Future Science at Next Generation Korean Synchrotron Workshop – Cheongju, Korea, June 25-27, 2024

Advanced Photon Source Upgrade

Commissioning, Initial science, & future outlook

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Associate Laboratory Director for S&T; Director X-ray Science Division
Advanced Photon Source
Argonne National Laboratory

ADVANCED PHOTON SOURCE

70

X-ray beamlines

6,000

Experiments
per year

2,000

Publications
per year

5,500

Unique users
in a typical year
~2000 grad students
~1000 postdocs

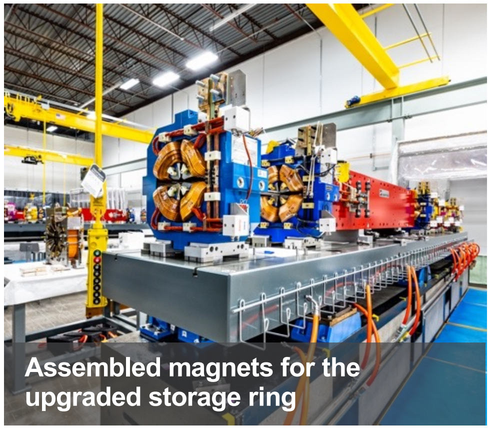
Countless
Societal impacts

APS UPGRADE

☼ **x500**

$815M

♻ **$1.5B**



Assembled magnets for the upgraded storage ring

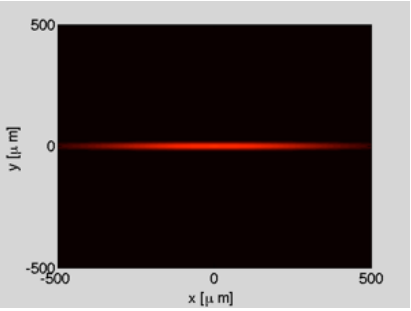
First new beamline instrument up and running

New front end systems to deliver X-ray beams to experiments

Long Beamline Building, which will house two of the nine feature beamlines

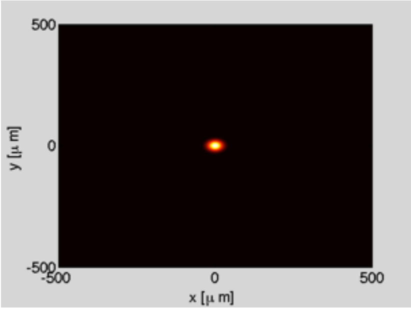
ADVANCED PHOTON SOURCE UPGRADE

Previous APS (7 GeV)



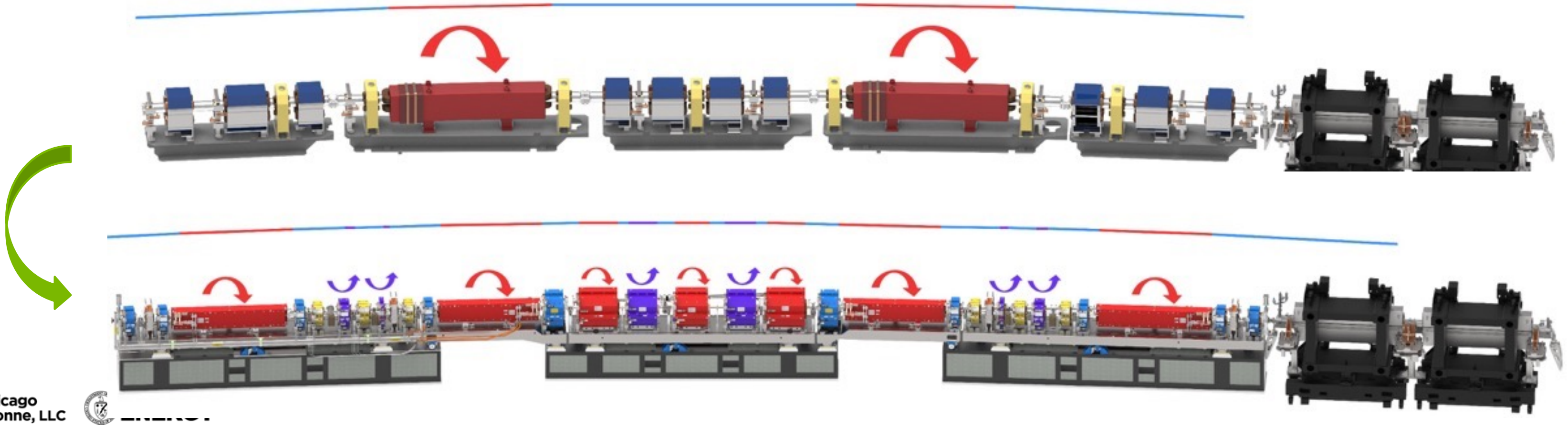
ε_o = 3100 pm

APS Today (6 GeV)



ε_o = 42 pm

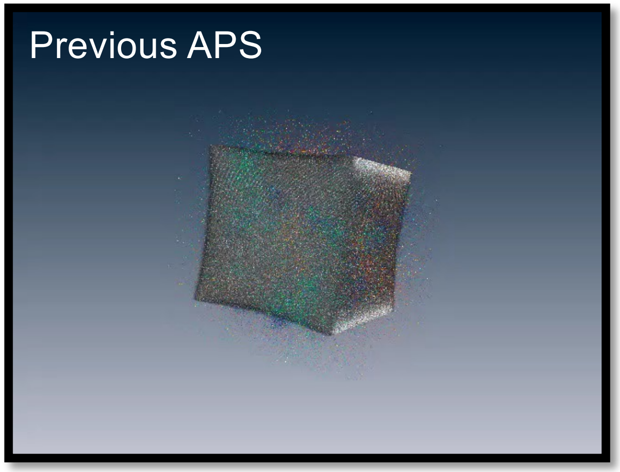
Replaced the storage ring decreasing electron source size



2BA

7BA+

HIGH BRIGHTNESS: HIGHER RESOLUTION, FASTER DYNAMICS



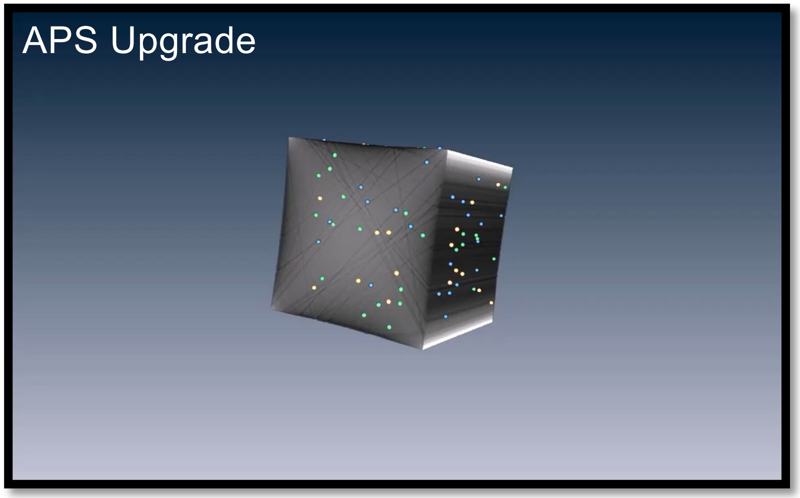
1 nm Cu (green), Co (blue), Ni (yellow); only photon noise, $(1\mu m)^3$ alumina support visible

Brightness – increasing the number of photons that hit the target – is key to:

- Visualizing nanoscale structure across macroscopic fields of view
- Electronic/magnetic/chemical contrast

APS-U's extreme brightness at high energies enables exploration of individual nanostructures/defects

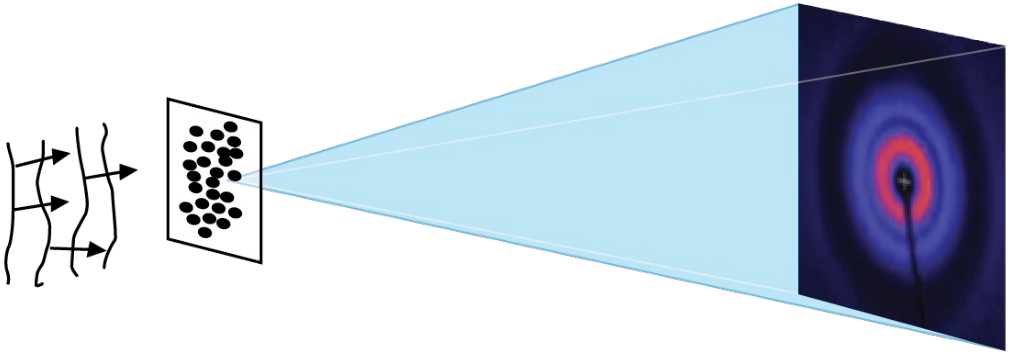
- Across length scales
- Deeply buried
- In real, complex environments
- Down to few-atom sensitivity



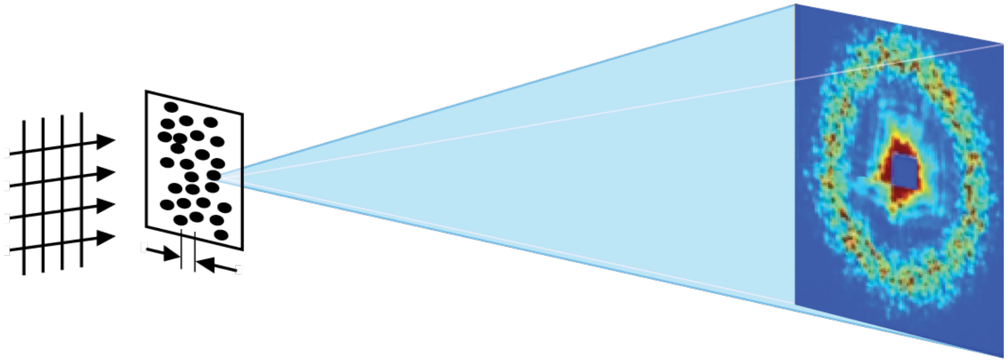
Catalytic nanoparticles clearly visible on alumina surface

COHERENT X-RAY STUDIES

Game-changing leap from average to local time/space information



Incoherent beam carries average information; resolution limited by optics



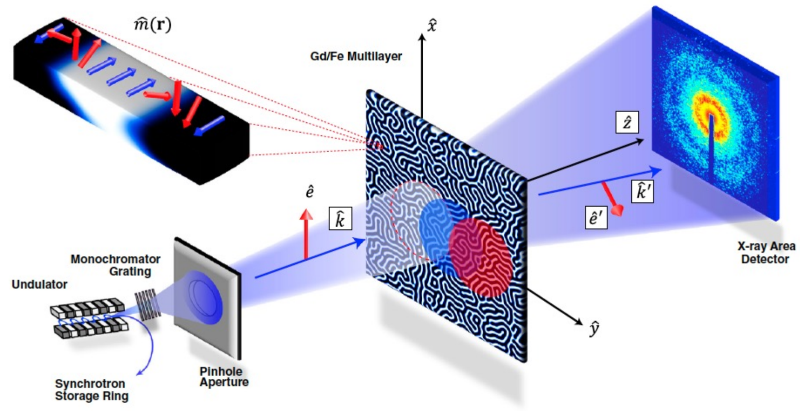
Scattering of coherent beam carries all microscopic, local information

non-periodic arrangements, correlations, dynamics

Spatial resolution limited only by x-ray wavelength, coherent flux

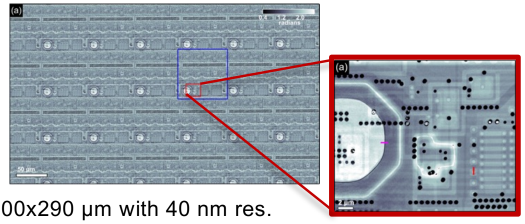
COHERENT DIFFRACTION IMAGING

Forward Scatting Ptychography

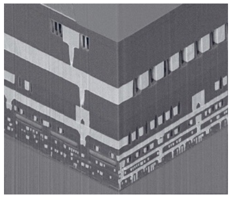


A. Tripathi *et al., PNAS* **108**, 13393 (2011)

Eiger "selfie"
M. Guizar-Sicairos et al., Optics Express 22,14859 (2014)

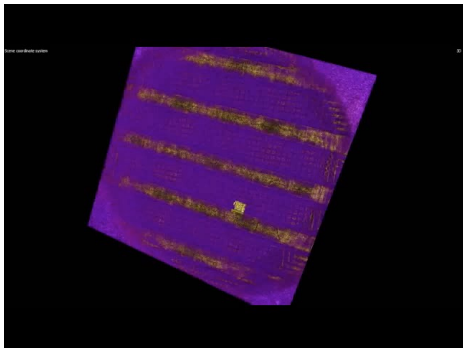


500x290 μm with 40 nm res.

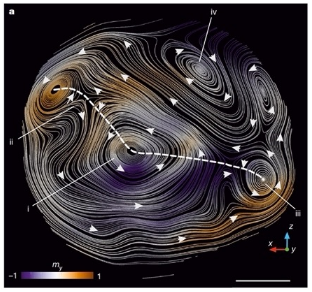


3D reconstruction with 10 nm resolution

3D movie of integrated circuit obtained at the APS



Reconstructed local magnetization of $GdCo_2$ Cylinder with 100nm resolution

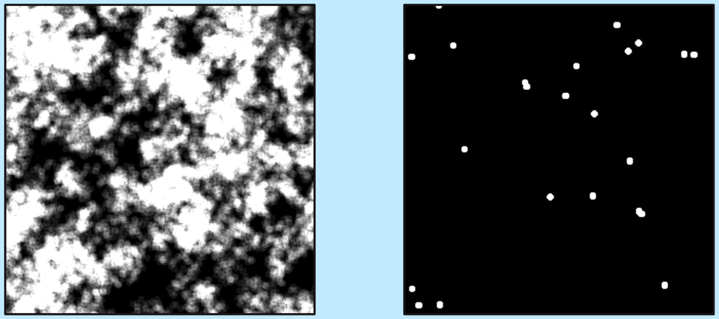


C. Donnelly *et al., Nature* **547**, 328 (2017)

APS-U: enough coherent flux to image $1mm^3$ of a microcircuit at 10 nm 3D resolution.

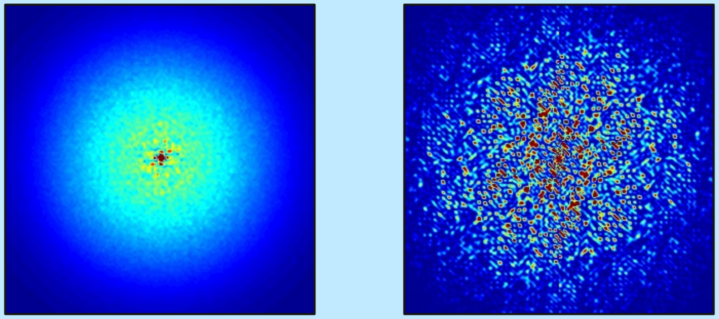
COHERENT FLUX: NON-EQUILIBRIUM PROCESSES

Ensemble (left) built up by fast particle dynamics (right)



Pre-APS-U: X-ray photon correlation spectroscopy time-averages to ms, faster trajectories are lost

APS-U: Speckle changes as sample evolves, dynamics are captured (simulation of 30x brightness)

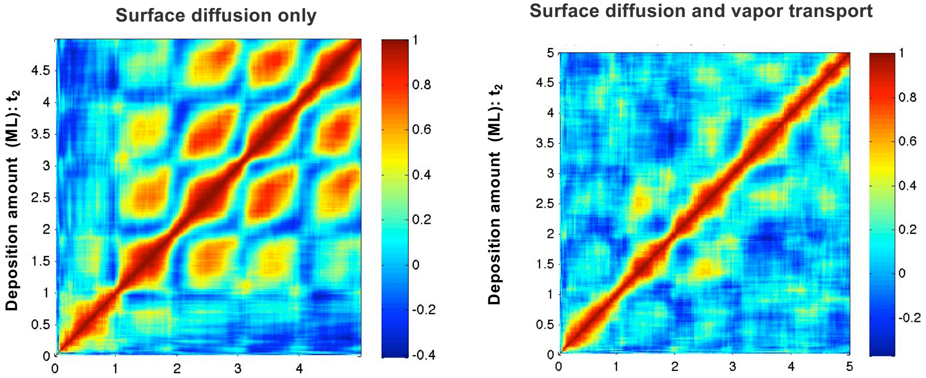


Sensitivity ~ (Coherent flux)^2

APS-U: increases *up to 1,000,000x*

Allows us to probe:

- Continuous, atomic-scale dynamics down to nanoseconds
- Beyond standard pair correlations
  - Deterministic insight into growth mechanisms and stability of materials, deformation vs. diffusive motion, stick-slip in microfluidic flow

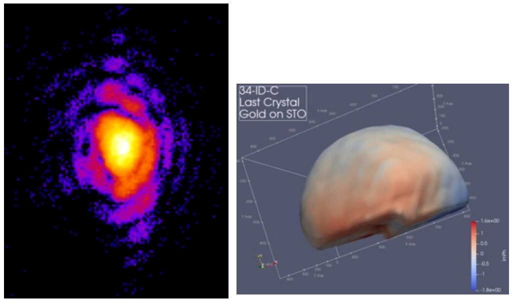


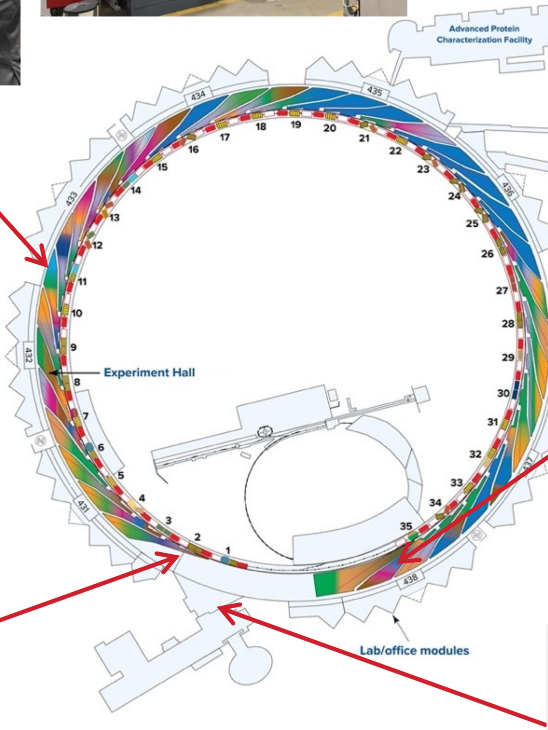
***APS-U:** Simulated time-time correlation functions during layer-by-layer crystal growth, for different adatom transport regimes*

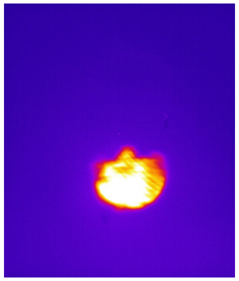
APRIL 17, 2023: END OF USER OPERATIONS

Last beam gathering at 11-ID/BM

Last light at 34-ID-C
Bragg-CDI Image of Gold nanocrystal on STO

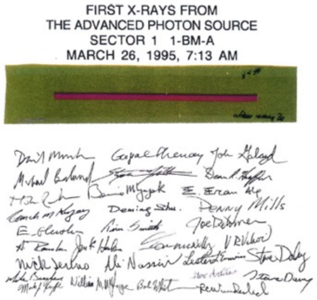






Last light at 6-ID-C

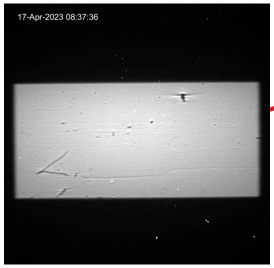
Control room for last beam



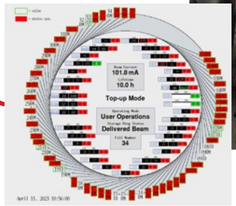
FIRST X-RAYS FROM
THE ADVANCED PHOTON SOURCE
SECTOR 1 1-BM-A
MARCH 26, 1995, 7:13 AM

Gopal Shenoy
Deming Shu.
Denny Mills
Ali Nassiri

First and last X-rays from
APS v.1.0



17-Apr-2023 08:37:36



= online
= shutter open

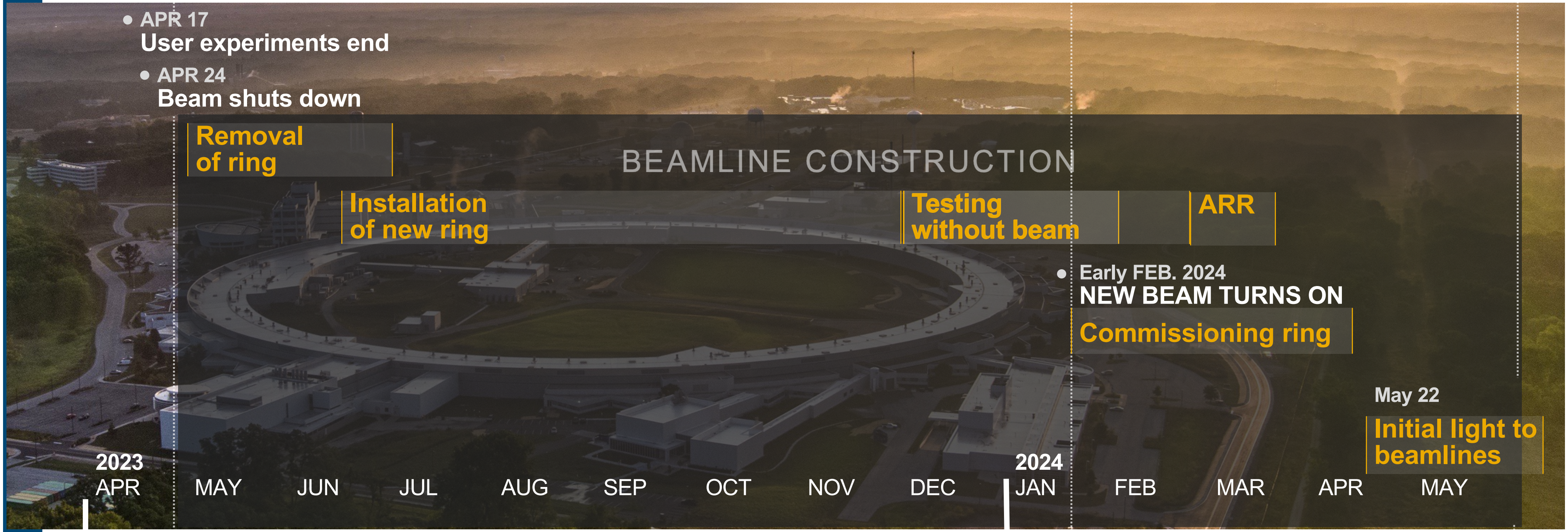
Beam Current
101.8 mA
Lifetime
10.0 h

Top-up Mode

Operating Mode
User Operations
Storage Ring Status
Delivered Beam
Fill Number
34

April 11, 2023 10:56:00

APS-U DARK TIME SCHEDULE



- APR 17
  User experiments end
- APR 24
  Beam shuts down

Removal of ring

BEAMLINE CONSTRUCTION

Installation of new ring

Testing without beam

ARR

- Early FEB. 2024
  NEW BEAM TURNS ON

Commissioning ring

May 22

Initial light to beamlines

2023 APR | MAY | JUN | JUL | AUG | SEP | OCT | NOV | DEC | 2024 JAN | FEB | MAR | APR | MAY

Initially planned to start of storage ring commissioning in early Feb. & beamlines early May ’24

Accelerator test and checkout, survey, & storage ring bake out took longer than expected

Injected electrons April 13th & first beamline x-ray June 17th

APS-U STORAGE RING REMOVAL

First girder of old APS storage ring coming out of ring in May, 2023

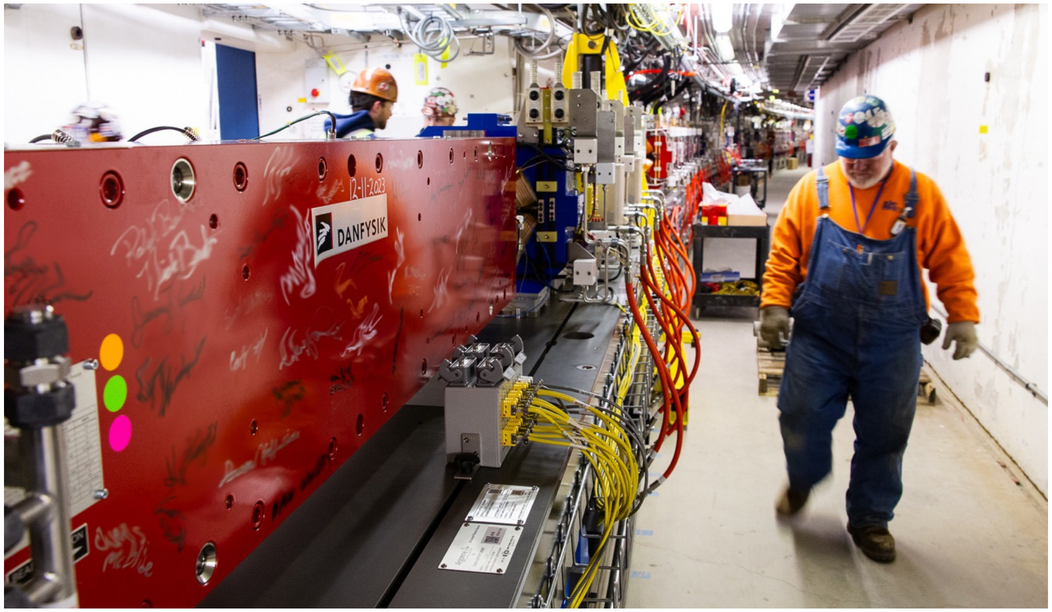
Empty storage ring tunnel in mid-June, 2023

- 1759 Tons of girders and magnets sent to BNL/JLAB (reusing for EIC)
- ~225 Tons of electronics, cabling, support equipment

MODULE INSTALLATION

First pre-assembled module installation – July 12, 2023

INSTALLATION OF LAST COMPONENTS



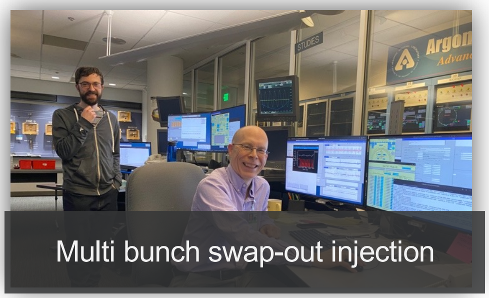
In December 2023, all 200 modules were in!

Feb. 2024, last piece being installed

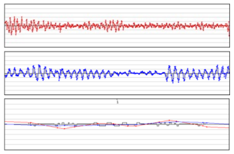
Vacuum, test & check out, & survey took slightly longer than expected.

APS-U ACCELERATOR COMMISSIONING

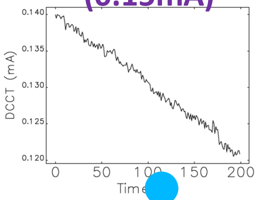

First stored beam in the storage ring


Multi bunch swap-out injection

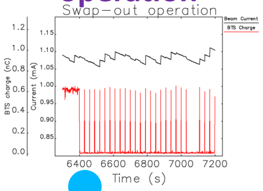
First turns



Stored beam (0.15mA)



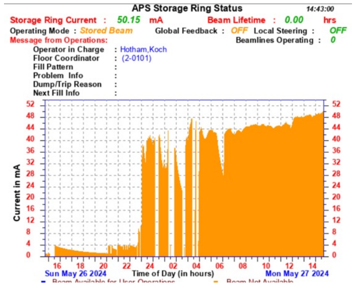
Swap-out operation



10 mA

25 mA

50 mA


APS Storage Ring Status 14:43:00

Storage Ring Current : 50.15 mA Beam Lifetime : 0.00 hrs

Operating Mode : Stored Beam Global Feedback : OFF Local Steering : OFF

Message from Operations: Beamlines Operating : 0

Operator in Charge : Hotham,Koch

Floor Coordinator : (2-0101)

Fill Pattern :

Problem Info :

Dump/Trip Reason :

Next Fill Info :

First light at user beamline @ 50 mA

April 13

April 20

April 29

May 12

May 17

May 27

June 17

Machine studies

Radiation studies

Machine studies

Septum failure

Machine studies

Septum failure

Machine studies

Beamline commiss

Machine studies

April 10

April 18

May 2

May 17

May 25

June 2

June 15

June 19

DOE authorizes start of commissioning

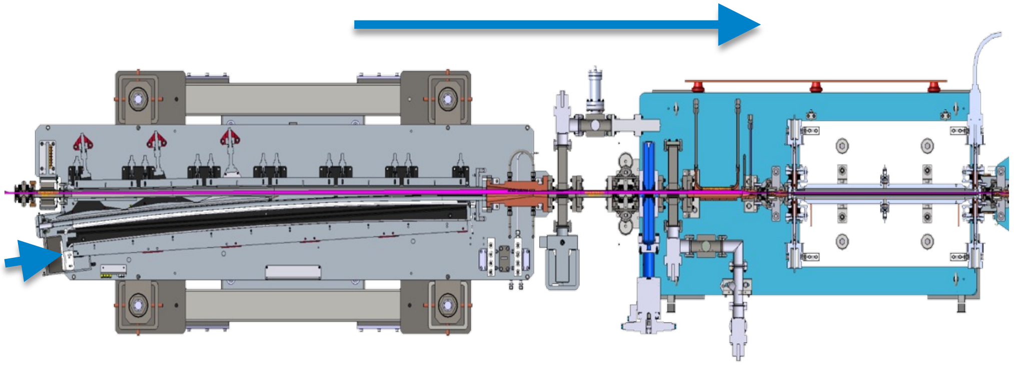
Vacuum conditioning started

Diagnostics beamline shutter opened with swap-out

INJECTION SEPTUM AND FIRST KICKER

On-axis injection needed due to small dynamic aperture

Beam Direction

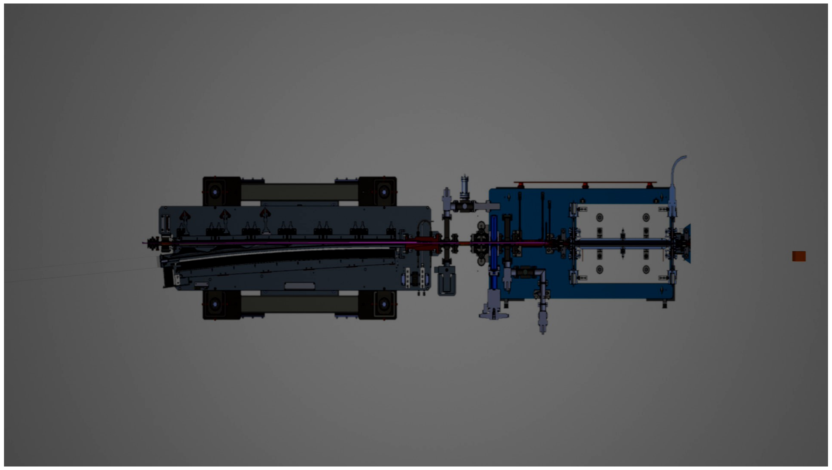


Septum

18 kA, 0.5 millisecond pulse

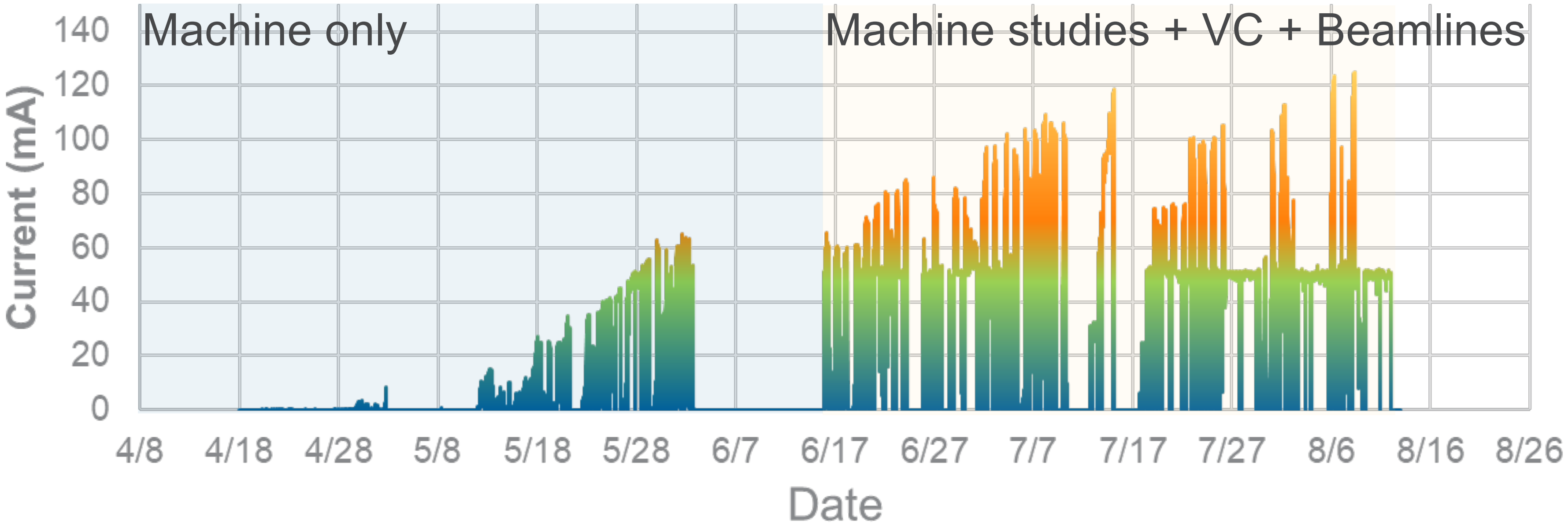
IK1 Kicker

27 kV, 20 nanosecond pulse



Swap out every 20-40s

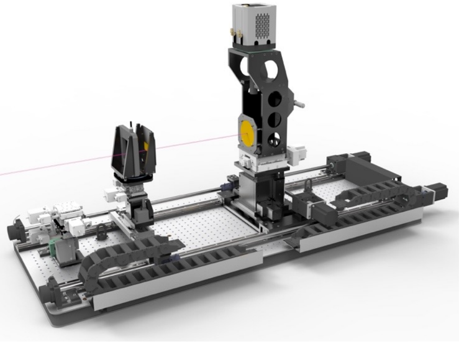
COMMISSIONING - CURRENT

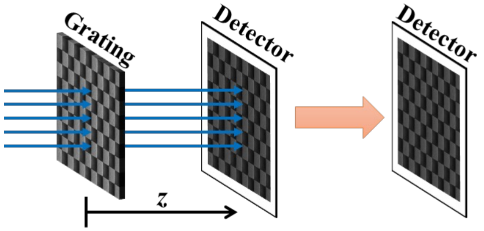


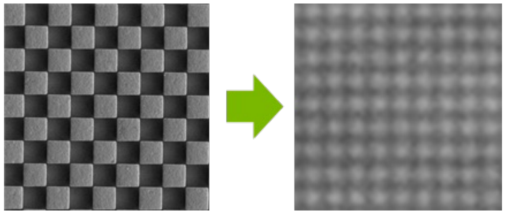
- <u>Operated in 3 shifts in the first operations run:</u>
  - User mode from 9am to 5pm (50 mA)
  - Machine study 5pm to ~1am
  - Vacuum conditioning at night (higher current)

EMITTANCE MEASUREMENT

Measured at 3-ID-B

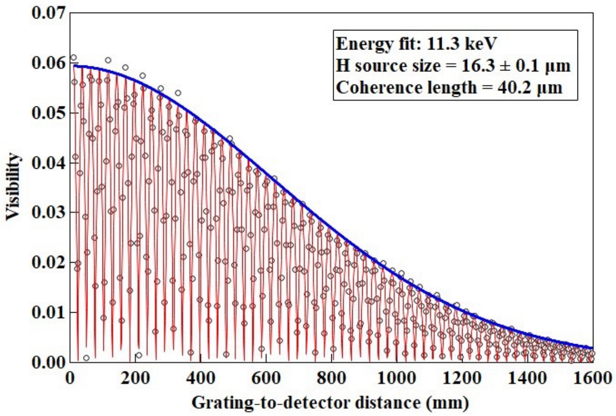


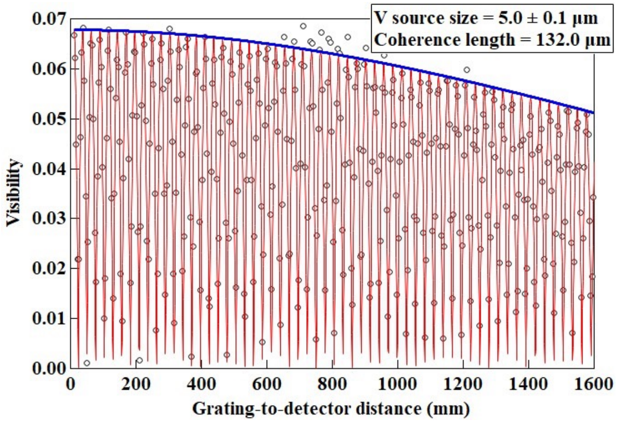




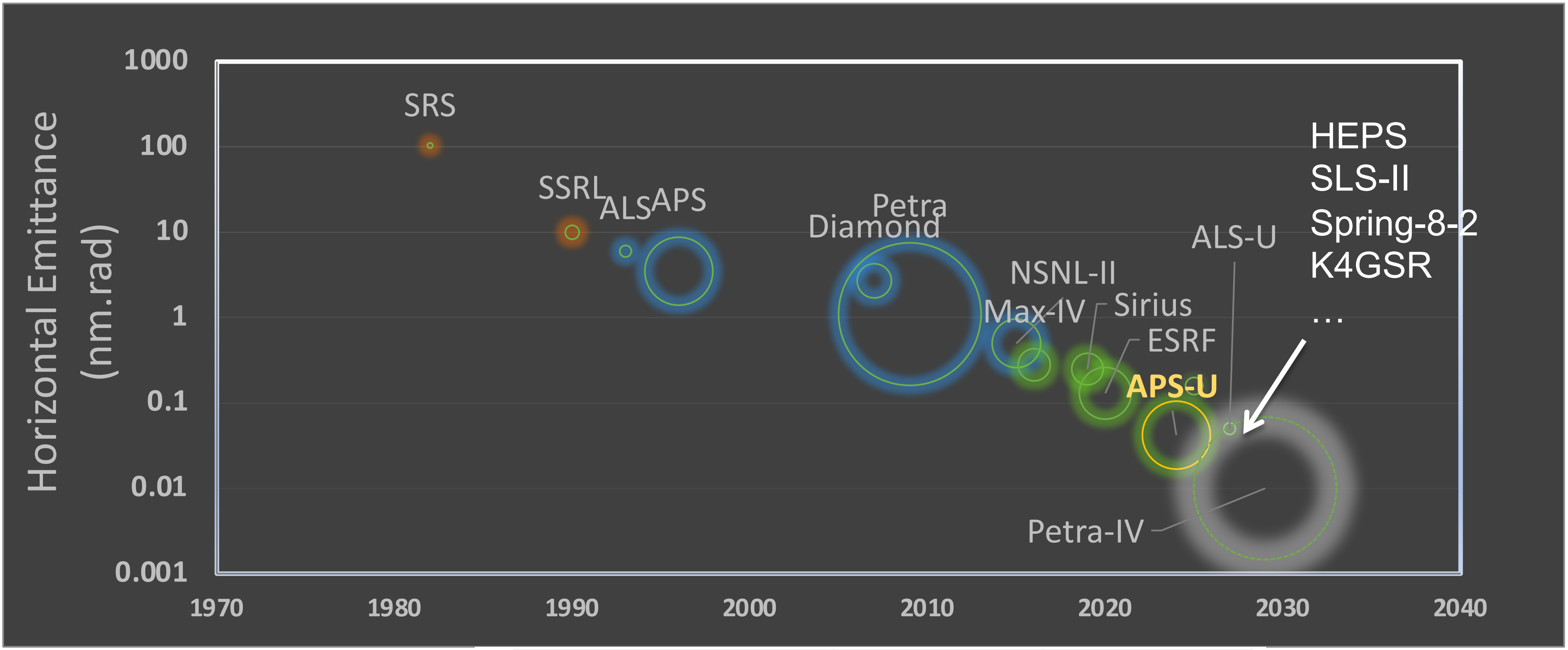
Fabricated at Center for Nanoscale Materials (ANL)

Low coupling, 48-bunch mode, 50 mA





APS-U HORIZONTAL EMITTANCE

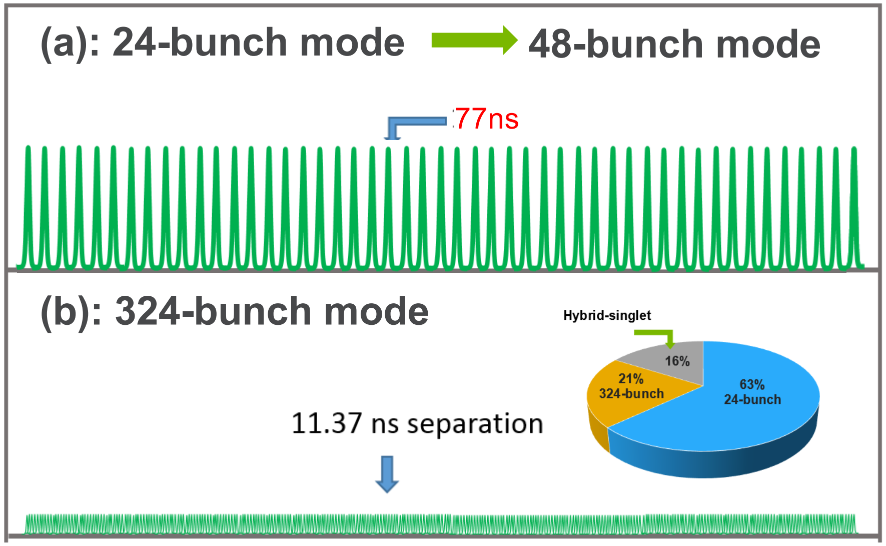


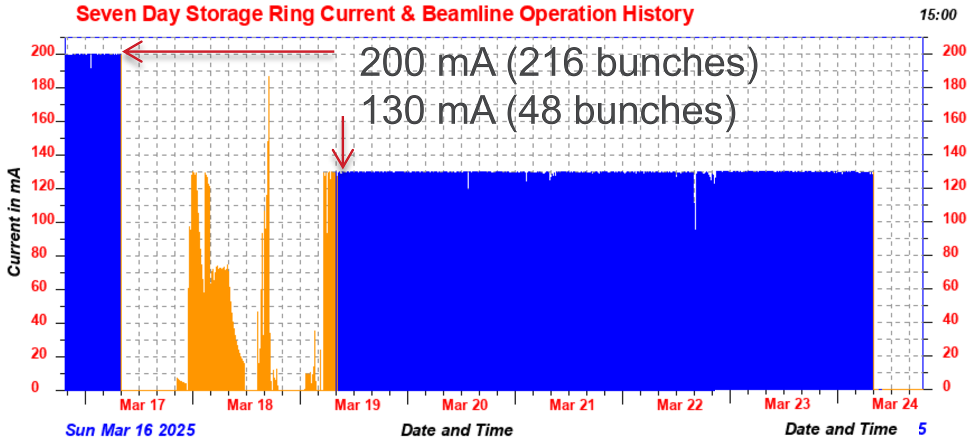
$\sigma_e\sigma_e'$ →

	Full coupling		Low coupling	
	H	V	H	V
Emittance ε (pm·rad)	**28**	**31**	**45**	**3.4**

Low: 10%, 324 bunch
Full: 100%, 48 bunch

APS/APS-U TIMING MODE

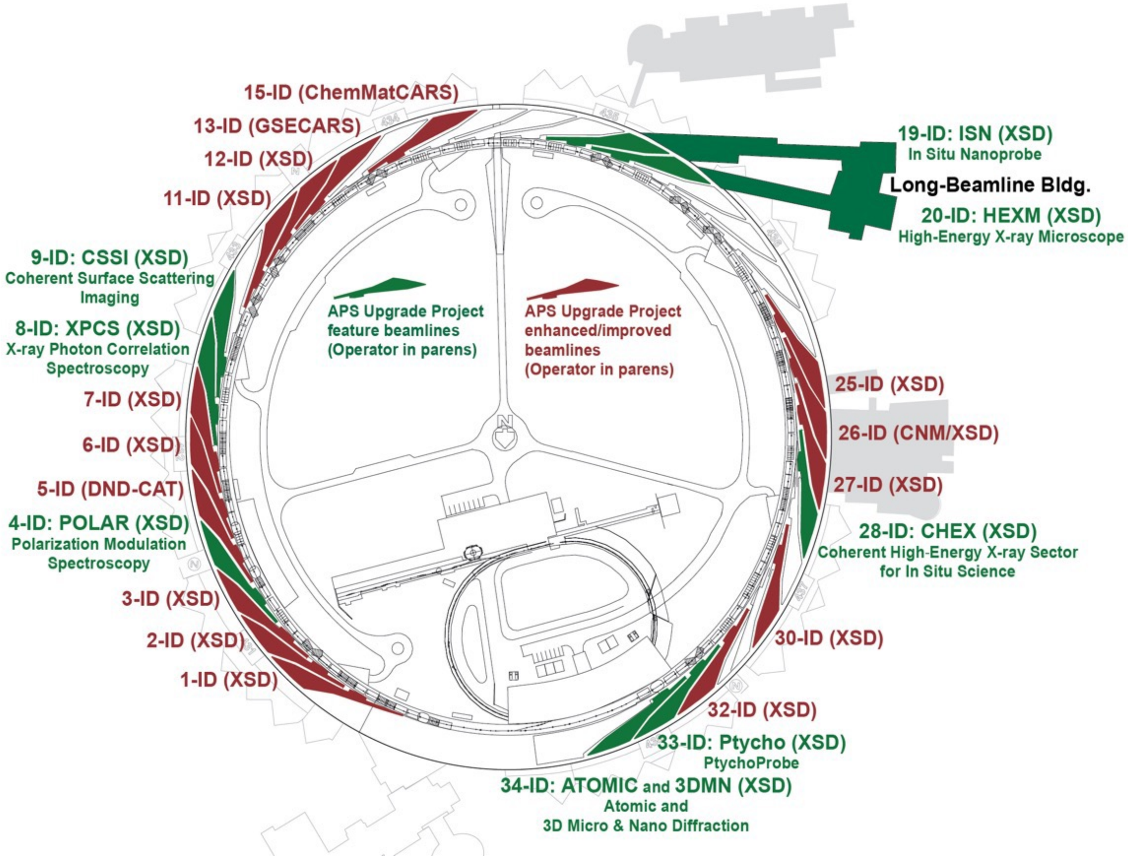




- APS operated ~80% in a fill pattern that enabled studies (24 bunch, 153 ns)
- APS-U designed for 48-buch “timing” mode (77 ns intra-bunch separation) as standard operating mode.

- Currently 48-bunch mode limited to <130 mA.
- Upgrading LINAC energy and Booster power supplies to provide needed charge per bunch (ETA one year).

APS UPGRADE PROJECT - BEAMLINES



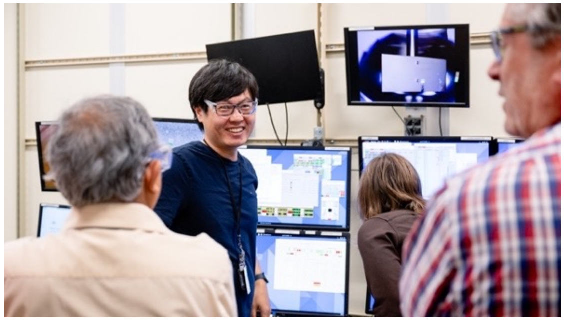
- New and updated insertion devices for optimum spectral performance.
- 9 new feature beamlines + Long Beamline Building (green)
- 15 enhanced and improved beamlines (red)
- Coupling with high performance computing & AI/ML for real-time data analysis and visualization (off project)

~2 Exaflop (2000 Petaflops)

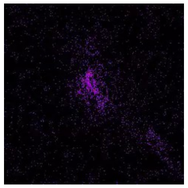
On-line spring 24’

RETURN BEAMLINES TO OPERATIONS

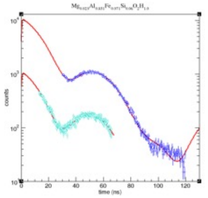
Time Increment in Weeks



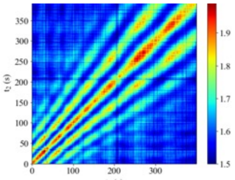
First light June 16, 2024



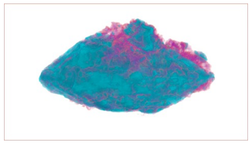
1-ID BCDI at 52 keV of single grain in polycrystal – S. Hruszkewycz - ANL



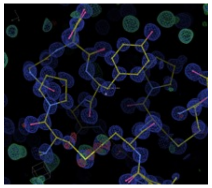
3-ID NRIS of Earth core materials at high PT – J. Jackson Cal. Tech.



8-ID XPCS polymer upcycling materials – M. Foster, U. Akron

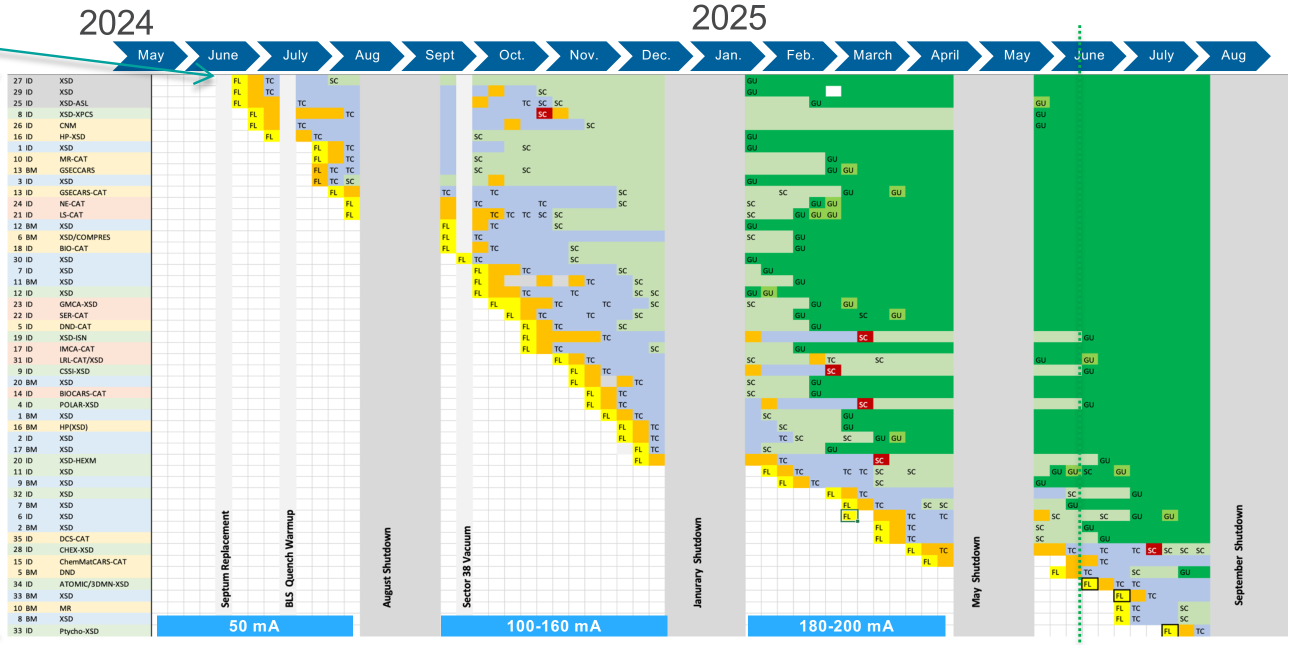


13-BM Tomogram of Olivine grain – P. Ruprecht (U. Nevada)



23-ID Structure of crambin with 1 μm beam – C. Chang (SBC)

Working on returning all beamlines back into scientific user program.



59 beamlines taken light as of **June 22**

🟨🟧 Shielding Verification - 4 beamlines
🟦 Technical Commissioning - 8 beamlines
▨ Scientific Commissioning - 23 beamlines
🟩 Accepting General Users - 24 beamlines

X-RAY PHOTON CORRELATION SPECTROSCOPY (8-ID)

Coherence optimized beamline for probing dynamics in soft and hard condensed matter

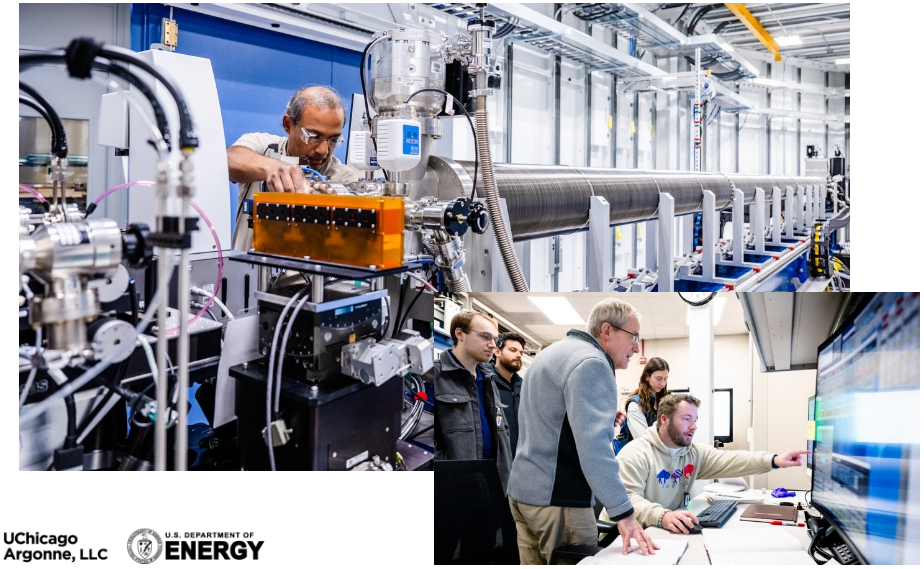
Leads: Suresh Narayanan, Qingteng Zhang & Eric Dufresne

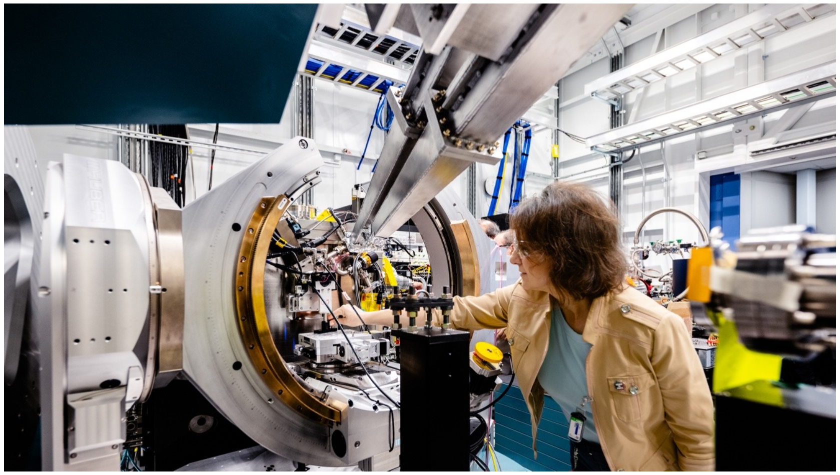
Small Angle Instrument

- Dynamical time scales: <1 microsec – 1000 sec with state-of-the-art pixel array detectors
- Coherence at higher energies for penetration into *in situ/operando* environments: 8-25 keV
- Wide range of sample environments

Wide Angle Instrument

- Spatio-temporal correlations to probe dynamical heterogeneities and intermittent fluctuations in hierarchical and energy materials
- Dynamic heterogeneity and structural transitions
- Structural dynamics in glasses and super-cooled liquids

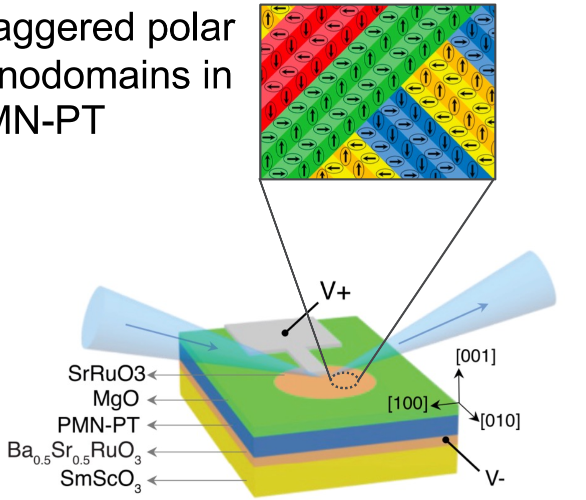




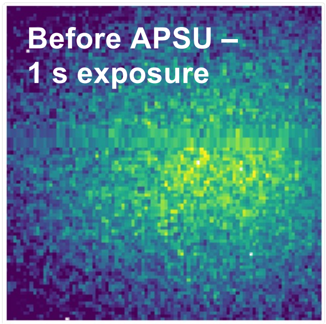
APS-U EARLY SCIENCE

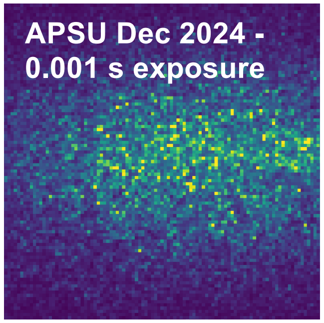
Electric-field response in relaxor ferroelectric nanodomains

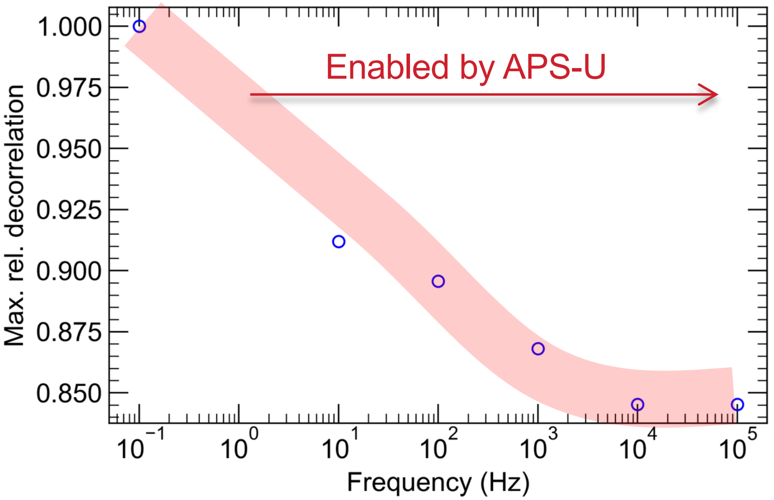
Staggered polar nanodomains in PMN-PT



PMN-PT: 0.68 $PbMg_{1/3}Nb_{2/3}O_3$-0.32$PbTiO_3$







“Flattening” of decorrelation vs E-field frequency, indicative of slowdown of domain response

Enhanced coherent photon flux enabled kHz operando XPCS studies of polar nanodomains in PMN-PT thin film devices, revealing possible latency in domain rotation at high electric field frequencies

Courtesy of Dr. Yue Cao ANL-MSD
Supported by DOE/BES/MSE X-ray Scattering Program

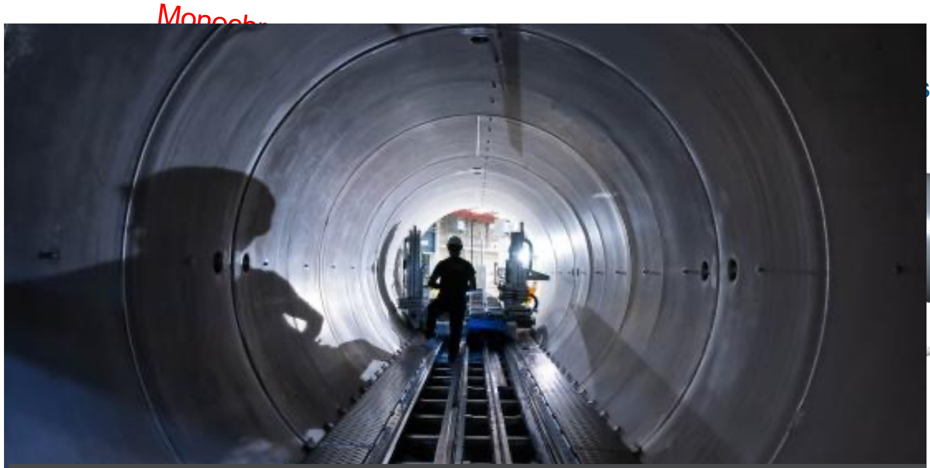
CSSI: Coherent Surface Scattering Imaging (9-ID)

Exploring structure and dynamics of low-dimensional mesoscale systems in 3D

Leads: Jin Wang, Zhang Jiang, Joseph Strazalka

- Grazing-incidence scattering with coherent beams
  - Diffraction limited beam size 0.5 μm to 10s μm
- Takes full advantages of the APS-U coherent flux
  - 10^{12-13} ph/s monochromatic coherent beam, 6 - 25 keV
- High spatiotemporal resolution
  - In plane 2 - 5 nm, out of plane < 1 nm, 1 ms

- Long large-diameter detector flight tube (20m, 2.75∅)
  - Long sample-to-detector distance (>23m)
  - Speckle oversampling
  - Large detector lateral motion for $\mathbf{Q}_x$ sampling
- Optimized optics to preserve wavefront
- Advanced reconstruction methods (HPC)

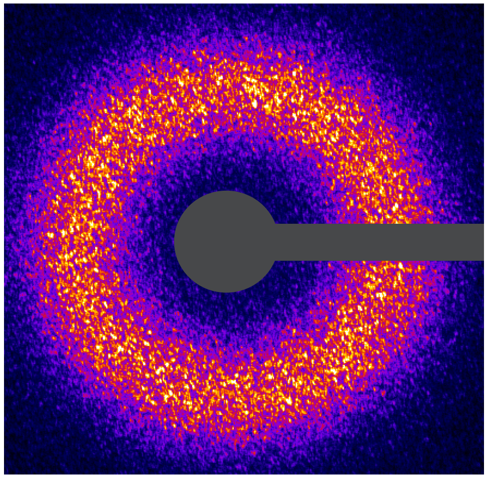


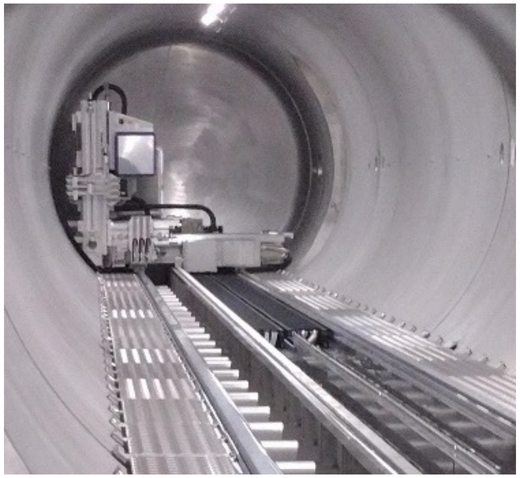
Installation of Flight Tube

First Users at the Beamline

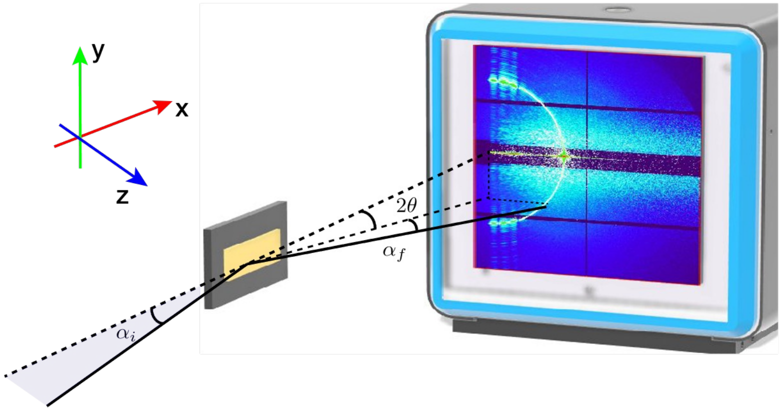
APS-U EARLY SCIENCE

Initial speckle measurements from a porous glass





Left: Small-angle transmission speckle pattern from porous glass measured at 11 keV with in-vacuum Eiger detector 21 m from the sample. Speckles are 3-4x bigger than detector pixels ("oversampled").
Right: Detector in vacuum flight path



Oversampling the speckle pattern is key to unlocking new imaging methods for inspecting 3D structures in semiconductor devices or tracking the dynamics of next-generation soft electronic materials.

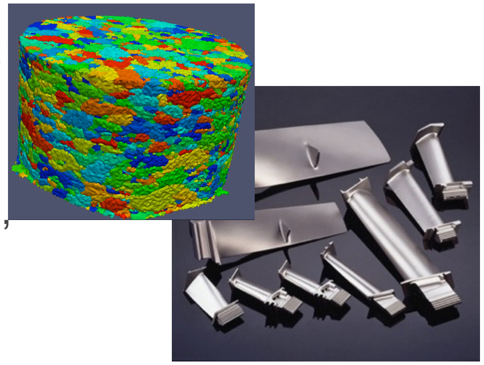
HEXM: High Energy X-ray Microscopy (20-ID)

Long beamline for 3D materials characterization of engineering materials

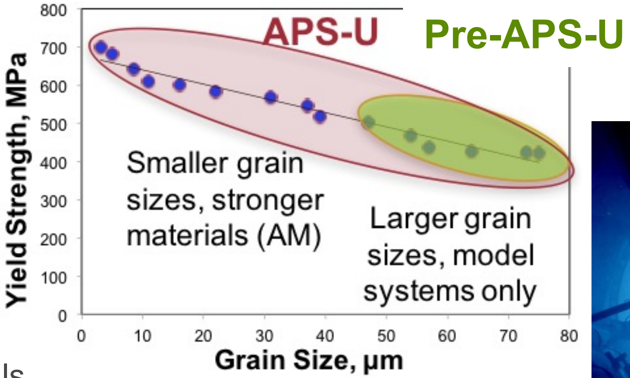
Leads: Jon Almer, Sarvjit Shastri, Jung-Sang Park, Peter Kenesei, Andrew Chuang

HEXM provides new information:

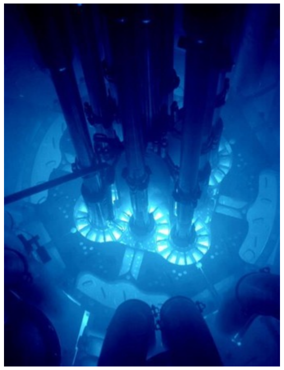
- Intra-granular structure (eg, ‘see’ crack initiation)
- Smaller grained materials (eg, energy storage, additive manufacturing)
- Dynamic processes (eg, fatigue)



Process-enhanced properties for airfoils



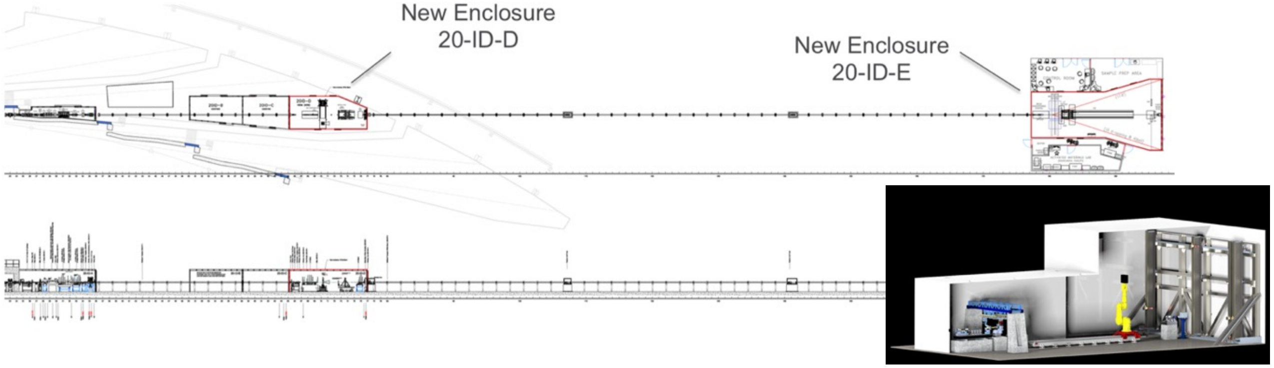
Advanced Test Reactor



nSUF Nuclear Science User Facilities

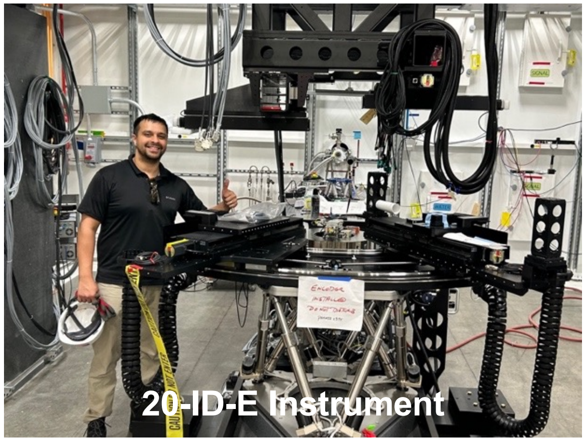
Activated Materials Laboratory (AML)

Layout and source properties (40 – 120 keV)



HEXM: High Energy X-ray Microscopy (20-ID)

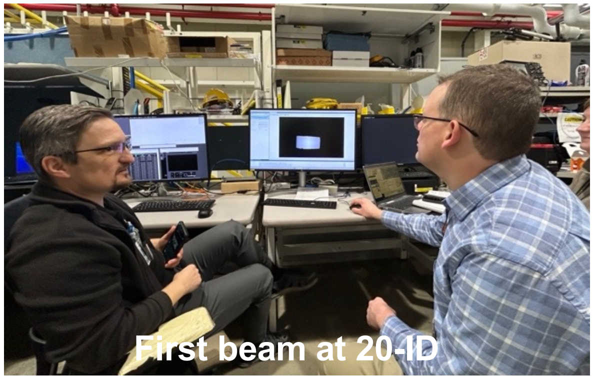
Recent progress & status: Received first x-rays Dec. 12, 2024, Started science comm.



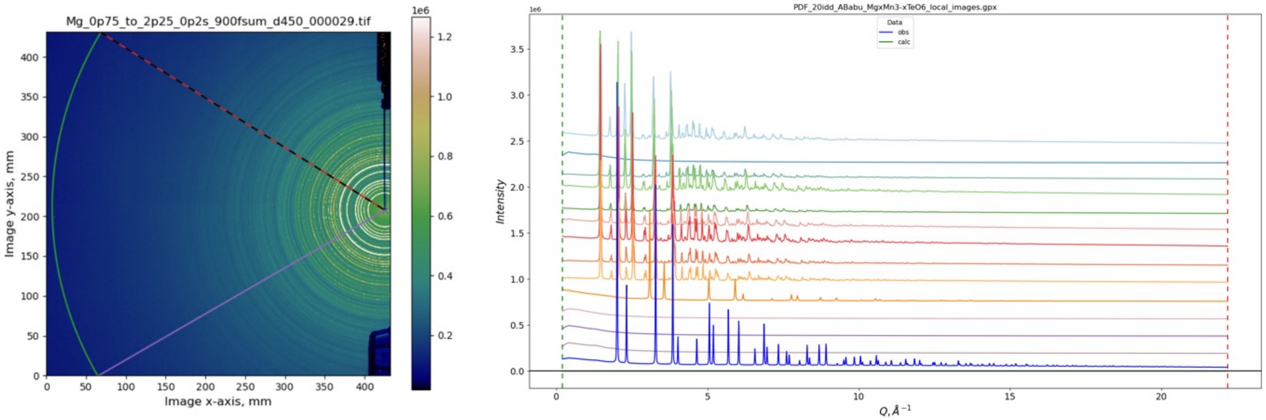
20-ID-E Instrument

Activated materials lab

Expected to be operational June ‘25



First beam at 20-ID



XRD from $Mg_xMn_{3-x}TeO_6$ @ 60 keV – T. Dominy, Clemson Univ.

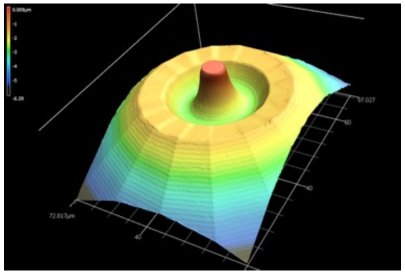
POLAR: Polarization Modulation Spectroscopy (4-ID)

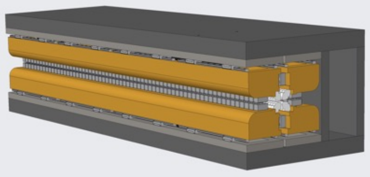
Exploring electronic and magnetic structure at extreme PT conditions

Leads: Joerg Stempfer, Gilberto Fabbris, Yong Choi, & Daniel Haskel

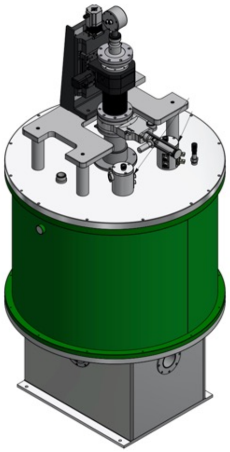
- Variable polarization (linear, circular)
  - Using phase retarding optics (direct from source ~2 years)
- Large bore superconducting magnet
  - 9-1-1 Tesla, 7 Mbar, 1.5 k
- Ptychography
  - Imaging electronic and magnetic structures with ~50 nm res.

- Developed capabilities at APS to produce toroidal anvils to achieve extremely high pressures in DAC– G. Fabbris & R. Hrubiak

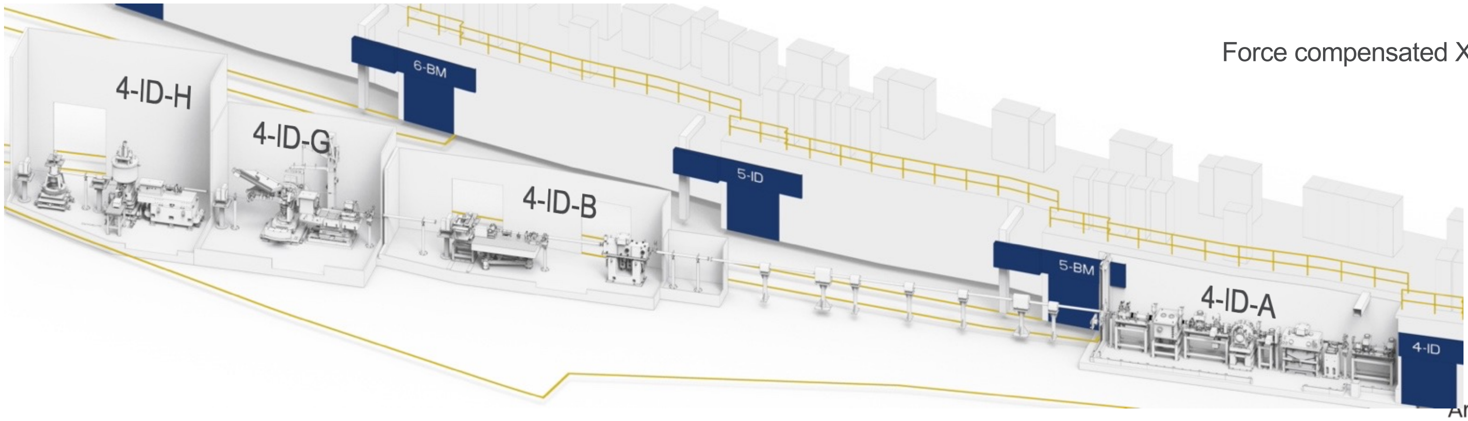




Force compensated X-undulator



Received first beam Nov. 23rd

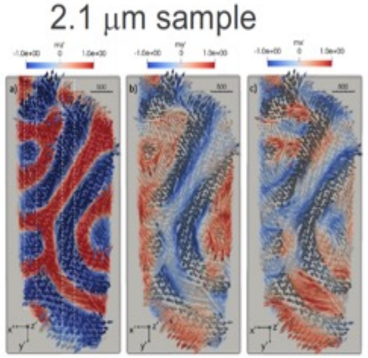


POLAR: Polarization Modulation Spectroscopy (4-ID)

Recent Progress and Status: First beam Nov. 23, 2024, Starting science commissioning

9-1-1 Magnet installed in station

9 Tesla; 7 Mbar; 1.5K



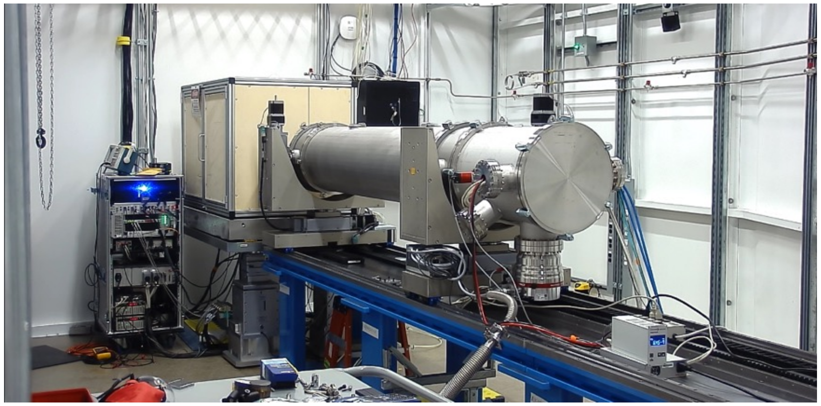
3D Magnetic domain imaging in NdFeB
S. Banerjee, J. *Synch Rad.* **31**, 877 (2024)

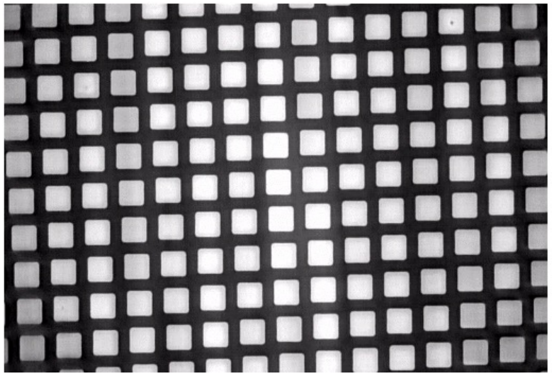
First users on diffractometer/imaging instrument

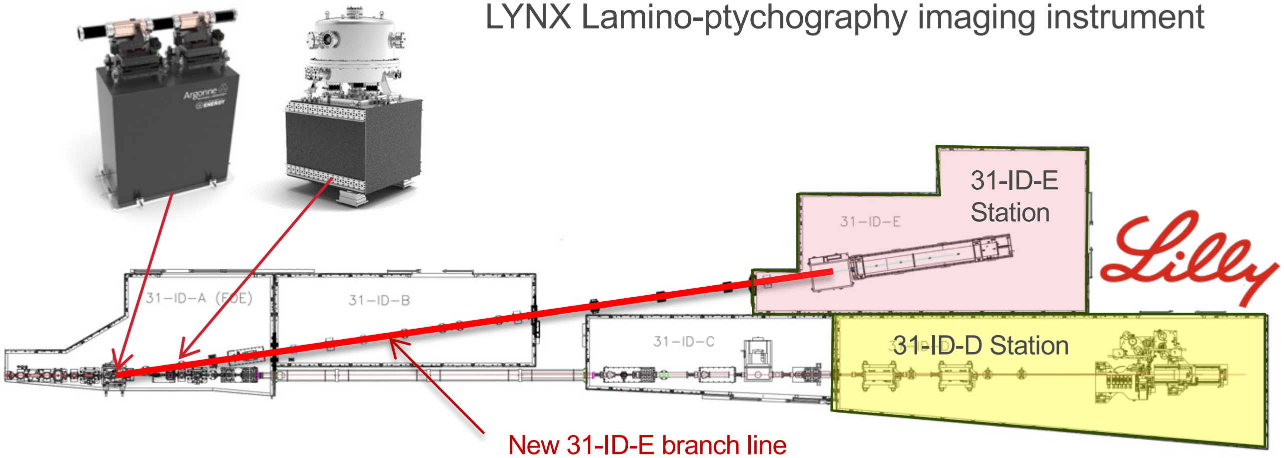
LYNX PTYCHOGRAPHIC IMAGING PROGRAM

Brilliance, High-Energy, External Partnerships

- Non-DOE funded program to demonstrate imaging of integrated circuits using x-ray ptychography
- Commissioned instrument pre-upgrade.
- Built dedicated beamline post-upgrade in un-used industrial MX station.


LYNX Lamino-ptychography imaging instrument

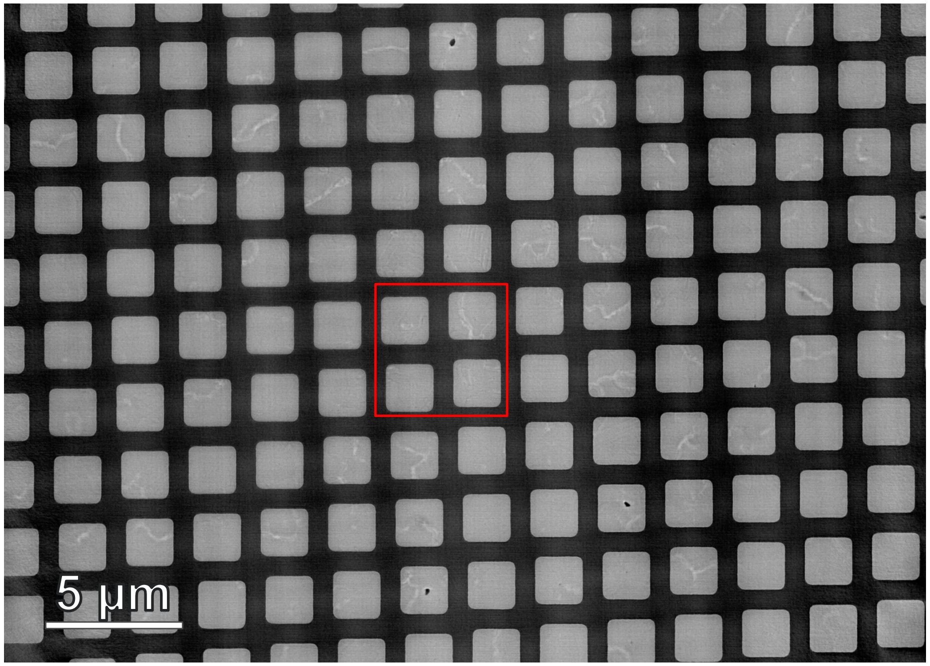

3D Image taken with APS-U



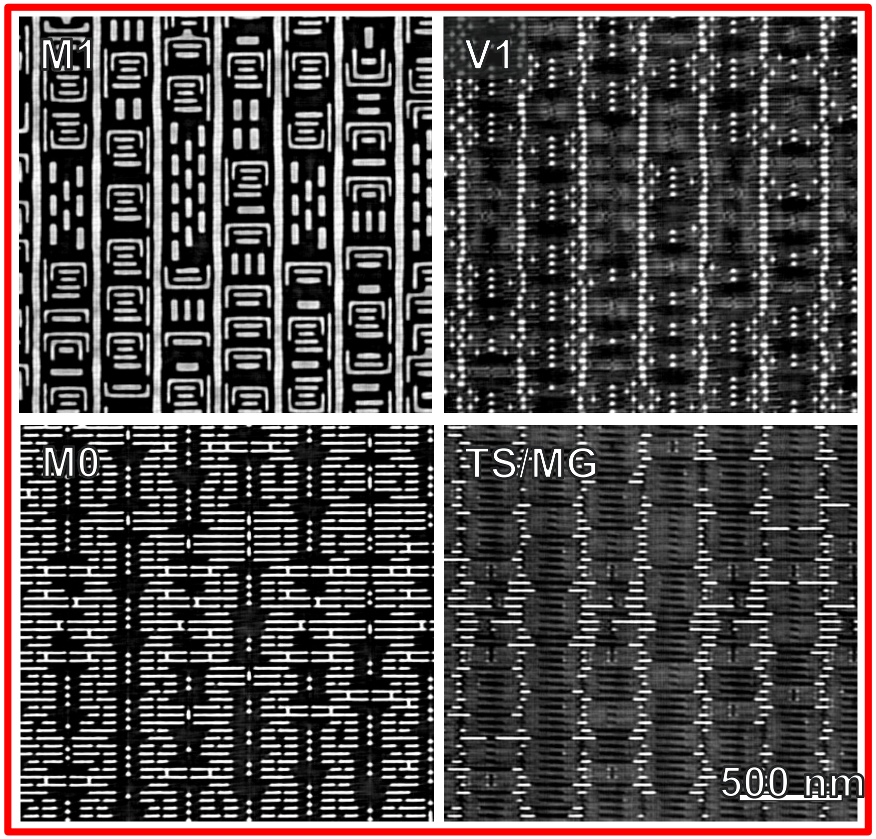
New 31-ID-E branch line

LYNX AT APS-U

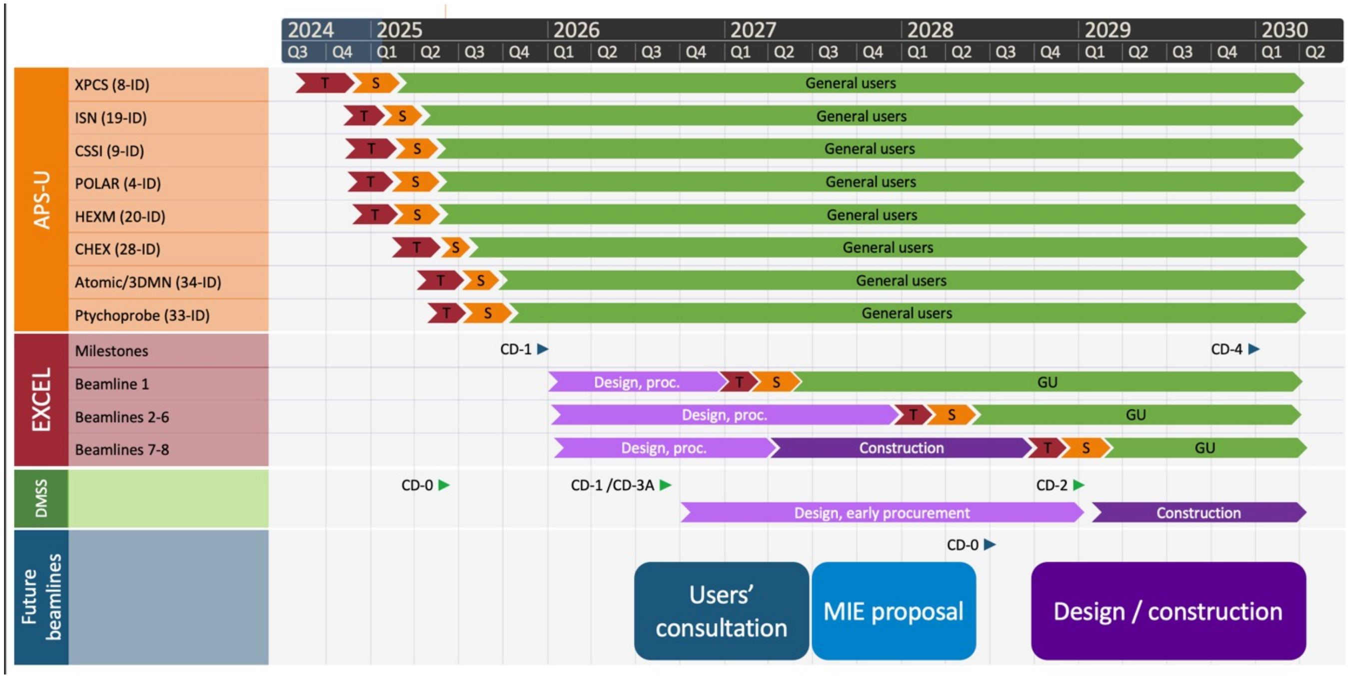
16nm FinFET device imaged at 31-ID-E



- 11nm voxel 3D reconstruction produced with APS tools: `pty-chi` (ptychography) and `pyxalign` (laminography)
- Credit: Yi Jiang (ptychography), Jeff Klug (measurement), and Hanna Ruth (laminography)



FUTURE APS-U BEAMLINE PROJECTS



CD-4 in ~ Aug. '25

CD-0 in ~ Oct. '24 ($60M)

CD-0 in FY25?

CD-0 in ~FY28

- EXCEL prepares additional beamlines to fully leverage high-brightness source
- Two additional beamline proposals in development DMSS (new long beamline) & "EXCEL-II" follow on to EXCEL to upgrade additional APS beamlines.

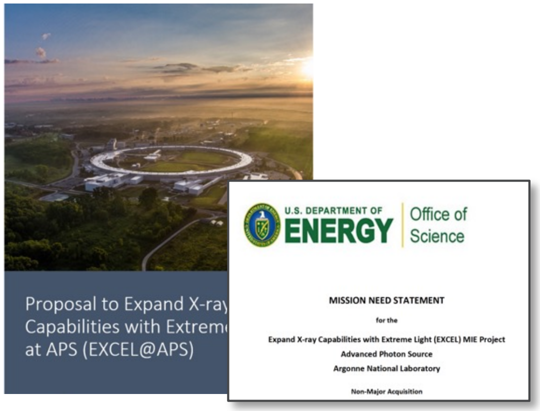
EXCEL@APS BASE SCOPE

Experimental Capability
Bragg CDI instrument (34-ID-F; ATOMIC)
Nano-Laue Diffraction Instrument (34-ID-E; 3DMN))
Engineering materials platform (20-ID; HEXM)
Rapid *in-situ* characterization (11-ID)
X-ray Raman microscopy (25-ID)
Advanced full field imaging (32-ID)
Broad bandpass microscopy (33-ID; PTYCHO)
High-resolution inelastic scattering (30-ID)
Computational Infrastructure

6 new instruments

2 optics upgrades

Computation package



Proposal to Expand X-ray
Capabilities with Extrem
at APS (EXCEL@APS)

U.S. DEPARTMENT OF ENERGY | Office of Science

MISSION NEED STATEMENT

for the

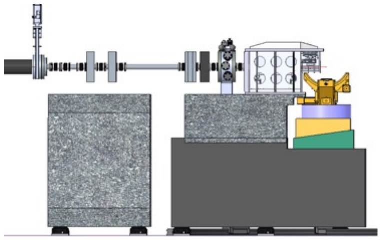
Expand X-ray Capabilities with Extreme Light (EXCEL) MIE Project

Advanced Photon Source

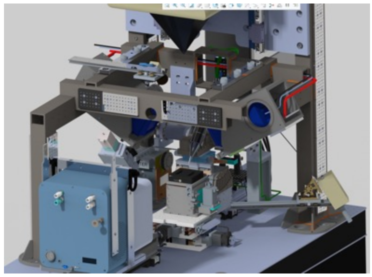
Argonne National Laboratory

Non-Major Acquisition

October 2024

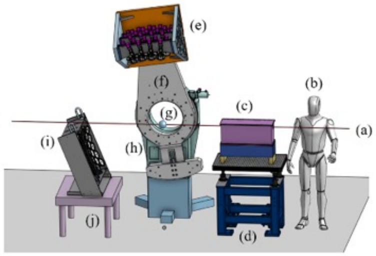


34-ID-F Atomic

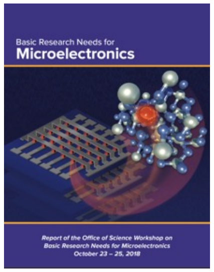


34-ID-E 3DMN

Compute infrastructure

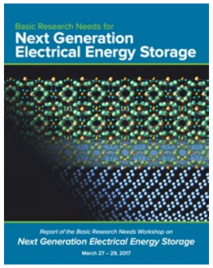


25-ID-D LERIX



Basic Research Needs for Microelectronics

Report of the Office of Science Workshop on Basic Research Needs for Microelectronics October 23 – 25, 2018



Basic Research Needs for Next Generation Electrical Energy Storage

Report of the Basic Research Needs Workshop on Next Generation Electrical Energy Storage March 27 – 29, 2017

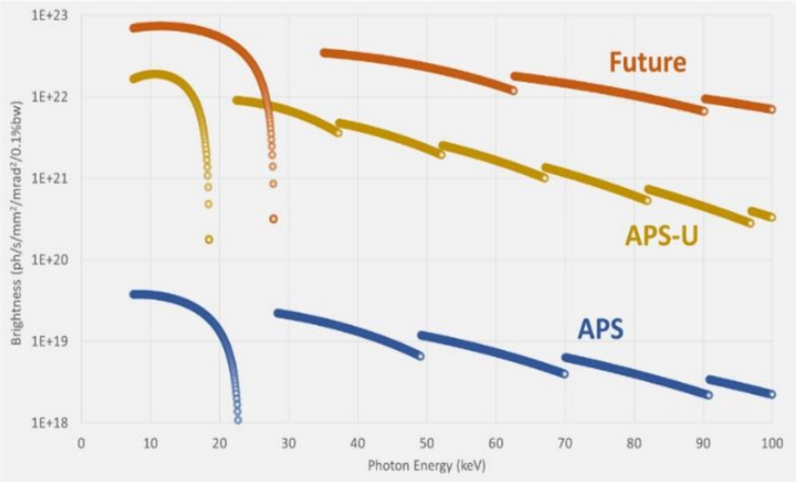
Basic Research Needs for Transformative Manufacturing

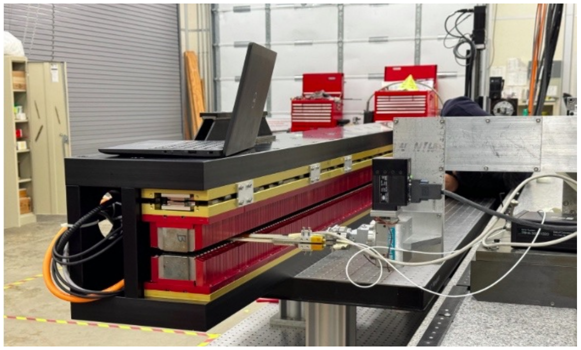
Report of the Basic Energy Sciences Workshop on Basic Research Needs for Transformative Manufacturing March 9 – 11, 2020

FUTURE ACCELERATOR IMPROVEMENTS

Continuing Push boundaries of X-ray brightness at APS

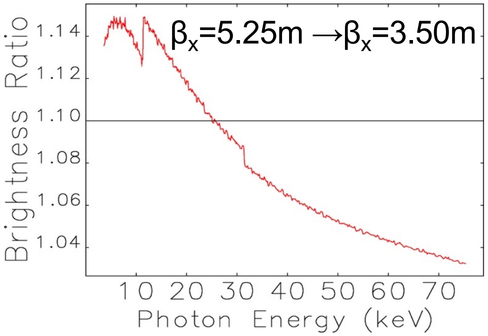
- Developing new PM small-gap and compact undulator technologies
- Developing cryo-free small-gap SCUs with high-temperature superconductors
- Electron optics to reduce beta functions
- Convert to solid state RF





2.4-m-long 27-mm period

SCU cores

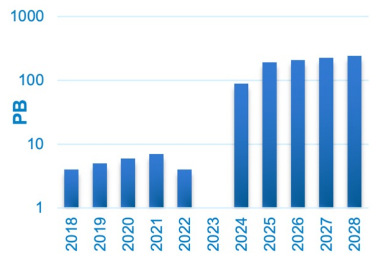


Brightness improvement ratio

Solid State RF

BIG-DATA PROBLEM (AND OPPORTUNITY):

The upgraded APS is expected to generate > 100 petabytes of data/year requiring up to 1 exaflop of peak computing power to process and analyze.



Cumulative data generation at APS by year

100 petabytes/year
= 150,000 Netflix movies every day

We need to look at every frame of every “movie,” analyze it in near-real time, and decide what to do

1 exaflop
= 500,000 servers

This will require ultrafast networks, archival storage, and a robust software infrastructure

Argonne Leadership Computing Facility (ALCF)

Coupling APS instruments with ALCF supercomputers to accelerate scientific discovery

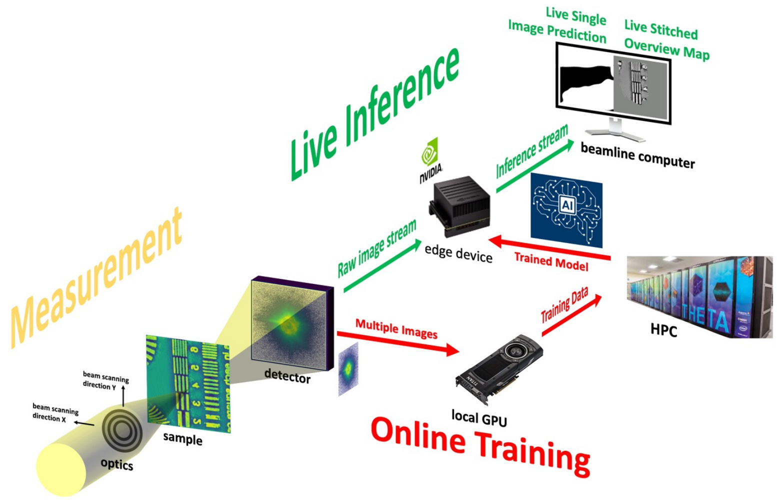
Polaris Supercomputer
44 petaflop/s peak performance

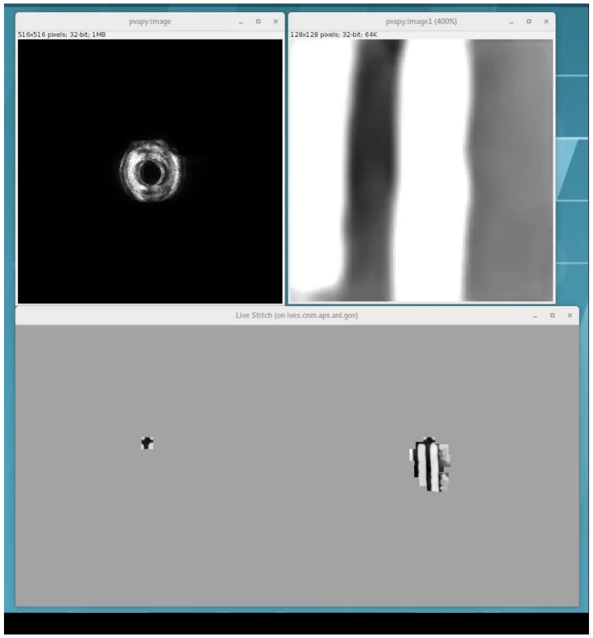
Aurora Supercomputer (early science 2025)
2 exaflop/s peak performance

- APS jobs can launch on-demand within seconds, preempting other running jobs
- Deployed a >1 Tbs network between the APS and the ALCF

HPC REAL TIME DATA PROCESSING

AI-enabled real-time ptychography reconstructions (~ 10 APS instruments)



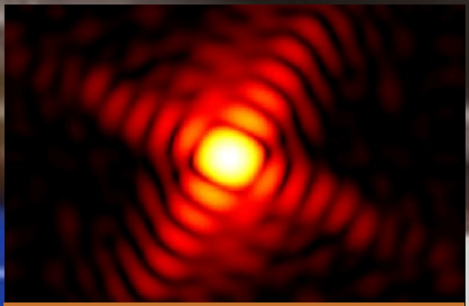


Computationally intensive phase retrieval methods are replaced with neural network models (PtychoNN) that learn to invert raw coherent imaging data to sample amplitude and phase in a single shot.

Babu, A.V., Zhou, T., Kandel, S. *et al.* “Deep learning at the edge enables real-time streaming ptychographic imaging”, *Nat Commun* **14,** 7059 (2023).

SUMMARY

APS-U successfully commissioned and initial science starting

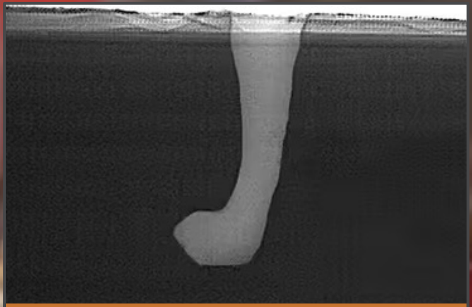


COHERENCE

Highest possible spatial resolution/dynamics

HIGH ENERGY

Penetrate bulk materials and operating systems



TIMING

Dynamic evolution on time scales from 250 ps to seconds

DATA SCIENCE

Real time analysis and decision making

- Coherence coupled with high-energies providing new possibilities for characterizing materials at new 4th generation synchrotrons.
- APS continuing to improve and exploit these source properties.
- Data sciences will play an increasing role in analysis/interpretation of experiments.