Argonne
NATIONAL LABORATORY

The Advanced Photon Source (APS):

current status and future needs from a materials science perspective

J. Murray Gibson

Associate Laboratory Director for Scientific User Facilities

Director, Advanced Photon Source

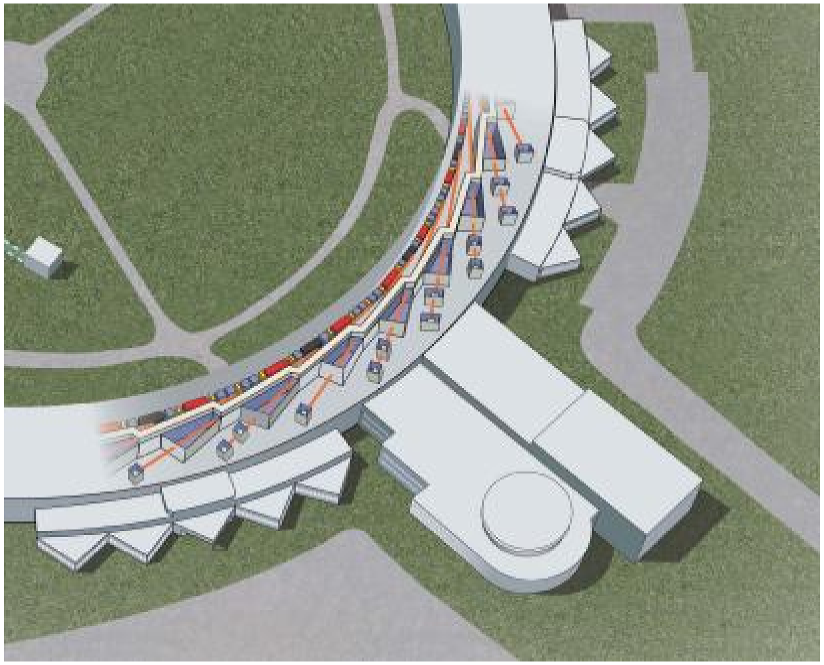
Presented to the SSSC Committee of the NRC, April 6th 2006 Washington DC

Outline

- What is the status of the APS today?
  - Overview of our successes and challenges
- Solutions and needs
  - From a one-year perspective
    - *Budget needs for APS in 2007*
  - From a five year perspective
    - *APS upgrade to maximize scientific impact*
- The APS in the national and international context

One of three in the world: the US's high-energy (7 GeV) third-generation x-ray synchrotron source

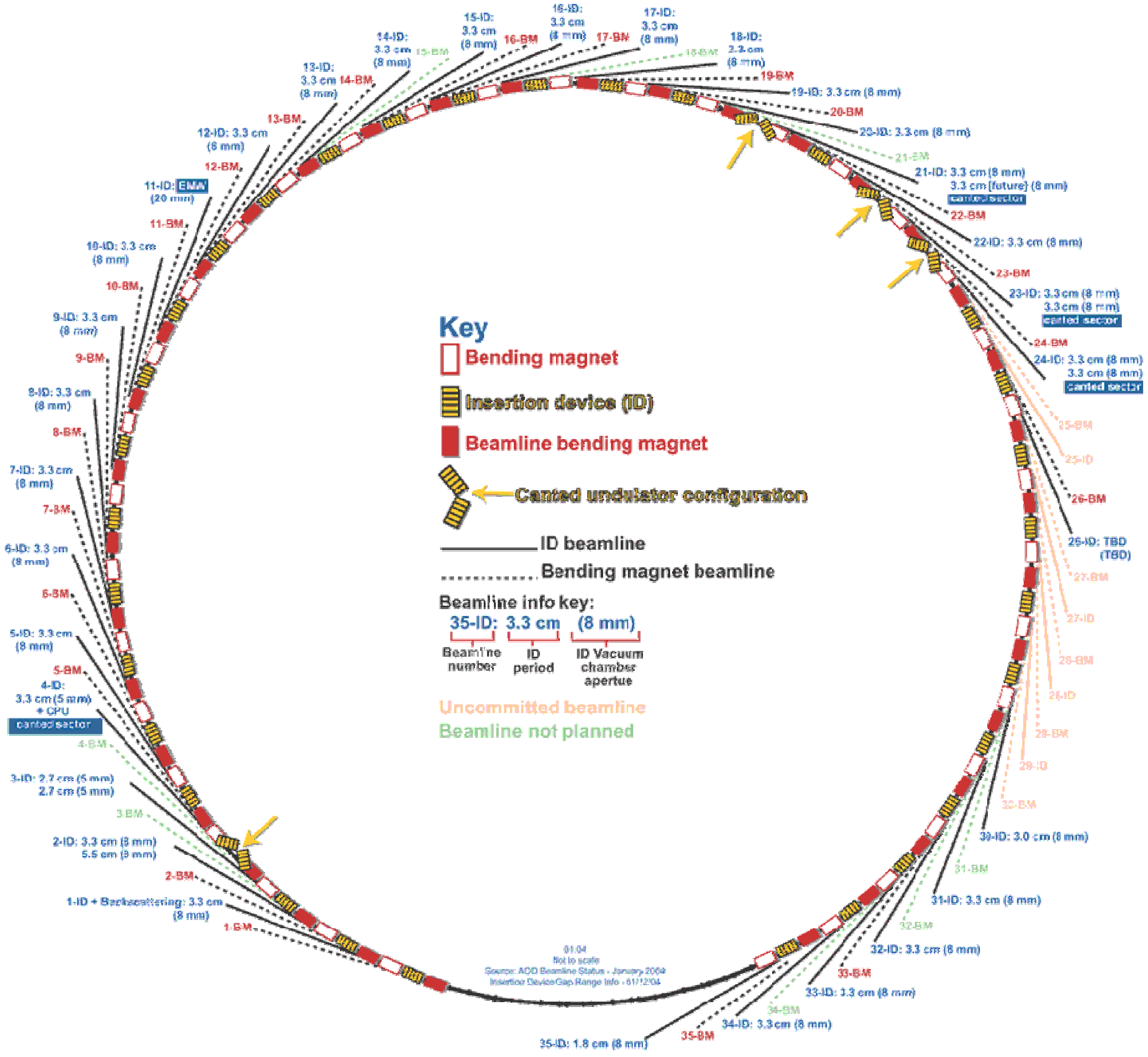
Making brilliant x-rays: synchrotron radiation



- High characteristic energies at APS ~25kV
- Relativity helps increase brilliance at high electron energies

Each insertion device or bending magnet creates at least one independent source of x-rays which permits many scientists to operate at the same time– so although the facility is large and relatively expensive to run, it is “massively parallel”

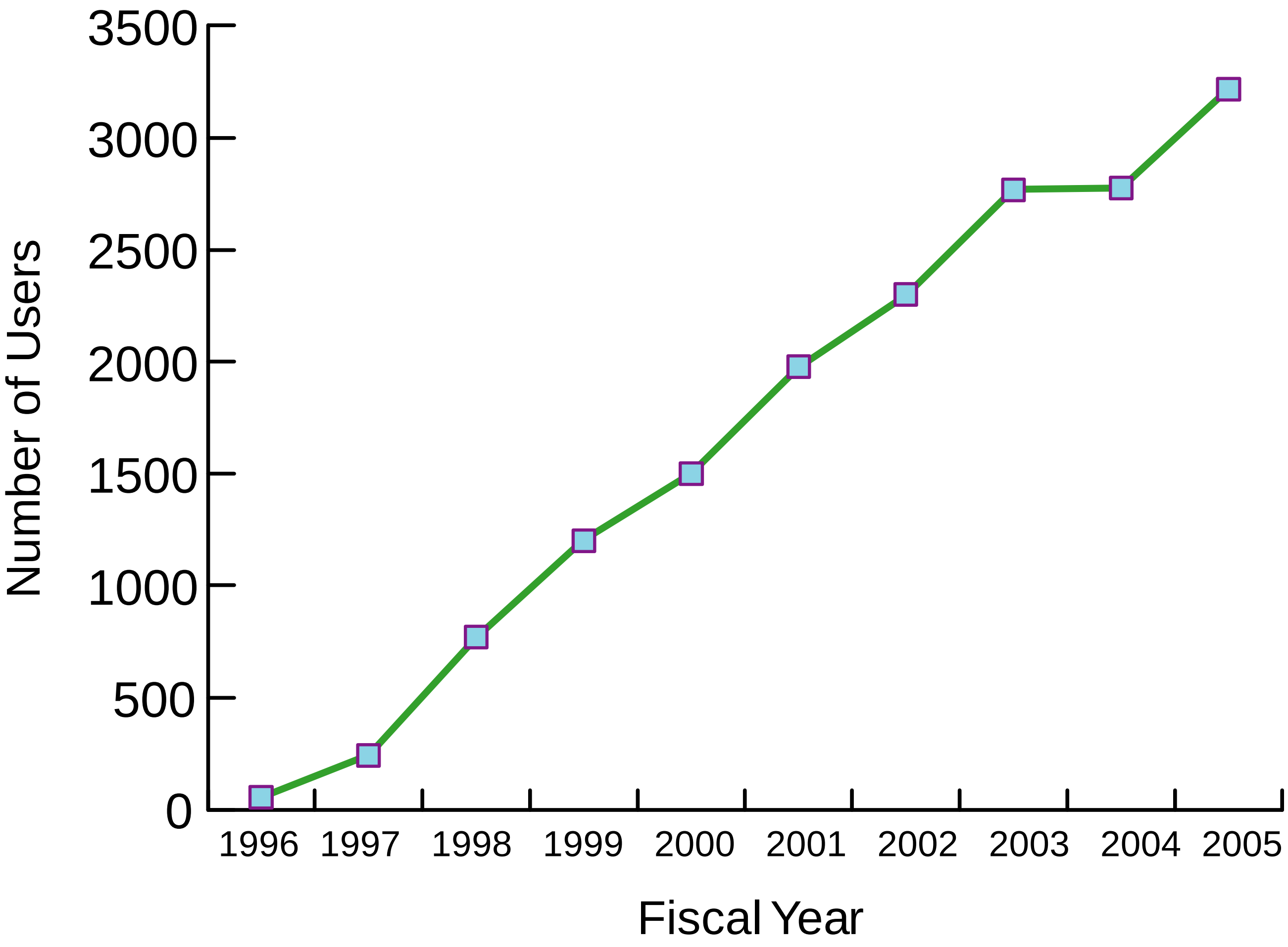
Beamlines at the APS



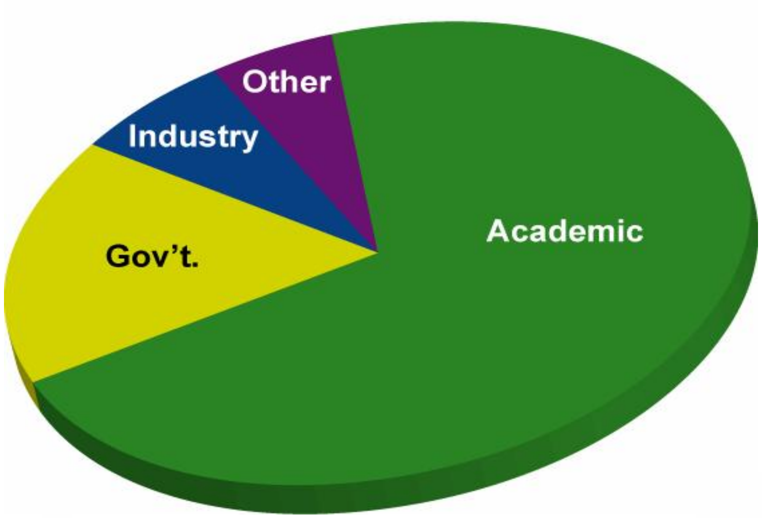
01/04
Not to scale
Source: AOD Beamline Status - January 2004
Insertion Device Gap Range Info - 01/12/04

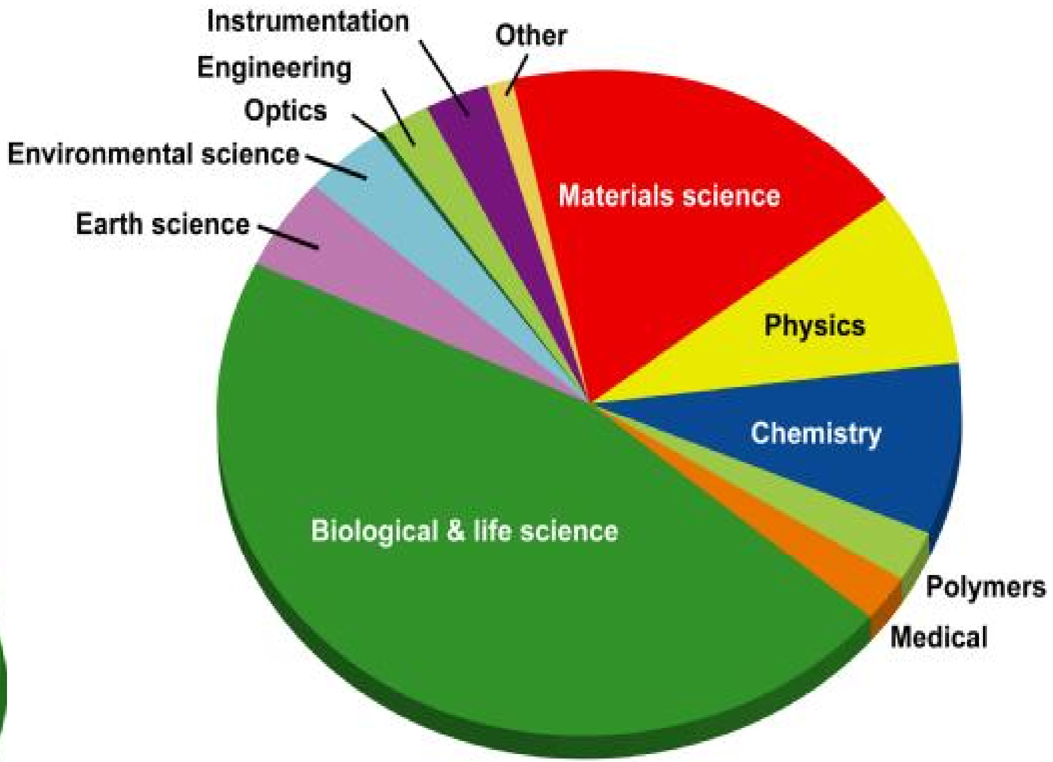
44 Operating in FY 2005; 12 Under Construction; >68 Possible;

APS Users: Number of unique users by fiscal year

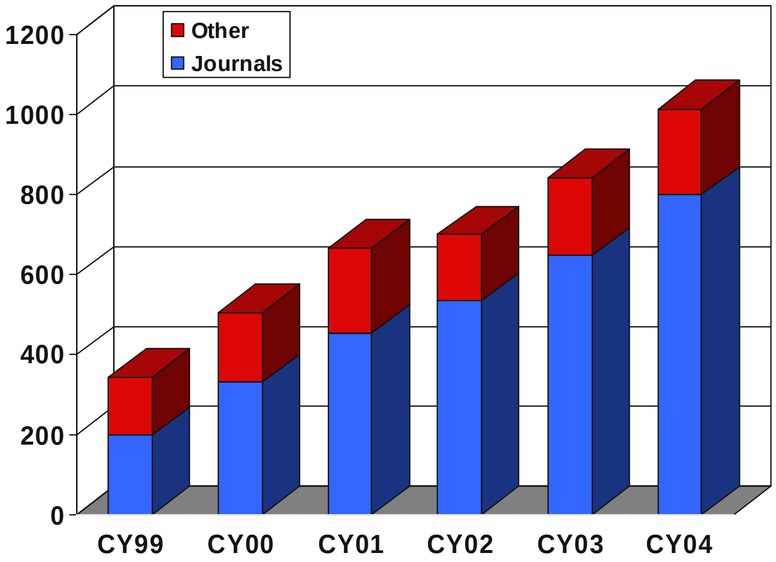


APS Users – who are they and what do they do?

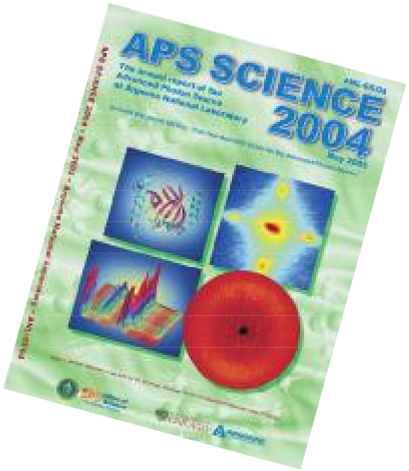




APS Scientific Impact

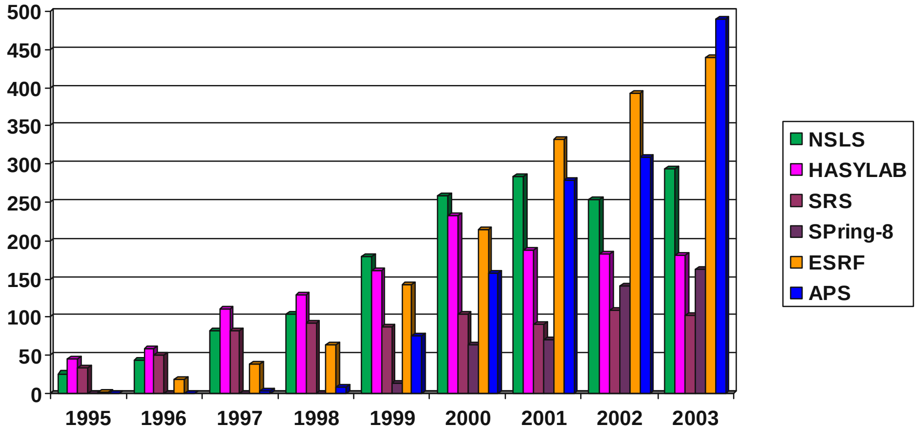


APS Refereed Publications by Calendar Year (CY)

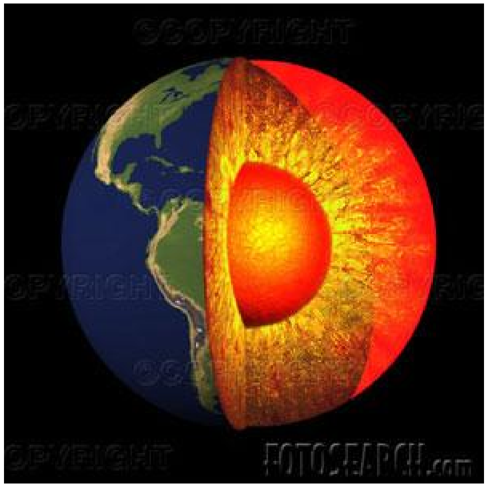


APS SCIENCE 2004

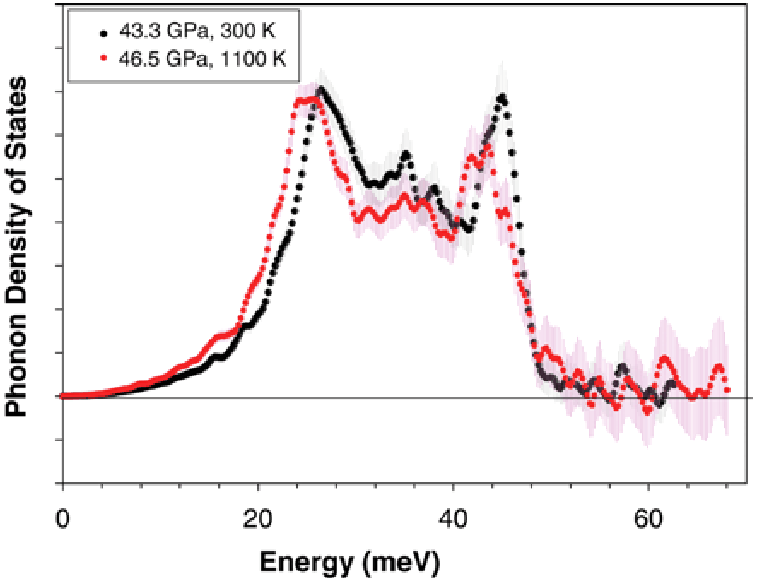
APS Protein Structures in International Databank



A Lighter Filling in Earth's Core



- Estimates of the density of earth's core depend on validity of Birch's law on how sound propagates through high pressure materials (sound velocities slow through less-dense material)
- APS research on iron shows significant impact of temperature on velocity/density relationship: Adding temperature decreases velocities of compression waves and shear waves
- Comparison of results with seismic-wave measurements shows more light elements in core iron than previously inferred from linear extrapolation at room temperature
- Major step toward predicting earthquakes, significant for new materials



DOS of hcp-Fe at 43.3 (±2.2) GPa and 300 K (black curve) and 46.5 (±2.8) GPa and 1100 K (±100) (red curve) shows high temperature softening.

J.-F. Lin et al., Science **308**, 1892 (24 JUNE 2005) (Sector 3)

Recent highlight emphasizes research under extreme conditions

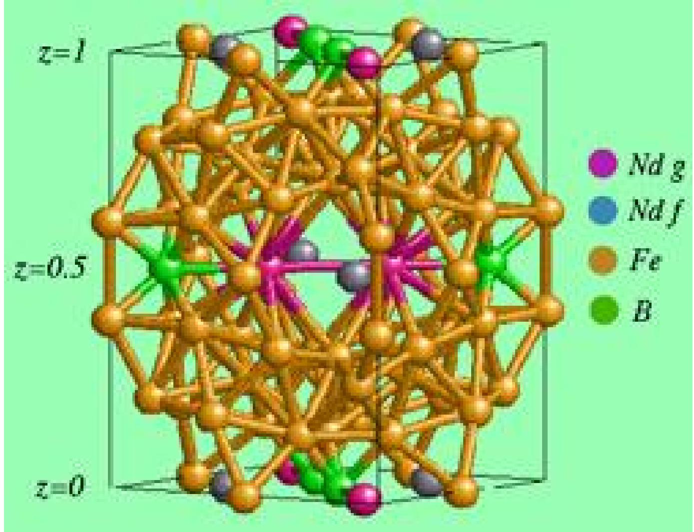
Rare Insights about Permanent Magnets

- Enhanced performance of permanent magnets impacts many areas: energy conservation, miniaturization of electronic devices, improving light-source magnet technology.

- APS researchers separated magnetic contributions of two types of rare-earth neodymium ions in dissimilar atomic environments.

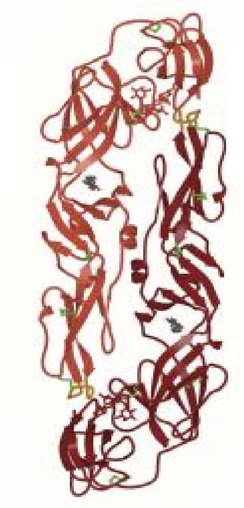
- This separation (not possible with other techniques) shows that one type of neodymium ion enhances magnetic stability of the best-performing magnet to date.

- Other type reduces magnetic stability providing important new clues into manipulation of local atomic structure for future optimization of permanent magnets.

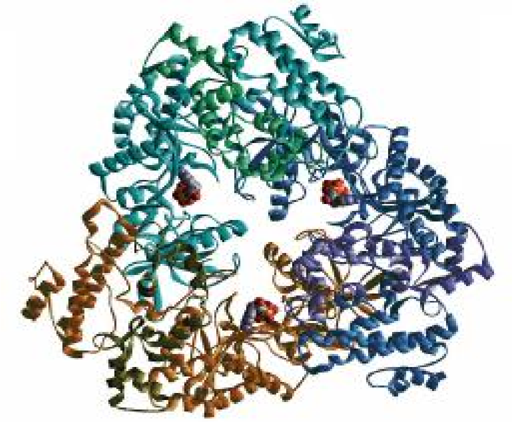


Unit cell of $Nd_2Fe_{14}B$ indicating the location of the two unequal Nd crystal sites that are the focus of this study.

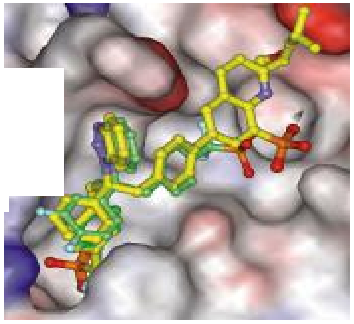
D. Haskel et al., Phys. Rev. Lett. **95**(21), 217207 (2005) APS Sector 4.



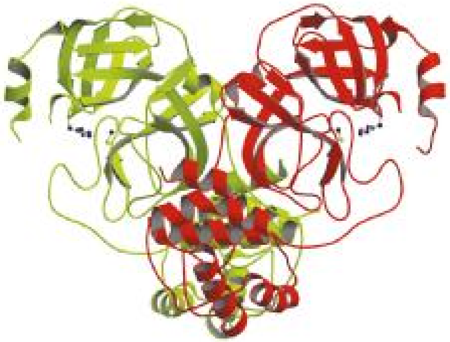
Cooling the Threat of Viral Infections



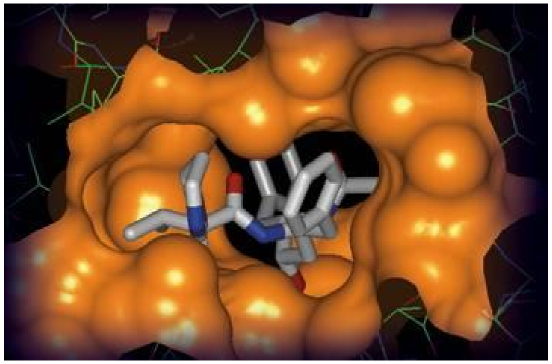
Piecing Together the Anthrax Puzzle



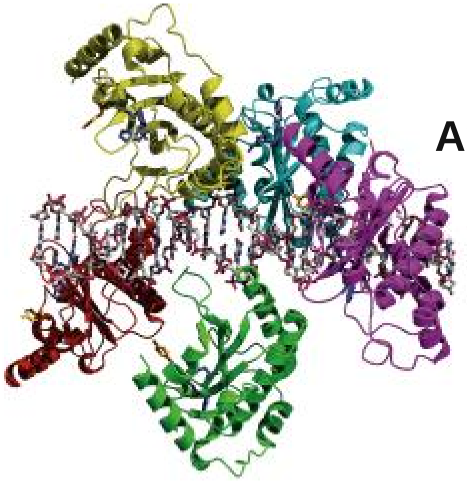
Homing in on Diabetes and Obesity



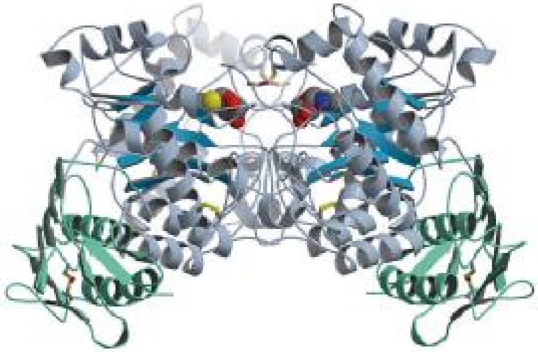
An Important Shot in the War on SARS



Kaletra ™ – a potent AIDS drug

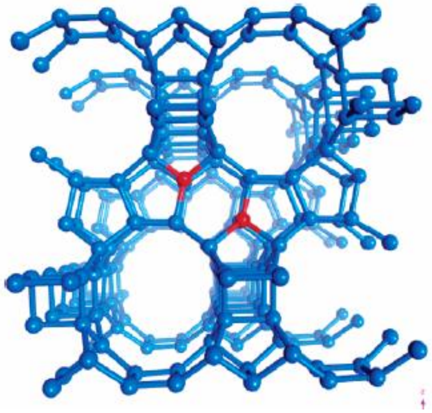


Targeting Hereditary Diseases



Attacking Tay-Sachs Disease

Importance of in-situ *work for Catalysis – comments from Bruce Gates (Cal Tech)*



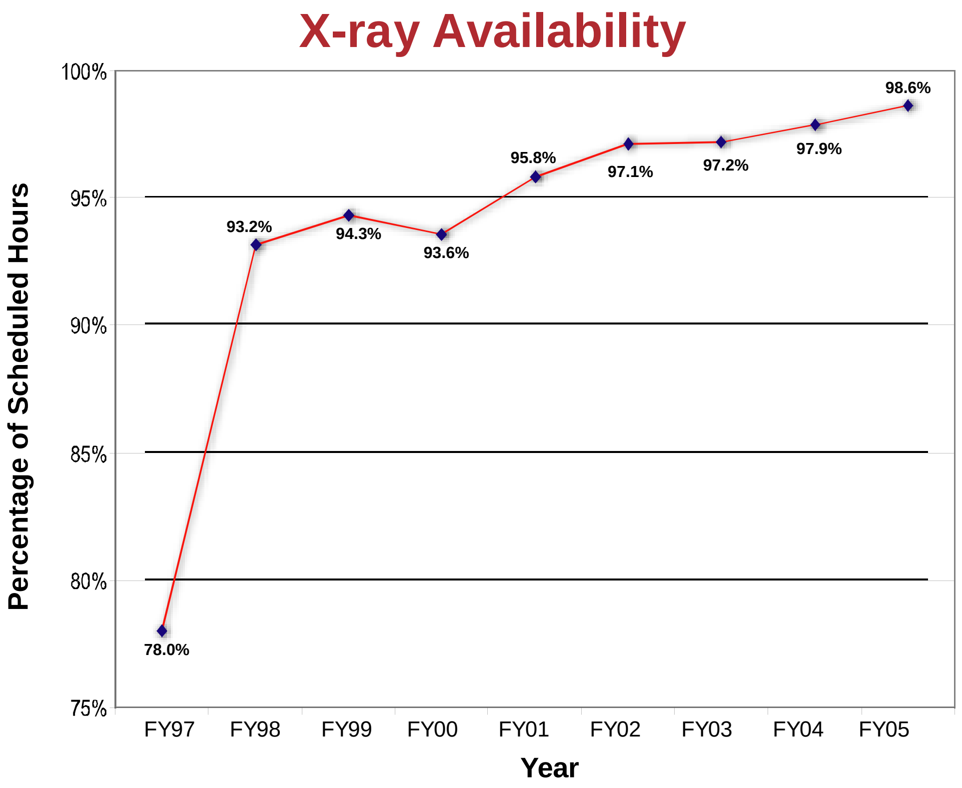
SOME CHALLENGES IN CATALYSIS RESEARCH – from recent APS workshop

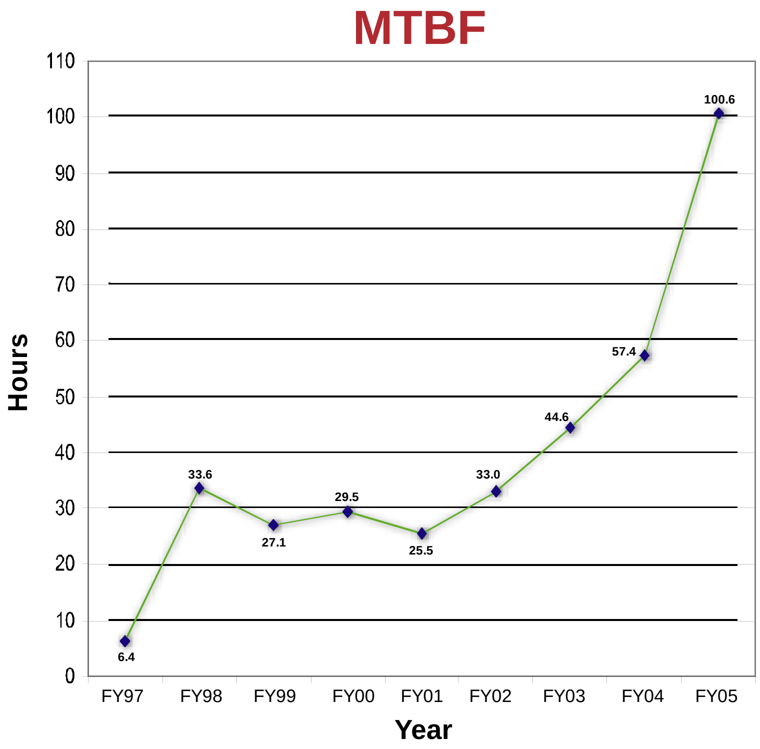
FIND STRUCTURES THAT DO THE CATALYSIS (**ELIMINATE RED HERRINGS**)

STRUCTURES CHANGE DEPENDING ON CONDITIONS SUCH AS TEMPERATURE & REACTIVE ATMOSPHERE

DETERMINE **RELATIONSHIPS** BETWEEN **STRUCTURE & CATALYTIC PROPERTIES**

Excellent Record of Improved APS Reliability and Availability – Critical for Users





At the same time accelerator innovation is essential

Innovations in APS Machine Performance

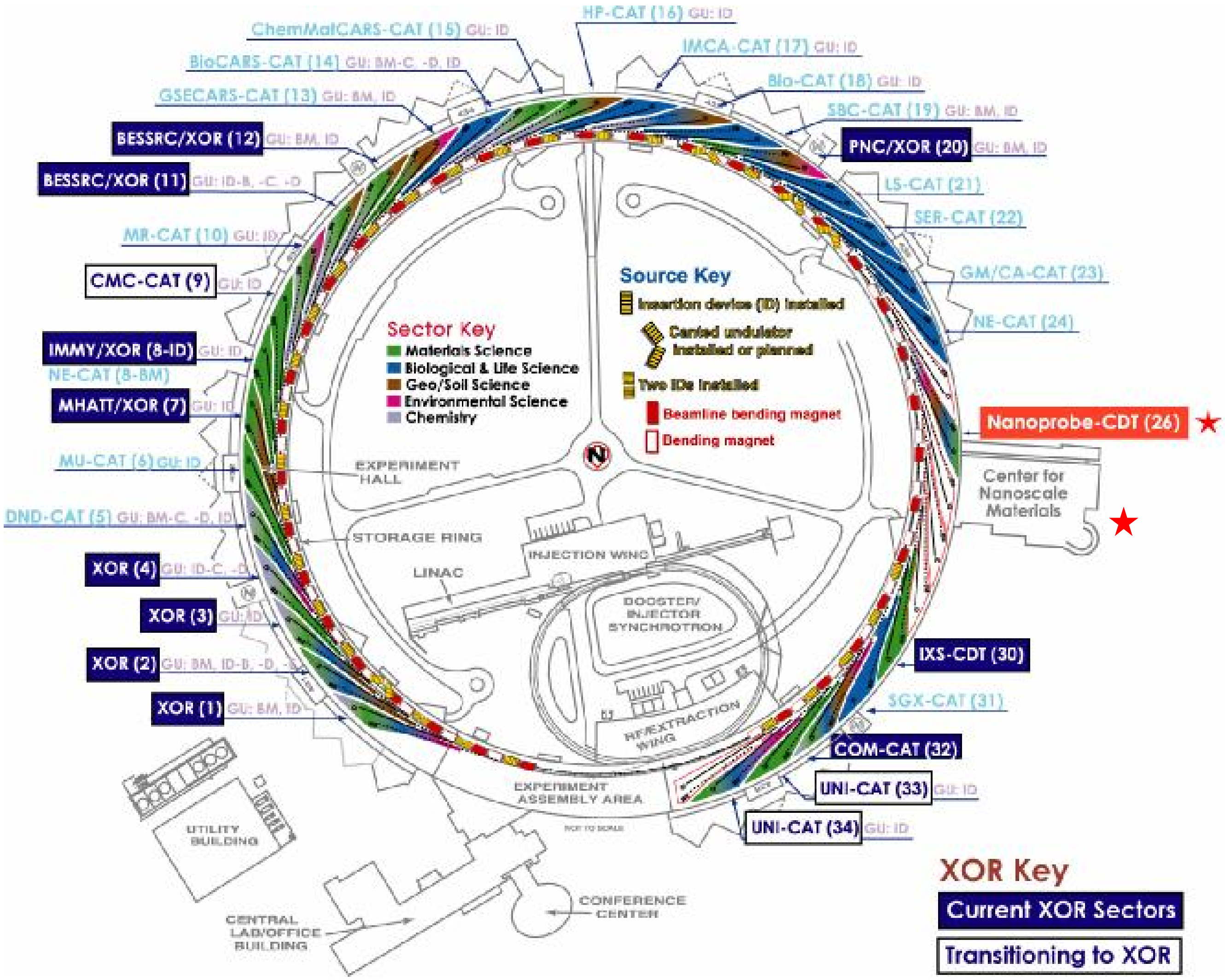
- Reduced electron emittance (improved x-ray brilliance) by over a factor of two in five years
- Introduced top-up operation mode
- Increased stability, improved x-ray optics
- More than doubled single bunch current
- Developing new insertion devices
  - e.g. superconducting ID

What is the optimal way to run a synchrotron source?

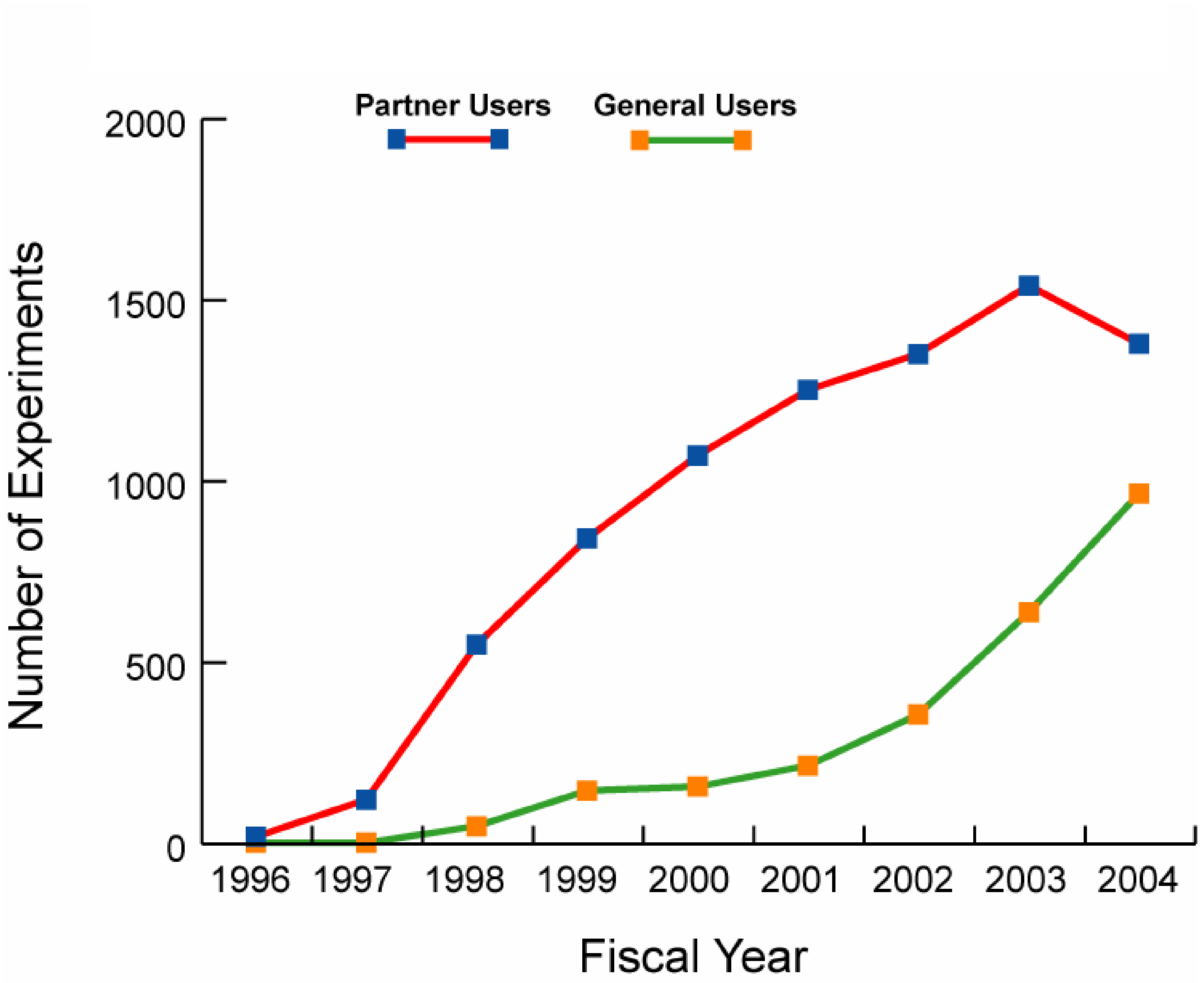
- Europe/Asia typically have a centralized model (e.g. ESRF/Spring-8)
- US synchrotron sources began with a distributed model: beamlines built and operated mostly be external entities (PRTs, CATs*)
  - **Advantage in strong partnerships (stakeholders)**
    - ***Increased intellectual input into facility development***
  - Advantage in leveraging of money
- Challenges with distributed model
  - Difficult to sustain stable operational support
  - More challenging for centralized general user access and support
  - **Smaller number of dedicated beamlines**
- US-DOE has moved to more centralized model
  - **With strong partnerships this can be the best of both worlds**
  - Need for resources at existing facilities to optimize beamline equipment and provide full staffing under new model

**__P__rogrammatic __R__esearch __T__eam; __C__ollaborative __A__ccess __T__eam*

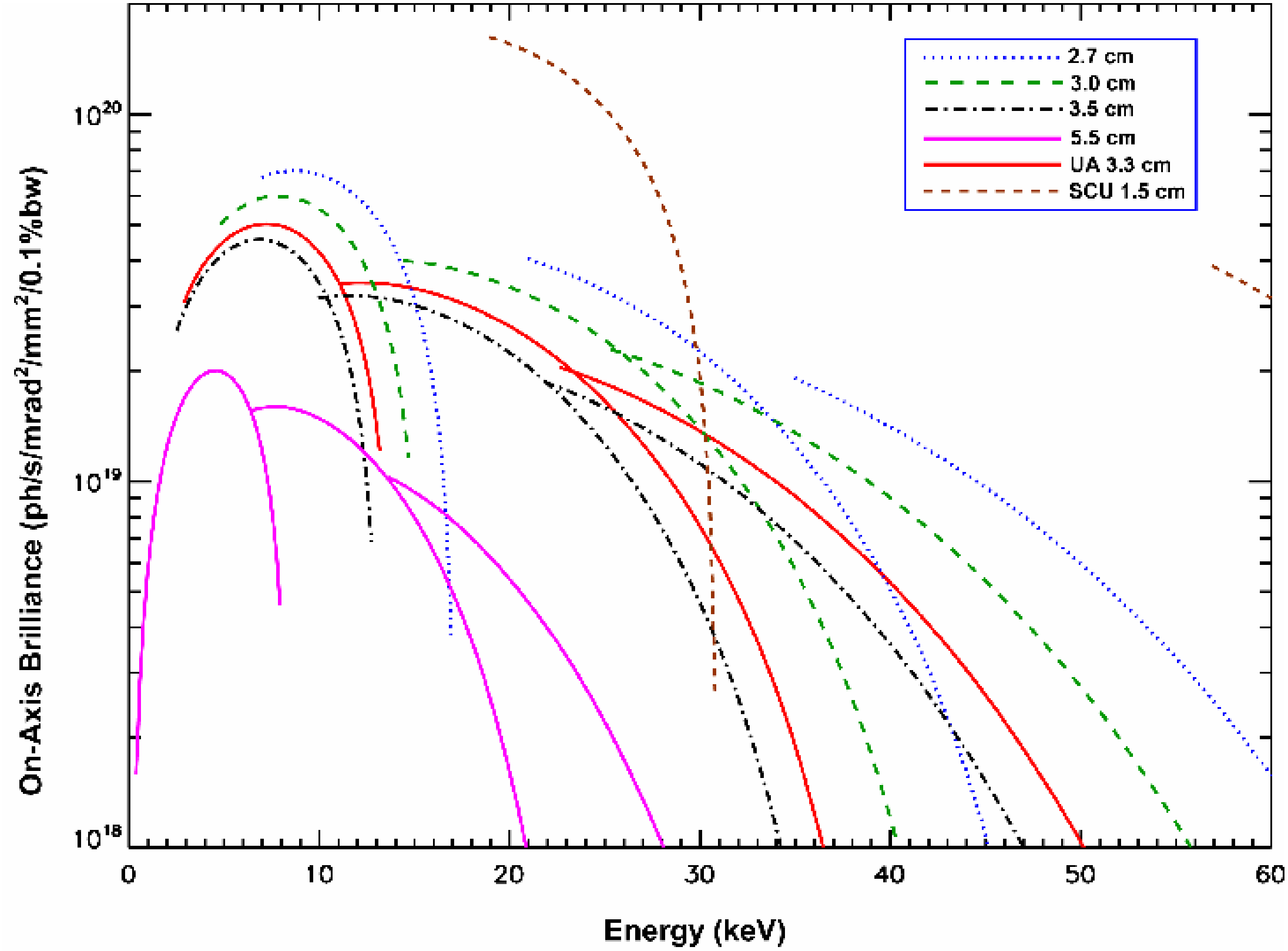
The Increasing Number of APS Operated (XOR) Beamlines



Access to APS by user type

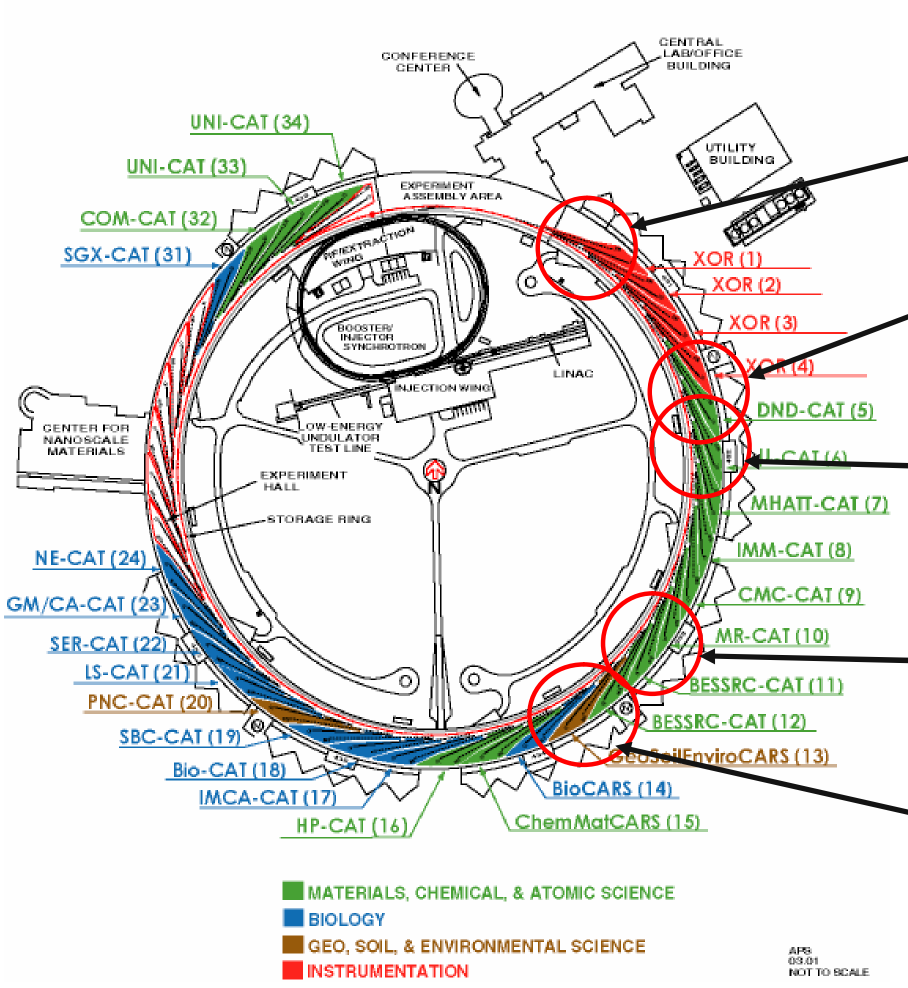


Tailoring the X-Ray Source for Dedicated Beamlines



XOR Strategic Plan to Dedicate Capabilities (e.g., High Energy)

APS Collaborative Access Teams by Sector & Discipline



1-ID (XOR)

Undulator

High Brilliance Optics

5-BM (DND-CAT)

Unoptimized bending magnet

6-ID (MU-CAT)

High-energy side station

11-ID (BESSRC/XOR)

Elliptical multipole wiggler

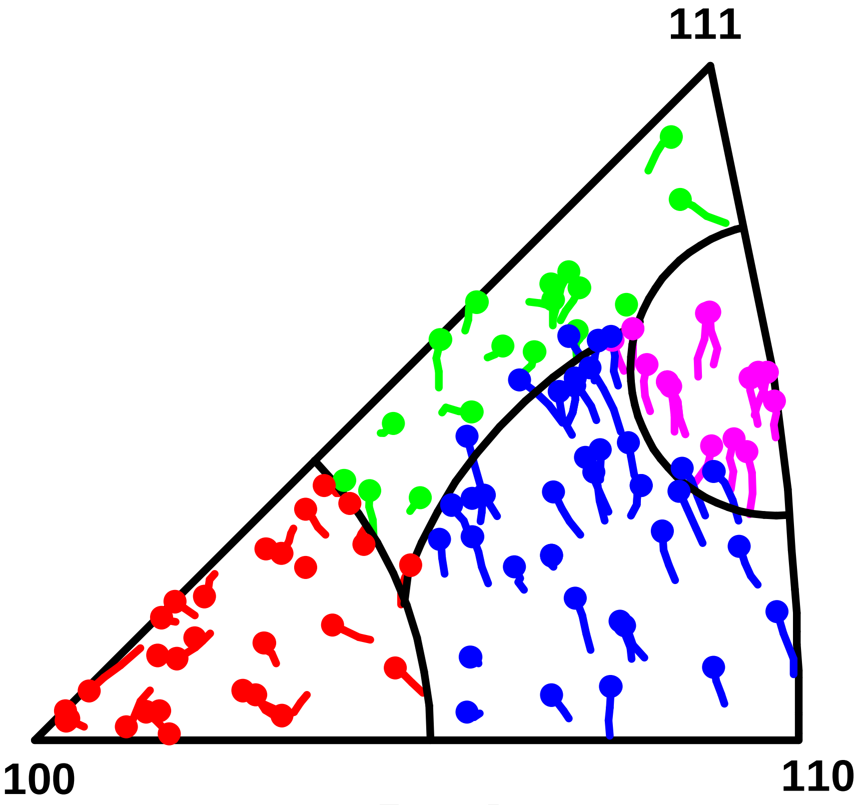
Triple-axis diffractometer

13-ID, 13-BM (GSECARS-CAT)

Geology/Earth Sciences

Tomography

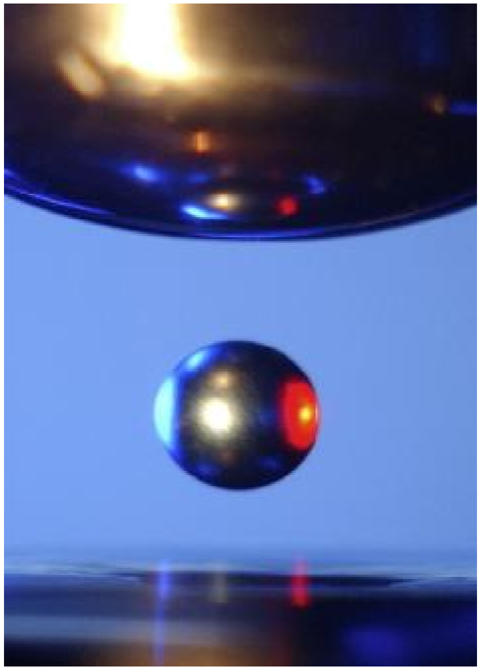
Dedicated high-energy x-ray capabilities



From Jensen

Winther, G. Margulies, L., Schmidt, S., Poulsen, H.F., 2004, Lattice rotations of individual bulk grain Part II: Correlation with initial orientation and model comparison. Acta. Mater. In press.

ESRF ID11



Icosahedral metals Goldman et. al.

Strategic plan for XOR optimized, dedicated beamlines

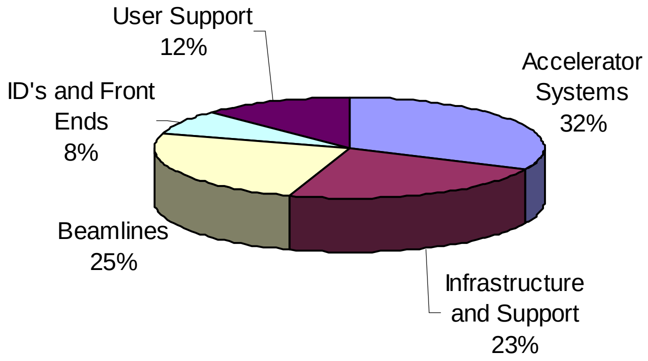
1-BM	Variable energy GISAXS, reflectivity, diffraction	MS, LS
1-ID	High-energy scattering, SAXS, powder diffraction, imaging	MS
2-BM	x-ray tomography	MS, LS
2-ID	2-32 keV STXM, microdiffraction, nanodiffraction	MS, LS, ES
3-ID	IXS, NRIXS	MS, LS, GS
4-ID-C	0.5 - 3 keV magnetic spectroscopy	MS
4-ID-D	2.6 - 45 keV magnetic spectroscopy	MS
7-BM	Ultra-fast imaging	Fluids
7-ID-B	Time-resolved white/pink beam imaging	MS, CS
7-ID-C	Time-resolved microbeam scattering	MS
7-ID-D	Laser pump/x-ray probe spectroscopy	CS, MS
8-ID-E	GISAXS	Thin films
8-ID-I	XPCS	Liquids, films
9-BM	XAFS	CS
9-ID-B	Liquid surface scattering	CS
9-ID-C	Resonant IXS	MS
11-BM	Powder diffraction	CS, MS
11-ID-B/C	High-energy powder diffraction, pdf, diffuse scattering	MS
11-ID-D	Laser pump/x-ray probe spectroscopy	CS
12-BM	XAFS, diffuse scattering, diffraction	CS, MS
12-ID-B	SAXS/WAXS	MS
12-ID-C	Time-dependant SAXS	MS, LS
12-ID-D	Surface/interface diffraction	MS
20-BM	XAFS, DAFS	ES, MS, CS
20-ID-B	Micro-XAFS	ES, MS, CS
20-ID-C	DAFS, XRR, surface-XAFS, laser pump-XAFS	ES, MS, CS
26-ID	Hard-x-ray nanoprobe	MS
30-ID	IXS, resonant IXS	MS
32-ID	Advanced full-field x-ray imaging	MS, LS
33-BM	Diffraction	MS
33-ID	Diffraction, surface/interface scattering	MS
34-ID-C	Coherent diffraction imaging	MS, LS
34-ID-E	3D-x-ray diffraction micro (and nano) scope	MS
New BM	Catalysis research (XAFS and WAXS)	CS
New ID	0.2 keV - 2.5 keV ARPES, resonant scattering, diffraction	MS
New ID	Hard-x-ray magnetic scattering (35 T magnet)	MS
New ID	ps-pulse science	CS
New ID	BioNanoprobe	LS

Short Term Needs (coming year)

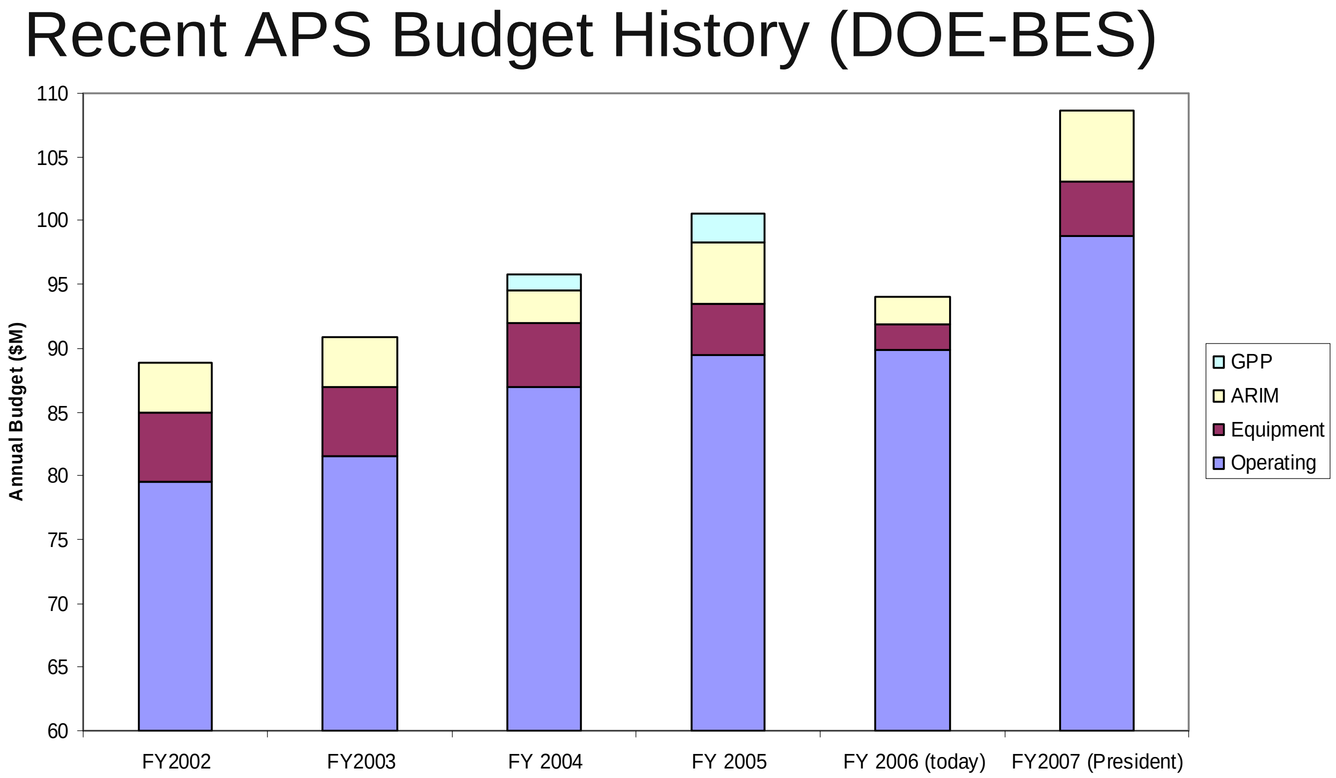
- Adequate staffing to operate beamlines
- Funds for routine maintenance and upgrading of accelerator
  - Dealing with obsolescence problem
- Capital funds to continue optimizing our beamlines

- *Without increases we would be forced to reduce staff, operating hours and beamline access*

The budget picture



where the money goes



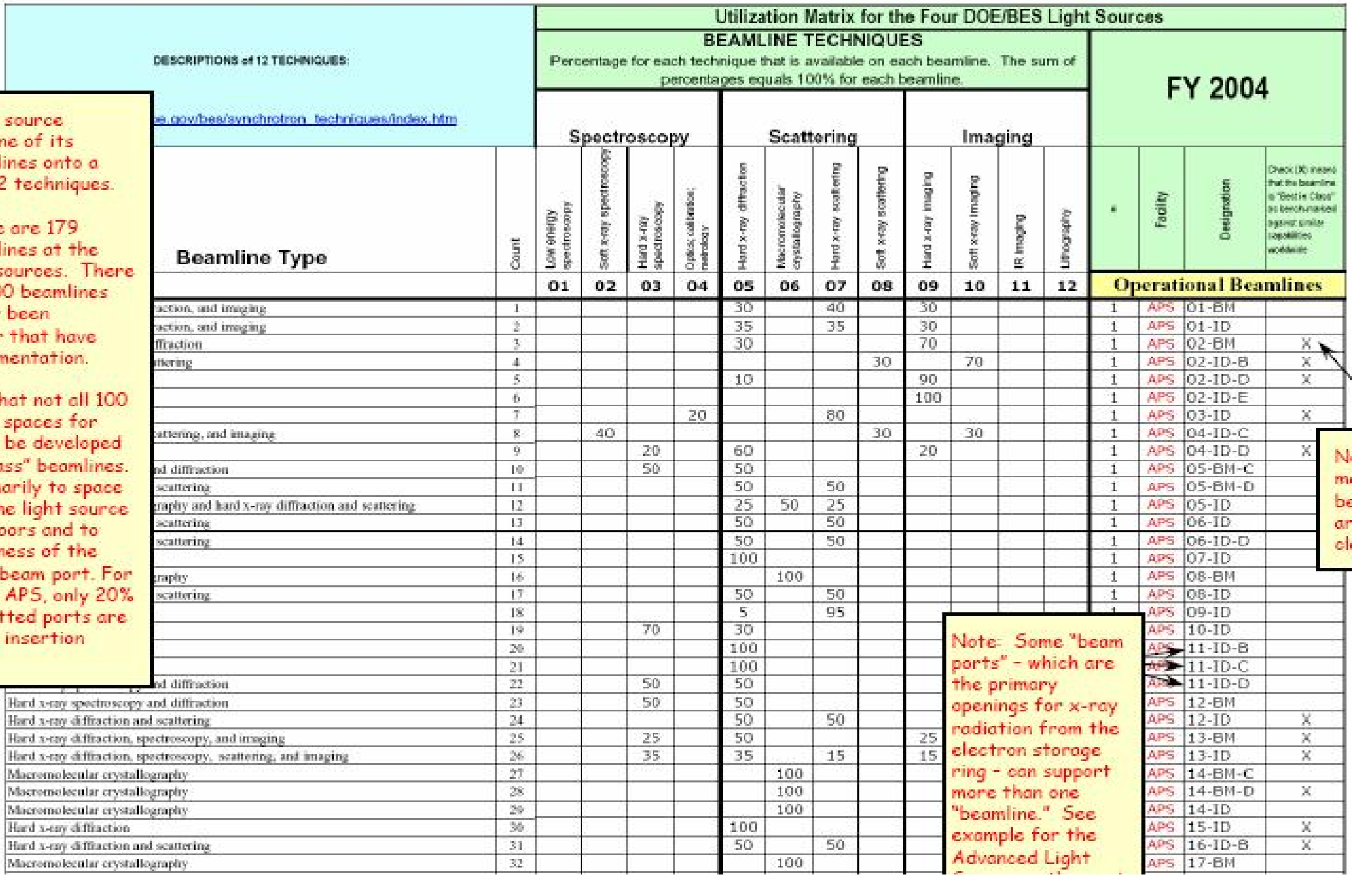
Longer term 3-5 Year Need to Begin ASAP a Major APS Upgrade

- Upgrade plans include:
  - Optimized and dedicated beamlines with state-of-the-art performance
    - *Opening new scientific communities and better supporting existing communities*
  - Unique accelerator improvements to enable new science
    - *e.g. picosecond pulses through RF crab cavities*
  - Dedicated insertion devices and long straight sections
    - *Build on unique characteristics of APS accelerator*
  - Take leadership in detector development
  - Expand user science expertise in house to enhance support
  - Work with partner users to leverage intellectual support
  - Build on synergy with other ANL facilities (nanocenter, IPNS, EMC..)
    - *"When you have a hammer everything looks like a nail"*

Upgrades beamlines and accelerator to bring world-leading new capabilities and accommodate larger and wider user community

Last year, DOE-BES looked at all their light sources and explored staffing and equipment upgrade needs…

Beamline Matrix – Advanced Photon Source (44)



DESCRIPTIONS of 12 TECHNIQUES:

e.gov/bes/synchrotron_techniques/index.htm

Utilization Matrix for the Four DOE/BES Light Sources

BEAMLINE TECHNIQUES

Percentage for each technique that is available on each beamline. The sum of percentages equals 100% for each beamline.

Beamline Type	Count	Spectroscopy				Scattering				Imaging				FY 2004			
		Low energy spectroscopy	Soft x-ray spectroscopy	Hard x-ray spectroscopy	Optics; calibration; metrology	Hard x-ray diffraction	Macromolecular crystallography	Hard x-ray scattering	Soft x-ray scattering	Hard x-ray imaging	Soft x-ray imaging	IR imaging	Lithography	*	Facility	Designation	Check (X) means that the beamline is "Best in Class" as benchmarked against similar capabilities worldwide
		01	02	03	04	05	06	07	08	09	10	11	12	Operational Beamlines			
action, and imaging	1					30		40		30				1	APS	01-BM	
raction, and imaging	2					35		35		30				1	APS	01-ID	
ffraction	3					30				70				1	APS	02-BM	X
ttering	4								30		70			1	APS	02-ID-B	X
	5					10				90				1	APS	02-ID-D	X
	6									100				1	APS	02-ID-E	
	7				20			80						1	APS	03-ID	X
cattering, and imaging	8		40						30		30			1	APS	04-ID-C	
	9			20		60				20				1	APS	04-ID-D	X
nd diffraction	10			50		50								1	APS	05-BM-C	
scattering	11					50		50						1	APS	05-BM-D	
raphy and hard x-ray diffraction and scattering	12					25	50	25						1	APS	05-ID	
scattering	13					50		50						1	APS	06-ID	
scattering	14					50		50						1	APS	06-ID-D	
	15					100								1	APS	07-ID	
raphy	16						100							1	APS	08-BM	
scattering	17					50		50						1	APS	08-ID	
	18					5		95						1	APS	09-ID	
	19			70		30									APS	10-ID	
	20					100										11-ID-B	
	21					100										11-ID-C	
nd diffraction	22			50		50										11-ID-D	
Hard x-ray spectroscopy and diffraction	23			50		50									APS	12-BM	
Hard x-ray diffraction and scattering	24					50		50							APS	12-ID	X
Hard x-ray diffraction, spectroscopy, and imaging	25			25		50				25					APS	13-BM	X
Hard x-ray diffraction, spectroscopy, scattering, and imaging	26			35		35		15		15					APS	13-ID	X
Macromolecular crystallography	27						100								APS	14-BM-C	
Macromolecular crystallography	28						100								APS	14-BM-D	X
Macromolecular crystallography	29						100								APS	14-ID	
Hard x-ray diffraction	30					100									APS	15-ID	X
Hard x-ray diffraction and scattering	31					50		50							APS	16-ID-B	X
Macromolecular crystallography	32						100								APS	17-BM	

Then each light source mapped every one of its operating beamlines onto a matrix of the 12 techniques.

Together, there are 179 operating beamlines at the four BES light sources. There are another ~100 beamlines that have never been instrumented or that have obsolete instrumentation.

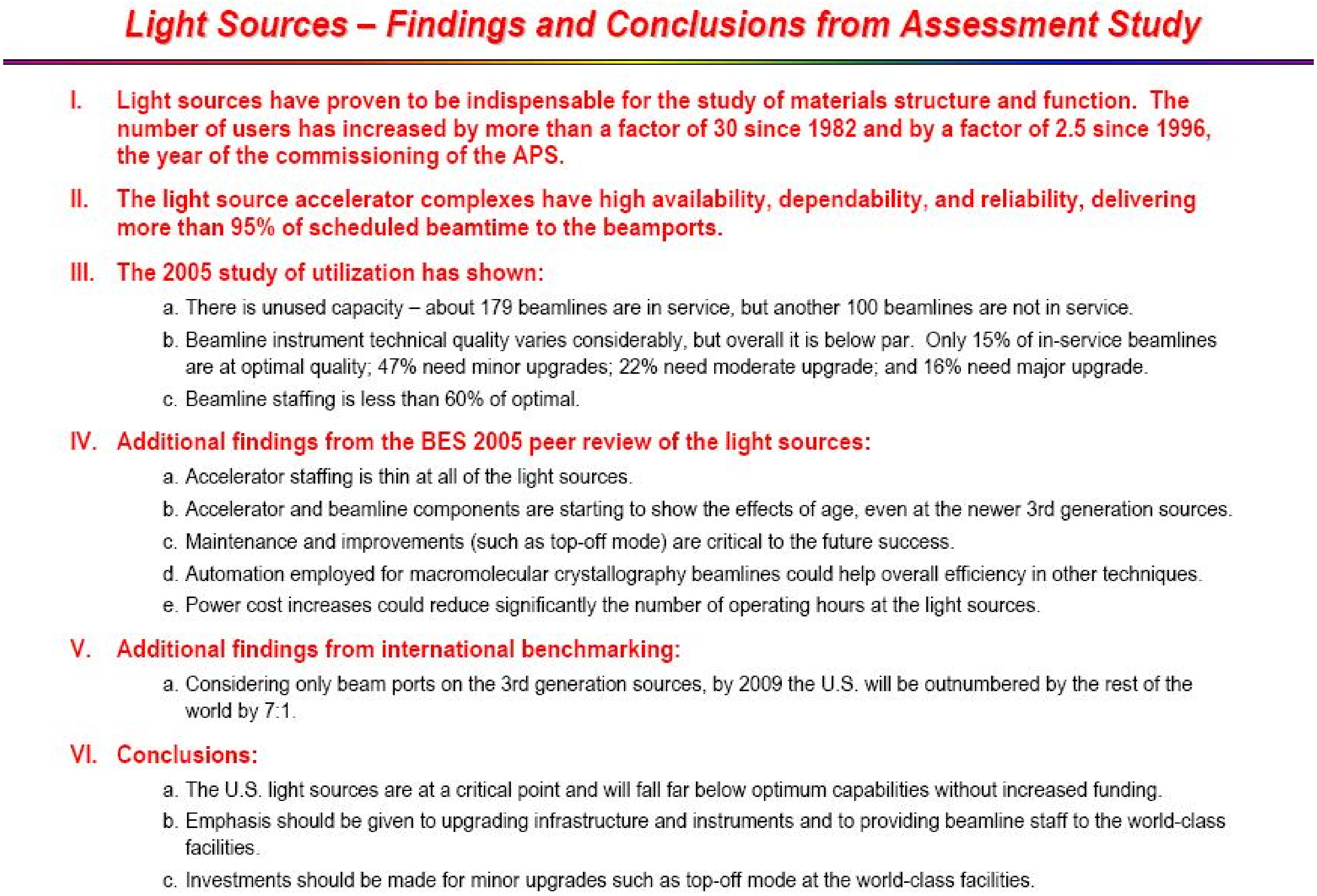
Note, though, that not all 100 of these "open" spaces for beamlines could be developed into "best-in-class" beamlines. This is due primarily to space limitations on the light source experimental floors and to ultimate brightness of the beam from the beam port. For example, at the APS, only 20% of the uncommitted ports are high brightness insertion device lines.

Note: The check marks indicate beamlines that are "best in class."

Note: Some "beam ports" – which are the primary openings for x-ray radiation from the electron storage ring – can support more than one "beamline." See example for the Advanced Light

Courtesy of Patricia Dehmer, DOE-BES

Courtesy of Patricia Dehmer, DOE-BES (SSRL User's Meeting)



Light Sources – Findings and Conclusions from Assessment Study

I. **Light sources have proven to be indispensable for the study of materials structure and function. The number of users has increased by more than a factor of 30 since 1982 and by a factor of 2.5 since 1996, the year of the commissioning of the APS.**

II. **The light source accelerator complexes have high availability, dependability, and reliability, delivering more than 95% of scheduled beamtime to the beamports.**

III. **The 2005 study of utilization has shown:**

   a. There is unused capacity – about 179 beamlines are in service, but another 100 beamlines are not in service.
   b. Beamline instrument technical quality varies considerably, but overall it is below par. Only 15% of in-service beamlines are at optimal quality; 47% need minor upgrades; 22% need moderate upgrade; and 16% need major upgrade.
   c. Beamline staffing is less than 60% of optimal.

IV. **Additional findings from the BES 2005 peer review of the light sources:**

   a. Accelerator staffing is thin at all of the light sources.
   b. Accelerator and beamline components are starting to show the effects of age, even at the newer 3rd generation sources.
   c. Maintenance and improvements (such as top-off mode) are critical to the future success.
   d. Automation employed for macromolecular crystallography beamlines could help overall efficiency in other techniques.
   e. Power cost increases could reduce significantly the number of operating hours at the light sources.

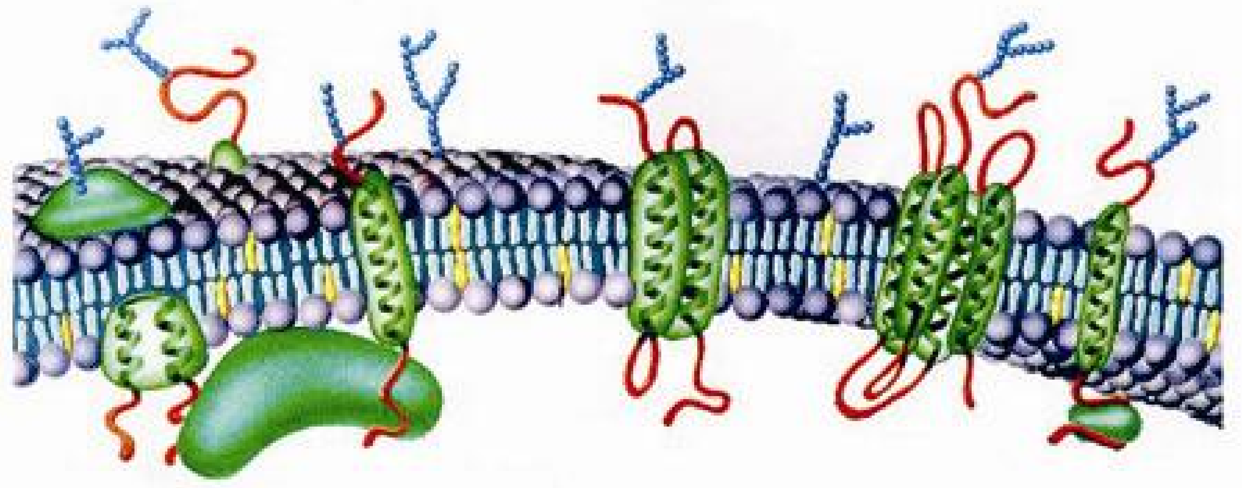
V. **Additional findings from international benchmarking:**

   a. Considering only beam ports on the 3rd generation sources, by 2009 the U.S. will be outnumbered by the rest of the world by 7:1.

VI. **Conclusions:**

   a. The U.S. light sources are at a critical point and will fall far below optimum capabilities without increased funding.
   b. Emphasis should be given to upgrading infrastructure and instruments and to providing beamline staff to the world-class facilities.
   c. Investments should be made for minor upgrades such as top-off mode at the world-class facilities.

New Directions: Membrane Science



Garrett & Grisham

Membrane technology useful for:

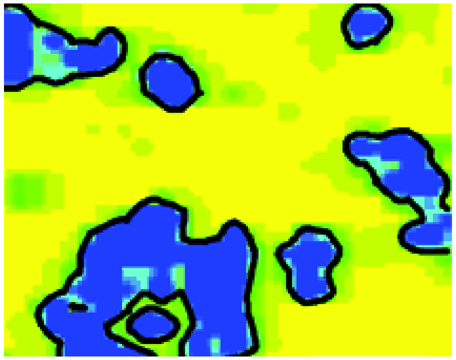
- **Water treatment and purification**
- **Electronics, semiconductors, chemicals, petrochemicals, pharmaceuticals**
- **Environmental applications**
- **Medical, biological processes (hemo-dialysis)**

Synchrotron-based techniques essential to molecular-level structural information about membranes

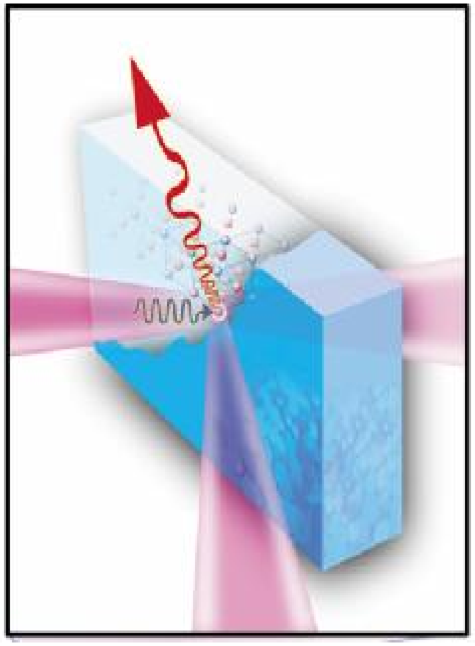
The Excitement of X-Ray Microscopy

New x-ray nanoprobe joint with the Center for Nanoscale Materials

- Third generation sources have sufficient brilliance and coherence for microfocussing and phase imaging
  - Complementary to electron microscopy
    - *Inferior spatial resolution and signal level*
    - *Superior, penetration, quantitation (e.g. kinematical), impurity sensitivity, resonant effects*
- Hard x-rays **focused to 30 nm ("Nanoprobe")**
  - Nanoscale strain measurement
  - Imaging of domains, *e.g.*, in ferroelectrics
  - Magnetism
  - Fluorescence spectro-microscopy

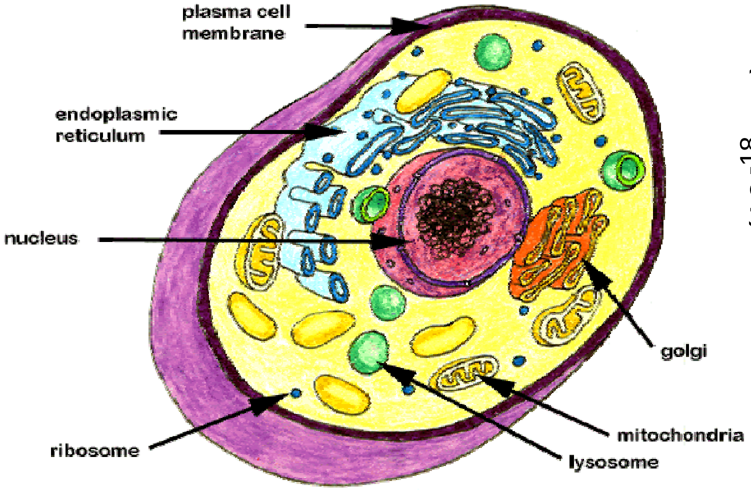


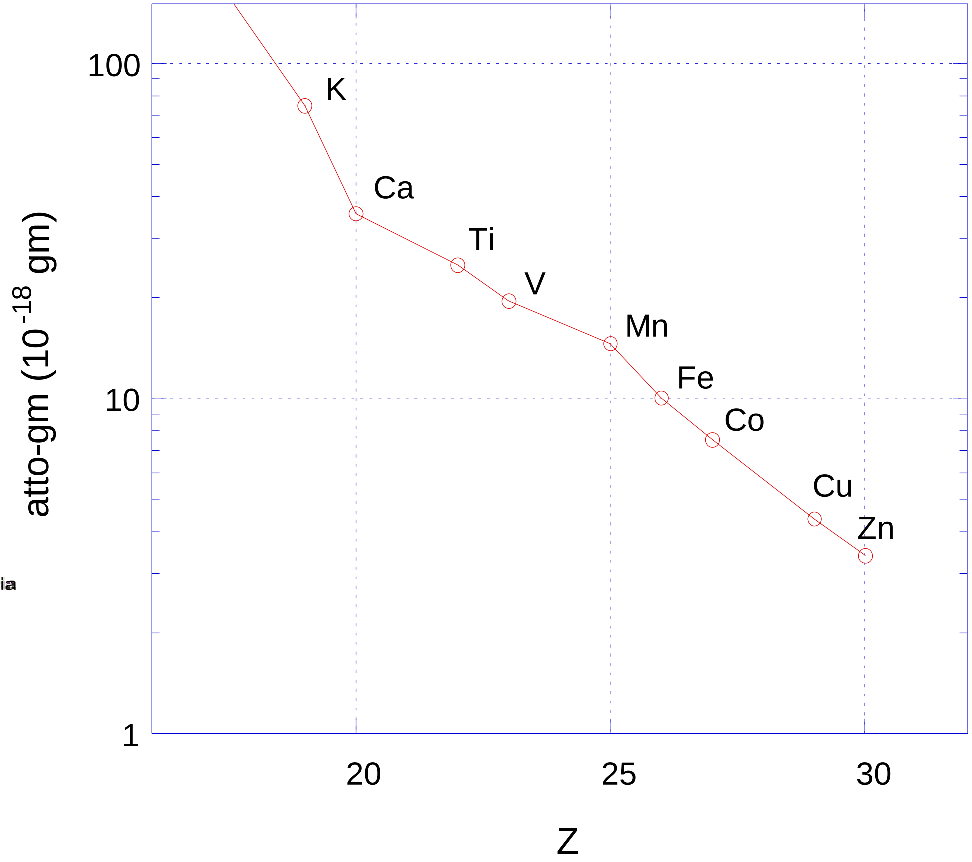
Evans et. al.



New fresnel zone plate developments at APS promise < 10nm spot size

Bio-Nanoprobe – Metals in Cell Biology

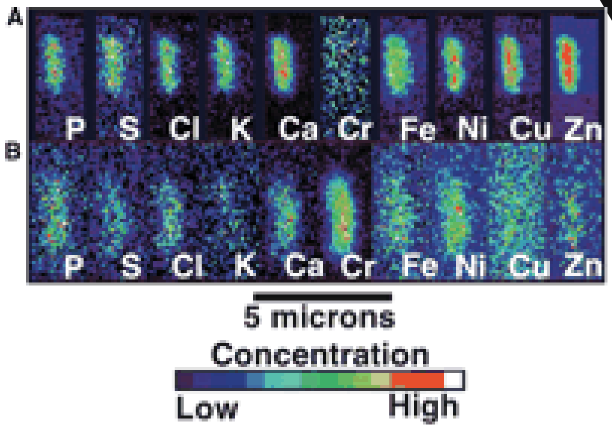




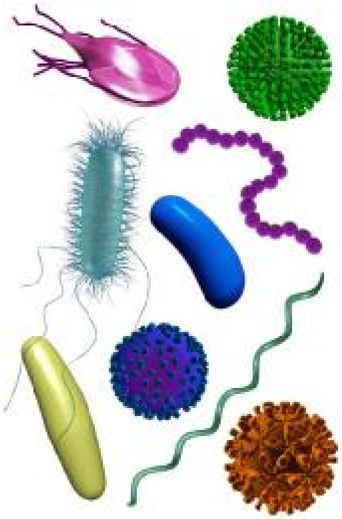
Detection Limit for Transition Elements:
for 1 s acquisition time, 0.2 x 0.2 μm^2 spot, E = 10 keV, 10^{10} ph/s

Studies of Living Bacteria Cells

- High-energy x-ray fluorescence “map” and chemical analyses of single free-floating and surface-adhered cells shows a large difference in the behavior of free and surface-adhered cells
- Implications to microbial remediation of environmental pollution and to understanding role of metals in human disease
- Only technique which has been able to study metal contaminants in individual cells



False-color micro-XRF maps of qualitative spatial distributions and concentration gradients of elements in and around planktonic microbes

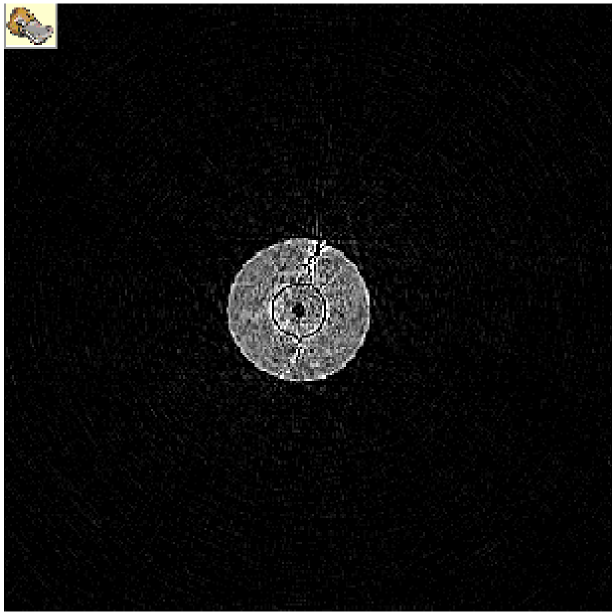


Kemner et al., *Science* **306**
(5696) 686 (22 October 2004)

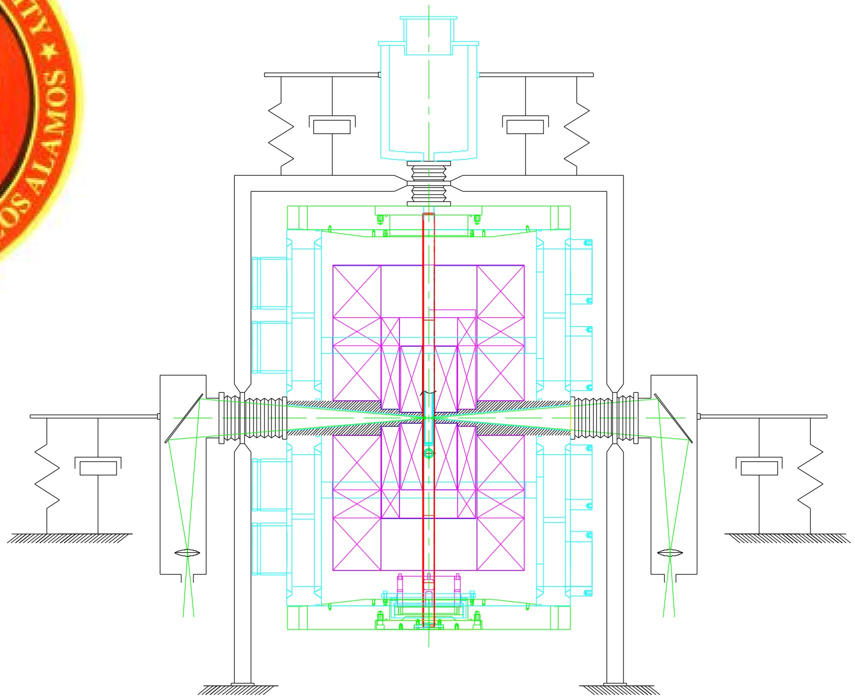
Growing interest in x-ray imaging – e.g. microtomography

Microtomography of ceramic matrix composites under applied stress

E. Ustundag – Caltech

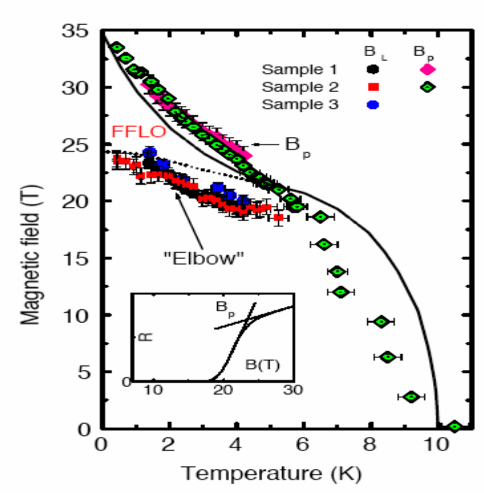


Proposed High magnetic field facility at APS



Aim for 35T with a hybrid design

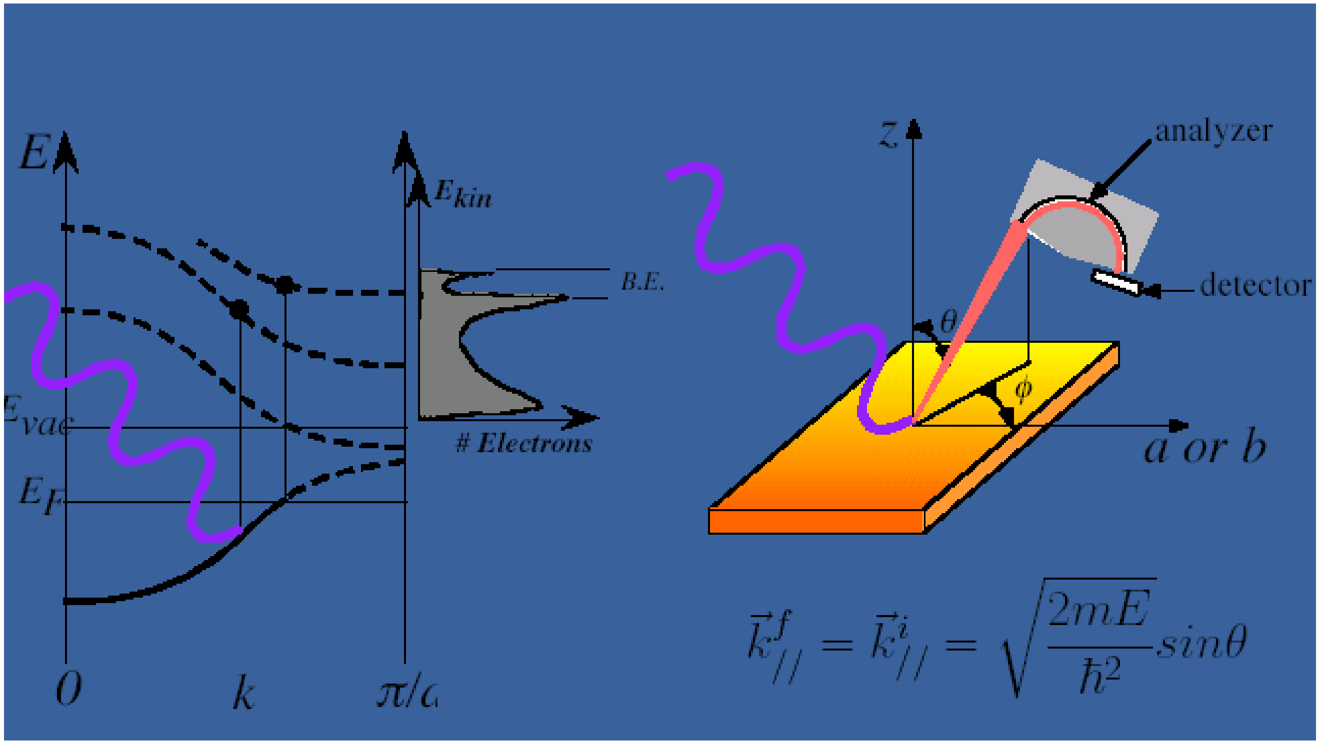
Modulated Collective States in High Magnetic Fields



Superconducting-phase modulated Fulde-Ferrell-Larkin-Ovchinnikov in κ-(BEDT-TTF)2Cu(NCS)2 JPCM, 12, 641

Improved soft x-ray capabilities proposed

Angle-resolved photoemission

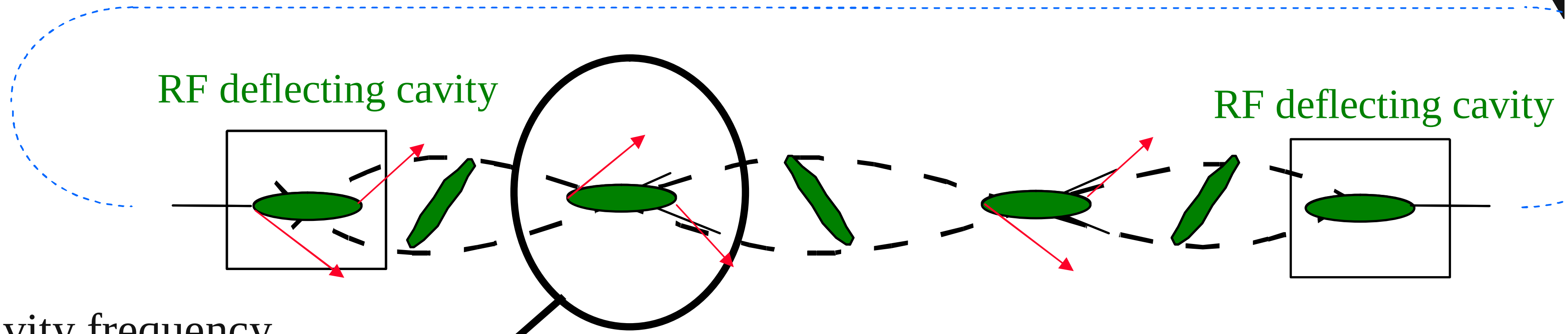


$$\vec{k}^{f}_{//} = \vec{k}^{i}_{//} = \sqrt{\frac{2mE}{\hbar^2}} sin\theta$$

Higher energy (1-3kV) offers deeper penetration and less surface sensitivity

Shorter pulse capabilities from the storage ring

(Adapted from A. Zholents' August 30, 2004 presentation at APS Strategic Planning Meeting.)



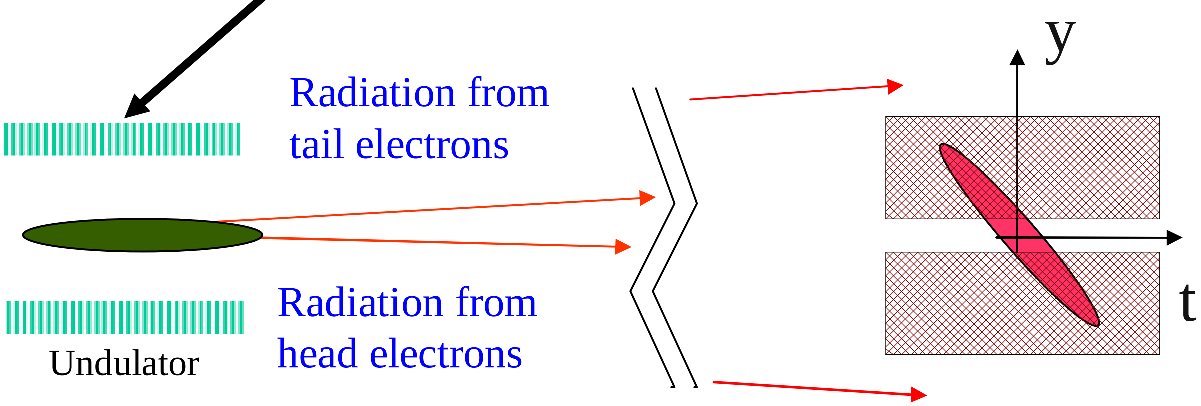
RF deflecting cavity

RF deflecting cavity

Cavity frequency
is harmonic *h* of
ring rf frequency

Application to
excited-state chemistry..

Ideally, second cavity
exactly cancels effect
of first



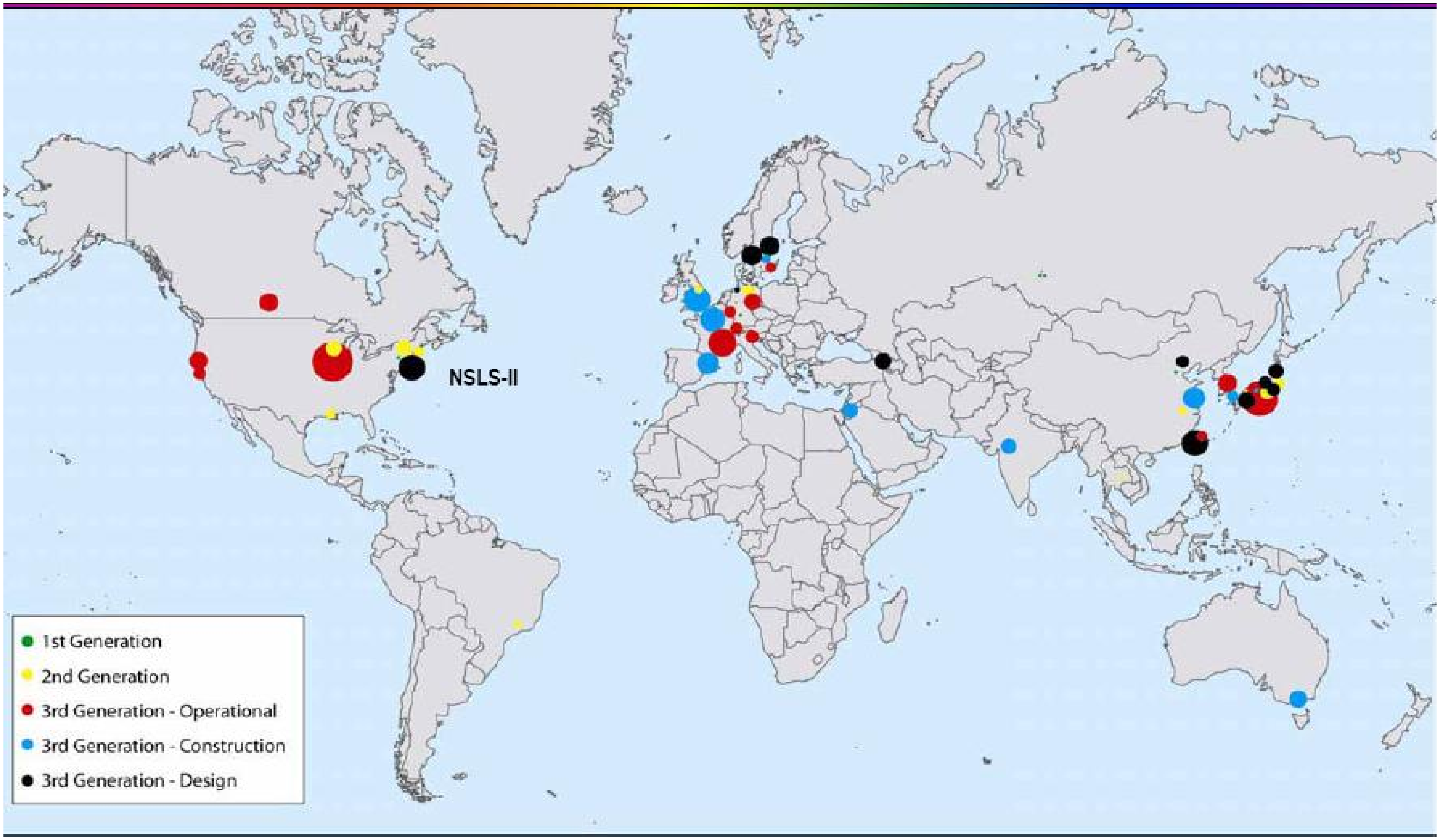
Radiation from
tail electrons

Radiation from
head electrons

Undulator

Pulse can be sliced
or compressed with
asymmetric cut
crystal

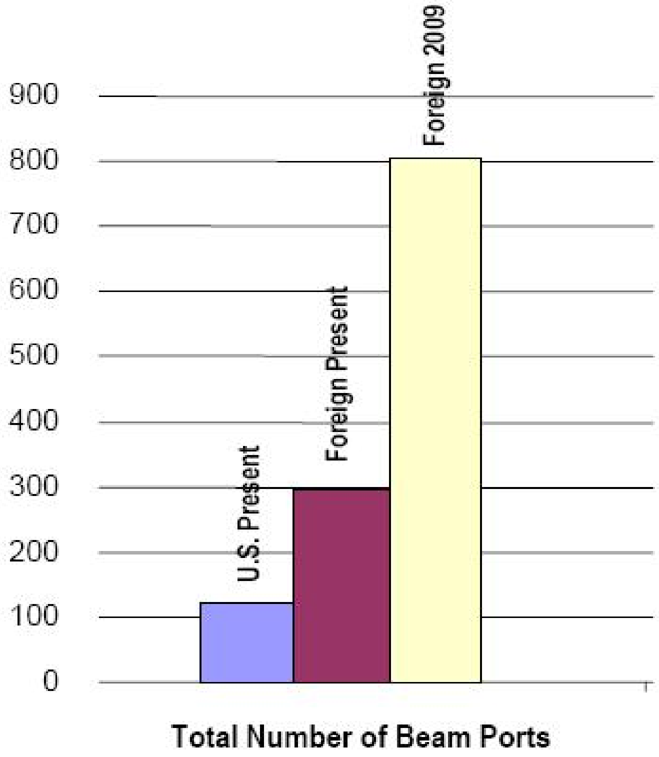
International Benchmarking: Synchrotrons Worldwide



Courtesy of Patricia Dehmer, DOE-BES

Courtesy of Patricia Dehmer, DOE-BES

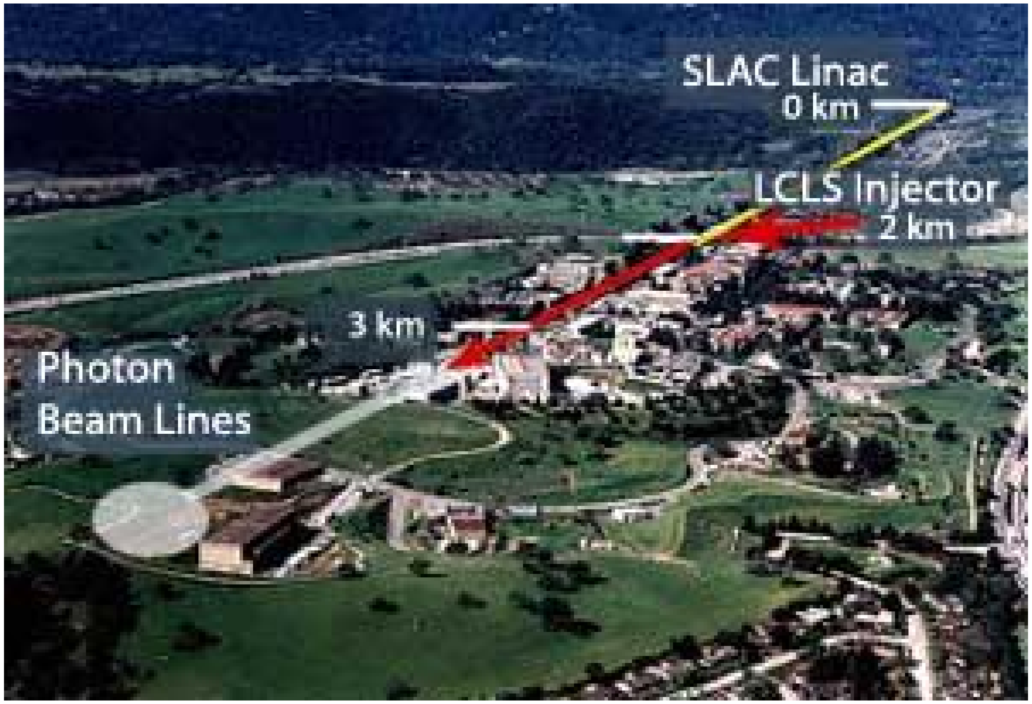
International Benchmarking: 3rd Generation Synchrotrons Worldwide



Considering only beam ports on the 3rd generation sources, this shows that by 2009 the U.S. will be outnumbered by the rest of the world by 7:1 (123 beam ports in the U.S. versus 806 beam ports in the rest of the world).

4-th Generation x-ray sources offer unique complementary capabilities

- X-ray lasers offer many orders of magnitude more brilliance for exciting new applications (complementary to third-generation sources)
- The first x-ray laser (LCLS) is being built at Stanford
- Future user facilities anticipated in US, Asia and Europe



Summary

- APS is the largest scientific user facility in the Western Hemisphere
- APS is evolving towards a model of facility supported, dedicated beamlines with strong outside partnerships
    - This offers the best opportunity for maximum scientific impact
- APS has the opportunity to greatly extend the quality and quantity of its impact through adequate staffing and instrument upgrades, leading to world leadership role
    - Heavily leveraged investment
    - Needs operating budget increases as reflected in the FY 2007 budget
        - *(estimated steady state $135M c.f. current $95M)*
        - *Because mission has changed to include most beamline operations (c.f. SNS)*
    - And major upgrade in next 5 years would bring best-in-class capabilities and double user community