Beamline Capabilities Ramp-up at NSLS-II

Paul Zschack
Photon Division Director (Interim)
NSLS-II Industrial Research Workshop
April 8-9, 2014

NSLS-II Beamlines

Beamlines may be typically characterized into 3 broad categories, and 12 separate techniques.

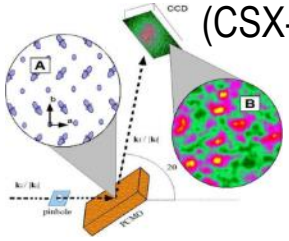
SPECTROSCOPY	SCATTERING	IMAGING
01 Low-Energy spectroscopy	05 Hard X-ray diffraction	09 Hard X-ray Imaging
02 Soft X-ray spectroscopy	06 Macromolecular X'tal	10 Soft X-ray Imaging
03 Hard X-ray spectroscopy	07 Hard X-ray scattering	11 Infrared Imaging
04 Optics/Calibration/Metrology	08 Soft X-ray scattering	12 Lithography

- Initial suite of beamlines at NSLS-II includes
  - Hard & Soft X-ray Spectroscopy (CSX-2, SRX)
  - Hard & Soft X-ray Scattering (CSX-1, CHX, IXS)
  - Hard X-ray Diffraction (XPD)
  - Hard & Soft X-ray Imaging (HXN, SRX, CSX-1)

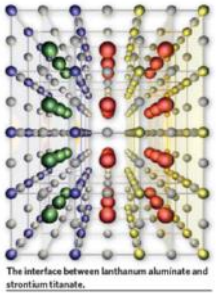
NSLS-II Project Beamlines

Commissioning Begins in 1QFY15

Coherent Soft X-ray Scattering (CSX-1)



World-leading coherent flux XPCS, CDI

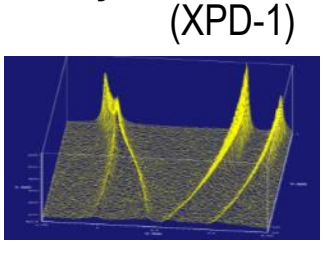


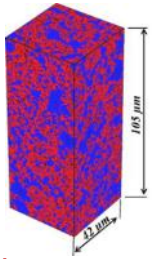
Fast Switching Polarization (CSX-2)

Resonant magnetic scattering, spectroscopy, XMCD

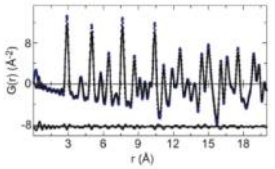
Imaging & dynamics in strongly correlated and magnetic materials

X-ray Powder Diffraction (XPD-1)





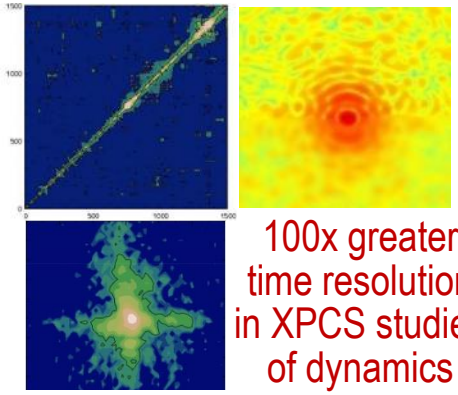
Provision for PDF (XPD-2)



Powder diffraction, scattering, PDF 30-80 keV

Time-resolved in-situ in-operando extreme conditions
Understanding complex nanostructured materials

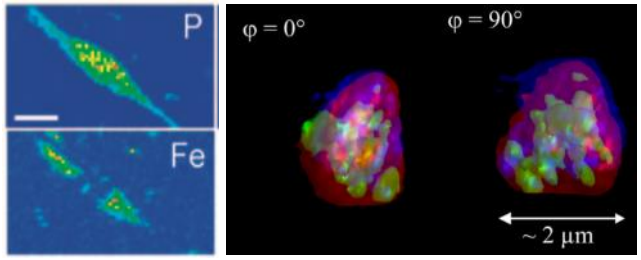
Coherent Hard X-ray Scattering (CHX)



100x greater time resolution in XPCS studies of dynamics

Non-equilibrium and heterogeneous dynamics in soft matter, at buried interfaces, biomaterials, glasses, driven systems

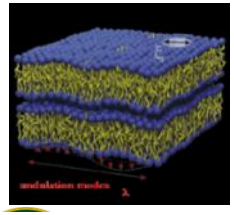
Sub-um Resolution X-ray Spectroscopy (SRX)

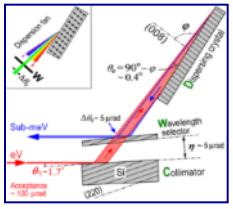


World-leading spectroscopy in sub-100 nm spot

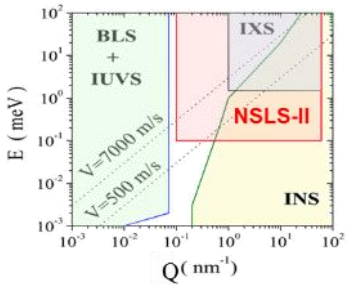
3D chemical imaging and speciation at the nanoscale

Inelastic X-ray Scattering (IXS)



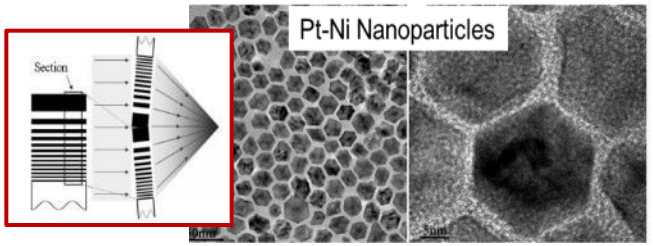


~1 meV baseline
~0.1 meV ultimate goal

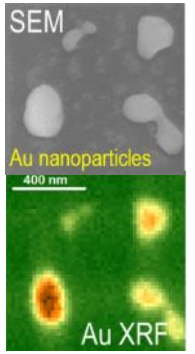


THz dynamics in liquid, glassy, and crystalline materials with nanoscale inhomogeneities

Hard X-ray Nanoprobe (HXN)



100m long beamline
~10 nm baseline
~1 nm ultimate goal



Nanoscale imaging with fluorescence and diffraction

NSLS-II Project Beamline Development Status

- Radiation enclosures installed on the NSLS-II experiment hall floor and outfitted with electrical and mechanical utilities.
- Beamline designs completed, fabrications nearly completed, and installations of major beamline components underway.
- Many installed components integrated into the beamline control systems.
- Personnel Protection System (PPS) and Equipment Protection System (EPS) now being deployed.
- Experimental endstation instrumentation and sample environments under development.
- Planning for start of beamline commissioning in September 2014

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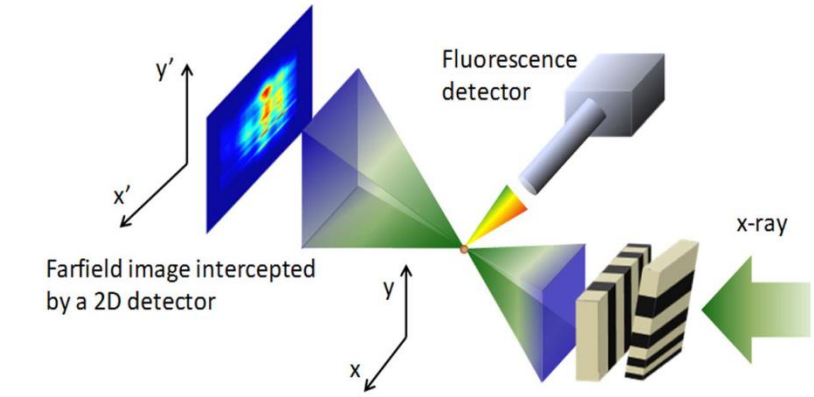
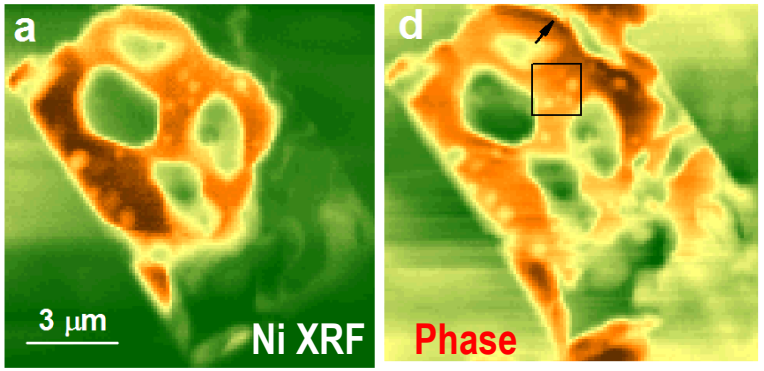
HXN Experimental Capabilities

- X-ray microscopy with high resolution and scientific flexibility:
  - 10 nm using MLLs (high resolution)
  - 30 nm using ZP (scientific flexibility)
- Simultaneous imaging of 2 or more techniques:
  - X-ray fluorescence imaging
  - X-ray diffraction microscopy
  - Differential phase contrast imaging
  - Absorption contrast imaging
  - Small-angle scattering
  - Transmission or Bragg ptychography
- Specimen Temperature regulation

Scientific Focus:
Materials science, environmental science, biology

World-leading ~1-10 nm nanoprobe for scanning fluorescence & diffraction imaging



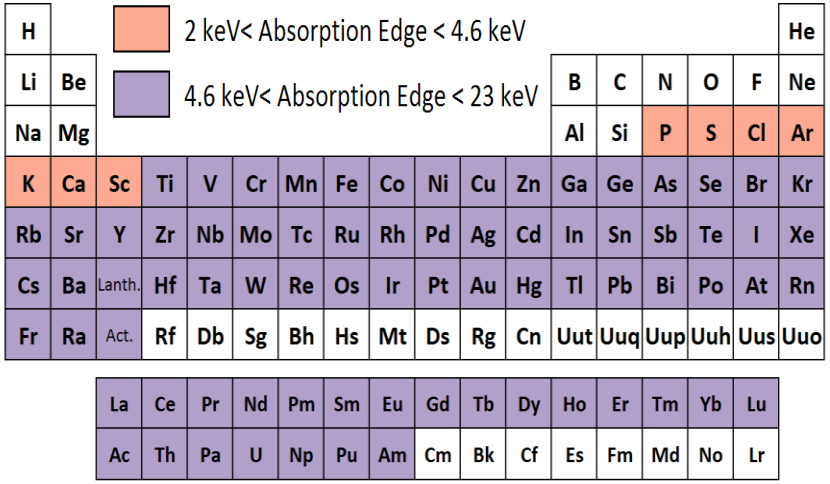


Simultaneous XRF and DPC using MLLs Yan et. al. Nature Sci. Reports 3, 1307(2013)

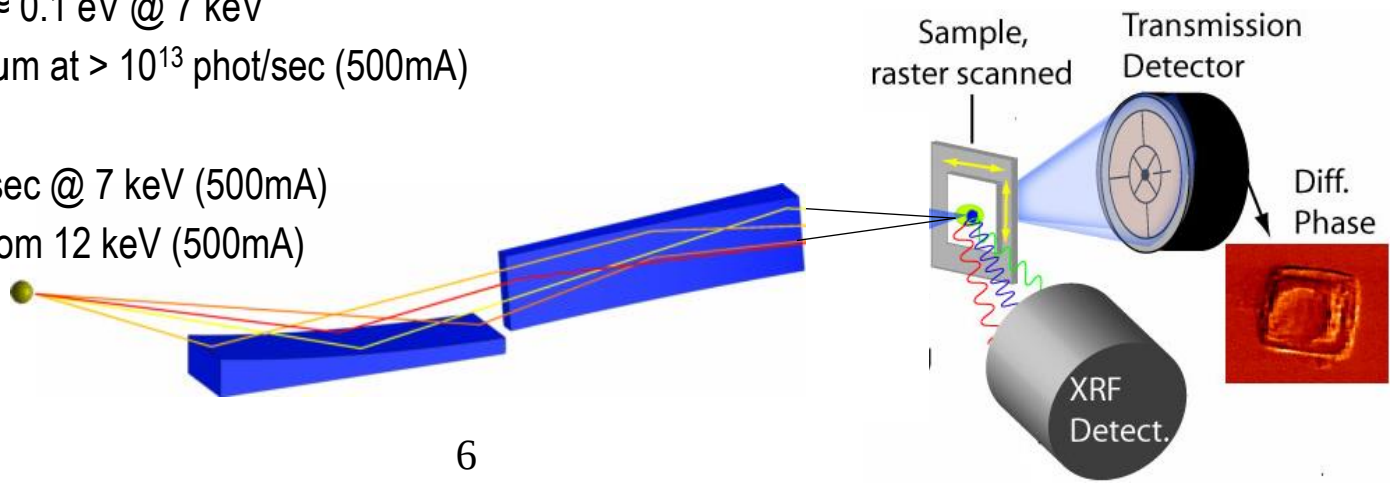
Submicron Resolution X-ray Spectroscopy (SRX)

Scientific Focus:

- Environmental science , life & biological science, material sciences, energy research, geosciences, and planetary sciences
- Spectroscopy with unprecedented high spatial resolution
- Imaging with absorption, fluorescence, or phase contrast
- Fluorescence trace element mapping & spectromicroscopy
- X-ray microdiffraction
- Fluorescence tomography



- ***Source***: In vacuum undulator, λ = 21 mm, L = 1.5m
- ***Energy range:*** 4.65 keV ≤ E ≤ 25 keV
- ***Energy resolution:*** ΔE ≈ 1.5-2.5 eV @ 12 keV
  Δ E ≈ 0.8 eV @ 7 keV
  (in collimating mode) Δ E ≈ 0.1 eV @ 7 keV
- High flux focus spot ≈ 0.5 µm at > 10^{13} phot/sec (500mA)
- High resolution focus spot:
  ≈ 70 nm at 10^{11}-10^{12} phot/sec @ 7 keV (500mA)
  ≈ 30 nm at 10^{11} phot/sec from 12 keV (500mA)



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X-ray Powder Diffraction Beamline (XPD)

Scientific Focus:

in situ or *in operando* studies with varying temperature, pressure, magnetic/electric/stress field, chemical environment, etc…

Hydrogen storage, CO2 sequestration, advanced structural ceramics, catalysis, and materials processing.

TECHNIQUES: medium angle scattering, tomography

Source: 1.8T Damping Wiggler – Ec = 11keV

ENERGY RANGE : 30 – 70 keV

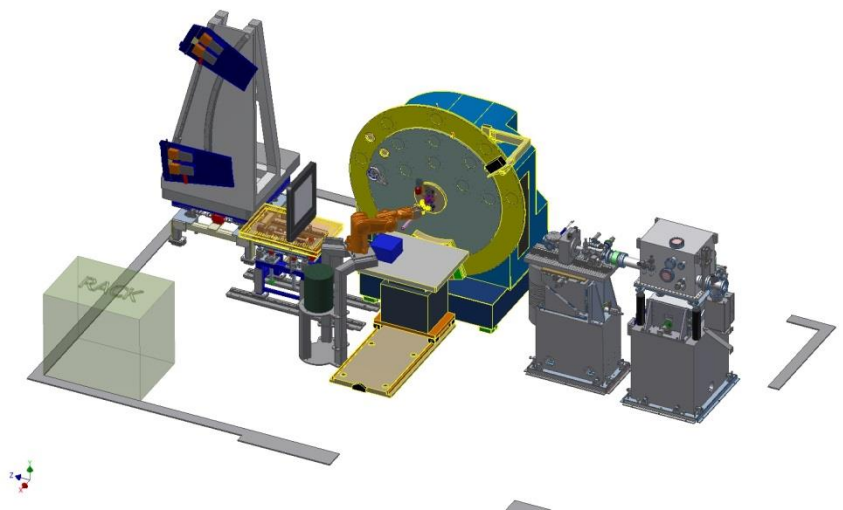
ENERGY RESOLUTION: $2x10^{-4}$ $\Delta E/E$

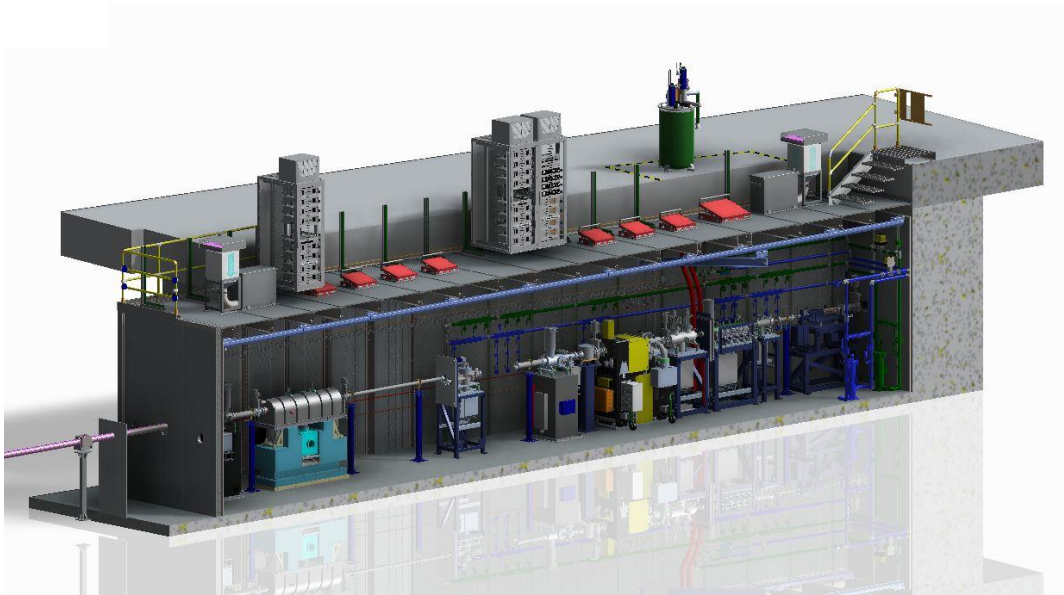
TIME RESOLUTION: sub-sec

DETECTOR: MAD and XPAD

Photon flux at 50 keV (10^{12} sec^{-1})

Ring current (mA)	10	50	100	300	500
Filtering	N	N	Y	Y	Y
No focus (1 mm)	0.7	4	7	16	20
Vertical focus (57 µm)	2	11	21	47	61
Power on optics (W)	60	300	440	470	470

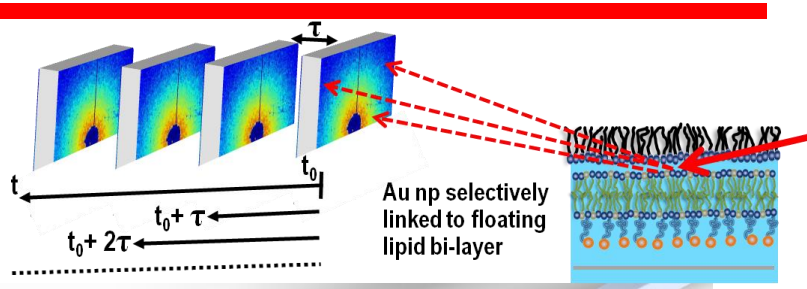




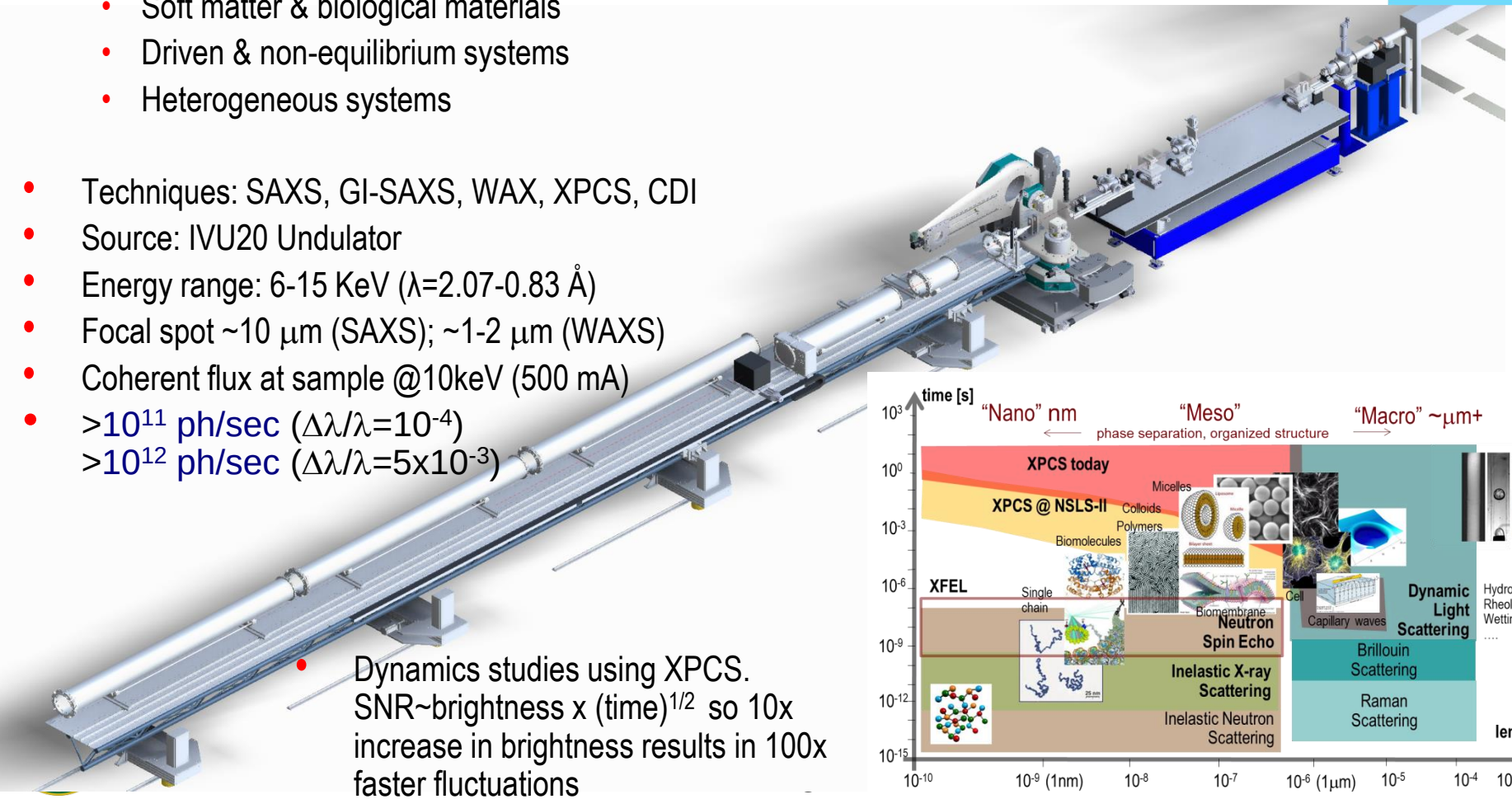
Coherent Hard X-ray Scattering (CHX)

Scientific Focus:

- Interplay between nano-scale dynamics, structure, and macroscopic properties in:
  - Inorganic materials (metallic glass, phase ordering crystals)
  - Soft matter & biological materials
  - Driven & non-equilibrium systems
  - Heterogeneous systems



- Techniques: SAXS, GI-SAXS, WAX, XPCS, CDI
- Source: IVU20 Undulator
- Energy range: 6-15 KeV (λ=2.07-0.83 Å)
- Focal spot ~10 μm (SAXS); ~1-2 μm (WAXS)
- Coherent flux at sample @10keV (500 mA)
- >10^{11} ph/sec ($\Delta\lambda/\lambda=10^{-4}$)
  >10^{12} ph/sec ($\Delta\lambda/\lambda=5\times10^{-3}$)

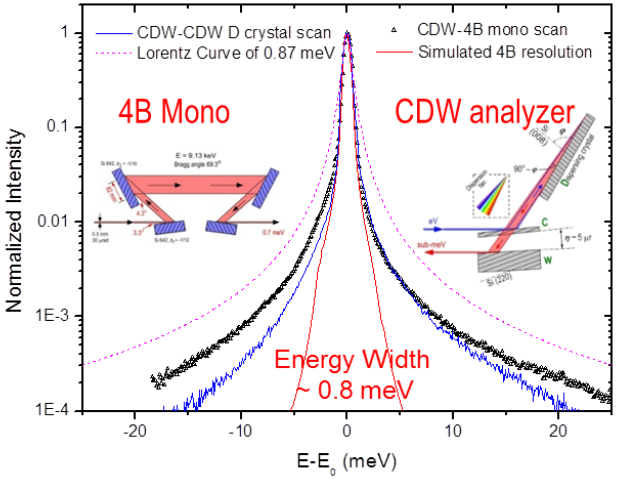


- Dynamics studies using XPCS. SNR~brightness x (time)$^{1/2}$ so 10x increase in brightness results in 100x faster fluctuations

Inelastic X-ray Scattering Beamline (IXS)

Scientific Focus:

- Ultrafast dynamics in liquids, soft matter, and biological systems
- Phonons in single crystals, surfaces and systems under extreme conditions
- Relaxation dynamics, sound propagation and transport properties in disordered systems such as glasses, fluids, polymers, etc.
- Collective dynamics of lipid membranes and other biological systems
- Dynamical studies on confined systems



Designed to Achieve Best-in-Class Performance for IXS :

- Angular dispersive crystal optics for cutting-edge resolution (**0.1 ~ 1 meV**) with **sharper tails** in resolution function and higher Q resolution.
- Medium operation energy (9.1 keV) capitalizing on NSLS-II's strengths in flux and brightness

Performance Comparison :

Facility (Beamline)	ΔE (meV)	ΔQ (nm^{-1})	E (keV)	$I_{inc.}$ @ ΔE (photons/sec)	Beam Size (V×H μm^2)	Flux Density (photons/sec/μm^2)	Sharp Res. Tails
ESRF (ID28)	1.6	0.3	21.7	6×10^9	7×12	7.1×10^7	--
APS (30-ID-C)	1.5	0.6	23.8	2×10^9	15×35	3.8×10^6	--
SPring-8 (43LXU)	1.5	0.3	21.7	$\sim5\times10^{10}$	20×35	$\sim7.1\times10^7$	--
NSLS-II (IXS)	1.0	0.2	9.1	$\sim1.6\times10^{10}$ (4B HRM)*	5×7	**$\sim5\times10^8$**	yes

* Performance for a IVU22-3 m at 500 mA (flux 8×10^{14} phs/sec/0.1% bw) and 30% spectral efficiency for the 4B monochromator.

Coherent Soft X-ray Scattering (CSX-1)

Scientific Focus:

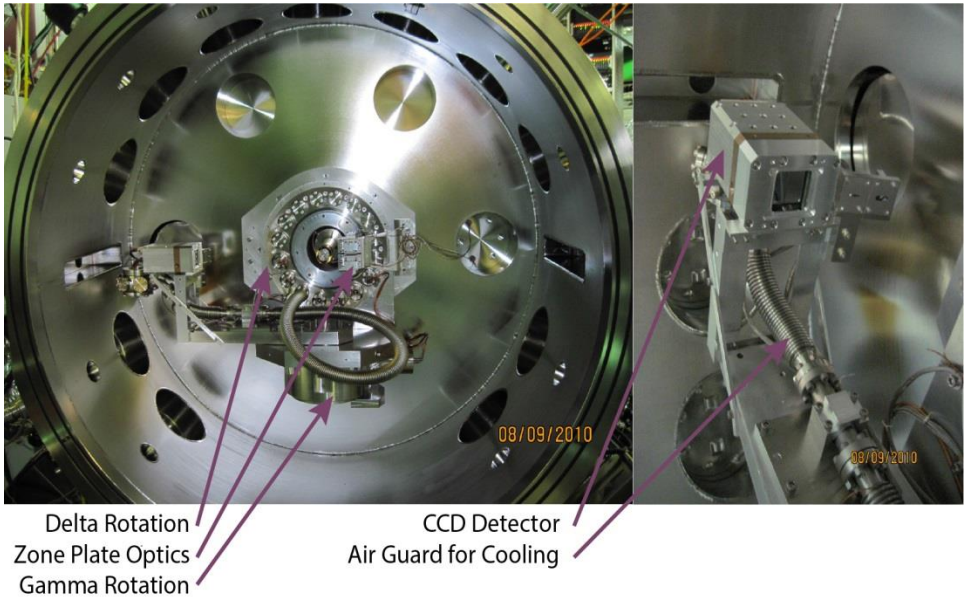
- Magnetic / Orbital / Stripe Domain structure
- Glassy Dynamics of Electronic Textures

Techniques: Coherent scattering, including CDI and XPCS; Soft X-ray Resonant Scattering

Zone-plate based soft x-ray nanodiffraction
50 nm (10 nm), 3 to 4mm working distance

Source: Dual EPU49 Undulators
Energy range: 0.27-2 KeV
Resolution: $\Delta E/E \sim 5 \times 10^{-3}$
Focal spot ~20 μm
Coherent flux at sample (500 mA)
$>10^{13}$ ph/sec

CSX-1 will have the highest soft x-ray coherent flux in the world and a unique endstation for combined scattering and imaging experiments.



Superconducting Cooper pairs in a background of charge order in a cuprate superconductor. Experiments at NSLS-II will take the first images of this charge order and measure the dynamics on ps timescales

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Full Polarization Control Beamline (CSX-2)

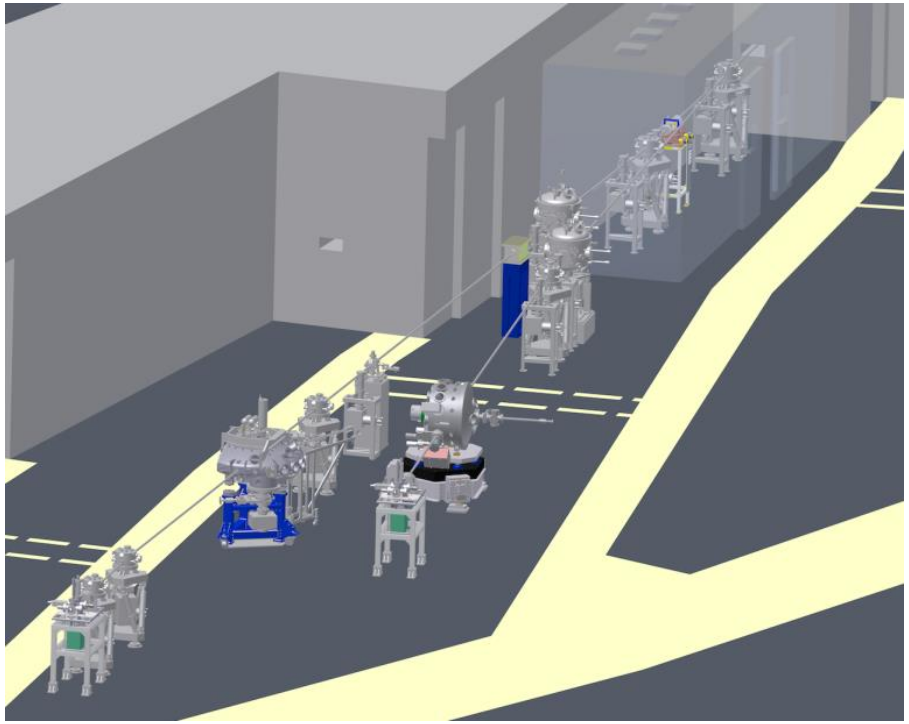
Scientific Focus:

- Characterization of (new) magnetic materials, spintronic devices, spin valves, spin ice, dilute magnetic semiconductors, exchange bias, multiferroics and ferroelectrics

Techniques:

- Spectroscopy (XAS, XMCD, MLD) and
- Resonant Magnetic Scattering,
- Element specific magnetometry
- Fast polarization switching to 1 kHz

Source: Dual EPU49 Undulators
Energy range: 0.27-2 KeV
Resolution: $\Delta E/E \sim 1 \times 10^{-4}$
Focal spot ~10 x 50 μm
Circularly polarized flux at sample (500 mA)
$>10^{13}$ ph/sec

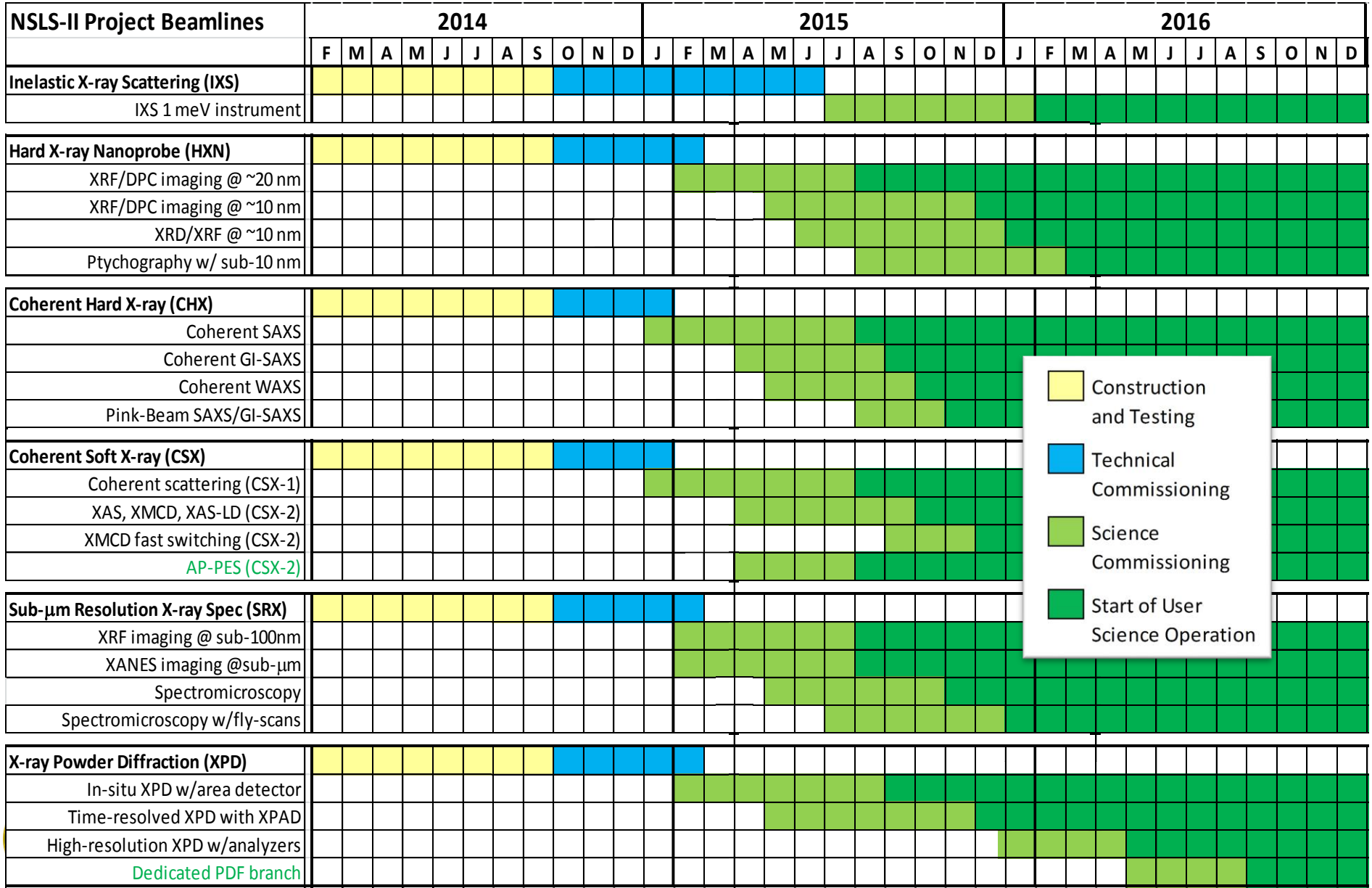


CSX-2 layout

Beamline Commissioning Steps

- **NSLS-II beamline commissioning will proceed in three steps**:
  - Integrated Testing (construction), technical commissioning, and science commissioning.
- **Integrated Testing** (construction) will be dedicated to installation and systematic testing without beam of all mechanical and control functions of installed beamline subsystems required to meet the project beamline installation criteria.
- **Technical Commissioning** will focus on beam delivery into the experimental endstation, with emphasis on characterizing the beamline performance parameters, including flux, focus, energy resolution & calibration, energy range, stability, etc…
- **Science Commissioning** will evaluate the beamline instruments and data acquisition systems for the planned science experiments, and may require measurements on standard systems or calibrated standards, followed by commissioning experiments selected through a review process.

Phased Ramp-up of Science Capabilities



Advanced Beamlines for Biological Investigations with X-rays

ABBIX Project - NIH funded $45M – Commissioning to begin 1QFY16

Frontier Macromolecular Crystallography (FMX)

Studies of enzymatic pathways of cellular and microbiological processes

Studies of drug-target interactions of new and improved pharmacologically effective compounds

Tunable 1μm beam of high intensity for micro-crystallographic studies of small crystals and large unit cells

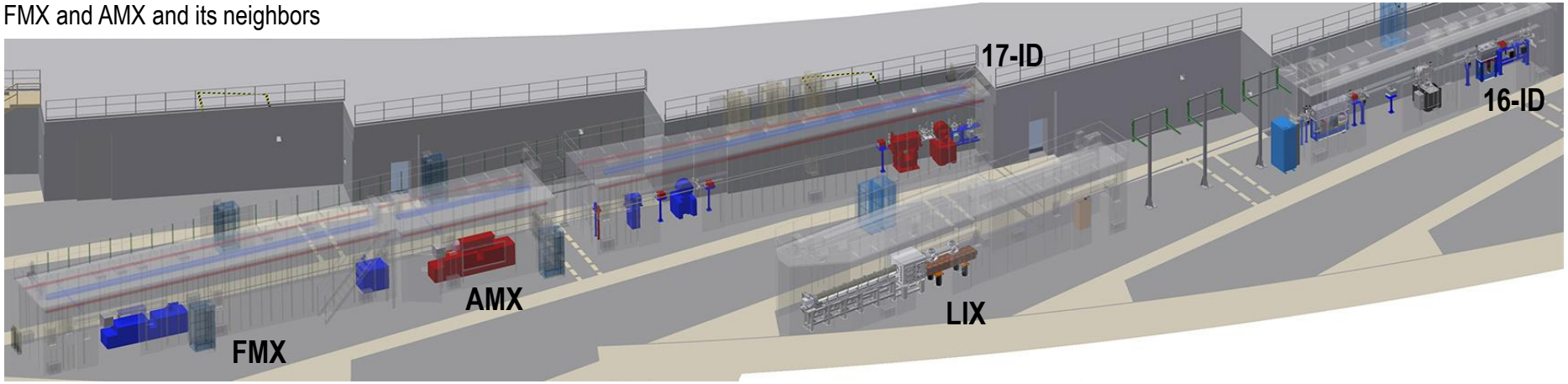
Highly Automated Beamline for Macromolecular Crystallography (AMX)

Atomic structure of large protein and nucleic acid complexes, including membrane proteins

Highly automated to support remote access and extensive experimental searches

Precise structure determinations with unprecedented throughput

FMX and AMX and its neighbors



High Brightness X-ray Scattering for Life Sciences (LIX)

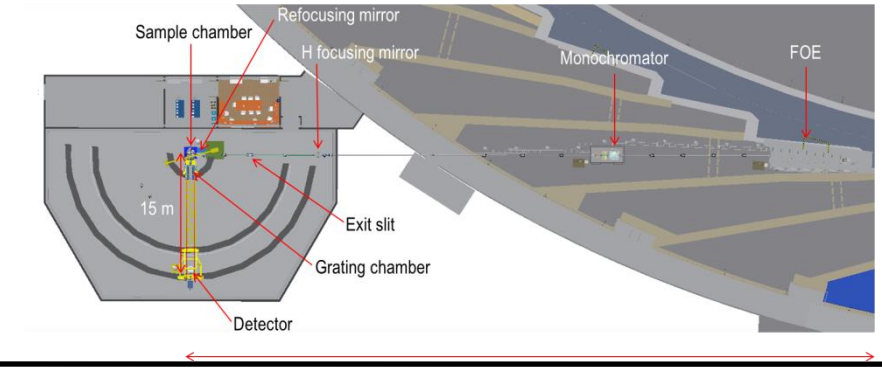
Grazing incidence scattering from 2D solutions of proteins embedded in near-native membranes

1μm beam scanning probe imaging and tomography of biological tissues

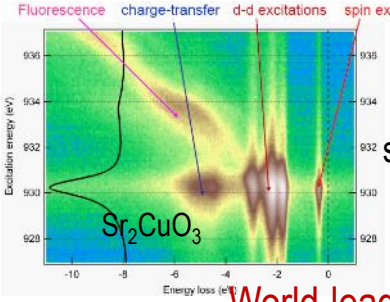
Time-resolved solution scattering down to 10μs

NSLS-II Experimental Tools (NEXT) Beamlines

DOE-BES funded $90M MIE project – Commissioning to begin 1QFY17



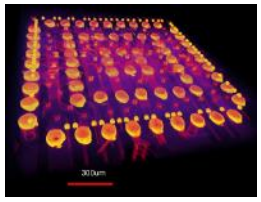
Soft Inelastic X-ray Scattering (SIX)



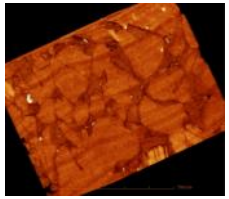
Elementary excitations (magnons, phonons and orbitons) in nanoscale samples $(100\ nm)^3$ w/ applications to superconductivity, nanocatalysts, energy storage materials

World-leading soft x-ray energy resolution

Full-field X-ray Imaging (FXI)



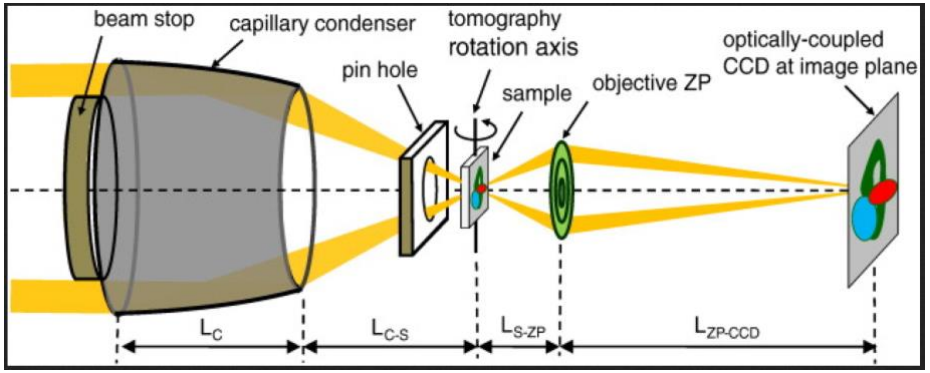
semiconductor failures

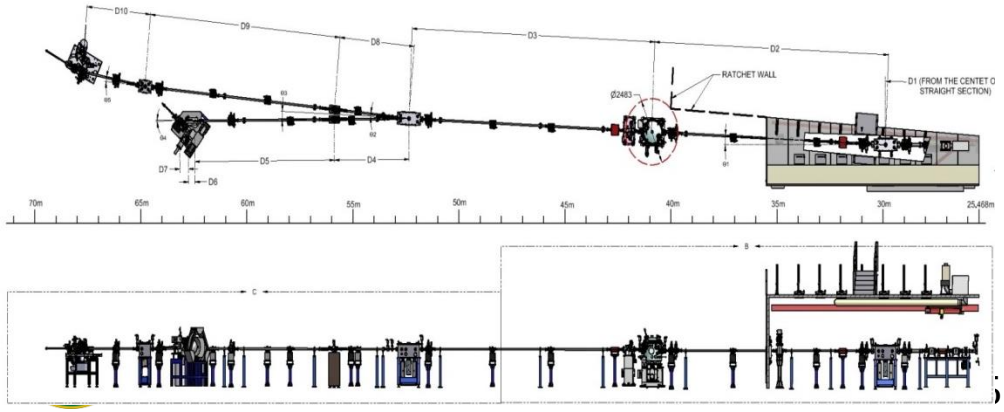


$CaCO_3$ drilling

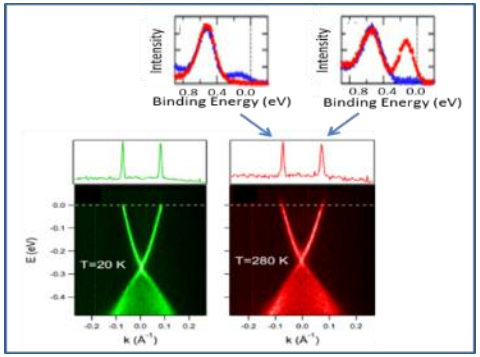
Real-time 3D imaging of natural and man-made materials in working environments

High speed TXM w/ 30 nm resolution





Electron Spectro-Microscopy (ESM)



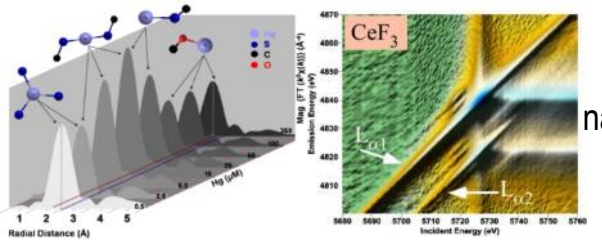
Advancing photoemission to characterize electronic structure of functional materials w/ high spatial resolution

Sub-meV nano-ARPES
LEEM/PEEM

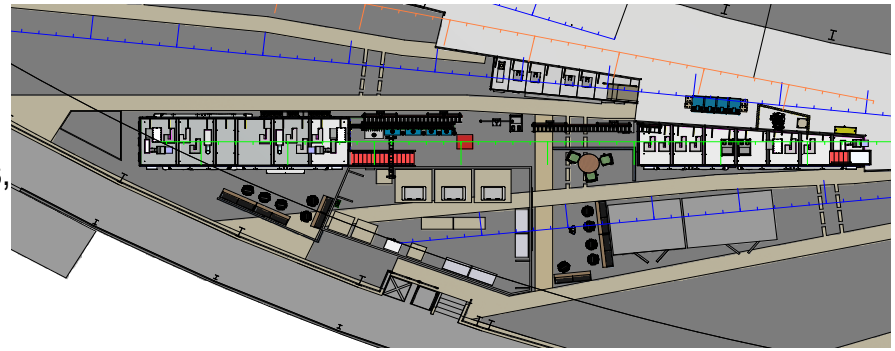
NSLS-II Experimental Tools (NEXT) Beamlines

DOE-BES funded $90M MIE project – Commissioning to begin 1QFY17

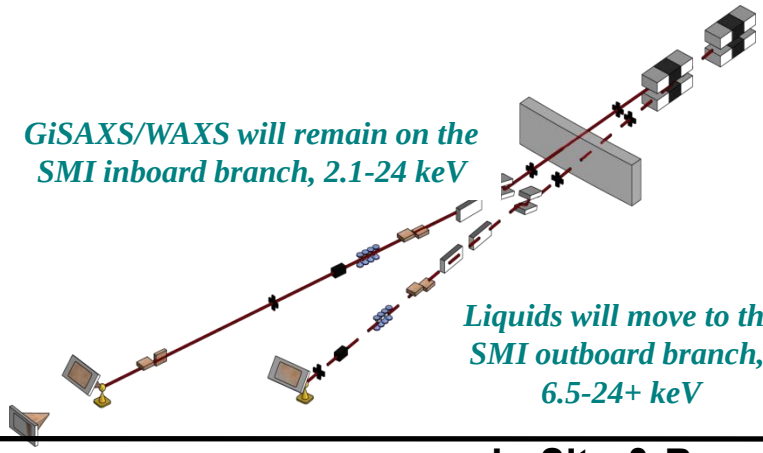
Inner Shell Spectroscopy (ISS)



In-situ, time-resolved, element specific studies of nanocatalysts, mettalloenzymes, environmental contaminants, batteries, and fuel cells

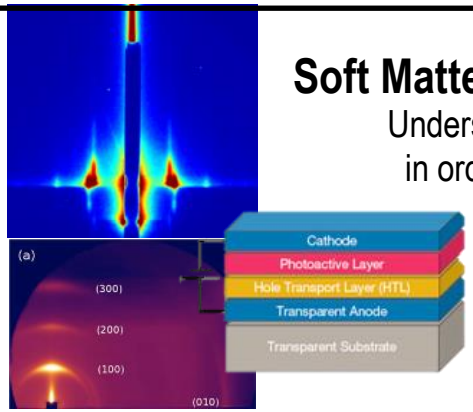


Time resolved XAS with high E-resolution and at ultra-dilute concentrations



GiSAXS/WAXS will remain on the SMI inboard branch, 2.1-24 keV

Liquids will move to the SMI outboard branch, 6.5-24+ keV

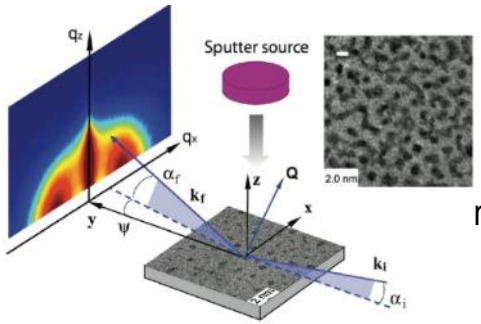


Soft Matter Interfaces (SMI)

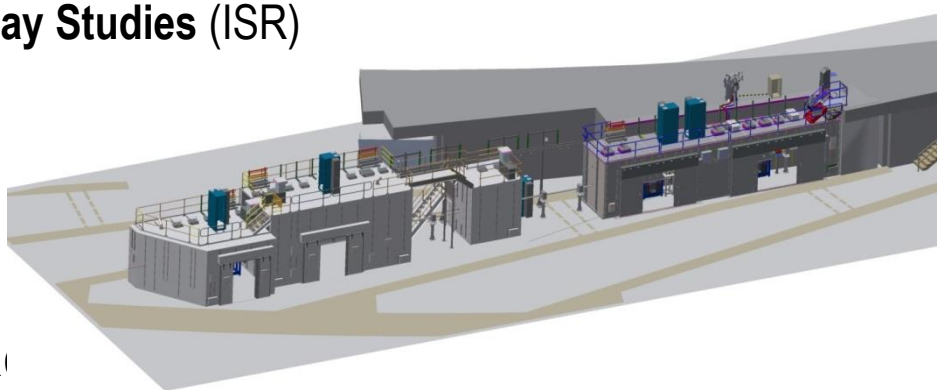
Understanding self-assembly of nanomaterials in order to create new hierarchical materials with tailored functionality

In-situ real-time studies of solid/liquid/vapor interfaces of complex materials

In-Situ & Resonant X-Ray Studies (ISR)



Powerful capabilities for in-situ, real-time growth, atomic structure of surface and interfaces, magnetic/orbital scattering, domain imaging, high magnetic fields

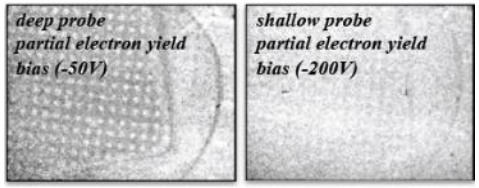


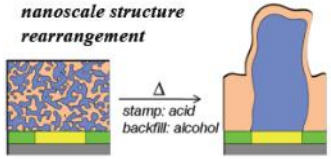
Integrated materials physics studies

Partner Beamlines

Operations to begin FY16

Spectroscopy Soft & Tender (SST-1, SST-2) - NIST





Nanoscale imaging of the structure and chemistry of buried layers and interfaces of real device architectures

6 unique world class NEXAFS/XPS stations (2 full field microscopes, 2 automated high-throughput, and 2 in-situ high pressure) with two undulators covering soft (100 eV – 2.2 keV) and tender (1 – 7.5 keV) x-rays

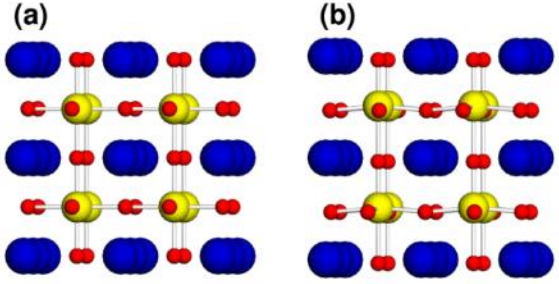
New X-ray Photoelectron Spectroscopy Microscope being developed for SST

NYSBC Microdiffraction Beamline (NYX) - NYSBC

Membrane proteins relevant to neurobiology and metabolic disorders, and protein-protein interactions in signaling complexes and protein-nucleic acid complexes in transcription or replication

Diffraction from micron sized crystals and optimized for anomalous scattering with high energy resolution at low energies (3.5 – 17.5 keV)

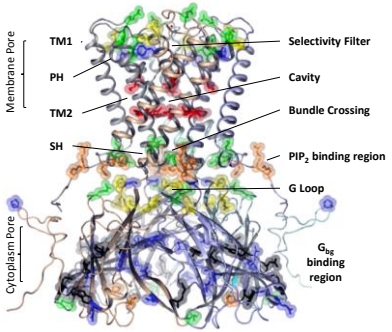
Beamline for Materials Measurements (BMM) - NIST



Strain engineering studies of electronic thin films, high throughput XAFS studies of chemical reactions and catalysts, phase transitions under controlled environmental conditions

High-throughput, high-quality hard x-ray absorption and diffraction

X-ray Footprinting (XFP) - CWRU



Steady state and time-resolved X-ray hydroxyl-radical mediated Protein and Nucleic Acid Footprinting

NxtGen Beamlines
Operations to begin FY15-FY17

- Bending magnet, three pole wiggler, and infrared beamlines are needed at NSLS-II to provide complementary capabilities, including high throughput, and add significant capacity
- These will also serve to transition much of the existing NSLS user community & their scientific programs to NSLS-II
- NxtGen will cost effectively transfer eight such beamlines from NSLS to NSLS-II by reusing components from one or more NSLS beamlines
- Staged plan for developing NxtGen beamlines during FY15-FY17 (schedule depends on annual funding level)

Complex Materials Scattering (CMS)
Magneto, Ellipso, High Pressure IR (MET/FIS)
Metrology & Instrum Development (MID)
In-situ X-ray Diffraction Studies (IXD)

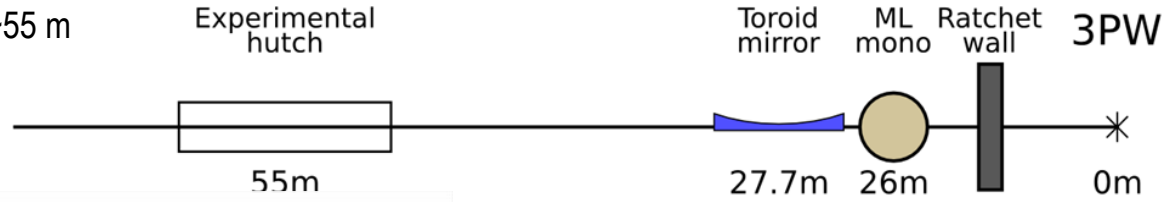
Materials Physics & Processing (MPP)
Quick X-ray Absorption and Scattering (QAS)
Tender X-ray Absorption Spectroscopy (TES)
X-ray Fluorescence Microscopy (XFM)

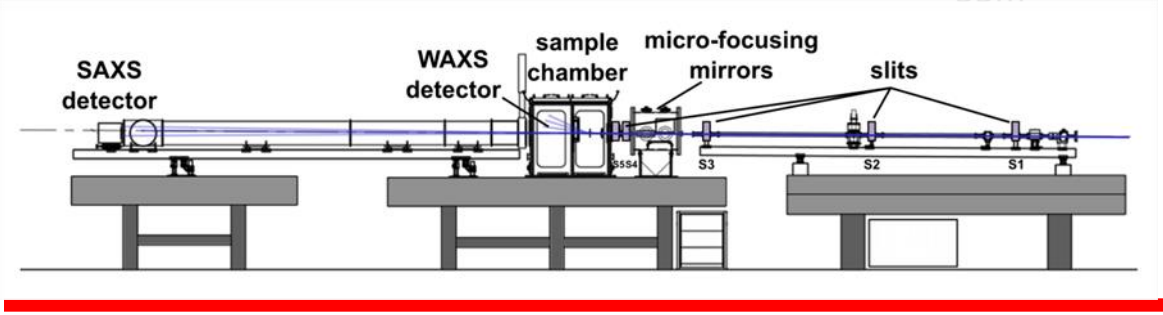
Complex Material Scattering - CMS

Probe structural order in hierarchical multicomponent materials

- study of hierarchical materials and next-generation nano- or meso- structures
- microfocusing for grazing-incidence (GISAXS/GIWAXS) experiments on surfaces and thin films

CMS with the X9 experimental hutch centered at ~55 m from the 3PW source. Multilayer monochromator (10 to 17 keV) and a toroidal mirror to provide 1:1 focusing onto the sample position.



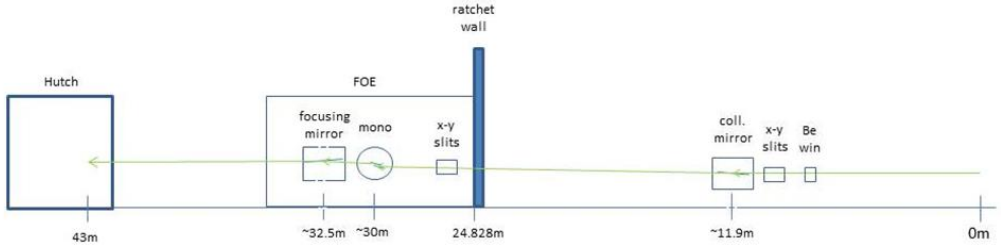


Based on X-9 design, a slit system (S1-S5) is used to collimate the beam. Microfocusing mirrors are optionally used to reduce beam size. Two area detectors are used simultaneously to capture a wide *q*-range.

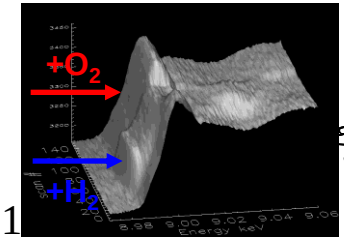
Quick X-ray Absorption and Scattering - QAS

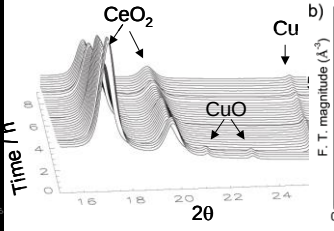
Spatial and temporal study of catalytic systems In situ and in operando

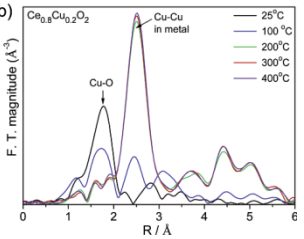
- fast kinetics (~10 ms time resolution) of working catalysts and fuel cells
- study size, shape, structure and morphology of metal nanocatalysts through the course of catalytic reaction



Water-Gas Shift catalyst: $Cu_{0.2}Ce_{0.8}O_2$







X-ray Fluorescence Microprobe - XFM

Characterization of chemically heterogeneous materials at the micron scale

- optimized for microfocus Extened X-ray Absorption Fine Structure spectroscopy
- includes microbeam x-ray fluorescence, diffraction and fluorescence computed microtomography

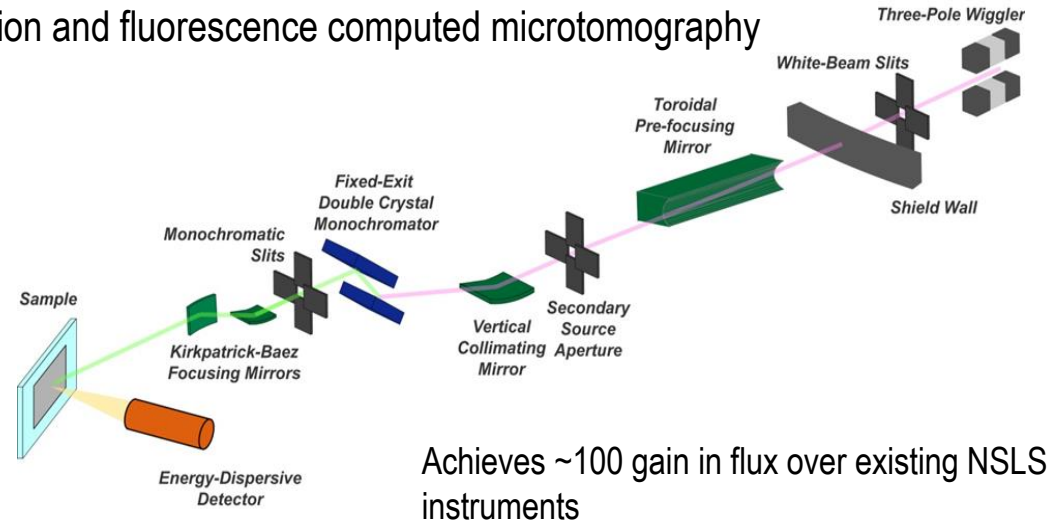
Beamline Capabilities:

TECHNIQUE(S): μm X-ray fluorescence (XRF), X-ray absorption fine structure (XAFS) spectroscopy, X-ray diffraction (XRD) and fluorescence computed microtomography (FCMT).

SOURCE: Three Pole Wiggler

ENERGY RANGE / RESOLUTION: 4 to 20 keV / 1 eV

SPATIAL RESOLUTION: 1 – 10 μm variable

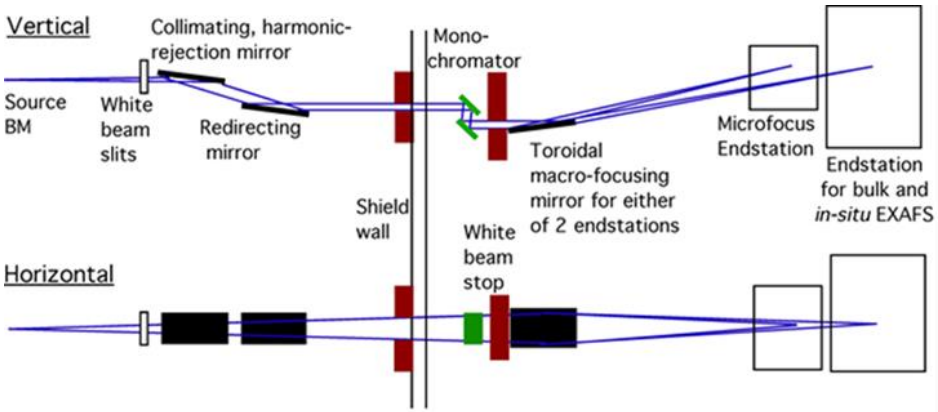


Achieves ~100 gain in flux over existing NSLS instruments

Tender Energy x-ray absorption Spectroscopy - TES

Tender-energy spatially resolved spectroscopy of multi-scale heterogeneous and dynamic systems

- mm to micrometer beam X-ray Absorption Spectroscopy from 1.2-8 keV
- *in situ*, *in operando* rapid-scanning XAS for chemistry & materials or XAS, GIXAS, XRF+XAS imaging

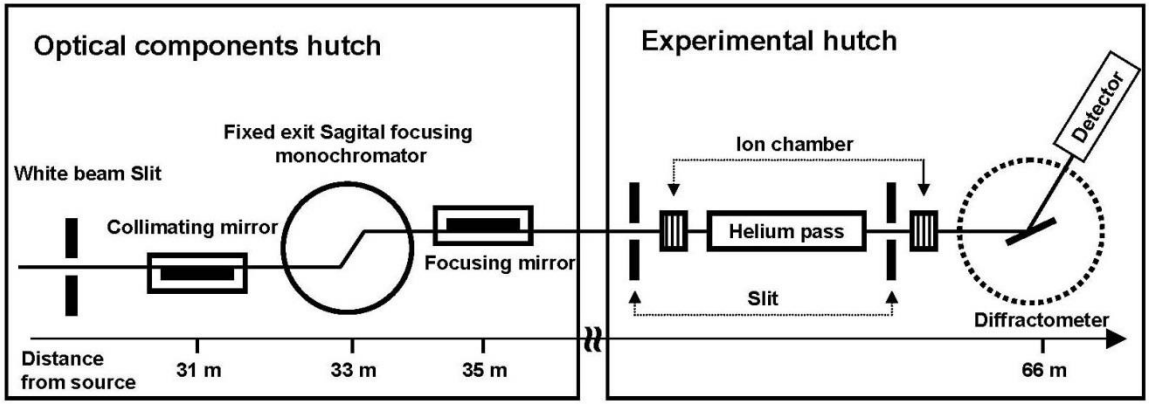


In-situ X-ray Diffraction - IXD

In situ and ex situ X-ray Powder Diffraction measurements in materials

- Structural and chemical changes of energy materials in their operating environments
- High q-resolution scattering with tunable energies up to 25 keV

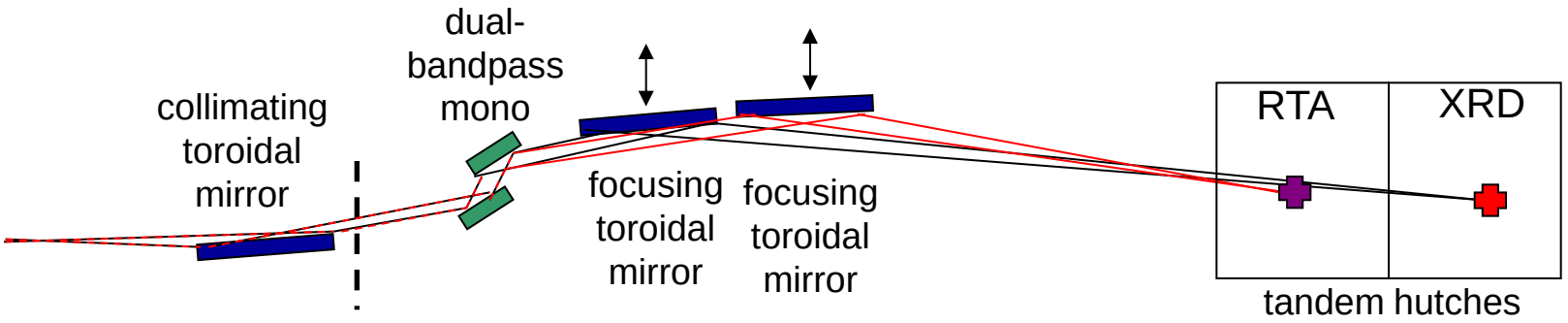
Supporting research on – batteries, supercapacitors, fuel cells, catalysis, high-temperature materials, light-metal production….



Materials Physics and Processing - MPP

Diffraction and scattering for study of materials (thin films, stacks, nanopatterned samples and bulk)

- high flux- low resolution mode for real-time in situ studies of phase transformations
- Medium-to-high resolution x-ray diffraction on samples in different environments



Frontier IR Spectroscopy / Magneto, Ellipsometric and Time Resolved IR – FIS/MET

Materials science and extreme conditions communities

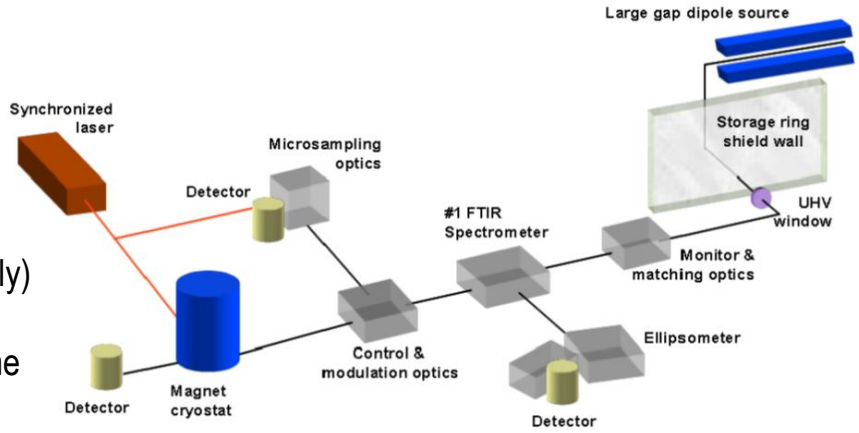
- high-brightness and pulsed THz, infrared and visible light for probing electronic properties and dynamics

Major Components:

New wide gap dipole chamber and extraction optics required

Key capabilities:

- 250 meV to 5 eV energy range
- Optics for small aperture diamond anvil cells to pressures ~250 Gpa
- Ellipsometry to directly extract optical constants (e and m independently)
- Samples in magnetic fields to 10T and temperatures to 1.5K
- Laser systems for photoexcitation (pump probe) and heating to extreme temperatures
- Photoconductivity capability from ~5Hz up to 1 GHz

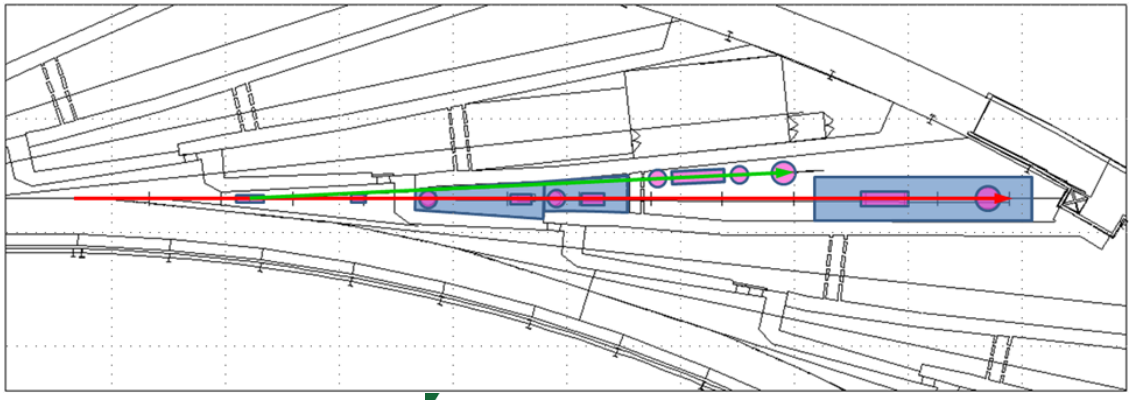


Note- source is 23BM, occupies sector 22 floor space

Metrology and Instrumentation Development - MID

Dedicated beamline for x-ray instrumentation development

- 3PW beam onto floor and up to three white beam capable hutches



Beamline Capabilities:

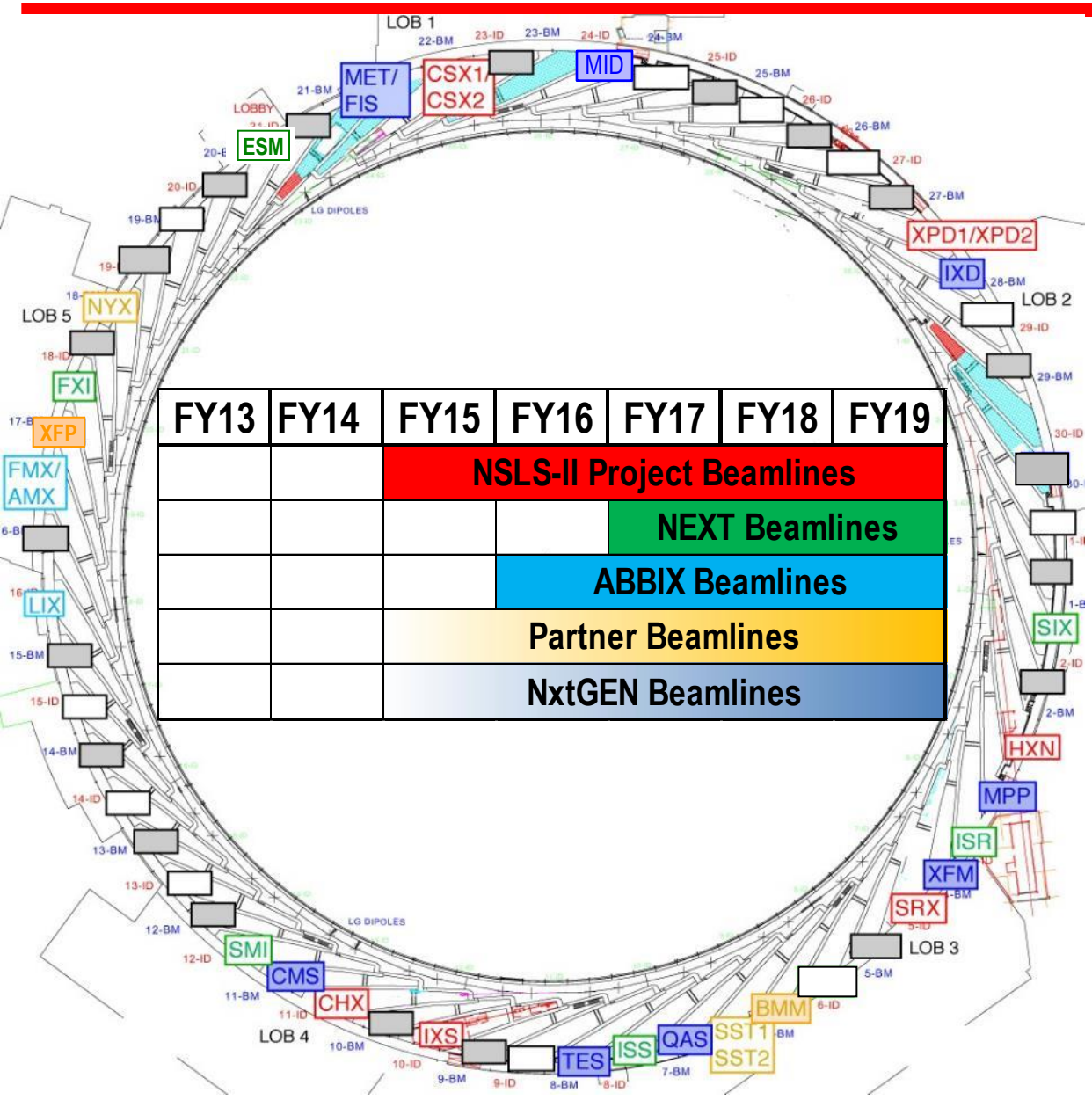
TECHNIQUE(S): White and monochromatic (focused & unfocused), soft and hard x-ray optics, and multiple optical benches for flexible test arrangements

SOURCE: 1.1 T 3-pole wiggler (and 0.3 T side-pole)

ENERGY RANGE: 50 eV – 50 keV

FAN SIZE: 2 mrad (130 mm at 65 m)

Developing the NSLS-II Beamline Portfolio



8 NSLS-II Project Beamlines

- Inelastic X-ray Scattering (IXS)
- Hard X-ray Nanoprobe (HXN)
- Coherent Hard X-ray Scattering (CHX)
- Coherent Soft X-ray Scat & Pol (CSX1, CSX2)
- Sub-micron Res X-ray Spec (SRX)
- X-ray Powder Diffraction (XPD1, XPD2)

6 NEXT Beamlines

- Photoemission-Microscopy Facility (ESM)
- Full-field X-ray Imaging (FXI)
- In-Situ & Resonant X-Ray Studies (ISR)
- Inner Shell Spectroscopy (ISS)
- Soft Inelastic X-ray Scattering (SIX)
- Soft Matter Interfaces (SMI)

3 ABBIX Beamlines

- Frontier Macromolecular Cryst (FMX)
- Flexible Access Macromolecular Cryst (AMX)
- X-ray Scattering for Biology (LIX)

5 Partner Beamlines

- Spectroscopy Soft and Tender (SST1, SST2)
- Beamline for Mater. Measurements (BMM)
- Microdiffraction Beamline (NYX)
- X-ray Footprinting (XFP)

8 NxtGen Beamlines

- Complex Materials Scattering (CMS)
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- Materials Physics & Processing (MPP)
- Quick X-ray Absorption and Scattering (QAS)
- Tender X-ray Absorption Spectroscopy (TES)
- X-ray Fluorescence Microscopy (XFM)

Summary

- NSLS-II beamline development continues to make excellent progress
- 30 beamlines are under development for NSLS-II to provide world leading capabilities
- Accelerator commissioning & early operations plans are well developed
- Looking forward to fast ramp up of operations & and exciting and productive science program at NSLS-II