25 APRIL 2018

APS ALL-HANDS MEETING

STEPHEN STREIFFER

DIRECTOR, ADVANCED PHOTON SOURCE

ASSOCIATE LABORATORY DIRECTOR, PHOTON SCIENCES

Argonne NATIONAL LABORATORY

AGENDA

- Safety
- APS Upgrade Project Update
- PSC News & Updates
- Questions
- Adjourn

Safety

SAFETY

- APS has done well since last summer – but can't lose focus!

  Plan the work. Work the plan. Be cautious. Talk to your line management.

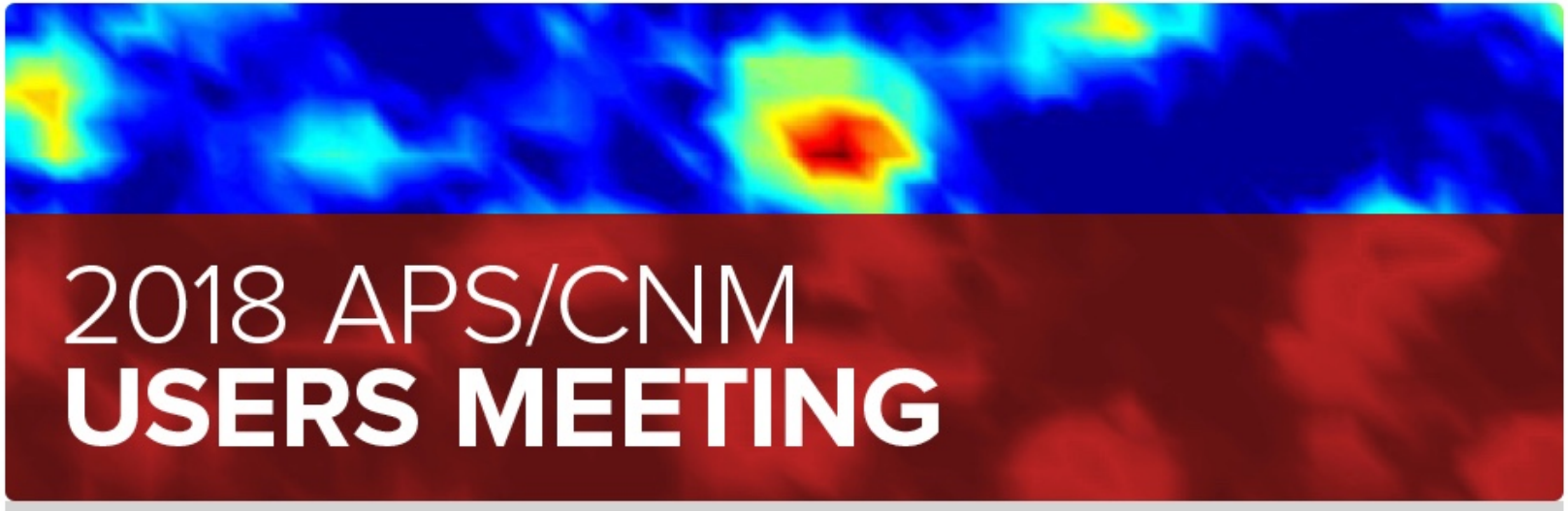
- DOE Office of Enforcement has completed assessment of last summer's events
  - Agreed to Consent Order rather than issuing a Notice of Violation
  - ANL currently reviewing Order
- Lab focusing on management awareness and engagement on high-hazard and high-risk work
- ANL is increasing its participation in Safety Academy For Excellence
  - Hands-on training for suprevisors
- Strengthening of APS Experimental Safety Review Board for ESAF review
  - Added 3 additional members with expertise in chemical and biological safety
- Improving APS tools and training for electrical equipment inspections
  - New process to request inspections that will allow tracking and trending
  - New training to allow all workers to identify NRTLs to limit workload on Designated Electrical Equipment Inspectors

PSC News

AWARDS

SERVICE AWARDS: 25+ YEARS

Michael Bracken
Dale Ferguson
Timothy Jonasson
Kevin Knoerzer
Steve LaBuda
Andre McKenzie
Kristine Mietsner
Glenn Moonier



MAY 7-10, 2018

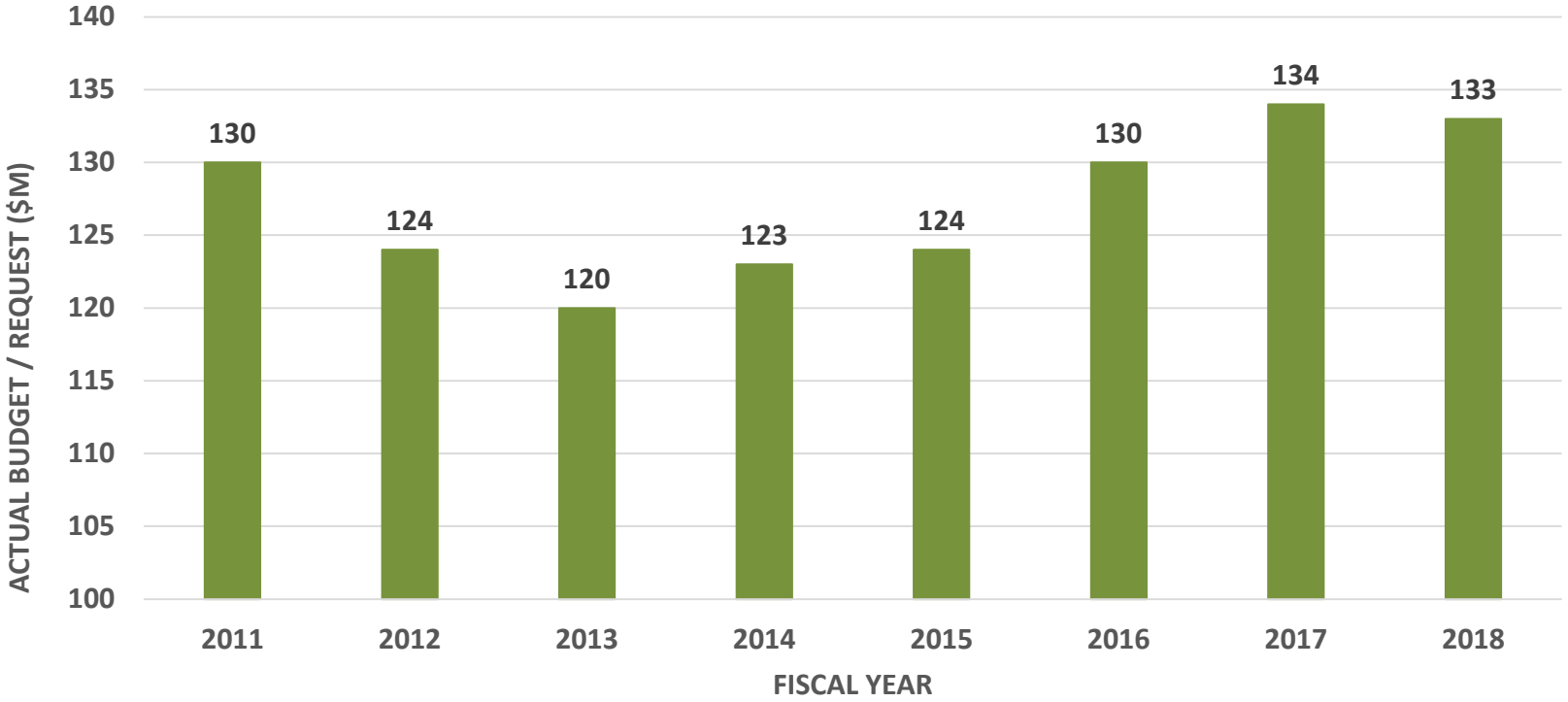
3-WAY MEETING AT APS, MAY 3RD AND 4TH

- The 3-Way Meetings are organized and attended by staff from the four high-energy storage ring sources (APS, ESRF, PERTA III, and SPring-8) from the three continents of Asia, Europe, and North America

- Information will be posted this week!
  - check https://www.aps.anl.gov/APS-Conferences-Workshops-Meetings/Upcoming

- These meeting, set up to facilitate discussions and collaborations between facility staff, have played a central role as a collaborative framework for discussing various scientific and/or technological issues as challenges for the four high-energy, large-scale, third-generation synchrotron radiation facilities

APS OPS FUNDING



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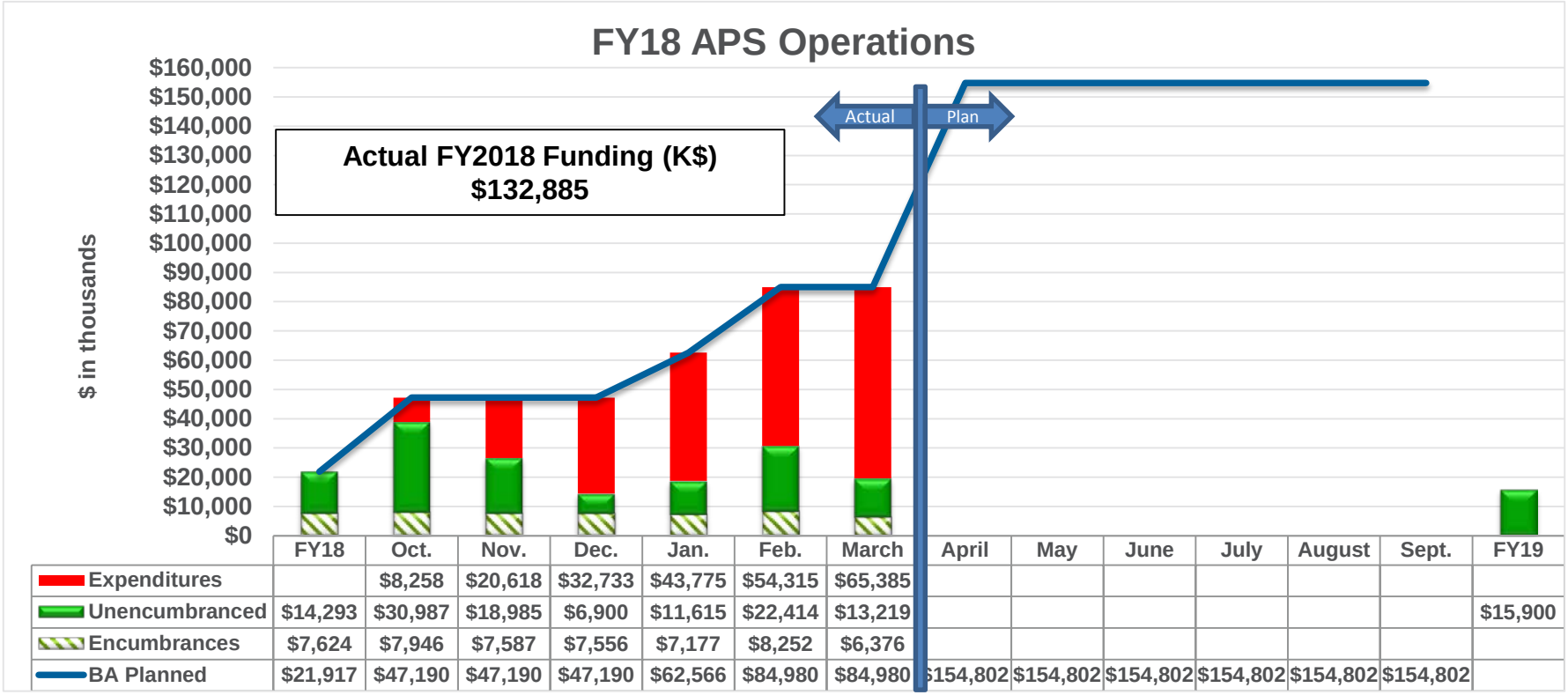
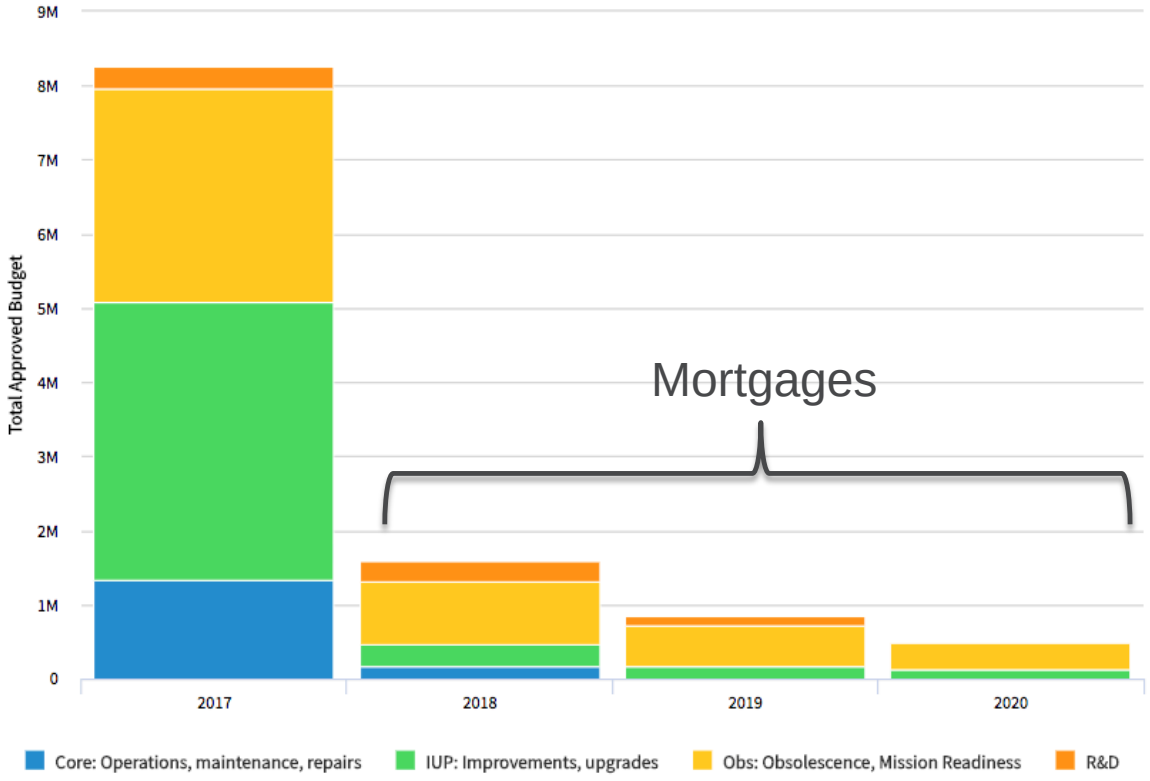
APS OPERATIONS – FY18 BUDGET: PLANNED VS ACTUAL SPENDING



	FY18	Oct.	Nov.	Dec.	Jan.	Feb.	March	April	May	June	July	August	Sept.	FY19
Expenditures		$8,258	$20,618	$32,733	$43,775	$54,315	$65,385							
Unencumbranced	$14,293	$30,987	$18,985	$6,900	$11,615	$22,414	$13,219							$15,900
Encumbrances	$7,624	$7,946	$7,587	$7,556	$7,177	$8,252	$6,376							
BA Planned	$21,917	$47,190	$47,190	$47,190	$62,566	$84,980	$84,980	$154,802	$154,802	$154,802	$154,802	$154,802	$154,802	

APS STRATEGIC PROJECTS SNAPSHOT

- **Total: $11.2M**



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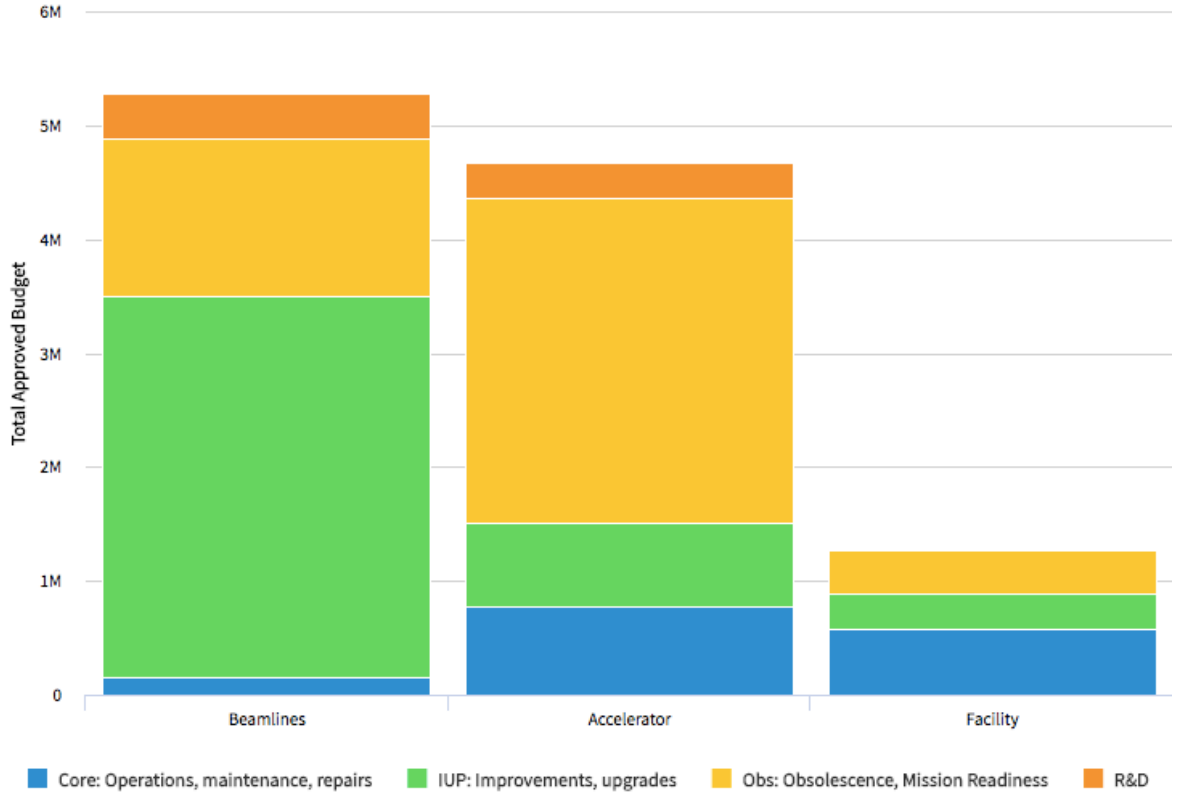
APS STRATEGIC PROJECTS: 2016-2020

- **Snapshot Total: $11.2M**



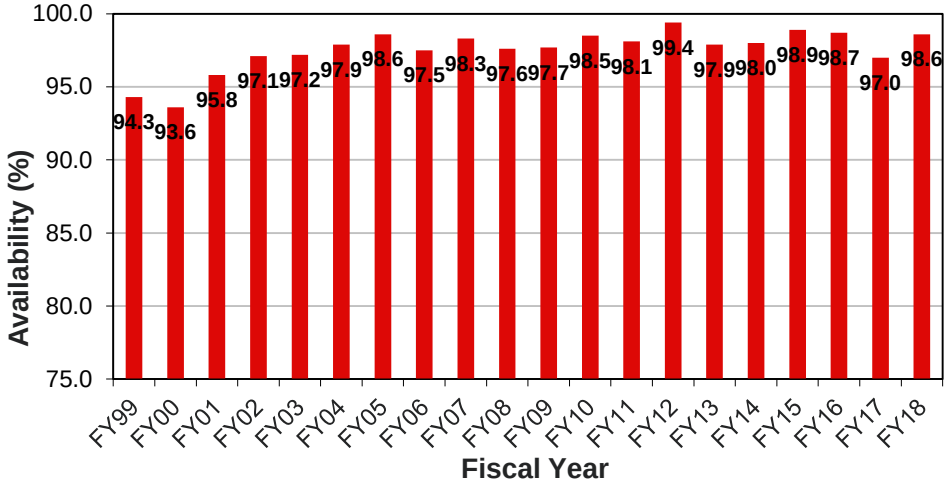
DIVERSITY AND INCLUSION UPDATE

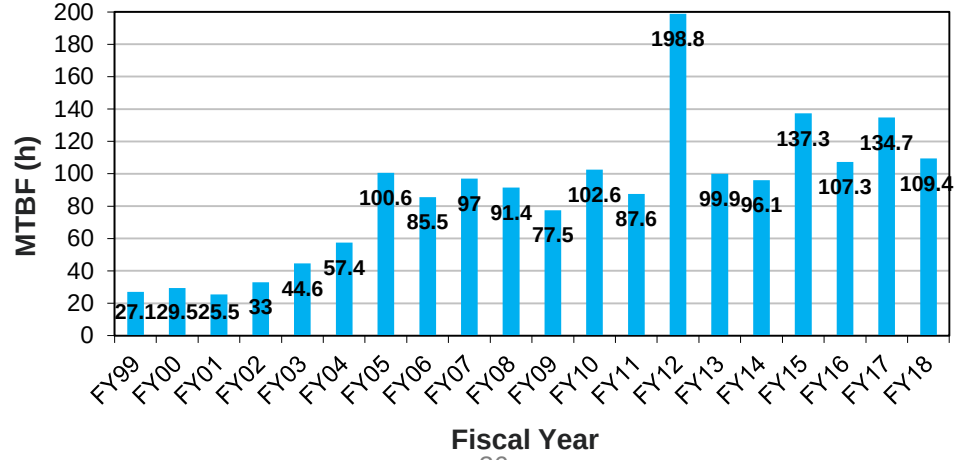
Respect your coworkers. Give everyone the chance to contribute.

- The Lab is updating the charter for its D&I initiative
- 2017 Next Step Climate Survey Follow Up
  - Paul Kearns presenting results to division directors today
  - Lab-wide All-Hands with discussion of results planned for May 15th
- PSC activities
  - Working with the Leadership Institute to schedule sharing PSC Climate Survey Follow Up results
  - Remember! PSC's D&I Working Group Meeting is at 1:30pm on the first Thursday of each month, in A5000. All are welcome!
  - Will update our D&I working group charter to dovetail with the Lab
  - Pairing D&I activities with those of Tom Padilla, our Human Resources Manager

Technical Highlights

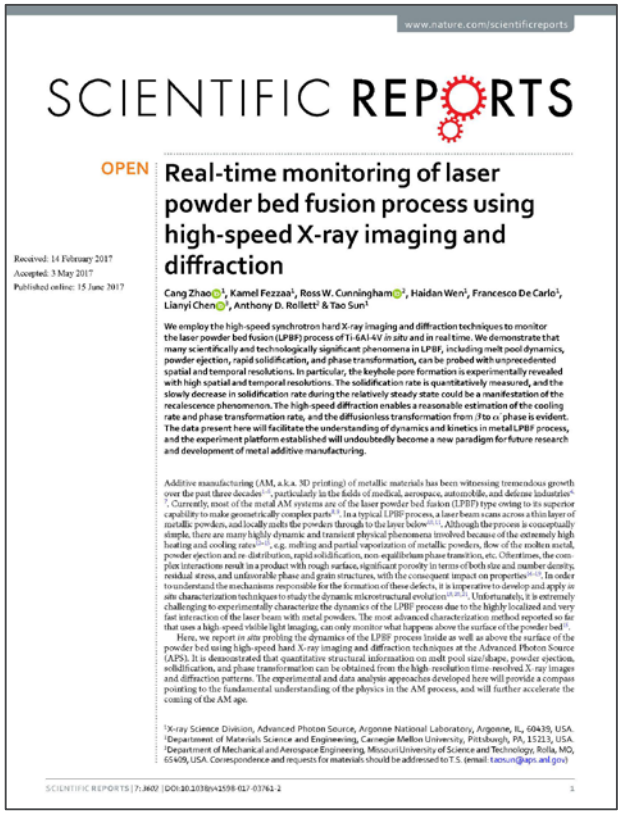
APS X-RAY AVAILABILITY AND MTBF, FY99-FY18 (RUN 2017-3)





APS PAPER ONE OF "SCIENTIFIC REPORTS" 2017 TOP 100

- *"Real-time monitoring of laser powder bed fusion process using high-speed X-ray imaging and diffraction"* (Cang Zhao et al., Sci. Rep. 7, 3602-1 [2017]) received 1079 article views in 2017, making it 1 of the top 25 highly read papers (out of more than 4500 materials science papers) for *Scientific Reports* in 2017.
- In addition to Zhao, other X-ray Science Division co-authors are Kamel Fezzaa, Haidan Wen, Francesco De Carlo, and Tao Sun, with Ross W. Cunningham and Anthony D. Rollett from Carnegie Mellon University, and Lianyi Chen from the Missouri University of Science and Technology.



www.nature.com/scientificreports

SCIENTIFIC REPORTS

OPEN

Real-time monitoring of laser powder bed fusion process using high-speed X-ray imaging and diffraction

Received: 14 February 2017
Accepted: 3 May 2017
Published online: 15 June 2017

Cang Zhao[1], Kamel Fezzaa[1], Ross W. Cunningham[2], Haidan Wen[1], Francesco De Carlo[1], Lianyi Chen[3], Anthony D. Rollett[2] & Tao Sun[1]

We employ the high-speed synchrotron hard X-ray imaging and diffraction techniques to monitor the laser powder bed fusion (LPBF) process of Ti-6Al-4V *in situ* and in real time. We demonstrate that many scientifically and technologically significant phenomena in LPBF, including melt pool dynamics, powder ejection, rapid solidification, and phase transformation, can be probed with unprecedented spatial and temporal resolutions. In particular, the keyhole pore formation is experimentally revealed with high spatial and temporal resolutions. The solidification rate is quantitatively measured, and the slowly decrease in solidification rate during the relatively steady state could be a manifestation of the recalescence phenomenon. The high-speed diffraction enables a reasonable estimation of the cooling rate and phase transformation rate, and the diffusionless transformation from β to α' phase is evident. The data present here will facilitate the understanding of dynamics and kinetics in metal LPBF process, and the experiment platform established will undoubtedly become a new paradigm for future research and development of metal additive manufacturing.

Additive manufacturing (AM, a.k.a. 3D printing) of metallic materials has been witnessing tremendous growth over the past three decades[1–5], particularly in the fields of medical, aerospace, automobile, and defense industries[6,7]. Currently, most of the metal AM systems are of the laser powder bed fusion (LPBF) type owing to its superior capability to make geometrically complex parts[8,9]. In a typical LPBF process, a laser beam scans across a thin layer of metallic powders, and locally melts the powders through to the layer below[10–13]. Although the process is conceptually simple, there are many highly dynamic and transient physical phenomena involved because of the extremely high heating and cooling rates[14–16], e.g. melting and partial vaporization of metallic powders, flow of the molten metal, powder ejection and re-distribution, rapid solidification, non-equilibrium phase transition, etc. Oftentimes, the complex interactions result in a product with rough surface, significant porosity in terms of both size and number density, residual stress, and unfavorable phase and grain structures, with the consequent impact on properties[16–18]. In order to understand the mechanisms responsible for the formation of these defects, it is imperative to develop and apply *in situ* characterization techniques to study the dynamic microstructural evolution[19,20,21]. Unfortunately, it is extremely challenging to experimentally characterize the dynamics of the LPBF process due to the highly localized and very fast interaction of the laser beam with metal powders. The most advanced characterization method reported so far that uses a high-speed visible light imaging, can only monitor what happens above the surface of the powder bed[22].

Here, we report *in situ* probing the dynamics of the LPBF process inside as well as above the surface of the powder bed using high-speed hard X-ray imaging and diffraction techniques at the Advanced Photon Source (APS). It is demonstrated that quantitative structural information on melt pool size/shape, powder ejection, solidification, and phase transformation can be obtained from the high-resolution time-resolved X-ray images and diffraction patterns. The experimental and data analysis approaches developed here will provide a compass pointing to the fundamental understanding of the physics in the AM process, and will further accelerate the coming of the AM age.

[1]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, 60439, USA. [2]Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, 15213, USA. [3]Department of Mechanical and Aerospace Engineering, Missouri University of Science and Technology, Rolla, MO, 65409, USA. Correspondence and requests for materials should be addressed to T.S. (email: taosun@aps.anl.gov)

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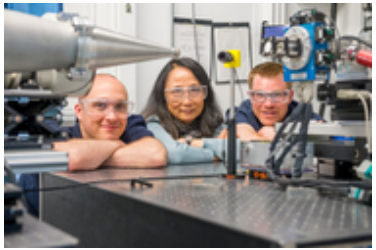
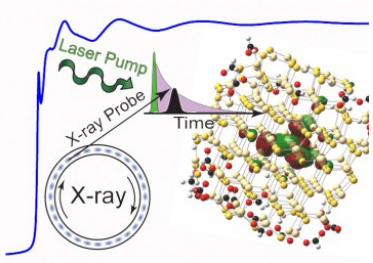
2017'S TOP STORIES FROM THE OFFICE OF SCIENCE: APS RESEARCH

- National Laboratory Articles (1 of 5 total)
  - "Chemical "dance" of cobalt catalysis could pave way to solar fuels" Argonne press release
    - "…using the Advanced Photon Source…researchers were able to directly measure cobalt oxidation states and use theory to calculate a quantity known as 'exchange coupling,' a quantum mechanical value that identifies the relationship between the spins of the electrons that are shuttled between the oxygen and cobalt atoms… found that these electrons spins are… antiferromagnetically coupled. "
      - "*In situ* characterization of cofacial Co(IV) centers in Co_4O_4 cubane: Modeling the high-valent active site in oxygen-evolving catalysts," March 27 edition of the *Proceedings of the National Academy of Sciences*.



- University Articles (1 of 5 total)
  - "Newly discovered semiconductor dynamics may help improve energy efficiency" University of Illinois at Chicago
    - **"**Using the Advanced Photon Source, they were able to capture X-ray images of what happens at the atomic level inside a semiconductor… [and] took very high energy X-ray photos of the semiconductors at millionths of a microsecond apart – which showed what was happening at the atomic level in real time as electrons flowed through the doped semiconductors."



https://science.energy.gov/news/featured-articles/2018/01-03-18/

SOLID-STATE POWER AMPLIFIER DEVELOPMENT IN PROGRESS

- Plan to transition from klystron-based rf source to solid-state is underway; currently seeking bids on design and fabrication of prototype “smart” 2-kW rf module
- Positive response from industry to build next-generation ”smart” rf module

- Specs for 2-kW smart modules have been issued
- Five industry partners have a positive response
  - Continental
  - R&K
  - Tomco
  - Pristine
  - Elite
- Expect to receive quotation on 14 modules in 4 weeks from all 5 vendors
- Current LDRD study shows good performance at 10 kW

Conceptual layout of 200-kW SSPA rf station occupying the same floor space as klystron.

EVIDENCE OF WATER DEEP IN EARTH'S MANTLE

Scientific Achievement

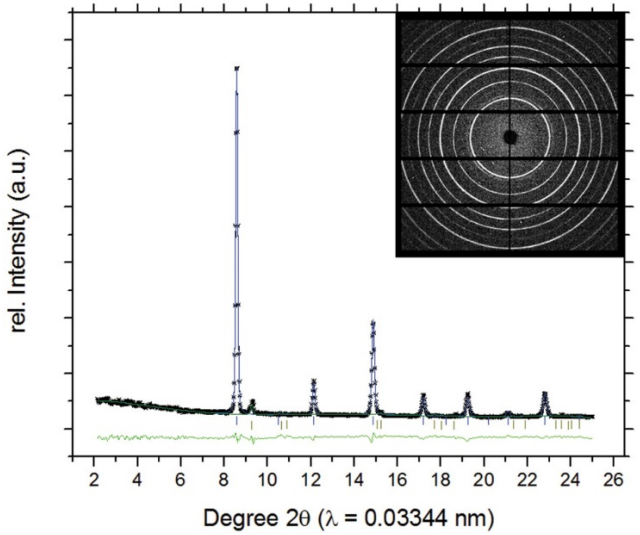
Scientists discovered first direct evidence that fluid water pockets may exist 500 miles deep in Earth's mantle.

Significance and Impact

Discovery underscores that water-rich regions in Earth's interior can play a role in global water budget and movement of heat-generating radioactive elements; and can help create new, more accurate models of what occurs inside Earth, specifically how and where heat is generated under Earth's crust.

Research Detail

- Diamonds pushed up in southern Africa (Orapa) from Earth's interior were examined by x-ray diffraction, x-ray micro-fluorescence, and infrared spectroscopy.
- Showed that diamonds had traces of unique crystallized water called Ice-VII, a high-pressure form of water ice that is stable above 2.4 GPa.



Diffraction pattern of ice-VII in diamond M57666 from Orapa.

O. Tschauner, S. Huang, E. Greenberg, V.B. Prakapenka, C. Ma, G.R. Rossman, A.H. Shen, D. Zhang, M. Newville, A. Lanzirotti, K. Tait, "Ice-VII inclusions in diamonds: Evidence for aqueous fluid in Earth's deep mantle," Science **359**, 1136 (9 March 2018). DOI: 10.1126/science.aao3030

Contact: olivert@physics.unlv.edu

HIGH-ENERGY COHERENT DIFFRACTION ENABLED BY EMULATING FINER PIXELS

Scientific Achievement

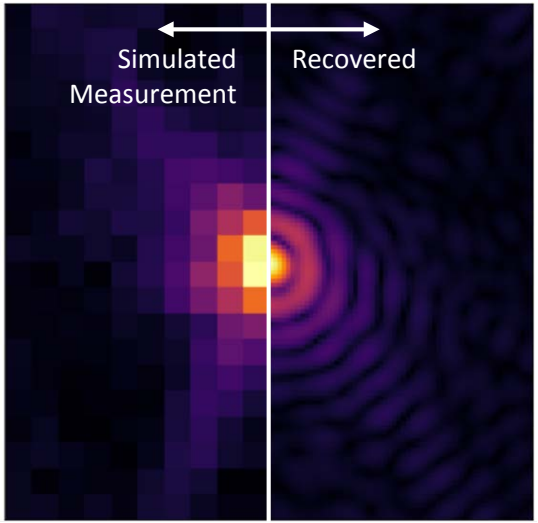
A sparsity-based numerical approach was developed that recovers intensity patterns suitable for coherent diffraction imaging of nanocrystals from high x-ray energy under-sampled coherent diffractions.

Significance and Impact

This work overcomes a significant challenge in enabling 3D coherent x-ray diffraction imaging at highly penetrating x-ray energies which will be one of the revolutionary capabilities of the Upgraded Advanced Photon Source.

Research Details

- Current coherent diffraction reconstruction algorithms fail when intensity patterns are under-sampled, as occurs at high x-ray energies (> 50 keV) due to reciprocal space scaling.
- The numerical method of emulating finer pixel utilizes multiple measurements of a Bragg peak offset by fractions of a physical pixel size, relieving experimental constraints.



A split image of a coherent x-ray Bragg diffraction intensity pattern simulation from a nanocrystal showing (left) the coarse pixelation expected due to the compression of reciprocal space at 54 keV, and (right) the recovered finely pixelated pattern recovered with our approach.

S. Maddali, I. Calvo-Almazan, J. Almer, P. Kenesei, J.-S. Park, R. Harder, Y. Nashed, S. O. Hruszkewycz. ***Scientific Reports***. *8, 4959 (2018)*

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PROTEIN STRUCTURE DETERMINATION WITH SPARSE SERIAL CRYSTALLOGRAPHY DATA

Recent news

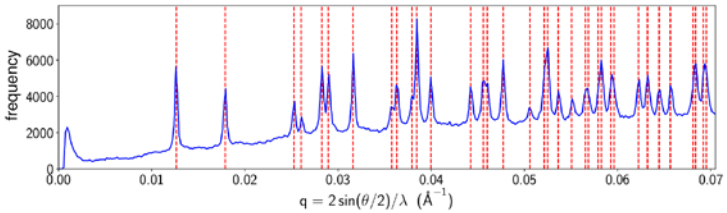
- EMC algorithm developed at Cornell (Elser and Gruner labs) and applied to serial crystallography data collected at GM/CA on lysozyme
  - Started with >300,000 frames where conventional methods found 124,800 frames with “hits”, but only 18,648 were indexable (ASU collaboration)
  - “Create” sparse data by excluding hits
  - Exclude noise (<3 peaks)
  - Reduces the data set to 120,000 frames
  - Create powder pattern to determine lattice parameters, and 3D reciprocal lattice
  - Identify possible crystal orientations for each frame by exhaustive 3D search
  - Refine the intensity and crystal size model with the EMC algorithm

Next 6-month milestones

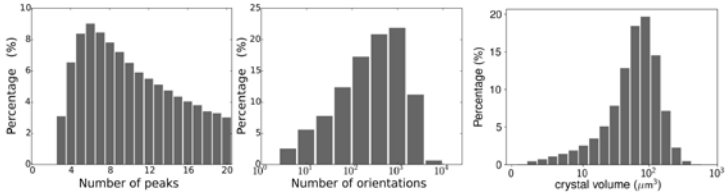
- Adapt code for real-time assessment
- Work with Cornell to determine structures of other proteins

Next 12-month milestones

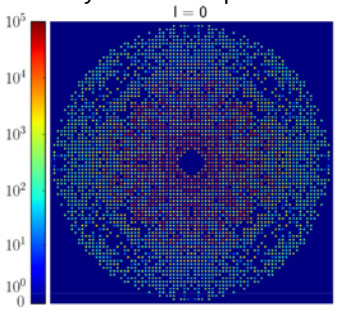
- Work with ALCF to deploy code
- Adapt code to work with “pink” beam data



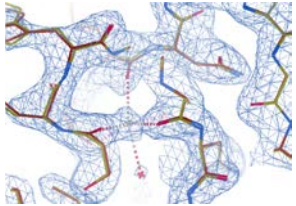
Powder pattern used to determine lattice parameters



Distribution of number of peaks, possible crystal orientations and crystal volume per frame



Central slice of the refined 3D intensity model along the l-axis



Comparison of protein active site with conventional Bragg analysis (Dark Red) and EMC sparse data (Yellow).

APS team: David Kissick, Robert Fischetti

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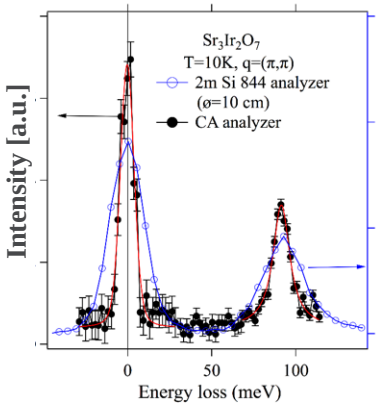
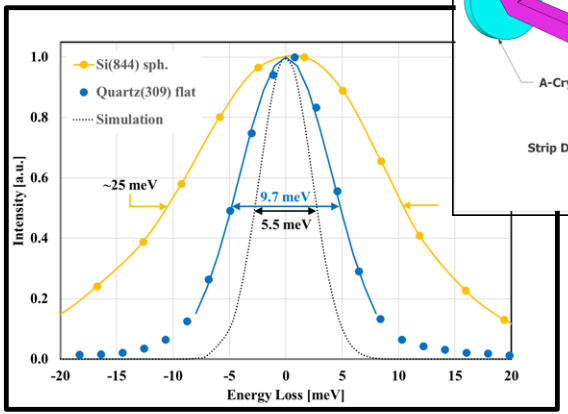
27-ID: HIGHEST ENERY RESOLUTION FOR RIXS MEASUREMENTS

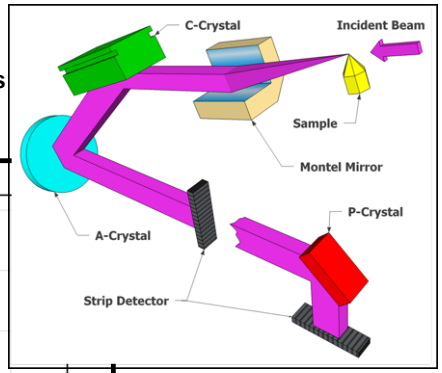
- RIXS is a powerful technique for study of electronic excitations in complex materials
- Extension to magnetic excitations ➡ requires much higher energy resolution
- Novel flat crystal spectrometer at 27-ID: reached sub-10 meV for the first time
  - **! New record for any hard x-ray RIXS measurement to date !**
- Also enables polarization analysis without loss of resolution



Magnon spectrum in $Sr_3Ir_2O_7$
Blue: 25 meV, Black: 9.7 meV
Dramatic sharpening of features and new spectral structures clearly visible with higher resolution

Flat-Crystal Optics

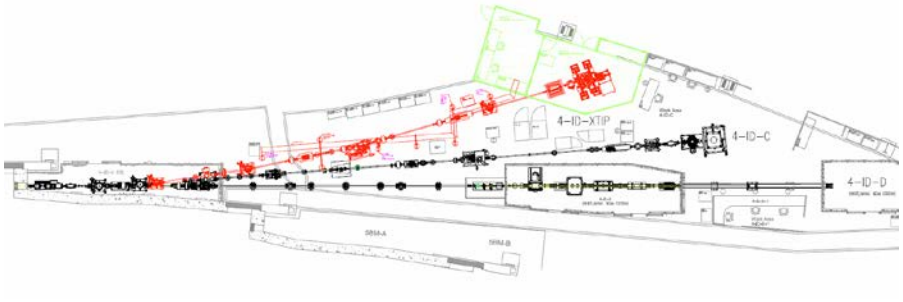


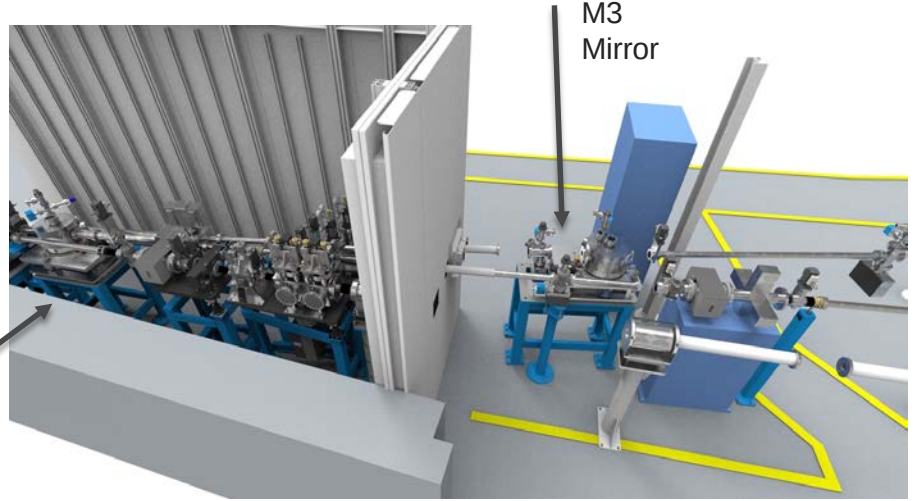


Resolution Functions
Yellow: previous
Blue: new spectrometer
Dashed: near-future option

X-TIP BEAMLINE AT 4-ID: STATUS UPDATE

- Revised schedule to complete
  - M2 + M3 deflecting mirrors currently in detail design
  - Run 2018-1: Install entrance slit, SGM, exit slit
  - May 2018 Shutdown: Install M2 + M3 Mirrors
  - Run 2018-2: Commission SGM using gas cell at end-station position (energy calibration, resolution)
  - Run 2018-3: Install M4 + M5 Mirrors for final focusing in end-station





XTIP beamline

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DATA WORKING GROUP

The Five Light Sources Have Formed a Data Working Group

- The purpose of the Data Working Group is to serve as a resource for the five BES light source directors to provide information and recommendations on working together in the areas of data and computing.
- Two charges for the first quarter of CY2018:
  - *Charge 1: Data Retention* - report that explores the topic of data retention, including the current data retention situation at the five light sources, and outlines ways for the light sources to work collaboratively towards a more uniform long-term approach to data retention.
  - *Charge 2: Real-Time Computing Needs* - report that explores the topic of real-time computing, including a summary of the current real-time computing situation at the five light sources, and projections of future user needs in terms of hardware, data analysis algorithms, and software resources.





Looking Forward…

ANNUAL LAB PLAN (ALP)

- ALP combined with the annual Performance Evaluation and Measurement Plan (PEMP) are the primary formal Lab engagement mechanisms with DOE Office of Science
- Annual submission due April 26th
  - Core Capabilities
  - Science Strategy for the Future / Major Initiatives
    - ***Hard x-ray sciences***
    - *Advanced computing*
    - *Universe as our laboratory (ULab)*
    - *Materials and chemistry*
    - *Manufacturing science and engineering*
  - Tech Transfer, Commercialization, and Partnership Strategy
  - Infrastructure
  - Human Resources
  - Cost of Doing Business
  - Strategic Partnership Project Report
  - LDRD Plan
- Lab Director and team present to DOE on June 4, 2018


Argonne NATIONAL LABORATORY

Annual Laboratory Plan:
Fiscal Year 2018

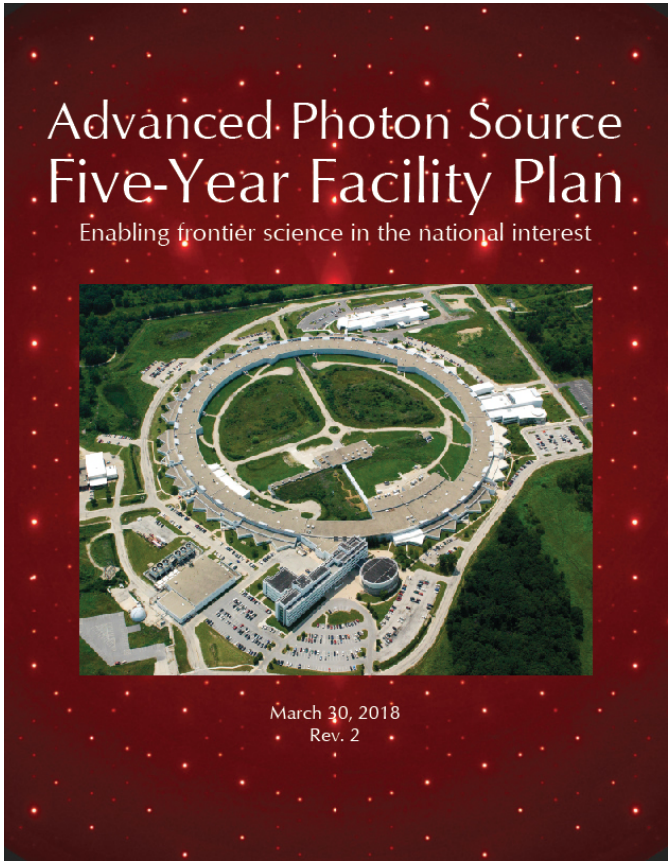
prepared for
U.S. Department of Energy Office of Science
by
Argonne National Laboratory
9700 South Cass Avenue, Argonne, Illinois 60439

Paul K. Kearns, Laboratory Director

April 26, 2018

UChicago ▸ Argonne LLC

APS STRATEGIC PLAN UPDATED MARCH 2018



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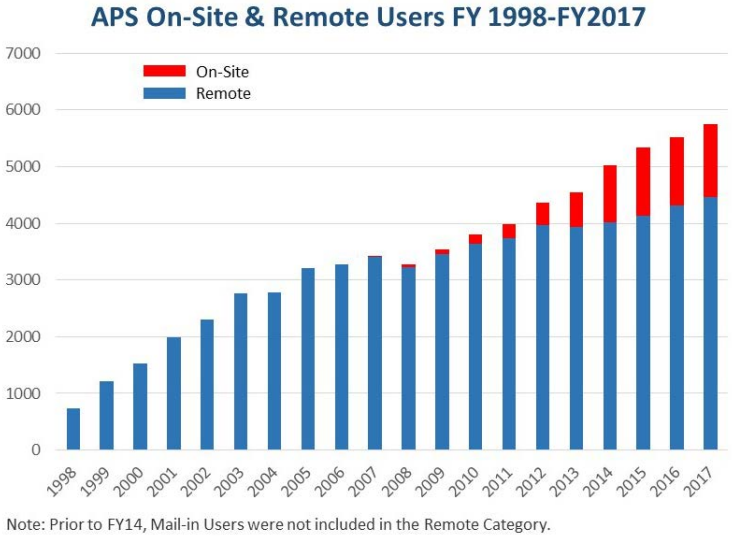
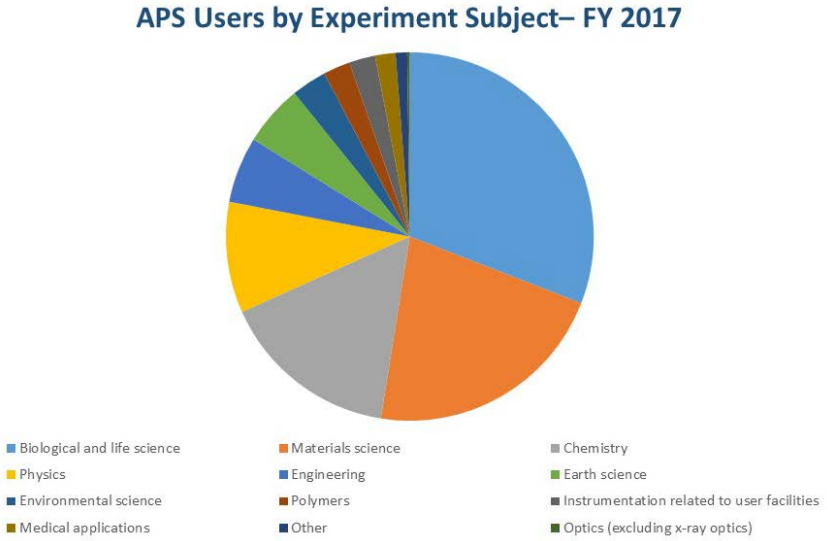
THE PATH TO APS-U (~MID-2022): FOCUS FOR THE NEXT 4-5 YEARS

- Redevelop Strategic Plan with an emphasis on Ops maintenance and obsolescence mitigation
  - We want to continue operating reliably the next 25 years
  - APS-U Project doesn't replace everything
- People! Work a staffing strategy that supports Ops & APS-U
- Keep the APS-U science case fresh
- Prepare the user community and collaborative access teams for the dark period

QUESTIONS?

SERVING A LARGE, GROWING, HIGHLY PRODUCTIVE, AND SCIENTIFICALLY DIVERSE USER COMMUNITY





In FY2017:

- >5,700 unique onsite/offsite users from >700 institutions
- The APS accounted for approximately half of all DOE-BES light source users and one-third of all DOE-BES facility users

ACCELERATOR OPERATIONS STATUS AS OF APRIL 9, 2018 17:05

- 2018-1 User Run started on January 30, 08:00

Total Amount of User Time	1415.0 Hours
Delivered Beam	1387.0 Hours
Percentage of Scheduled Time	98.02%
Mean Time Between Faults (MTBF)	77.1 Hours
Downtime During Period	28.0 Hours
Mean Fill Duration in Period	73.0 Hours
Faults per Day of Delivered Beam	0.3
Total Number of Faults	18 (and 2 delayed starts)

- Most of the faults were due to power supplies, PSS and controls
- Last 2 weeks: perfect run; no downtime

BES Triennial Review of the APS

- BES Triennial Review was held Tuesday, August 15 to Thursday, August 17, 2017
- Review report received on November 29, 2017. The reports (76pp) are very positive, while still noting areas for improvement.
  - "The APS appears to be performing very well. Staff is highly motivated, experienced, and knowledgeable."
  - "As the largest synchrotron facility in the US, the scientific output of APS is outstanding, and its impact on science is profound."
  - "The APS facility has been exceptionally productive – in quantity and quality of publications and other measures from the facility and CAT beamlines; the accelerator operations has been with excellent reliability, and the number of users is very high and continues to grow. APS is to be congratulated for these excellent achievements."
  - "The APS accelerator team has a strong international reputation for accelerator research, in particular for their computational simulation capabilities, superconducting undulator development, solid state RF and beam stability/feedback."
  - "There is a challenge in the extensive matrixing of staff, in particular between the APS and APS-U, and management needs to ensure that both activities prosper in parallel until the APS-U is complete."
- Five recommendations to address on staffing skill distributions, continuing to find efficiencies in operations, cost structure, LDRD activities, and safety

USER MEETING AWARDS

- **Joshua Riback** (The University of Chicago), APS user and graduate student in the Biophysical Sciences at The University of Chicago, earned the 2018 APSUO Rosalind Franklin Young Investigator Award for his work using small-angle x-ray scattering techniques at the APS to study biophysical interactions.

- **Hua Zhou** (XSD-SSM) was named the recipient of the 2018 Gopal K. Shenoy Excellence in Beamline Science Award for his critical work in the field of synchrotron radiation studies of complex oxide heterostructures, where he is a world-recognized leader both in terms of performing hard x-ray studies and in promoting the use of hard x-ray techniques for oxide investigation.