NSLS-II Current Status and Plans

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Joint BNL/SBU NSLS-II Workshop
May 18, 2011

U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY
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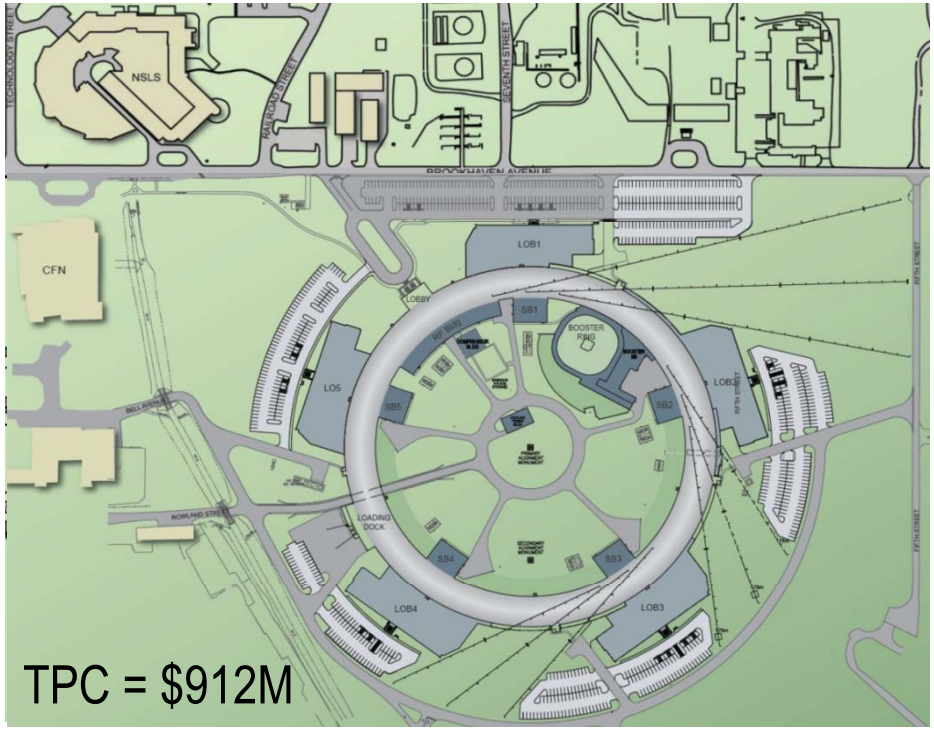
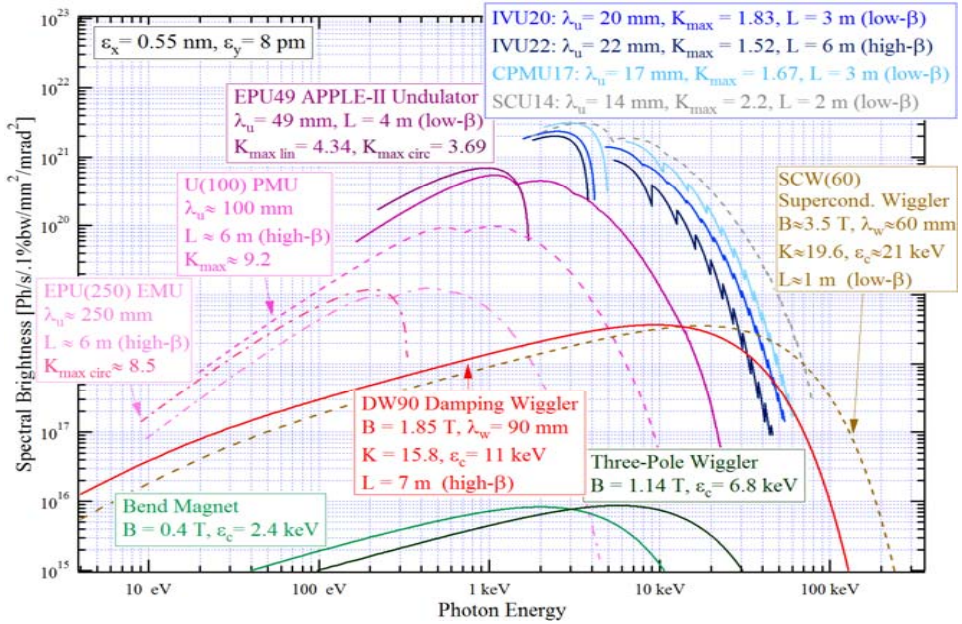
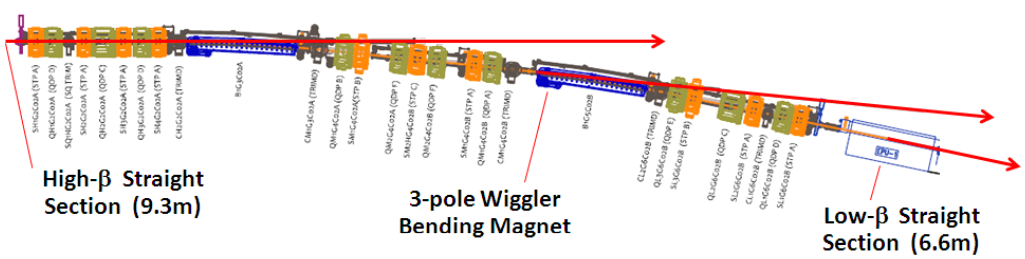
Outline

- NSLS-II Overview
- NSLS-II Project Beamlines and Capabilities
- Photon Sciences R&D Programs
- Beamline Advisory Teams
- Beamline Development beyond NSLS-II Project
- NSLS-II User Access Policy update
- Early Science Experiments

NSLS-II: Optimized 3rd Generation SR







- 3 GeV, 500 mA, Circumference 791 m
- Emittance: ε_x= 0.55, ε_y= 0.008 nm-rad
- High brightness from soft to hard x-rays
- Small beam size: σ_y=2.6 μm, σ_x=28 μm
- Pulse length (rms) ~15 psec
- 27 insertion device beamlines
- 31 BM / 3PW / IR beamlines
- High brightness, small source size, long beamlines – unique design features

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NSLS-II Key Project Milestones

Aug 2005	CD-0, Approve Mission Need	(Complete)
Jul 2007	CD-1, Approve Alternative Selection and Cost Range	(Complete)
Jan 2008	CD-2, Approve Performance Baseline	(Complete)
Jan 2009	CD-3, Approve Start of Construction	(Complete)
Feb 2009	Contract Award for Ring Building	(Complete)
Aug 2009	Contract Award for Storage Ring Magnets	(Complete)
May 2010	Contract Award for Booster System	(Complete)
Feb 2011	1st Pentant Ring Building Beneficial Occupancy	(Complete)
Mar 2011	Start Accelerator Installation	(Complete)
Feb 2012	Beneficial Occupancy of Entire Experimental Floor	
Apr 2012	Start LINAC Commissioning	
Jun 2012	Beneficial Occupancy of 1st LOB	
Oct 2012	Start Booster Commissioning	
May 2013	Start Storage Ring Commissioning	
Mar 2014	Projected Early Completion; Beamlines Ready for Beam	
Jun 2014	Early Project Completion; Beamlines Ready for Beam	
Jun 2015	CD-4, Approve Start of Operations	

NSLS-II Construction Progress

- Ring building construction progressing on budget and ahead of schedule
- LOB construction started
- Pentant 1 beneficial occupancy received; Accelerator installation in progress

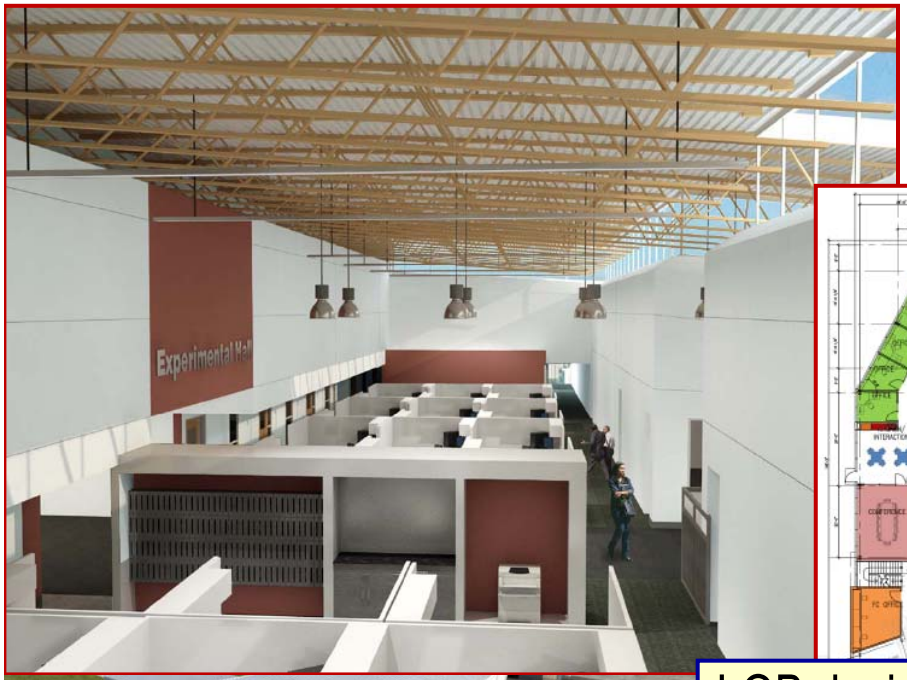
Construction Progress Cont'd

Electrical
Mezzanine in P-1

Pentant -1 –Finished
Experimental Floor

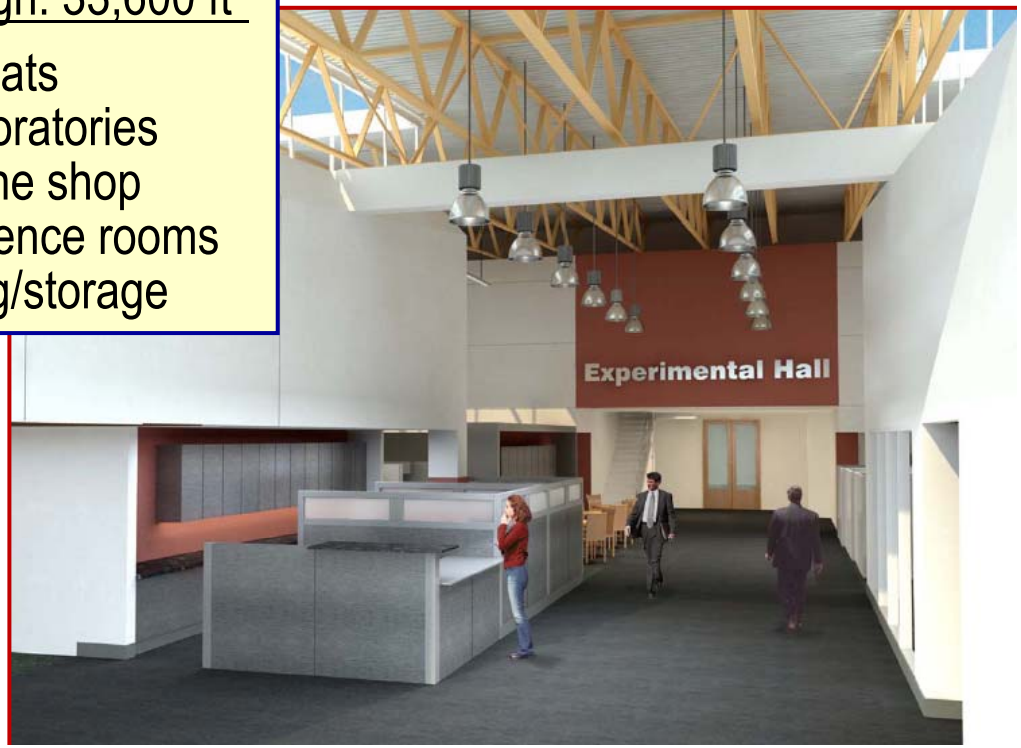
Pentant 5 - Last Section of
Experimental Floor - Rebar
Ready for Concrete

Laboratory Office Bldg.

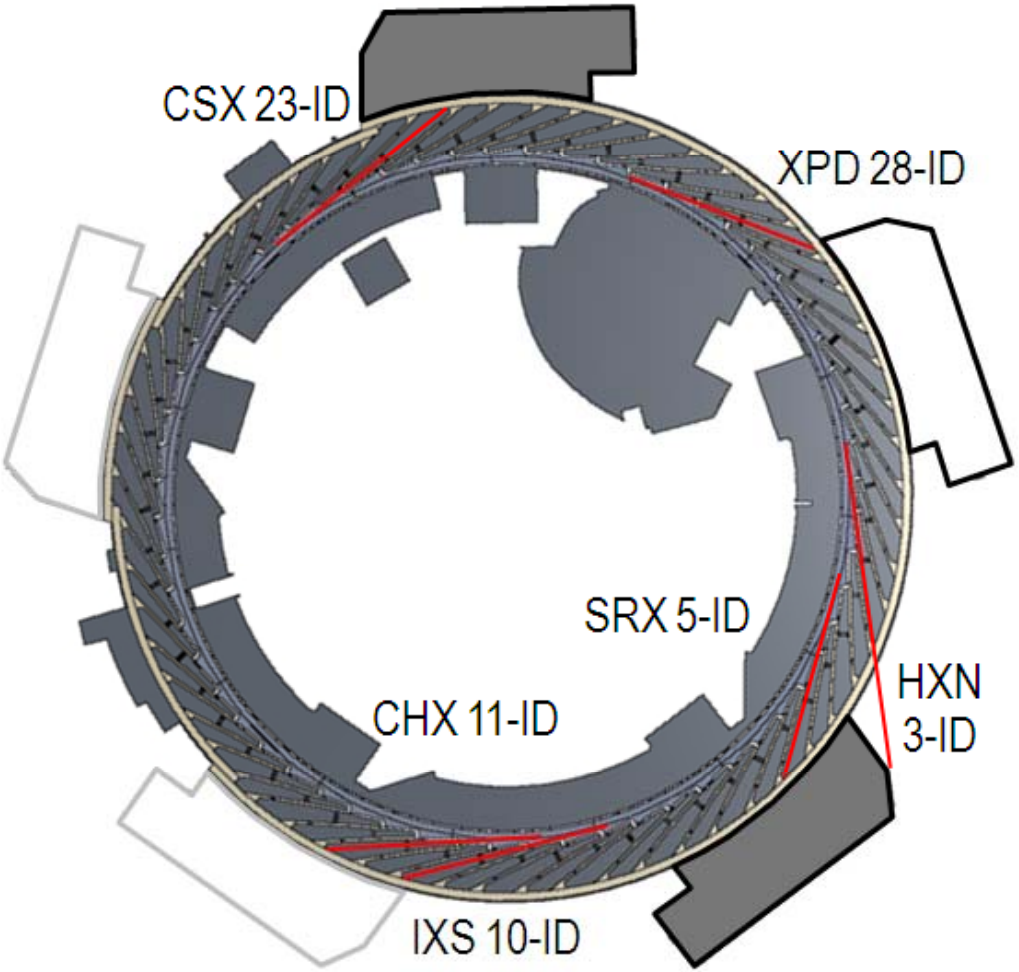


LOB design: 33,600 ft^2

- 120 seats
- 10 laboratories
- machine shop
- conference rooms
- loading/storage area



Six Beamlines in Construction Project



- Inelastic X-ray Scattering (IXS)
- Hard X-ray Nanoprobe (HXN)
- Coherent Hard X-ray Scattering (CHX)
- Coherent Soft X-ray Scattering & Polarization (CSX)
- Sub-micron Resolution X-ray Spectroscopy (SRX)
- X-ray Powder Diffraction (XPD)

- *Beamline locations finalized for the six project beamlines*
- *Preliminary designs completed; Procurement of long-lead-time components in progress*
- *Beamline commissioning & ramp-up of ops projected to start March 2014*

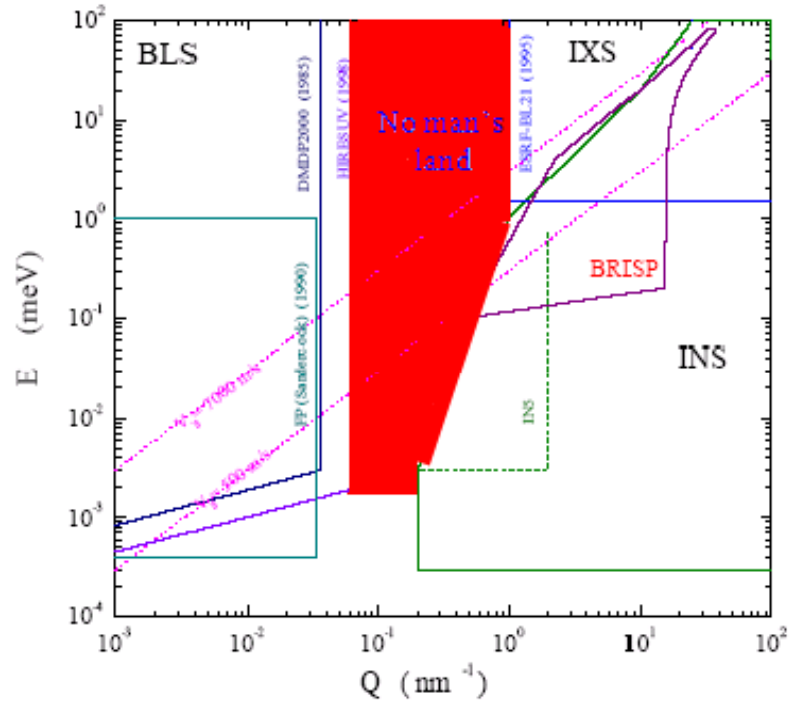
Inelastic X-ray Scattering (IXS)

IXS at NSLS-II:

- Will enable studies of THz dynamics in liquids, glassy, and crystalline materials with nanoscale inhomogeneities
- A novel monochromator/analyzer concept will provide a sub-meV broad resolution function with sharp tails
- Analyzer with a collimating multilayer mirror will provide narrow momentum (Q) resolution
- IXS will open up access to an unexplored dynamic region, which bridges the “no man’s land” in between THz and GHz (visible light) spectroscopic techniques

Examples of Science Areas & Impact:

- RELAXATION IN HIGHLY VISCOUS FLUIDS : relaxation processes in these systems are slow and out of the reach with current IXS spectrometers.
- BIOPHYSICS: studies of dynamics of water in hydrated proteins usually occurs within time-scales hardly accessible by existing IXS instrumentation.



Beamline Capabilities:

TECHNIQUE(S): Inelastic X ray Scattering with sub-meV resolution

ENERGY RESOLUTION: < 1 meV (baseline), 0.1 meV (ultimate goal)

Q RESOLUTION: < 0.5 nm^{-1} (baseline)

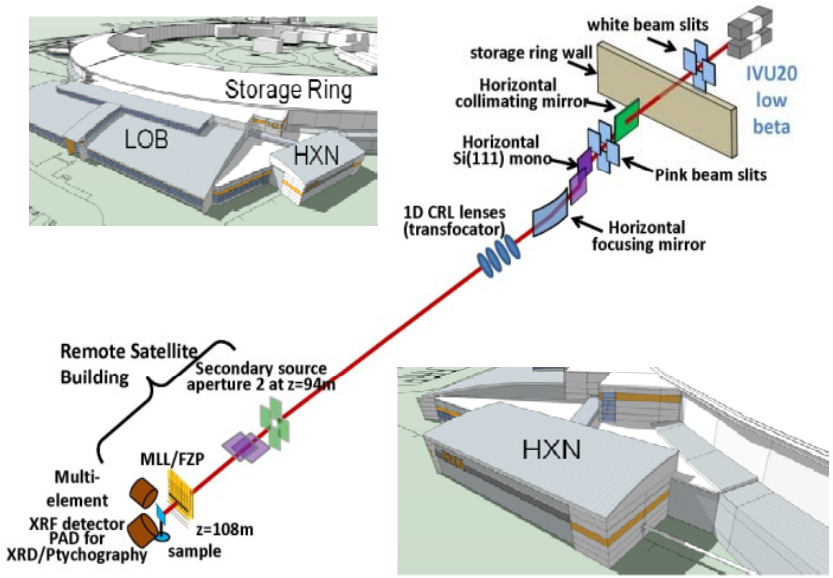
Hard X-ray Nanoprobe (HXN)

Scanning Microscopy at Nanometers at NSLS-II:

- Enable new frontiers of hard x-ray microscopy with the highest achievable spatial resolution.
  - initial goal: 10 nm using MLLs and 30nm using ZP, as initial goal
  - long-term goal: 1~10nm using MLLs
- Image structural inhomogeneity of buried interfaces using x-ray fluorescence and diffraction.
- Cutting-edge x-ray microscope in a vibration-isolated satellite building

Examples of Science Areas & Impact:

- Material Science: Investigation of a wide variety of buried interfaces for composition, morphology, and crystalline ordering
- Nano-catalysis: Investigation of composition profile and morphology of heterogeneous nanoparticles.
- Environmental Science: Investigation of reactivity, bioavailability, toxicity of environmental particulates, and interaction of organisms with contaminants.
- Biology: Imaging and quantification of metal distributions in cells and tissue to understand metal-mediated biological processes including many diseases and their potential treatments.



Beamline Capabilities:

TECHNIQUE(S):

Nanodiffraction & fluorescence (primary)

Differential phase contrast & Ptychography (supporting)

Source: low beta, IVU20

ENERGY RANGE / RESOLUTION: 6-25 keV/ 2 eV

SPATIAL RESOLUTION: 1~10nm (MLL), 30nm (ZP)

Coherent Hard X-ray Scattering (CHX)

XPCS at NSLS-II:

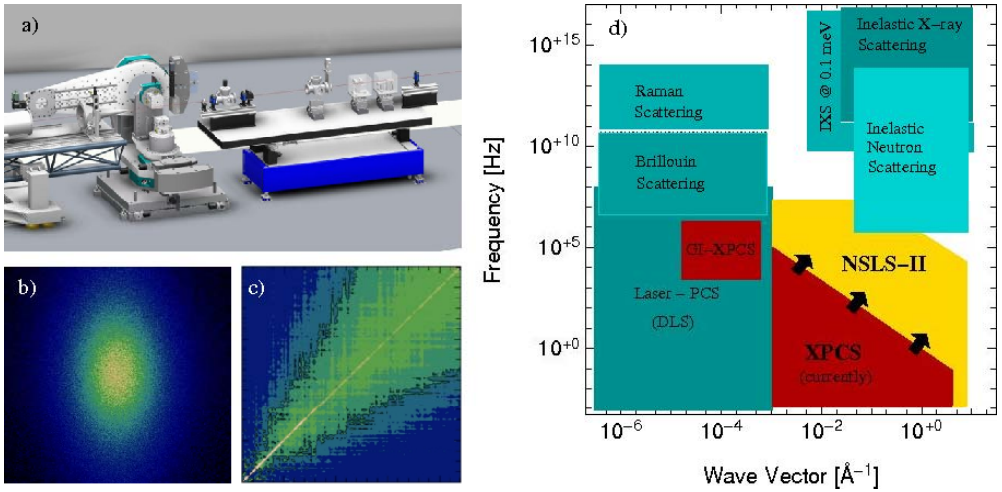
- The unprecedented brightness of the NSLS-II source will enable studies of dynamics with X-ray Photon Correlation Spectroscopy (XPCS) on faster time scales (100 x) and shorter length scales than was ever possible before.

Examples of Science Areas & Impact:

"How do we characterize and control matter away- especially very far away- from equilibrium?"

Directing Matter and Energy: Five Challenges for Science and Imagination (BESAC)

- SOFT MATTER: non-equilibrium and heterogeneous dynamics in colloids, polymers, gels and glasses, driven systems (e.g. complex fluids under shear); interplay between dynamics and rheology
- SOFT MATTER INTERFACES: studies of dynamics at buried interfaces; fast surface dynamics
- BIOLOGICAL MATERIALS: dynamics in protein crystals, proteins in solution; protein aggregation. Understanding the dynamics of e.g. cataract formation in the eye crystalline
- INORGANIC MATERIALS: dynamics in metallic glasses, phase ordering crystals



a) Preliminary design of the CHX end station; b) speckles from a phase-ordering Cu_3Au alloy and c) two-time correlations measuring the dynamics of fluctuations; d) The NSLS-II source will enable studies of dynamics on faster time scales and shorter length scales than is possible at current sources

Beamline Capabilities:

TECHNIQUE(S):

- X-ray Photon Correlation Spectroscopy (XPCS)
- Coherent X-ray Diffraction (SAXS, WAXS)
- Full-field Coherent Diffraction Imaging (CDI)

Source: IVU20 Undulator ENERGY RANGE: 6 -15 keV

COHERENT FLUX: $>10^{11}$ photons/sec $(\Delta\lambda/\lambda)=10^{-4}$

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Coherent Soft X-ray Beamline (CSX)

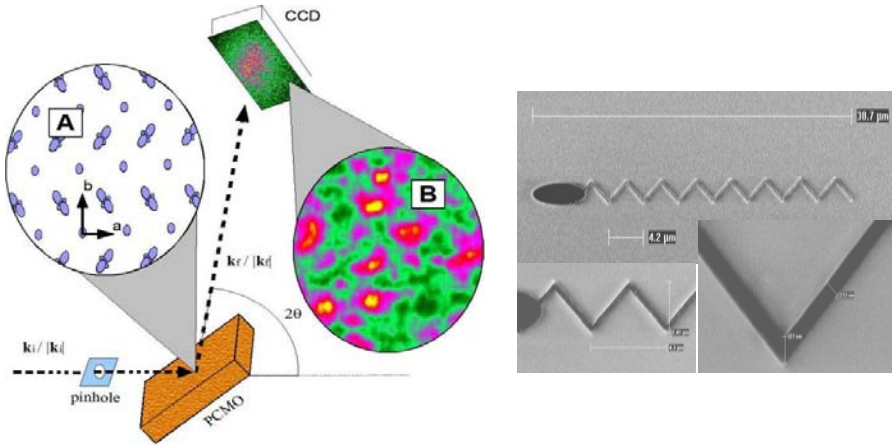
CSX at NSLS-II

The beamline design (source and optics) has been optimized to the NSLS-II parameters with two branches, to provide the highest possible flux for experiments requiring either high coherence flux (HCF) or full control of the polarization (PC).

- Coherent scattering / diffraction / imaging
- Polarization dependent scattering /spectroscopy
- Ultrafast dynamics

Examples of Science Areas & Impact:

- MATERIAL SCIENCE (MAGNETISM) coherence and fast polarization switching to study polarization dependent properties in materials. For example the magnetic structure in energy storage spring magnets, spin torque dynamics and anti-ferromagnetic clusters.
- MATERIAL SCIENCE / PHYSICS by using highly coherent beams the imaging of phase segregation in strongly correlated materials
- MATERIAL SCIENCE / SOFT MATTER by using the polarization/coherence to study the molecular orientation/ order in soft matter systems.



Left: Coherent x-ray scattering from PCMO. The scattering geometry is set to measure the orbital-order Bragg reflection in $Pr_{0.5}Ca_{0.5}MnO$. (J.J. Turner, et. al, New Journal of Physics)$_3$. Right: Example of nanowire to study dynamics and propagation of magnetic domain walls . T. Hase, Univ. of Warwick

Beamline Capabilities:

SOURCE: Dual 49 mm period EPU

ENERGY RANGE: 250 – 1700 eV

RESOLVING POWER: 2000 (HCF), 10000 (PC)

SPOT SIZE: 20x20 µm (HCF), 10x50 / 5x5 µm (PC)

FLUX (max): $2x10^{13}$ ph/s/0.1%bw at 500 eV (HCF / PC)

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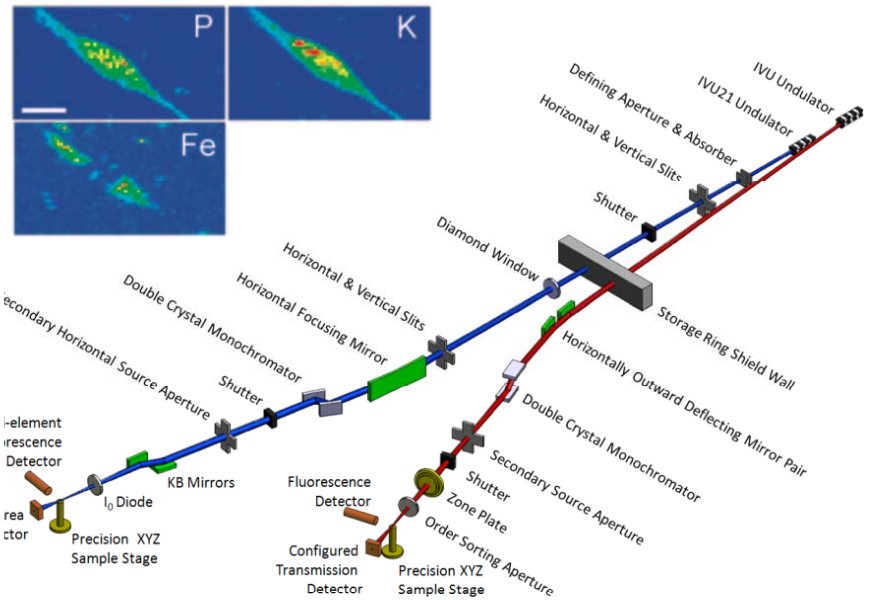
Sub-Micron Resolution X-Ray Spectroscopy (SRX)

SRX at NSLS-II:

- Beamline with versatile sample setup for experiments in environmental, life, and material sciences.
- Beamline with two branches, each optimized to perform spectroscopy with very high flux and high spatial resolution.
- Branch with KB mirrors optimized for E = 4.65 - 25 keV. Two sets of KB optics will create either a sub-µm focal spot at > 10^{13} ph/s or a sub-100 nm spot > 10^{11} ph/s.
- Branch using zone plates is optimized for E = 2 - 15 keV focal spot < 30 nm. *Not in the baseline scope.*



Beamline performance of KB branch:

Source: In vacuum undulator, λ = 21 mm, L = 1.5 m
Energy range: 4.65 keV ≤ E ≤ 25 keV
Monochromator: Horizontal DCM, Si (111), Si (311)
Energy resolution: $\Delta E \approx$ 1.5-2.5 eV @ 12 keV
$\Delta E \approx$ 0.9 eV @ 7 keV

✓ **Performance at the focal spot:**

Focal spot size and flux with high flux setup:
≈ 0.5 x 0.5 µm^2 at > 10^{13} ph/sec

Focal spot size and flux for high resolution setup
≈ 60 x 60 nm^2 (H x V) at 10^{11}-10^{12} ph/sec @ 7 keV
≈ 30 x 30 nm^2 (H x V) at 10^{11} ph/sec @ 18 keV

Techniques available:

X-ray absorption imaging
X-ray fluorescence imaging
X-ray microtomography
XANES absorption spectroscopy
XANES fluorescence spectroscopy
X-ray spectromicroscopy
X-ray microdiffraction

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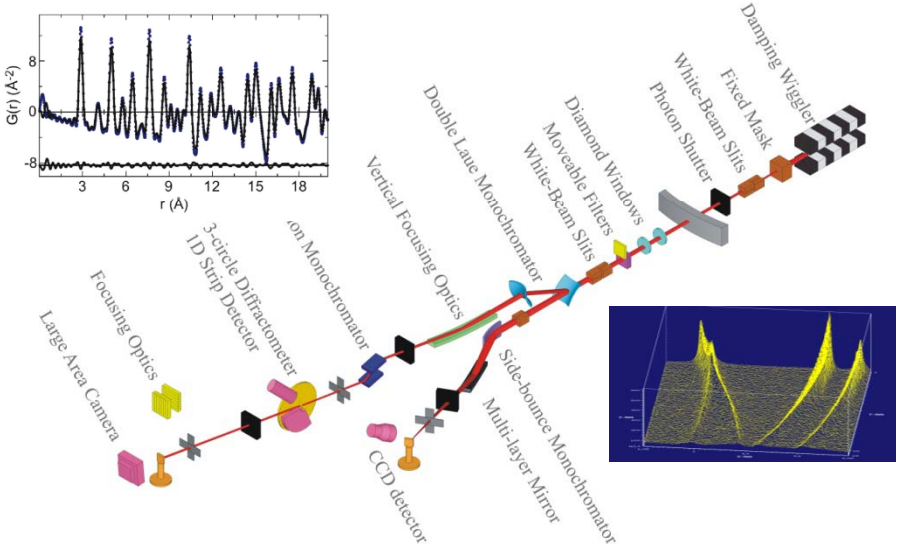
X-Ray Powder Diffraction (XPD)

XPD at NSLS-II:

- powder diffraction of complex materials using high energy x-rays either in high photon flux mode or high angle resolution mode.
- *in situ* and *in operando* structural science (variety of sample environments, materials in working conditions or in operating devices).
- dynamics, rapid acquisition, time-resolved (msec to sec scale).
- total structure diffraction studies: high Q-space resolution (average, long-range structure) combined with high real-space resolution (pair distribution function: local structure or nanostructure).

Examples of Science Areas & Impact:

- STRUCTURAL AND IN SITU MATERIALS SCIENCE: high T synthesis, structural ceramic composites, thermal barrier coatings…
- MATERIALS CHEMISTRY AND ENERGY SCIENCE: hydrogen storage, fuel cells, catalysis, cements, batteries, porous materials…
- EARTH AND PLANETARY SCIENCES: ices and clathrates, new phases or structurally modified earth materials…
- ENVIRONMENTAL SCIENCE: sequestration of pollutants, sorption of contaminants, CO_2 sequestration, speciation in solution…
- CONDENSED MATTER PHYSICS: magneto-resistance, charge ordering, magnetic frustration, superconductors, Negative Thermal Expansion materials, multiferroic materials…



The layout of XPD features two independent branches served by Laue-crystal monochromators and three in-line endstations fitted with 0, 1 and 2D detectors. XPD is capable of collecting data at high energies ideal for high-Q data and in situ and time resolved studies in environmental cells.

Beamline Capabilities:

TECHNIQUE(S): powder diffraction, total scattering, medium angle scattering, tomography

Source: 1.8T Damping Wiggler

ENERGY RANGE : 30 -80 keV

ENERGY RESOLUTION: 10^{-3} to 2×10^{-4} $\Delta E/E$

SPATIAL RESOLUTION: ~mm horizontal beam (powder averaging) down to ~ 50 μm

TIME RESOLUTION: ~ms

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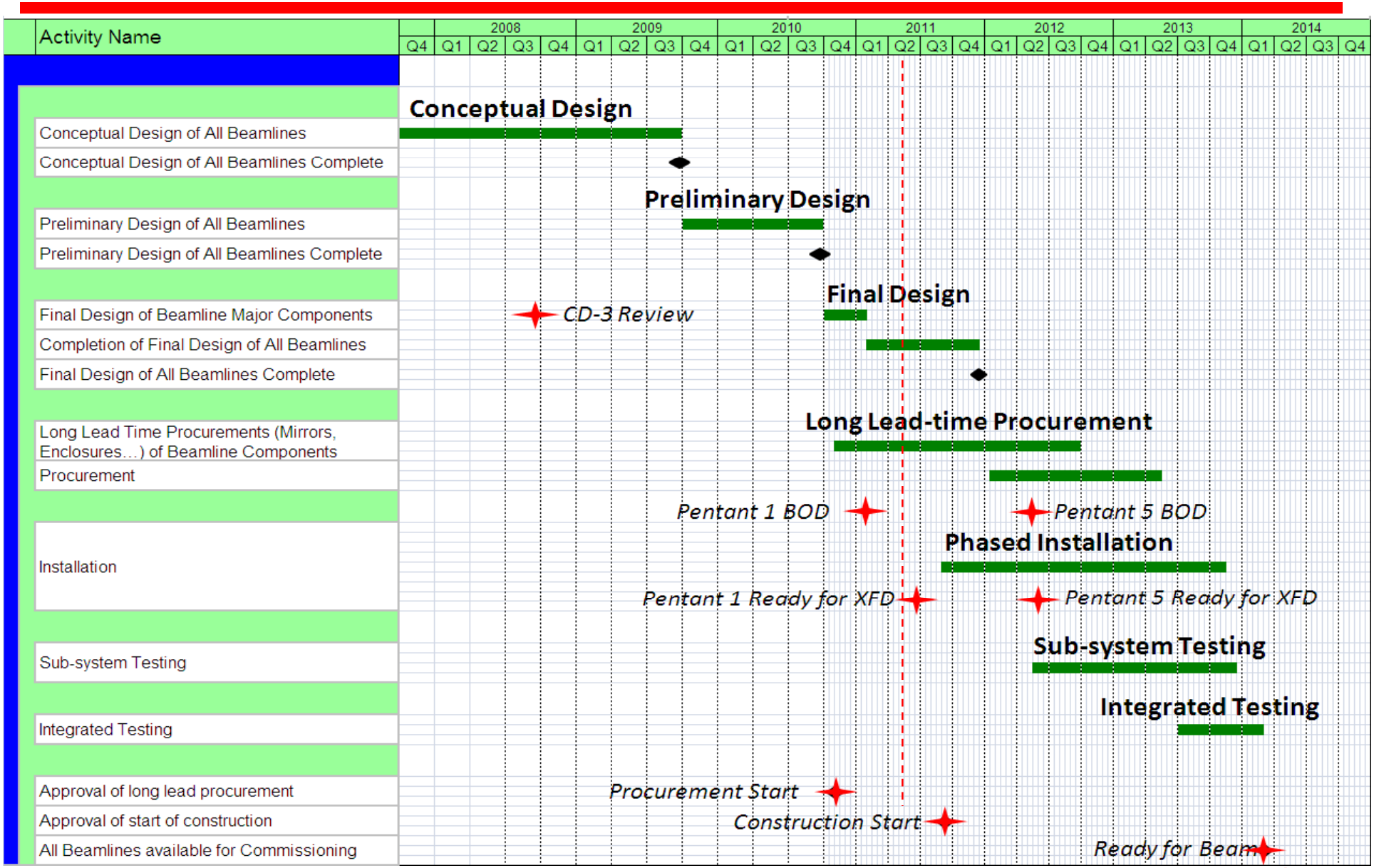
NSLS-II Project Beamline Schedule

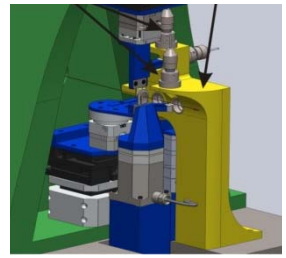


March 2014

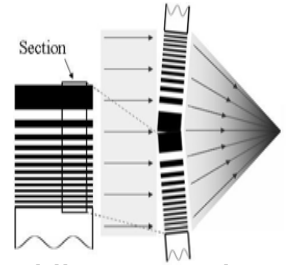
Photon Sciences R&D Programs

Four focus areas:

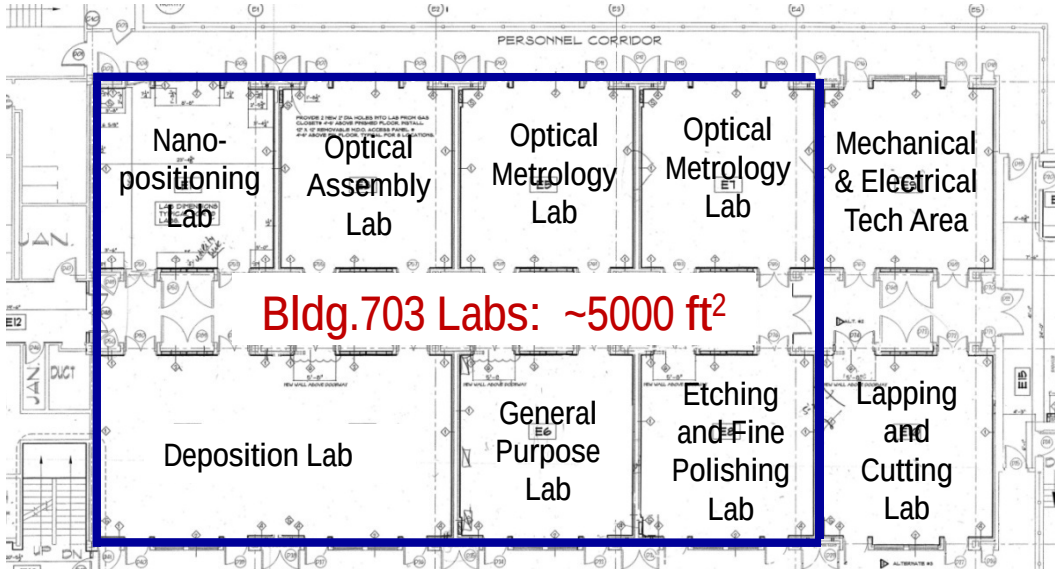
- Beamline design & precision engineering
- Optics R&D – 1 nm & 0.1 meV
- Optics metrology & coherence
- Advanced detectors R&D

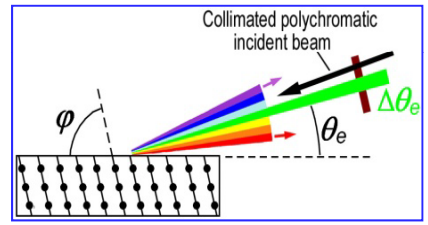


Nanopositioning



Multilayer Laue lens





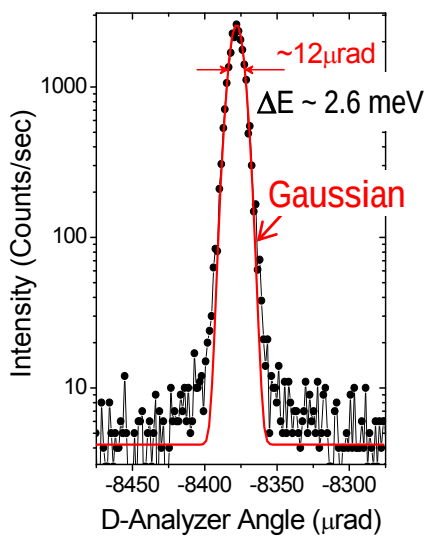
Asymmetric back-reflection

Advanced detectors

- R&D space & facilities: Recent development of NSLS-II R&D programs has led to much greater footprint in R&D portfolio in PS, with much enhanced & enabling capabilities

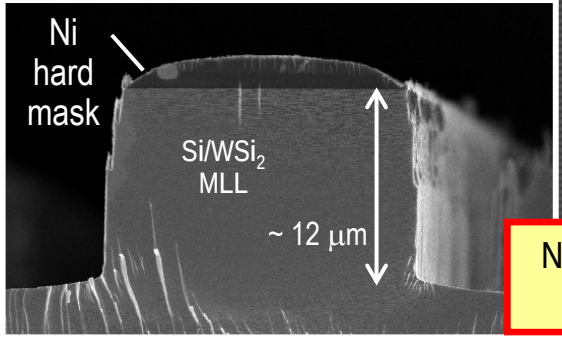
Nanofocusing & Dispersive Optics R&D

- MLL deposition laboratory established and operational in Bldg 703 at BNL
- First MLL deposition using the new system completed: consisting of 6,510 layers, 43 μm thick, of WSi2/Si and 4 nm outmost zones, with system running continuously for 5 days
- This was the largest MLL ever grown
- ML deposition also enables fabrication of ML mirrors – promising alternative approach for sub-10 nm focusing
- High energy-resolution optics group observed for the 1st time Gaussian like sharp tails in the resolution function – critical result for 0.1-1 meV IXS program



Ray Conley received 2010 BNL Engineering Award

SEM of 1st MLL grown in new deposition system



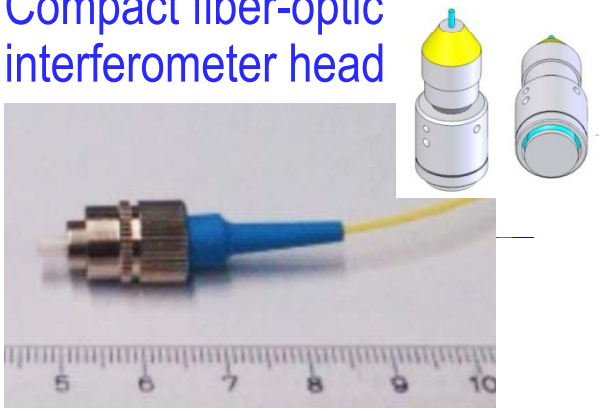
Nathalie Bouet received 2010 BNL Engineering Award

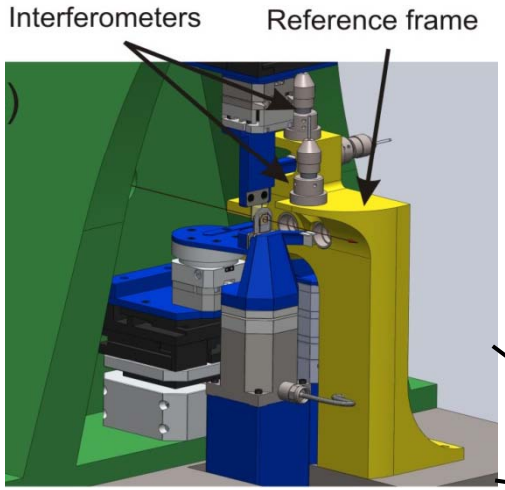
XRF imaging at resolution 23nm x 27nm using 2D MLLs (APS 26-ID)

Nanopositioning R&D for MLL-Based Microscope

- Conceptual design of HXN baseline microscope has been completed
- It includes innovative design features based on compact nanopositioning system

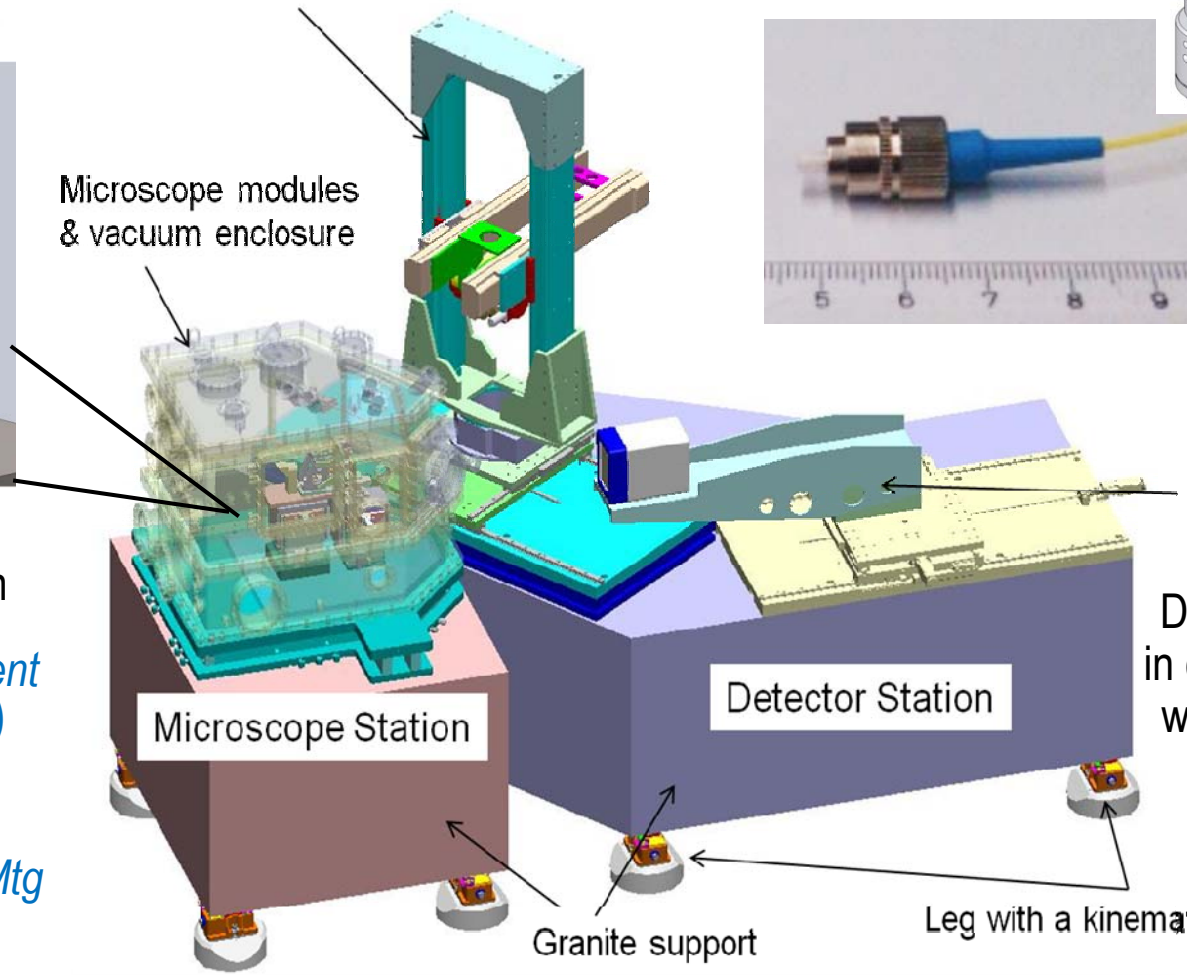
Compact fiber-optic interferometer head





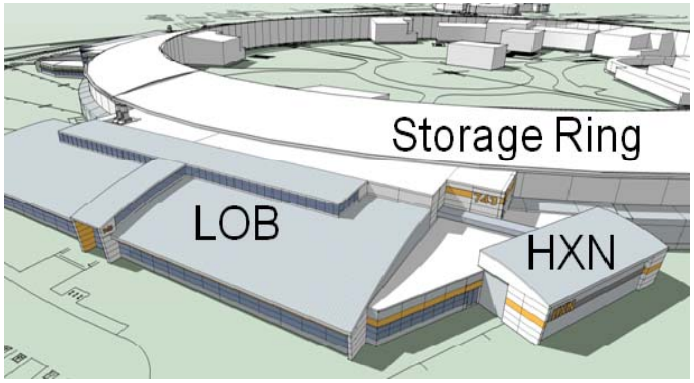
MLL mount with compact laser interferometer system

Rafael Lozano (GEM student working with E. Nazaretski) won 1st Place Award in Technical Presentation at 2010 GEM Annual Board Mtg



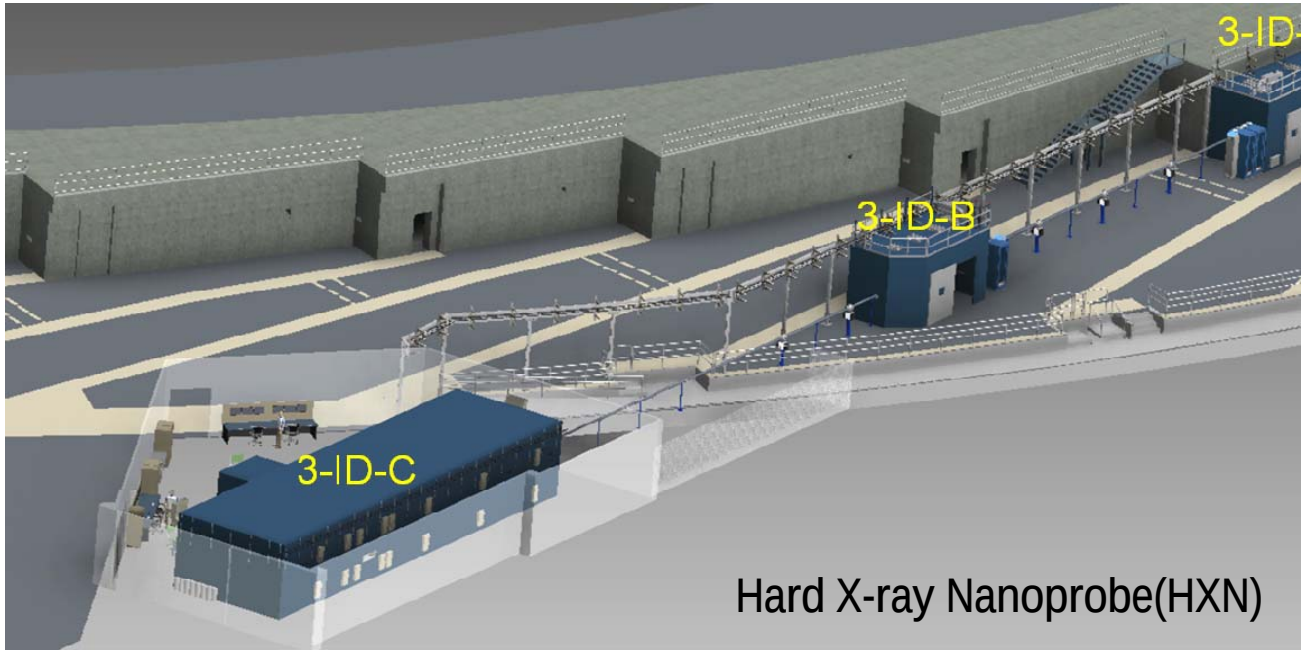
Development in collaboration w/ APS/CNM

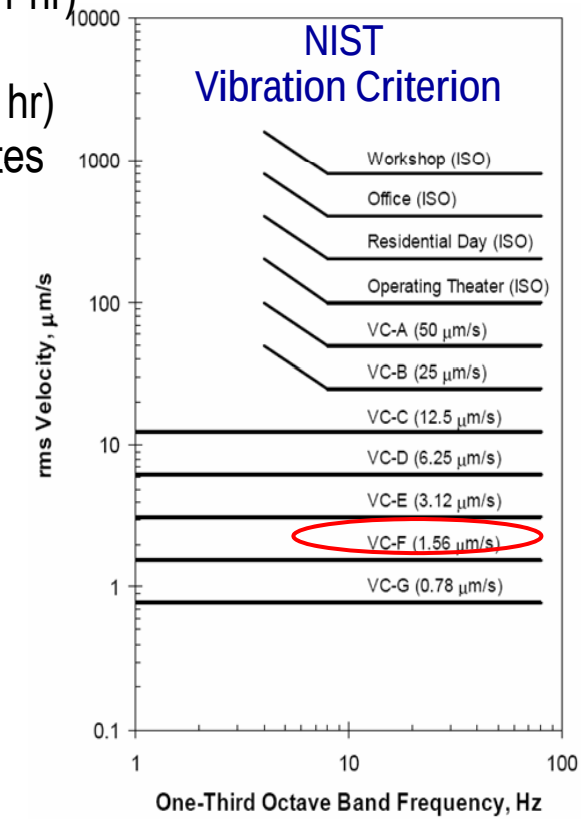
Beamline Design Progress – Hard X-ray Nanoprobe



Satellite Bldg. Stabability Specifications:

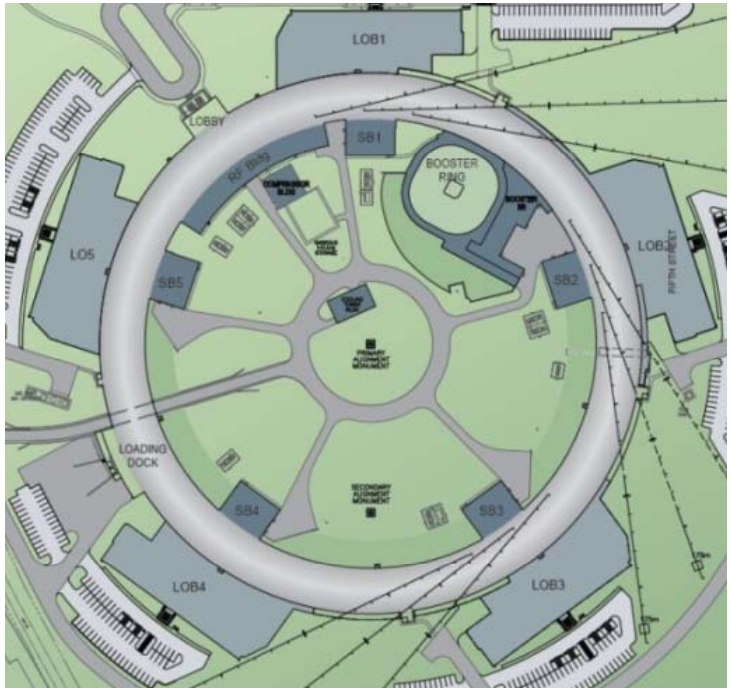
- Vibration: VC-F minimum; goal to achieve VC-G
- Temperature Inside hutch:
  ±0.1 C (long term), ±0.05 C (~1 hr)
- Temperature Outside hutch:
  ±1.0 C (long term), ±0.5 C (~4 hr)
- Equilibrium T reached in 30 minutes





Beamline Advisory Team (BAT) Concept

- In order to foster engagement of the scientific community, to encourage novel ideas, and to ensure that every beamline built at NSLS-II will best serve the interests of the user community, the design and construction of every beamline will be overseen by a Beamline Advisory Team (BAT)

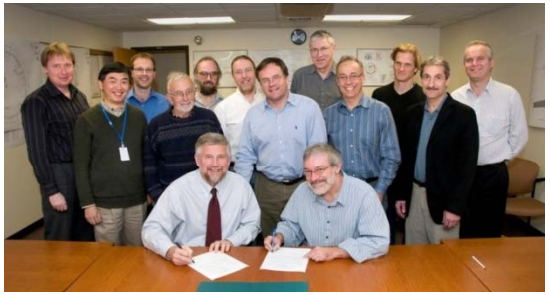


- BAT is defined as a small group of scientists who
  - represent a segment of the scientific community
  - advise PS staff and management on the development of a beamline or a suite of beamlines based on a common set of experimental techniques and/or scientific mission

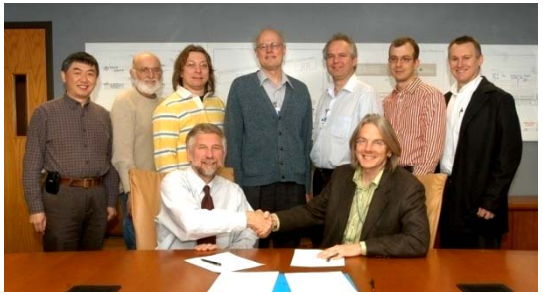
BAT Roles and Responsibilities

- BAT will work with the Beamline Development Group to provide feedback and input on the design of the beamline to ensure that it optimally enables the science mission and includes innovations to achieve best-in-class performance
- BAT roles:
  - represent the interests of each scientific community that has a significant interest in using the beamline as described in the Beamline Development Proposal or identified in the review process
  - advise the Beamline Group on the scientific mission and technical requirements, and on the design, construction, and commissioning of, the beamline
- BAT responsibilities:
  - participate in periodic BAT meetings, and in project & design reviews as requested
  - communicate to the community about the beamline and its associated science capabilities and opportunities

Six Project Beamline Advisory Teams



SRX BAT



XPD BAT

IXS BAT

CHX BAT

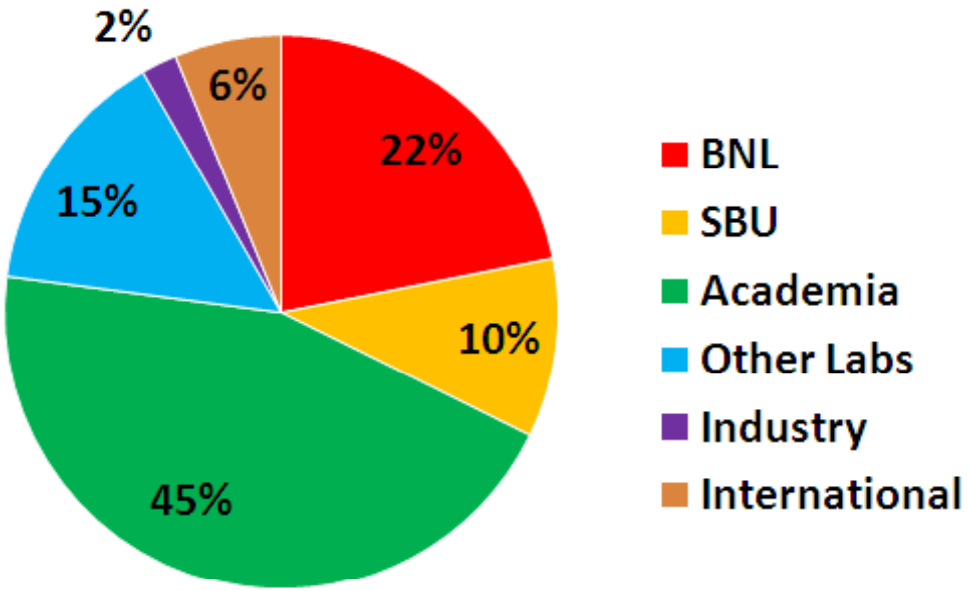
CSX BAT

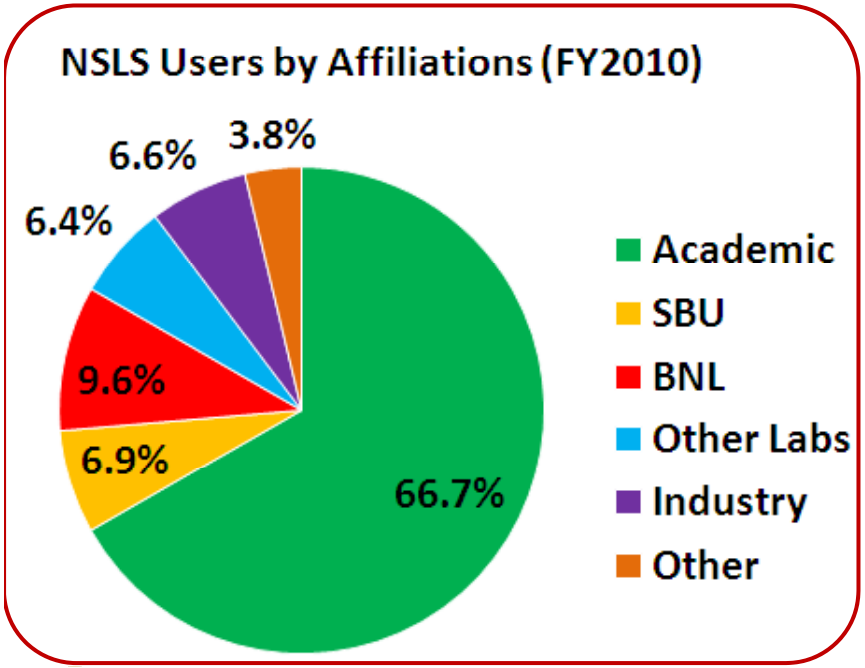
HXN BAT

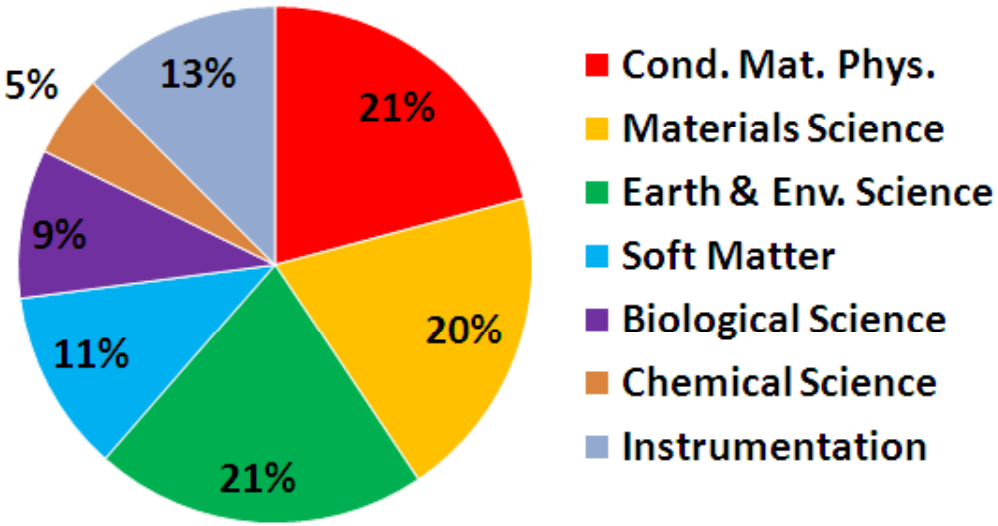
- Each project beamline BAT has been meeting at least twice a year
- BAT meeting topics may include scientific and technical scope of the beamline, updates on beamline planning and near-term issues, and technical reviews of beamline design for construction and upgrades

BAT Membership of Six Project Beamlines

- BNL/SBU representation ~32%
- Majority membership from other US academic institutions and research laboratories
- Compared to current NSLS user community, BNL/SBU representation is greater in current NSLS-II BATs







Development of Additional Beamlines

2010 Call for Beamline Development Proposals
National Synchrotron Light Source II

March 26, 2010

- Scope
  - All areas of science and beamline types – ID, BM, 3PW, IR
  - Independent of funding source or implementation approach
- Science case and technical requirements
- Results
  - 54 Beamline Development Proposals received by Jun 21
  - Reviewed by Science Advisory Committee & Study Panels
  - 34 BDPs approved; Results announced Oct 4, 2010

Critical Dates

Call for proposal issued
March 26, 2010

Informational session
Wednesday, April 14, 2010
Agenda | Video (RealPlayer)

Letter of Intent due Monday, April 26, 2010
(submitted LOIs)

Beamline development workshops
April-June 2010

Beamline proposal due Monday, June 21, 2010

SAC review
Summer 2010

Related Materials

Proposal template

NSLS-II Beamline Development Policy

NSLS-II Source Properties

NSLS & NSLS-II User Access Policy (draft)

Conceptual Design Report for Six Project Beamlines

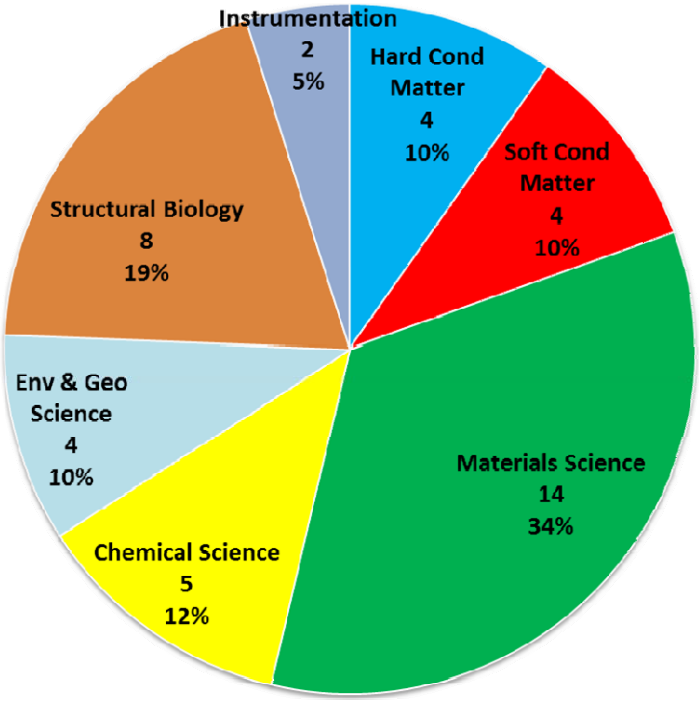
Background Beamline Information

Approved Beamline Development Proposals

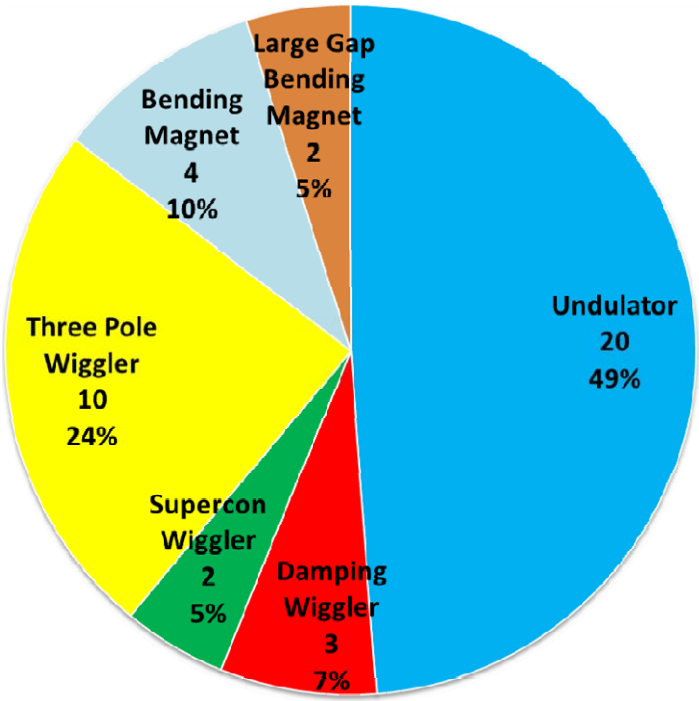
http://www.bnl.gov/nsls2/beamlines/2010BeamlineProposal-Approved.asp

Acronym	Title	Spokesperson	Type
4DE	4-Dimensional Studies in Extreme Environments	Donald J. Weidner, Stony Brook U.	1
ABS	A Highly Automated Instrument for Static X-ray Scattering Measurements of Biological Molecules in Solution	Lin Yang, BNL	1
AIM	Advanced Infrared Microspectroscopy	Lisa Miller, BNL	1
AMX	Flexible Access Macromolecular Crystallography at an Undulator Beamline	Dieter Schneider, BNL	1
BMM	Hard X-ray Abs. Spectro. & Diffraction - Beamline for Materials Measurements	Daniel Fischer, NIST	2
CDI	Coherent X-ray Diffraction	Ian Robinson, U. College London	1
CMS	Complex Materials Scattering	Kevin Yager, BNL	1
ESM	Electron Spectromicroscopy for Fundamental Studies of the Physics & Chemistry of Materials	Elio Vescovo, BNL	1
FIS	Frontier Synchrotron Infrared Spectro. Beamline Under Extreme Conditions	Zhenxian Liu, Carnegie Institute	1
FMX	Frontier Macromolecular Crystallography at an Undulator Beamline	Robert Sweet, BNL	1
FXI	A Superconducting Wiggler Long Beamline for Full-field Imaging	Jake Socha, Virginia Tech	1
HIX	Hard X-ray - Inelastic X-ray Scattering	Young-June Kim, U. of Toronto	1
IRI	Full-field Infrared Spectroscopic Imaging	Lisa Miller, BNL	1
ISR	Integrated In-situ & Resonant Hard X-ray Studies	Karl Ludwig, Boston U.	1
ISS	Inner-shell Spectroscopy	Bruce Ravel, NIST	1
IXD	Powder Diffraction Beamline for In-situ Studies of Structural & Chemical Transformations	Jianming Bai, U. of Tennessee	1
LIX	A High-brightness X-ray Scattering Instrument for Biological Applications	Lin Yang, BNL	1
MET	Infrared & THz Beamline for Magnetospectro., Ellips. & Dynamical Studies	Larry Carr, BNL	1
MID	Dedicated Beamline for X-ray Instrumentation Development	Jeff Keister, BNL	1
MPP	Materials Physics & Processing	Jean Jordan-Sweet, IBM	1
MXD	Multiscale X-ray Diffraction	Kenneth Evans-Lutterodt, BNL	1
NYX	NYSBC Microdiffraction Beamline	Wayne Hendrickson, Columbia U.	2
OFT	At-wavelength Metrology & In-situ Figuring	Konstantine Kaznatcheev, BNL	1
QAS	In-situ Studies of Chemical Transformations by Combined Quick X-ray Absorption & Scattering Measurements	Anatoly Frenkel, Yeshiva U.	1
SIX	Soft Inelastic X-ray Scattering	Kevin Smith, Boston U.	1
SM3	Correlated Single-crystal Spectroscopy & Macromolecular Crystallography	Allen M. Orville, BNL	1
SMI	Soft-Matter Interfaces	Ben Ocko, BNL	1
SSS	Soft X-Ray Spectroscopy & Scattering	Joseph Dvorak, BNL	1
SST	Soft & Tender X-ray Spectroscopy & Microscopy	Daniel Fischer, NIST	2
TEC	Time-resolved X-ray Diffraction & Spectroscopy Under Extreme Conditions	Alexander Goncharov, Carnegie Inst.	1
TES	Tender Energy X-ray Spectroscopy	Paul Northrup, Stony Brook U.	1
XAS	X-ray Abs. Spectroscopy for Biological, Environmental & Energy Sciences	Mark Chance, Case Cent. for Syn. Bio.	1
XFM	X-ray Fluorescence Microprobe	Antonio Lanzirotti, U. of Chicago	1
XFP	X-ray Footprinting	Mark Chance, Case Cent. for Syn. Bio.	1

Beamline Distributions (Project + Approved Beamlines)



Science



Source

NSLS & NSLS-II Beamline Portfolios

Experimental Technique	NSLS BLs*	NSLS-II BLs
SPECTROSCOPY	22	11
Low-Energy Spectroscopy	6	3
Soft X-ray Spectroscopy	3	1
Hard X-ray Spectroscopy	9	5
Optics/Calibration/Metrology	4	2
SCATTERING	31	22
Hard X-ray Diffraction	11	6
Macromol. Crystallography	10	5
Hard X-ray Scattering	7	8
Soft X-ray Scattering	3	3
Imaging	9	8
Hard X-ray Imaging	5	6
Soft X-ray Imaging	2	0
Infrared Imaging	2	2
TOTAL	62	41

IF all of these are eventually built out, they would provide a world-class and well balanced portfolio and a smooth transition path for existing NSLS beamlines

41 = 6 Project + SRX-2 + 31 Type I + 3 Type II

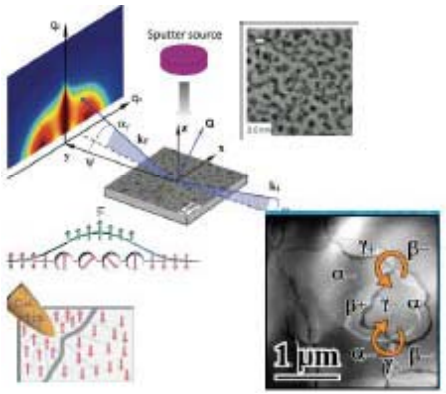
*Includes 3 Diagnostics/Instrumentation beamlines that provide only limited user support due to insufficient staffing

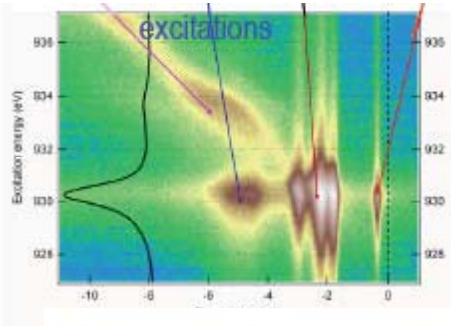
Funding for Additional Beamline Projects

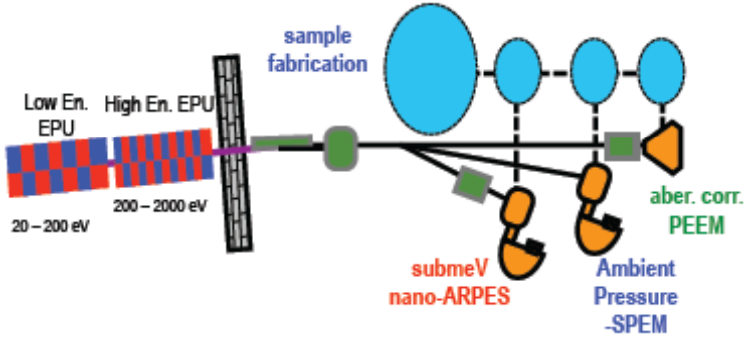
- Discussions of funding for additional beamlines at NSLS-II have been pursued with DOE, NIH, and other funding agencies
- Beamline projects that received funding commitments:
  - NEXT: 6 ID beamlines (DOE/BES-MIE), $50-90M
  - NIH: 3 ID beamlines (NIH), $45M
  - Type II: 3 ID beamlines funded by external independent groups
- On-going discussions:
  - NxtGen: 3PW/BM/IR beamlines (DOE/BES), number of beamlines TBD
  - NEXT-II: 5-6 ID beamlines (DOE/BES-MIE), to follow NEXT project
  - DOE/BER
  - DOE/NNSA
  - NSF

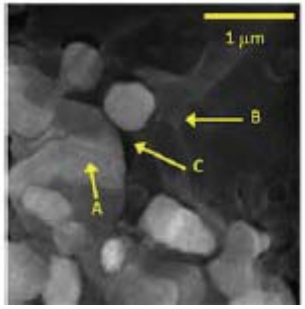
NEXT Beamlines Project

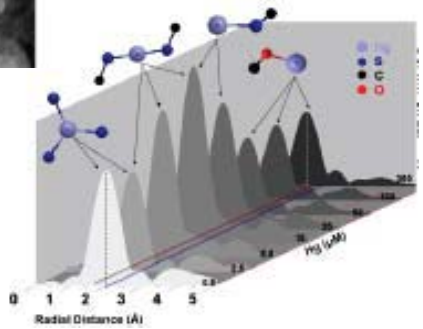
ESM -- Electron Spectro-Microscopy
FXI -- Full-field X-ray Imaging from µm to nm
ISS -- Inner Shell Spectroscopy
ISR -- Integrated In-Situ & Resonant X-Ray Studies
SIX -- Soft Inelastic X-ray Scattering
SMI -- Soft Matter Interfaces

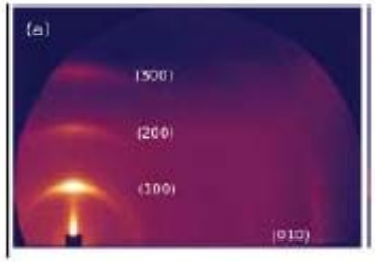












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BROOKHAVEN SCIENCE ASSOCIATES

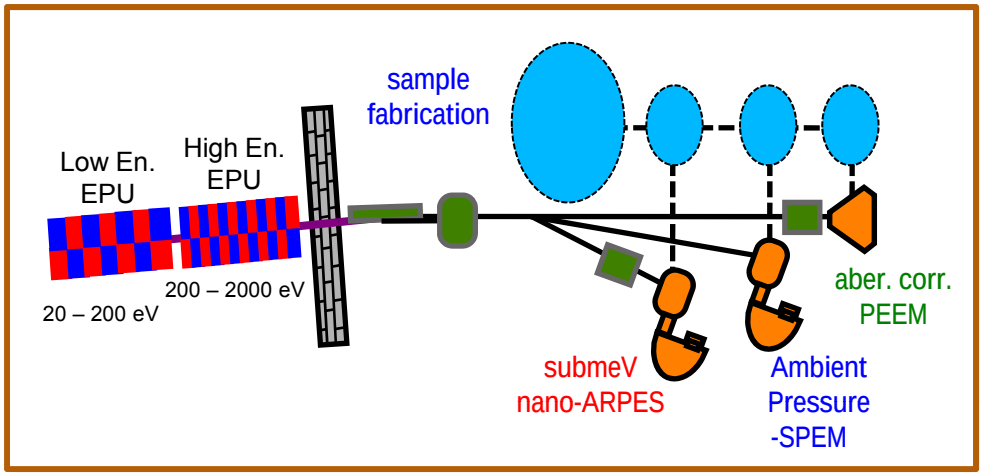
Photoemission-Microscopy Facility for Fundamental Studies of the Physics and Chemistry of Materials (ESM)

ESM at NSLS-II

- A suite of instruments to probe, characterize and design functional materials based on their electronic structure
- Overcoming traditional barriers: spatial averaging & ambient pressure
- Advancing photoemission to make contact with real devices and applications

Examples of Science Areas & Impact

- ARPES from ~ 300 nm samples (inside polycrystalline grains)
- SP-ARPES from multi-domain samples in zero applied field (sampling of single magnetic domains)
- Catalysis @ relevant partial pressures
- Chemical composition maps at ambient pressure
- Combinatorial investigation of multi-parameter samples
- Photoemission from real (micro-)devices (spintronics, fuel cells, etc.)



Schematic of proposed ESM beamline

Beamline Capabilities

TECHNIQUE(S): nano-ARPES, SP-ARPES, AP-SPEM, XPEEM

SOURCE: two EPUs

ENERGY RANGE / RESOLUTION: 20 – 2000 eV
< 1 meV to 70 eV (0.2 meV @ 20 eV)
< 10 meV to 1000 eV
< 100 meV to 2000 eV

FLUX: > 10^{12} ph/sec @ 10000 resolving power

SPATIAL RESOLUTION: ~200x300 nm (KB), ~50 nm (ZP)

U.S. DEPARTMENT OF ENERGY

Spokesperson: Elio Vescovo, Brookhaven National Laboratory

BROOKHAVEN NATIONAL LABORATORY
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Full field x-ray imaging from micron to nanometer scales (FXI)

FXI at NSLS-II

- Full-field configuration will enable 2D and 3D dynamic imaging of centimeter-scale samples with micron resolution
- Transmission x-ray microscope (TXM) will achieve high-speed imaging with 30 nm resolution
- Large user community serving national needs and addressing fundamental issues across many fields

Examples of Science Areas & Impact

- ENERGY: Real-time imaging 3D imaging of solid oxide fuels, biofuels, and energy storage materials under real operating conditions
- MATERIALS SCIENCE & ENGINEERING: In situ imaging of functional nano-materials and materials in extreme environments
- BIOLOGY & BIOMIMETICS: Deriving inspiration from nature, such as structural biological materials or internal flows in insects, for novel engineering solutions
- PALEONTOLOGY: Unlocking ancient secrets in rare or fragile fossils

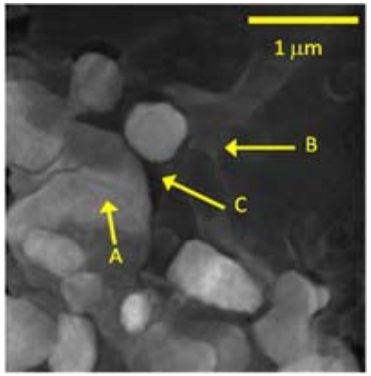
Beamline Capabilities

TECHNIQUE(S): full-field imaging; transmission x-ray microscopy (TXM)

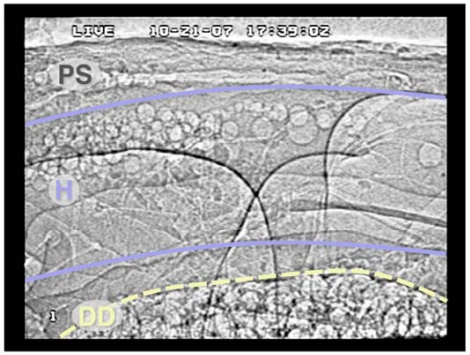
SOURCE: superconducting wiggler

ENERGY RANGE: 5-60 keV (TXM: 5-11 keV)

SPATIAL RESOLUTION: ~1–5 μm (full-field); 30 nm (TXM)



Tomographically reconstructed 3D volumetric data of a Ni-YSZ cermet sample. Enhanced contrast between the Ni and YSZ phases are achieved by tuning the incident x-ray energy just above the Ni K-edge. A: Ni phase (anode), B: YSZ phase (electrolyte), C: porous TPB between the anode and electrolyte. Wilson et. al. *J. Electrochemical Society*, 157 (6) B783-B792 (2010). The NSLS-II will enable a larger field of view and faster imaging.



Particle tracking in a section of the tubular heart of a grasshopper, demonstrating the feasibility of synchrotron PIV of biological flows. FXI at NSLS-II would enable visualization of the entire heart at once, elucidating how exactly flows are created for possible biomimetic microfluidic applications. W.-K. Lee & J.J. Socha., *BMC Physiology* 9:2 (2009).

U.S. DEPARTMENT OF ENERGY

Spokesperson: Jake Socha, Virginia Tech

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BROOKHAVEN SCIENCE ASSOCIATES

Integrated *In-Situ* and Resonant X-ray Studies Beamline (ISR)

Physics of Materials for the 21st Century

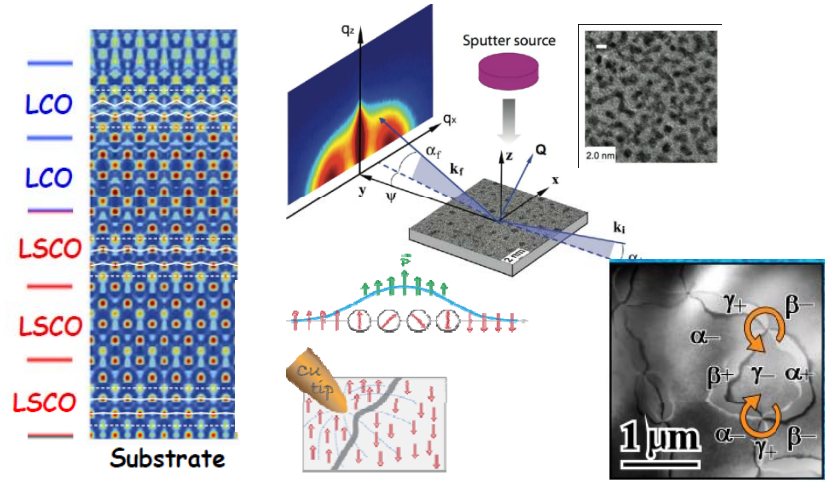
ISR at NSLS-II

Combination of NSLS-II brilliance with powerful capabilities for *integrated* materials physics studies unique in the world:

- Highly flexible range of sample environments
- Fully controllable incident polarization
- Micro/nanofocusing (100 nm) w/good focal distance
- Resonance studies with energies 2.1-23 keV
- Coherent studies (XPCS,CDI,XRIM)
- 12 T magnetic field

Examples of Science Areas & Impact

- CORRELATED ELECTRON MATERIALS: Combine magnetic/orbital-sensitive scattering with domain imaging and high magnetic fields.
- FUNCTIONAL SURFACES AND INTERFACES: Probe *in-situ* the atomic structure of surfaces and interfaces needed for energy conversion and information processing needs.
- SURFACE AND THIN-FILM GROWTH PROCESSES: Study in real time fundamental surface processes in PLD, MBE, ALD, sputter deposition and other techniques.



POWERFUL COMBINATION OF MATERIALS PHYSICS CAPABILITIES ENABLED BY ISR

Left: Sub-Angstrom resolution electron density map from CTR measurements of a $LaSrCuO_4$ epitaxial film showing interfacial superconductivity (Zhou *et al*. PNAS 2010).

Top: Real-time GISAXS patterns during first stages of WSI_2 film growth showing nanoparticle formation and corresponding TEM image (Zhou *et al*. PRB 2010).

Right and Bottom: In-situ imaging of evolving magnetic and orbital domains with 100 nm resolution - important for exploring the physics of magnetic wall motion controlled by electric field in magnets and multiferroics (T. Choi *et al*., Nature Materials 2010).

).

Beamline Capabilities

TECHNIQUE(S): RXS; Polarized XRD; GID; CTR; TXRF; GISAXS; *in-situ* XPCS; *in-situ* CDI; *in-situ* XRIM

SOURCE: 3m undulator in high-β straight section

ENERGY RANGE: 2.1-23 keV

POLARIZATION CONTROL: Dual phase plates

U.S. DEPARTMENT OF ENERGY

Spokesperson: Karl Ludwig, Boston University

BROOKHAVEN NATIONAL LABORATORY
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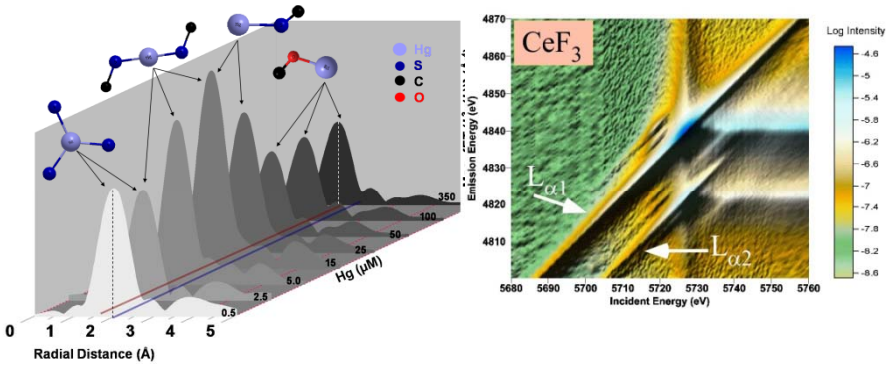
Inner Shell Spectroscopy (ISS)

ISS at NSLS-II

- XAS of samples with very low absorber concentration
- Resonant and non-resonant x-ray emission spectroscopy
- XAS with resolution below the natural core-hole lifetime
- Low energy absorption edges (below 1keV) using non-resonant inelastic scattering to measure x-ray energy loss spectroscopy

Examples of Science Areas & Impact

- MATERIALS DEVELOPMENT: Technologically relevant thin films and buried layers measured by XAS with high throughput
- ENVIRONMENTAL SCIENCE: Fate and transport of contaminants studied at environmentally relevant concentrations
- BIOCHEMISTRY: Time resolved XES of Cytochrome P450 intermediates in heme mediated alkane hydroxylations to follow heme oxidation, spin state, and ligation throughout the catalytic cycle
- ENERGY SCIENCE: Fields ranging from battery and fuel cell development to petroleum processing benefit by XELS measurements of soft x-ray edges using hard x-ray probe



Left: Fourier transformed Hg L_3 EXAFS data measured for Hg adsorbed to *S. oneidensis MR-1* as a function of Hg concentration ranging from 0.5 μM (a concentration that cannot be measured on a dipole source) to 0.4 mM (a simple experiment for a dipole source). At the environmentally relevant lowest concentrations, the binding environment of the Hg is quite different from the higher concentrations.

Right: A resonant XES study of the Ce Lα emission from CeF_3. We observe a strong splitting of the pre-edge emission at ~5719 eV incident energy. This yields insight into the *f*-orbital ground states of such systems which are unavailable by other inner-shell techniques.

Beamline Capabilities

TECHNIQUE(S): x-ray absorption spectroscopy, x-ray emission spectroscopy, x-ray energy loss spectroscopy

SOURCE: damping wiggler

ENERGY RANGE/RESOLUTION: 5–45 keV / 1-2x10^{-4} ΔE/E

SPATIAL RESOLUTION: unfocused beam, 500 μm (preliminary focus), 30 μm (secondary focus)

U.S. DEPARTMENT OF ENERGY

Spokesperson: Bruce Ravel, NIST

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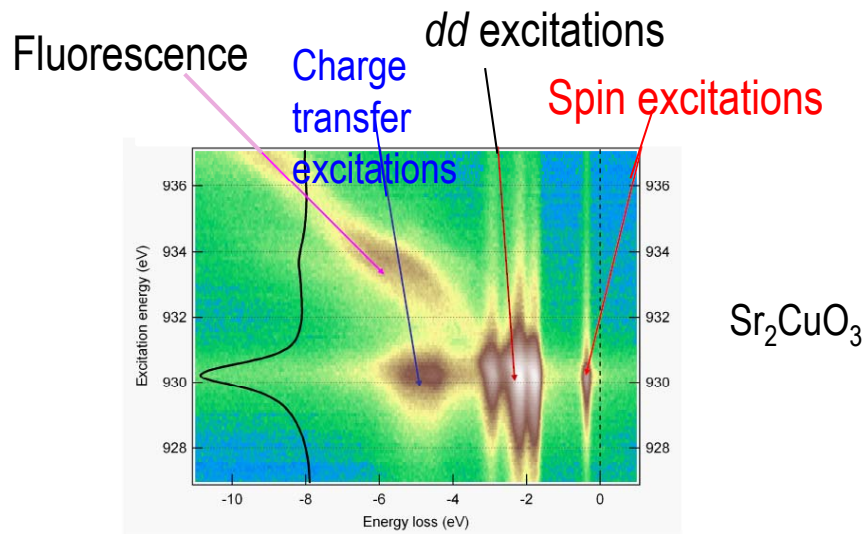
Soft Inelastic X-ray Scattering (SIX)

SIX at NSLS-II

- Will take advantage of the unique combination at NSLS-II of high brightness in the soft x-ray regime and ability for beamlines to go "long" to produce world-leading energy resolving power of 10^5 (factor of x10 better than anywhere else today)
- Will enable measurements of elementary excitations (magnons, phonons and orbitons) in condensed matter samples with extremely small volumes: surfaces, devices, nanoscaled systems *for the first time*

Examples of Science Areas & Impact

- SUPERCONDUCTIVITY: "Game changing" studies of electronic and lattice excitations in 3d transition metal oxides: "neutron scattering from 100 nm of material"; allows studies of excitations in devices and nanoscaled systems
- CATALYSIS: *In situ* studies of electronic structure of catalytic nanoparticles – facilitating rational design of next generation catalysts
- ENERGY STORAGE: *In situ* studies of Li-ion transport and electronic structure in next generation batteries



Excitation spectrum of a cuprate observed with soft RIXS. Data taken with 100 meV resolution. At NSLS-II this will be improved to an unprecedented 10 meV, allowing low energy excitations to be resolved in 3d transition metal compounds for the first time. (Data from J. Schlappa et al., unpublished)

Beamline Capabilities

TECHNIQUE(S): resonant inelastic x-ray scattering

SOURCE: elliptically polarized undulators

ENERGY RANGE: 50 eV – 1000 eV

ENERGY RESOLUTION: 10 meV

U.S. DEPARTMENT OF ENERGY

Spokesperson: Kevin Smith, Boston University

BROOKHAVEN NATIONAL LABORATORY
BROOKHAVEN SCIENCE ASSOCIATES

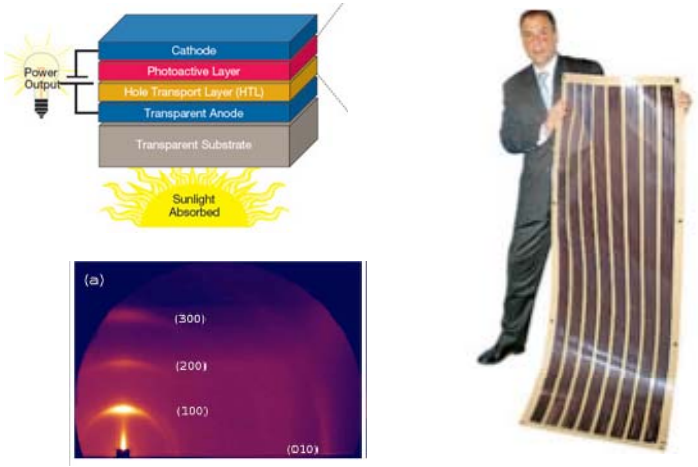
Soft Matter Interfaces (SMI)

SMI at NSLS-II

- Will enable in-situ studies of the structure of soft-matter interfaces using a variety of x-ray scattering methods
- Two different configurations will allow studies to be carried out at the solid/vapor, solid/liquid, liquid/vapor, liquid/solid and liquid/liquid interfaces
- The high brightness of NSLS-II will allow both very small x-ray beams and new opportunities for resonant studies in the tender x-ray regime

Examples of Science Areas & Impact

- ENERGY: To understand the microphase behavior and orientation of materials in thin film organic photovoltaic devices, a promising new class of energy materials
- ENERGY: To understand gas hydrate formation at the gas-water interface
- ENVIRONMENT: To improve our understanding of the extractant-mediated transfer of metal ions from an aqueous to an immiscible organic phase
- BIOMOLECULAR MATERIALS: To develop a fundamental understanding of self-assembly in order to create new materials with a range of architectural tailorability



(top) Organic photovoltaic (OPV) device configuration. (bottom) Diffraction pattern from OPV polymer materials. (right) Roll-to-roll prepared OPV sheet manufactured by Konarka with 4% efficiency. Research may to lead to 10% efficiency in the next 5-10 years.

Beamline Capabilities

TECHNIQUE(S): x-ray reflectivity, grazing incidence x-ray scattering, and anomalous/resonance techniques

SOURCE: undulator

ENERGY RANGE / RESOLUTION: 2-22 keV

SPOT SIZE: ~2 – 5 μm using compound refractive lenses

U.S. DEPARTMENT OF ENERGY

Spokesperson: Ben Ocko, Brookhaven National Laboratory

BROOKHAVEN NATIONAL LABORATORY
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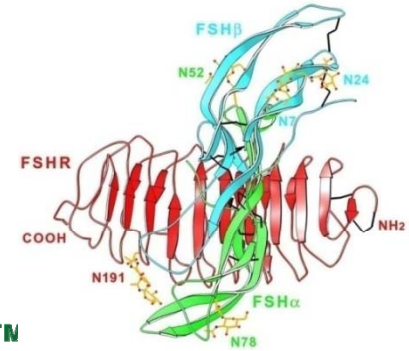
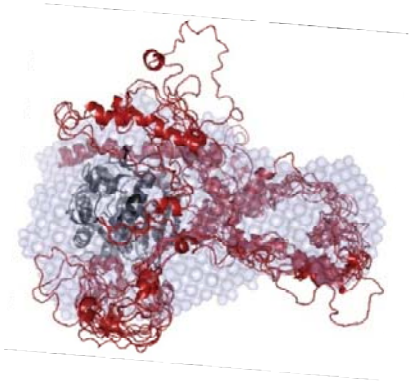
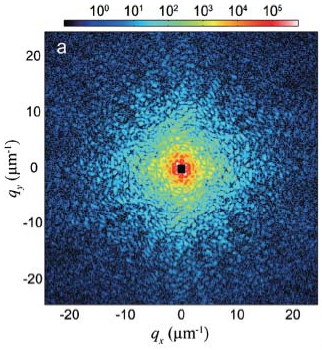
NIH Beamlines

- NIH Advisory Panel for Biomedical Beamlines at NSLS-II formed in May 2010, to advise NIH about beamline development at NSLS-II
- NSLS-II recommended 4 beamlines be supported by NIH as result of 2010 SAC review; NIH Advisory Panel met on Feb 24, and recommended to pursue 3 beamlines:
  - 2 MX beamlines: Frontier MX (FMX), Automated MX (AMX)
  - 1 scattering beamline: X-ray scattering for life sciences (LIX)
  - Imaging beamline has considerable potential at NSLS-II due to high brightness and small horizontal source size, but funding is insufficient







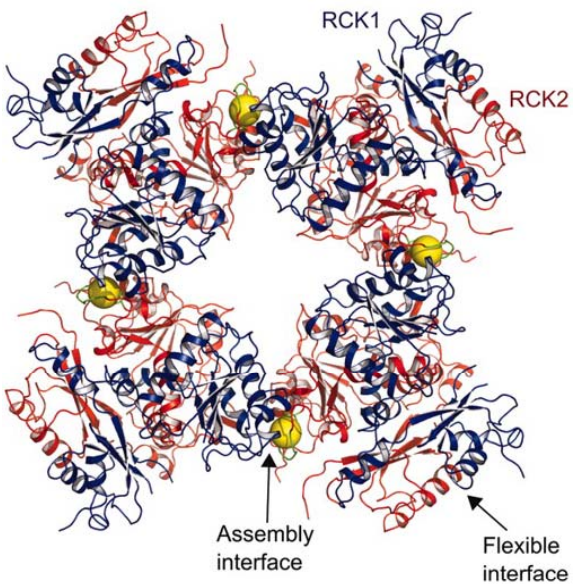
Flexible Access and Highly Automated Beamline for Macromolecular Crystallography (AMX)

AMX at NSLS-II

- Will provide structural biologists with ready access to an advanced facility for precise structure determinations at unprecedented rates
- Will optimally exploit unique source characteristics and deliver a very high flux in a suitably small focused beam
- Will be highly automated to support remote access and extensive experimental studies

Examples of Science Areas & Impact

- STRUCTURAL BIOLOGY: Atomic structures of large protein and nucleic acid complexes, including membrane proteins, are prerequisites to gaining insights into their function, and interactions, thus creating molecular movies
- BIOCHEMISTRY: Structural analysis of all intermediates in entire enzymatic cycles and pathways will expand our understanding of cellular and microbiological processes
- PHYSIOLOGY AND MEDICINE: Crystallographic studies of the interactions of drugs with their targets are essential in the development of improved and new pharmacologically effective compounds



Ribbon diagram of the gating ring of the human BK channel Ca-activation apparatus. This channel encodes negative feedback regulation of membrane voltage and Ca-signaling, which plays a central role in numerous physiological processes.

P.Yuan, MD Leonetti, AR Pico, Y Hsiung and Roderick MacKinnon, *Science 329, 182-6 (2010).*

Beamline Capabilities

TECHNIQUE: macromolecular crystallography

Source: canted U20 In-vacuum undulator

ENERGY RANGE / RESOLUTION: 5-20 keV; $\Delta E/E \sim 5\times10^{-4}$

SPATIAL RESOLUTION: beam size from 6x5 to 300 μm^2 (diffraction resolution to < 1 Å)

U.S. DEPARTMENT OF ENERGY

Spokesperson: Dieter Schneider, Brookhaven National Laboratory

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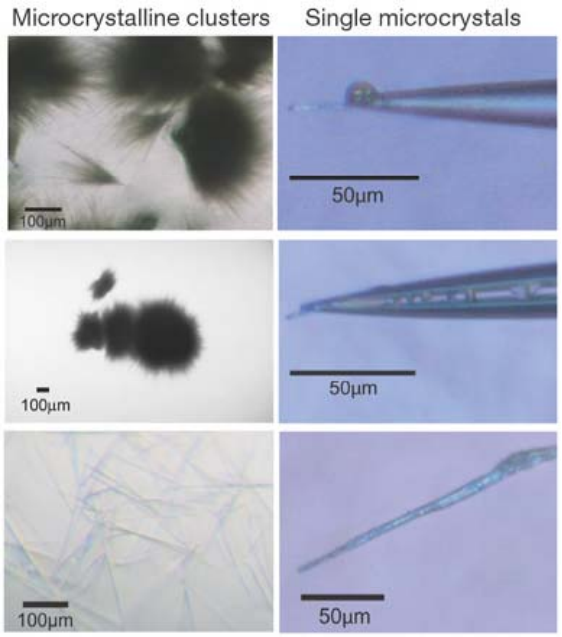
Frontier Macromolecular Crystallography (FMX)

FMX at NSLS-II

- This MX beamline will exploit the finest properties of NSLS-II and push the state of the art in x-ray optics.
- The tunable, one micron, variable divergence beam handles small crystals, and very large unit cells.
- Preserving beam coherence makes new experiments possible.
- Cryogenic automation at the state of the art provides convenience for users.

Examples of Science Areas & Impact

- STRUCTURAL BIOLOGY: The most interesting structures are often the most difficult. This beamline will push new limits in crystal size.
- BIOCHEMISTRY: Knowledge of intermediates in enzymatic pathways expands our understanding of cellular and microbiological processes.
- PHYSIOLOGY AND MEDICINE: Knowing how drugs interact with their targets is essential to development of improved and new pharmacologically effective compounds.



Crystals of β amyloid, which are always long and very thin

From: Sawaya MR, Sambashivan S, Nelson R, Ivanova MI, Sievers SA, Apostol MI, Thompson MJ, Balbirnie M, Wiltzius JJ, McFarlane HT, Madsen AØ, Riekel C, Eisenberg D. Nature 447, 453-7 (2007)

Beamline Capabilities

TECHNIQUE: macromolecular crystallography

SOURCE: canted U20 in-vacuum undulator

ENERGY RANGE / RESOLUTION: 5-20 keV; $\Delta E/E \sim 5\times10^{-4}$

BEAM SIZE: from 1x1 to 100x100 μm^2; diffraction resolution to 1 Å

U.S. DEPARTMENT OF ENERGY

Spokesperson: Robert Sweet, Brookhaven National Laboratory

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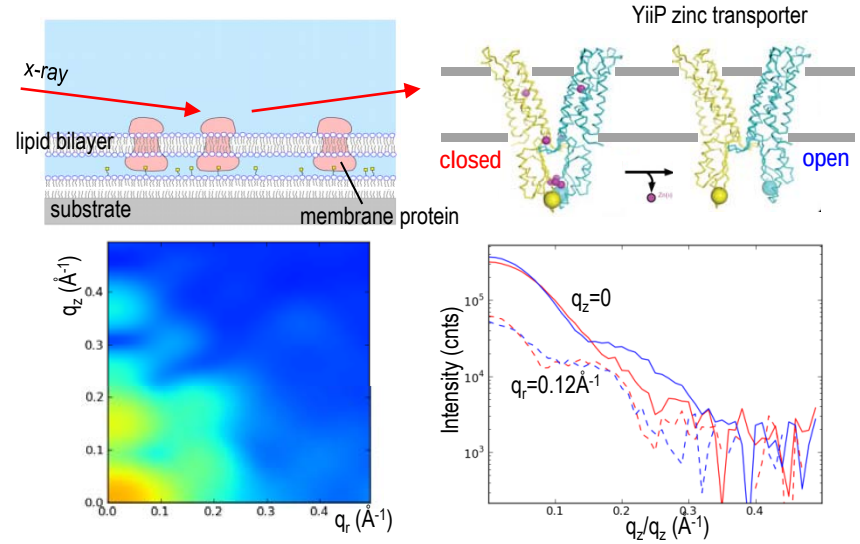
High Brilliance X-ray Scattering for Life Sciences (LiX)

LiX at NSLS-II

- Time-resolved x-ray scattering measurements of proteins and DNA/RNA in solution using flow cells on time scales down to 10μs
- Grazing incident scattering from 2D solutions of membrane proteins embedded in near-native membranes
- 1μm beam scanning probe imaging and tomography of biological tissues

Examples of Science Areas & Impact

- PROTEIN DYNAMICS: Help understand the dynamic processes of protein conformation change (e.g. folding) and enzymatic reaction
- MEMBRANE PROTEINS: Resolve the structure of membrane proteins at low resolution; Reveal how the structures of these proteins change in response to external stimuli
- TISSUE ENGINEERING: Help elucidate the relationship between the hierarchical structure in natural and engineered tissues and their functional properties.



A unique capability of the LiX beamline is to collect scattering data from membrane proteins embedded in near native membranes. This is the two-dimensional analogue of the solution scattering technique that has been very successful for soluble proteins in recent years. This figure shows simulated data from YiiP in DOPC bilayer in open and closed states. Simulated noise, based on estimated scattering cross-section, has been added in the line cuts (lower right).

Beamline Capabilities

TECHNIQUES: micro-beam, simultaneous small and wide angle x-ray, transmission and grazing incidence

SOURCE: undulator (U23)

ENERGY RANGE / RESOLUTION: 2-20keV @ 0.01%

Q RANGE: 0.002-3.0Å^{-1} @ 12keV

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Spokesperson: Lin Yang, Brookhaven National Laboratory

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NYSBC Microdiffraction Beamline (NYX)

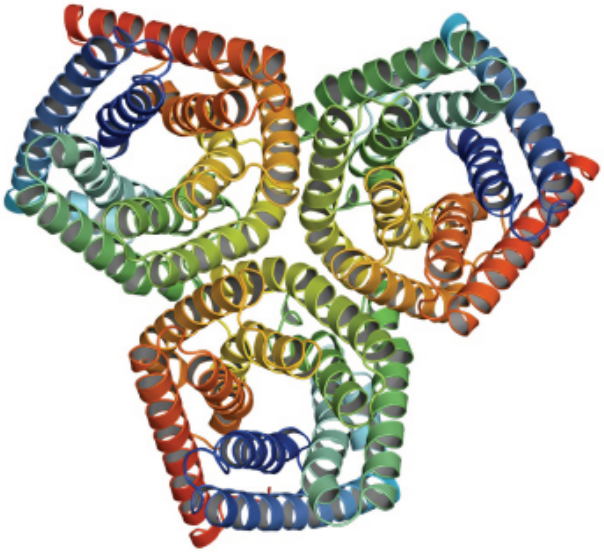
Opportunities for NYSBC Science at NSLS-II

- Diffraction from micron-sized crystals and rastered scans for optimized diffraction from larger crystals of challenging biological macromolecules and complexes
- Access to a broad range of resonant edges for anomalous diffraction (MAD and SAD) phasing, from U M_V (3.5 keV) to Se K (12.7 keV) to U L_{III} (17.2 keV)
- Optimization of anomalous scattering from high energy resolution for sharp transitions at resonant edges and lower energy for increased f '' with light elements (sulfur)

Example Science Areas and Impact

- MEMBRANE PROTEINS: Challenging structural problems with high relevance in neurobiology & metabolic disorders
- MACROMOLECULAR COMPLEXES: Protein-protein interactions in signaling complexes and protein-nucleic acid complexes in transcription or replication
- METHODS DEVELOPMENT: Supports efforts for methods to improve phase evaluation and enhance resolution

New York Structural Biology Center (NYSBC) hosts dozens of investigator groups at ten premier institutions



Homolog structure of the SLAC1 anion channel for closing stomata in leaves. Here the trimeric channel protein is shown as viewed from outside the membrane of a guard cell. Each protomer is colored spectrally from the amino-terminus (blue) to carboxy-terminus. Chen et al., *Nature* **467**,1074 (2010).

Beamline Capabilities

TECHNIQUE: macromolecular crystallography

Source: undulator on a low-β straight section

BEAM CROSS-SECTION: 5-50 μm

ENERGY RANGE: 3.5 – 17.5 keV

ENERGY RESOLUTION: $\Delta E/E \sim 5 \times 10^{-5}$

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Spokesperson: Wayne Hendrickson, Columbia University

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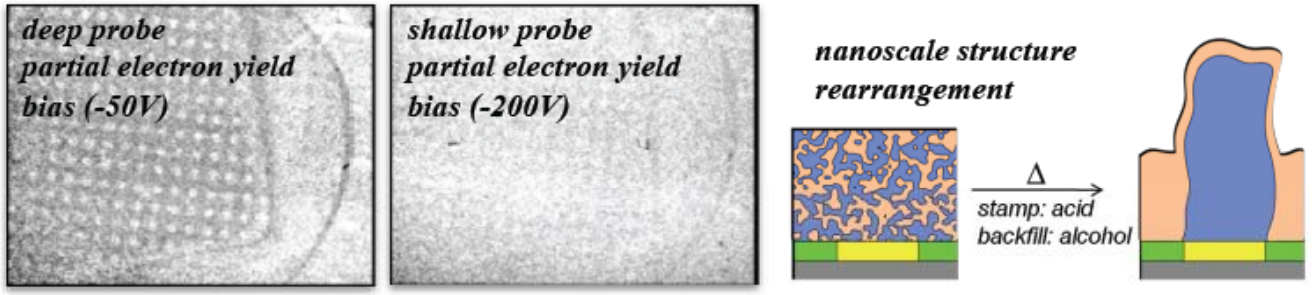
Spectroscopy Soft and Tender (SST)

SST at NSLS-II

- Structure function relationships in advanced materials, often at the nanoscale, for promoting innovation and enhancing US industrial competitiveness



NIST's NEXAFS microscope (NSLS U7A) reveals the structure of an OPV film structured "by design" in collaboration with University of Washington (Ginger). Lighter areas are fullerene-rich; contrast is generated by split π resonance of fullerene.*

- XPS Full Field Magnetic Projection Microscope: (3D) chemical mapping of the structure of nanomaterials and nanodevices at all points within their volume
- Large Area Full Field NEXAFS Microscope: highly efficient, depth selective, spectroscopic chemical and orientation maps of gradient samples, combinatorial arrays

Examples of Science Areas & Impact

- BIOMATERIALS: Structure and chemistry sensitive imaging to enable development of next generation of biomedical arrays using high-throughput screening
- ORGANIC PHOTOVOLTAICS: Precise measurements of materials composition and molecular orientation with sub-100 nm spatial resolution
- MICROELECTRONICS: Imaging structure and chemistry of buried layers and interfaces of real device architectures towards ultimate CMOS Scaling

Beamline(s) Capabilities

TECHNIQUE(S): 6 unique world class NEXAFS/XPS experimental stations (2 full field microscopes, 2 automated high-throughput, and 2 in-situ high pressure)

SOURCE: canted undulator sources; (1) soft x-rays (100 eV - 2.2 keV) and (2) tender x-rays (1 - 7.5 keV)

ENERGY RANGE / RESOLUTION: continuous 100 eV to 7.5 keV (at two common focal points) /10,000

SPATIAL RESOLUTION: XPS microscope, 1nm; NEXAFS microscope, 1um

Spokesperson: Daniel Fischer, NIST

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

Beamline for Materials Measurements (BMM)

BMM at NSLS-II

- Will enable materials studies of both local and long-range atomic structure
- High throughput, high quality x-ray absorption fine structure (XAFS) measurements for materials studies
- High throughput, high quality x-ray diffraction (XRD) measurements for materials studies
- Advanced spectroscopy techniques combining both XAFS and XRD

Examples of Science Areas & Impact

- MICROELECTRONICS: Strain engineering studies of electronic thin films and materials
- CATALYSIS AND CHEMICAL SCIENCES: High throughput XAFS studies of chemical reactions and catalysts
- PHASE TRANSITIONS AND ENVIRONMENTAL SCIENCE: Quantitative XRD and XAFS from same samples under identical environmental conditions

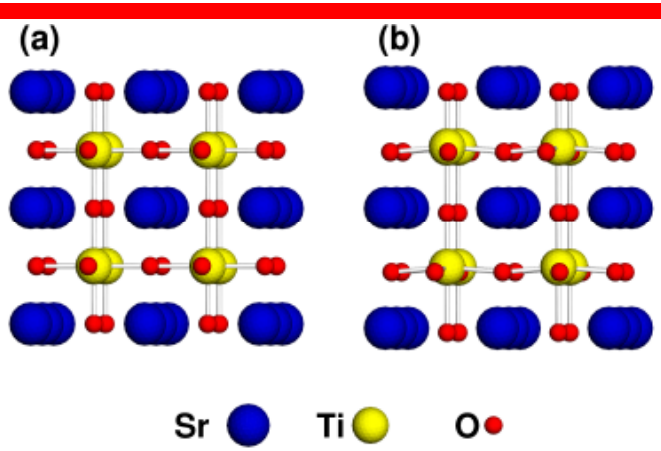


*Figure 3: (a) Structure of cubic $SrTiO_3$. (b) Structure of strained $SrTiO_3$ on Si(001) as calculated by density functional theory. The structure in (b) reveals both AFD and FE distortions and has been confirmed by both XAFS and XRD. Woicik et al., Phys. Rev. B **75**, Rapid Communications, 140103 (2007). Warusawithana et al., Science **324**, 367 (2009).*

Beamline Capabilities

TECHNIQUE(S): x-ray absorption fine structure (XAFS) and x-ray diffraction (XRD)

SOURCE: three-pole wiggler

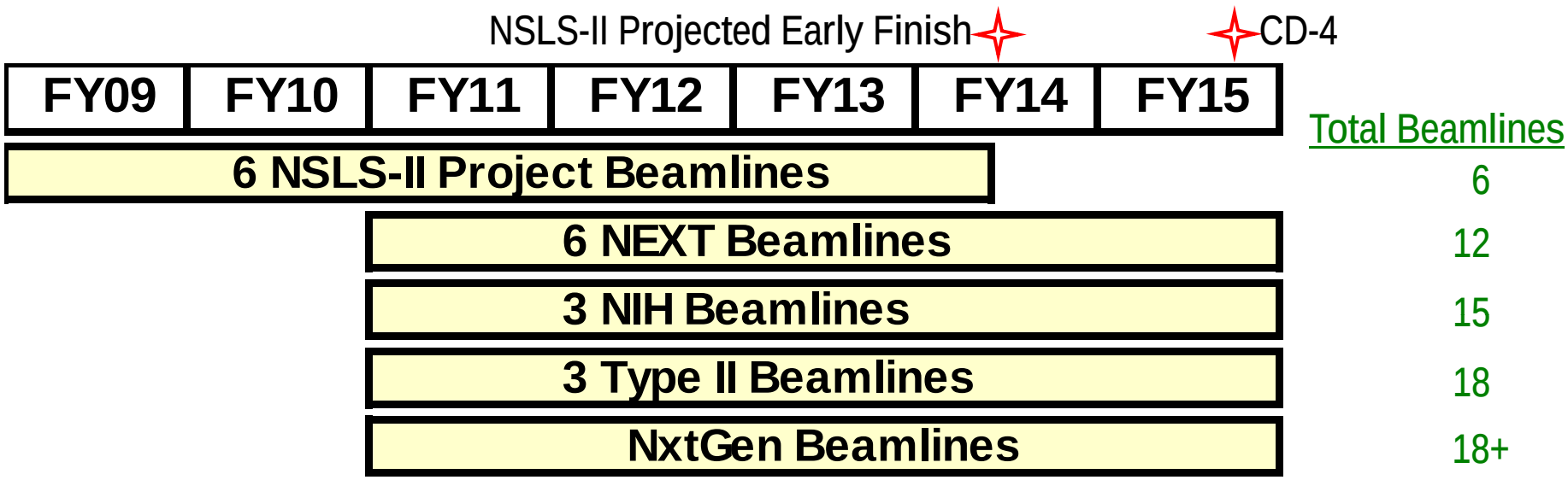
ENERGY RANGE / RESOLUTION: 4.9 keV – 30 keV / 1 eV – 5 eV

SPATIAL RESOLUTION: 100 μm x 100 μm

Spokesperson: Daniel Fischer, NIST

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

Overall Beamline Development Schedule



- Aggressive schedule is being planned to ramp up a good number of beamlines at the first year of NSLS-II operations, both for delivering enabling capabilities and for accommodating existing communities at NSLS
- NEXT and NIH funding are reasonably assured
- Funding for NxtGen (3PW/BM/IR) beamlines is under discussion with DOE

2011 Call for Beamline Development at NSLS-II

2011 Call for Beamline Development Proposals
National Synchrotron Light Source II

February 16, 2011

The National Synchrotron Light Source II (NSLS-II), currently under construction at the U.S. Department of Energy's Brookhaven National Laboratory on Long Island, NY, is pleased to announce the 2011 Call for Beamline Development Proposals for experimental facilities to be implemented at NSLS-II.

NSLS-II is a highly optimized third-generation synchrotron facility that will provide excellent

Critical Dates

Call for proposal issued
Thursday, February 17, 2011

Letter of Intent due
Monday, March 28, 2011

Beamline proposal due
Monday, June 6, 2011

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Photon Sciences User Access Policy

- Evolve User Access Policy (UAP) to NSLS-II:
  - First draft of new UAP developed and reviewed by SAC in 2010, to be finalized in 2011
  - Includes general user, partner user, and long-term general user access modes to allow flexibility and encourage community involvements
  - SAC review in Aug. 2010 made important recommend-ations to improve flexibility in UAP

- User Access Policy Taskforce established
  - Review SAC comments and concerns
  - Solicit and consider stakeholder/community input
  - Identify specific issues and make recommendations
  - Draft a revised UAP
- Taskforce chaired by Tony Lanzirotti (UEC Chair), include members of the user community and facility staff with broad representation of different background and research interests
  - Taskforce discussed with various stakeholders, and held Town Meeting on March 15 to solicit additional community input
  - New draft UAP includes GU, PU, and staff access, with minimum 50% GU access
  - New draft UAP (Apr 2011) reviewed by SAC Apr. 4-5, 2011

NSLS-II User Access Policy (draft Apr 2011)

- Three modes of scientific user access:
  - General User (GU) access (min. 50%)
  - Partner User (PU) access (up to 30%)
  - Beamline staff access (up to 20%)

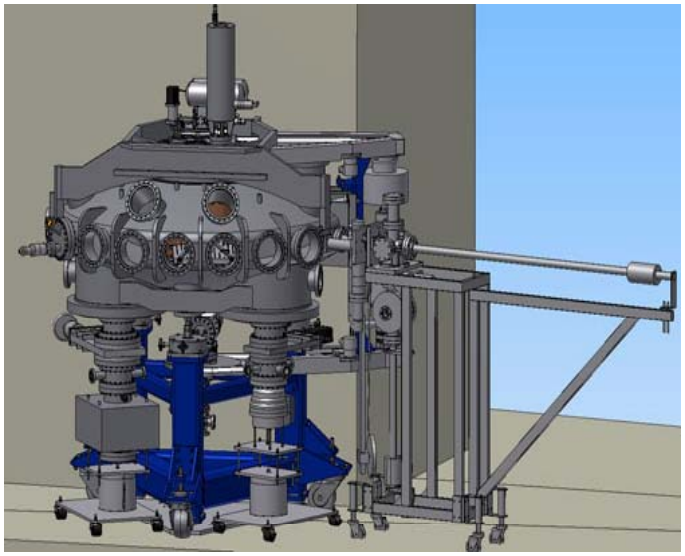
- General User (GU) Proposal
  - Valid for up to 2 years
  - May request multi-cycle status, remote access, or mail-in access
- Partner User (PU) Proposal
  - Must indicate PU contributions to enhance capabilities or contribute to operations
  - Each PU proposal may request up to 30% of the available user beam time per run cycle
  - Valid for up to 3 years
- Examples of PU Contributions:
  - contributing a sophisticated endstation
  - contributing staff & equipment to provide user support for a given program
  - design and construction or operation of a beamline

Proposal Evaluation and Review

- Beam time proposals are peer reviewed by Proposal Review Panels (PRPs) through a central review process managed by PS
- Evaluation Criteria:
  - Scientific and/or technical innovation and originality
  - Scientific, technical and/or industrial importance
  - Education and/or outreach importance
  - Capability of the proposal group and quality of past performance based on track record (e.g., publications, patents, or corporate impact statements)
  - Experimental plan and technical feasibility
- In addition to being reviewed and rated by PRPs, PU proposals will also be reviewed by the SAC, for the potential of the PU proposal to have a positive impact on the overall scientific program, such as:
  - contributing to the development of technical capabilities at the beamline
  - providing technical assistance and support for use of a sophisticated endstation that the PU is willing to let general users access

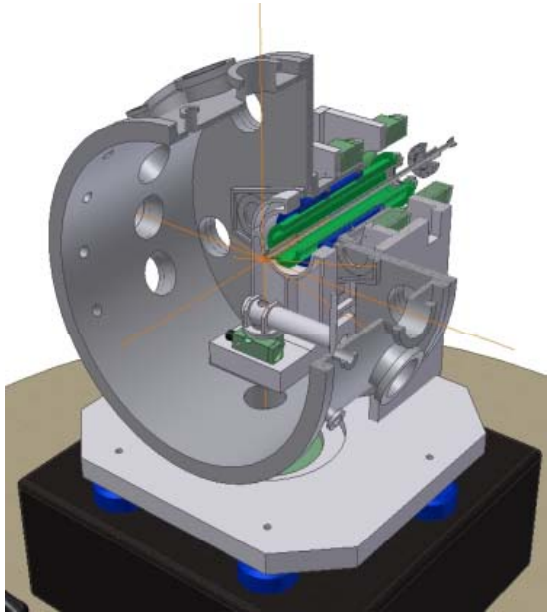
GU Proposal with Multi-Cycle Status

- GU proposal may request *multi-cycle status* for guaranteed access each run cycle to a beamline or beamlines over the life time of the proposal
- PRPs may grant multi-cycle status to GU proposals requesting it if they have a high overall rating and meet one or more of the following criteria:
  - Development of a new experimental capability or a new scientific application that clearly requires assured access in multiple run cycles in order to achieve results
  - Clearly demonstrated scientific or technical needs for assured access for a single experiment over multiple run cycles



Partner User Agreement

- For approved PU proposals, rights and obligations of the PU will be negotiated on a case-by-case basis and written out in the PU Agreement
- PU Agreement will define the responsibilities of the PU in developing and/or operating the beamline and the governance model for how the PU participates in decisions regarding the stewardship of the beamline, including decision-making process on future beamline upgrades and improvements



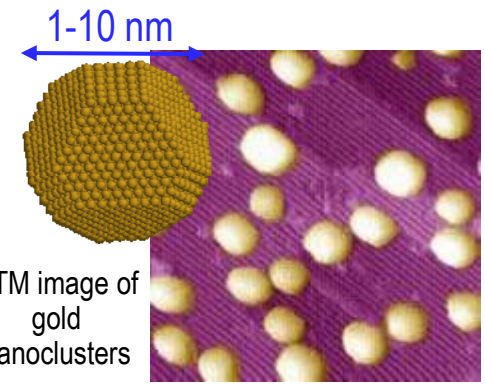
- Recognizing the need for early commitment of investments by prospective PUs in the development of a beamline, PS plans to work with prospective PUs and encourage them to submit PU proposals well before start of operations
- Detailed procedure in the pre-operation period is being developed

Science Village

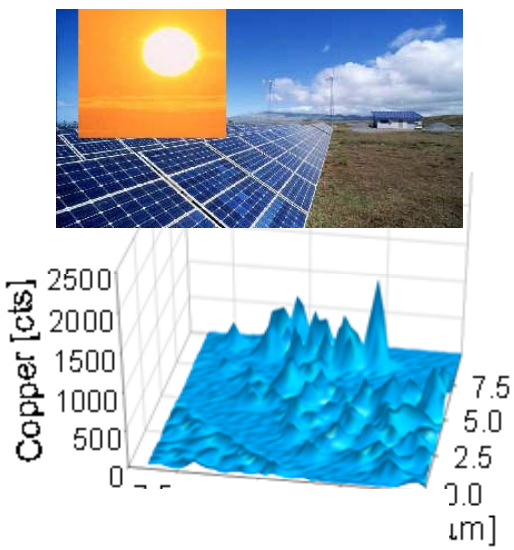
- Traditionally, facilities tend to foster using the facilities of a single beamline and interacting primarily with the staff and users of that beamline
- "Science Village" concept:
  - Facilitate access to multiple capabilities throughout the facility
  - Encourage broader interaction between users and communities throughout the facility
- NSLS-II will support this in several ways:
  - Beam time proposal, allocation, and usage will support access to multiple beamlines in a single visit if required by experiment
  - Beamlines that are likely to have overlapping user communities will be located near to one another to the maximum extent allowed by physical constraints
  - Laboratories in LOBs will be shared among beamlines and will include some ancillary instruments
  - User office space in LOBs will be "open plan" to encourage interaction
  - LOBs will each contain several "interaction areas" to facilitate contact and discussions among users and staff

HXN and SRX: Structural & Chemical Imaging of Nanoscale Heterogeneous Materials

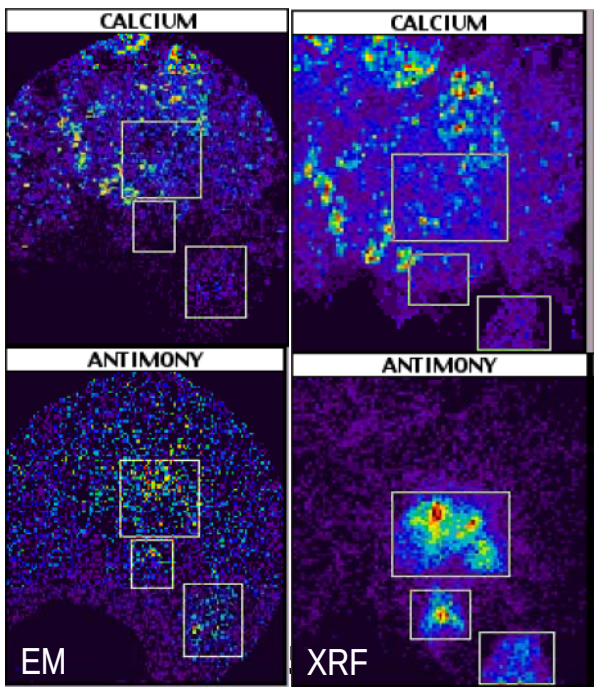
- Structural and chemical imaging at nm-scale resolution in broad areas of science from nano-materials and technology to biology and environmental sciences
- X-ray nanoprobe complements existing electron microscopy capabilities with higher elemental sensitivity, and allow nanoscale *in-situ* imaging in variety of realistic environmental conditions

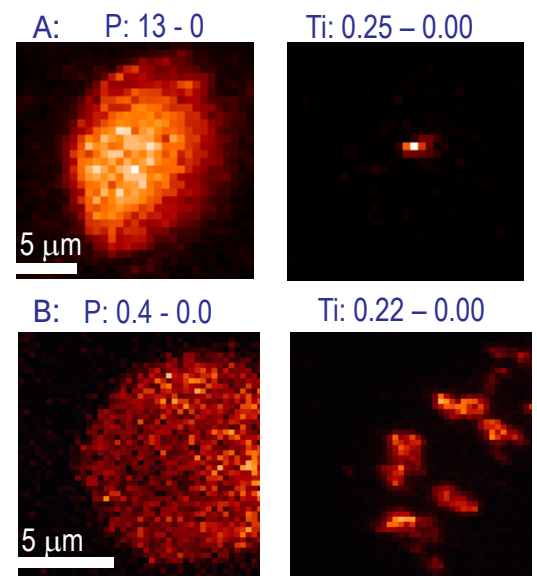


X-ray nanoprobe allows in-situ imaging of structure and chemical state of single nanoparticles in realistic environment



Nanoscale imaging of defects distribution and chemical state in solar cell materials leads to higher efficiency devices

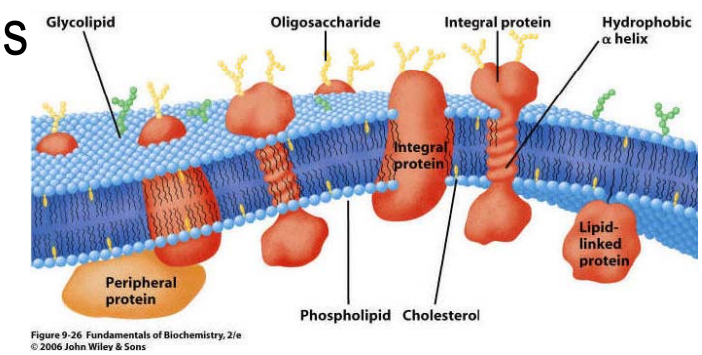


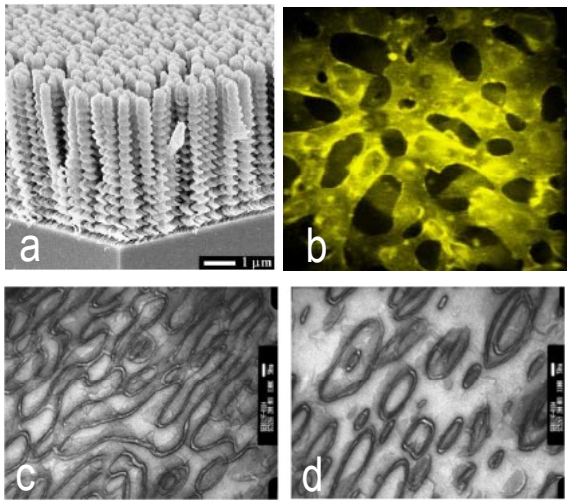


XRF elemental map of TiO_2 nanoparticles distribution in biological cells

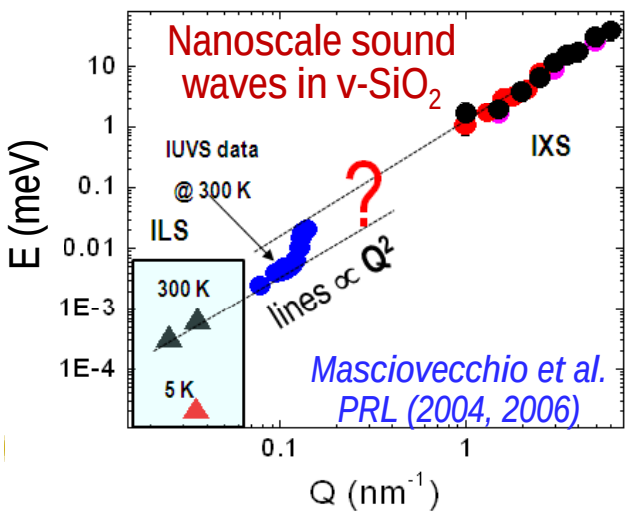
IXS and CHX: Dynamics of Nanoscale Inhomogeneities in Disordered Systems

- Strong scientific interest in studying elastic properties and collective atomic motions due to naturally occurring nanoscale inhomogeneities in disordered condensed matter and biological systems
- Example: CHX enables study of elastically connected membrane protein conformational dynamics at ~ 10's nm





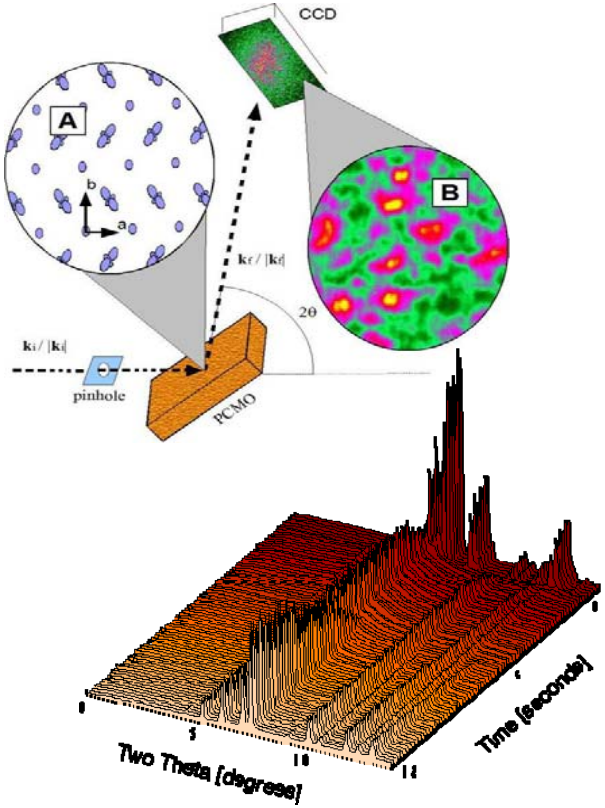
(a) Porous silicon; (b) bicontinuous micro-structure formed by interfacial colloidal jamming; (c-d) sponge phase in polymer blend

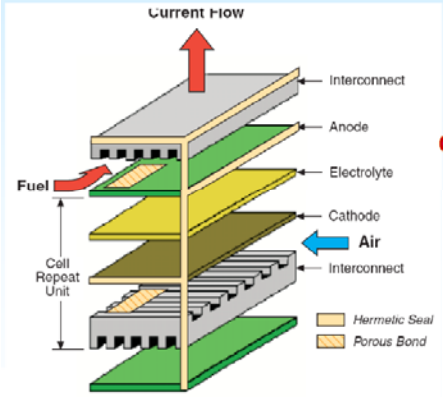


- Example: Propagation of acoustic waves is controlled by local density and elastic constants, which are affected by inhomogeneities
  - Crossover at given Q corresponds to characteristic length scale of static density fluctuations
  - IXS aims to to provide critical knowledge on the dynamics in systems with ~nm inhomogeneities

CSX: Molecular/Charge/Orbital/Spin Orders in Materials
XPD: Structural Science in Real Time & Real Conditions

- Order/disorder in systems with competing degrees-of-freedom by using coherent scattering to image domain interactions in strongly correlated materials
- Studies of molecular orientation/order in soft matter systems by using polarization/coherence
- Multi-length structure solution becomes possible on transient phases or in complex engineering environments (in toxic gases, under stress, inside a casing, in a pressure cell)
- Structure and kinetics of complex materials under real conditions, *e.g.*, cathode degradation, catalytic activity and cycling failure in a planar solid oxide fuel cell at 600-900° C, using time-resolved XRD





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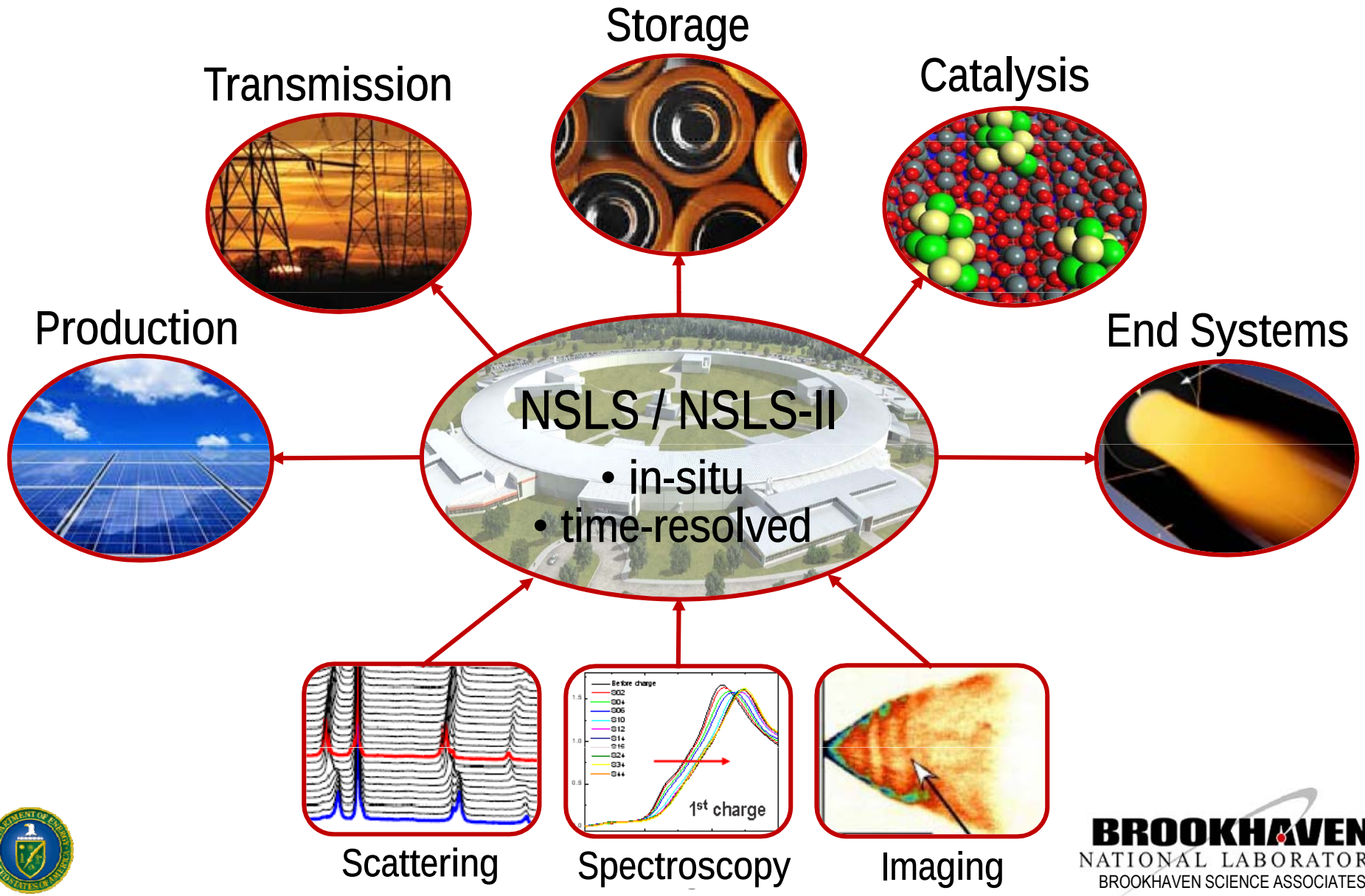
Example: Energy Research at NSLS/NSLS-II



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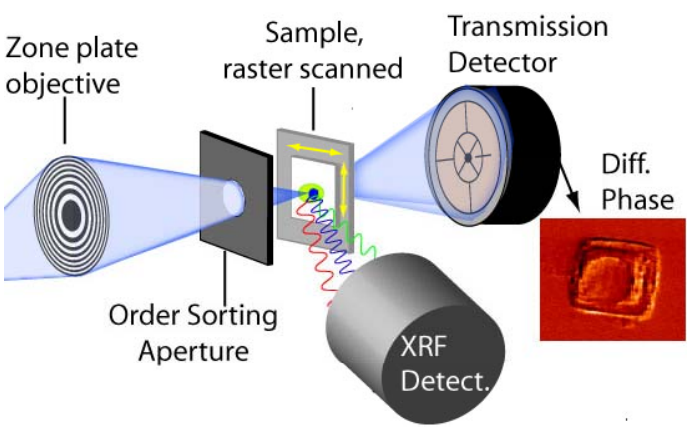
NSLS-II Data Rates & Data Volume

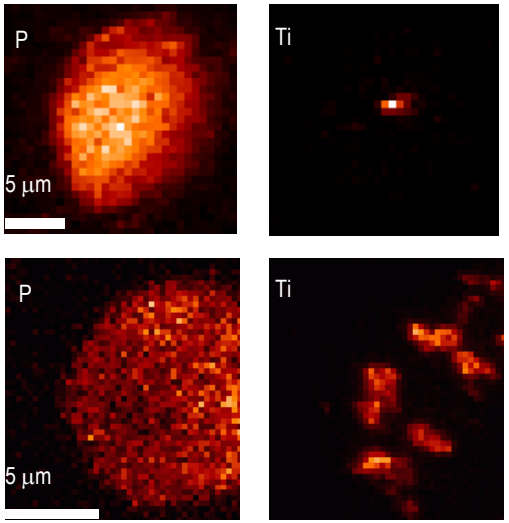
Experiments at NSLS-II	Approved Beamlines	Typical Dataset (TB)	Daily Data Rate (TB)	Notes	Number of BLs	Total Daily Data Rate (TB)	Weekly Archive (TB)
Coherent Scattering SAXS/WAXS (2x 6M 16-bit @ 1 kHz x6000)	CHX, CDI, CSX	1	2	12 hrs/dataset limited by signal at high Q	3	6	36
X-ray fluorescence microscopy (400x 12-bit 1K A/D @ 10 kHz x10^9	SRX, HXN, TES, XFM	4	3	Daily rate limited by counting time	4	12	72
High-speed x-ray tomography (2K x 2K 12-bit @ 4 kHz x3000)	FXI	0.015	4	300 s/dataset limited by data-bus rate	2	9	52
Macromolecular crystallography (6M 16-bit @ 10 Hz x360 3 λ's)	FMX, AMX, NYX, SM3	0.01	4	3-400 datasets /day limited by robotics	4	16	96
High-throughput u-XRD (6M 16-bit @ 10 Hz 100x100 pxl)	MXD, XPD, IXD	0.1	3	20 min./datasets 30 datasets/day	3	9	54
Time-resolved SAXS/WAXS/GISAXS (2x 6M 16-bit @ 10 Hz x100)	SMI, LIX, ABS, ISR, MPP, CMS	0.002	9	20 sec / dataset limited by robotics	6	52	311
Estimated NSLS-II Total					**22**	**103**	**621**

- Assuming maximum data rate, only limited by data acquisition hardware; Sample issues and duty cycles are ignored
- Modern high-thruput beamlines already approach above data rates (e.g. APS 2BM)
- Such data volume could be handled by local beamline system (e.g. local Raid Array)

Scanning XRF Microscopy & Tomography

- X-ray fluorescence microscopy offers high elemental sensitivity (<10^{-21}gm at NSLS-II), easy quantification, chemical state mapping, & 3D tomographic imaging;
- Optimized experiment on a 10 μm biological multi-cell complex at 10 nm resolution may make use of a 400 element fluorescence detector array that covers 30% of 4π solid-angle;
- Each detector element gives rise an energy spectrum which is digitalized to 1024 channels at 12 bit dynamic range, with 0.1 ms dwell time;
- This leads to a peak data rate of 400x1024x 12x10000 = 50 Gb/sec;
- Complete 3D dataset on the 10 μm cell complex at 10 nm resolution will consist of 1000x1000 x1000 pixels, leading to 4 TB per 3D dataset;
- Such 3D dataset may be collected in ~ 1.2 days.

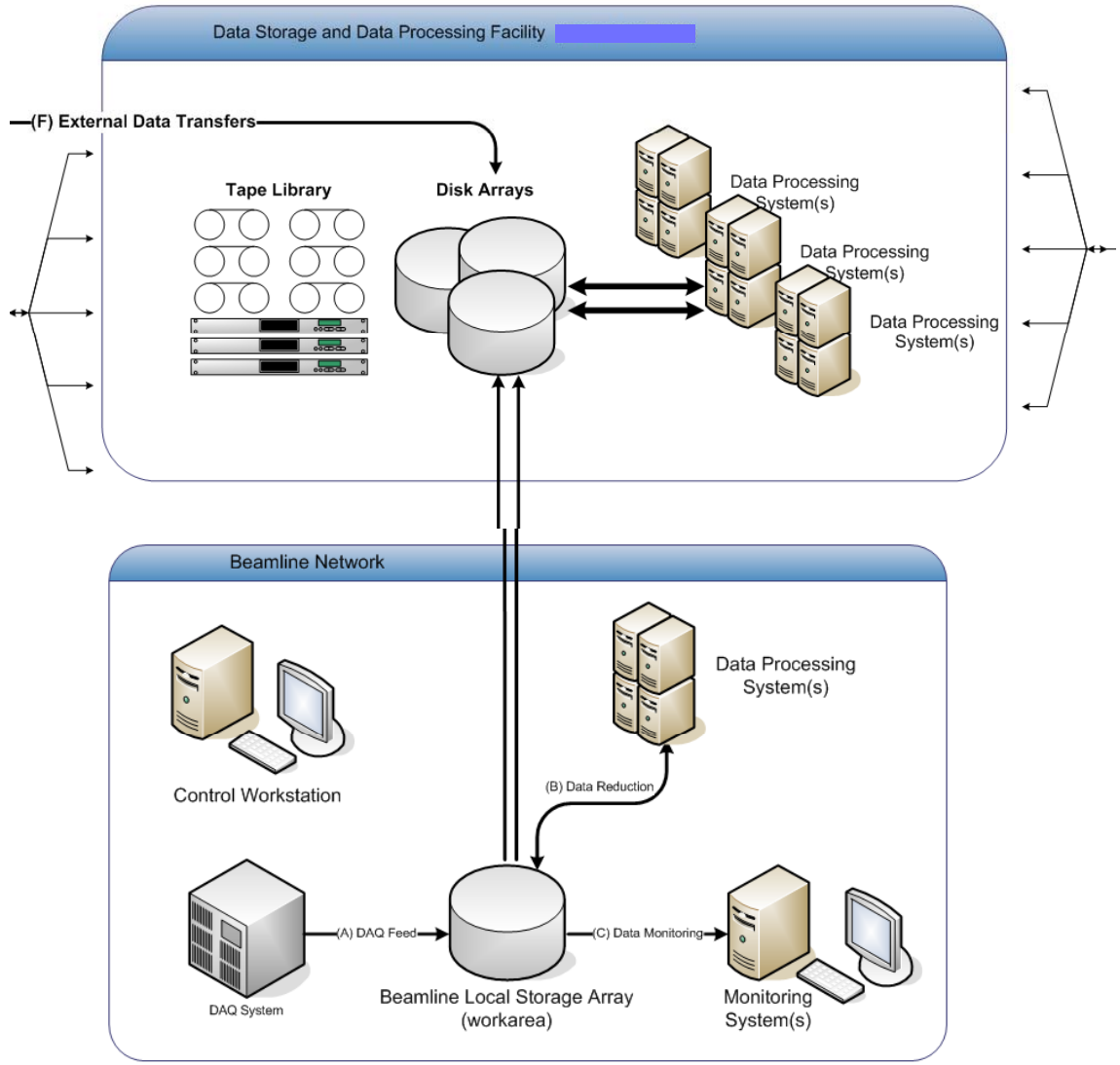




Scientific Computing at NSLS-II

- World-leading capabilities, coupled with modern detectors, expected to lead to high data rates and large data quantities for many types of experiments at NSLS-II
- Discussions on-going at BNL to plan in advance the appropriate computing facilities to adequately support user science experiments and enhance scientific productivity and impact at NSLS-II
- Collaborative LDRD proposal on prototype data management system in preparation

R. Popescu (BNL/PS)



Summary

- NSLS-II construction project (including 6 project BLs) progressing well
- Additional beamline projects getting started (NEXT, NIH, Type-II)
- Photon Sciences staff are excited to work with the community to define and pursue cutting-edge beamlines and science programs at NSLS-II
- Active, innovative, and engaged BNL/SBU community crucial to successful NSLS-II
- Looking forward to interesting discussions at this workshop