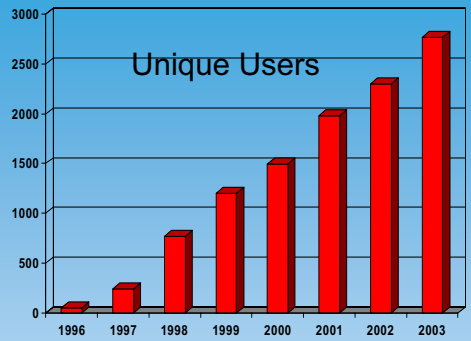
Advanced
Photon
Source

APS Update for the 2004 Users Meeting

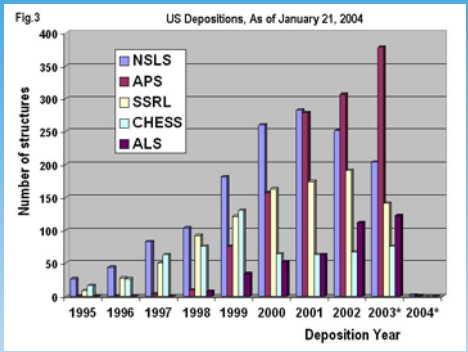
J. Murray Gibson
Associate Laboratory Director
Argonne National Laboratory

APS at the APS

Milestones

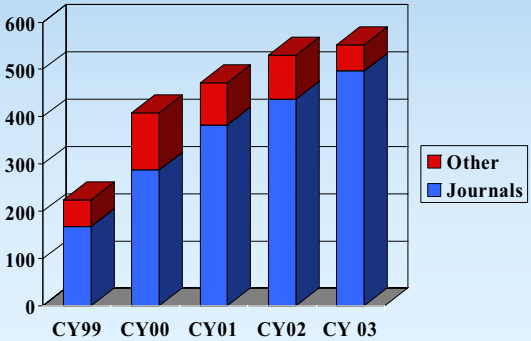


Protein Databank History (US)



Median distance to home of a US APS user has increased from 400 miles in 1999 to 660 miles in 2003

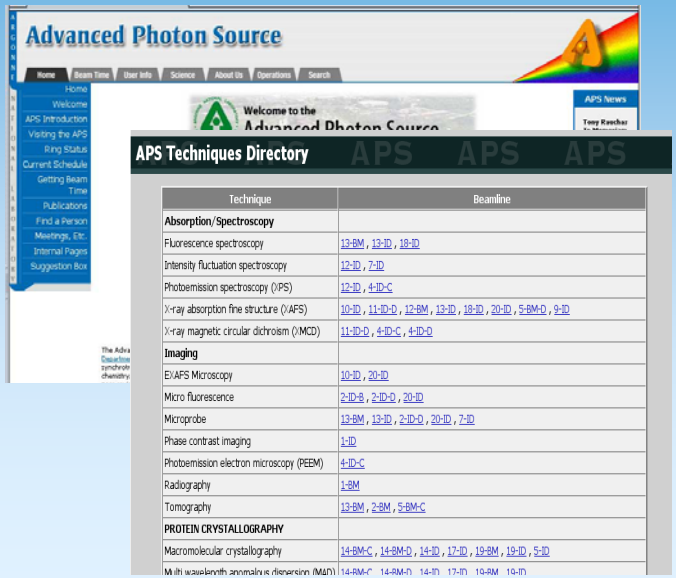
Publications



Thriving general-user program

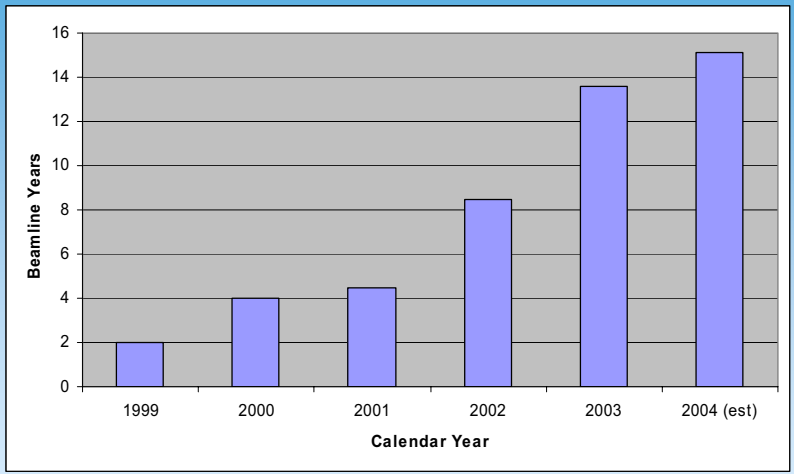
Web-based submission (www.aps.anl.gov)
8 Independent Proposal Review Panels
2 Beamtime Allocation Committees

1270 beamtime requests (890 proposals) submitted in 2003
~ 8500 8 hr shifts allocated (>**13 beamline years**)
~ 60% proposal success rate



Technique	Beamline
Absorption/Spectroscopy	
Fluorescence spectroscopy	13-BM , 13-ID , 18-ID
Intensity fluctuation spectroscopy	12-ID , 7-ID
Photoemission spectroscopy (UPS)	12-ID , 4-ID-C
X-ray absorption fine structure (XAFS)	10-ID , 11-ID-D , 12-BM , 13-ID , 18-ID , 20-ID , 5-BM-D , 9-ID
X-ray magnetic circular dichroism (XMCD)	11-ID-D , 4-ID-C , 4-ID-D
Imaging	
EXAFS Microscopy	10-ID , 20-ID
Micro fluorescence	2-ID-B , 2-ID-D , 20-ID
Microprobe	13-BM , 13-ID , 2-ID-D , 20-ID , 7-ID
Phase contrast imaging	1-ID
Photoemission electron microscopy (PEEM)	4-ID-C
Radiography	1-BM
Tomography	13-BM , 2-BM , 5-BM-C
PROTEIN CRYSTALLOGRAPHY	
Macromolecular crystallography	14-BM-C , 14-BM-D , 14-ID , 17-ID , 19-BM , 19-ID , 5-ID
Multi wavelength anomalous dispersion (MAD)	14-BM-C , 14-BM-D , 14-ID , 17-ID , 19-BM , 19-ID

Number of beamline years available for general users



Partnerships

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- Many of our productive beamlines are built on strong partnerships with outside institutions
- We appreciate successful collaborative access teams, and provide a flexible model for involving partner users now and in the future
- Example of new partner user proposals:
  - IXS Collaborative Development Team (new sector - 30)
  - Enhanced Sensitivity of X-ray Magnetic Circular Dichroism Measurements Using Phase Lock-in Detection (Sector 4, 15% , 2 yrs)
  - Ultrafast X-Ray Science (Sector 7, 20%, 3 years)

SCIENTIFIC IMPACT

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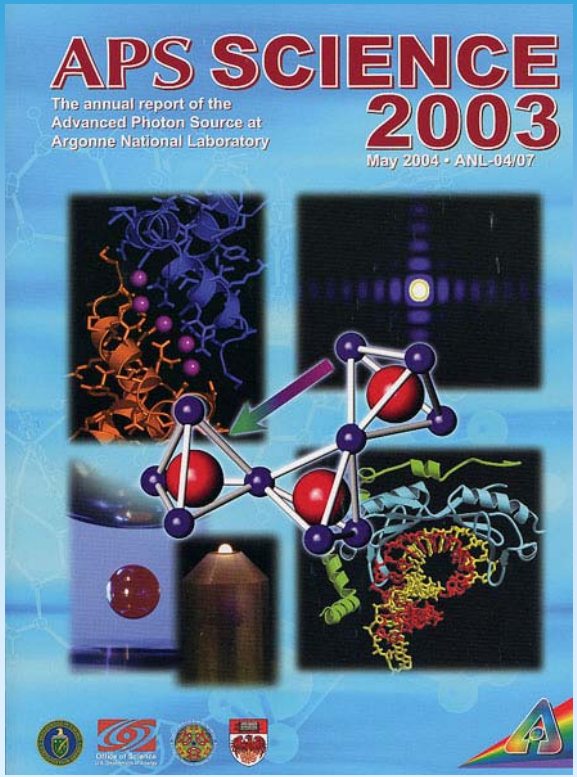
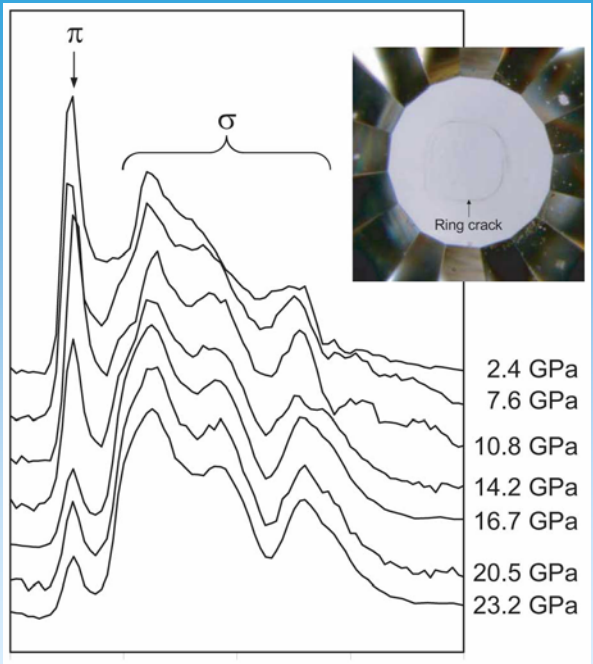


Soft graphite becomes superhard under high pressure

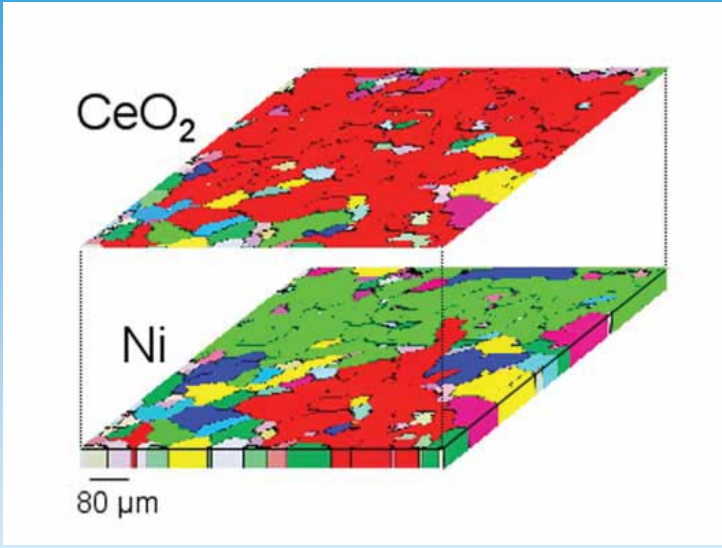


IXS spectra for compressed graphite plotted as normalized intensity (i.e., scattered intensity normalized to the incoming intensity) versus energy loss (incident energy minus analyzer energy). The spectra were taken in the vertical direction, which probes the c plane. The lower energy peak corresponds to transitions associated with π bonding and the higher energy portion corresponds to transitions associated with s bonding. After the transition at ~17 GPa, the s bonds increase at the expense of the π bonds. The insert shows a photomicrograph of the indentation of a diamond anvil by the compressed, superhard graphite sample.

HP-CAT 16-ID

W.L. Mao et al., "Bonding Changes in Compressed Superhard Graphite," Science **302**(17), 425-427 (October 2003).

Two growth modes for oxide films on textured metal substrates

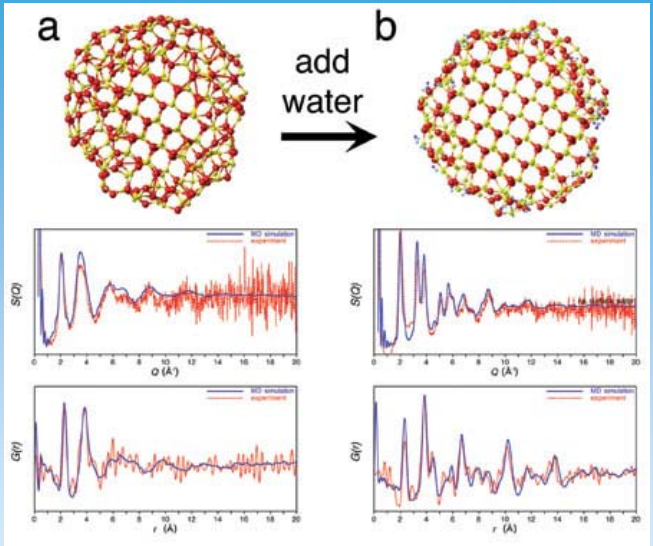


Orientation maps from a deposited oxide film and a textured Ni substrate obtained by using x-ray Laue microdiffraction. Black lines within each map indicate boundaries where the total misorientation is greater than 5°. Each colored area shows a percolative region connected by boundaries of less than 5°. The oxide film exhibits larger percolation distances than the substrate, due to crystallographic tilts induced during epitaxial growth.

UNI-CAT 34-ID and MHATT/XOR 7-ID

J.D. Budai et al.,, "X-ray microdiffraction study of growth modes and crystallographic tilts in oxide films on metal substrates," Nat. Mater. **2**, 487-492 (July 2003).

With nanoparticles, a little water on the outside can rearrange the atoms on the inside



Water binds to the surface of zinc sulfide nanoparticles in methanol and drives a transition from structural disorder (a) to order (b). From wide angle x-ray scattering data acquired versus diffraction vector, Q, the researchers calculate the structure factors, S(Q), and the real-space pair distribution functions, G(r) of the nanoparticles before and after the transformation. Molecular dynamics simulations reproduce the x-ray scattering data and provide specific predictions of the nanoparticle structure.

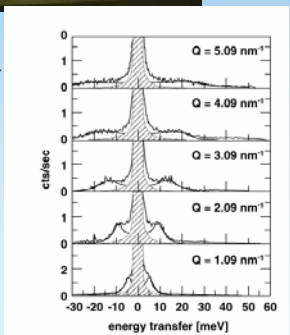
BESSRC/XOR 11 ID-C

Z.H. Zhang, B. Gilbert, F. Huang, and J.F. Banfield, "Water-driven transformation of nanoparticle structure at room temperature," Nature **424**, 1025-1029 (23 August 2003)

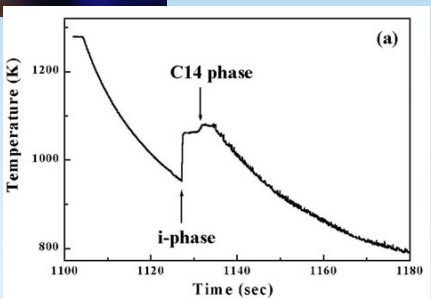
There's a whole lot of levitating going on…

Liquid TiZrNi crystallization inhibited by icosahedral order
MU-CAT 6-ID

Liquid alumina at 1800°C
IXS shows anomalously low damping
XOR 3-ID

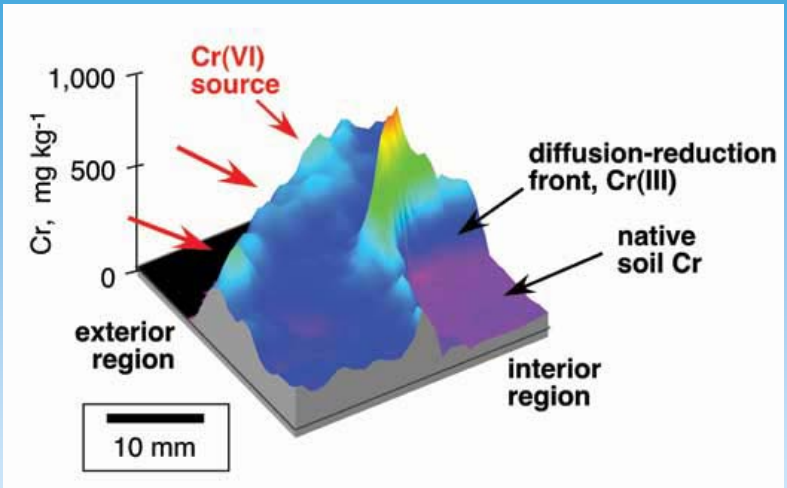


H. Sinn et al., Science **299**, 2047-2049 (2003)



K.F. Kelton et al., Phys. Rev. Lett. **90**(19), 195504-1 (2003)

Distribution of chromium contamination and microbial activity in soil aggregates

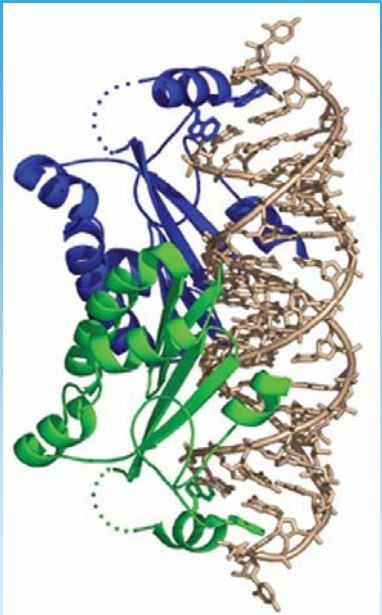


Chromium distribution in a quarter-section slice through a natural soil aggregate, 31 days after exposure. Chromium occurs primarily as Cr(VI) along the exterior , and primarily as Cr(III) at the diffusion-reduction front.

GSECARS 13-ID

T.K. Tokunaga et al., "Distribution of Chromium Contamination and Microbial Activity in Soil Aggregates," J. Environ. Qual. **32**, 541-549 (March-April 2003).

Plant virus defends itself with tiny caliper

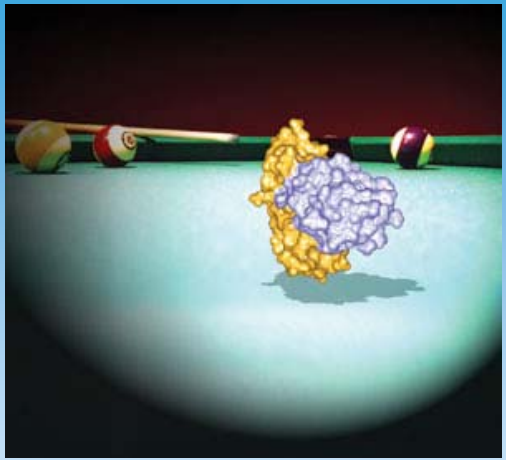


Two viral p19 protein molecules (green, blue) join to form a long groove for binding RNA fragments that would destroy the virus if left alone.

SER-CAT 22-ID

J.M. Vargason et al., "Size Selective Recognition of siRNA by an RNA Silencing Suppressor," Cell **115**, 799–811 (26 December 2003).

How ubiquitin takes its cue



The CUE domain (gold) joins in pairs to form a basket-like pocket that cups the ubiquitin protein (blue). (Image by G. Prag.)

SBC-CAT 19-ID and SER-CAT 22-ID

G. Prag et al., "Mechanism of Ubiquitin Recognition by the CUE Domain of Vps9p," Cell **113**, 609–620 (30 May 2003).

APS research on human diseases..

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- SARS
  - protease structure determined (SGX)
- Tay Sachs
  - protein changes which lead to neurological disorders (BIOCARS)
- Drug addiction
  - a promiscuous enzyme recognizes cocaine and heroin, but could detoxify sarin (SERCAT)
- Osteoporosis
  - how osteocalcin controls Ca in bones (IMCA)
- Cystic fibrosis, bacterial infections, lupus..

These and other highlights in the 2003 annual report…

Recognizing APS users…..

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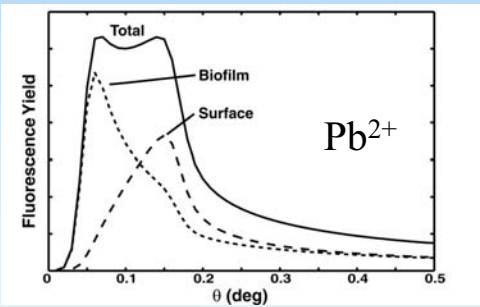
Amy Rosenzweig (DND-CAT & Northwestern University) received a prestigious MacArthur grant

For her studies of metalloproteins, which contain metal ions (iron, copper or zinc) in addition to carbon, oxygen, nitrogen, hydrogen and sulfur atoms

Only Illinois resident chosen; one of 12 women and 12 men across all intellectual endeavors who were awarded no-strings-attached 2003 "genius grants"

The Rosalind Franklin Award

Alexis Templeton (PhD Stanford 2002) studies biofilms at the Scripps Institute of Oceanography; and their role in changing the chemical form of impurities – important in understanding deep-sea landforms and environmental remediation



“The accelerator performance is outstanding”

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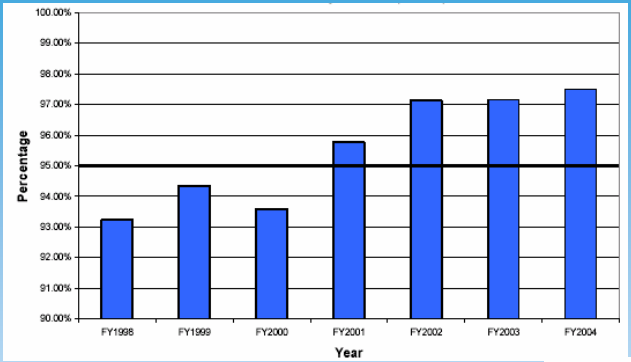
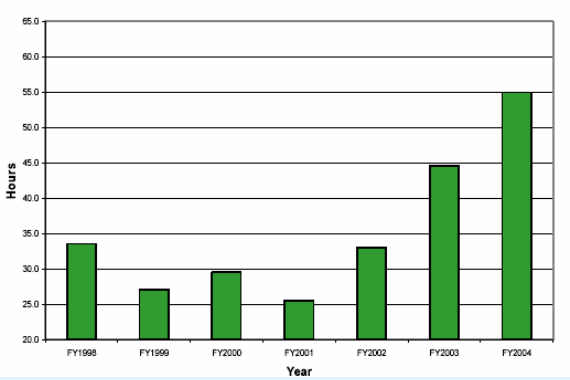
UC Review Committee

Machine reliability



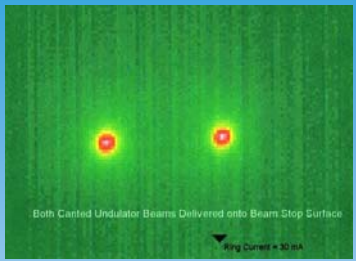
Availability in %
to date (goal is 95%)

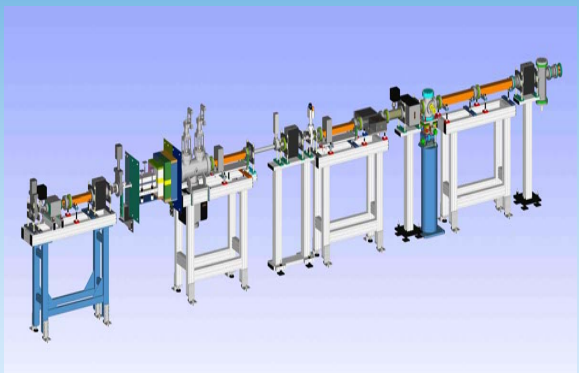
Mean time between
faults in hours
(stretch goal is 48 hours)



Machine improvements

- Stability is outstanding
- New canted-undulators delivering light

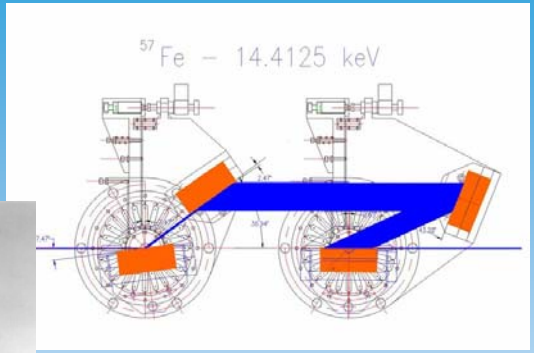


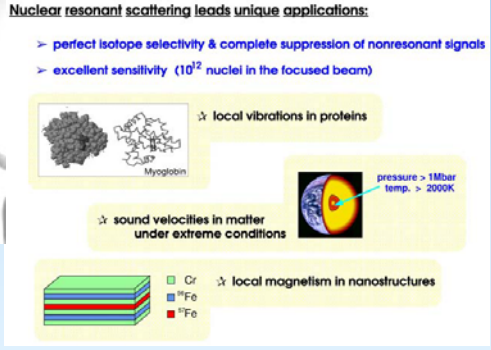


Higher power front ends developed

Great science from great instruments

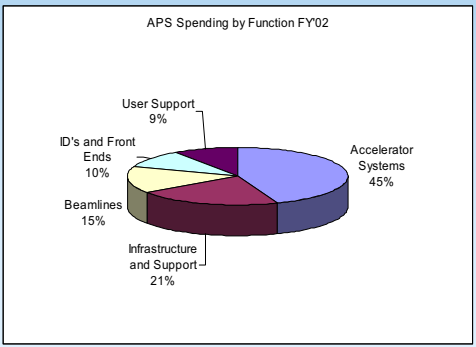
- Wolfgang Sturhahn and Thomas Toellner win the 2004 University of Chicago Distinguished Performance Award

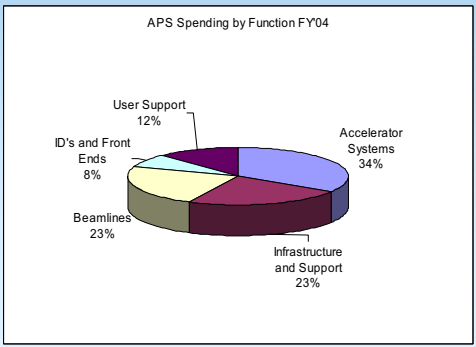




Growing mission for the APS

- APS has growing responsibility for BES sectors
  - offering stability of support
  - optimization of dedicated beamlines
- Opportunity to retain appropriate existing partners and encourage future partnerships
- Enhancing user support for all users and sectors





X-ray Operations and Research increases responsibility for BES sectors

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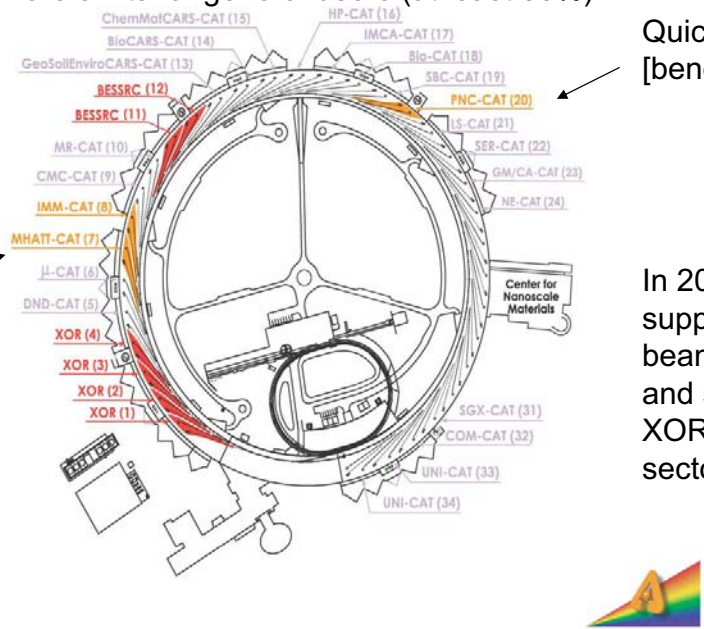
More shifts for general users (at least 50%)

Quick EXAFS [bending magnet]

Photon Correlation Spectroscopy

Time-Resolved Program



In 2004 we will support 26 beamline scientists and staff on new XOR/BES sectors

also new sectors, IXS(30), Nano(26), and Powder Diffraction(11BM)

The challenge – developing a suite of dedicated beamlines

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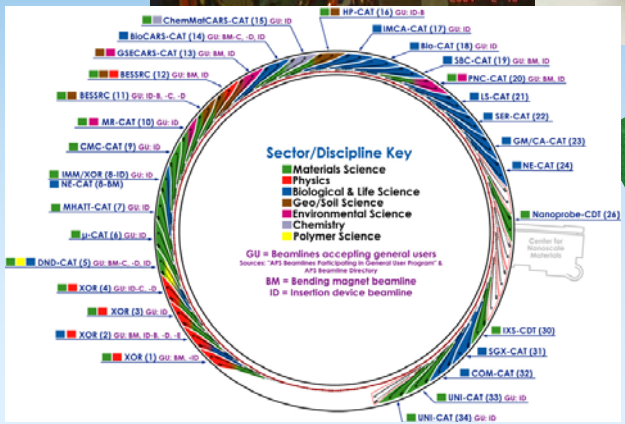
Enhanced user support

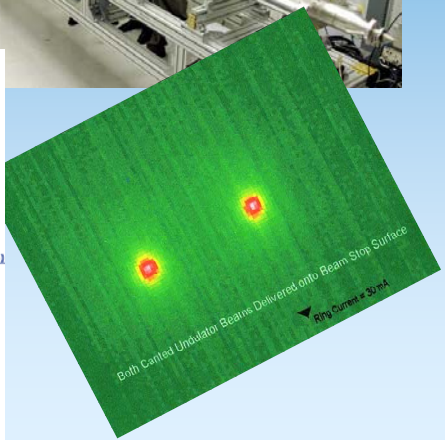
Enhanced user support

- Detector pool
- Beamline controls
- Computing
- Database management
- Mechanical and electrical engineering
- User program administration
- Environment, safety, and health

New sectors

2004 2 18


ChemMatCARS-CAT (15) GU: ID
HP-CAT (16) GU: ID-B
BioCARS-CAT (14) GU: BM-C, -D, ID
IMCA-CAT (17) GU: ID
GSECARS-CAT (13) GU: BM, ID
Bio-CAT (18) GU: ID
BESSRC (12) GU: BM, ID
SBC-CAT (19) GU: BM, ID
BESSRC (11) GU: ID-B, -C, -D
PNC-CAT (20) GU: BM, ID
MR-CAT (10) GU: ID
LS-CAT (21)
CMC-CAT (9) GU: ID
SER-CAT (22)
GM/CA-CAT (23)
IMM/XOR (8-ID) GU: ID
NE-CAT (8-BM)
NE-CAT (24)
MHATT-CAT (7) GU: ID
Nanoprobe-CDT (26)
μ-CAT (6) GU: ID
DND-CAT (5) GU: BM-C, -D, ID
XOR (4) GU: ID-C, -D
XOR (3) GU: ID
IXS-CDT (30)
XOR (2) GU: BM, ID-B, -D, -E
SGX-CAT (31)
XOR (1) GU: BM, -ID
COM-CAT (32)
UNI-CAT (33) GU: ID
UNI-CAT (34) GU: ID
Sector/Discipline Key
Materials Science
Physics
Biological & Life Science
Geo/Soil Science
Environmental Science
Chemistry
Polymer Science
GU = Beamlines accepting general users
Sources: "APS Beamlines Participating in General User Program" & APS Beamline Directory
BM = Bending magnet beamline
ID = Insertion device beamline
Center for Nanoscale Materials


Both Canted Undulator Beams Delivered onto Beam Stop Surface
Ring Current = 30 mA

Center for Nanoscale Materials

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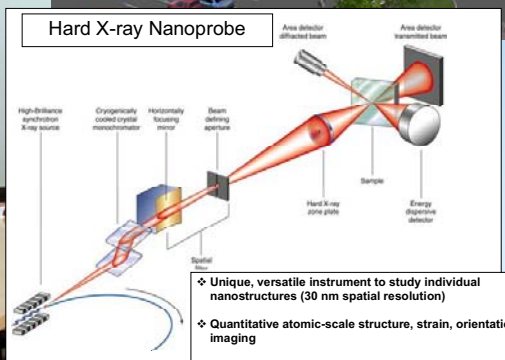

- Unique, versatile instrument to study individual nanostructures (30 nm spatial resolution)
- Quantitative atomic-scale structure, strain, orientation imaging
- Sensitive trace element and chemical state analysis
- Ability to penetrate overlayers, environments, fields

4th Generation Light Sources

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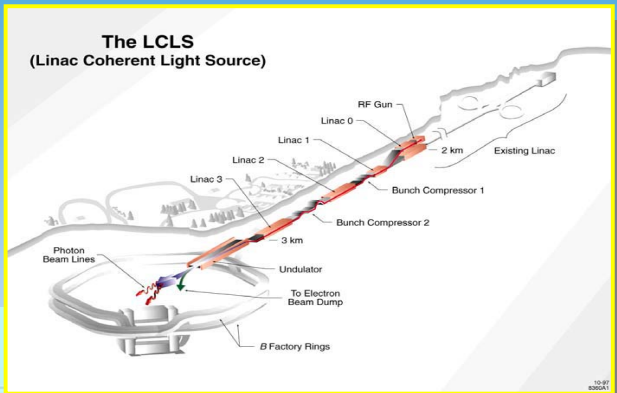
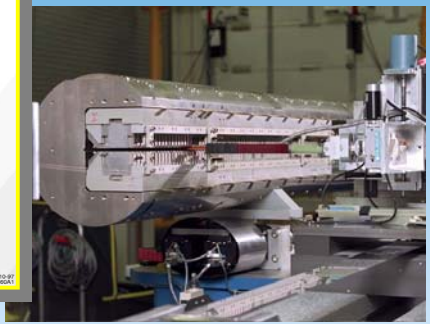
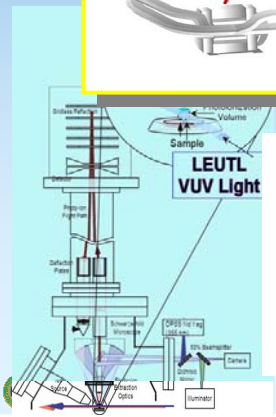
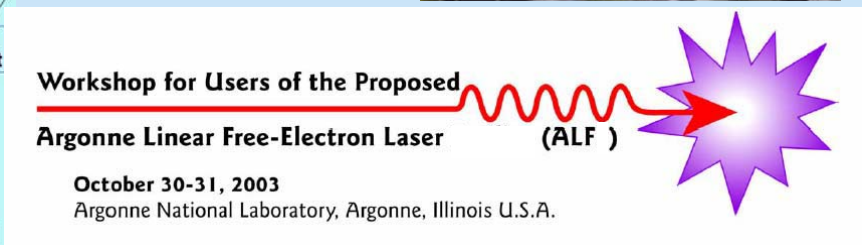
LCLS









Partners and friends…

Partner User Council chair Jim Viccaro spends a day with high-school students

APS Science Advisory Committee during cross-cut review on "Science with Microbeams," 1/04

Biological resident users sharing ideas for improved technical collaboration

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Informal Workshop for Protein Crystallography CATs
Bldg. 401, Advanced Photon Source, January 13, 2004

Argonne community

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- New Regional Biocontainment Laboratory
  - and plans for a protein production facility (DOE Genomes to Life)
- Strategic emphasis on accelerators
  - APS, RIA, HEP…
- Shared interest in femtosecond science in chemistry, materials science and biology
- Strengthening connections with IPNS (Pulsed Neutron Source) and EMC (Electron Microscopy Center)

APS and the outside community

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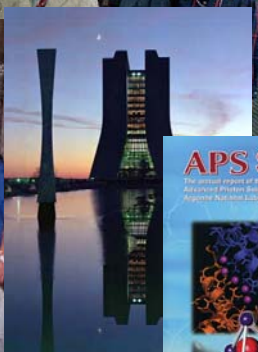

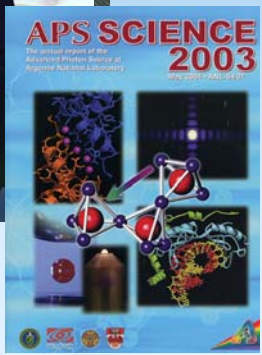

Selected APS Employee Goals for FY'04

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- **Increase the output and impact of user science**
  - Expand the size, scientific scope and national character of our user base
  - Provide advice and support for general users
  - Enhance support to sectors
  - Increase productivity of BES beamlines
  - Perform cross-cutting reviews
  - Encourage and support development of specialized beamlines
  - Foster theory activities
- Invest in the future:
  - Increase the number of graduate students and postdocs
  - Foster training in beamline and accelerator research

Pacesetters!!

For exemplary support of the mission of the Advanced Photon Source: To explore new materials, to seek out new structures, to boldly go where no light source has gone before...

Greg Banks (left, ASD) & Daniel Hausermann (right, HP-CAT) were the first to receive "Beam Me Up, Scotty" T-shirts. Banks nominated Hausermann in recognition of his tutorials on user science given to APS Main Control Room operations staff.

APS Diversity Committee

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Julie Alderman (AOD)

Joann Brown (XFD)

Kathy Harkay (ASD) – Chair

Leonard Morrison (ASD)

Nena Moonier (AOD)

Liz Moog (XFD)

Rod Salazar (AOD)

Greg Wiemerslage (XFD)

Building a working environment where everyone can contribute equally

Challenges for the future

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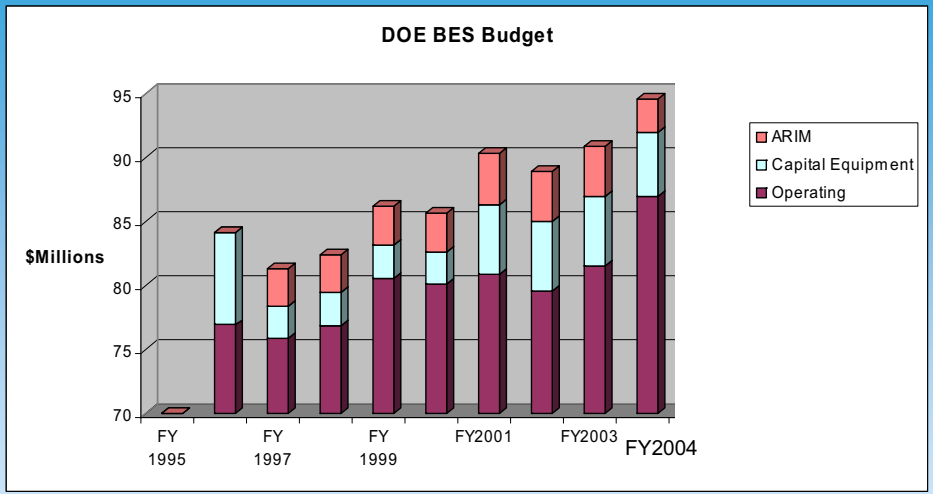
- Evolving the best set of well-supported and productive beamlines, with strong general and partner user access
- Maintaining a *state-of-the-art* machine
- Securing resources for our new mission
- Developing plans for future science directions at the APS
- Fostering detector development
- Enhancing closer interactions and support amongst biological CATs

Budget update



We received $2.4M of the $8M congressional facilities increment

Additional $3M operating income came from LCLS, CNM..

FY2005 will be challenging..

Strategic Planning: State-of-the-Art 3rd-Generation Science in 20 Years?

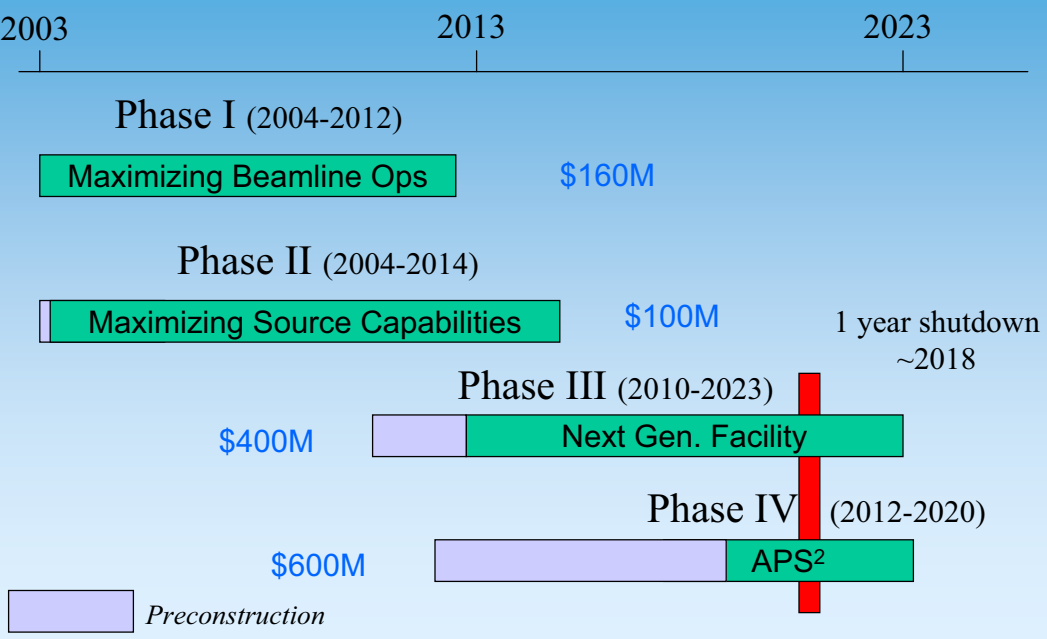
Advanced Photon Source
ARGONNE NATIONAL LABORATORY

From the 20-year Upgrade Plan:

- *Individual nanoscale objects can be observed in real time.*
- *Electronic, dynamic, and magnetic properties of a single nanostructure can be measured.*
- *A few atoms can be chemically identified.*
- *A full dataset for protein structure analysis can be collected in less than a second.*
- *X-ray imaging of objects with nm resolution is routine.*

Leads to a phased plan to upgrade APS effective performance by 3-4 orders of magnitude.

APS Upgrade Plan



A STUDY ON THE FUTURE SCIENTIFIC DIRECTIONS FOR THE ADVANCED PHOTON SOURCE

Advanced Photon Source
ARGONNE NATIONAL LABORATORY

PURPOSE: *to explore future science directions for the Advanced Photon Source (APS) users that will expand their scientific leadership and push the boundaries of the scientific frontiers in the next decade*

Gopal Shenoy, Advanced Photon Source (Chair)
Sunil Sinha, University of California San Diego (Co-chair)
sanctioned by APS Scientific Advisory Committee

Seven workshops planned, culminating in a strategic planning meeting in Fontana, WI , Sept. 2nd-3rd 2004

APS² Is on the DOE-SC Roadmap

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U.S. Department of Energy

	Priority	Program	Facility
	1	FES	ITER
	2	ASCR	UltraScale Scientific Computing Capability
Near-Term	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
	12	HEP	BTeV
	13	HEP	Linear Collider
Mid-Term	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 Facility:

Background:

What's New:

Applications:

PHASE IV – APS² – LINAC Augmented Light Source

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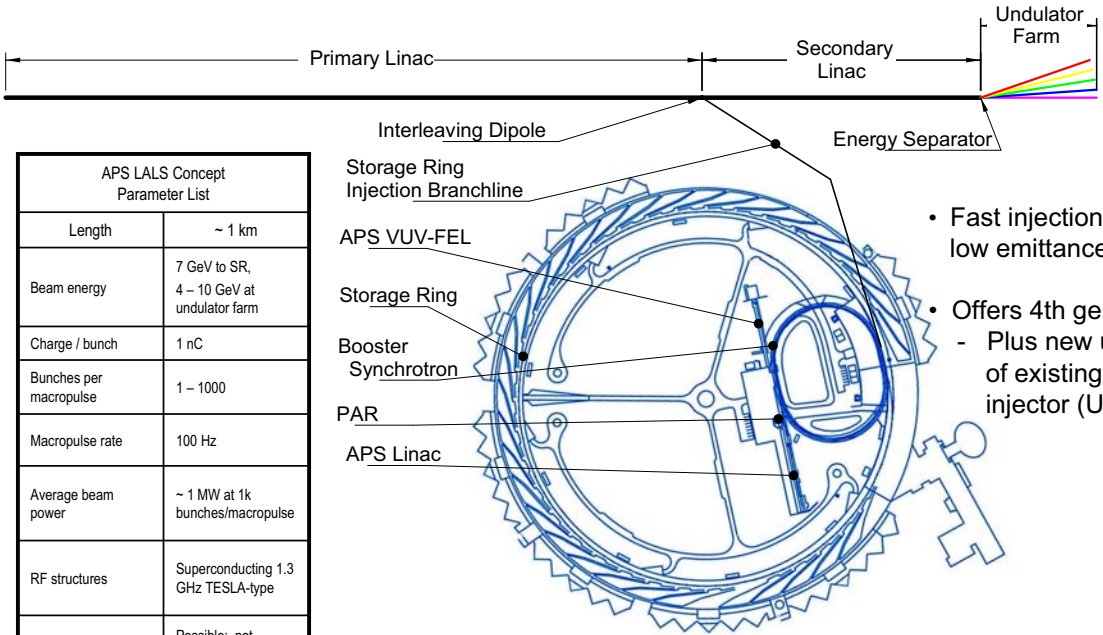

APS LALS Concept Parameter List	
Length	~ 1 km
Beam energy	7 GeV to SR, 4 – 10 GeV at undulator farm
Charge / bunch	1 nC
Bunches per macropulse	1 – 1000
Macropulse rate	100 Hz
Average beam power	~ 1 MW at 1k bunches/macropulse
RF structures	Superconducting 1.3 GHz TESLA-type
Recirculation?	Possible; not required for low beam power operation

- Fast injection, low emittance
- Offers 4th gen.
  - Plus new use of existing injector (UV,IR)

One possibility…

Courtesy of J. Lewellen, APS/ANL

The ingredients of our success

- Outstanding machine performance
- Accessibility and responsiveness to users
- Partnerships
- Great people working at the APS – employees and resident users