The Advanced Photon Source (APS):
current status and future needs
from a materials science perspective

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Director, Advanced Photon Source

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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

The Advanced Photon 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

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 Protein Structures in International Databank

APS SCIENCE 2004
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

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

Recent highlight emphasizes research under extreme conditions

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.
Rare Insights about Permanent Magnets


• 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.

Cooling the Threat of Viral Infections

Piecing Together the Anthrax Puzzle

Targeting Hereditary Diseases

An Important Shot in the War on SARS

Homing in on Diabetes and Obesity

Attacking Tay-Sachs Disease

Kaletra™ – a potent AIDS drug
Importance of in-situ work for Catalysis – comments from Bruce Gates (Cal Tech)

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

Some challenges in catalysis research – from recent APS workshop
Excellent Record of Improved APS Reliability and Availability – Critical for Users

X-ray Availability

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 by 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

*Programmatic Research Team; Collaborative Access Team*
The Increasing Number of APS Operated (XOR) Beamlines

X-ray Operations and Research
Access to APS by user type

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Number of Experiments

Fiscal Year
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- **Partner Users**
- **General Users**
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


ESRF ID11

Icosahedral metals Goldman et. al.
### Strategic plan for XOR optimized, dedicated beamlines

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

Recent APS Budget History (DOE-BES) where the money goes

<table>
<thead>
<tr>
<th>Year</th>
<th>GPP</th>
<th>ARIM</th>
<th>Equipment</th>
<th>Operating</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY2002</td>
<td></td>
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<td>FY2003</td>
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<td>FY2004</td>
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<tr>
<td>FY2005</td>
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<td>FY2006 (today)</td>
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<td>FY2007 (President)</td>
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</table>

- Accelerator Systems: 32%
- ID's and Front Ends: 8%
- Beamlines: 25%
- User Support: 12%
- Infrastructure and Support: 23%
 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)

<table>
<thead>
<tr>
<th>Beamline Type</th>
<th>FY 2004</th>
</tr>
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<tbody>
<tr>
<td>Spectroscopy</td>
<td>Scattering</td>
</tr>
<tr>
<td>01</td>
<td>02</td>
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*Note: The check marks indicate beamlines that are “best in class.”*

There 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 beam 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.

*Courtesy of Patricia Dehmer, DOE-BES*
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.
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

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

Evans et. al.
Detection Limit for Transition Elements:
for 1 s acquisition time, 0.2 x 0.2 µm² spot, E = 10 keV, 10¹⁰ 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.

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 \( \kappa \text{-}(BEDT-TTF)_{2}\text{Cu(NCS)}_{2} \)

JPCM, 12, 641
**Improved soft x-ray capabilities proposed**

Angle-resolved photoemission

Higher energy (1-3kV) offers deeper penetration and less surface sensitivity
Shorter pulse capabilities from the storage ring

Cavity frequency is harmonic $h$ of ring rf frequency

Ideally, second cavity exactly cancels effect of first

Application to excited-state chemistry..

Pulse can be sliced or compressed with asymmetric cut crystal
International Benchmarking: Synchrotrons Worldwide

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