Argonne NATIONAL LABORATORY

Scientific Opportunities with Improved Coherence and Imaging at APS

Qun Shen, Alec Sandy, Wah-Keat Lee
Advanced Photon Source

- *Two planning meetings: June 15 & July 11*
- *Coherent & phase contrast imaging*
- *X-ray photon correlation spectroscopy*
- *New opportunities with APS upgrade*
- *ERL – exciting prospects !*

Planning Meetings on Coherence/Imaging

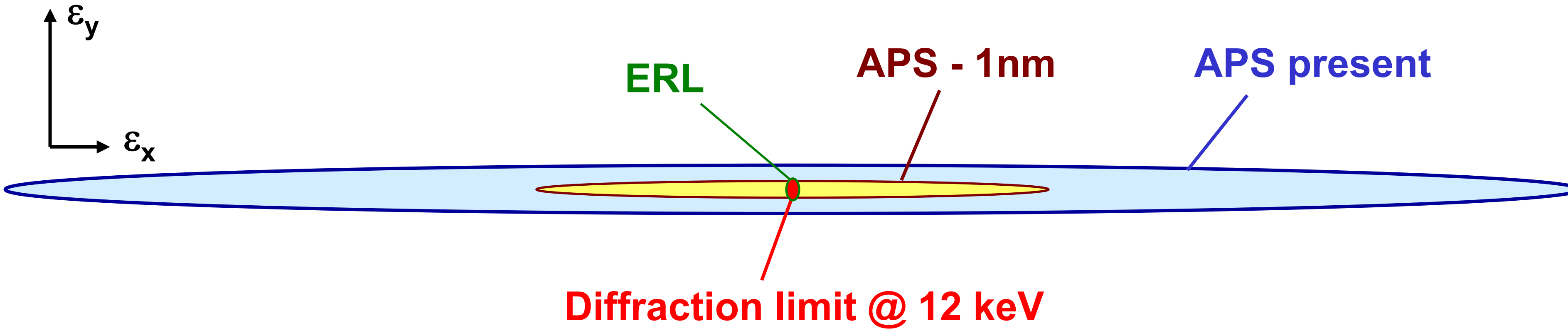
Tuesday, July 11, 2006	
1:30–1:35 pm	Introduction – **Alec Sandy, Advanced Photon Source**
1:35–2:00 pm	Possible technical specifications for an upgraded APS storage ring **Michael Borland, Advanced Photon Source**
2:00–2:25 pm	How x-ray intensity fluctuation spectroscopy can push the boundaries of materials science **Mark Sutton, McGill University**
2:25–2:50 pm	Coherent diffraction plans for Diamond **Ian Robinson, University College London and Diamond Light Source**
2:50–3:10 pm	Prospects for x-ray photon correlation spectroscopy on biological materials in water **Larry Lurio, Northern Illinois University**
3:10–3:30 pm	Break
3:30–3:55 pm	Coherent diffraction imaging: APS upgrade and future prospects **Qun Shen, Advanced Photon Source**
3:55–4:15 pm	If I had a trillion photons: coherent flux and new possibilities in quantum dynamics **Oleg Shpyrko, Center for Nanomaterials**
4:15–4:40 pm	A long imaging beamline: scientific and technical aspects **Wah-Keat Lee, Advanced Photon Source**
4:40–4:50 pm	Prospects for studying surface dynamics at an upgraded APS **Michael Sprung, Advanced Photon Source**
4:50–5:05 pm	Fluctuation x-ray microscopy – future perspectives **Lixin Fan, Advanced Photon Source**
5:05–5:30 pm	Discussion

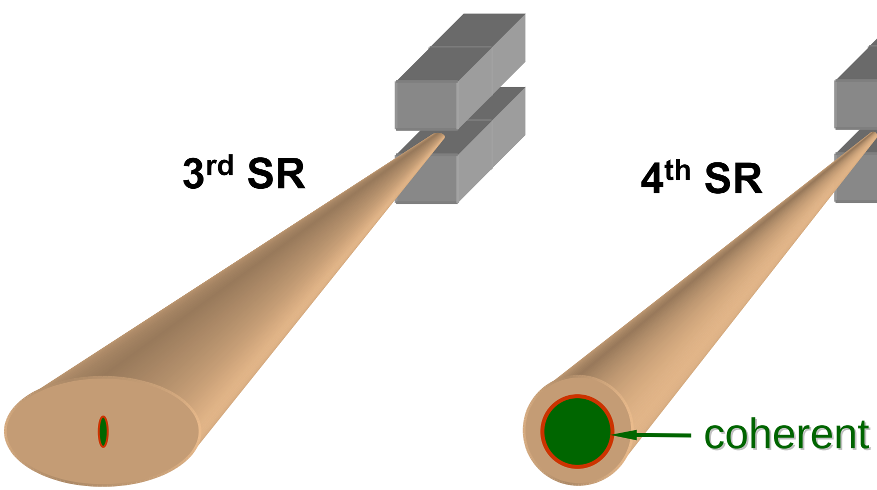
Other Communications

Simon Mochrie (Yale)
Sunil Sinha (UCSD)
Jyotsana Lal (IPNS, ANL)
Steve Wilkins (CSIRO)
Keith Nugent (Melbourne)
John Miao (UCLA)
John Spence (Arizona State)
Chris Jacobsen (Stony Brook)
Ben Larson (ORNL)
Jon Tischler (ORNL)
Veit Elser (Cornell)
Linda Young (ANL-CHM)
Brian Stephenson (ANL-MSD)
Eric Isaacs (ANL-CNM)
Paul Fenter (ANL-CHM)
Yukwang Hwu (Taiwan)
Giorgio Margaritondo (EPFL)
Kyeong Ook Lee (ANL-CTR)
Mark Westneat (Field Museum)
Jon Harrison (Arizona State)
Elaine Backus (USDA)
Melina Hale (Chicago)
David Hung (Visteon Corp.)
… …

X-ray Source Properties with APS Upgrade

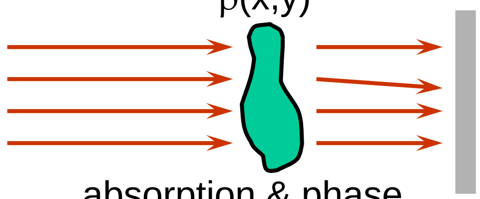
Transverse properties:





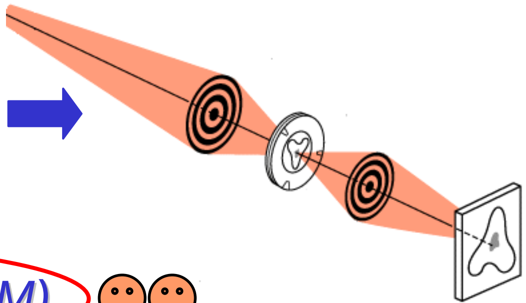
- Substantial portion of undulator central cone is spatially coherent
- Ideal source for coherent diffraction, imaging, and nanofocusing

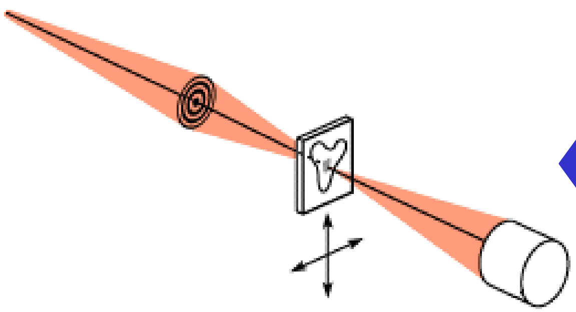
X-ray Imaging and Coherence



Direct imaging (radiography)

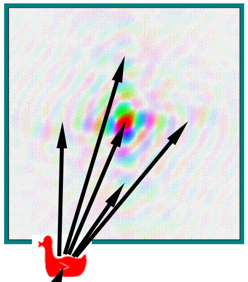
Transmission microscope (TXM)

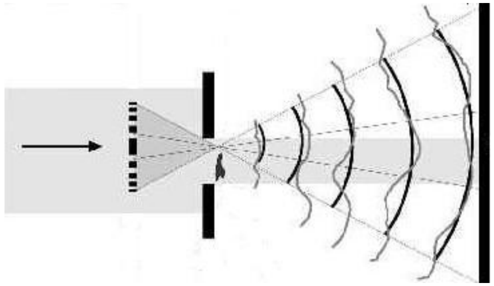




Scanning microscope (SXM)

Far-field diffraction

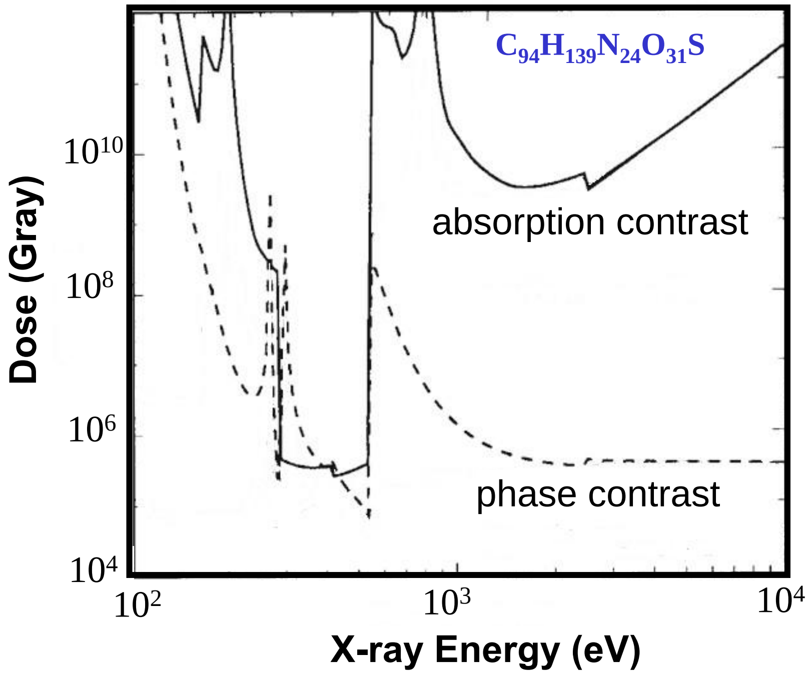




Holography

XPCS: photon correlation spectroscopy

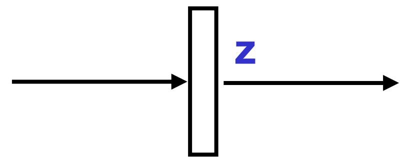
Phase Contrast vs. Absorption Contrast Imaging



Kirz (1995): *0.05μm protein in 10μm thick ice*

Refraction index:

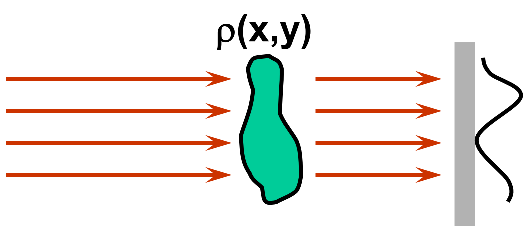
$$n = 1 - \delta - i\beta$$



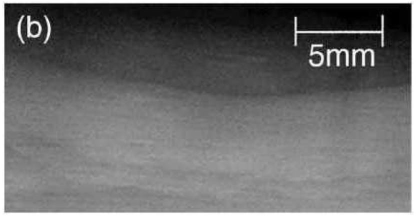
- **Phase contrast is 10^3-10^4x greater than absorption contrast for hard x-rays**
- **Phase contrast imaging may lead to reduction of dose required**

⇒ ***Absorption contrast:***

$$\mu z = 4\pi\beta z/\lambda \sim \lambda^3$$

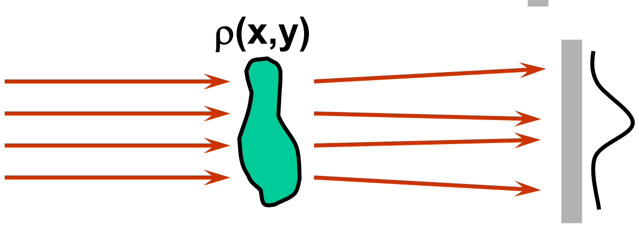


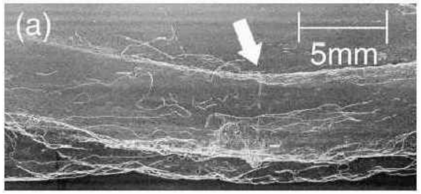
Mori et al. (2002): broken rib with surrounding soft tissue



⇒ ***Phase contrast:***

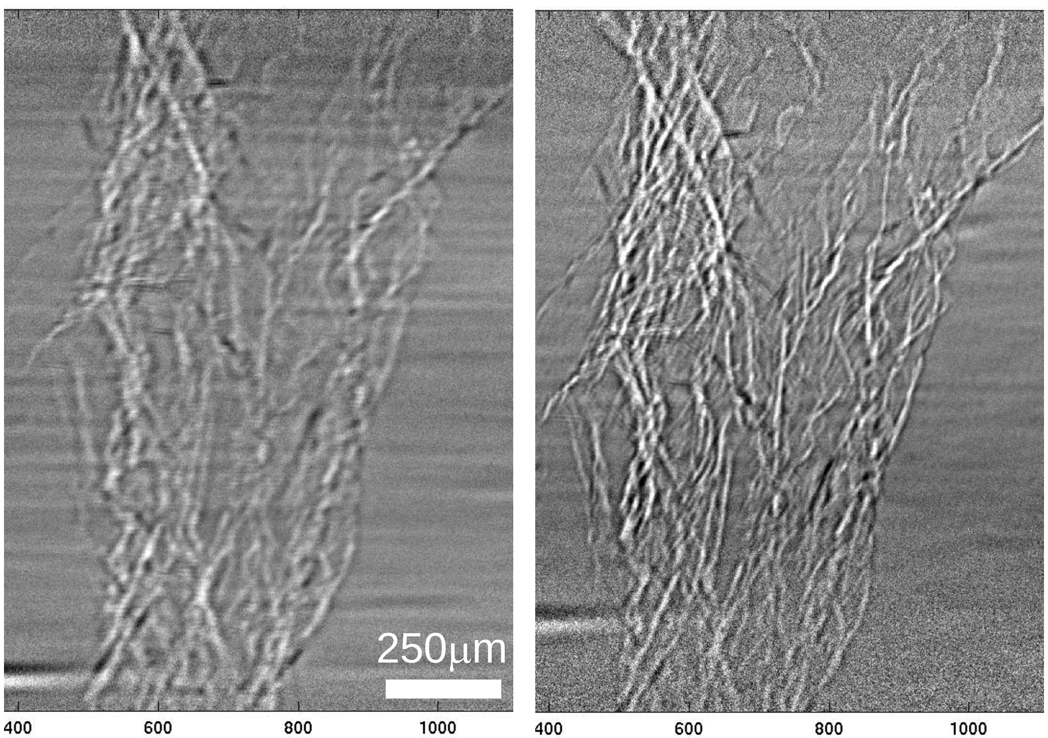
$$\phi(z) = 2\pi\delta z/\lambda \sim \lambda$$

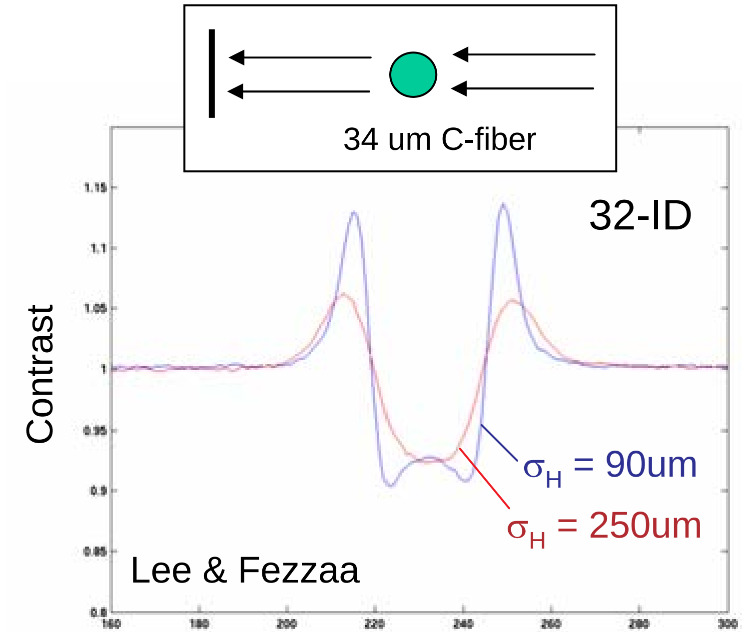




Phase-Contrast Imaging (PCI) ➔ Local Coherence

- ***<u>Small source size</u> with APS upgrade would greatly enhance observable phase contrasts for weak density differences***



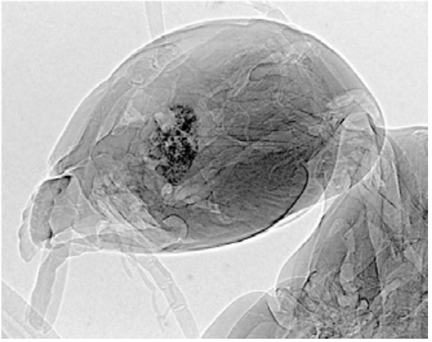


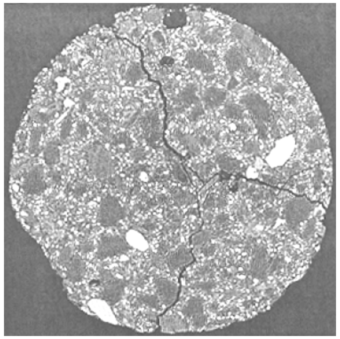
🡐 Stress cracks in Aluminum
t = 3 mm, 30 keV, D = 1m

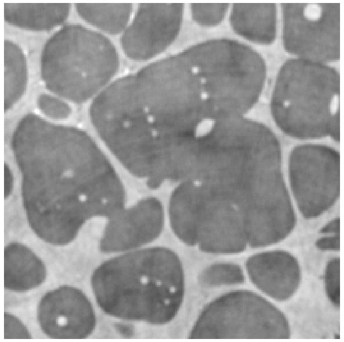
PCI Applications in Materials Science and Biology

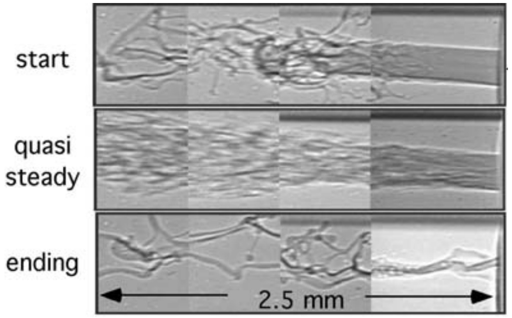
APS Strategic Planning Workshop on X-ray Imaging (2004)

- fracture mechanics of composites and biomaterials
- materials deformation and sintering
- bone and cartilage growth and formation
- small animal and soft tissue research
- vascular and pulmonary functions
- structure and development of plant seeds
- geological structures and microfossils
- cement mortar curing
- structure and development of metal and polymer foams
- granular packing of non-equilibrium systems
- time-resolved studies of internal complex fluid flow and sprays
- in-situ observation of chemical reactions
- shock-wave propagations

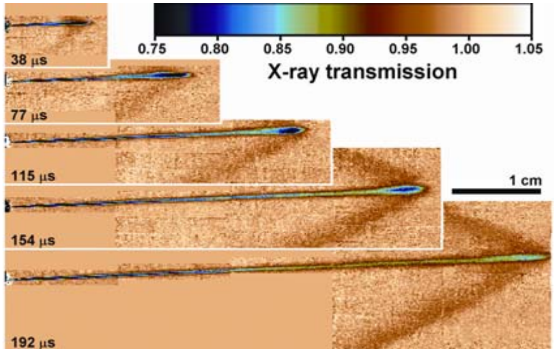


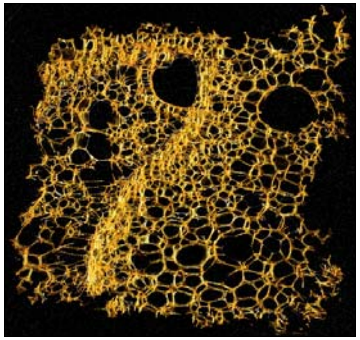






X-ray flash imaging @ 300ns!



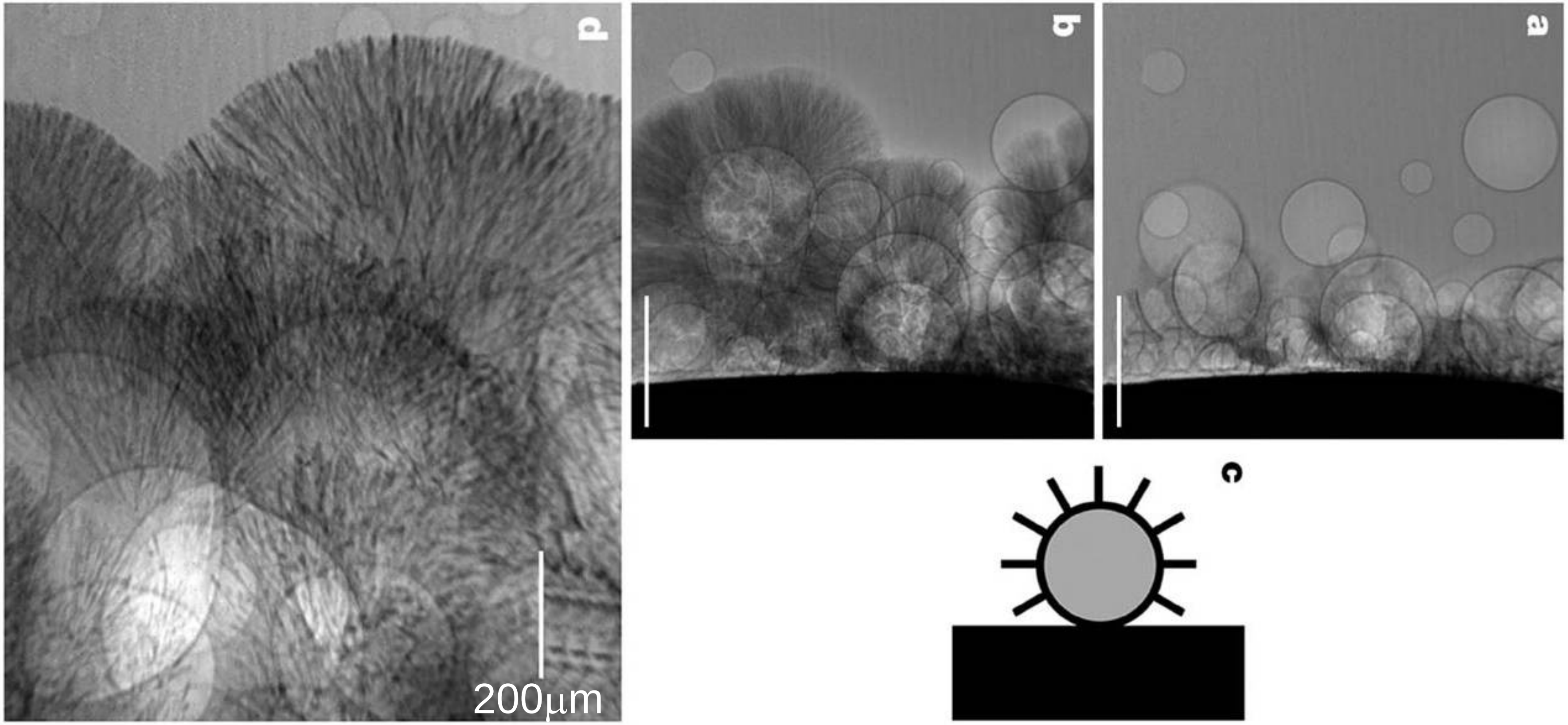


In-situ X-ray Imaging of Electrodeposition

Tsai et al, "Building on bubbles in metal electrodeposition", Nature 417, 139 (2002)

In the electrodeposition of metals, a widely used industrial technique, bubbles of gas generated near the cathode can adversely affect the quality of the metal coating. Phase-contrast imaging is used to witness directly and in real time the accumulation of zinc on hydrogen bubbles.

Pohang Light Source

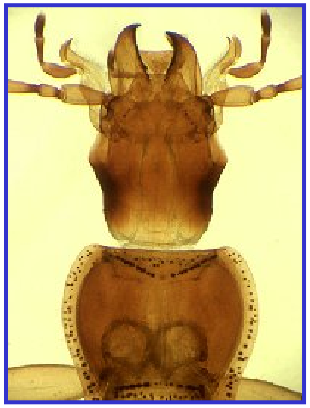


Phase Contrast Imaging with APS Upgrade

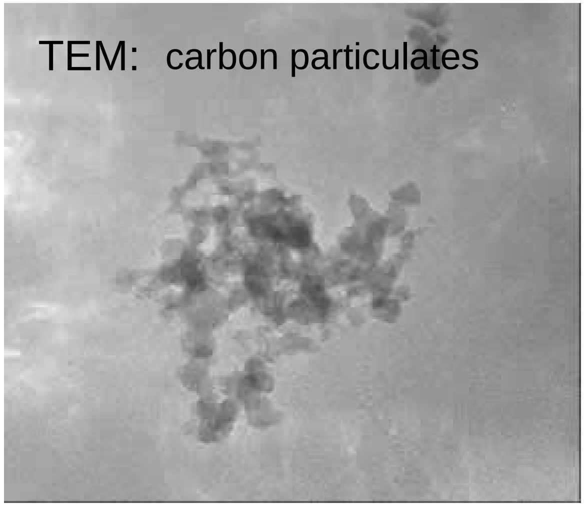
- ***In-situ real-time imaging of low-contrast materials processing and depositions, e.g. formation of carbon particulates in engines, polymer aggregates and polymer thin-film coatings***

- ***Time-resolved imaging at few-ps temporal resolution with sub-μm microscopic details, e.g. nanoparticles in chemical reactions, limited only by sound velocity ~ 1 nm/ps***

- ***Biological imaging of soft tissues, small animal physiology, and biomechanics with much enhanced contrasts for hard-to-detect internal features***



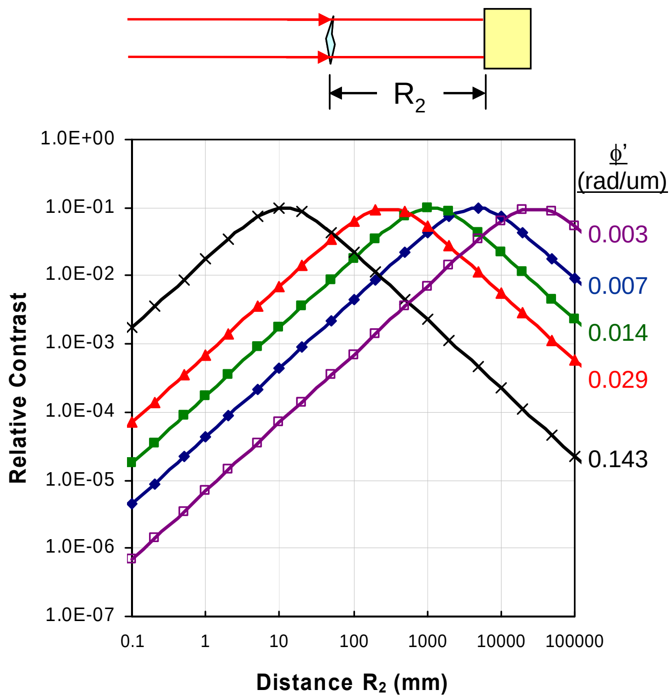
wood beetle

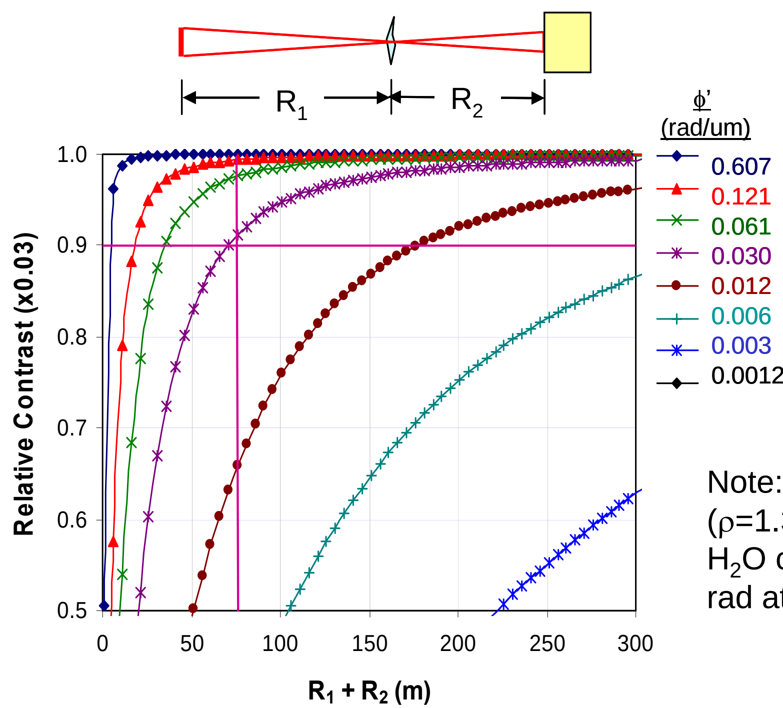


Phase Contrast Imaging Wish List

Wah-Keat Lee (APS)

- Small round source size (< 50 μm FWHM) – ERL would be great!
- Larger vertical beam size (electron tumbling?)
- BEAM STABILITY!! Currently ~0.5 μrad fluctuations at 50-200 Hz
- Long beamline (>150m) for weak phase objects & larger field of view
- Efficient area detectors with fast readout & small pixels
- Coherence preserving x-ray optics

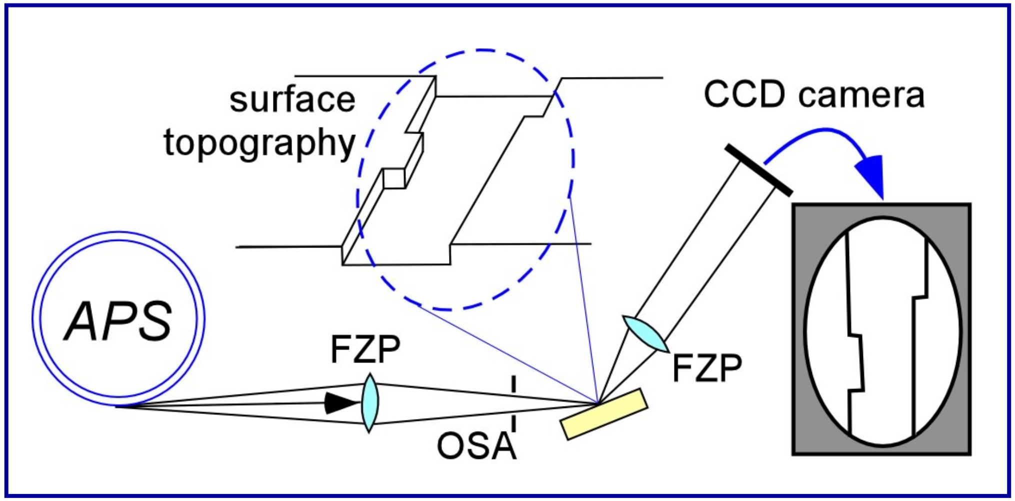




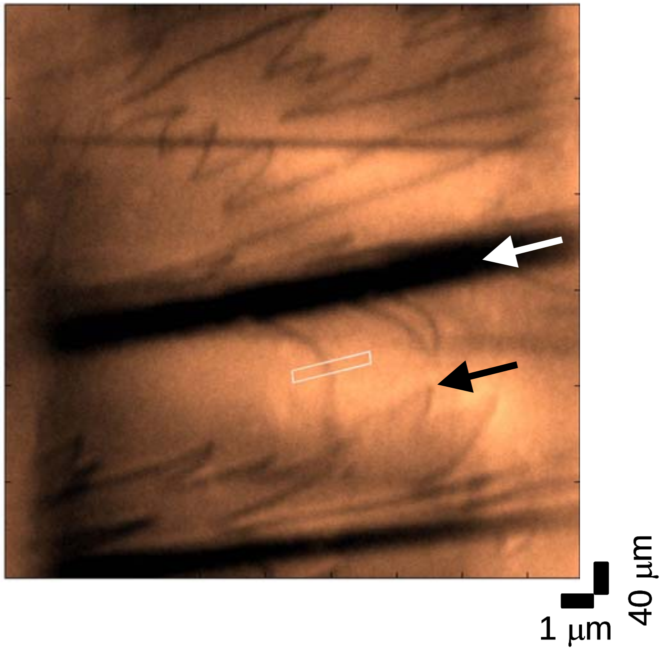
Note: 3um thick biomatter (ρ=1.35) in 30um thick H_2O corresponds to ~0.03 rad at λ = 1 A

Phase-Contrast X-ray Diffraction Microscopy

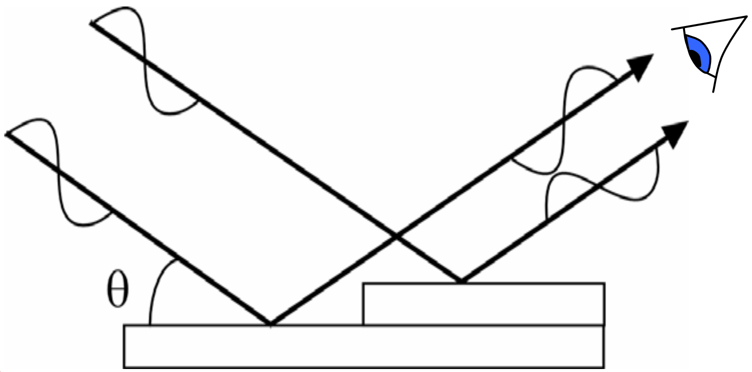
*P. Fenter, C. Park, Z. Zhang, and S. Wang, submitted (2006)



Step distributions on $KAlSi_3O_8$ (001)

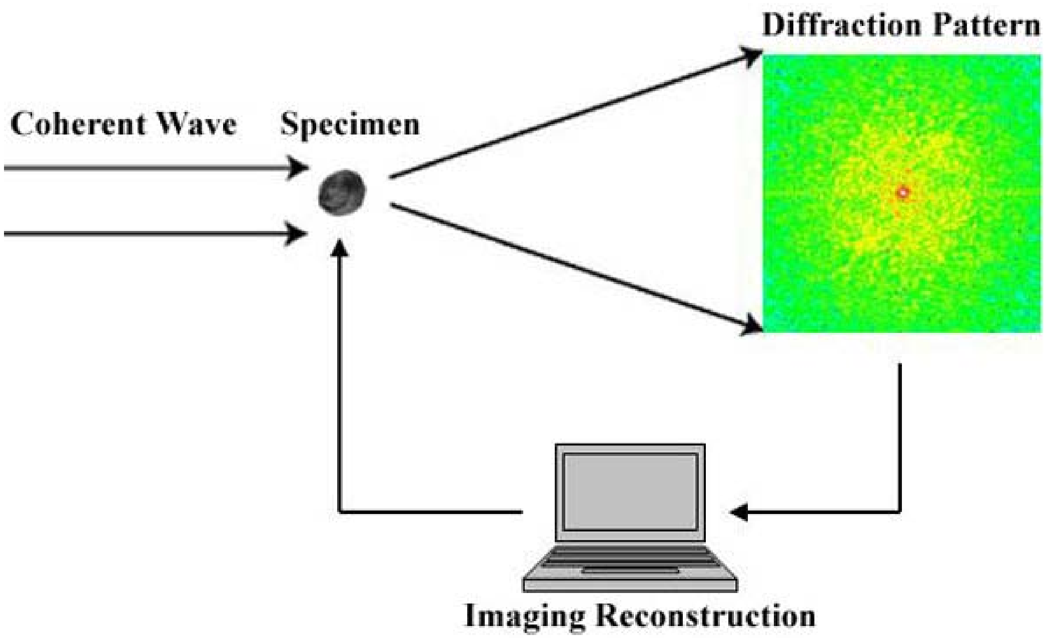


X-ray Reflection Interface Microscopy



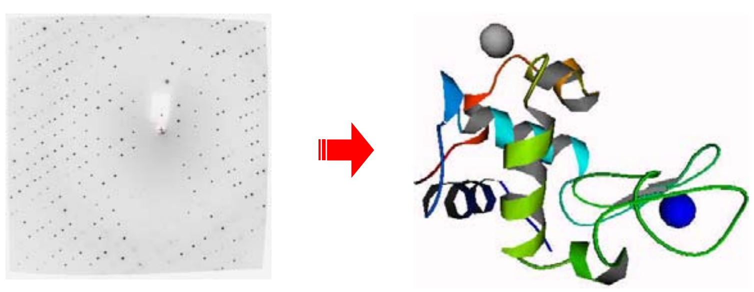
Non-invasive structural tool (no probe tip):
- reactions in aggressive chemical conditions
- extreme pH, corrosive gases
- elevated temperature
- buried interfaces
- in-situ, real-time observations of interfacial reactions at nm scale

Coherent X-ray Diffraction Imaging

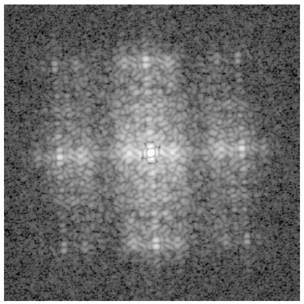


- Coherent diffraction imaging is much like crystallography but applied to noncrystalline materials
- First proposed by David Sayre in 1980, and first experimental demonstration by John Miao et al in 1999 using soft x-rays
- Requires a fully coherent x-ray beam

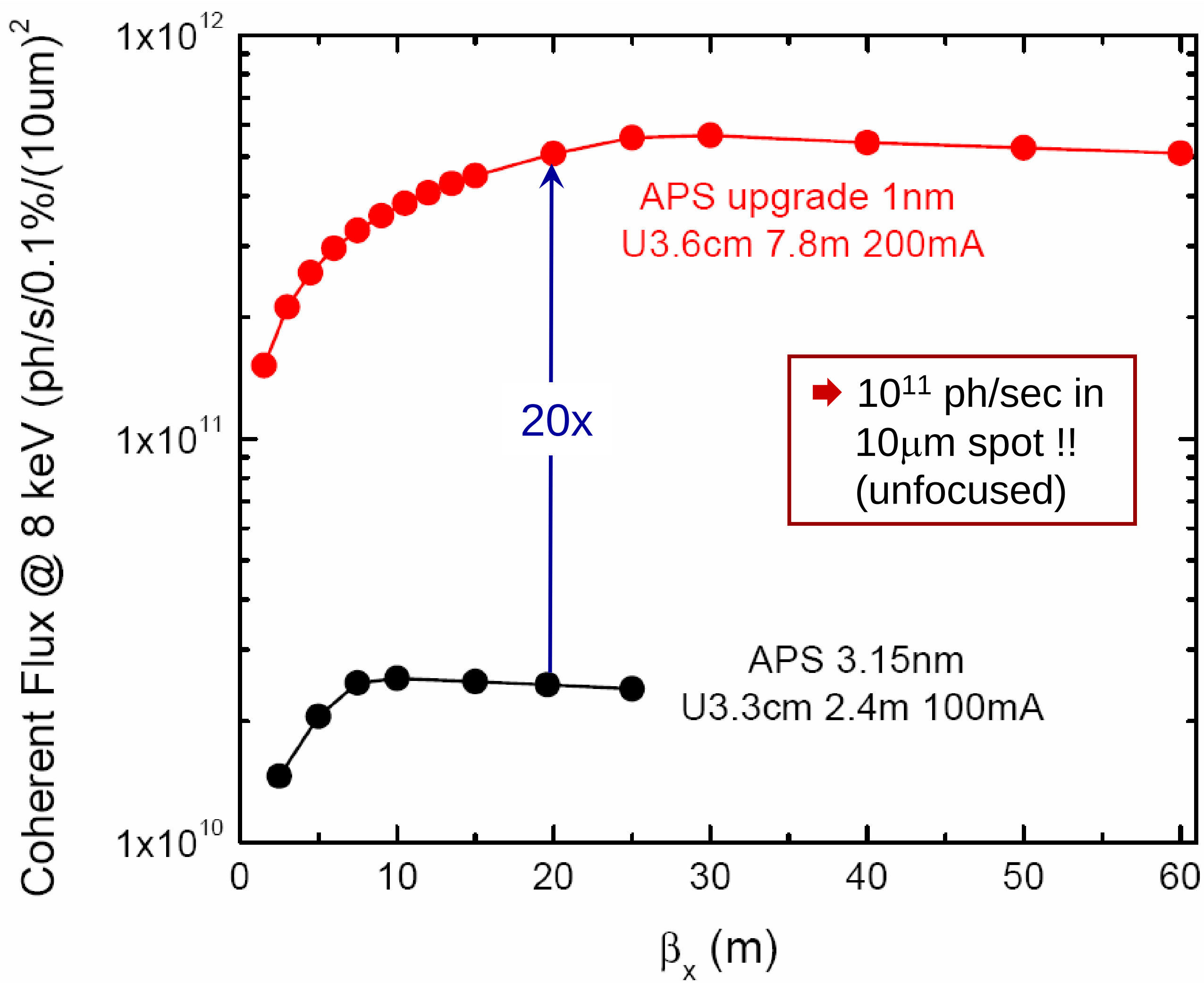
Analogous to crystallography



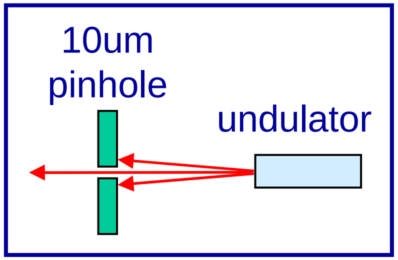
Miao et al. (1999)



Effects of APS Upgrade on Coherent Diffraction



- 10^{11} ph/sec in 10μm spot !! (unfocused)



$$\sigma_x = \sqrt{\varepsilon_x \beta_x}$$

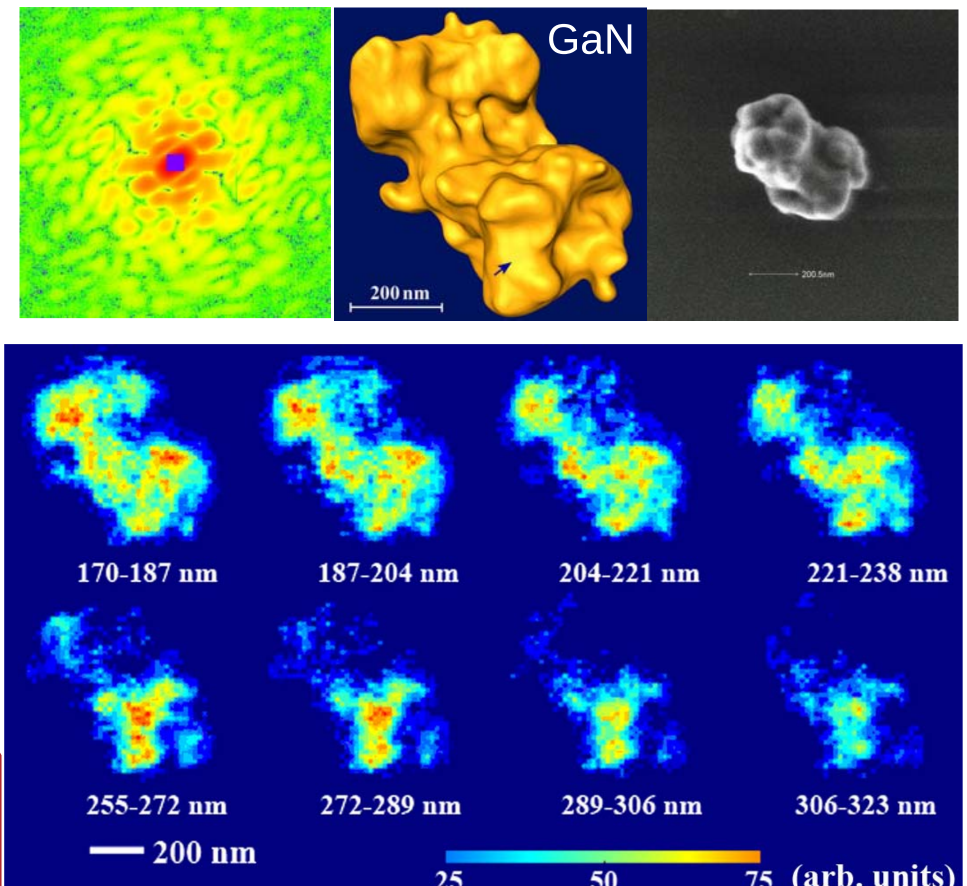
$$\sigma_{x'} = \sqrt{\varepsilon_x / \beta_x}$$

In addition:

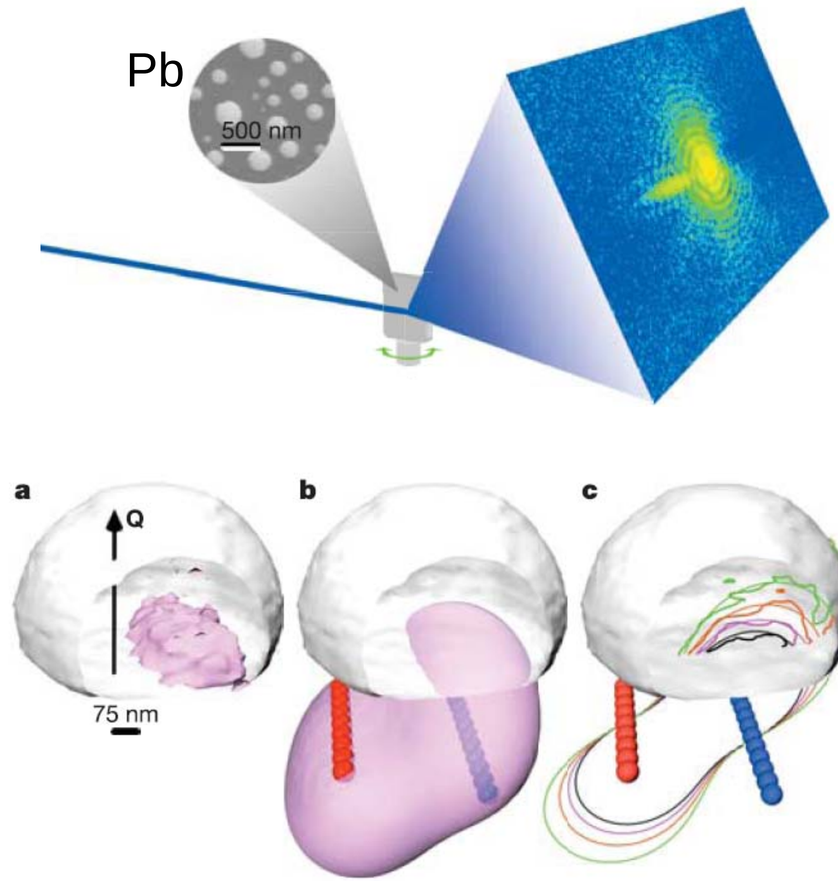
- Detectors: faster readout, high sensitivity & dynamic range
- Improve S/N by reducing background

Internal Structure and Strain of Nanoparticles

Miao et al, "Quantitative Image Reconstruction of GaN Quantum Dots from Oversampled Diffraction Intensities Alone", *Phys. Rev. Lett.* (2005)



M.A. Pferfer et al., "Three-dimensional mapping of a deformation field inside a nanocrystal", *Nature* 442, 63 (2006)



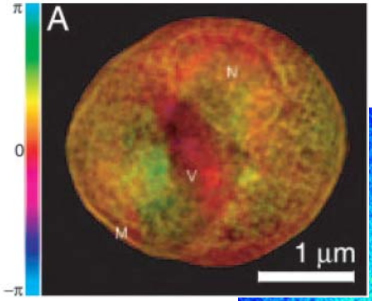
Coherent Diffraction Imaging with APS Upgrade

- ***Coherent X-ray Diffraction Imaging*** *is an exciting research field with many potential applications that would open up structural science from mostly* ***crystal-based*** *today to* ***noncrystalline*** *materials*

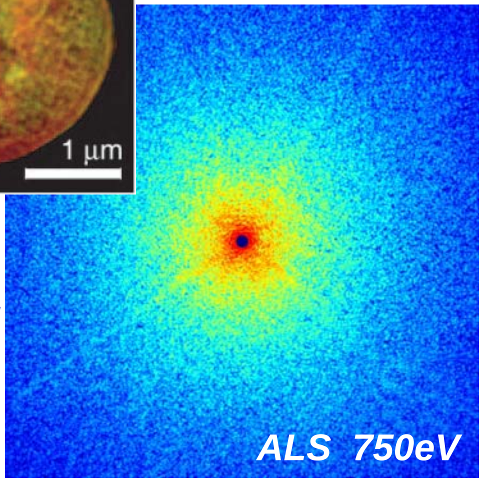
- ***Lack of intense fully coherent x-rays*** *has been one of main limitations for rapid advances in this field, along with* ***dedicated beamlines***. ***ERL @ APS*** *will change this completely.*

- ***Radiation damage*** *may limit spatial resolution to ~ few nm for biological specimens*

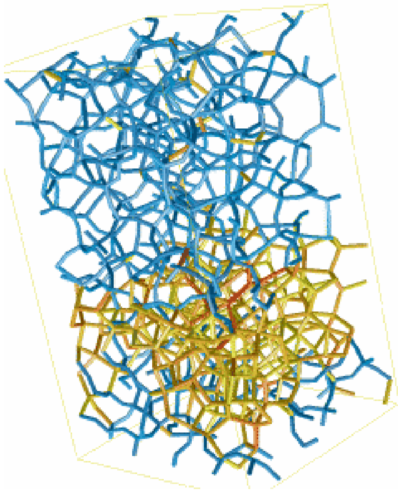
- ***Emerging Applications:***
  - -- *structure and strain in nanoparticles*
  - -- *atomic structure of amorphous materials*
  - -- *2D crystallography e.g. membrane proteins*
  - -- *few unit-cell crystals*
  - -- *subcellular organelle structures in cells*
  - -- *laser-oriented macromolecules*
  - -- *bio-organic-inorganic hybrid structures*



Shapiro et al. PNAS (2005)



Freeze-dried yeast cell: reconstructed to ~30nm



Amorphous Silicon (α-Si):

→ structure at atomic resolution?

→ one of grand challenges in solid state physics

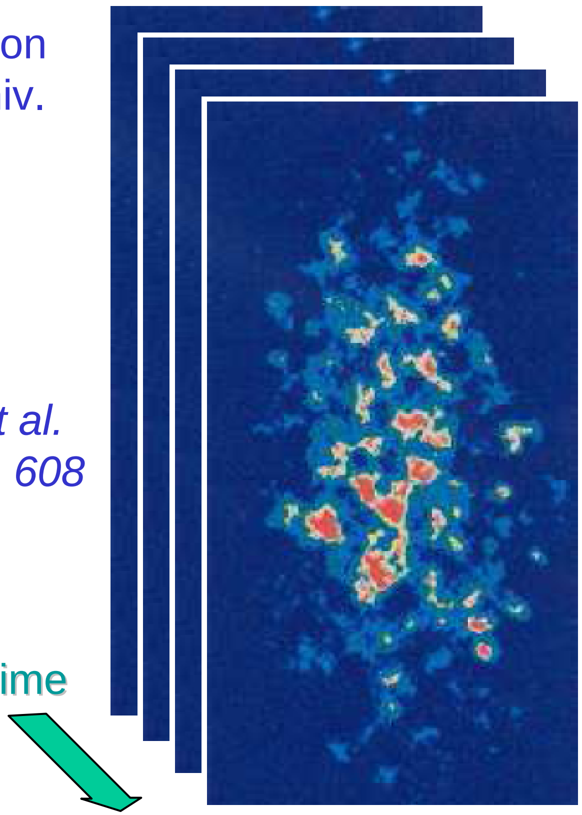
-- Veit Elser (Cornell)

Structural Dynamics by Looking at Intensity vs. Time

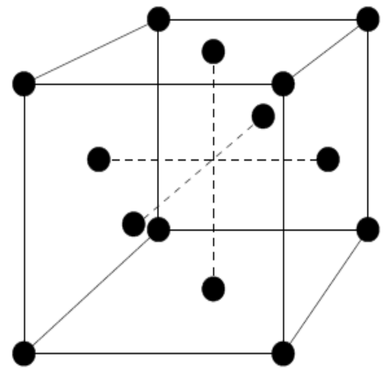
Mark Sutton
McGill Univ.

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

(001) Cu_3Au peak

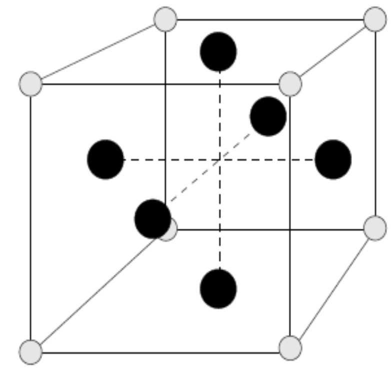


Disorder:



$f = 0.75\, f_{Cu} + 0.25\, f_{Au}$

Order:



f_{Cu}, f_{Au}

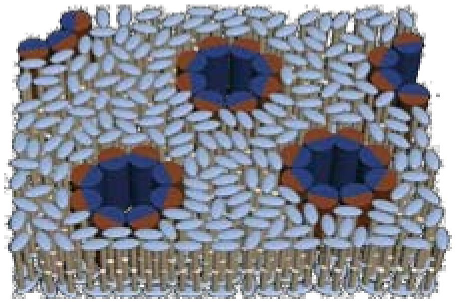
XPCS: x-ray photon correlation spectroscopy

- Fluctuating x-ray speckle yields autocorrelation decay and characteristic sample fluctuation times
  - SNR ~ Brilliance * $\sqrt{\text{(fastest time scale)}}$
  - n× increase in source brilliance → n^2× faster processes for same SNR
  - B → B × 30 (source) × 10 (focusing)
    > improves fastest times: 10 ms → 1 μs
    > overlaps slow limit of neutron spin echo

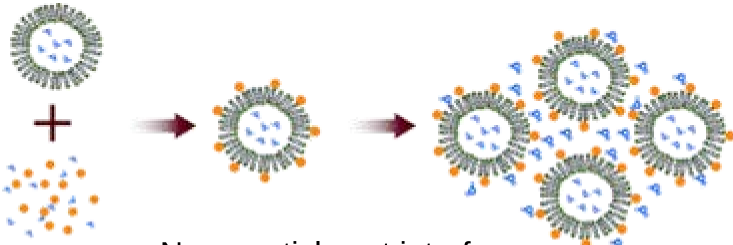
XPCS Scientific Opportunities

Alec Sandy (APS)

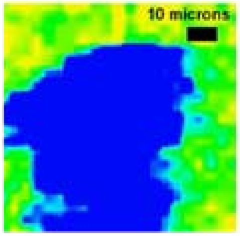
- Current: dynamics of particles in viscous solutions
  - e.g., latex, silica, gold particles in glycerol
  - Time scales: 0.1–10 s
- Dynamics of proteins in aqueous solution
  - I.e., liquid-glass transition in eye lens protein solutions
  - Time scales: 0.1–1 μs
- Dynamics of / within biological membranes in water
  - Protein diffusion within membranes
  - Lipid raft motion along membranes
  - Anti-microbial pore dynamics in membranes
  - Time scales: 1 μs–1 ms
- Nanoparticle dynamics
  - Nanoscale particle dynamics versus enhanced macroscopic physical properties
  - Nanoparticles confined to interfaces
  - Time scales: 0.1–1 μs
- Non-equilibrium dynamics
  - Micro-/nanoscale dynamics during structural evolution
    e.g. domain boundaries, grain boundaries, defects
  - Block copolymer melts under shear
  - Microscopic dynamics within flow
- Hard condensed matter
  - Magnetic: cross section $10^{-6}\times$ less than charge scattering
  - Quantum-mechanical effects in metals, alloys, oxides, …



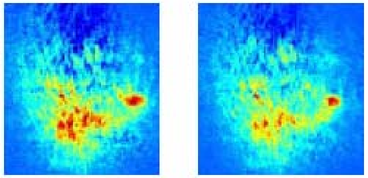
AMP Pores
(Huey Huang, Rice University, website)



Nanoparticles at interfaces
Zhang & Granick, Nano Lett. **6**, 694 (2006)



Spin domains in chromium



t   t + Δt

Shpyrko & Isaacs (CNM)

XPCS Technical Needs

Alec Sandy (APS)

- **Suitable detectors are a critical need:**

Today	Tomorrow??
Photon counting	Photon counting
≥ 10^6 pixels per chip	≥ 10^6 pixels per chip and tiling
≈ 20 μm per pixel	≈ 50–100 μm per pixel
17 ms time resolution (≈ 1 ms for small subset of pixels)	0.1 μs time resolution
Posthumous data reduction	Onboard pixel-by-pixel reduction to autocorrelation decays
50% efficient @ 7 keV	100% efficient @ 20 keV

- **Radiation damage mitigation**
  - Flow cells
  - Higher energy operations

Summary

❖ ***APS Upgrade*, particularly ERL option, is an exciting opportunity to expand well beyond the current capabilities (coherence, small round source, short pulse) to satisfy growing interests in physical & biological science communities**

❖ ***These interests* include:**
- in-situ imaging of chemical reactions and materials processing;
- imaging of internal biomechanics and physiology in small animals;
- structural studies of non-crystalline or nanocrystalline materials;
- 3D mapping of strain and grain structures & defects at nm-scale;
- flash imaging of chemical reactions and transient fluids at ps to sub-ps;
- dynamics of nanoparticles and biomacromolecules in solutions;
- domain wall fluctuations in condensed matter systems;
……

❖ ***Overall* this workgroup believes that APS upgrade, especially ERL option, would truly open up new scientific possibilities in x-ray imaging, structural science, and materials dynamics.**

Acknowledgments:

Many Thanks to all planning meeting participants and others who have provided comments and inputs through email and other forms of personal communications.

APS is supported by the U.S. DOE, BES, under Contract No. W-31-109-Eng-38.