

APS Update

G. Brian Stephenson
APSUOSC – PUC Meeting
November 18, 2011

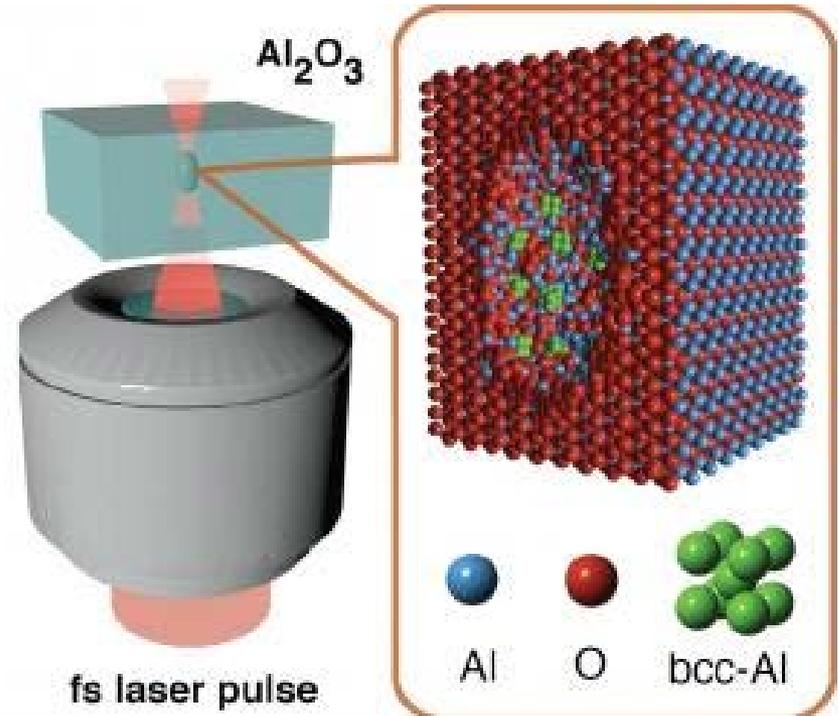
Outline

- Science Highlights
- Activities and News
 - Safety
 - FY11 Stats
 - User Survey
 - DOE Triennial Review
 - Advance Protein Crystallization Facility
 - Dynamic Compression Sector
 - Budget Outlook
- Planning
 - Sector Reviews
 - Space
 - Upgrade



Creating the Heart of a Planet in the Heart of a Gem

- Researchers at HP-CAT beamline 16-BM-D found a novel form of aluminum
- Table-top laser device at Shizuoka University (Japan) that penetrates crystals and sets off interior micro-explosions was used to blast tiny bits of sapphire creating powerful shock waves that compressed surrounding material
- Under extreme conditions—terapascals of pressure, temperatures of 100,000K—warm dense matter formed
- Because sapphire is an alumina researchers expected to find evidence of various phases of high-pressure alumina inside gem
- Instead examination at 16-BM-D of sapphire interior showed minuscule amounts of surprisingly stable, highly-compressed body-centered cubic elemental aluminum

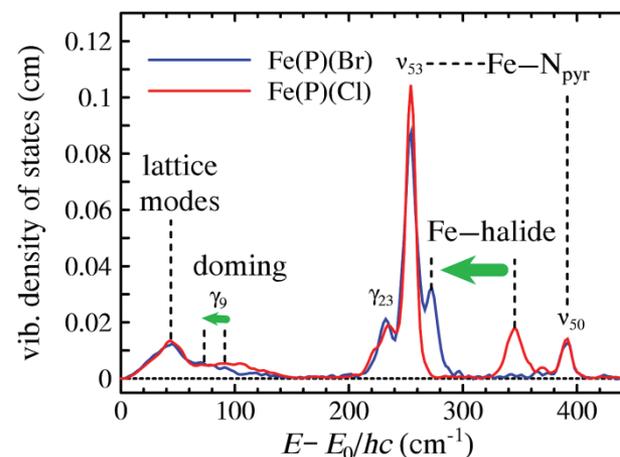
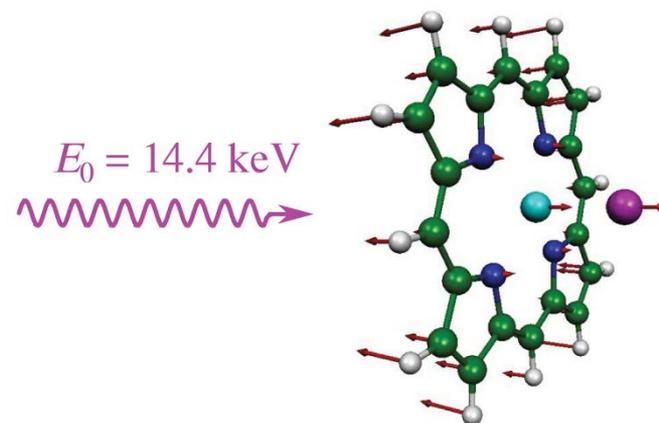


Left: A tightly focused femtosecond pulse generates hot plasma in sapphire, which in turn produces a strong shock wave, which compresses the material against the surrounding pristine Al_2O_3 crystal into a densified amorphous phase A and forms a void V in the centre of a laser-induced microexplosion. The superdense bcc-Al phase was found within this compressed material. Right: A sapphire crystal with a laser-carved cavity. (Image by Arturas Vailionis.)

Ringing the Hemoglobin Bell

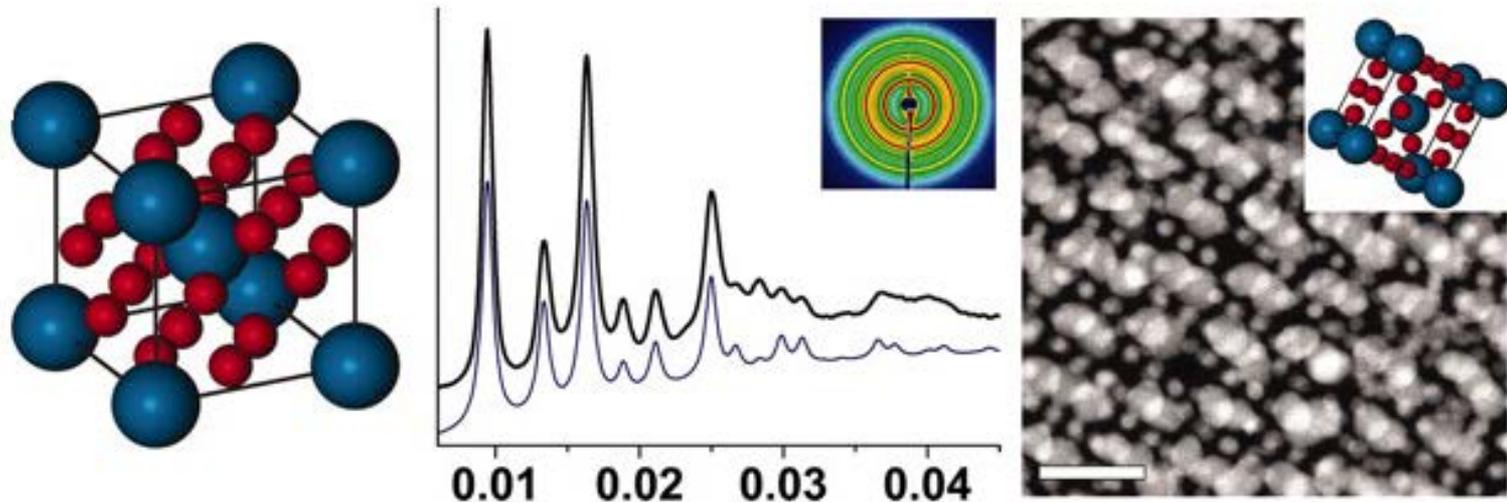
- Most available techniques for studying vibrational properties of a protein have limitations, especially when probing lower frequencies at which proteins actually function
- Researchers using XSD 3-ID beamline found a way around problem by employing new nuclear resonance vibrational spectroscopy technique to investigate iron-based heme molecules at the reactive core of a multitude of proteins such as hemoglobin
- The work provides new information about the vibrational dynamics of hemes
- Beamline 3-ID pioneered the applications of nuclear resonance techniques

Alexander Barabanschikov et al., [J. Chem. Phys. 135, 015101 \(7 July 2011\)](#)



Iron is the reactive core of the heme molecule responsible for essential biological processes. The ⁵⁷Fe nucleus recoils upon absorption of precisely tuned high-energy x-ray photons available at the APS, enabling measurement of the resulting molecular oscillations. These include the heme "doming" motion shown here, which controls the reaction of oxygen with heme-containing proteins, such as hemoglobin.

Emulating – and Surpassing – Nature



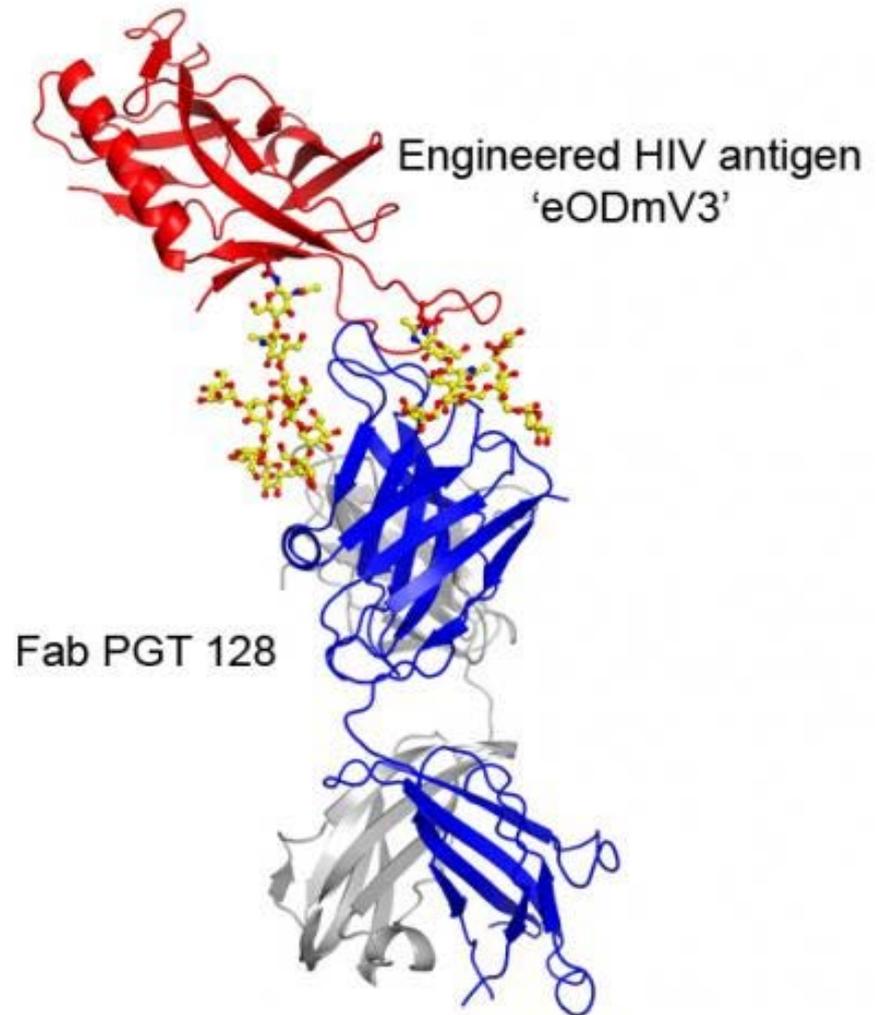
Example of an isostructural superlattice, Cs_6C_{60} lattices. L. to r.: model unit cell (not to scale); 1-D and 2-D (inset) SAXS diffraction patterns; TEM image of resin-embedded superlattices, with the unit cell viewed along the appropriate projection axis (inset). (From Macfarlane et al., *Science* **334**, 204 [2011]).

- Researchers using DND-CAT beamline 5-ID learned to build crystalline materials from nanoparticles and DNA, same material that defines genetic code for all living organisms
- Using nanoparticles as "atoms" and DNA as "bonds," they created crystals with particles arranged in same types of atomic lattice configurations as some found in nature
- Have also have built completely new structures that have no naturally occurring mineral counterpart
- Basic design rules established for this approach to nanoparticle assembly promise possibility of creating a variety of new materials that could be useful in catalysis, electronics, optics, biomedicine and energy generation, storage and conversion technologies



How a Powerful Antibody Neutralizes HIV

- Details of how a powerful HIV antibody grabs hold of the virus have been uncovered by researchers using a GM/CA-CAT beamline at the APS and an SSRL beamline at SLAC National Accelerator Laboratory
- Findings highlight a major vulnerability of HIV and suggest a new target for vaccine development
- Determined structure of new antibody (PGT 128) joined to its binding site on molecular mockups of the virus
- By experimentally mutating, altering viral target site, could see that PGT 128 works in part by binding to glycans on the viral surface



The PGT 128 antibody in action. (Image courtesy of the Wilson lab, The Scripps Research Institute.)

Increased Focus on Safety

- APS and Argonne safety statistics not as good in FY11 as FY10
- We need to refocus our attention on safety

Subject: Labcast: Message from Bill Brinkman, Director, DOE-SC / Argonne's safety record

To: Argonne Lab Employees
Subject: SC-1 Safety Message

Argonne National Laboratory has a rich history of delivering transformational research across the globe. But the lab's ability to sustain its scientific contributions is directly linked to its ability to conduct its research and supporting operations safely. [Accordingly, I am quite disappointed with the number of recent injuries at the laboratory.](#) I spoke this week with your Director and the Argonne Site Office about the lab's current safety record and the necessity to identify causes, show improvement, and thereby demonstrate accountability.

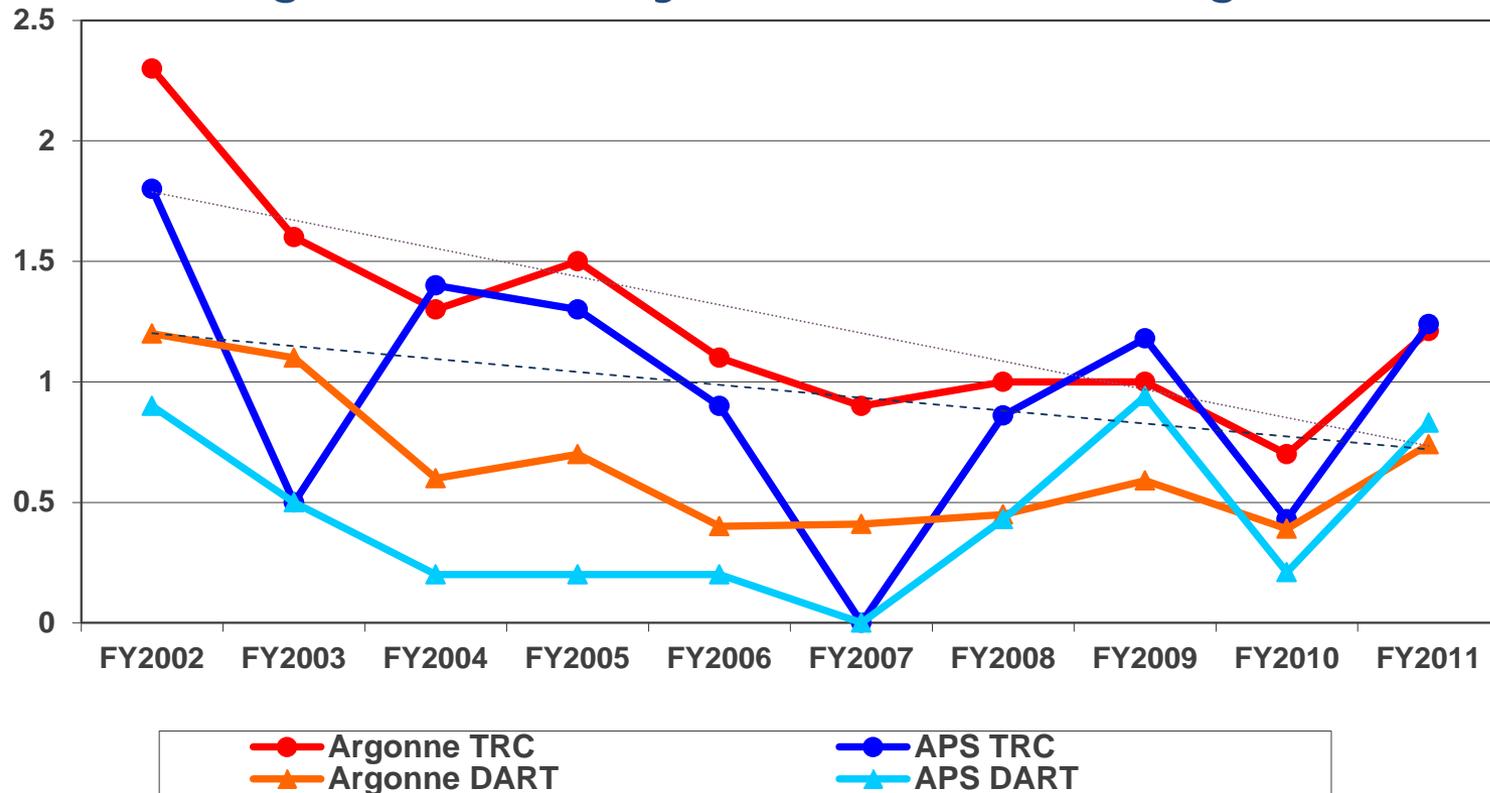
Safety is everyone's responsibility, and one that must be felt personally. [Industry's safety leaders commit to the belief that all accidents are preventable and that a realistic goal is one of zero injuries.](#) I strongly encourage each of you to plan your work carefully, consider and mitigate hazards thoughtfully, and strictly conduct your work in accordance with documented laboratory practices.

"Safety is our full-time job, don't make it a part-time practice."

Bill Brinkman, Director
Office of Science



APS and Argonne Safety Statistics through FY11



TRC = Total OSHA Recordable Case Rate per 200,000 Hours Worked

DART = Days Away, Restricted Duty, or Job Transfer Case Rate per 200,000 Hours Worked

FY2002-4 APS Divs.

FY2005-8 SUF (APS Divs.+ IPNS)

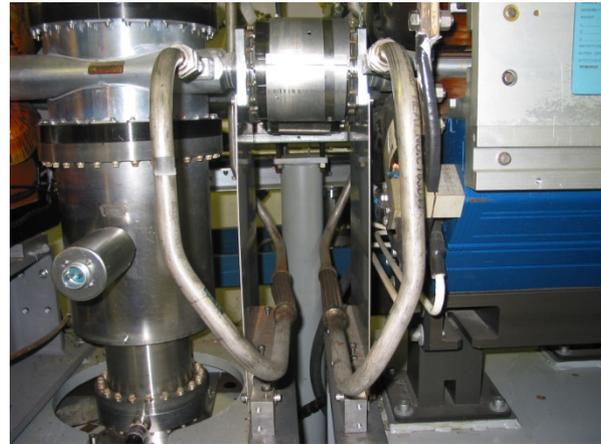
FY2009-10 PSC (APS Divs. Only)

FY2011 PSC (APS Divs) data thru 9/11



Lifting Injury

- APS technician suffered a partially torn tendon in right forearm while replacing lead bricks on a local shield stand:
 - Picked up lead bricks (22 lbs) from floor to stack on stand using only right hand and felt loss of strength in right forearm
 - Initial diagnosis was strain, subsequent tests revealed tendon partially torn
 - Required surgery to repair as did not heal on own
- Lessons Learned from injury
 - Use two hands in lifting lead bricks or use lifting device if it will fit
 - Full extent of injury may not be evident for several days or weeks



APS Safety Action Plan - Group Meetings

- We must constantly improve our work practices and communicate safety awareness to all staff
- Last month each group had a discussion about the application of Integrated Safety Management in their everyday work
- Have not heard from the following: MR-CAT, GSE/Bio/ChemMatCARS, HP-CAT, IMCA-CAT, & NE-CAT
- We need to follow up with continued focus, communication, awards

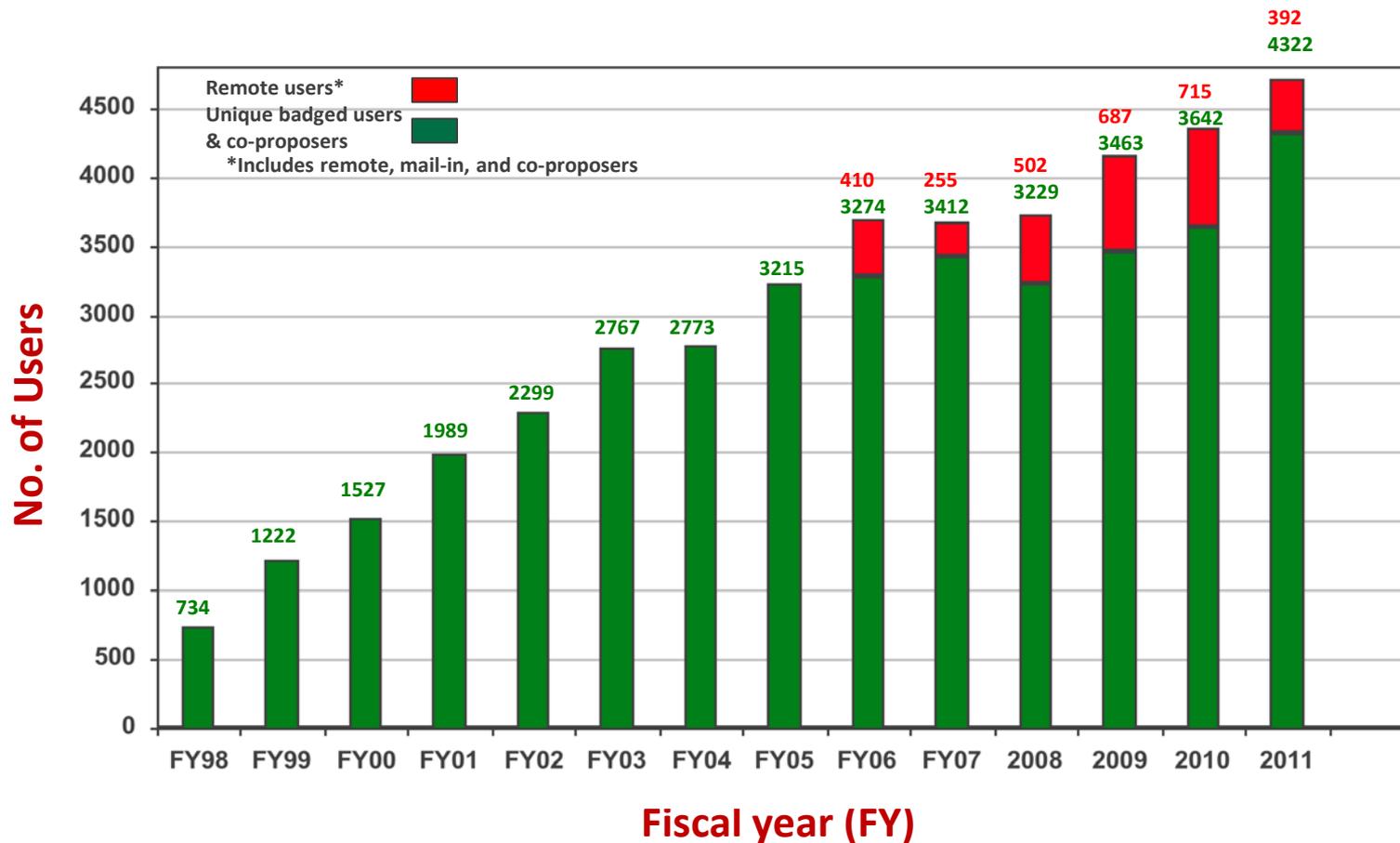


Electrical Equipment Inspections

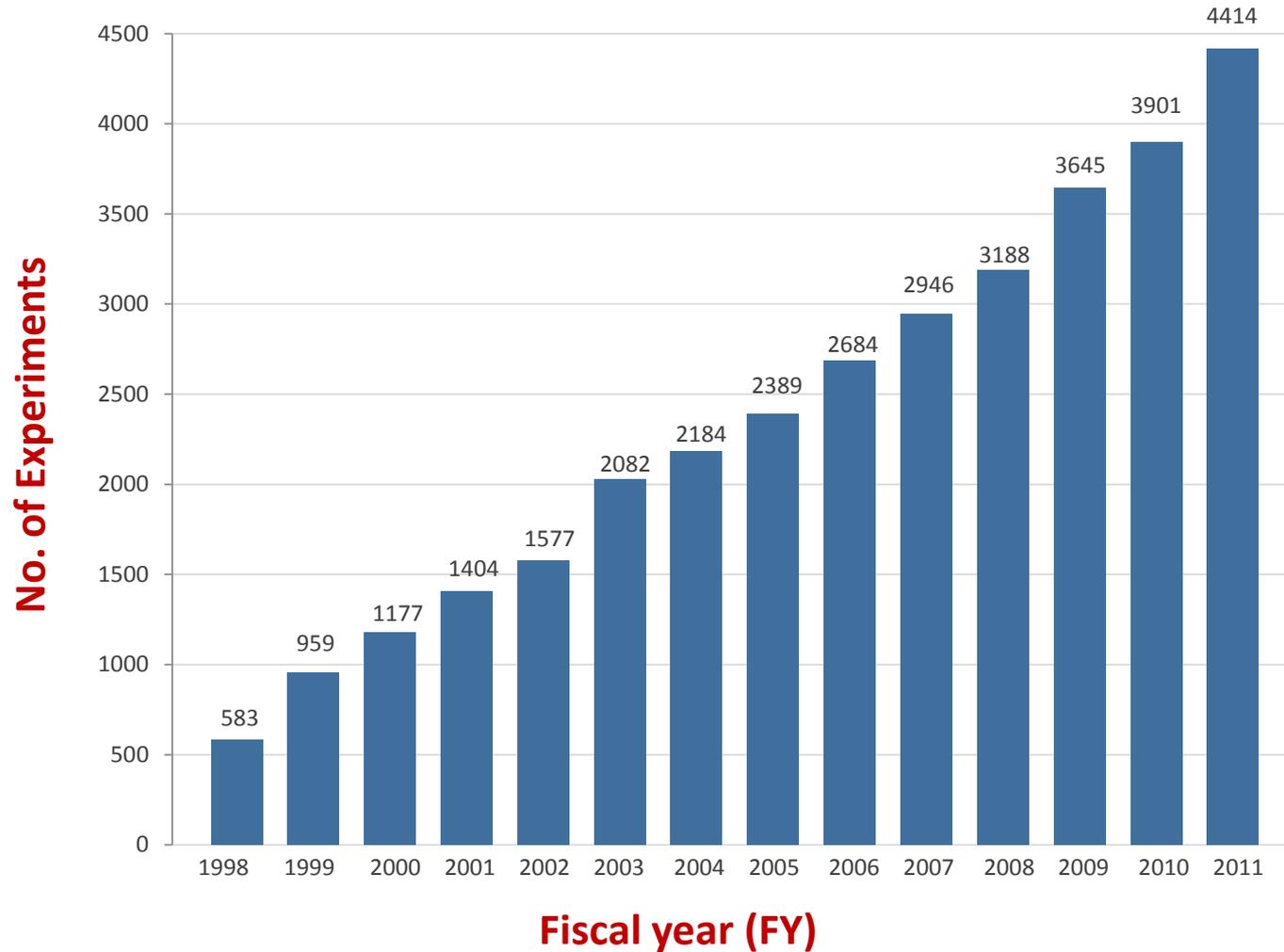
- Five-year program to inspect all existing non-NRTL electrical equipment completed in September
- Thanks for making it a success
- Please continue to inspect newly-arrived equipment



Number of APS users participating in experiments (on-site and remote), FY1998-FY2011

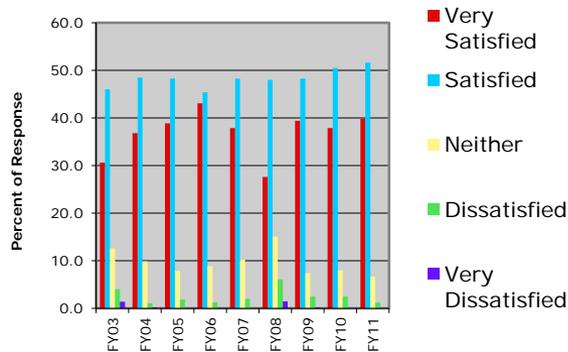


Number of experiments by APS users, FY1998-FY2011

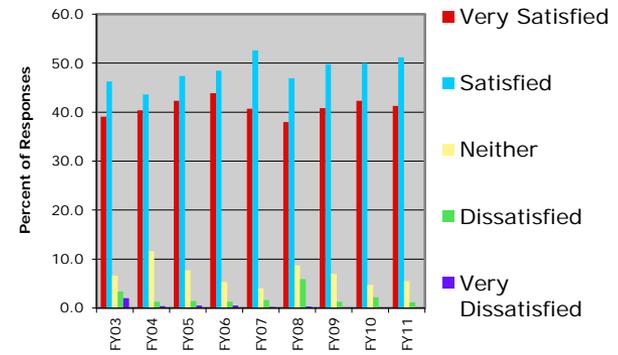


Response to DOE Questions on User Survey

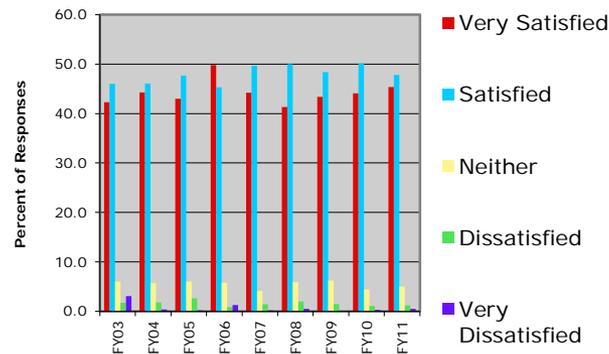
1. How satisfied were you with the fraction of the year that the facility operates?



2. How satisfied were you with the schedule or service?

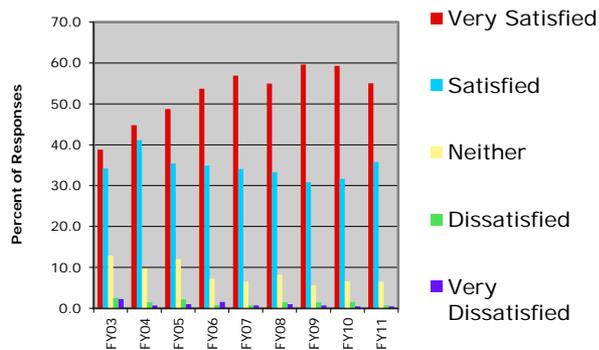


3. How satisfied were you with the performance?

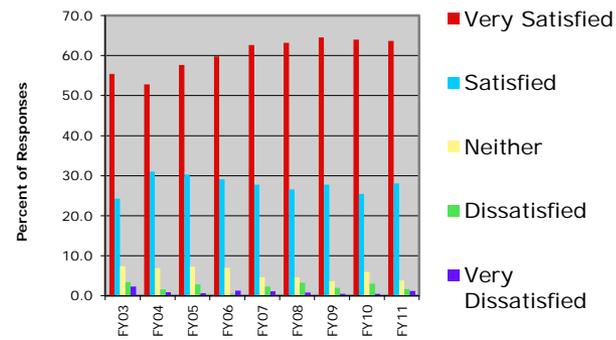


Response to DOE Questions on User Survey

4a. How satisfied were you with the support for users provided by the facility staff?



4b. How satisfied were you with the support for users provided by the beamline staff?



Responses from the User Survey Question: What would you like this facility to do differently?

- Improve/Change the General User proposal process
 - GUP-information (statistics) about ... each beamline should be available
 - Easier and more straightforward access to industry users
- Improve Documentation/Training/Education
 - One thing that would help me and my students would be a workshop (in-person once per year, or on-line) to help novices learn how to process and interpret data gathered during our experiments.
 - Provide more education for new users on experimental procedures
 - The neutron community has new-user workshops, frequently, at major conferences. This needs to be done for SR also.
- Misc
 - Bring back the CAT systems (or similar system) where the science and facilities are driven by users and not by insiders.
 - For time-sensitive experiments, it's unfortunate that most down/maintenance periods seem to be synchronized with other synchrotrons (e.g. NSLS) rather than distributed, so that there is year-round availability
 - I believe that trikes are dangerous
 - Improve the radioactive material review and safety procedures. They should be brought in line with actual risk



APS Reviews

- The Office of Basic Energy Sciences triennial review of the APS took place September 12-15
 - The review consisted of presentations by APS management and users, but also included a number of informal meetings between the reviewers and staff
 - The close-out was encouraging;
 - A theme of the comments was a desire for more communication of an informal nature; transparency in setting priorities; need for regular reviews of scientific productivity and management of each sector
 - The written report is expected next month
- We have received the written report (held July 2011) from the UChicago Argonne LLC Review Committee.
 - Comments overall were very positive and constructive
 - Many of the recommendations dealt with the APS-U project, e.g. use of contingency funds will need to be communicated in a transparent fashion

Scientific Advisory Committee Meeting October 12-13

- Charge Item: Future Beamline Reviews
 - In the future, all APS sectors will be occupied
 - New programs can only be created by the evolution or replacement of existing programs
 - What process should be used to review the tenure of each beamline?
- SAC agreed to take lead in beamline reviews
- Process is being drafted
- Expect to start with APS-operated beamlines next year



BES Facility Directors Meeting November 8

Agenda:

- Industrial user programs, potential changes to master user agreements
- Definition of high-impact publications
- Data analysis, storage, and distribution



Staffing and Budget Planning

- We are developing a comprehensive staffing plan that includes Upgrade and operations activities, for FY12 and for future years
- Will involve significant new hiring, both directly for the Upgrade and to backfill positions in operations
- Staffing plan will provide a main basis for our budget planning, along with needs for M&S and non-Upgrade-related projects
- We will have to plan for multiple possible funding scenarios
- Matrix organization of Upgrade will require significant management planning and attention this year

Budget and Staffing

- We are operating under a continuing resolution, expected to last to December 16
- After the CR, we expect funding for both operations and Upgrade preliminary design this year
- Have active searches underway for 64 personnel openings

"Educate the Director" meetings

- Over the next year, I am meeting with a different APS group each week
 - Mainly educational for me, to meet people, understand what they do
 - Includes a tour of workplace
- Could extend to meetings with every CAT

APS Space Planning

- With Upgrade, we will run out of 'unused' floor space for staging construction, temporary storage, etc.
- Clutter and poor housekeeping are a safety concern
- First step – APS Space Use Guide drafted
- Part of a long term plan being developed to expand and organize office, lab, staging, and storage space
- Want to get feedback from all on both Guide and long term plan as we develop them

Advanced Photon Source

	Page 1 of 9
Revision #:	0
Issue Date:	6/8/11
Review Period:	3 years
Supersedes:	N/A
Last Reviewed:	6/8/11

APS Space Use Guide

All areas occupied by the APS shall be assigned to and overseen by one of the APS Divisions or the ALD Office (see [Appendix A](#)). Oversight is the responsibility of the designated Division Director/ALD and responsibilities include:

- Ensuring space is used effectively (e.g., as programs and staffing change, the ALD-appointed APS Space Committee is notified of changes in space needs requirements—including when space is no longer needed—and ensuring that spaces are not used to store materials that are of little value to the APS); and
- Maintaining a professional, uncluttered appearance, and
- Maintaining a safe work environment, that meets Argonne ESH standards.

Site-specific Standards

Experiment Hall

Sector Boundaries — Each sector is bounded by the storage ring, the sector dividing egress aisles (see Experiment Hall Layout, Sector Beamline Areas insert, APS document number [APS_1418307](#)), and three line segments defined by lines connecting the out-board faces of the I-beam columns at the end of the sector. Unless approved by the AES Division Director (AES-DD) as part of a beamline design review process and the APS Deputy Director for X-ray



Advanced Protein Crystallization Facility

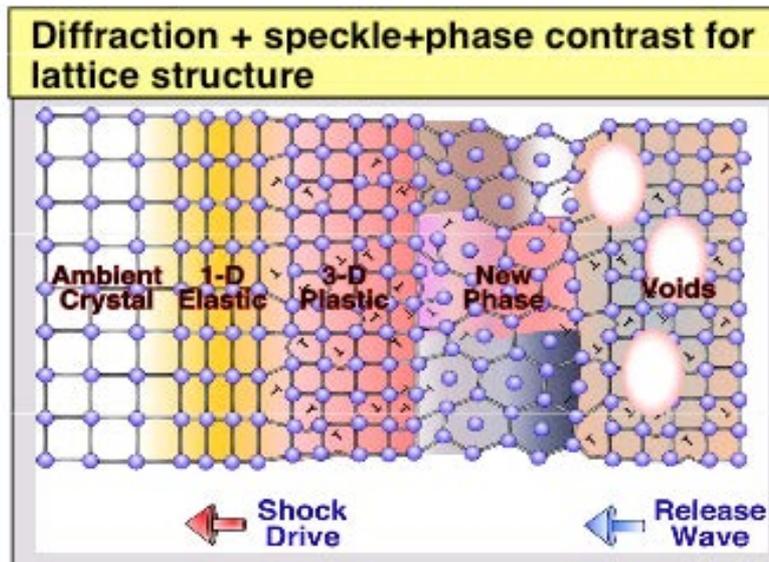


- Groundbreaking ceremony for APCF was August 30
- State of Illinois-funded facility will establish highly automated laboratories and user facilities for the production of proteins and protein crystals from gene sequence data
- Unique state-of-the-art resource for academic and industrial biotechnology and biomedical researchers, serving as a focus for launching new opportunities made possible by large-scale molecular biology, biochemistry, and protein engineering

Dynamic Compression Sector

NNSA-supported beamline organized by Y. Gupta (WSU) to study materials in real time under extreme conditions of pressure (e.g. shock waves)

- Diffraction and imaging, 10 – 100 keV
- Time resolution down to 100 ps
- X-ray source, optics, hutches built by APS
- Drivers built and operated by WSU



Two stage gun (~7 km/s)

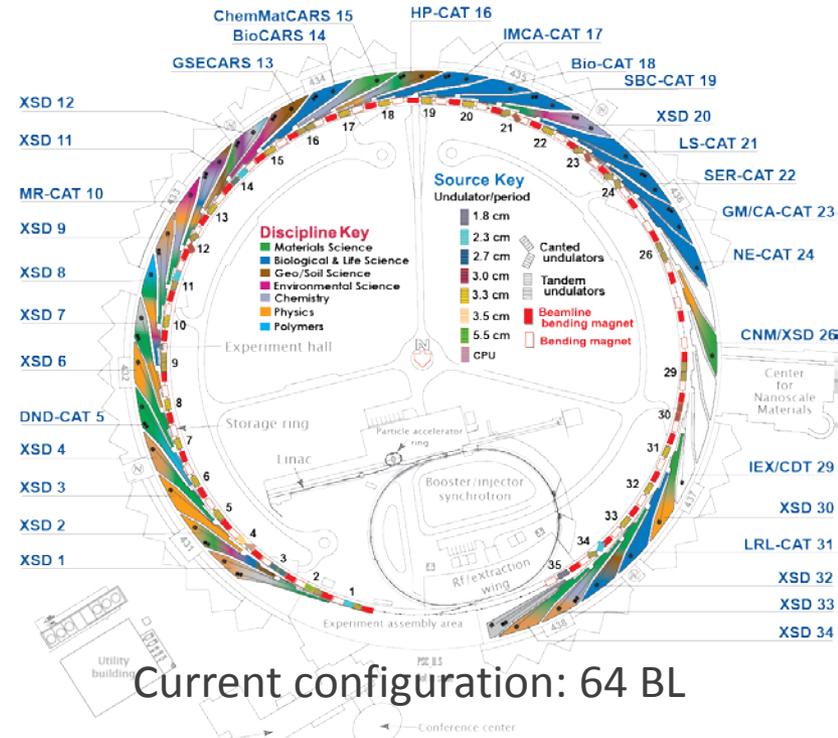


Laser Shock

Roadmap for APS Beamlines

- We are currently developing a "roadmap" for the future location of APS beamlines that includes anticipated beamlines:

	New BL	Upgr. BL
Underway	2	1
APS-U baseline	6	8
APS-U contingent	8	7
Other SAC-approved Biological Science	3	1
Other SAC-approved Physical Science	2	6
Future	1	



- Optimizing the location of all beamlines may involve moving some existing programs, and our decision process will include close consultation with all stakeholders
- We are working to help secure funding for new beamlines where needed

