximum thickness ~10 μm;

X-ray: λ =1Å; Maximum phase difference ~1.87 rad;

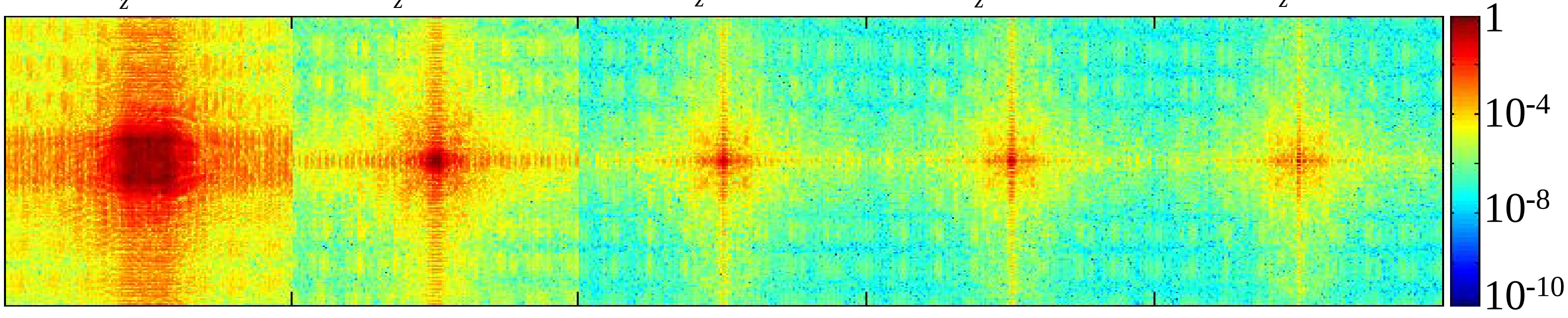
Absorption contrast ~0.1%;

Oversampling factor: 2x2;

Statistical noise included with 4.4x10^7 photons integrated.

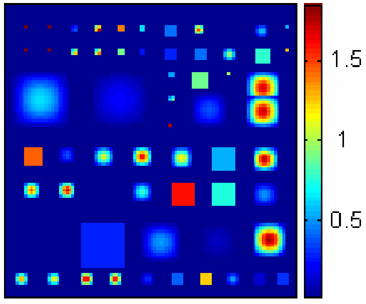


$z = 5$ cm $N_z = 5$ | $z = 20$cm $N_z = 1.25$ | $z = 50$cm $N_z = 0.5$ | $z = 100$cm $N_z = 0.25$ | $z = \infty$ $N_z = 0$

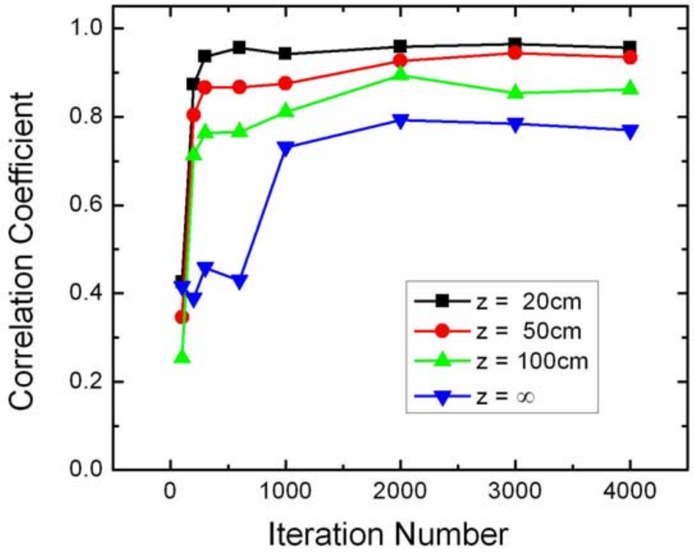


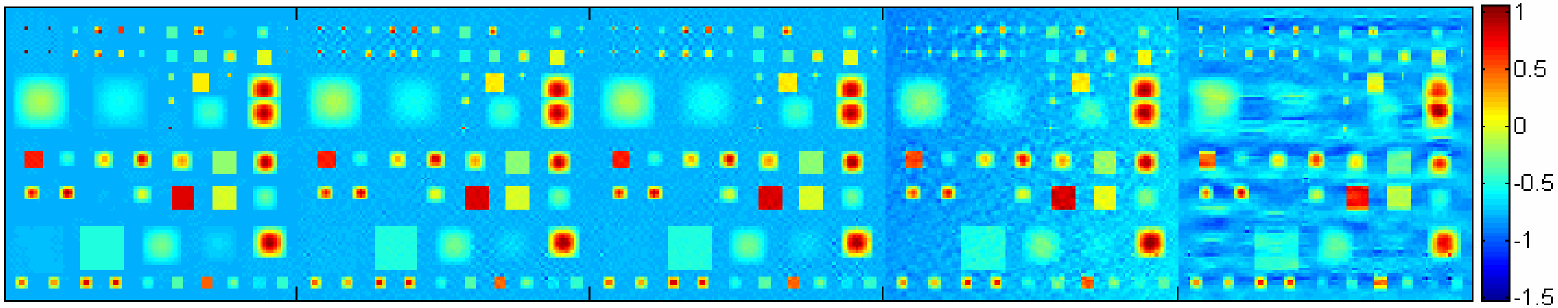
$\Delta X = 0.25$ um | $\Delta X = 1$ um | $\Delta X = 2.5$ um | $\Delta X = 5$ um | $\Delta X \propto z$

Phasing Results

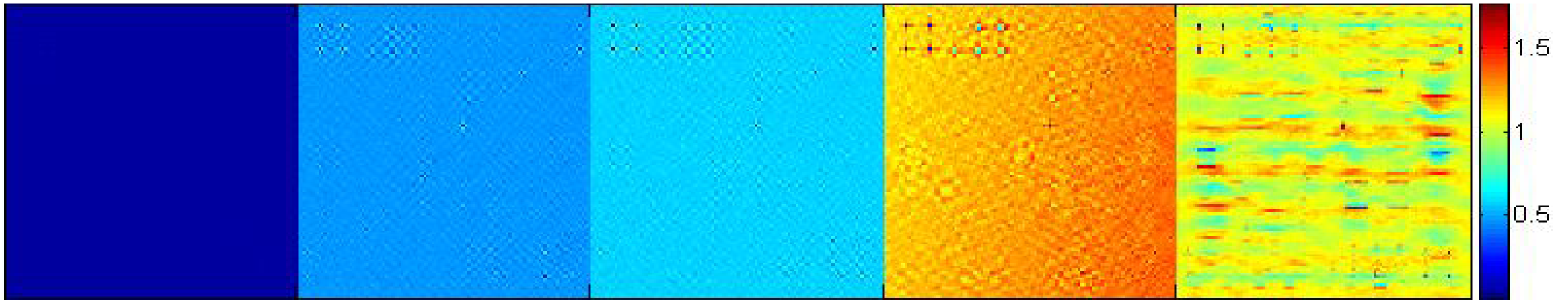


Xiao & Shen, PRB 72, 033103 (2005).





Twin image in far-field ??

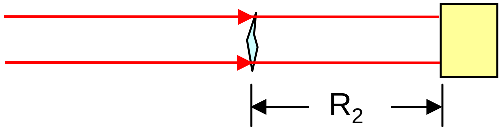


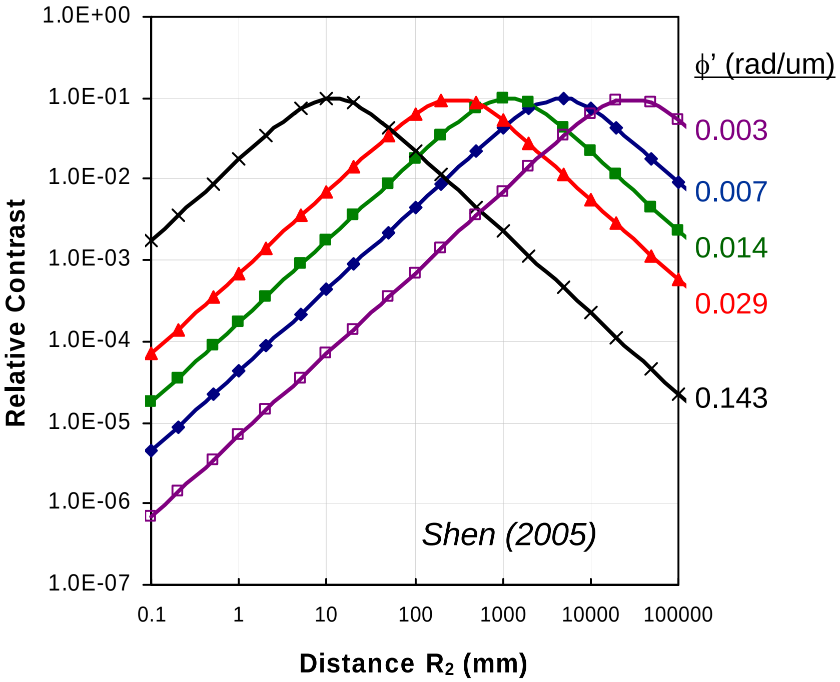
$R = 0.9998$ $R = 0.9954$ $R = 0.9943$ $R = 0.9639$ $R = 0.9248$

Other Applications of Distorted Object

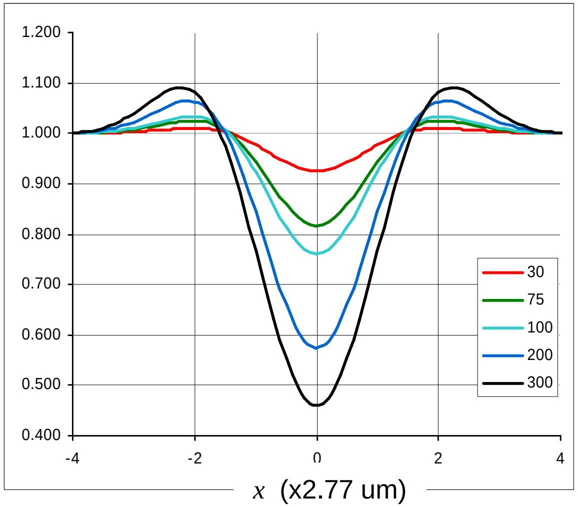
2D Gaussian phase object
→ Analytical expressions

- ❑ Phase imaging sensitivity study



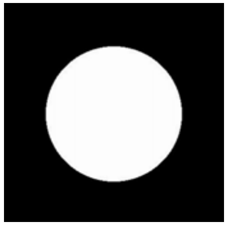


- ❑ Phase-contrast XRD topography

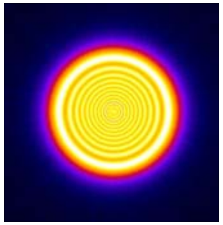


- ❑ Coherent optics & expt. design

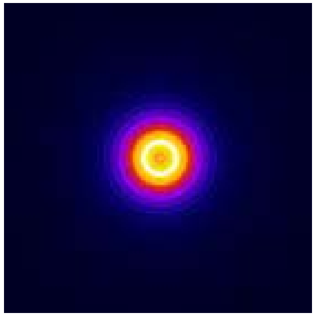
Question: Sample position in coherent diffraction experiments ?



pinhole



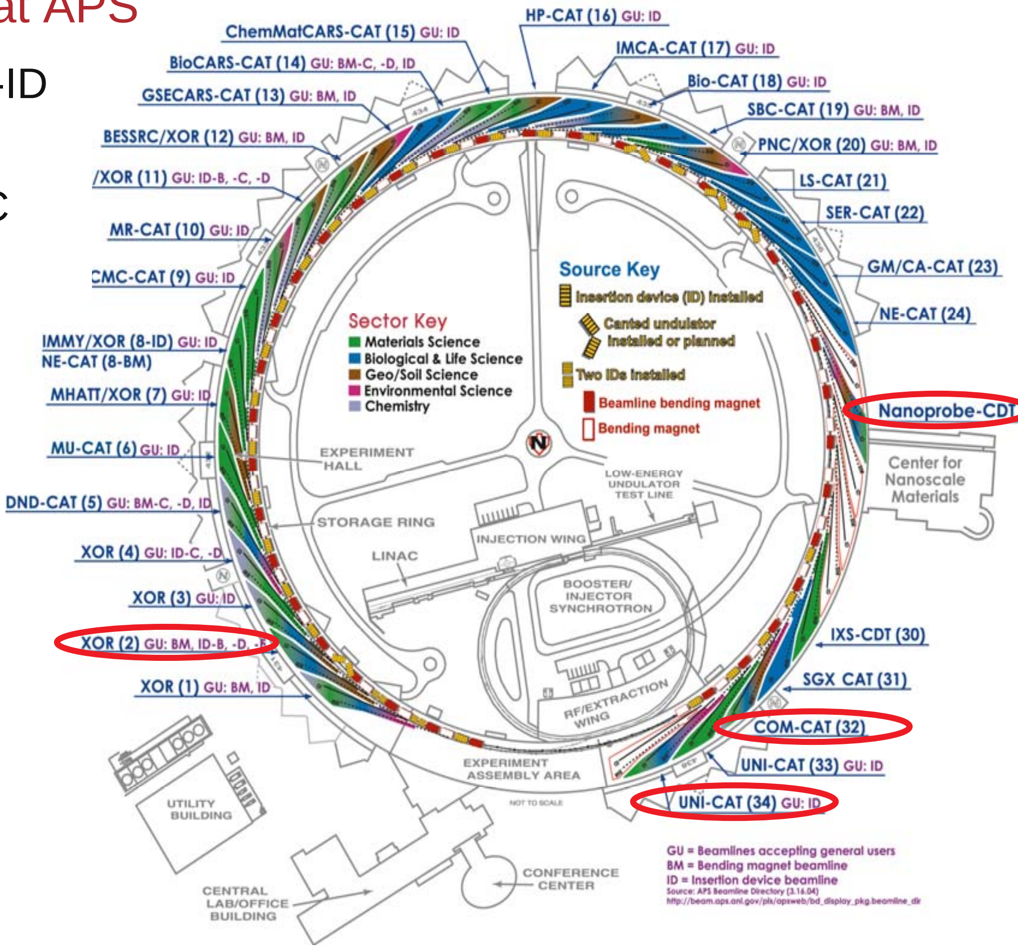
near-field ?



far-field ?

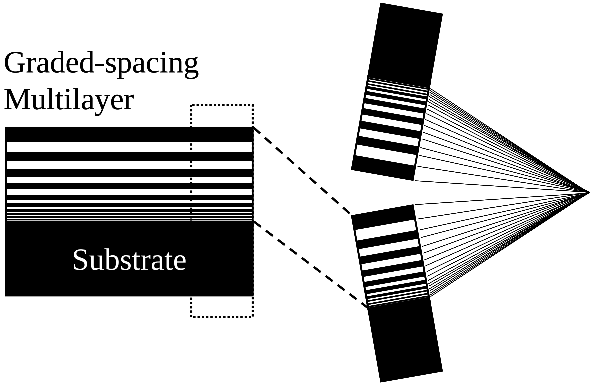
Outline

- Overview: imaging & x-rays
- X-ray microscopy & imaging group at APS
  - → Scanning x-ray microscopy: 2-ID, 26-ID
  - → Full-field x-ray imaging: 2-BM, 32-ID
  - → Coherent diffraction imaging: 34-ID-C
- Dedicated x-ray imaging beamline
  - → Phase-contrast imaging
  - → Diffraction-enhanced/USAXS imaging
  - → Full-field x-ray microscope
  - → Coherent diffraction in near-field
- Future upgrade paths
  - → 200m long beamline ?
  - → Optimized machine parameters & IDs
  - → R&D activities
- Summary

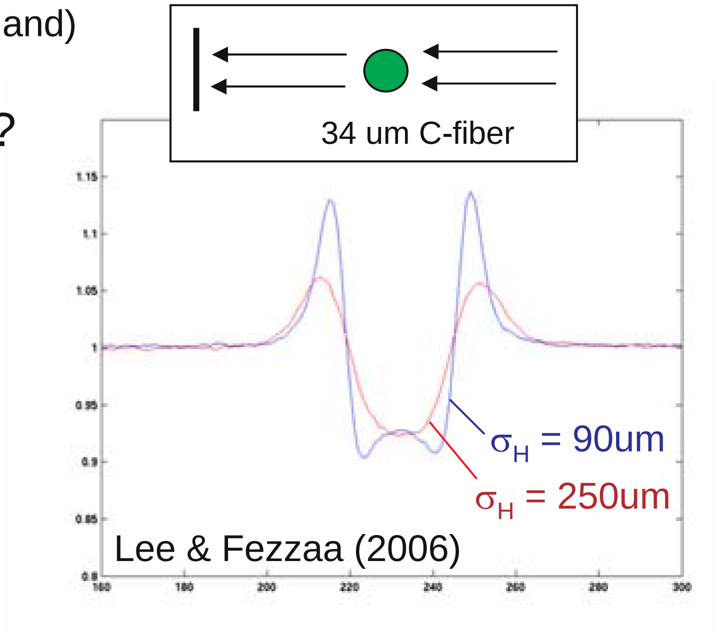


R&D Activities in X-ray Microscopy & Imaging

- Low-β machine lattice: better coherence (M. Borland)
- Multilayer zone plate: x-ray focusing to few nm?

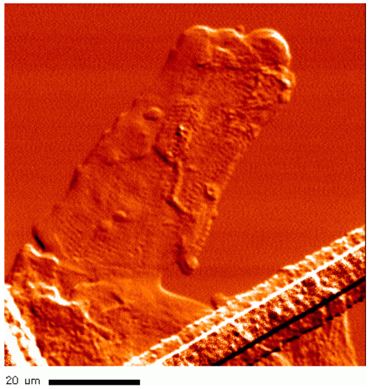


Maser, Macrander, Stephenson, et al. (2006)



Lee & Fezzaa (2006)

- Differential phase contrast: simultaneous XRF & phase-contrast imaging → XRF tomography?



Vogt, Jacobsen, et al.

Summary

- X-ray Microscopy & Imaging is an exciting research field with many on-going and potential applications, in both scanning x-ray microscope and full field imaging areas.
- Dedicated X-ray Imaging Sector at APS will offer a range of advanced x-ray imaging tools for studies such as real-time biomechanics and physiology in small animals, ultrafast imaging of fuel sprays and fluid dynamics, defect formation and propagation in engineered materials, etc.
- Research and Developments aim to push the envelope in several technology areas, such as coherent focusing optics, phase contrast mechanisms, and accelerator improvements, promising an exciting future in x-ray imaging at APS.

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Thank You !