Argonne NATIONAL LABORATORY

... for a brighter future

Research Possibilities at ANL's Large Scientific User Facilities

Presented to the ANL Postdoc lunch group, August 24th, 2007

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U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

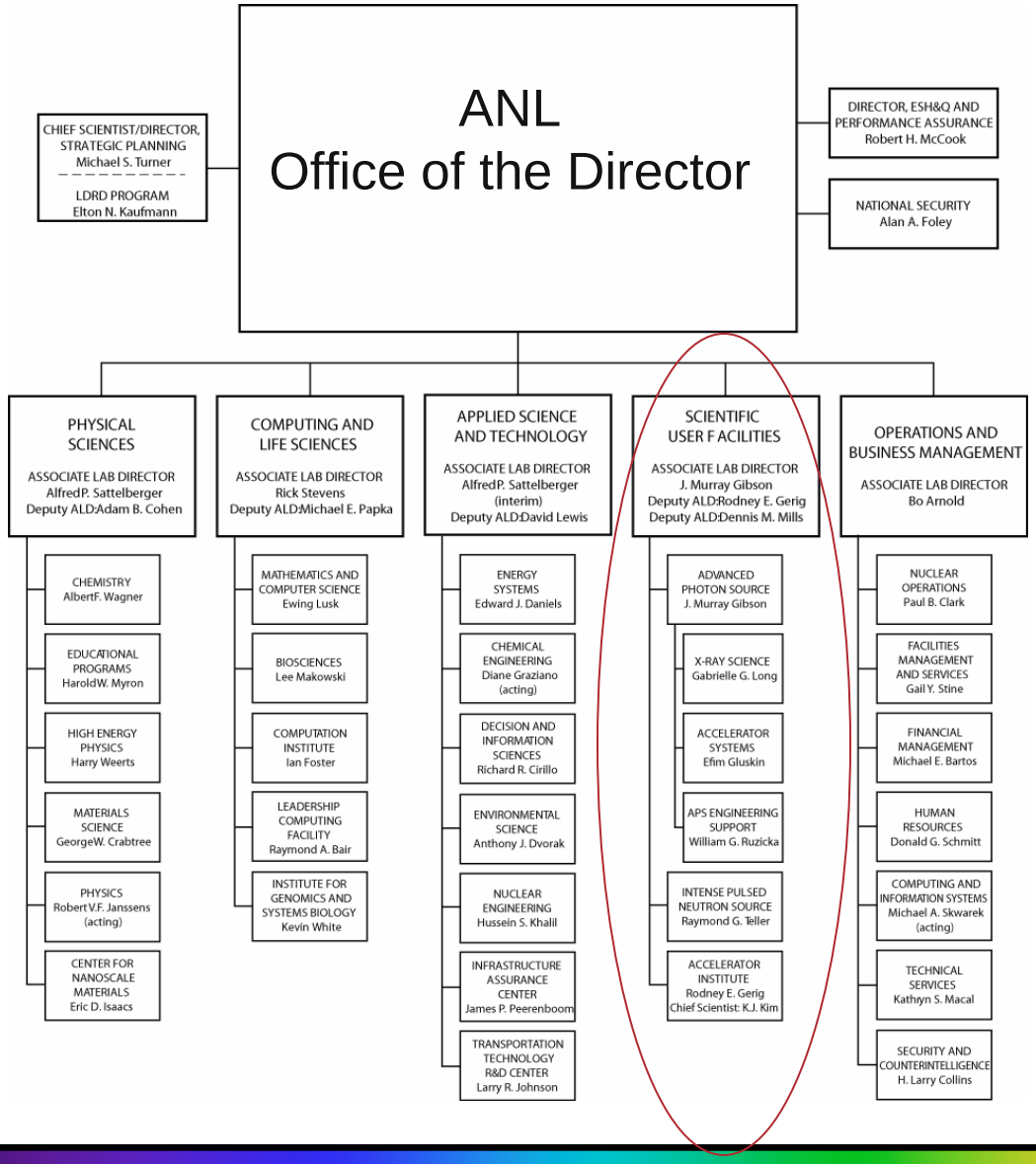
Office of Science
U.S. DEPARTMENT OF ENERGY

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

What I will try to accomplish

- Short overview of SUF
  - APS
  - IPNS
- Scientific areas of interest
- Future development plans
- Getting beam time
- Career possibilities
- Questions, discussion, career advice??..

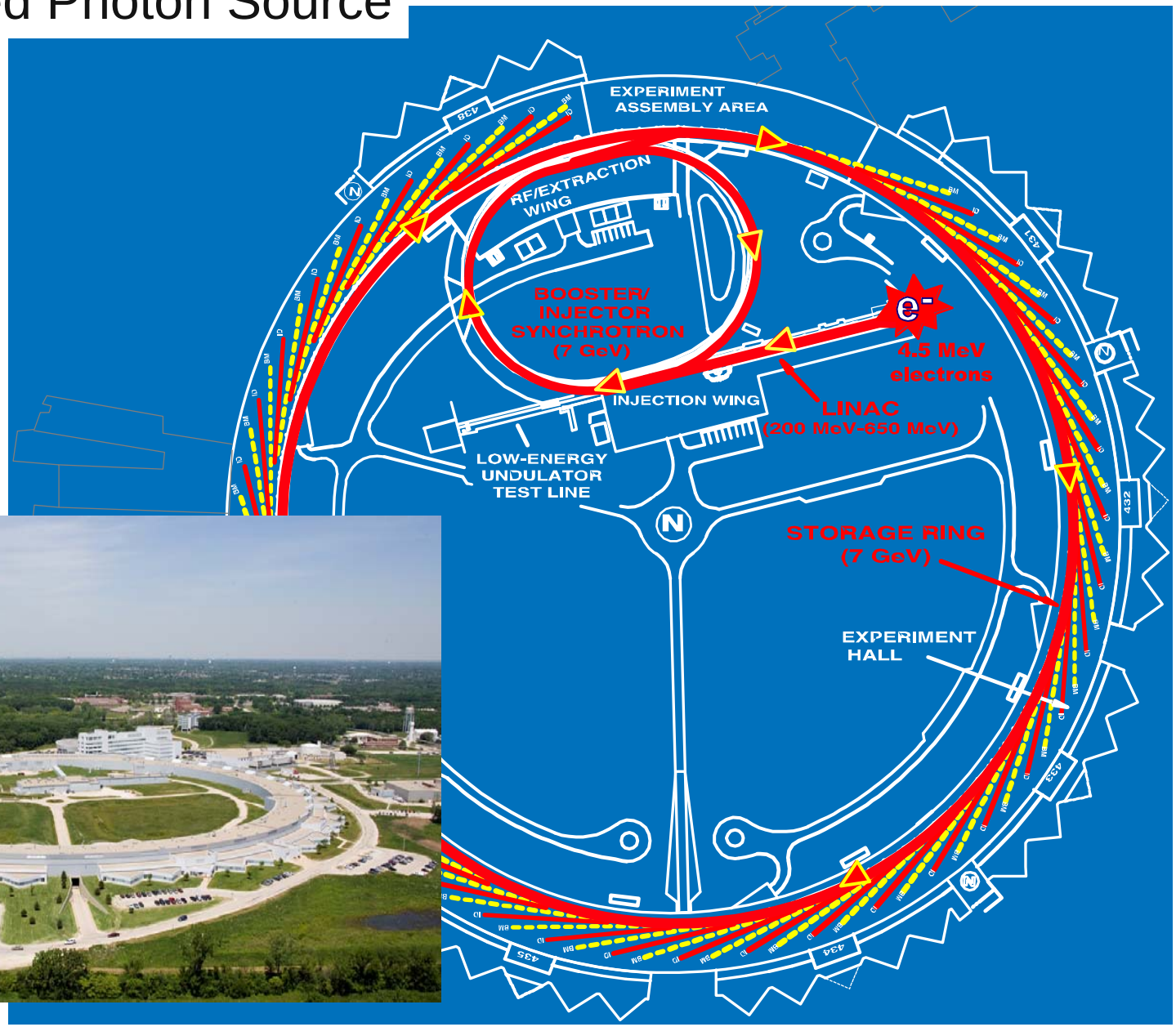
Scientific User Facilities within Argonne



ATLAS, CNM, EMC outside SUF

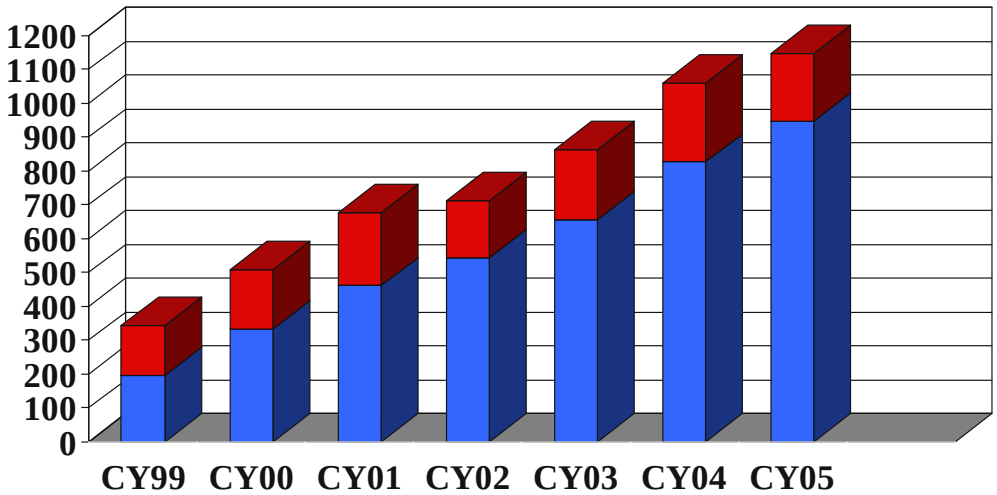
The Advanced Photon Source

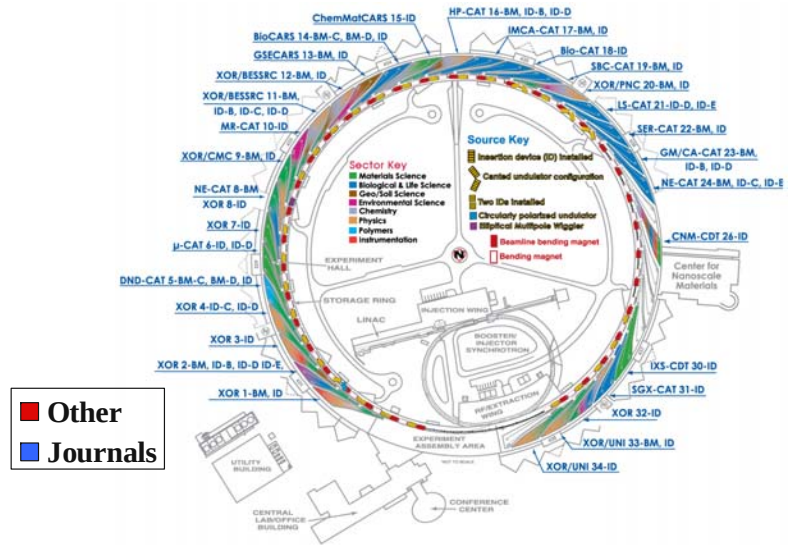
APS x-ray beams are emitted from 34 undulator and bending magnet ports to users

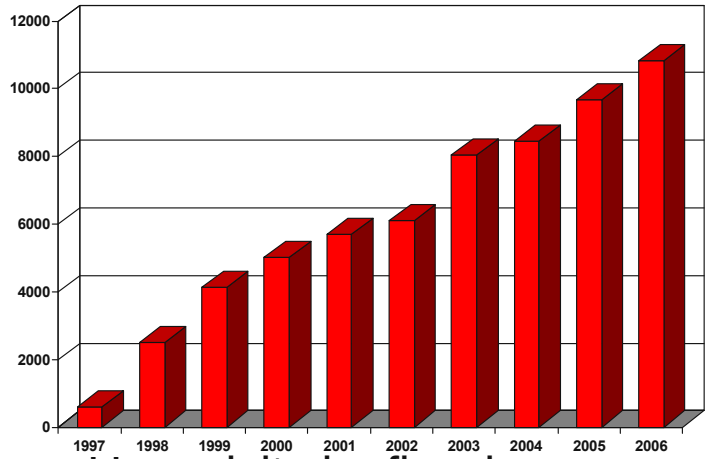


. . . the largest scientific user facility in the US, and growing

Refereed publications by calendar year

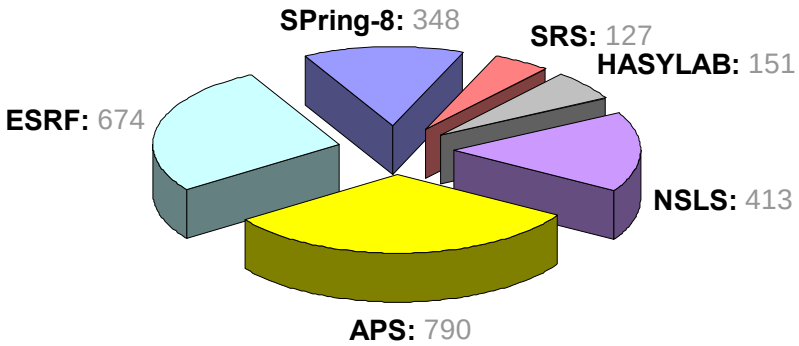




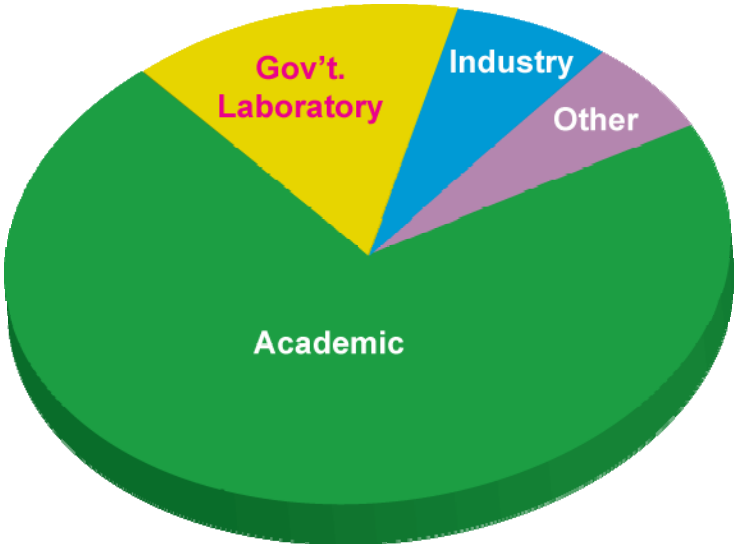


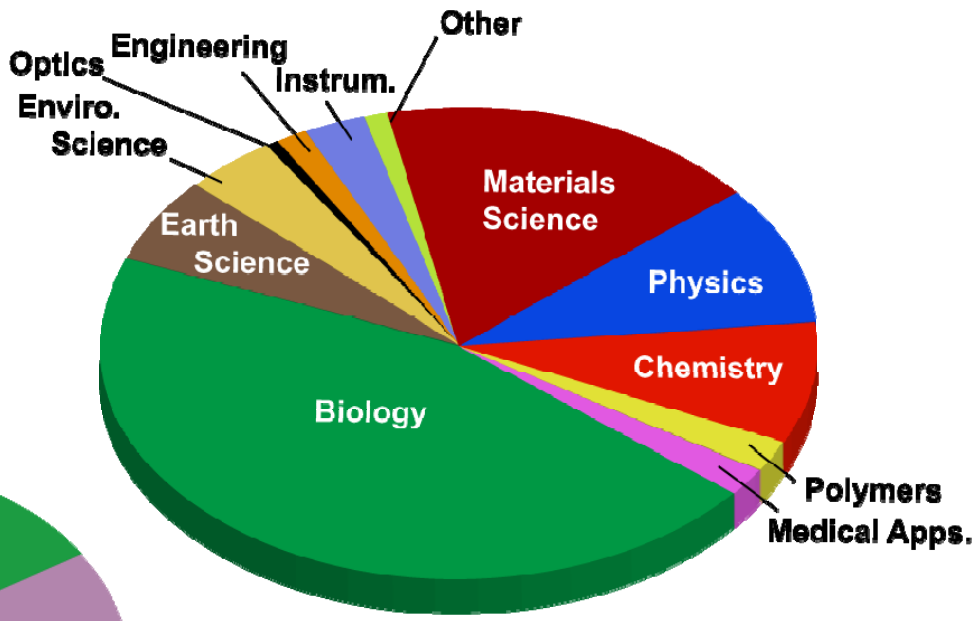
User visits by fiscal year

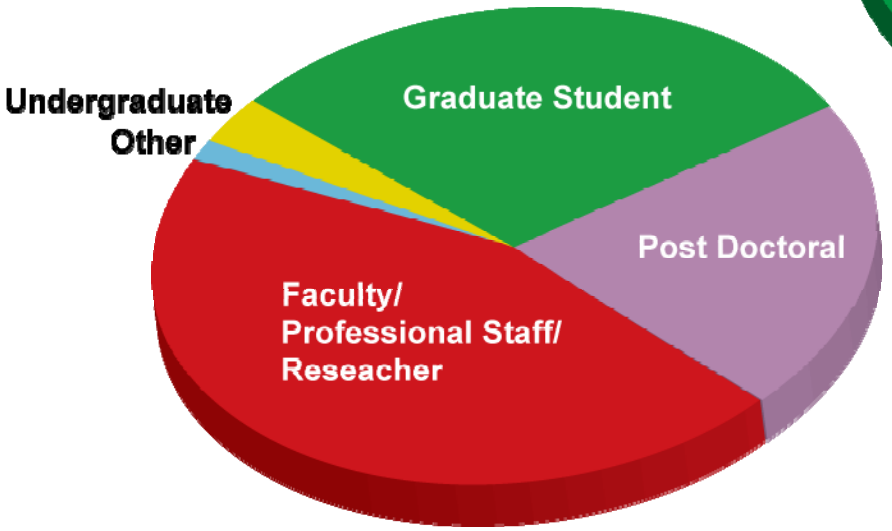
Protein structures in 2005



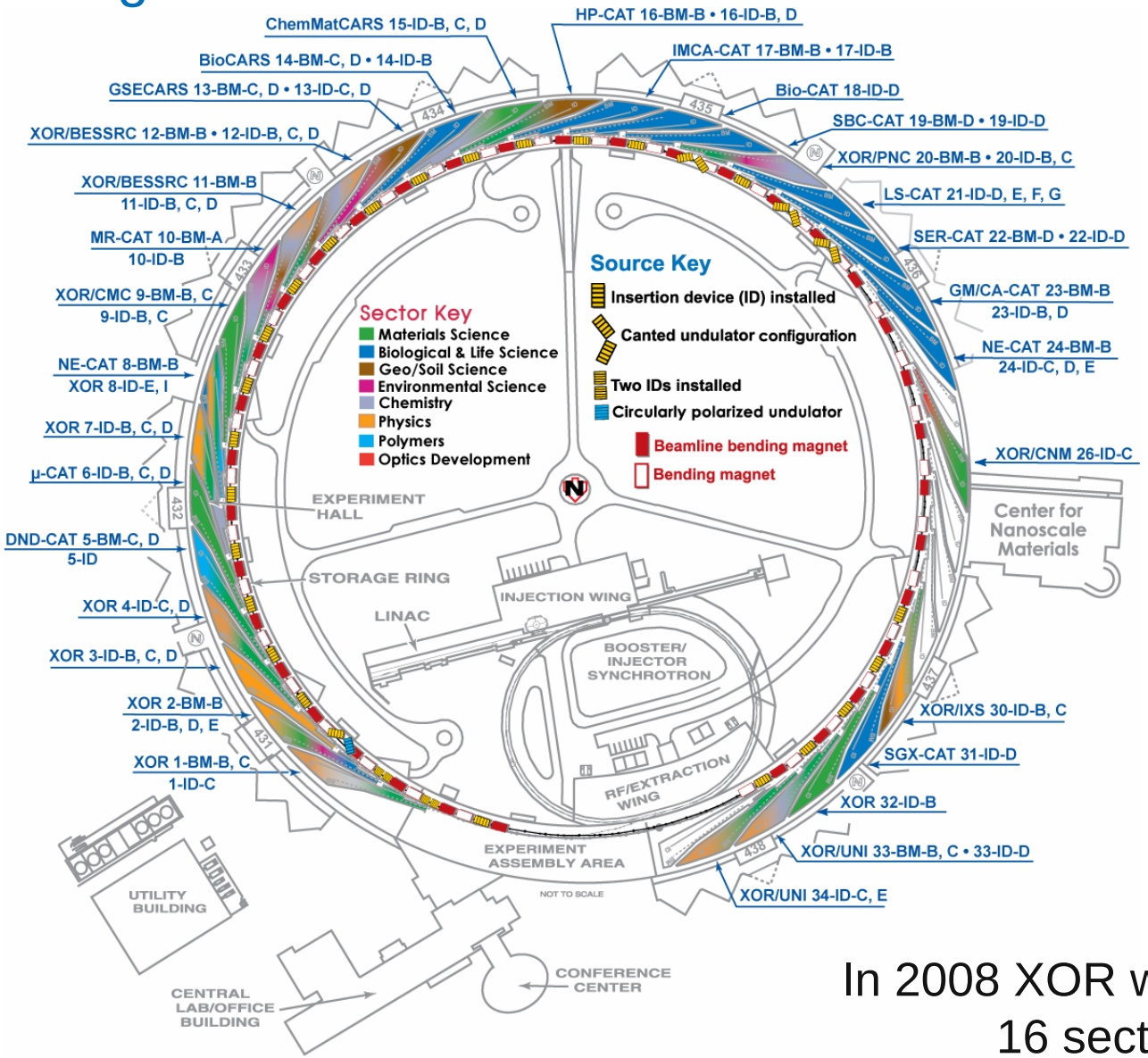
APS users – who are they and what do they do?







Around the ring

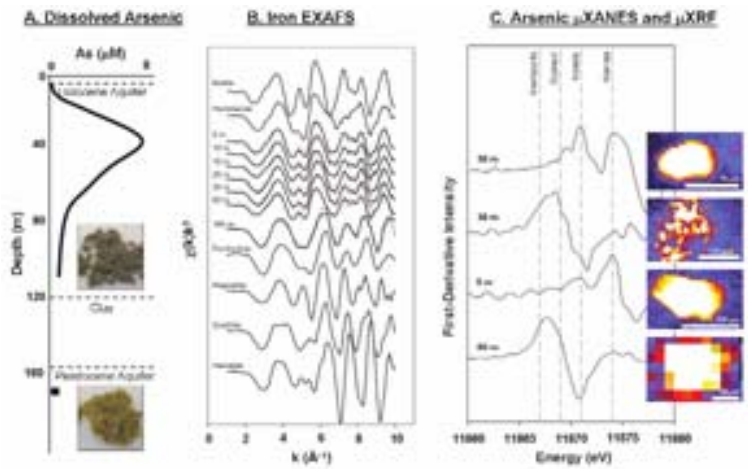


In 2008 XOR will operate 16 sectors

Some scientific highlights

How arsenic enters a water supply

- Arsenic contamination of ground water in Bangladesh is largest environmental disaster world has seen: ~57 million inhabitants are at risk of drinking dangerous levels of arsenic from wells
- Source of arsenic understood; critical question is: How did arsenic migrate to water supply?
- Researchers using GSECARS 13-ID-C have obtained data suggesting that arsenic is released near the surface via redox cycling and is later transported to well-depth
- Researchers propose that:
  - ~15% of solid-phase arsenic is rapidly desorbed, 60% is bound in sulfides unreactive in the strongly reducing aquifer
  - Arsenic released from the surface binds weakly to silicate minerals that dominate aquifer sediments, are easily transported to well depth.
- Study indicates that remediation requires arsenic monitoring of soil environments above aquifers & developing better understanding of arsenic transport

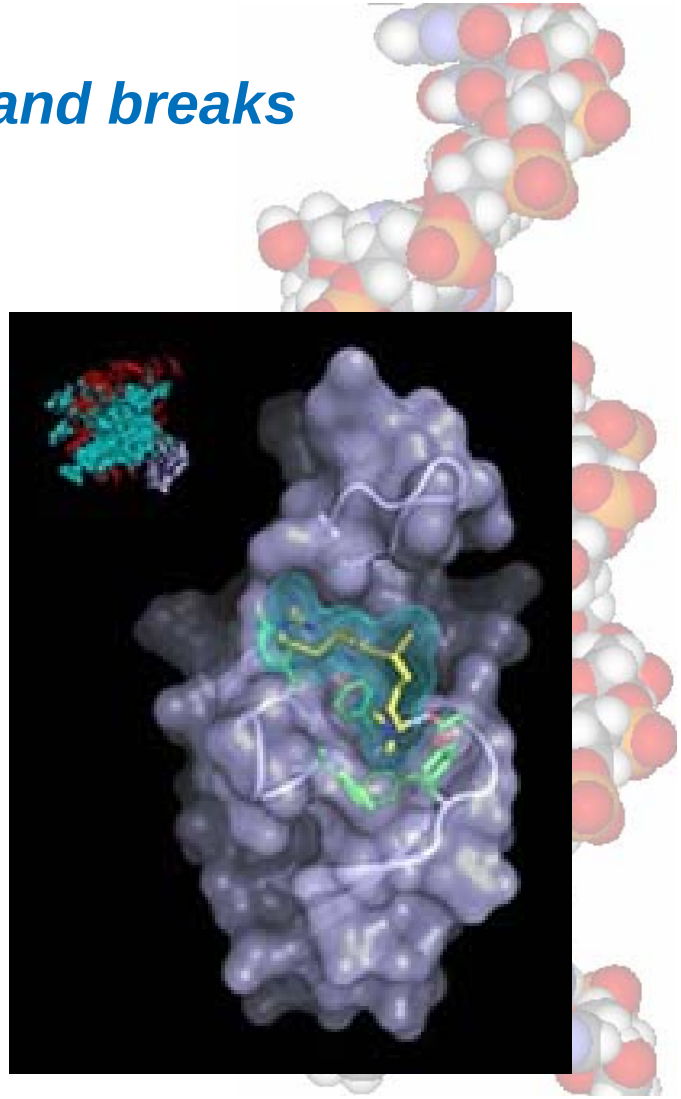


(A) Dissolved arsenic peaks at 30-40-m depth in a Holocene aquifer at the field site. They are not detected in a deeper Pleistocene aquifer. (B) Iron EXAFS linear-combination fitting of aquifer sediment samples indicate that Fe mineralogy is constant with depth within the Holocene aquifer, but Fe(III) (hydr)oxides are not detected, despite the fact that they have been suggested as a source of arsenic. (C) Arsenic is found in a host of oxidation states within the solid-phase. Arsenic-bearing sulfide minerals, a previously unrecognized source of arsenic, are found throughout the sediment profile, most commonly as 10-35-μm grains, and may account for up to 60% of the total solid-phase arsenic.

Matthew L. Polizzotto et al., Chem. Geol. 228, 97 (2006). DOI: 10.1016/j.chemgeo.2005.11.026

A key step in repairing DNA double-strand breaks

- Double-strand breaks in DNA can result from external agents such as UV radiation or mutagenic chemicals
- Unrepaired, a single DNA double-strand break can lead to cell death or cancer
- So cells have evolved elaborate machinery made of proteins to detect, repair DNA lesions
- Atomic-level understanding of how this DNA repair machinery functions is important for correcting malfunctioning DNA double-strand break repair process
- Mayo research team using SBC-CAT 19-ID showed that a human protein essential for repairing DNA double-strand breaks is recruited to the sites of DNA damage by direct interaction with histone H4, a protein constituent of the DNA packaging structure called chromatin

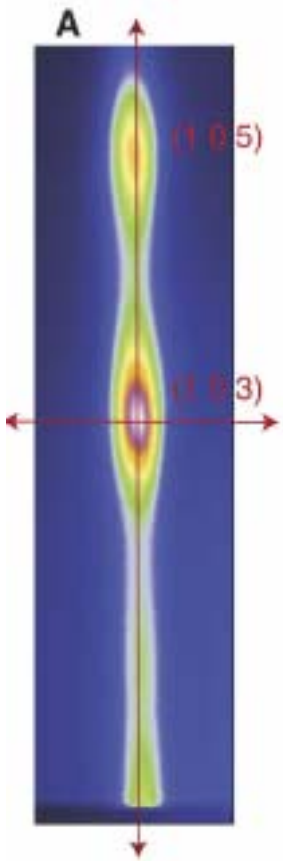


The atomic structure of the protein 53BP1 identified by Mayo researchers. (Courtesy: Mayo Clinic)

Maria Victoria Botuyan et al., Cell **127**, 1361 (29 December 2006).

An insulating breakthrough

- A new insulating material with the lowest thermal conductivity ever measured for a fully dense solid has been created at the University of Oregon and tested at XOR/UNI 33-BM
- While not having immediate application, the principles involved could lead to improved insulation for a wide variety of uses
- Used a novel approach to synthesize various thicknesses of tungsten diselenide, yielded a random stacking of tungsten-diselenide planes (WSe_2), possibly leading to a localization of lattice vibrations
- Resulting synthesized material yielded thermal conductivity 30 times smaller than that for single-crystal WSe_2 and factor of six smaller that minimum level predicted by theoretical computations for the cross-plane thin films used in the experiments

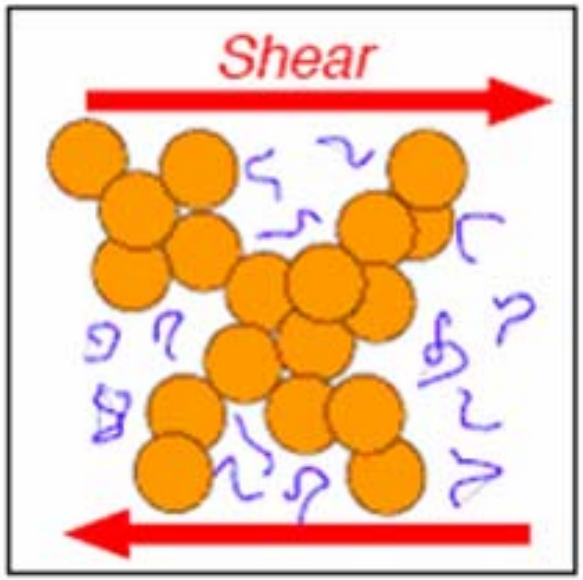


False-color depiction of the x-ray diffraction intensities for a 32.5 nm thick WSe_2 film collected at 33-BM using 18.5 keV photons collected by the area detector in the vicinity of the (1 0 3) and (1 0 5) reflections. The vertical direction is normal to the sample surface and the horizontal direction is in the plane of the sample

Catalin Chiritescu et al., Science **315**, 342 (Jasnuary 2007). DOI: 10.1126/science.1138067

Watching gels get the stress out

- Macroscopic flow properties of a wide assortment of disordered soft materials (foams, concentrated emulsions, colloidal suspensions) can change dramatically from fluid-like to solid-like with subtle changes in microscopic characteristics
- This behavior bears strong resemblance to liquid-glass transition in molecular fluids
- Microscopic mechanisms of recovery from shear in disordered soft solid materials studied and compared to aging in glasses viaUniversity of Illinois, and Florida State University have combined
- Multispeckle x-ray photon correlation spectroscopy at XOR and diffusing wave spectroscopy studies on concentrated colloidal gels subjected to strong shear combined
- Studies call into question connection between aging in glasses and slow equilibration that various disordered soft solids display
- Should motivate a rethinking of models that seek to unify these phenomena

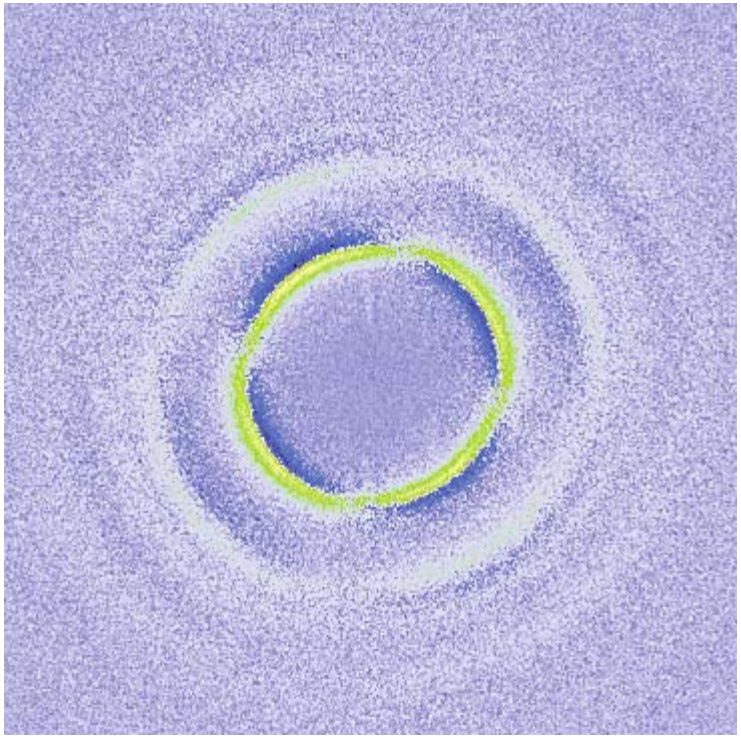


Cartoon of gels under shear

B. Chung et al., “Microscopic Dynamics of Recovery in Sheared Depletion Gels”, Phys. Rev. Lett. **96**, 228301 (2006).

Looking into metallic glass

- **Metallic glass is an amorphous metal that does not crystallize when cooled from liquid to solid**
- **Atomic-scale structure is highly disordered, much like a liquid, gives metallic glasses unique properties of high strength and elasticity that make them ideal for a wide range of applications, incl. military hardware, spacecraft, sporting equipment**
- **The ability to measure elastic strain in glasses thought to be limited by material's structural randomness, difficulties in collecting and analyzing data**
- **Researchers used XOR 1-ID to measure elastic strain on a bulk amorphous metallic alloy**
- **Study shows that elastic strain in metallic glass can be measured accurately with high-energy x-ray scattering**

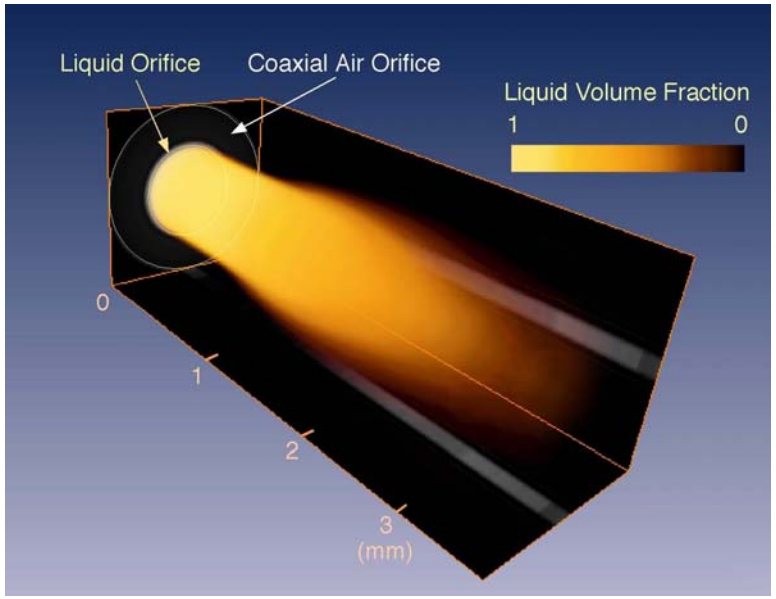


Change in x-ray scattering between loading and unloading for a specimen tested in pure shear. The distortion of the scattering rings reflects the principal strains (which are oriented approximately ± 45°from vertical)

T.C. Hufnagel et al., Phys. Rev. B 73, 064204 (2006). DOI: 10.1103/PhysRevB.73.064204

Beneath the surface of high-speed industrial sprays

- "Seeing" beneath the surface of a jet from ubiquitous high-speed industrial paint sprayer can yield important new information needed to optimize the sprayers themselves
- Researchers and engineers from Argonne and Illinois Tool Works (ITW), Inc. (Glenview, IL) using XOR 7-ID beamline have captured first images of complex and transient multiphase spray flow just millimeters from a high-speed industrial spray nozzle
- First-ever visualization of near-nozzle high-speed coaxial flows can be used to develop and validate liquid breakup models and is indispensable for understanding downstream spray formation



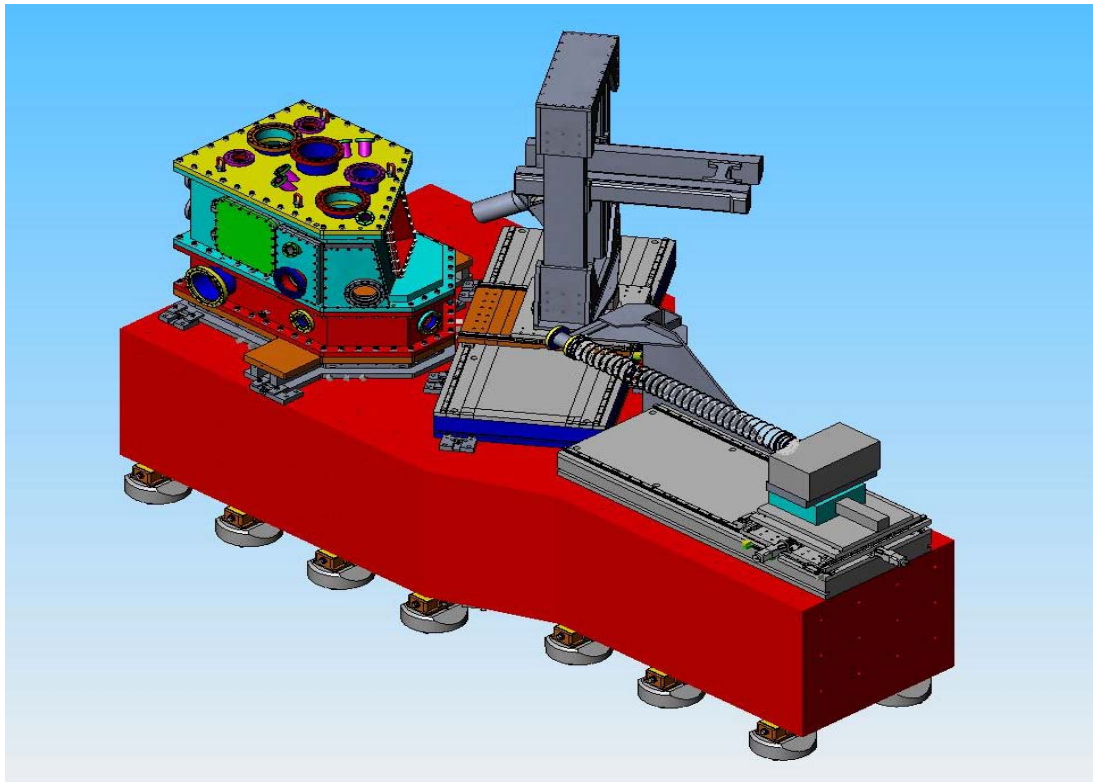
Three-dimensional rendering of air-assisted coaxial spray in near-nozzle region with an air pressure of 137 kPa (corresponding to a Weber number of 380). False color intensity represents liquid volume fraction, which was quantified for first time with the x-ray phase-contrast imaging.

Y. J. Wang et al., "Quantitative x-ray phase-contrast imaging of air-assisted water sprays with high Weber numbers," Appl. Phys. Lett. **89**, 151913 (9 October 2006).

The Linac Coherent Light Source (at ANL)

- A matrixed partnership - Stanford Linear Accelerator Center and ANL are building the world's first x-ray free electron laser
  - ANL experts design and produce 130 meters of undulator systems (33+ spares) for installation in new underground tunnel at SLAC
  - ANL (APS) undulator system TPC ~$45M
  - FY 06 & 07 - Undulator system construction
  - FY 08 - Installation, commissioning, and 1st light

Center for Nanoscale Materials (CNM)



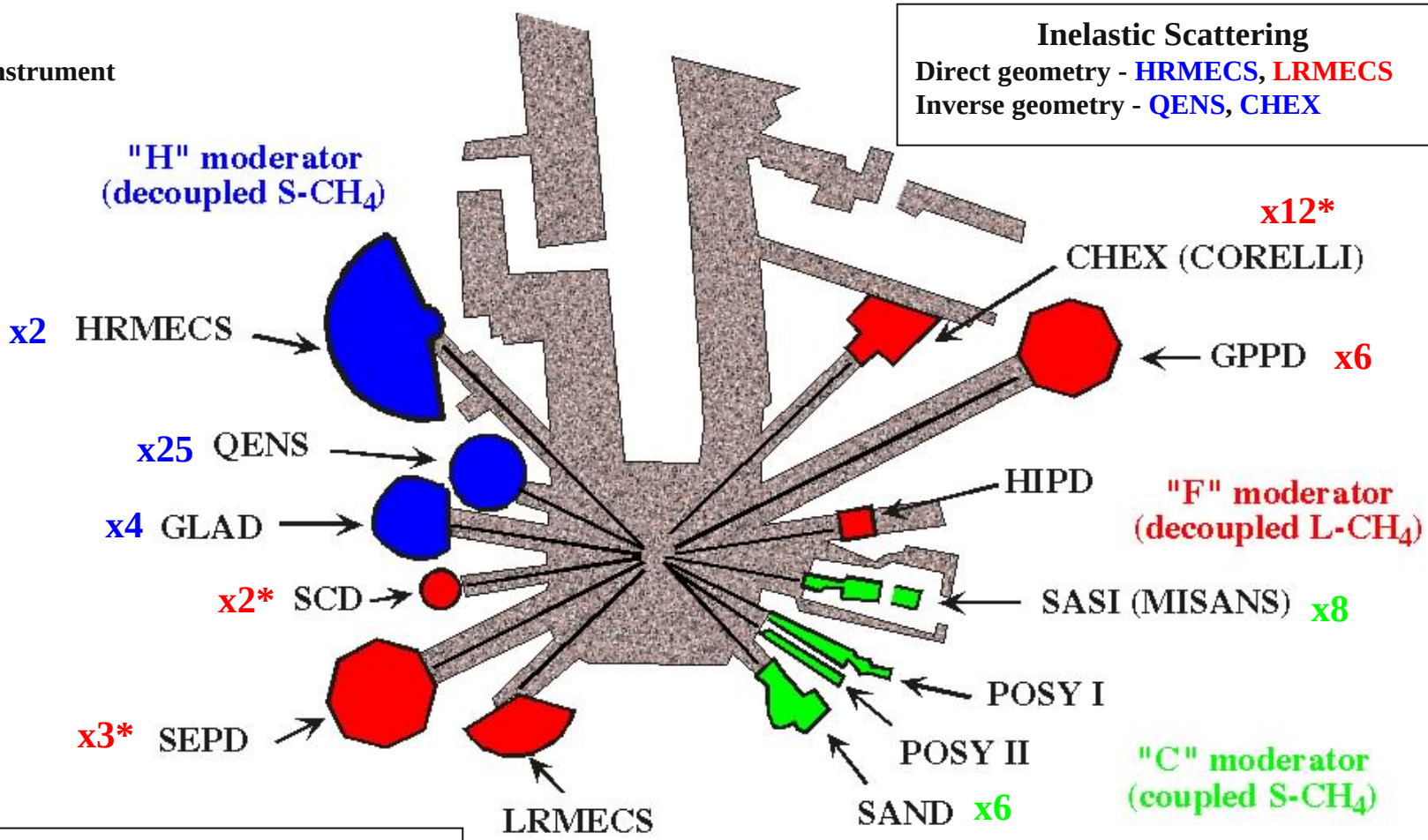
Partnership

Nanoprobe finishing construction
at 26-ID will be jointly operated by CNM and APS

Aiming for a 10-nm-resolution x-ray microscope

IPNS Instrument Suite

* New instrument



Inelastic Scattering
Direct geometry - HRMECS, LRMECS
Inverse geometry - QENS, CHEX

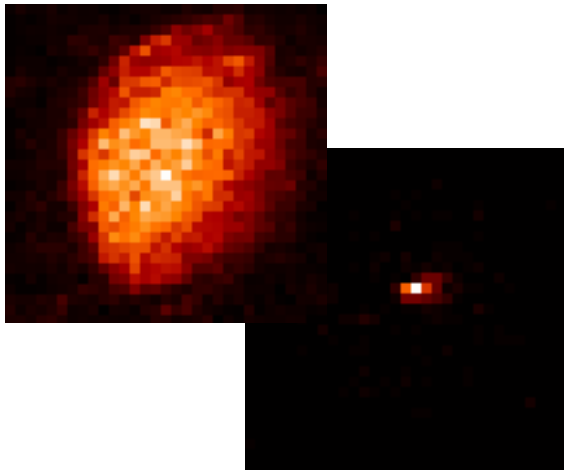
Diffraction
Powder diffraction - SEPD, GPPD, HIPD
Single crystal - SCD
Liquids and Amorphous Materials - GLAD

Large Scale Structures
Small Angle Scattering - SAND, SASI
Reflectometry - POSY I, POSY II

Future development plans

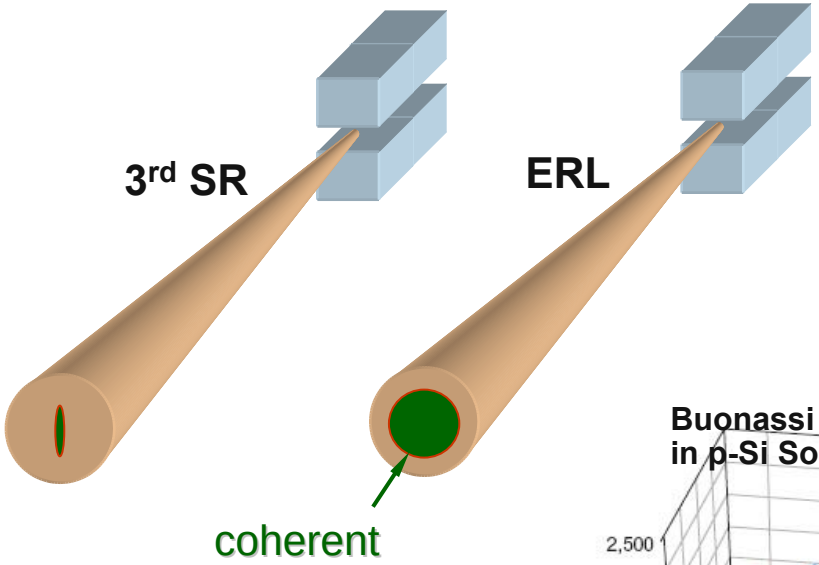
Future for APS – an Energy Recovery LINAC?

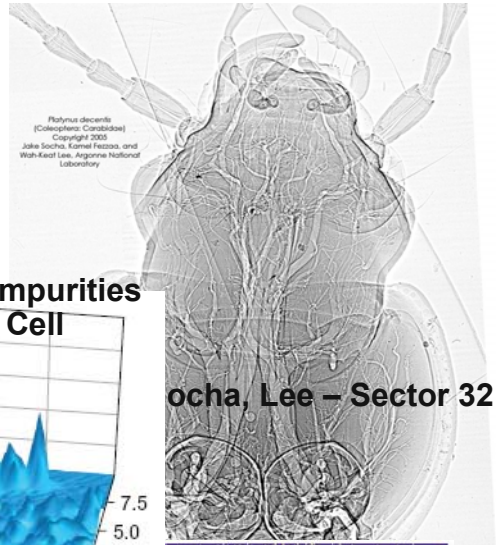
110 years



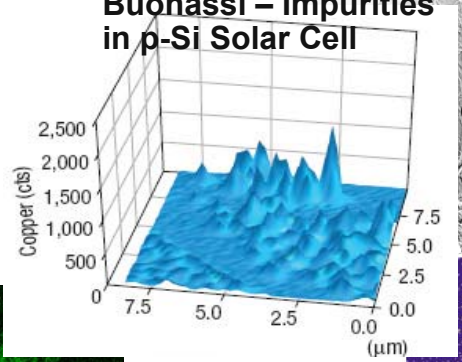
- Imaging is back at the forefront of x-ray science!
- Next generation sources offer full coherence which will revolutionize x-ray imaging and related coherent applications
- What is happening in x-ray imaging today at APS and elsewhere?
- Plans to develop ERL sources

ERL: Ideal source for imaging and nano-probes

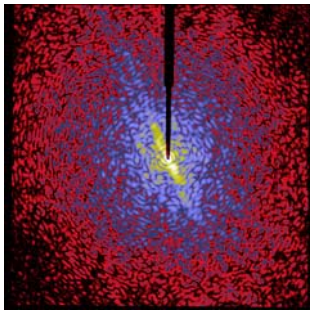


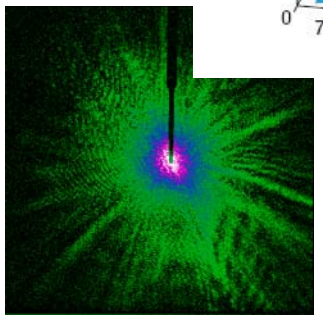


Buonassi – Impurities in p-Si Solar Cell

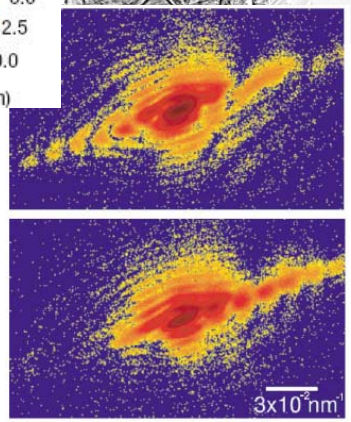


ocha, Lee – Sector 32

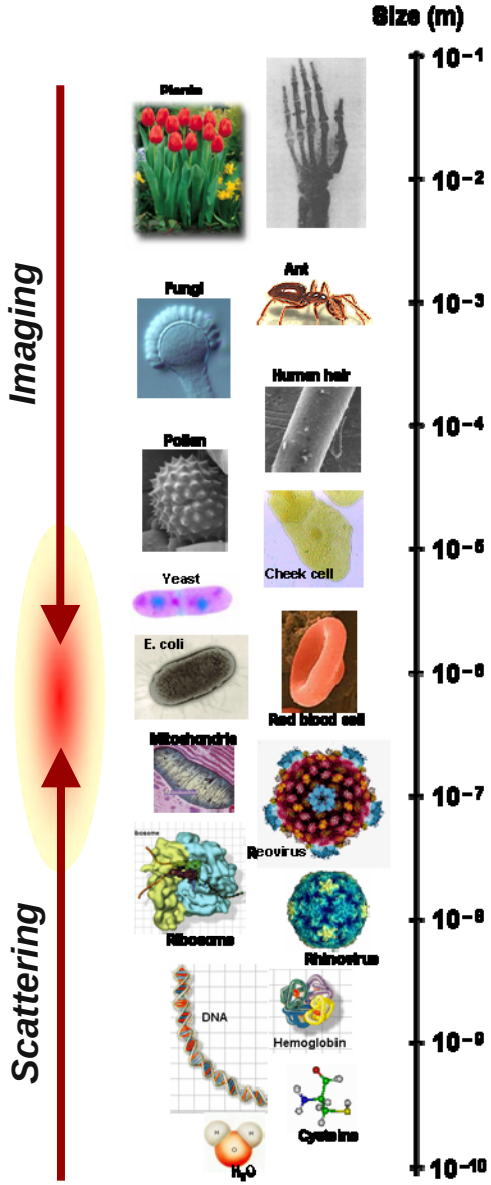




Miao – actin filaments, 2-ID-B



Robinson – Au particles 34-ID-C



The Advanced Photon Source has been operating for 11years, and a major upgrade is expected in the next decade

U.S. Department of Energy

	Priority	Program	Facility
Near-Term	1	FES	ITER
	2	ASCR	UltraScale Scientific Computing Capability
	Tie for 3	HEP	Joint Dark Energy Mission
		BES	Linac Coherent Light Source
		BER	Protein Production and Tags
		NP	Rare Isotope Accelerator
	Tie for 7	BER	Characterization and Imaging
		NP	CEBAF Upgrade
		ASCR	ESnet Upgrade
		ASCR	NERSC Upgrade
		BES	Transmission Electron Achromatic Microscope
Mid-Term	12	HEP	BTeV
	13	HEP	Linear Collider
	Tie for 14	BER	Analysis and Modeling of Cellular Systems
		BES	SNS 2-4 MW Upgrade
		BES	SNS Second Target Station
		BER	Whole Proteome Analysis
	Tie for 18	NP/HEP	Double Beta Decay Underground Detector
		FES	Next-Step Spherical Torus
		NP	RHIC II
Far-Term	Tie for 21	BES	National Synchrotron Light Source Upgrade
		HEP	Super Neutrino Beam
	Tie for 23	BES	Advanced Light Source Upgrade
		BES	Advanced Photon Source Upgrade
		NP	eRHIC
		FES	Fusion Energy Contingency
		BES	HFIR Second Cold Source and Guide Hall
		FES	Integrated Beam Experiment

Facilities for the Future of Science available from http://www.science.doe.gov/Sub/Facilities_for_future/20-Year-Outlook-screen.pdf

Priority: Tie for 23
Advanced Photon Source (APS) Upgrade

The APS upgrade will greatly enhance the brilliance and power of the facility to enable scientists to study very small sample crystals—important for nanoscience research.

The Facility: The Advanced Photon Source (APS) upgrade will create a "super storage ring" of electrons that will greatly enhance the brilliance of the facility, increasing the power of the device and enabling scientists to work on very small sample crystals. Small samples are important: many current experiments are limited by the fact that the subject materials will not grow into large enough crystals for study.

Background: The APS at Argonne National Laboratory was commissioned in 1996. It currently provides the brightest x-ray beams available in the Western Hemisphere for a wide range of research from materials science to structural biology. The 1,104-meter circumference storage ring of the APS, which is large enough to house a baseball park in its center, produces, accelerates, and stores a beam of subatomic particles that is the source of the x-ray beams that feed numerous experimental stations. The APS will support more than 4000 users on 70 beamlines.

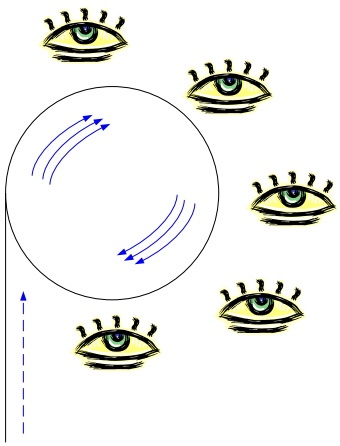
What's New: This eventual APS upgrade will replace and upgrade major components of the accelerator to further increase performance in the hard x-ray region of the spectrum, most notably x-ray photon correlation spectroscopy, coherent imaging, inelastic scattering, and x-ray nanoprobe microscopes. The upgrade will be necessary to keep the APS among the best of the hard x-ray facilities, and ensure that its performance and scientific output continue to be ground-breaking.

Applications: Using high-brilliance x-ray beams from the APS, members of the international synchrotron-radiation research community have achieved major advances in basic and applied research in the fields of materials science; biological science; physics; chemistry; environmental, geophysical, and planetary science; archeology; and innovative x-ray instrumentation.

What is the fourth generation revolution in x-ray sources?

$\tau_{lifetime} >> \tau_{relaxation}$

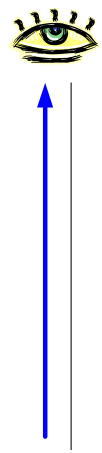
Storage ring



- Many users
- High flux
- Low brilliance
- Long pulses

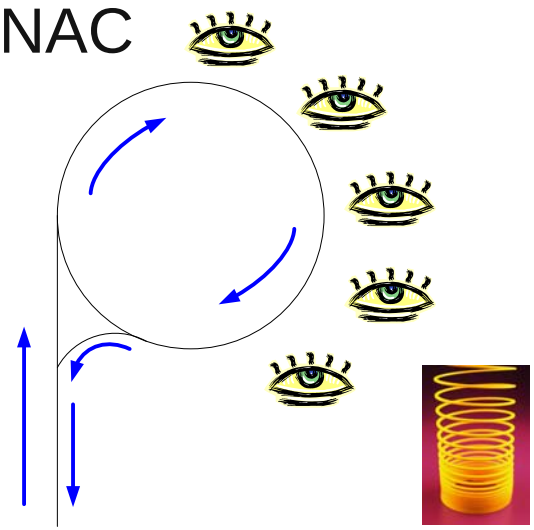
$\tau_{lifetime} << \tau_{relaxation}$

LINAC source (=> FEL)



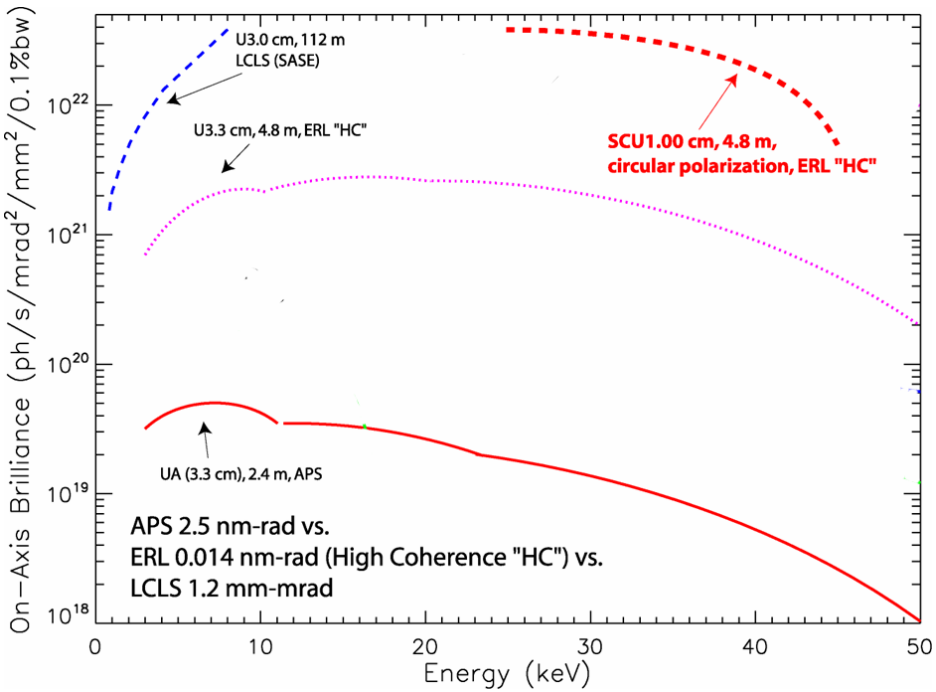
- Extremely high peak brilliance
- Full spatial coherence
- Ultrashort pulses
- Temporal coherence?
- Low rep rate
- Few users

Energy-Recovery LINAC



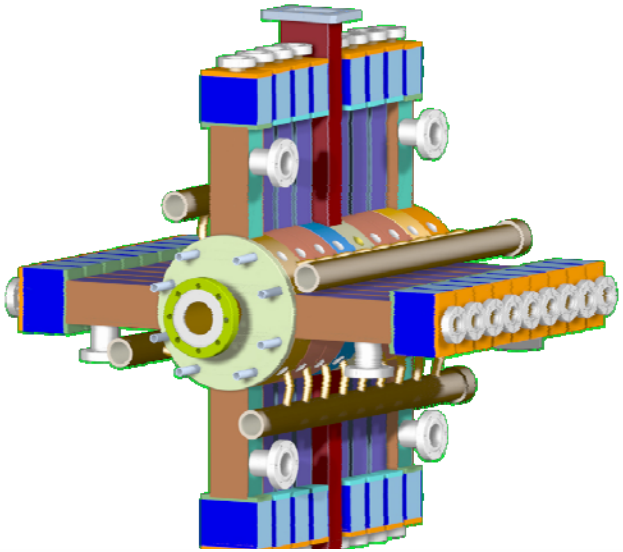
- High average brilliance
- Full spatial coherence
- Many users
- High flux
- Short pulses but closely spaced and lower # of photons per pulse

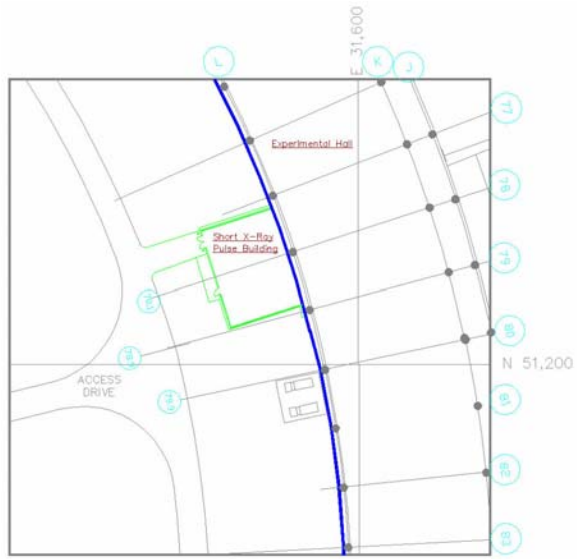
What does an ERL offer?

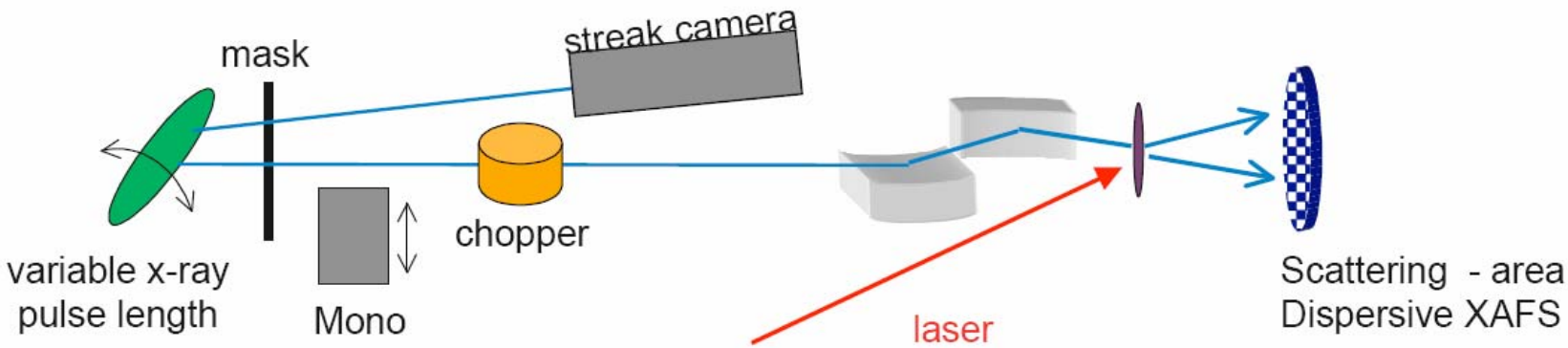


- Substantially spatially-coherent source
  - It can put >100 times more flux into a <10nm probe and improve phase contrast compared with a storage ring
  - And deliver to many users
- It offers pulses 100 times shorter or less (in the sub-ps regime)
  - Does not rival FEL for peak brilliance
  - But compatible with FEL upgrade as well
- Proposed and developed by Cornell
- Natural upgrade path for storage ring such as APS
  - Can be done without compromise or major disruption

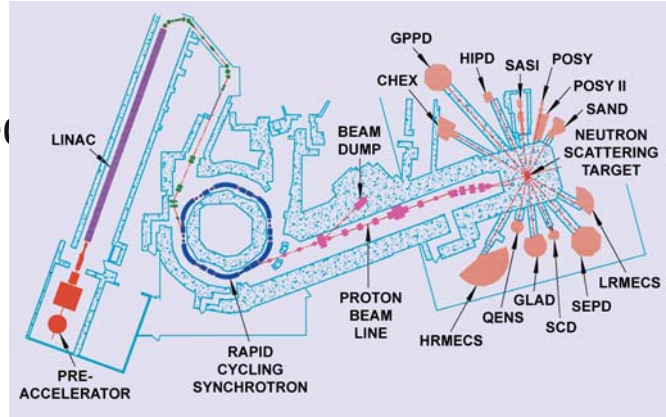
Short pulses at APS in the shorter term
A million photons in a trillionth of a second at sector 7 in 2008





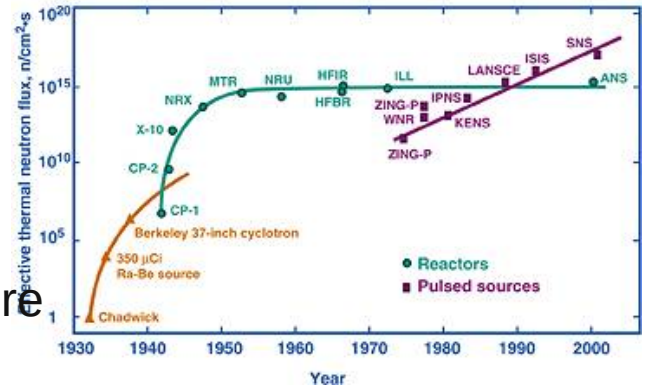


What does the future hold for IPNS?



- Instruments performing at highest capacity ever
  - Enhancements for all major instruments completed over past 5+ years
  - World-class special environment capabilities, reasonably well-integrated
  - But, no funding for further improvements
- Future operations
  - Uncertain beyond FY08-09
- Desired outcomes
  - Retain key personnel for the benefit of Argonne
    - *: beamline staff, accelerator expertise*
    - *Transitions to APS - accelerator group moved Feb. 2007*
  - Preserve IPNS collaborative research heritage for APS and SNS
  - Participate in enhancement of APS science and linkage between photon and neutron user bases in US
  - Create Argonne Scattering and Imaging Institute (ASI^2)

What will ASI² be?

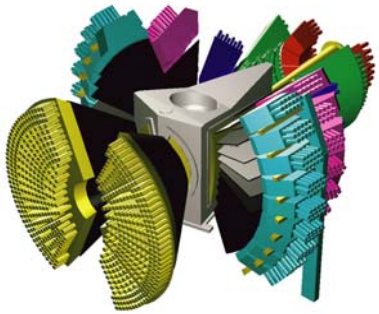


- ASI² aspires to:
  - Become a driver for new discoveries through more effective use of scattering data
  - Become a leading innovator in scattering theory, simulation and analysis, data visualization, and instrumentation design
  - Become home of US community scattering data analysis development through creation of large group of dedicated scientists and programmers
  - Create strong but flexible interfaces with major US facilities and scattering research groups at DOE laboratories and universities
  - … cture that maintain … ific … gr

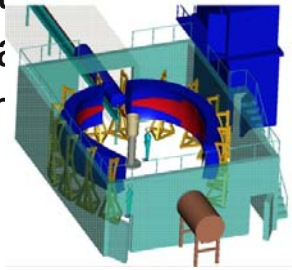
D1a (ILL) 1978

12 detectors
0.1m²

GEM (ISIS) 2000



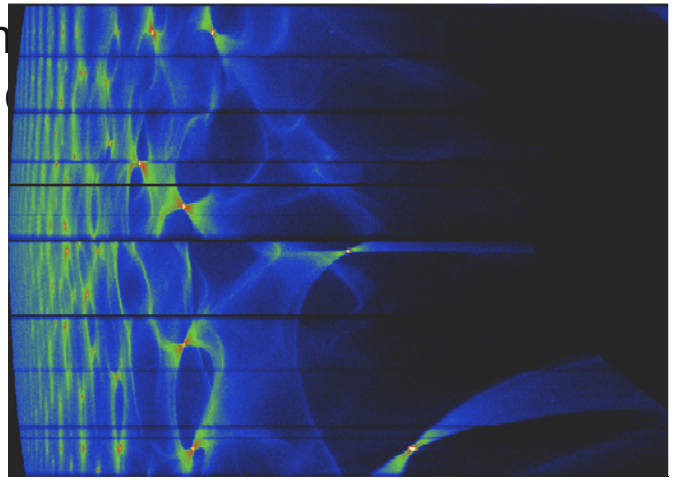
10,000 detectors
10m²



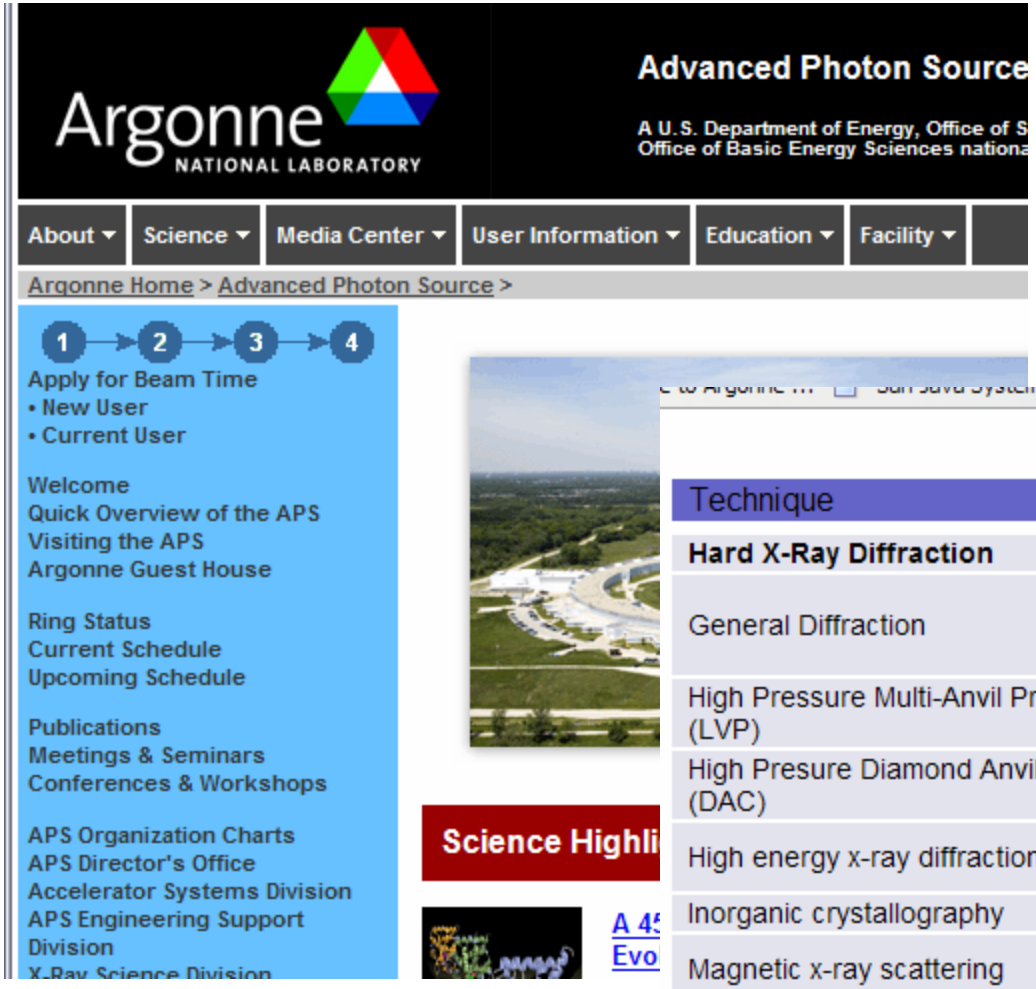
POWGEN3 (SNS) 2006

240,000 detectors
47m²

Si single crystal on GPPD - 1.8 Mpixels



Getting beam time



Web-based
Also for IPNS, CNM, EMC

SCATTERING

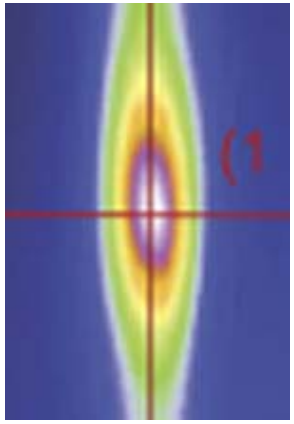
Technique	Beamline
Hard X-Ray Diffraction	
General Diffraction	XOR/UNI-33-ID-D , XOR/BESSRC-11-ID-D , XOR/UNI-33-BM-C , XOR-2-BM-B , XOR/BESSRC-12-BM-B , HP-CAT-16-ID-D
High Pressure Multi-Anvil Press (LVP)	GSECARS-13-BM-C,D , GSECARS-13-ID-C,D
High Presure Diamond Anvil Cell (DAC)	GSECARS-13-BM-C,D , XOR-3-ID-B,C,D , HP-CAT-16-ID-B , GSECARS-13-ID-C,D , 16-ID
High energy x-ray diffraction	DND-CAT-5-BM-D , XOR/BESSRC-11-ID-C , XOR/BESSRC-11-ID-B , MU-CAT-6-ID-D
Inorganic crystallography	DND-CAT-5-ID
Magnetic x-ray scattering	MU-CAT-6-ID-B,C , XOR-4-ID-C , MU-CAT-6-ID-D , XOR-4-ID-D
Micro - diffraction	GM/CA-CAT-23-ID-B , GM/CA-CAT-23-ID-D , XOR/UNI-34-ID-C , ChemMatCARS-15-ID-B,C,D , Bio-CAT-18-ID-D* , HP-CAT-16-ID-B , XOR-2-ID-D , XOR-2-BM-B , GSECARS-13-ID-C,D , 16-ID

Career possibilities

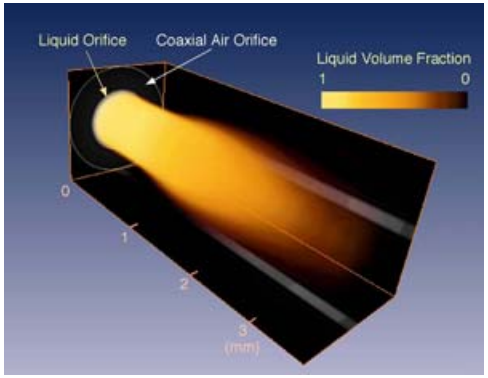
- APS is expanding the # of beamline staff in the next few years
- *ASI2 may be looking for staff if funded in theory/software development for neutron and x-ray scattering*
- *The Center for Nansocale Materials is recruiting scientific staff*

Questions?

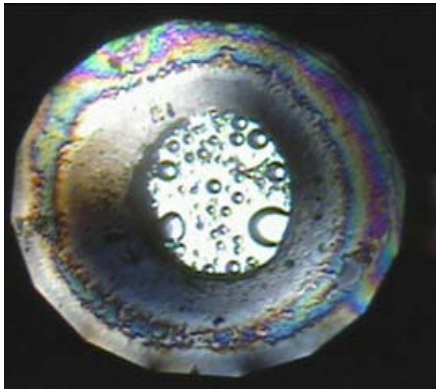
Third generation sources like the Advanced Photon Source have had broad impact on science



WSe_2 - a material with lowest κ due to deliberate random layer stacking
Chiritescu et. al. Science, January 2007



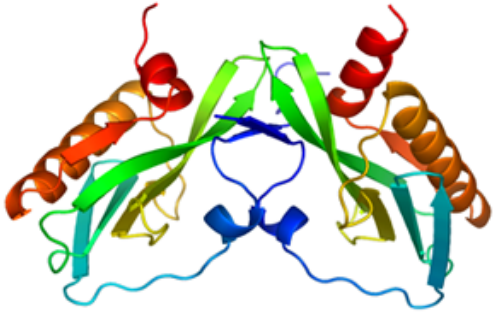
Inside a paint-spray
Wang et. al. Appl. Phys. Lett. ***89****, 151913 (2006).*



New H_2:O_2 alloy at high P-T
Mao et al., Science 314, 636 (2006).

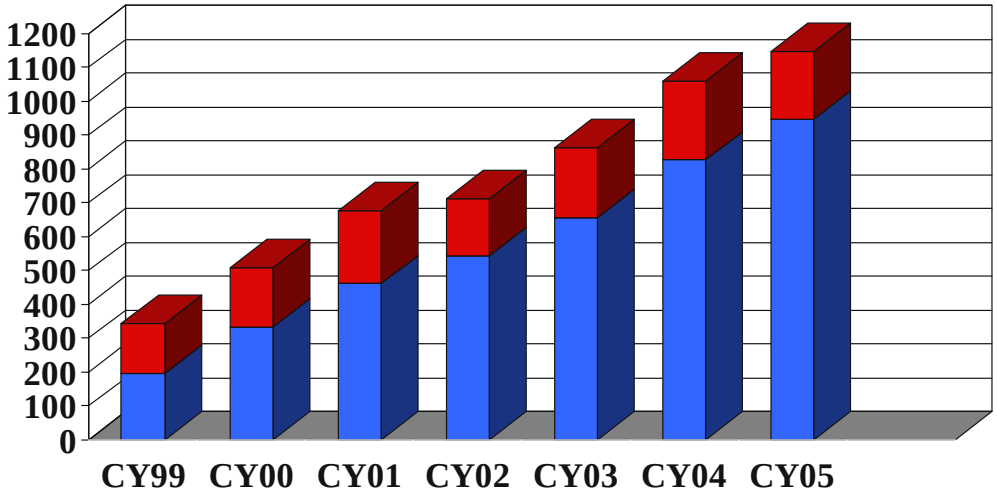
Individual atomic steps on orthoclase
Fenter et. al. Nat. Phys. ***2****, 700 (2006).*

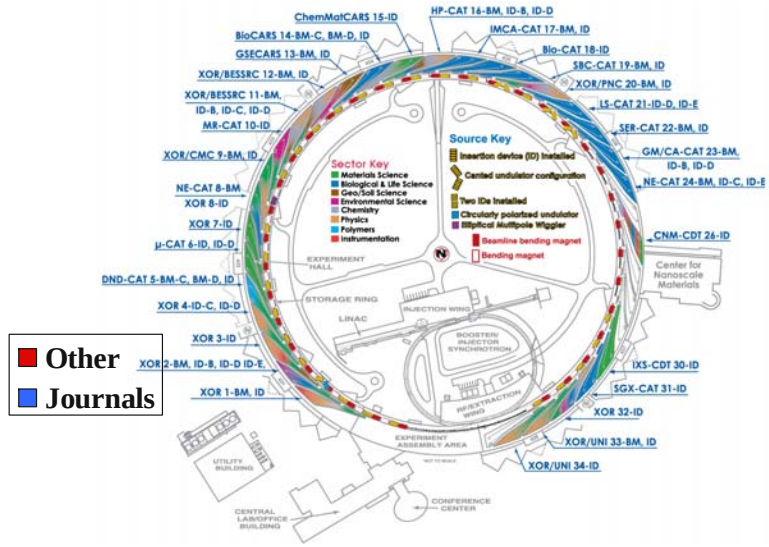
The protein that gives avian flu its virulence
Bornholdt et. al. Nature Struct. Mol. Biol. ***13****, 559 (2006)*

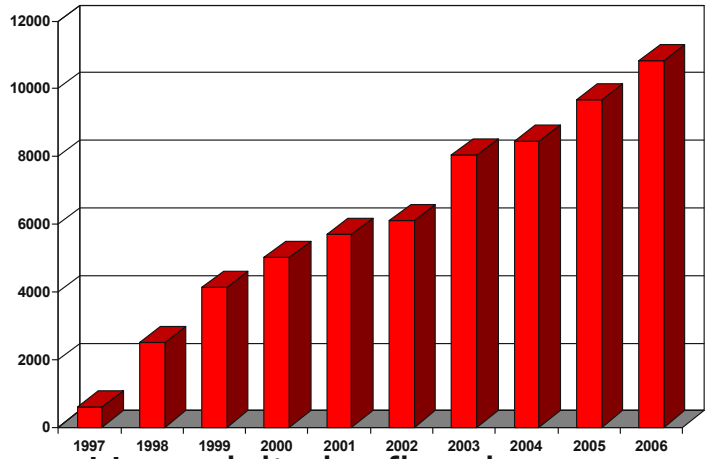


. . . and cater to large user demand

Refereed publications by calendar year

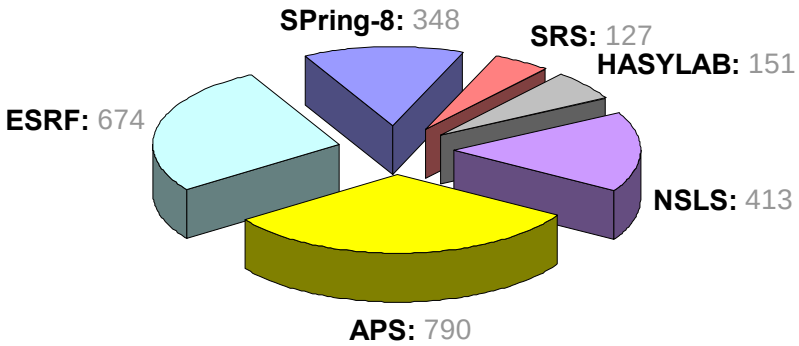




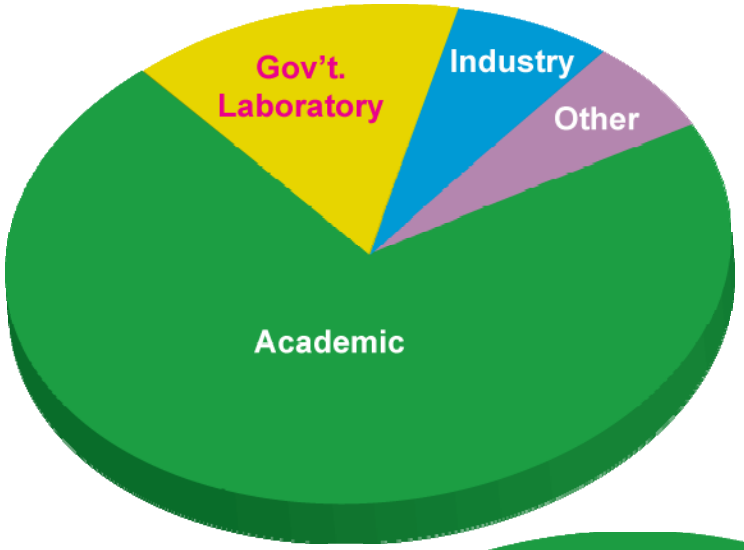


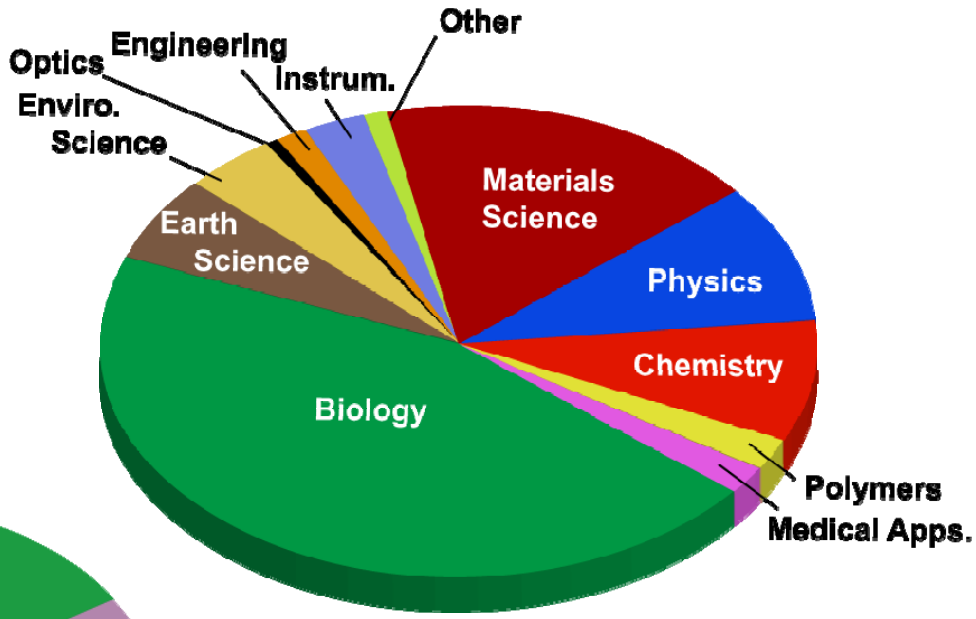
User visits by fiscal year

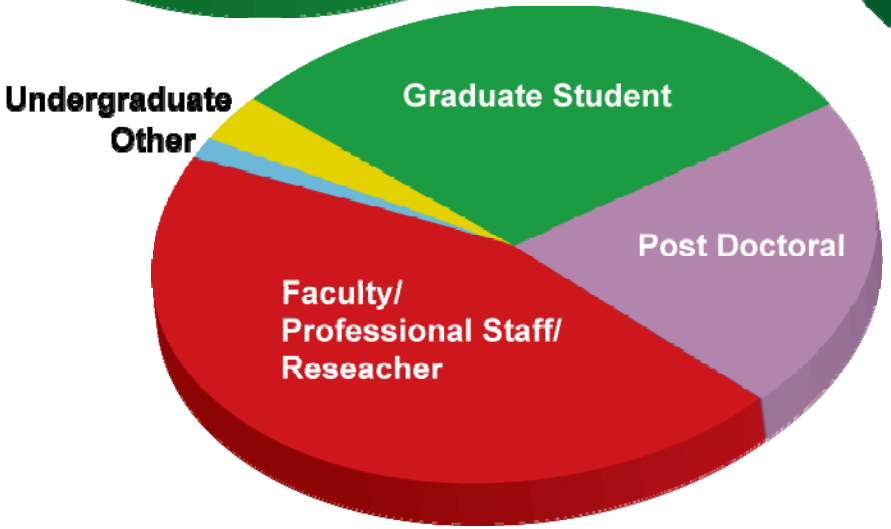
Protein structures in 2005



The majority of our users are from academia







and a significant fraction of their research support comes from NSF

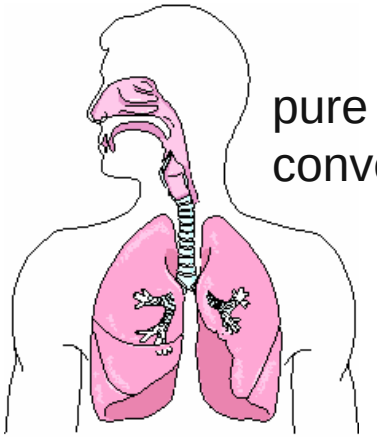
Full-field imaging: Biomechanics and animal physiology

pure diffusion

very small critter

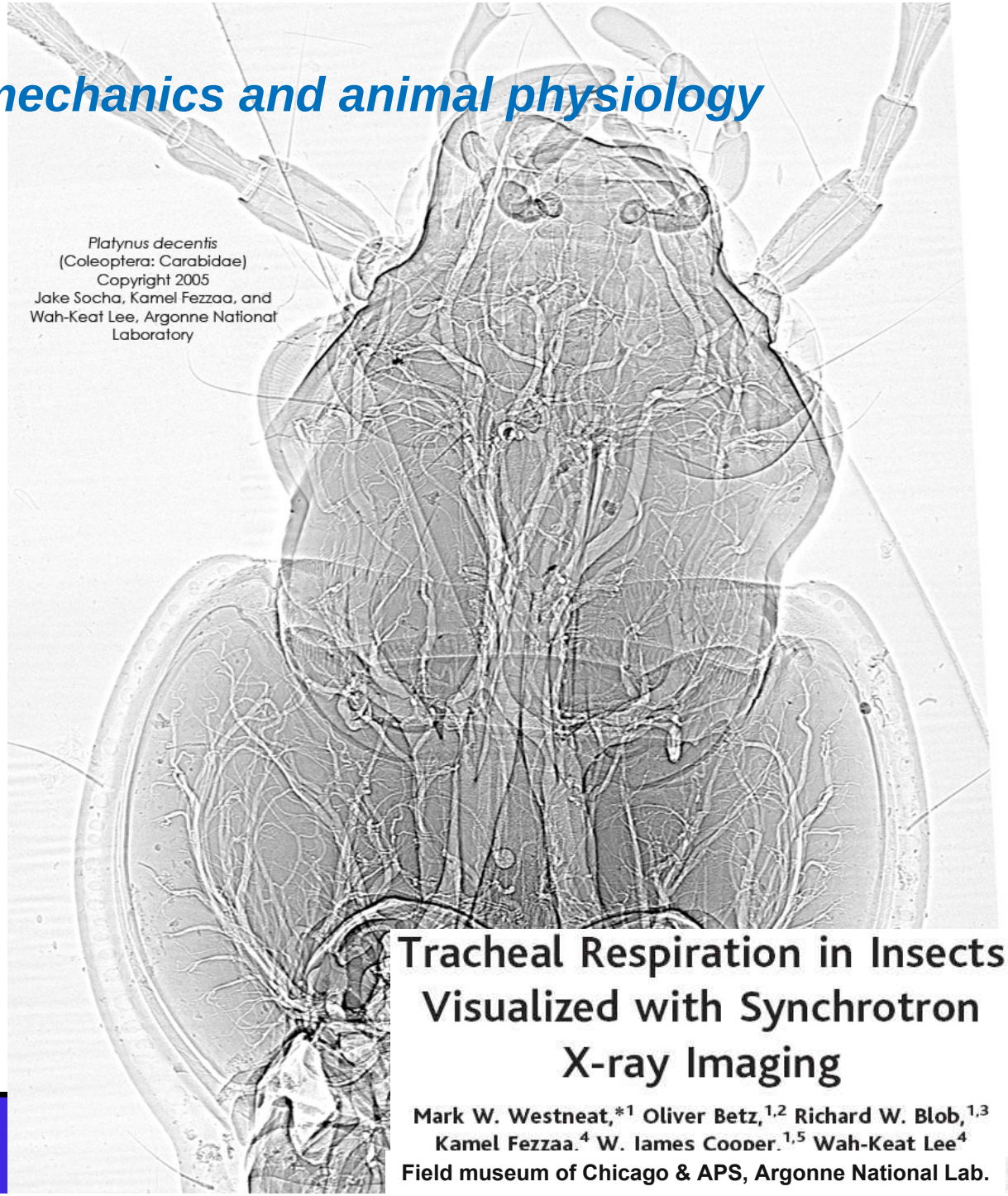
?

insect



pure convection

human



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]

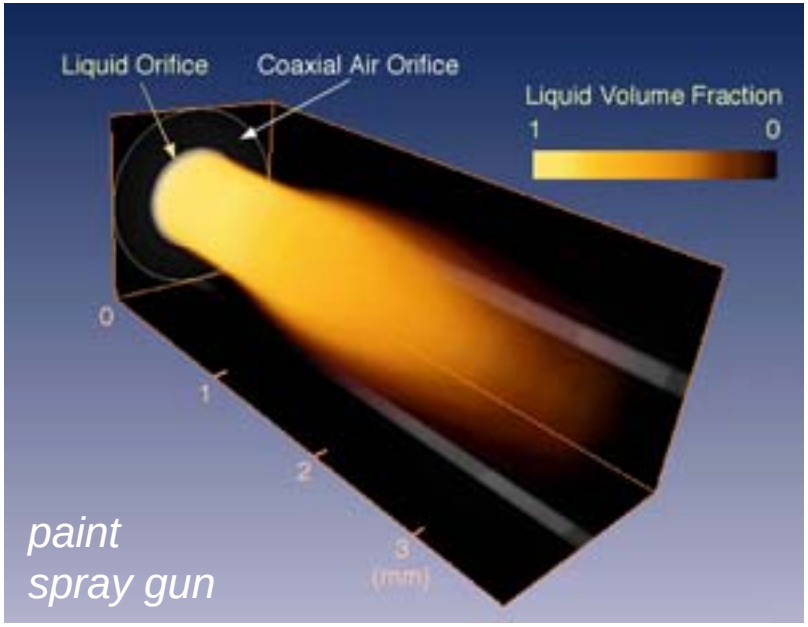
Field museum of Chicago & APS, Argonne National Lab.

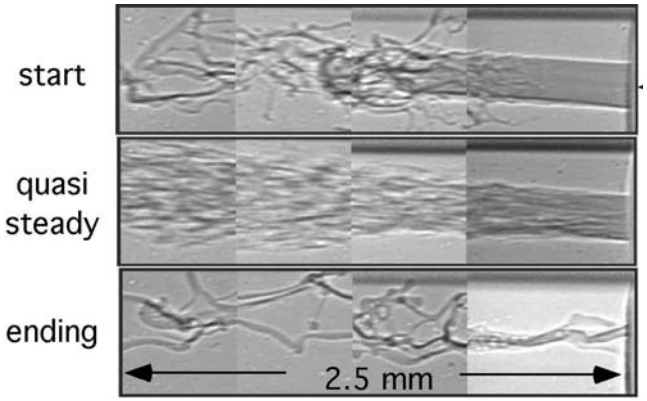
Argonne NATIONAL LABORATORY

High-speed imaging of fuel and liquid sprays

Y. J. Wang, Kyoung-Su Im, K. Fezzaa, W. K. Lee, J. Wang, P. Micheli, and C. Laub, "Quantitative x-ray phase-contrast imaging of air-assisted water sprays with high Weber numbers," Appl. Phys. Lett. **89**, 151913 (9 October 2006).

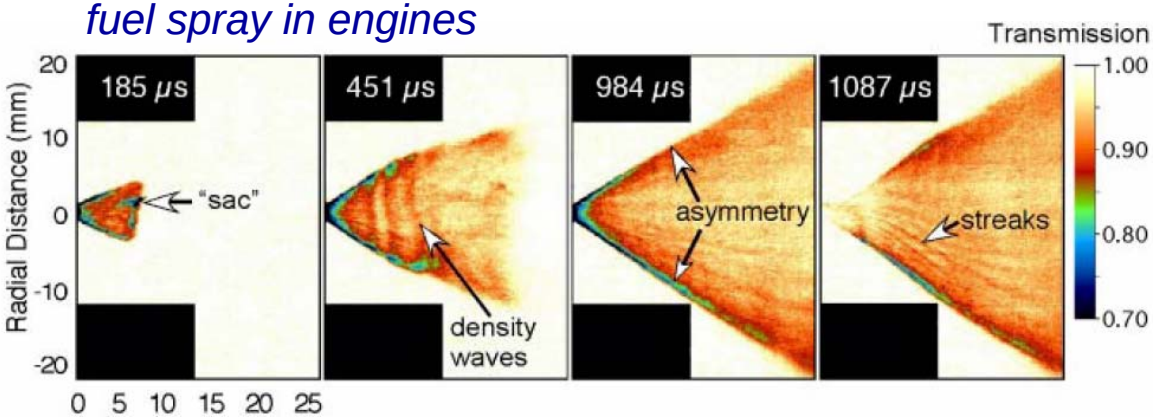
Left: Three-dimensional rendering of the air-assisted coaxial spray in the near-nozzle region of an industrial paint spray gun (Illinois Tool Works, Inc.) with an air pressure of 137kPa. The false color intensity represents the liquid volume fraction, which was quantified for the first time with the x-ray phase-contrast imaging. (Courtesy of Francesco De Carlo of the APS.)



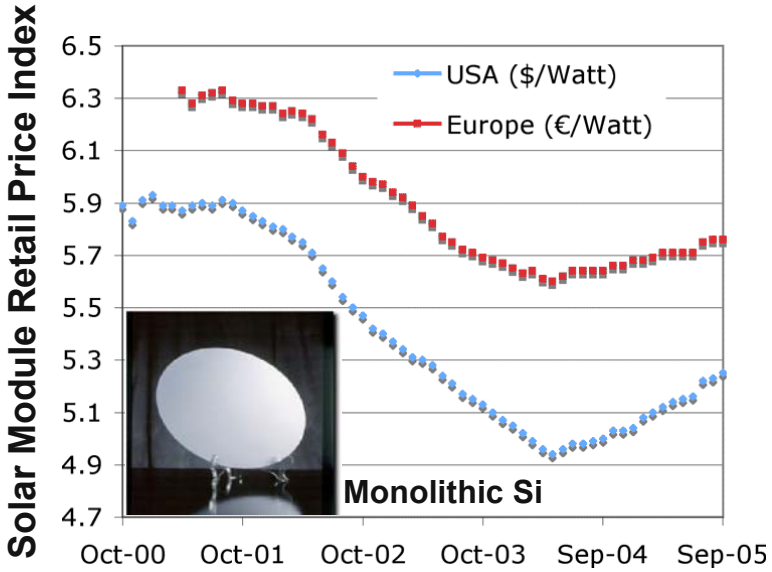


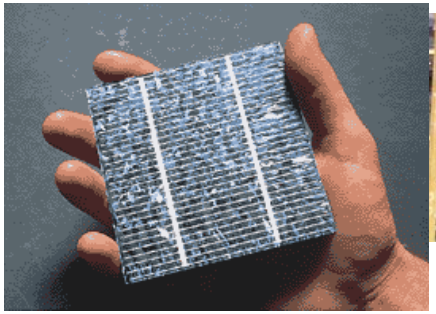
X-ray flash imaging at 300ns !!

fuel spray in engines



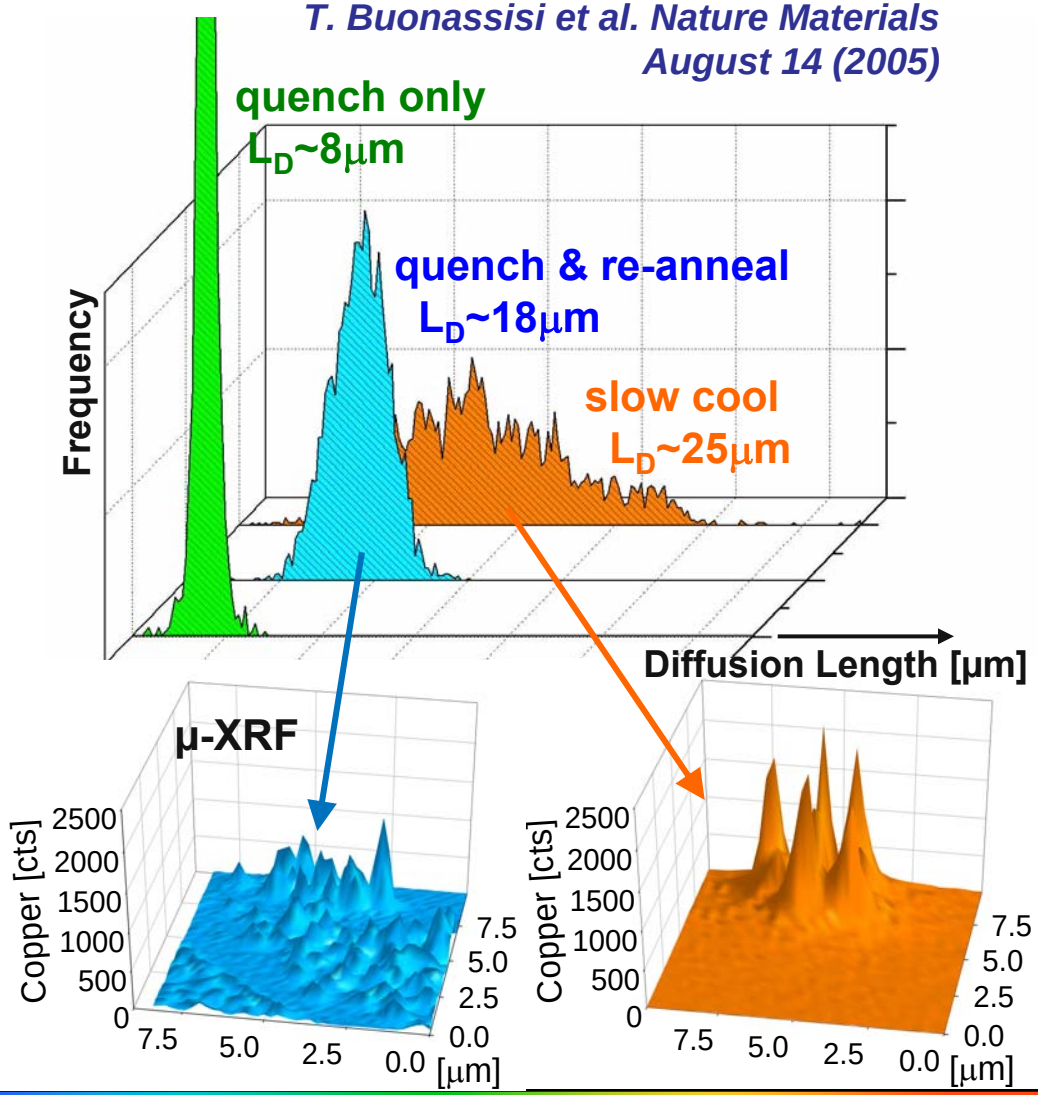
STXM example - Defect engineering for less-costly solar cells





Multicrystalline mc-Si

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



- **Metal impurities in mc-Si**

➔ **Device performance?**

➔ **Defect engineering?**

X-Ray fluorescence imaging of single bacterial cells

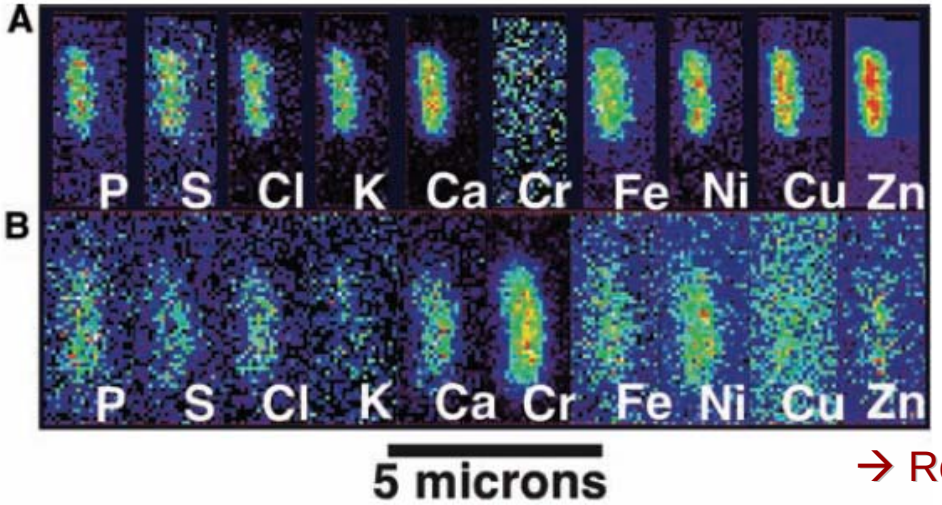
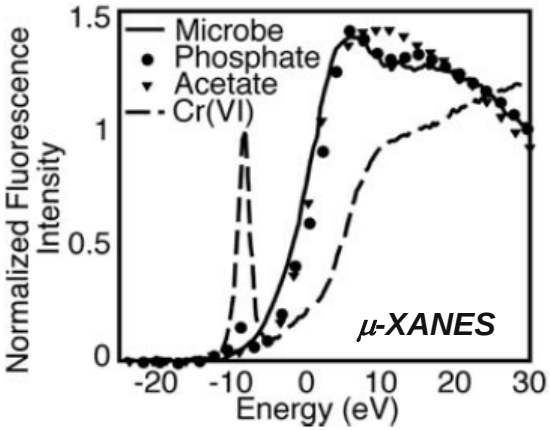
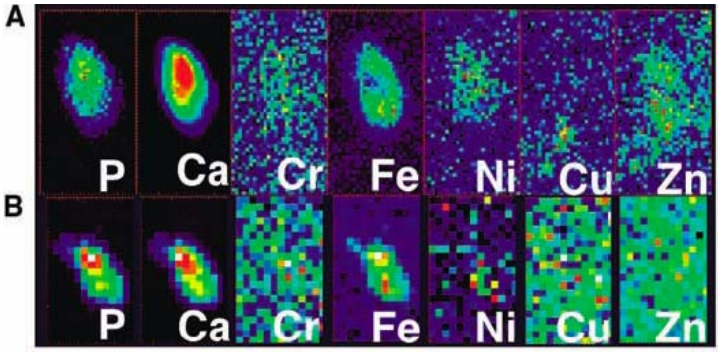


Fig. 1. False-color micro-XRF maps of qualitative spatial distributions and concentration gradients of elements in and around planktonic *P. fluorescens* microbes harvested before (**A**) and after (**B**) exposure to potassium dichromate [Cr(VI)] solution (1000 ppm) for 6 hours.

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



→ Redox states Cr(III)



A: planktonic bacterium cell before exposure to Cr

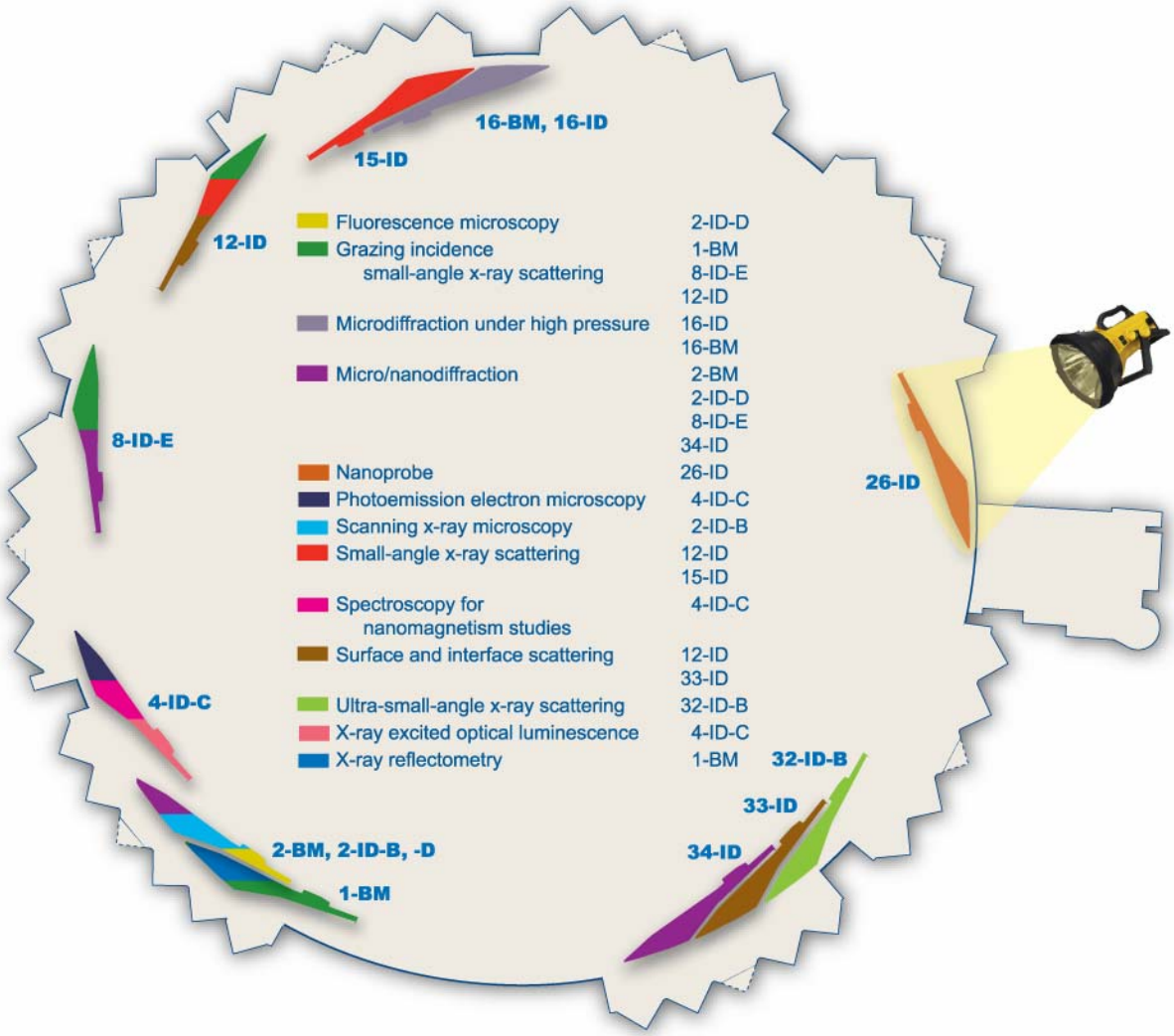
B: planktonic cell after exposure to 1000 ppm Cr(VI)

Isolated planktonic cell accumulates Cr, looses 'typical' cellular elements, and stains 'dead'

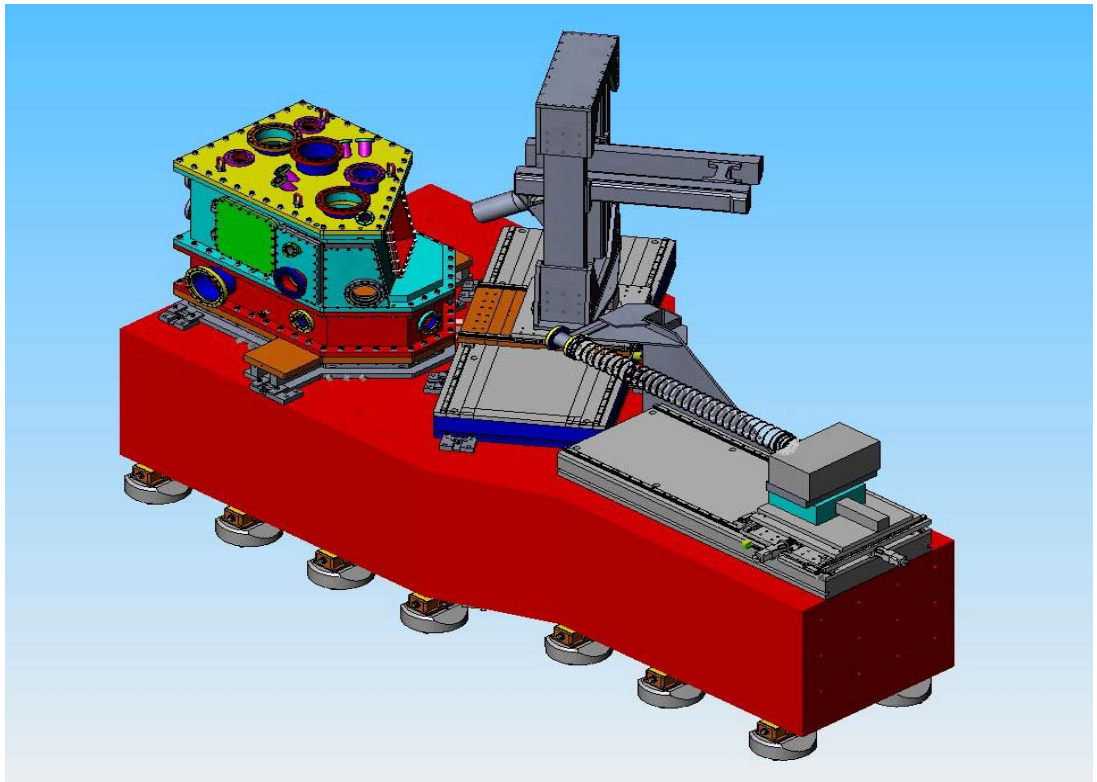
Surface adhered cell does not take up Cr, shows no change in elemental content, and remains alive

Attachment of prokaryotic cells to surfaces modulates elemental content and response to environmental challenges

APS science at the nanoscale



Center for Nanoscale Materials (CNM)

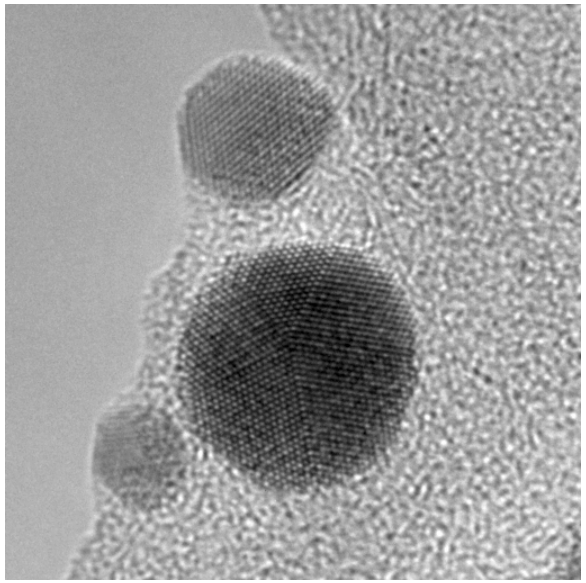


Nanoprobe finishing construction
at 26-ID will be jointly operated by CNM and APS

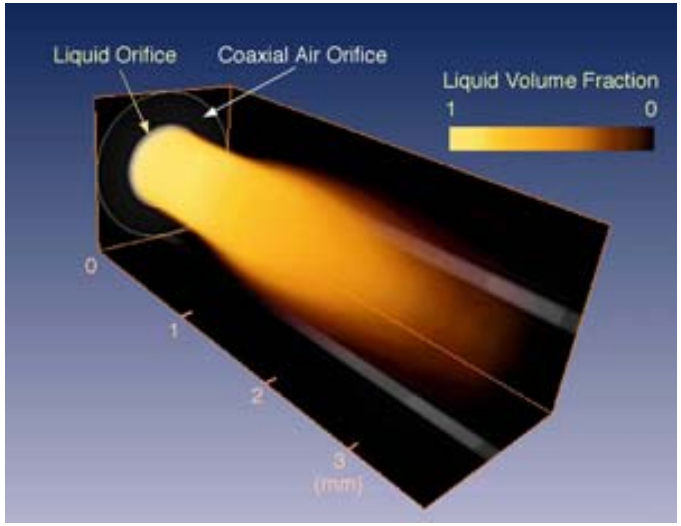
Aiming for a 10-nm-resolution x-ray microscope

X-rays complementary to other imaging techniques….

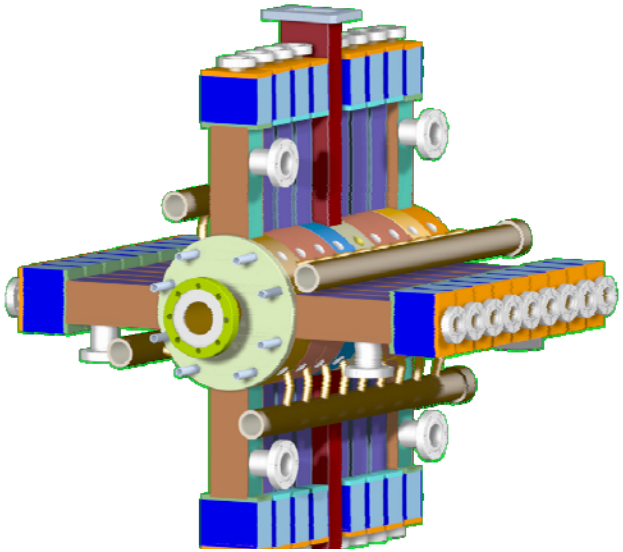
- X-ray sources better suited for studying large volume samples and doing some averaging (scattering cross section is low relative to electrons, radiation damage is comparable)
  - Precision measurements of structure, lattice spacing and strain, magnetization..
  - Higher spectroscopic sensitivity to low concentration
- Or, *in-situ* experiments where penetration is needed

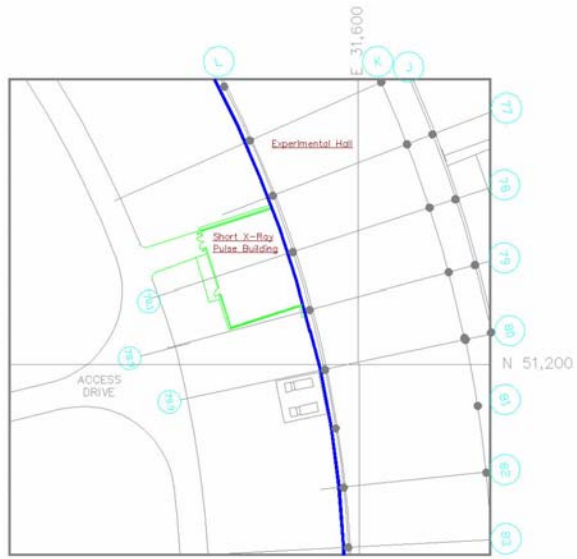


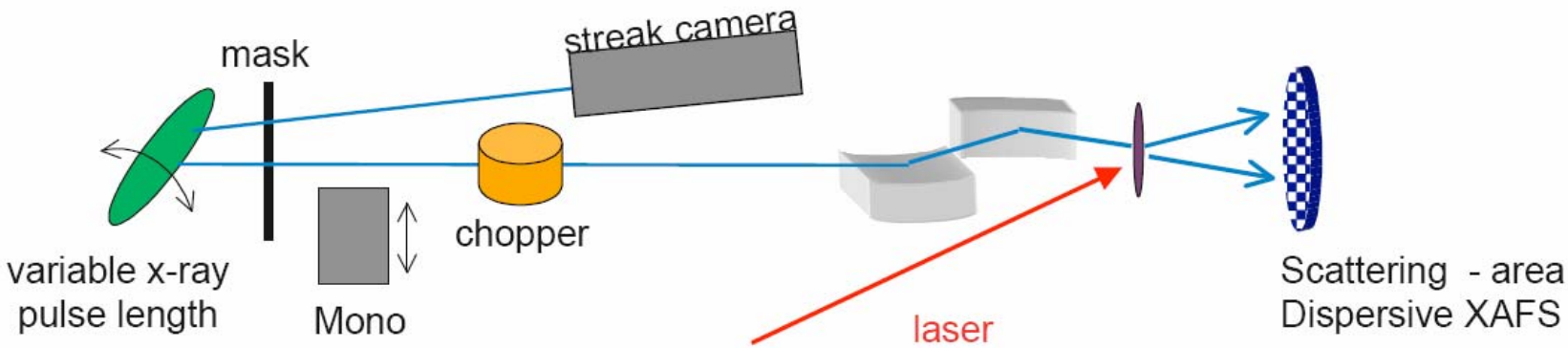
Transmission Electron Microscopy



Short pulses at APS
A million photons in a trillionth of a second at sector 7 in 2008

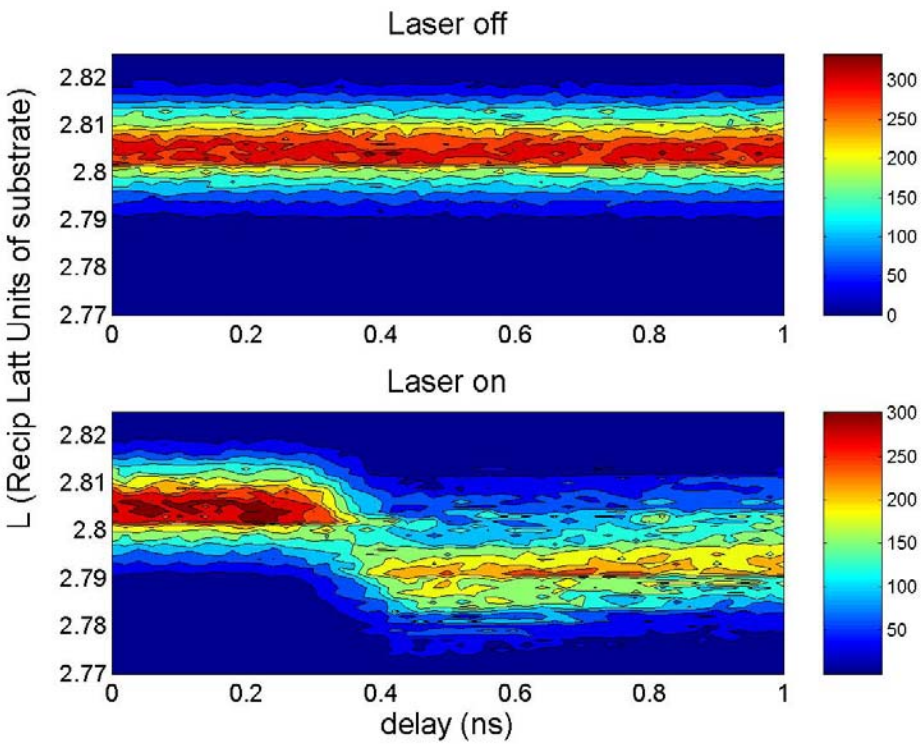




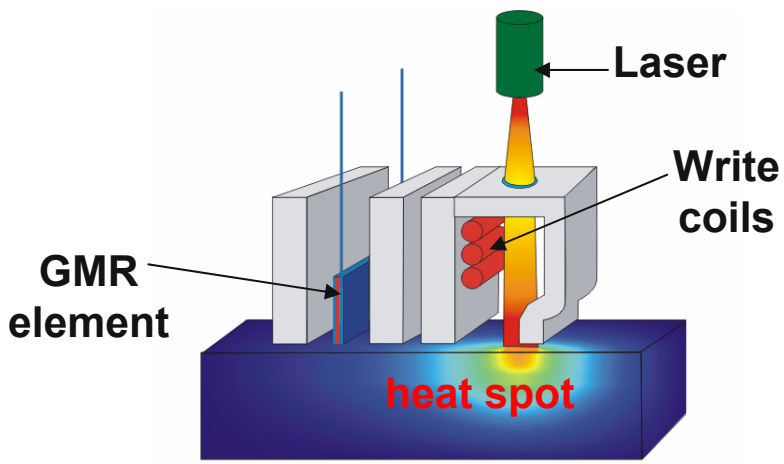


Fast dynamics: FeRh lattice-expansion phase transition

Motivation: Explore correlated magnetic and structural phase transitions in a material of technological interest

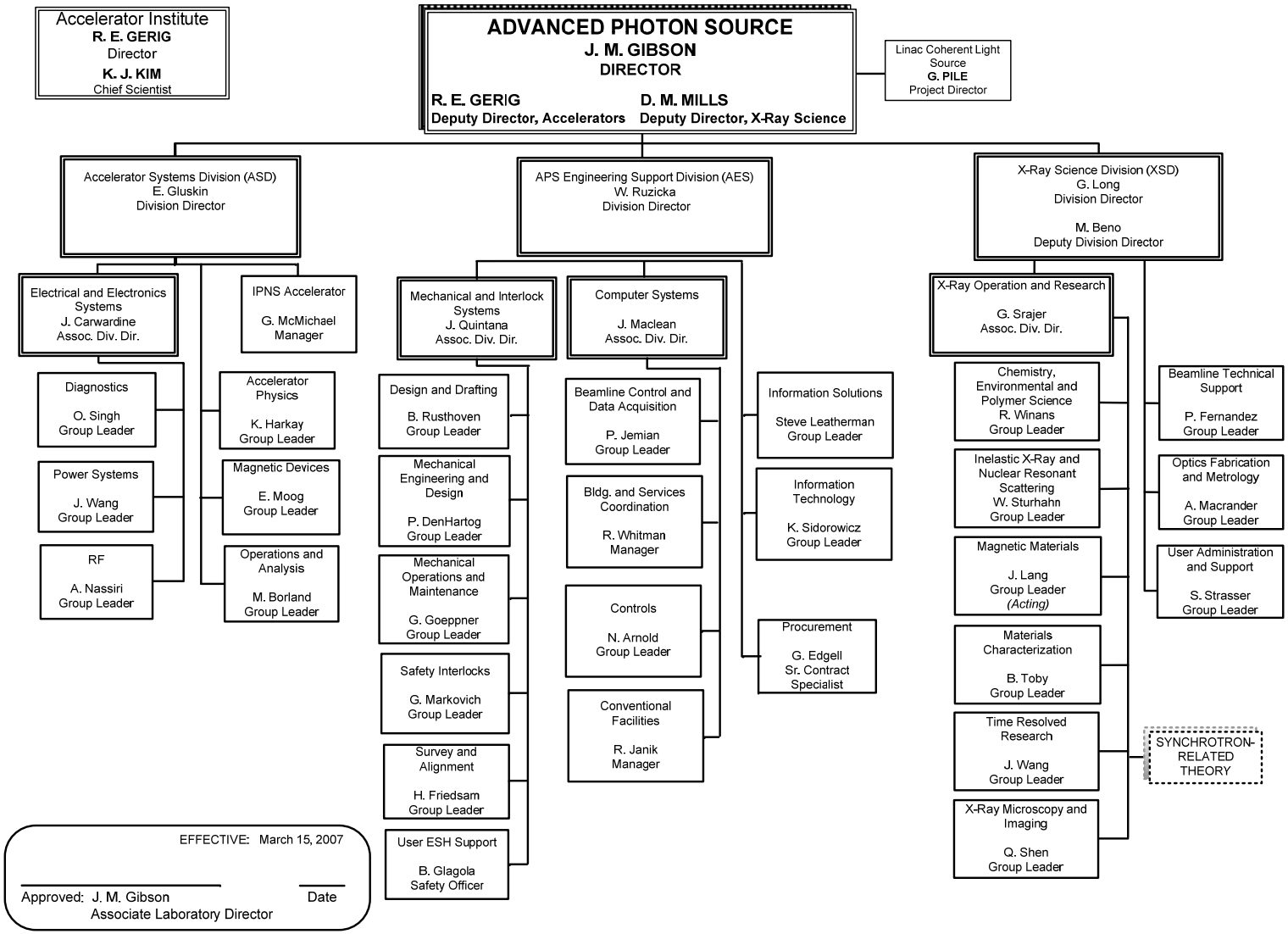


- Ultrafast laser induces magnetic phase transition (~500 fs) and anomalous lattice expansion
- Present measurements on homogeneous thin films
- Material may have applications in laser assisted recording:

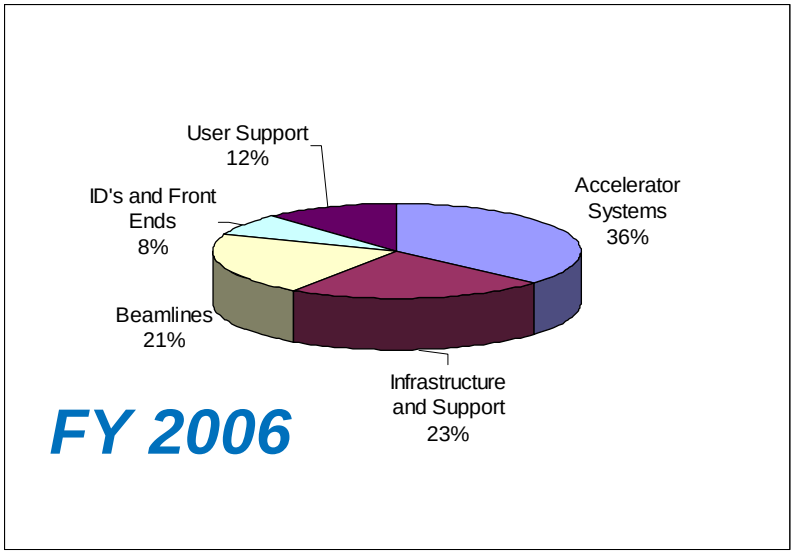


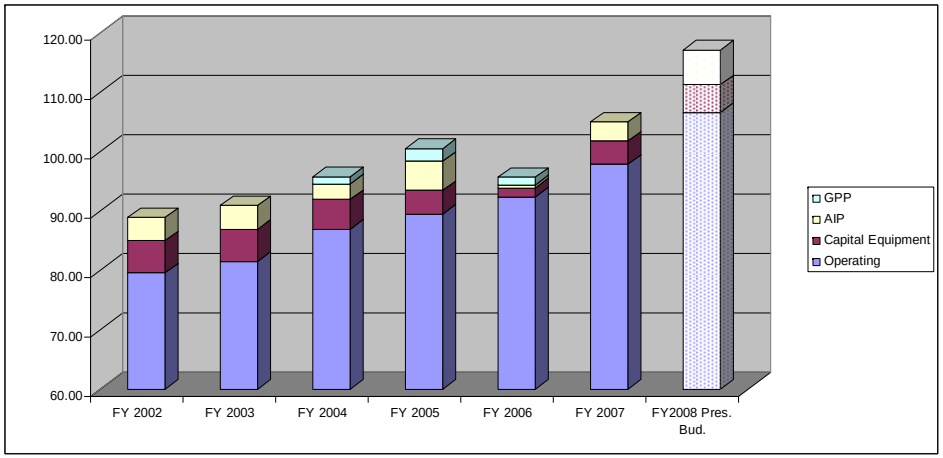
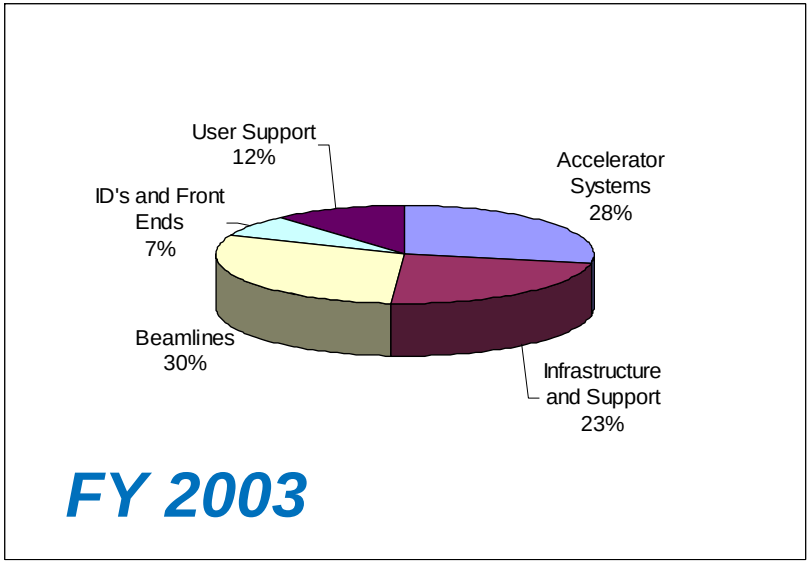
Phase contrast imaging hits Times Square last week…

APS Internal Structure



APS has been allocating more towards beamline research and operations





Budget has grown, but we also had to reallocate resources internally