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LIGHTING THE WAY UTILIZING ULTRABRIGHT X-RAYS: THE ADVANCED PHOTON SOURCE

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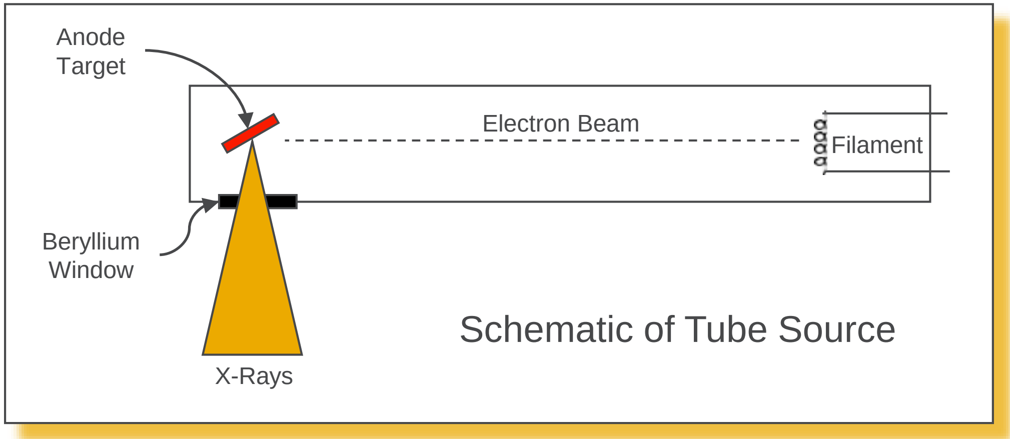
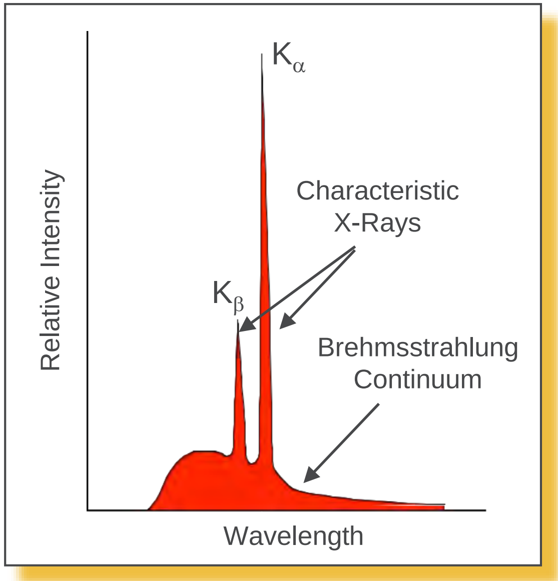
Argonne NATIONAL LABORATORY

AGENDA

- Introduction to storage ring light sources
- Introduction to the Advanced Photon Source
- Science Examples
- Upgrading the Advanced Photon Source

TUBE SOURCE AND BRAGG'S LAW

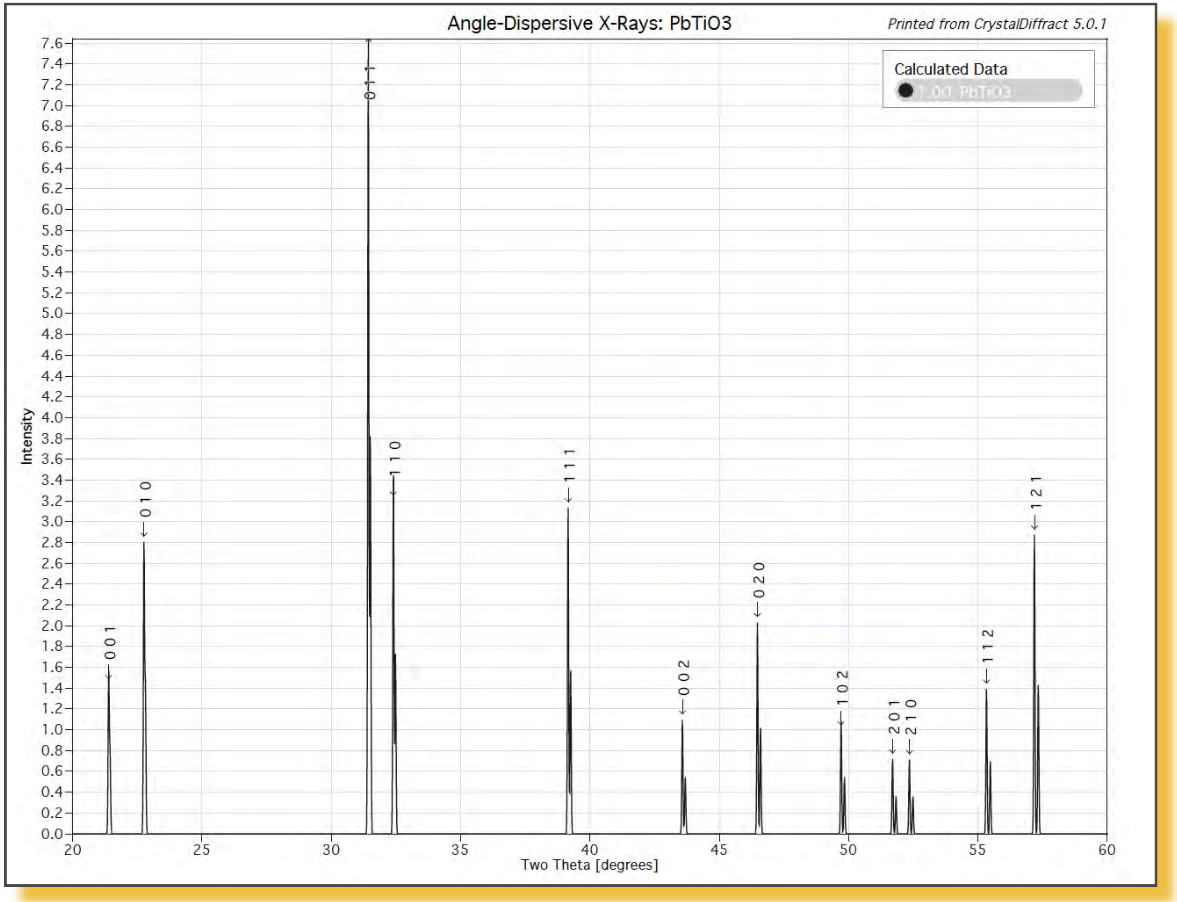




TUBE SOURCE AND BRAGG'S LAW

Bragg's Law

$$n\lambda = 2d\sin\theta$$



WHY USE A SYNCHROTRON X-RAY SOURCE?

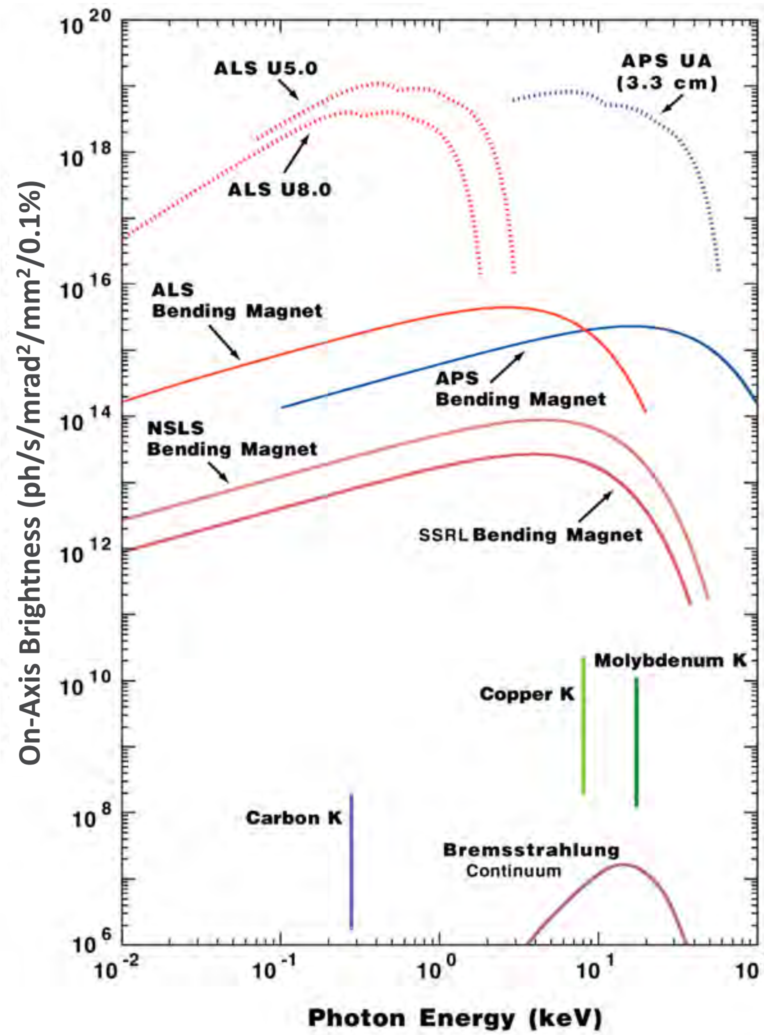
Synchrotron Radiation (SR) - radiation from the acceleration of a charged particle

$$\text{Brightness} = \frac{\text{Photons/second}}{(\text{mrad})^2(\text{mm}^2 \text{ source area})(0.1\% \text{ bandwidth})}$$

beam collimation

size of beam source

monochromaticity

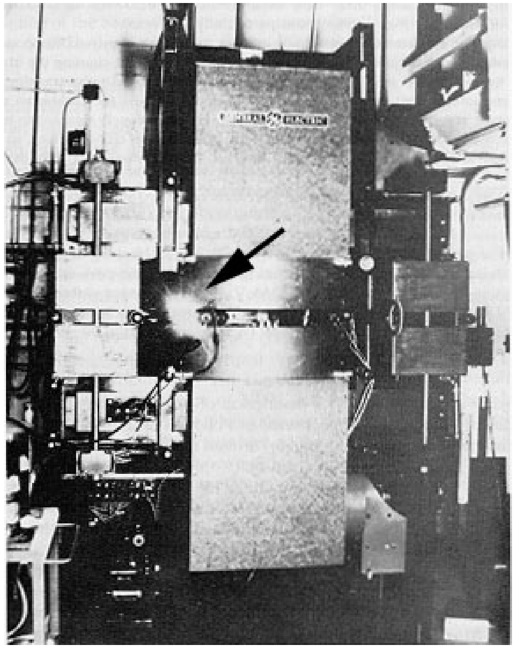


$\lambda[\text{Å}] = 12.4 / E[\text{keV}]$

WHY USE A SYNCHROTRON X-RAY SOURCE?

- **High brightness:** synchrotron light is extremely intense and highly collimated.
- **Coherence:** synchrotron x-ray wavefronts have a high degree of order
- **Wide energy spectrum:** synchrotron light is emitted with energies ranging from the infrared to hard, energetic (short wavelength) x-rays
- **Tunable:** through sophisticated monochromators and insertion devices it is possible to obtain an intense beam of any selected wavelength
- **Highly polarized:** the synchrotron emits highly polarized radiation, which can be linear, circular or elliptical
- **Emitted in very short pulses:** pulses emitted are typically less than a nanosecond (a billionth of a second)

HISTORY OF SYNCHROTRONS



Synchrotron light from the 70-MeV electron synchrotron at GE

- Accelerator-based synchrotron light was seen for the first time at the General Electric Research Laboratory in the USA in 1947
  - Considered a nuisance because it caused the accelerated particles to lose energy
- 1960's: First Generation (CHESS and SSRL)
  - Synchrotron light recognized in the 1960s as being useful as a research tool
  - Parasitic operation on synchrotron colliders
- 1970's: Second Generation (e.g. NSLS)
  - Storage rings designed for and dedicated to the production of synchrotron radiation, dedication of time from high-energy-physics facilities
  - Realization that higher brightness (as opposed to flux) could be realized with better sources (i.e. the way the electron beam is circulated in the storage ring) and using dedicated magnet assemblies (insertion devices)
- 1990's: Third Generation (ALS, APS, NSLS II)
  - New generation of storage rings with a lower emittance (product of beam size and divergence) and long straight sections for undulators, that permit achieving even higher brightness, and with it a considerable degree of spatial coherence
- For more detail, see Arthur L. Robinson, http://xdb.lbl.gov/Section2/Sec_2-2.html
- See also www.lightsources.org

FROM SYNCHROTRONS TO STORAGE RINGS

THE REVIEW OF SCIENTIFIC INSTRUMENTS

Letters to the Editor

Prompt publication of brief reports of NEW ideas in measurement and instrumentation or comments on papers appearing in this Journal may be secured by addressing them to this department. No proof will be sent to the authors. Communications should not exceed 500 words in length. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents.

Use of Synchrotron Orbit-Radiation in X-Ray Physics*

L. G. Parratt

Cornell University, Ithaca, New York

(Received December 1, 1958)

IT is well known by now that intense x-radiation is emitted by the centripetally accelerated electrons in the orbit of a high-energy synchrotron.[1] Comparison is made here of the prospective usefulness of this radiation in the range of wavelengths 0.1 to 20 A with the x-rays obtainable from a conventional x-ray tube.

I. Calculations of the spectral distribution for three typical synchrotron energies and orbit radii are shown in Fig. 1.[2,3] The spectral power is shown averaged over one-half of an acceleration cycle in which the electron energy is taken as proportional to the square of a sinusoid.[4] The power is expressed in ergs per second per 4π solid angle per x unit per electron, and must be trimmed

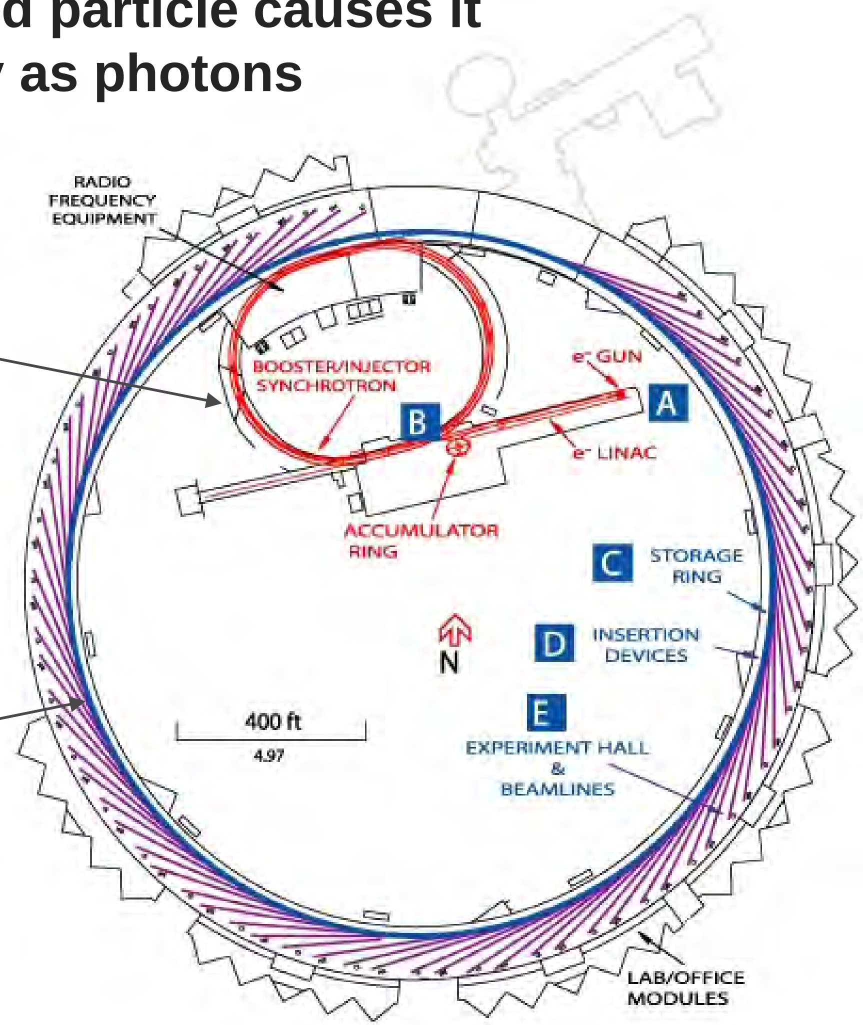
- Synchrotrons were first used as sources of SR. However, the particles' constantly changing energy was not attractive and the advent of storage rings provided a far more attractive source.
- We now use the name synchrotron radiation to describe radiation that is emitted from charged particles traveling at relativistic speeds, regardless of the accelerating mechanism and shape of the trajectory.
- Although synchrotron radiation can cover the entire electromagnetic spectrum, we are interested in radiation in the x-ray regime.

WHAT IS A SYNCHROTRON?

Acceleration of a charged particle causes it to give off energy as photons

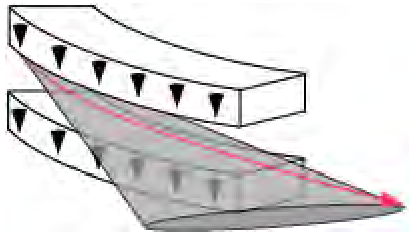
- Electrons (or positrons) are accelerated to almost the speed of light by a linear accelerator (linac) and booster ring. They are then transferred to an outer storage ring.

- The electrons are confined to the “circular” orbit by a series of bending magnets separated by straight sections.



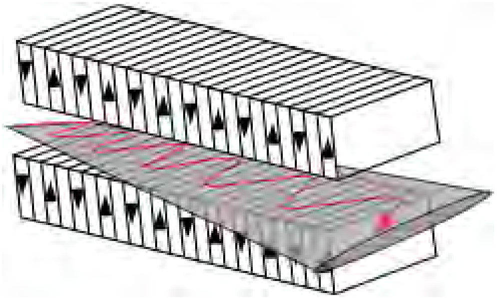
WHAT IS A SYNCHROTRON?

- As the electrons are deflected through the magnetic field created by the bending magnets, they give off electromagnetic radiation, so that at each bending magnet a beam of synchrotron light is produced.



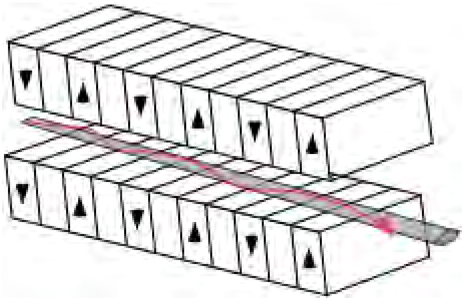
Bending Magnet: Deflection of the electron path yields a fan of radiation with a broad energy spectrum

- Electrons passing through "insertion devices" in the straight sections of the ring give off an extremely intense beam of light



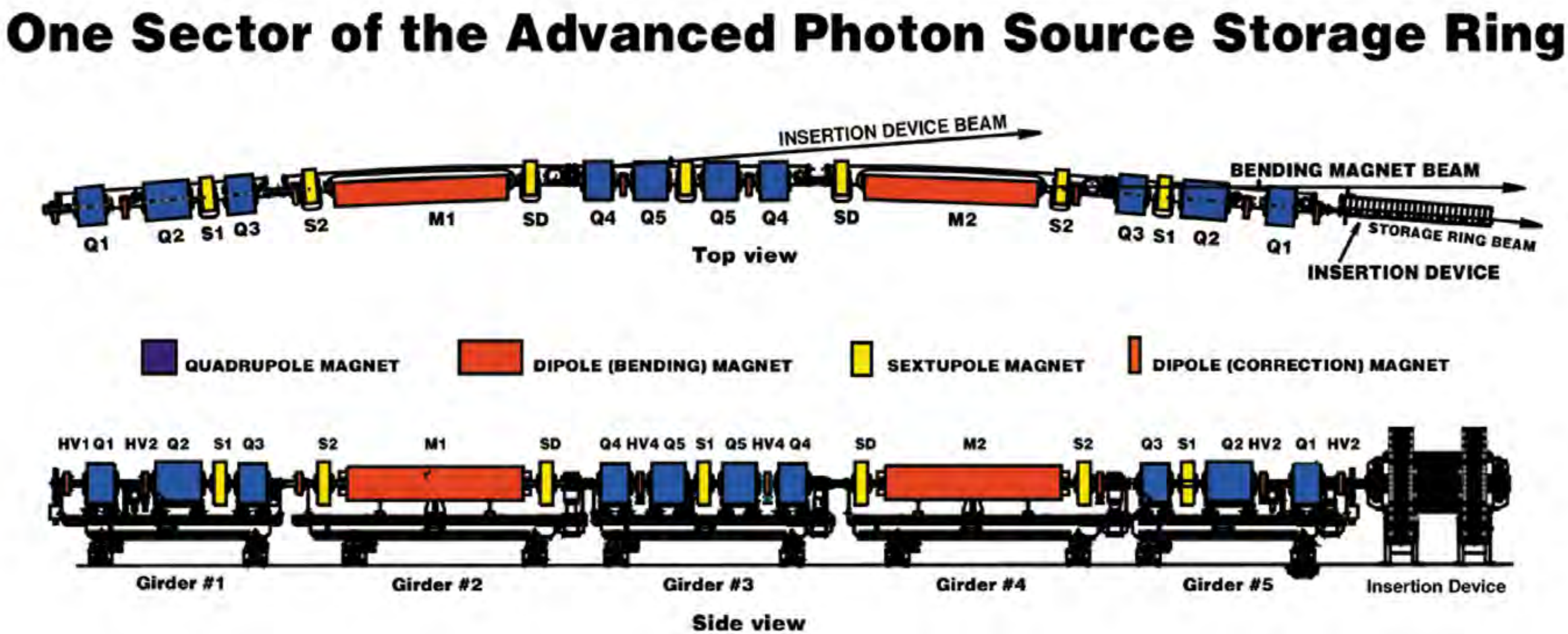
Wiggler: Intensities add with the number of wiggles

- Energy is added back to the electron beam using rf cavities



Undulator: Radiation from each undulation interferes constructively, yielding a narrow energy spectrum with high brightness

TYPICAL STORAGE RING SECTOR



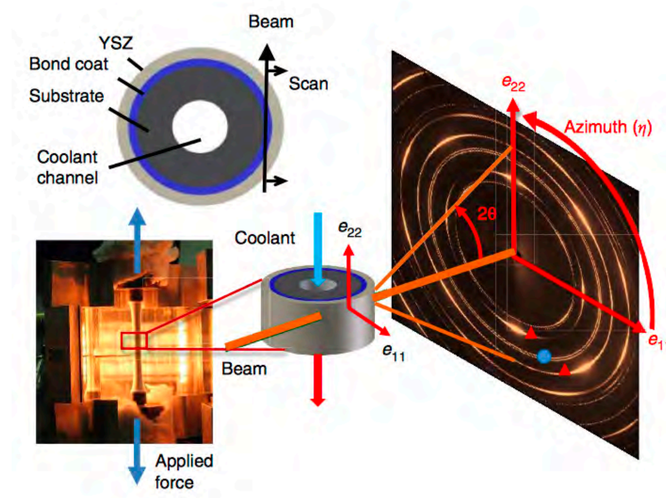
Magnets and vacuum chambers are mounted on girders,
which are aligned in the storage ring tunnel to a tolerance of ± 0.1 mm.

TYPICAL STORAGE RING SECTOR

UNDULATOR INSERTION DEVICES

TYPES OF SYNCHROTRON X-RAY METHODS

- Scattering and Diffraction
  - Very high resolution
  - Penetration into sample can be tuned by the incidence angle
  - Tunable wavelength: anomalous scattering - element specific
  - High energy - penetrating
  - Dynamical scattering
  - Small-angle scattering
  - Magnetic scattering
- Spectroscopy
  - Penetration into sample can be tuned by the incidence angle
  - Fluorescence
  - X-ray absorption fine structure
  - Inelastic scattering
- Microscopy and Imaging
- Time-Resolved Measurements



Technology Implications: Accurate lifespan estimates of materials, wider adoption of thermal barrier coatings, increased fuel and energy efficiency for autos, airplanes, boats, energy generation facilities. For example, 1 % increase in operating temperature at a single electric generation facility can save up to $20 million a year

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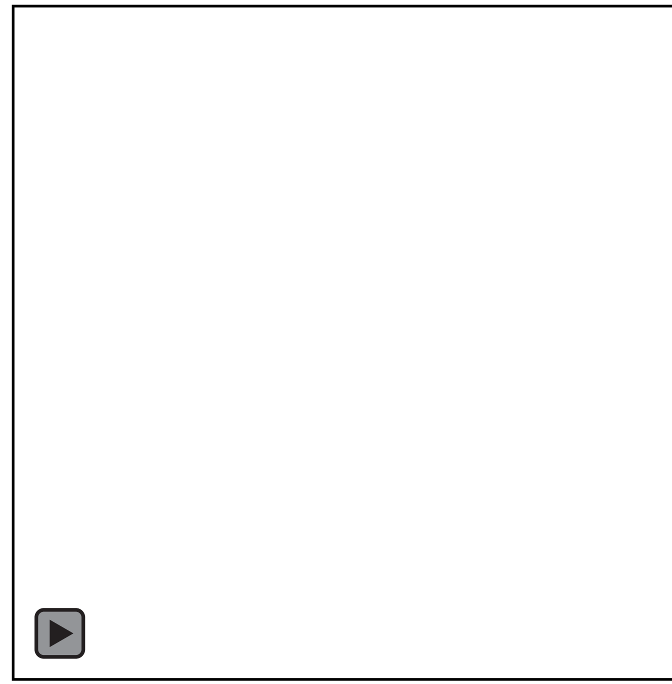
Growth of Al-rich dendrite in Al-Cu alloy
Cooling rate 1K/min from 550 K
3D tomographic dataset in 1.6 s



J. W. Gibbs, K. A. Mohan, E. B. Gulsoy, A. J. Shahani, X. Xiao, C. A. Bouman, M. De Graef & P. W. Voorhees, "The Three-Dimensional Morphology of Growing Dendrites,"
Sci. Rep. 5, 11824 (03 July 2015).| DOI: 10.1038/srep11824

HOW TO BUILD A SYNCHROTRON

- Ring radius: Cost is linear with circumference
- Electron beam energy: Sets performance as a function of photon energy (higher is better), but power requirements go up really fast with energy
- Magnets are only so strong, so can steer the electron beam only so much
- Fill current: determines the photon flux, but limited by packing of electrons in the storage ring and how much power you're willing to pay for.
- Storage ring design gives the emittance (size x divergence) of the electron beam
- Emittance sets brightness and coherent flux

Storage Rings and Free-Electron Lasers

Storage Rings

Near continuous sources with high average brightness, wide tunable energy range, and high stability enable:

- Imaging and spatially resolved spectroscopies of complex systems and processes
- Study of systems evolving on hierarchical time and length scales
- Probing intrinsic atomic fluctuations with un-clocked correlation spectroscopies
- Balanced flux on sample to follow processes (interact but do not destroy)
- Diverse, highly optimized, multiplexed end stations solving critical problems for a wide range of scientific and technological communities and numerous user groups

Free-Electron Lasers

Pulsed sources with ultra-high peak and average brightness with full spatial coherence enable:

- Resolving ultrafast processes critical for emergent properties, excited-state transient phenomena, bond breaking and formation
- Development and application of non-linear x-ray techniques
- Near-instantaneous snapshots of processes in isolated areas (diffract before destroy)
- A small number of end stations addressing carefully selected, high-profile problems

DOE's Light Source Network

Impact by the Numbers

- ~ 12,000 users each year
- From all 50 states, ~33 countries
- Oversubscribed by factor of 3 or 4
- More than 250 universities
- More than 200 companies, many Fortune 500
- 4 Nobel Prizes

Product breakthroughs:

HIV & cancer drugs, green refrigerants, improved LEDs, green fracking, thin films, industrial batteries, gasoline injector system

Government partnerships:

DOE, NIST, NSF, NIH, NNSA, DOD, NASA

Soft(est) X-Rays	Intermediate Wavelength X-Rays	Hard X-Rays & X-Ray Lasers	Hard(est) X-Rays
ALS Best for surface chemistry and electronic structure	NSLS-II & SSRL High flux for diverse range of characterization and exploration	LCLS Ultrabright X-Ray Laser best for probing ultrafast dynamics in molecules and materials	APS Best for studies of real materials, systems, and processes in real time under real operating conditions
BERKELEY LAB Lawrence Berkeley National Laboratory	BROOKHAVEN NATIONAL LABORATORY SLAC NATIONAL ACCELERATOR LABORATORY	SLAC NATIONAL ACCELERATOR LABORATORY	Argonne NATIONAL LABORATORY

Each has unique characteristics as well as tailored overlap of certain capabilities, to cover the entire discovery space for a broad user base

ACCELERATOR-BASED RADIATION SOURCES AROUND THE WORLD

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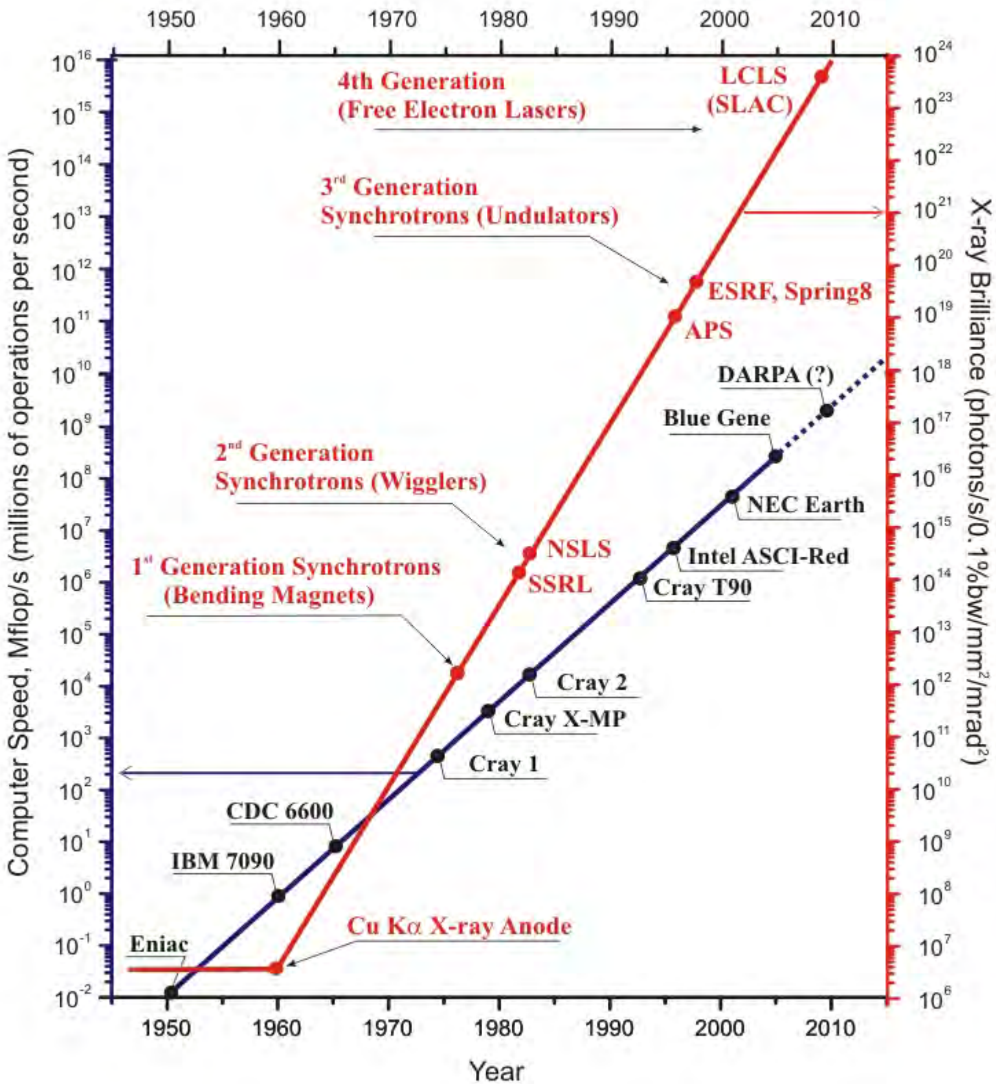
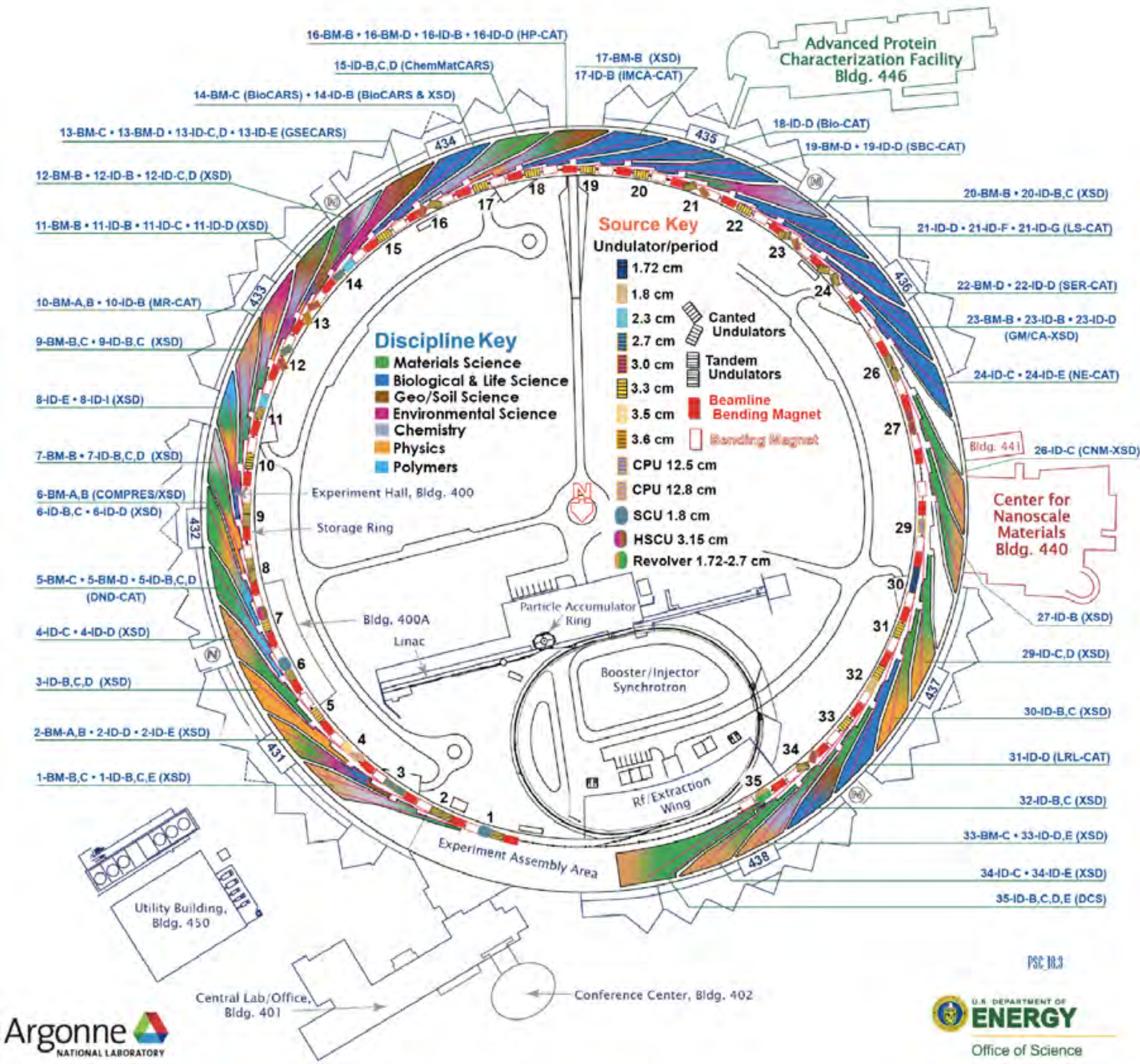
Moore's Law for X-ray Source Brightness



Computer speed: 12 orders of magnitude in 6 decades

X-ray source brightness: 18 orders of magnitude in 5 decades!

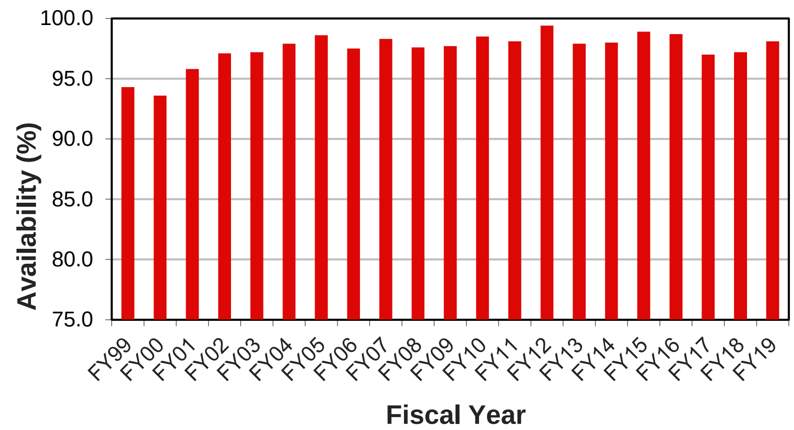
THE ADVANCED PHOTON SOURCE OVERVIEW



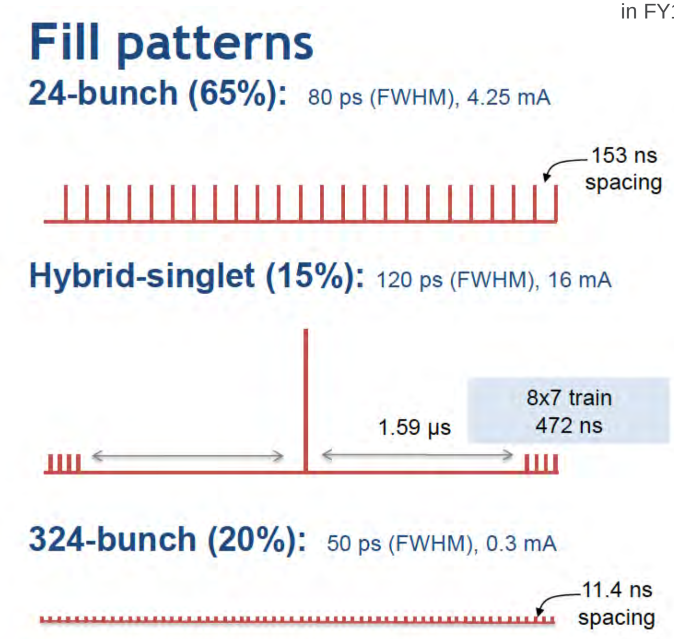
- 68 simultaneously operating endstations
  - 46 undulator beamlines
  - 22 bending magnet beamlines
  - 35 APS-operated with BES funding
  - 33 partner beamlines, principally CATs
- Two sectors (25,28) being developed by APS-U

APS OPERATIONS OVERVIEW

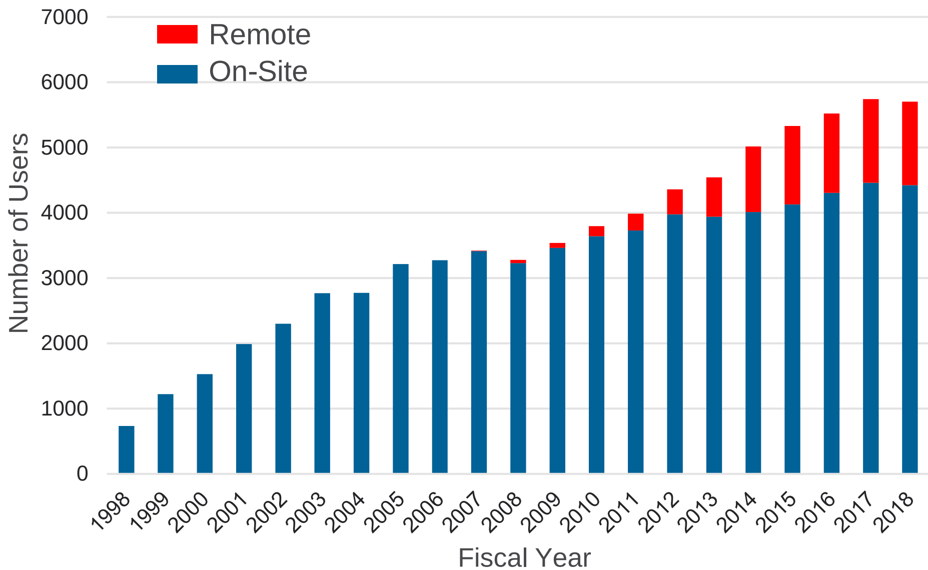
- Commissioned in 1995, first top-up operation in 1999
- 7 GeV light source operating at 102 mA
  - 1104 m circumference
  - 40 sectors, 35 ID straights
  - Effective emittance of 3.1 nm
  - Vertical emittance of 40 pm, 1.3% coupling
- Two fill modes support timing studies
  - 102 mA, 24 bunch mode:
    - 65% of time (~9 h lifetime)
  - 102 mA, hybrid mode
    - 15% of time (~6 h lifetime)
  - Both require top-up
- 102 mA, 324 bunch mode does not require top-up (~60h lifetime)

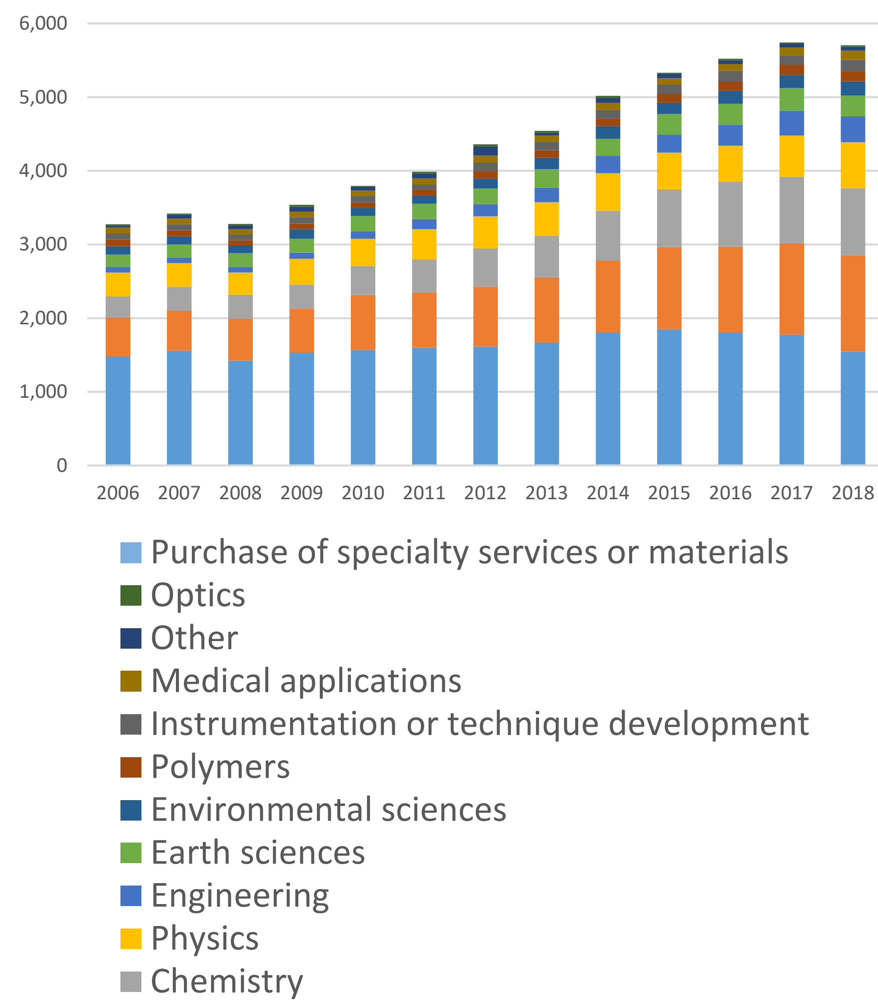


*2 runs in FY17



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





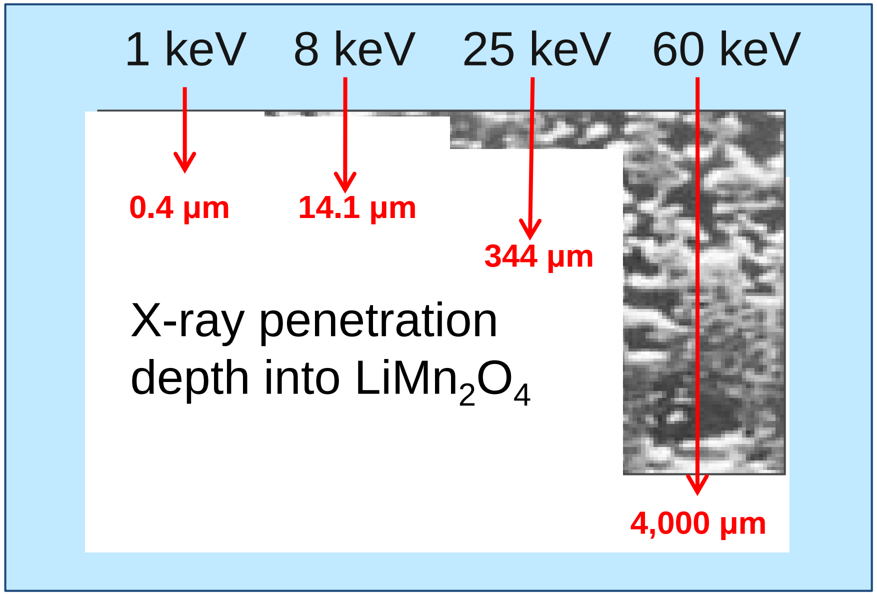
In FY2018:

- >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

High energy: Necessary to probe deeply into real materials in realistic environments

High-energy x-rays enable deep penetration, making it possible to probe:

- Samples behind thick-walled chambers of reaction vessels
- Buried structures in real materials
  - Turbine blades, commercial batteries
- Materials in extreme conditions, including high pressure, high temperatures



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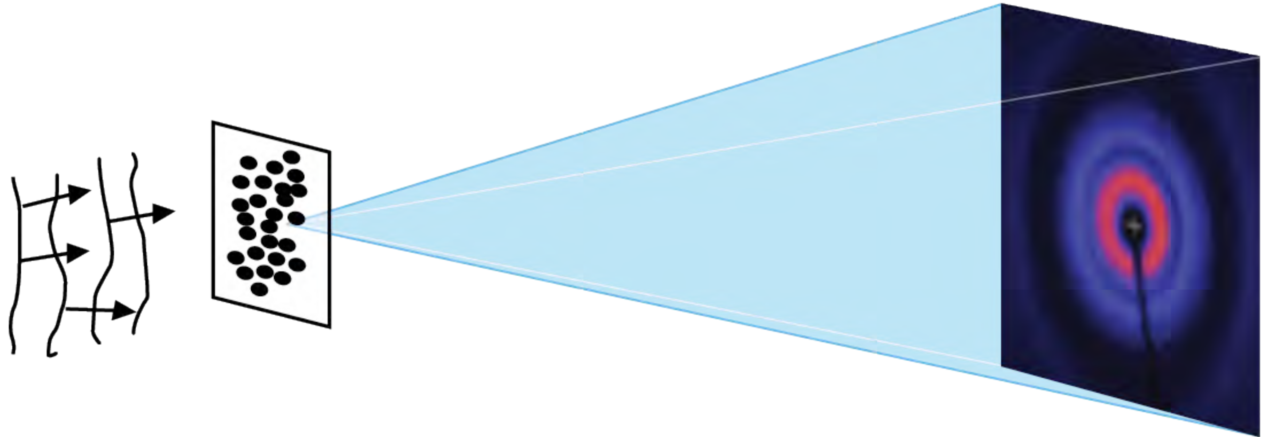
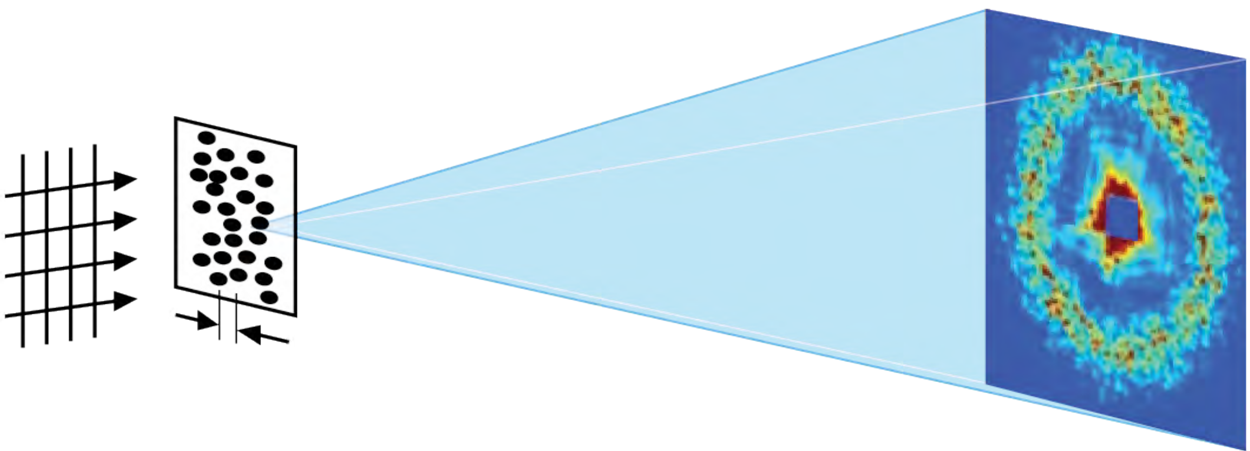
Coherent x-ray studies: Game-changing leap from average to local time/space information



Incoherent beam carries average information; resolution limited by optics



Scattering of coherent beam carries all microscopic, local information – non-periodic arrangements, correlations, dynamics

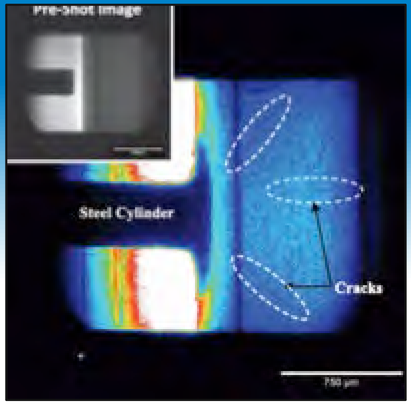
Spatial resolution limited only by x-ray wavelength, coherent flux

The Advanced Photon Source:
The Hard X-Ray 3D Microscope

High Energy

Penetrating bulk materials and operating systems

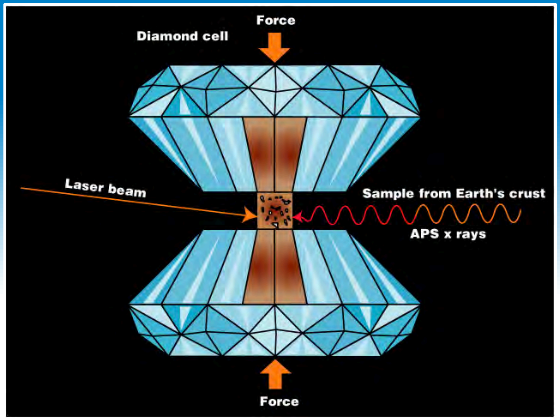
- U.S.' brightest source of hard X-rays
- 3D mapping, deep inside samples
- X-ray cinematography



Brightness

Providing large fields of view with high resolution

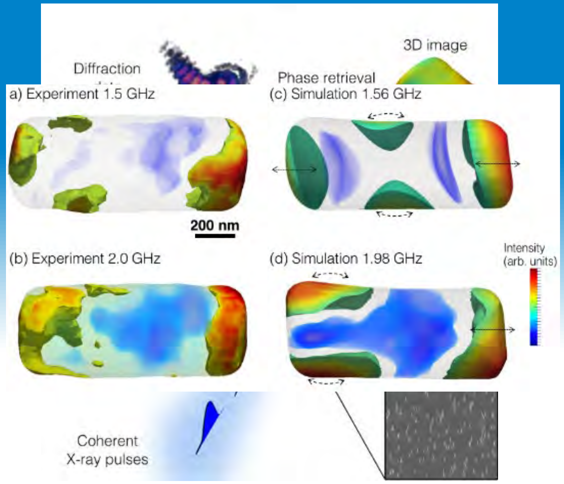
- Multi-scale imaging – connecting microscale features across macroscopic dimensions
- Fast sampling with chemical, magnetic, electronic sensitivity



Coherence

Enabling highest spatial resolution even in non-periodic materials

- Extends lensless imaging with resolution down to 10 nm
- Correlation spectroscopy methods allow time resolution down to microseconds



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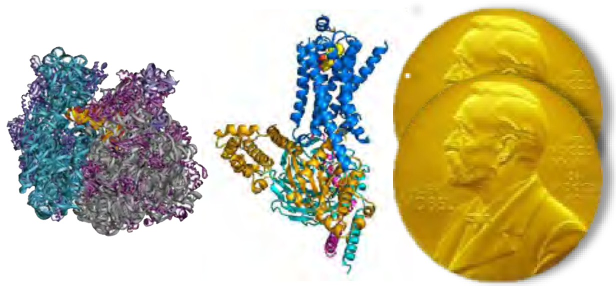
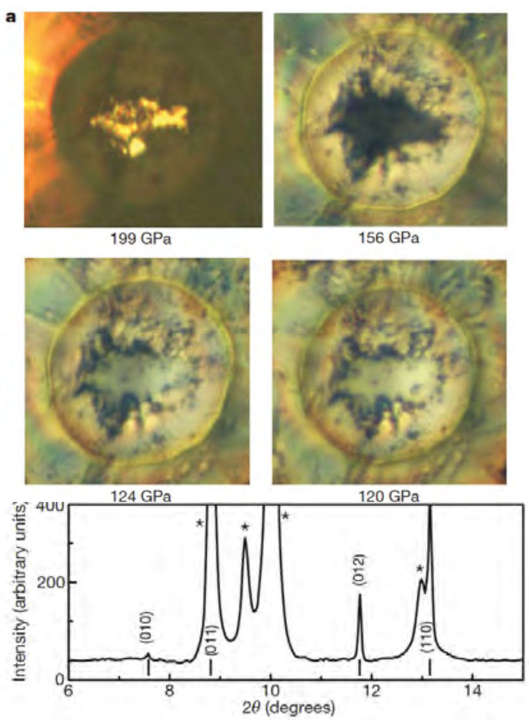
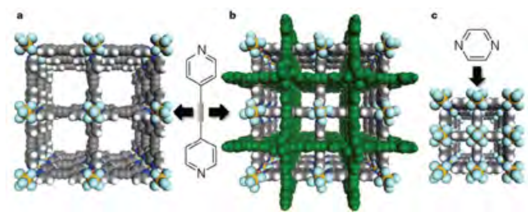
APS research: Significant impacts in science, industry



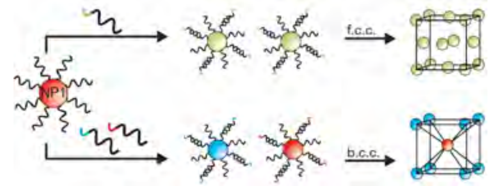
Nobel Prizes in Chemistry, 2009 (structure of ribosome) and 2012 (GPCRs)



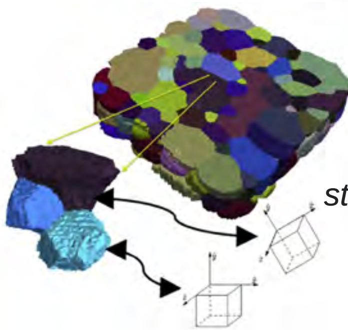
Equations of state under pressure: transparent dense sodium



Reticular chemistry: CO_2 separation

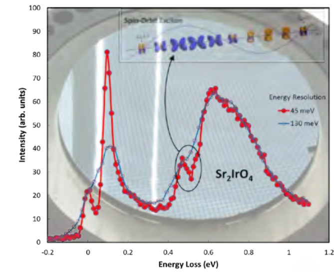


DNA-programmable nanoparticle crystallization

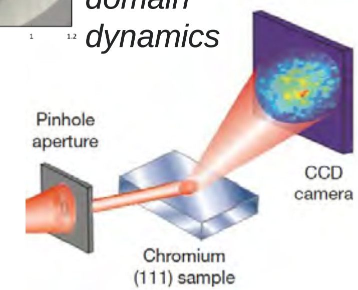


Unexpected evolution of intergranular stresses in creep deformation

Role of Zn in fertilization

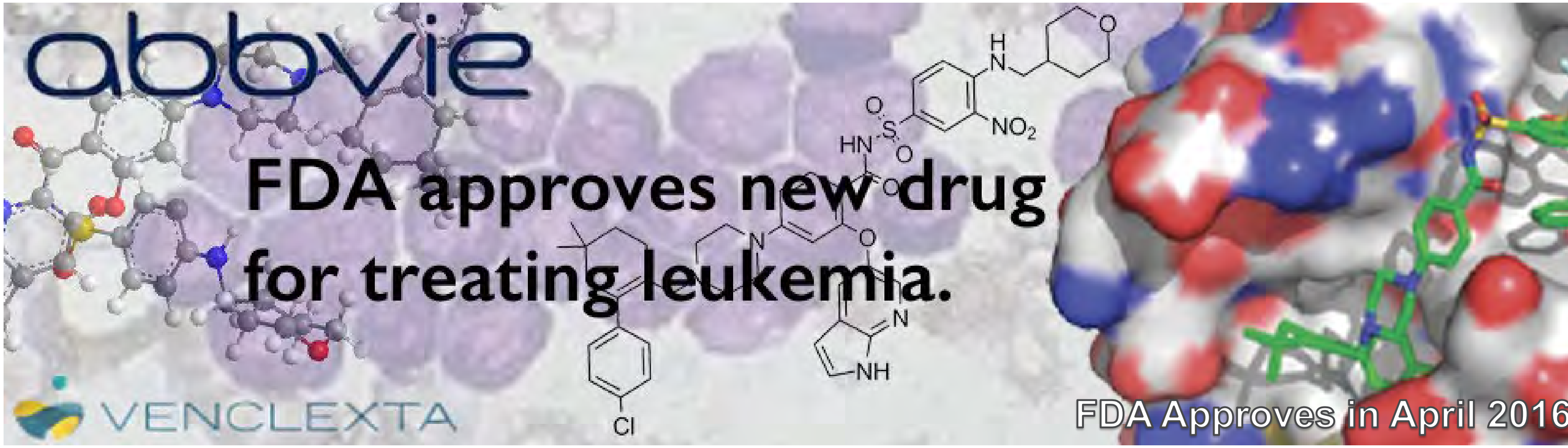


Magnon physics, quantum phase transitions, anti-ferromagentic domain dynamics



Industrial impacts

- Drug development: Januvia (diabetes, Merck), Kaletra (HIV, AbbVie), Votrient (kidney cancer, GlaxoSmithKline), Zelboraf (melanoma, Genentech), Venclexta (leukemia, AbbVie)
- Cummins: fuel injectors
- Dow: solar shingles
- Chevron: improved catalysts for recovery of oil, natural gas
- DuPont: Suva^{TM} refrigerants
- Chevrolet: batteries



AbbVie developed important new drug, Venclexta® (venetoclax) for treating leukemia

- First FDA-approved drug that targets B-cell lymphoma 2 (BCL-2) protein
- FDA granted
  - ‘breakthrough therapy’ designation
  - priority review
  - accelerated approval
- For treatment of patients with chronic lymphocytic leukemia (CLL) who have a chromosomal abnormality called 17p deletion (lack of protein p53 that suppresses cancer growth)

- Pipeline was 20 years
- X-ray crystallography was critical
- AbbVie is member of IMCA
- Proprietary research was conducted @ IMCA-CAT beamline 17-ID

IMCA-CAT
Industrial Macromolecular Crystallography Association
Collaborative Access Team

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EXAMPLE: SHIFTING THE METAL ADDITIVE MANUFACTURING R&D PARADIGM

Trial & Error

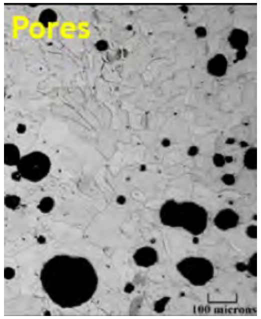
Parameters

?

- Dimension
- Microstructures

- Property
- Performance

Modelling & Simulation



D. Gu, et al., International Materials Reviews, 57, (2012) 133

Parameters → *In situ* characterization →

- Dimension
- Microstructures

→

- Property
- Performance

Modelling & Simulation

Tao Sun et al.

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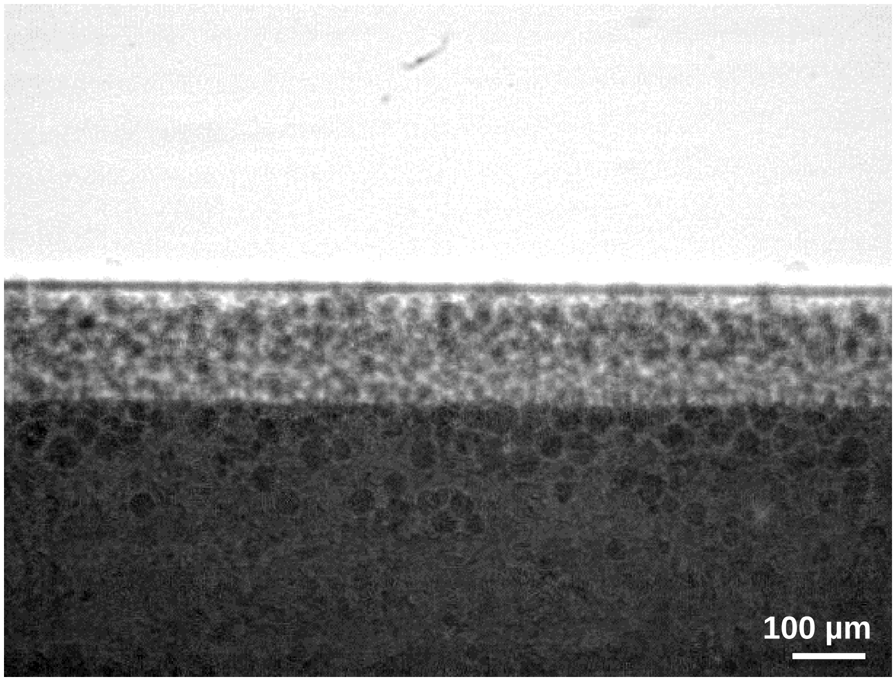
HIGH-SPEED X-RAY IMAGING

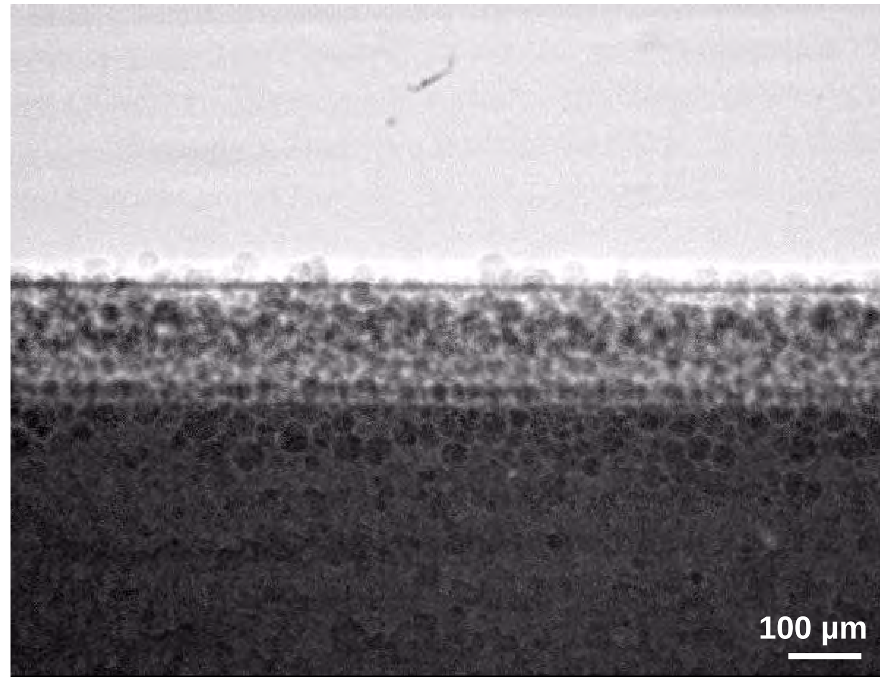
Laser powder bed fusion process (selected laser sintering)

Conduction melting mode



Frame rate: 45 kHz
Exposure: 100 ps
Laser power: **150 W**
Scan speed: 0.3 m/s
Laser spot: ~100 µm

"Keyhole" melting mode



Frame rate: 45 kHz
Exposure: 100 ps
Laser power: **300 W**
Scan speed: 0.3 m/s
Laser spot: ~100 µm

(unpublished)

COMING IN 2023*: THE APS UPGRADE

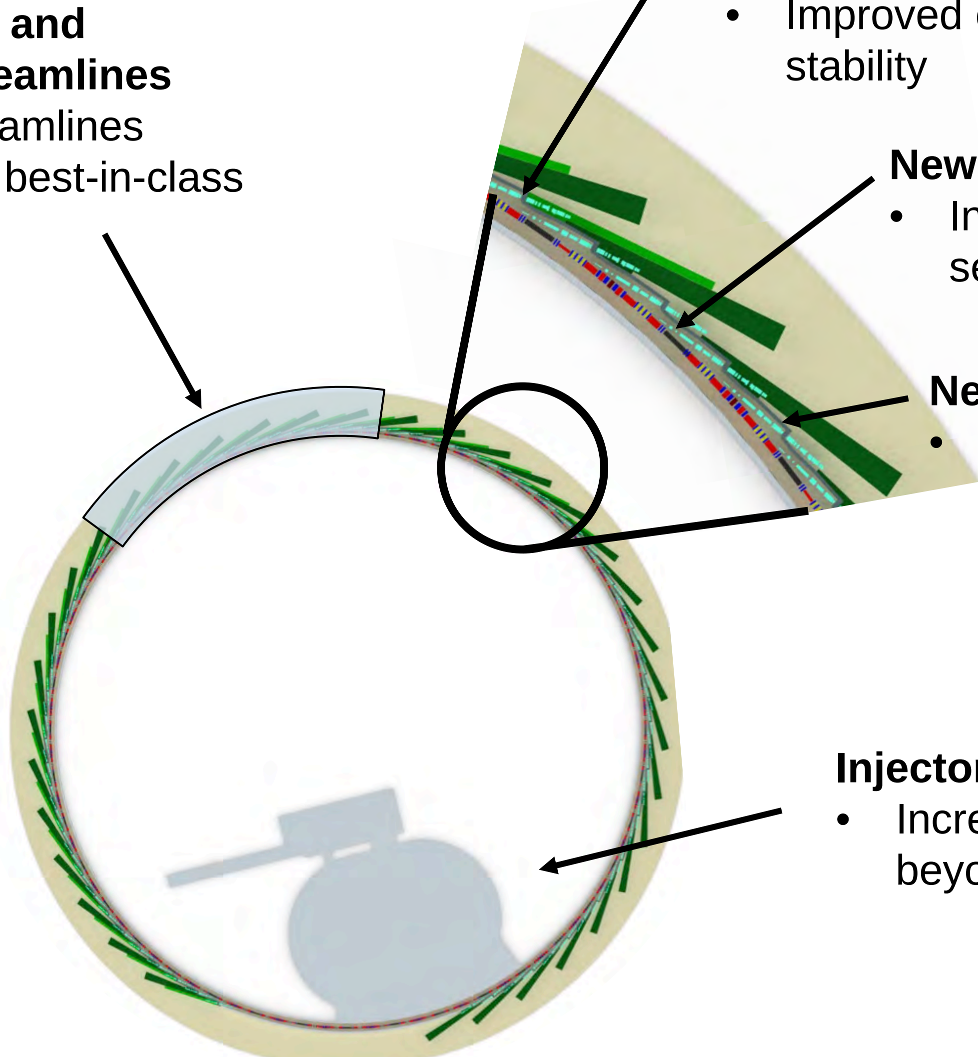
New Storage Ring
- 6 GeV MBA lattice
- 200 mA current
- Improved electron/photon stability

New, rebuilt and upgraded beamlines
Suite of 8 beamlines designed for best-in-class performance

New Insertion Devices
- Incorporate SCUs on selected beamlines

New/upgraded Front-ends
- Common design for maximum flexibility

Beamline Enhancements: improvements to make beamlines "Upgrade Ready"



Injector improvements
- Increase performance beyond present capability

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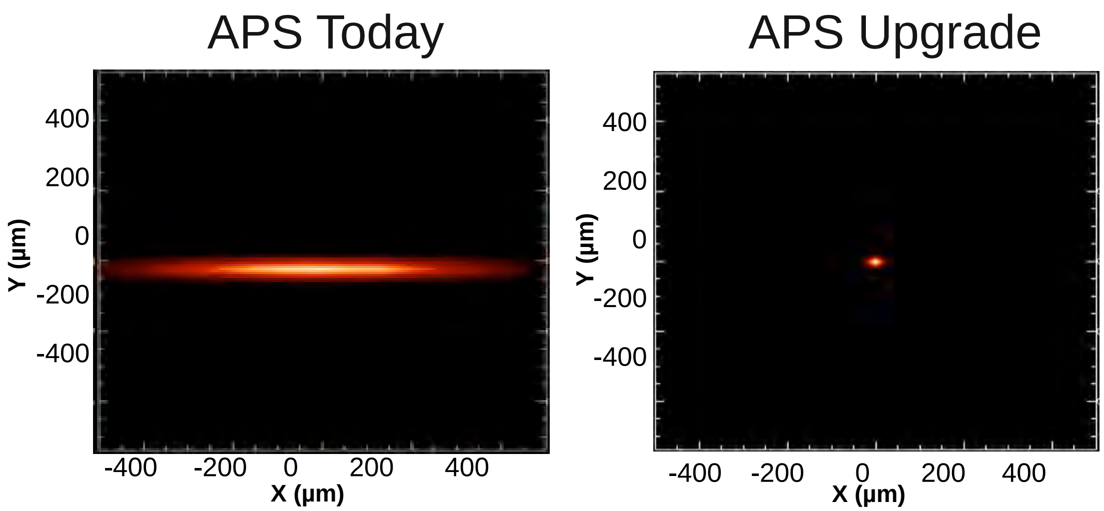
Coming in 2023* – The APS Upgrade:
The world's leading high-brightness hard x-ray storage ring



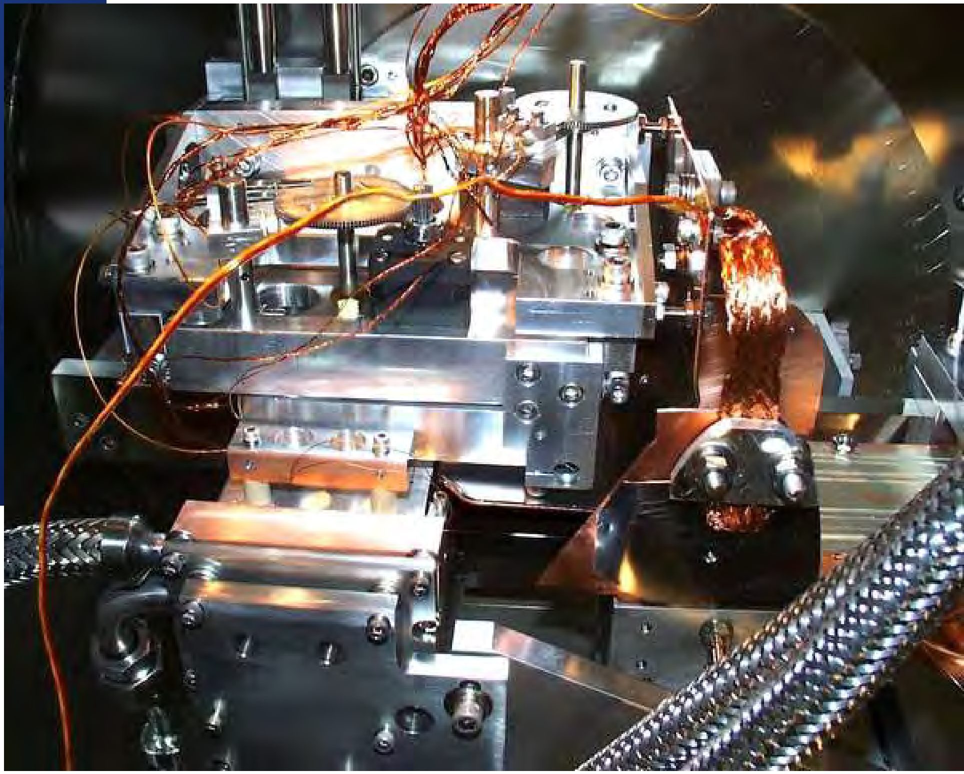
APS Upgrade will exceed the capabilities of today's synchrotrons by **2 to 3 orders of magnitude** in brightness, coherent flux, and nanofocused flux

World's brightest storage ring light source above 4 keV

Argonne NATIONAL LABORATORY


Thanks!

Monochromators for Wavelength Selection



Monochromator used to select x-ray energy

In vacuum and LN_2 cooled

Important to align monochromator (angle) and undulator (gap) energy

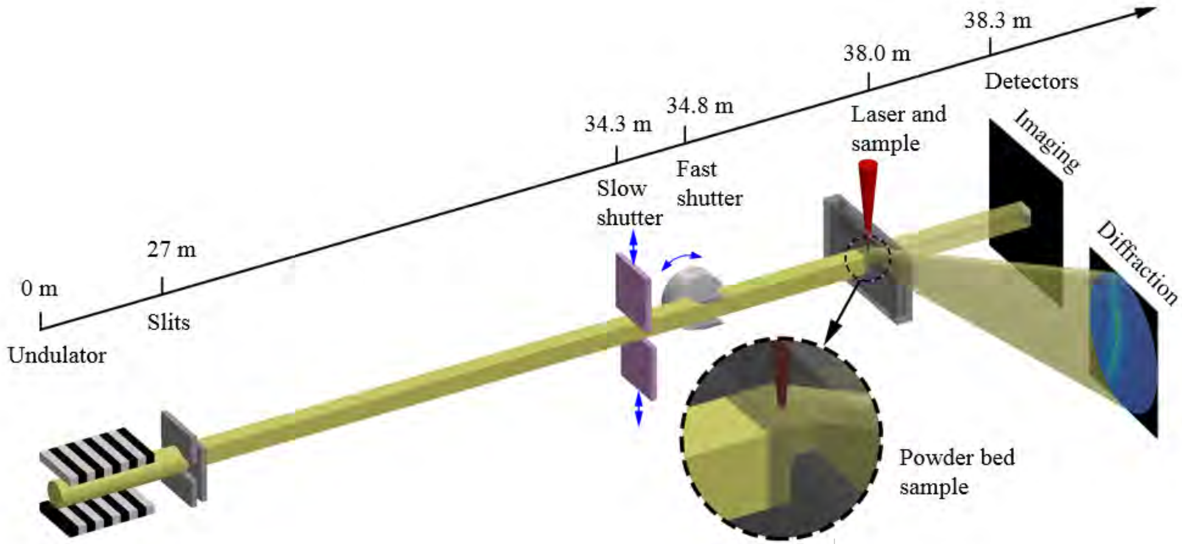
Collaborative Assess Teams (CATs) at the APS

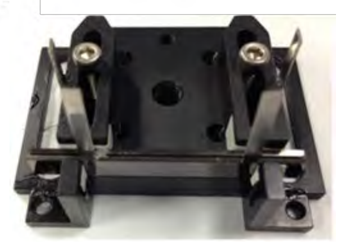
- CATs are made up of teams of researchers who have raised funds to build and operate a beamline or sector at the APS.
- CATs provide <u>at least</u> 25% of time to General Users through competitive process.
- Some CATs are funded as "National User Facilities" (NUFs) where all beam time is provided to their community (no set-aside time for member institutions or staff).
- Two CATs at APS are supported by NNSA:
  - High Pressure CAT
  - The Dynamic Compression Sector

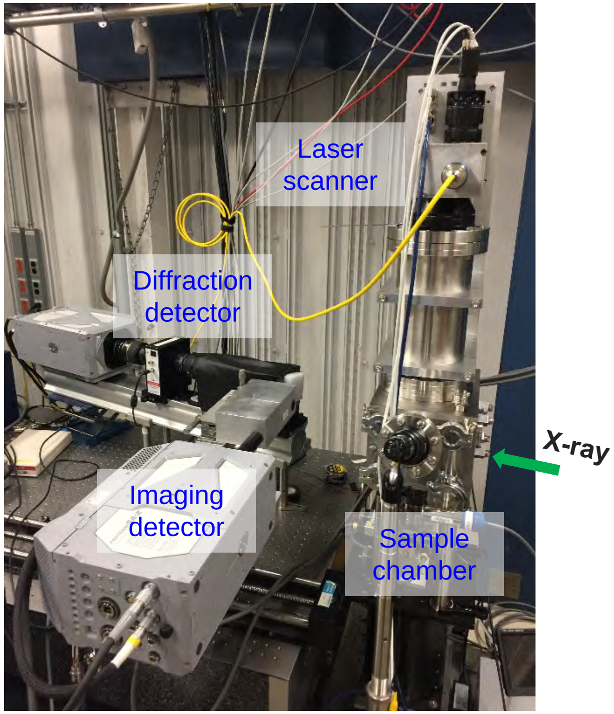
- Sector 5 – DuPont-Northwestern-Dow (DND) CAT
- Sector 10 – Materials Research (MR) CAT
- Sector 13 – GeoSoilEnviro (GSE) CARS
- Sector 14 – BioCARS*
- Sector 15 – ChemMatCARS
- **Sector 16 – High Pressure (HP) CAT**
- Sector 17 – Industrial Macromolecular Crystallography Association (IMCA) CAT
- Sector 18 – BioCAT
- Sector 19 – Structural Biology Center (SBC) CAT
- Sector 21 – Life Sciences (LS) CAT
- Sector 22 – South East Regional (SER) CAT
- Sector 23 – General Medicine/Cancer (GM/CA) CAT*
- Sector 24 – Northeastern (NE) CAT
- Sector 26 – Nanoprobe (CNM)*
- Sector 31 – Lilly Research Labs (LRL) CAT
- **Sector 35 – Dynamic Compression Sector in commissioning***

*operational involvement by APS

EXPERIMENT SETUP



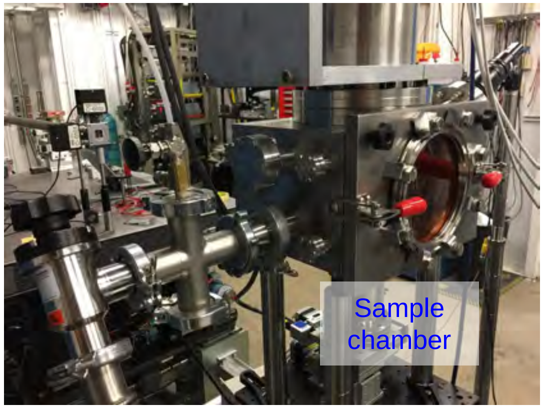




- ❑ **Beamline**
  - 32-ID-B at APS
  - Source: ~24 keV (4% bandwidth)
  - Max spatial resolution: 1 µm
  - Max temporal resolution: 100 ps

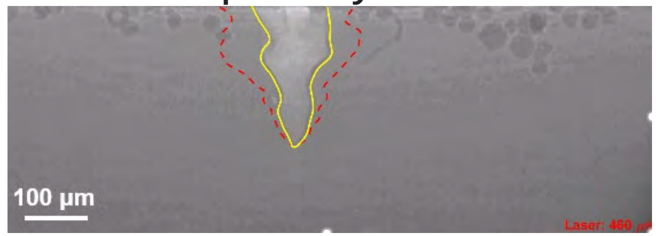
- ❑ **Laser**
  - Ytterbium fiber
  - Wavelength: 1070 nm
  - Max power: 500 W
  - Max scanning speed: 2 m/s

- ❑ **Sample:**
  - Material: Ti-6Al-4V
  - Thickness: 0.5 or 1 mm
  - Protection gas: Ar
  - Container: glassy carbon

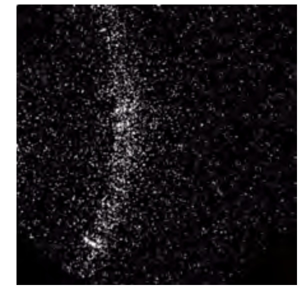


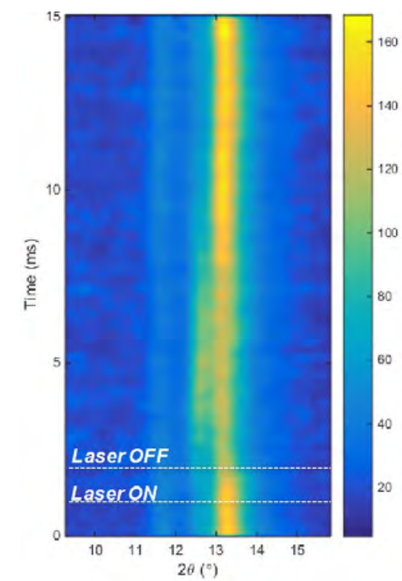
UNIQUE CAPABILITIES OF HIGH-SPEED X-RAY TECHNIQUES

Melt pool dynamics

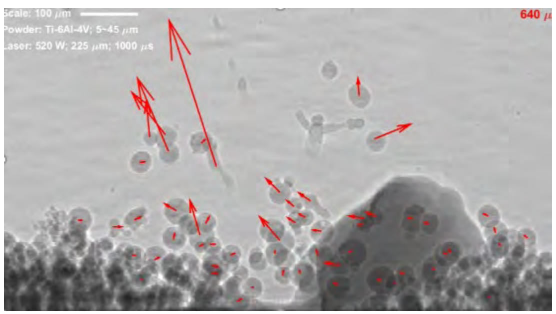


Phase transformation

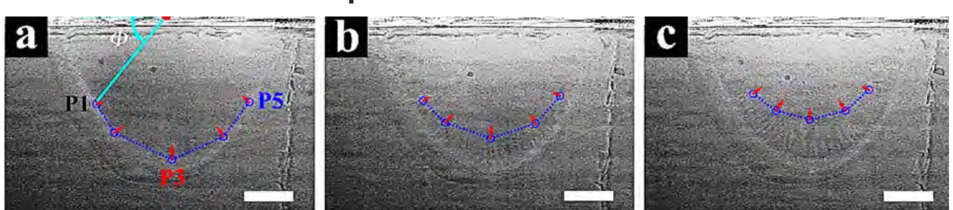




Powder spatter ejection



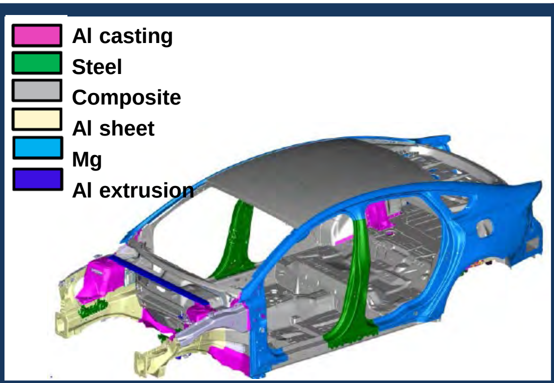
Rapid solidification



C. Zhao, et al., Submitted

APS-U: Developing new, more durable structural materials

The Challenge



Global market for advanced materials (energy/environment) **$90 billion yearly by 2020**

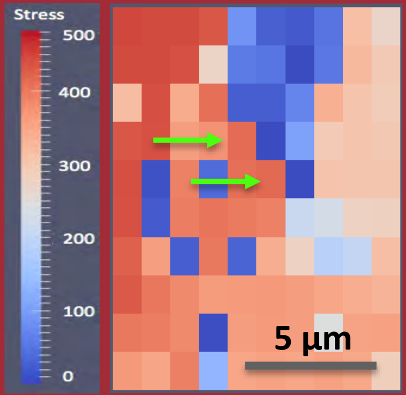
- Deformation and failure of advanced materials are not sufficiently understood, leading to costly over-design
- Use of lightweight, advanced materials in ¼ of U.S. vehicles could save more than 5 billion gallons of fuel annually by 2030
- 10% life extension of jet turbine engine disks = $600K savings per aircraft

The Science Problem

Lack of predictive models validated by experiment prevents microstructure-sensitive design

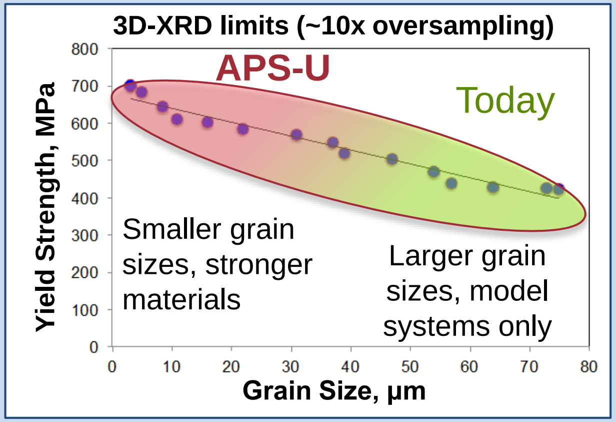
- Information needed from subgrain level to macroscale
- Initial crack growth (a rare event) not understood, occurs at length scales not accessible today

State of the art today:
1 μm 2D focus to study 30 μm grains



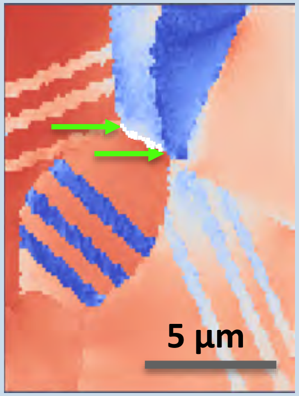
Simulation of deformation and crack formation in a superalloy; arrows show location of unresolved crack initiation

APS Upgrade



With APS-U:

- **80 keV brightness to penetrate bulk materials, measure strains with 50nm resolution**



- **Coherent imaging to measure intragrain & grain boundary properties**

With APS-U, twin bands and initial crack are resolved