News from the NSLS-II Beamline Community

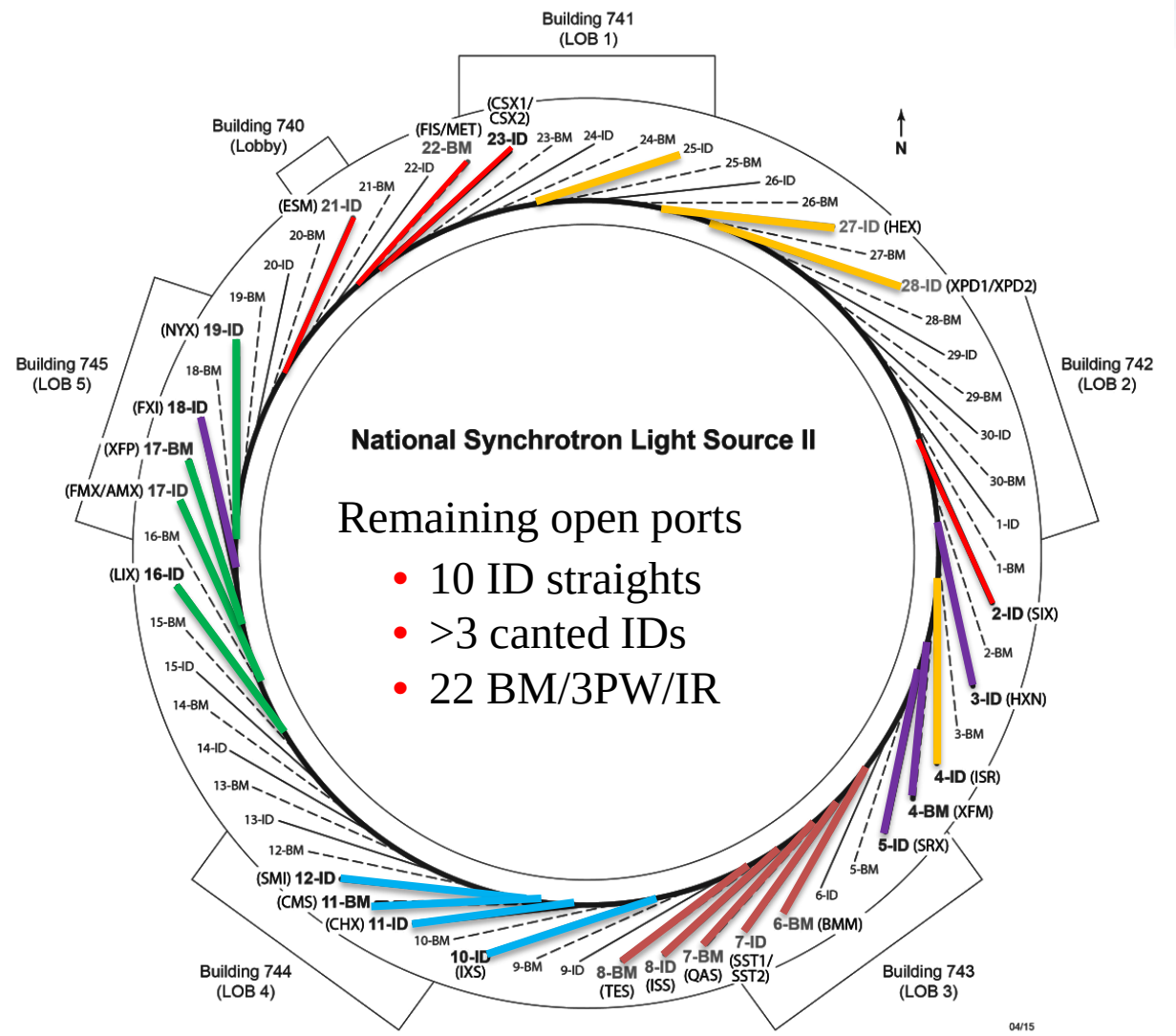
P. Zschack

High-Brightness Synchrotron Light Source Workshop, 26 April 2017

NSLS-II Beamline Development Projects

- 7 NSLS-II Project funded beamlines ($107M)
- NEXT Project: DOE-BES funded $90M MIE project to design 6 and build 5 insertion-device beamlines
- ABBIX Project: Design and build 3 NIH-funded state-of-the-art insertion-device beamlines ($48M)
- Partner Beamline Developments: NSLS-II partnering with NIST, Case-Western Reserve University, and NY Structural Biology to develop 5 beamlines ($64M)
- New York State Beamline Development: NY state investing $25M for development of High Energy X-ray Diffraction (HEX) beamline at NSLS-II
- Beamlines Developed through NSLS-II Operating funds. ($17.5M in FY17)

NSLS-II Beamline Portfolio



Soft X-Ray Scattering & Spectroscopy

23-ID-1: Coherent Soft X-ray Scat (2015)
23-ID-2:Coherent Soft X-ray Spectr & Pol (2015/2016)
21-ID: Photoemission-Microscopy Facility (2017)
2-ID: Soft Inelastic X-ray Scattering (2017)
22-BM: Magneto, Ellipso, High Pressure IR (2018)

Complex Scattering

10-ID: Inelastic X-ray Scattering (2015)
11-ID: Coherent Hard X-ray Scattering (2015)
11-BM: Complex Materials Scattering (2016)
12-ID: Soft Matter Interfaces (2017)

Diffraction & In Situ Scattering

28-ID-1: X-ray Powder Diffraction (2015)
28-ID-2: X-ray Powder Diffraction (2017)
4-ID: In-Situ & Resonant X-Ray Studies (2017)
27-ID: High Energy X-ray Diffraction (2020)
25-ID: Materials in Radiation Environments (2020?)

Hard X-Ray Spectroscopy

8-ID: Inner Shell Spectroscopy (2017)
7-BM: Quick X-ray Absorption and Scattering (2016)
8-BM: Tender X-ray Absorption Spectroscopy (2017)
7-ID-1: Spectroscopy Soft and Tender (2017)
7-ID-2: Spectroscopy Soft and Tender (2017)
6-BM: Beamline for Mater. Measurements (2017)

Imaging & Microscopy

3-ID: Hard X-ray Nanoprobe (2015)
5-ID: Sub-micron Res X-ray Spec (2015)
4-BM: X-ray Fluorescence Microscopy (2017)
18-ID: Full-field X-ray Imaging (2018)

Structural Biology

17-ID-1: Frontier Macromolecular Cryst (2016)
17-ID-2: Flexible Access Macromolecular Cryst (2016)
16-ID: X-ray Scattering for Biology (2016)
17-BM: X-ray Footprinting (2016)
19-ID: Microdiffraction Beamline (2017)

Beamlines: Current Status

General User Operations
CSX-1, CSX-2, XPD, HXN, SRX
IXS, CHX, LIX, AMX, FMX, ISS

Science Commissioning
XFP, TES, CMS, ISR

Technical Commissioning
ESM, SMI, NYX, SIX

Completion* in FY17
BMM, SST-1, SST-2, QAS, XFM

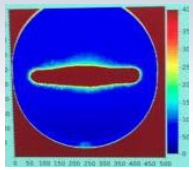
Completion* in FY18
PDF, FXI, FIS, MET

19 beamlines now taking beam!

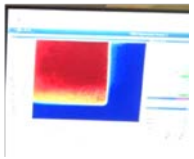
* Completion defined as having completed IRR – First Light

First Light Images: FY16

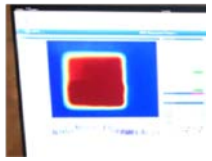
LIX Nov 16, 2015



ISS April 5, 2016

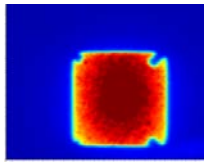


FMX March 8, 2016

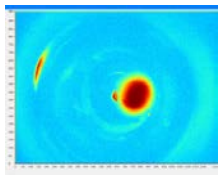


AMX March 8, 2016

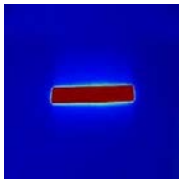
XFP July 11, 2016



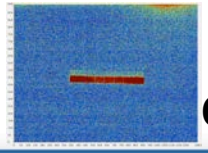
ISR July 11, 2016



ESM July 25, 2016

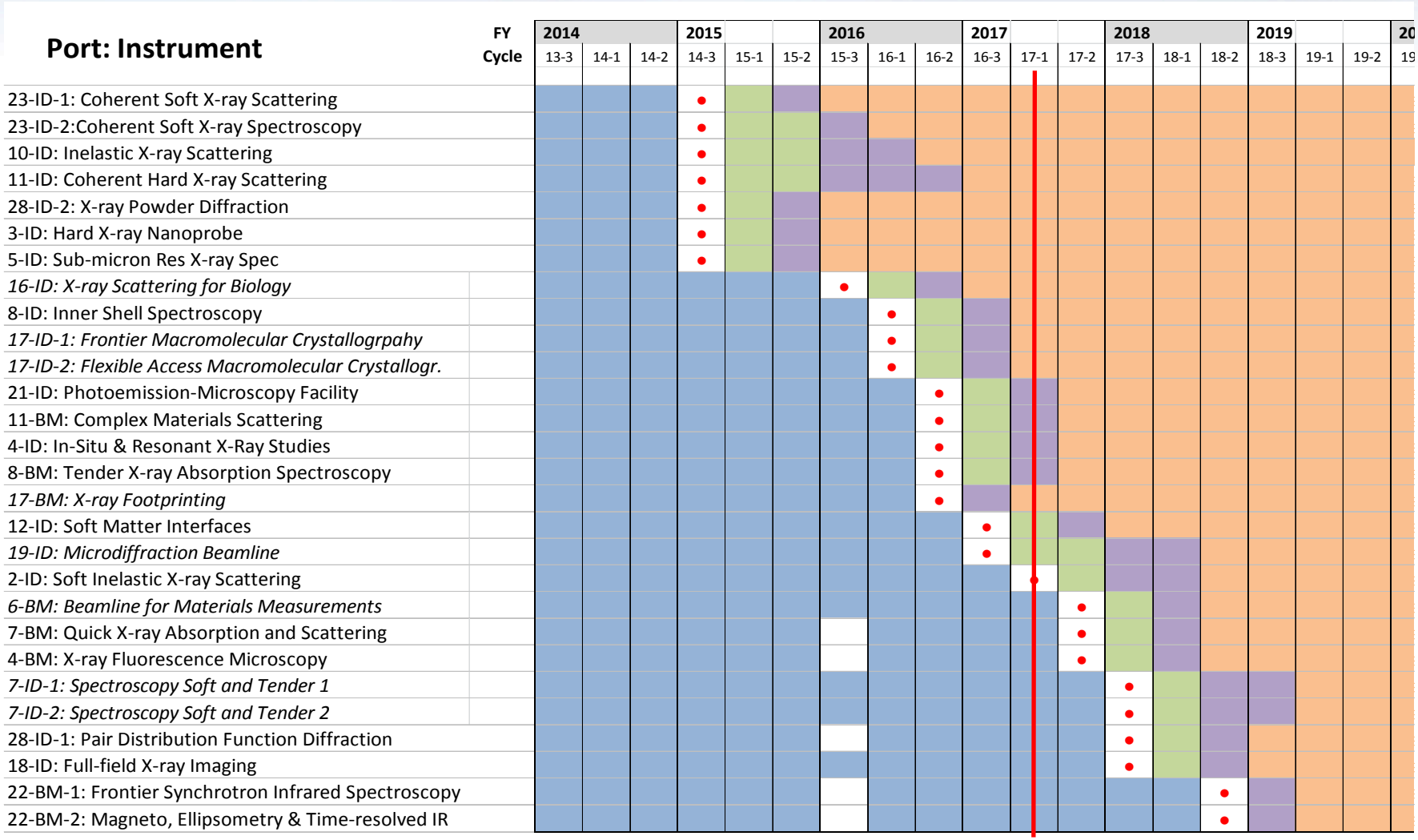


TES Aug 19, 2016



CMS Aug 29, 2016

NSLS-II Beamline Buildout

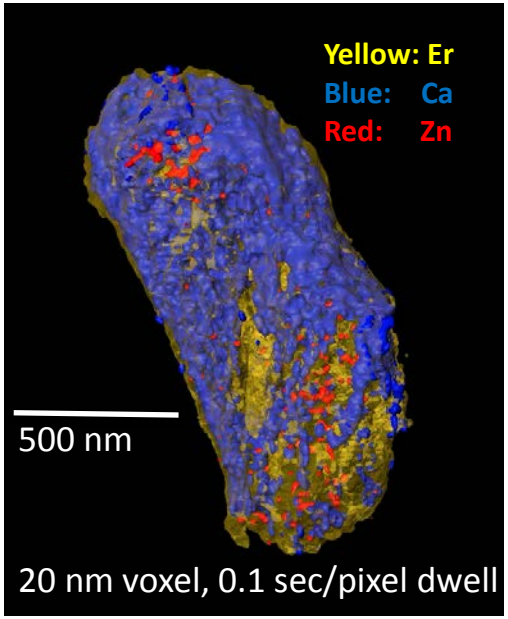


- First light date

Imaging and Microscopy Program Beamlines (1)

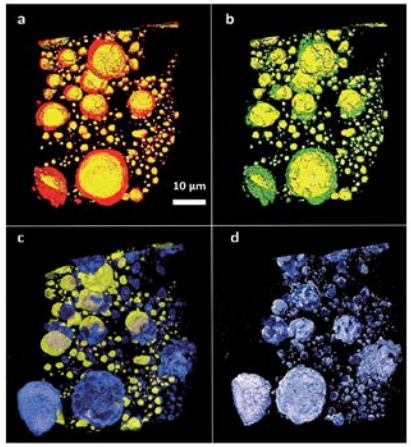
HXN – Hard X-ray Nano-probe

- World-leading resolution for hard x-rays (~13 nm) with exceptional measurement sensitivity offering multimodality imaging (XRF, DPC, ptychography, XRD, XANES, tomography).
- Highly optimized for nanofluorescence and nanodiffraction imaging.



FXI – Full-field X-ray Imaging

- World's fastest transmission X-ray microscopy beamline with opportunity to be a world leader for in-situ/in-operando TXM studies
- Designed to accommodate sample environment cells with a 20-40 um field of view, and better than 30 nm resolution.



In situ 3D morphological changes in Li-ion battery tin electrode. J. Wang et al, Angewandte Communications 53, 2014

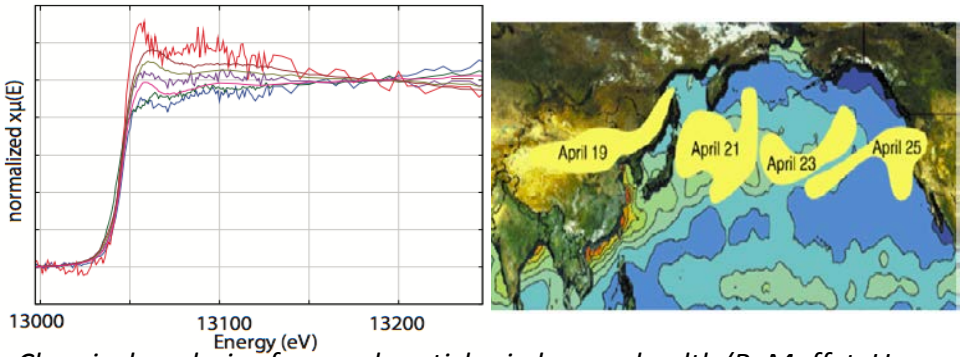
Imaging and Microscopy Program Beamlines (2)

SRX – Submicron Resolution X-ray Spectroscopy

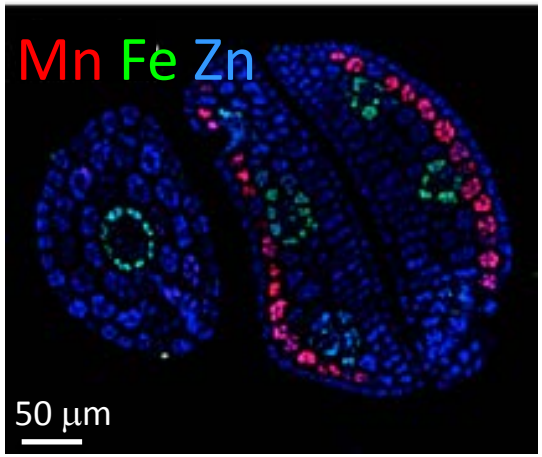
- Dedicated to X-ray spectroscopy (XANES) and X-ray fluorescence imaging in 2D and 3D with sub-µm and sub-100nm spatial resolution
- Nanoscale resolution EXAFS capability
- Versatile sample setup for experiments in environmental, life, geo-, planetary, energy and material sciences.
- World-leading flux, very fast data acquisition, allowing for large scale samples, in-situ and in-operando studies

XFM – X-ray Fluorescence Microscopy

- High throughput XRF imaging at the micron scale in 2D and 3D, micro-XRD
- Spatially-resolved XAS spectroscopy (2-23 KeV) for heterogeneous systems
- Low-energy spectroscopy (P, S, Cl, Ca K-edges)
- Versatile endstation for high throughput and large field of view XRF imaging



Chemical analysis of aerosol particles in human health (R. Moffet, U Pacific; M. Schoonen, BNL)

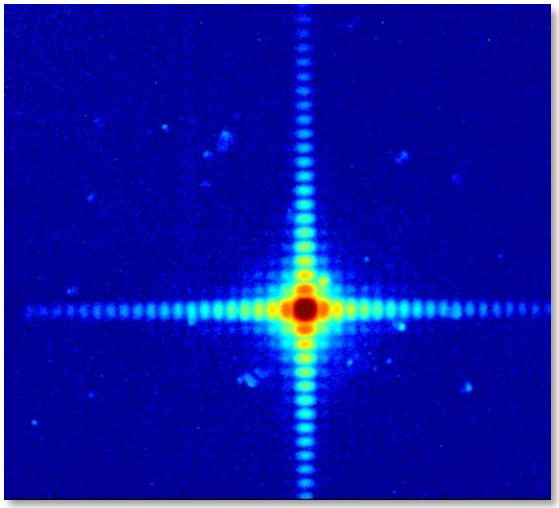


Trace element uptake in plants for nutrition, phytomining, and phytoremediation (R. Tappero, BNL)

Complex Scattering Program Beamlines (1)

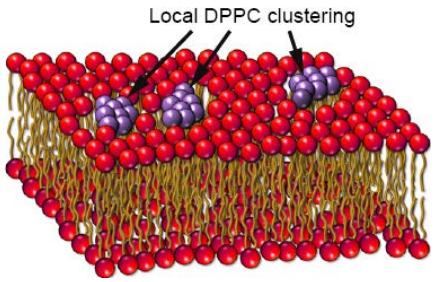
CHX – Coherent Hard X-ray Scattering

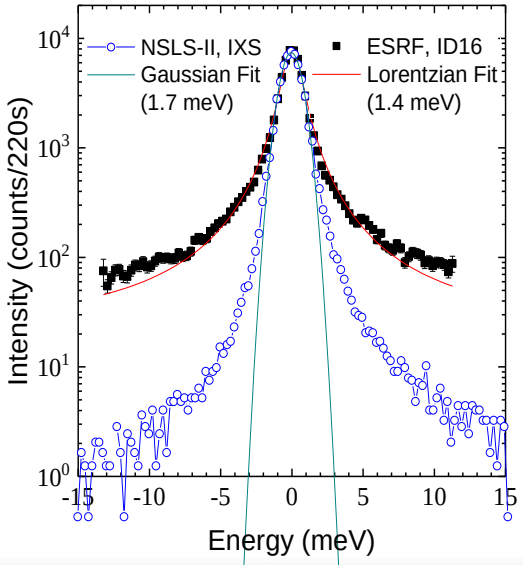
- XPCS with highest available brightness in the 6-16 keV range to access usec timescale.
- Widest accessible q-range (Angstroms to microns), suited for soft and hard matter systems
- Only existing setup for simultaneous SAXS/WAXS with a coherent beam.
- Beam size ~10 um (SAXS) and ~1 um (WAXS)



IXS – Inelastic X-ray Scattering

- Designed to deliver an initial energy resolution of ~1 meV and a fine (<10 um) focus.
- Lower operation energy and sharp tails are unique in the world and the design offers high Q-resolution
- This combination of features provides unique strengths for the study of THz dynamics in heterogeneous, disordered, and low-Z materials





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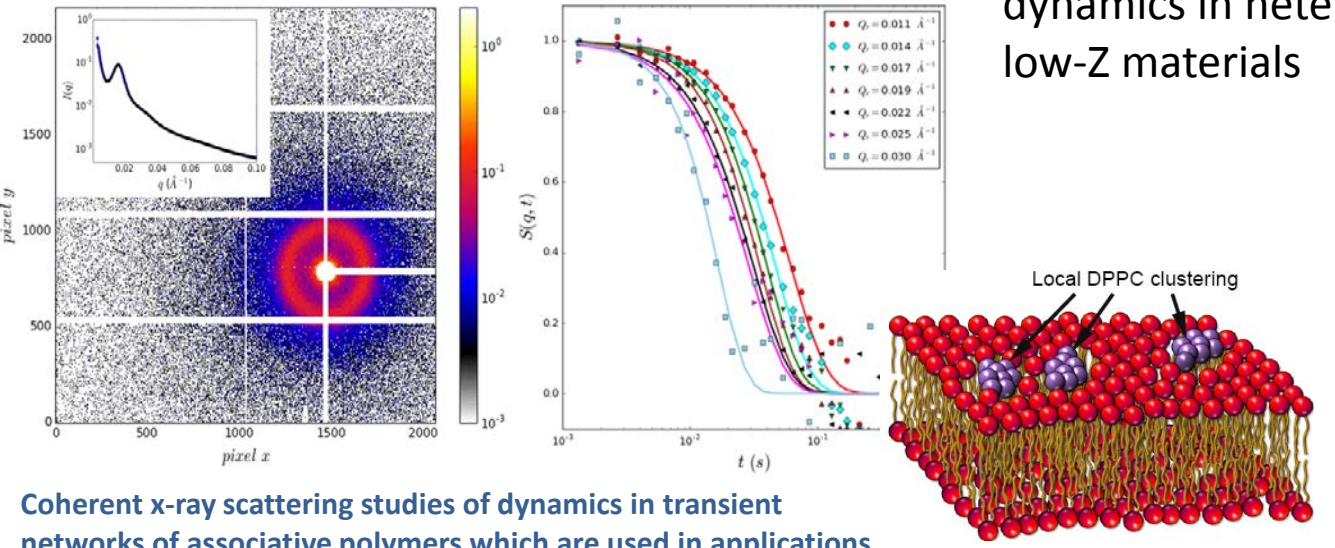

Coherent x-ray scattering studies of dynamics in transient networks of associative polymers which are used in applications such as artificial skin and self-healing gels

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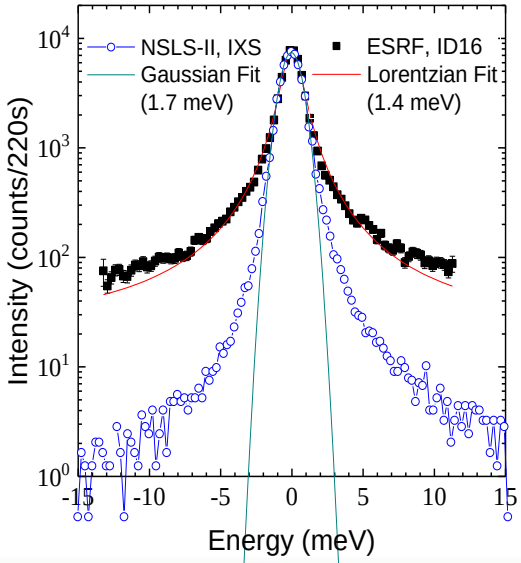
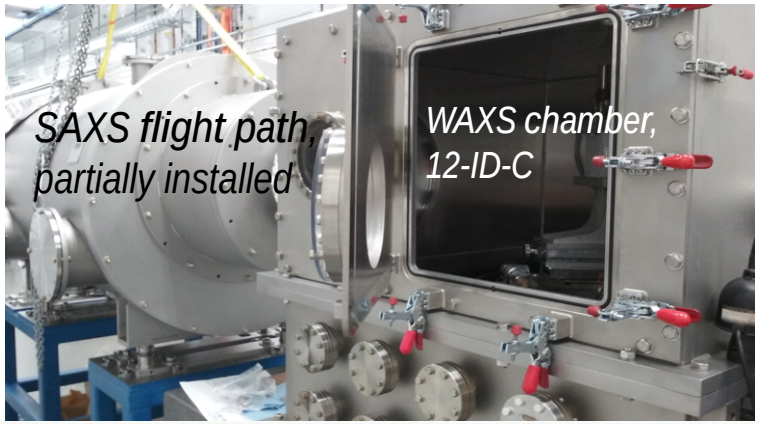


Complex Scattering Program Beamlines (2)

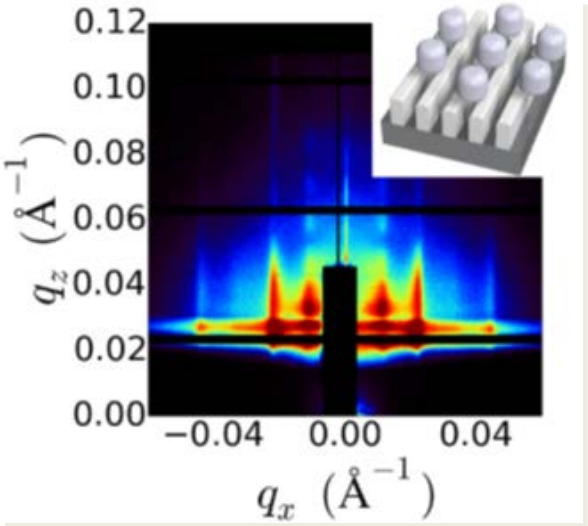
SMI – Soft Matter Interfaces

- Time-resolved SAXS, WAXS, GISAXS, GIWAXS studies at 500 Hz
- Broad energy range (2.1-24 keV) covers S, K, P, Cl, and Ca edges that are important in soft matter; a tender (2.1-4.5 keV) x-ray $q_{max} \sim 1 Å^{-1}$ is a *unique* capability.
- High energy for liquid/liquid interfaces.
- Incorporates a spectroscopy-grade DCM for resonant scans and flyscans
- Provides a variable beam focus



CMS – Complex Materials Scattering

- Simultaneous SAXS/WAXS on 3PW source
- GISAXS/GIWAXS for interfaces and thin films, including liquid surfaces; accommodates scanning-probe SAXS/WAXS.
- Tunable energy (10-17 keV) to enhance q resolution (low E) or to probe dense materials and buried interfaces (high E)

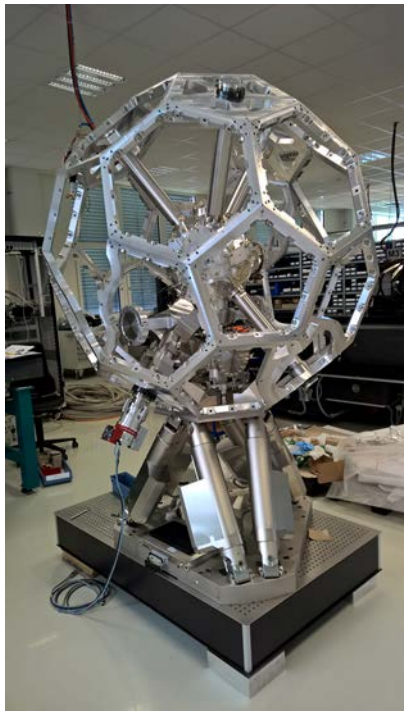


Scattering from multilayered structures via block copolymer self-assembly - A. Rahman *et al*. Nature Comm. (2016)

Hard X-Ray Spectroscopy Program Beamlines (1)

ISS – Inner Shell Spectros.

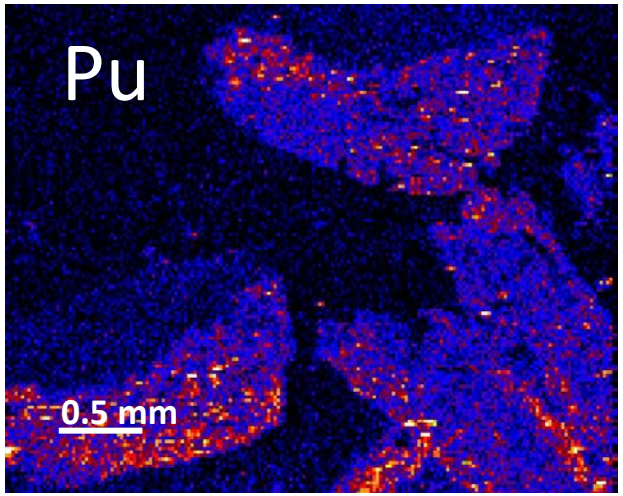
- High throughput hard X-ray spectroscopy on a DW
- Low to medium energy resolution detection
- Optimized for in-situ and operando experiments



TES – Tender Energy Spectros.

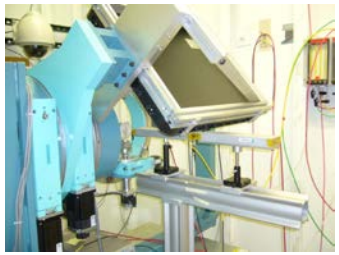
- Micro-spectroscopy beamline in tender energy range (1-8 KeV) with 10 um – 1 mm focus
- Low energy resolution detection Optimized for environmental samples; In-situ and operando end station is planned

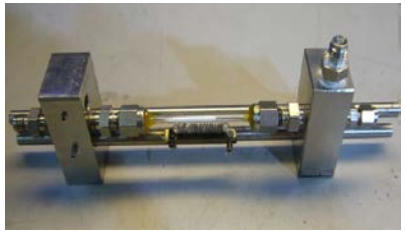
R. Tappero, P. Northrup, M. Maloubier & B. Powell



QAS – Quick Absorp. & Scatter.

- QEXAFS with powder diffraction capabilities
- Focus on low energy resolution but fast detection
- Optimized for in-situ and operando experiments
- Flexible sample environments integrated into data-acquisition system



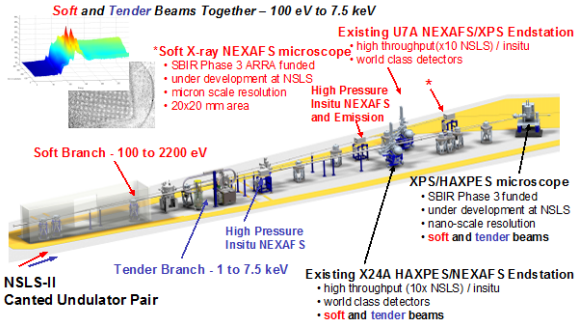


Hard X-Ray Spectroscopy Program Beamlines (2)

Structure/function relationships in advanced materials, often at the nanoscale; development of new materials into devices and systems with advanced functionality

SST-1, SST-2 – Spectroscopy Soft & Tender

- Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy
- SST1 and SST2 will have 6 unique world class NEXAFS/XPS experimental stations: 2 full field microscopes, 2 automated high-throughput stations, and 2 in-situ high pressure stations.
- Continuous selection of X-rays from 100 eV to 7.5 keV at a common focal point



BMM – BM for Materials Measurement

- X-ray Absorption Spectroscopy (XAS) and X-ray Diffraction (XRD) over the 4.7 – 22 keV energy range with tunable spot size
- End-station is equipped to provide high-quality, high-throughput XAS coordinated with an eight-circle goniometer for XRD and constant-q spectroscopy measurements such as refflexafs or DAFS.

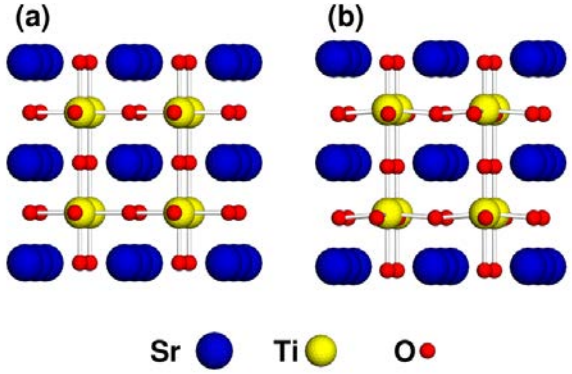


Figure 3: (a) Structure of cubic $SrTiO_3$. (b) Structure of strained $SrTiO_3$ on Si(001) as calculated by density functional theory. The structure in (b) reveals both AFD and FE distortions and has been confirmed by both XAFS and XRD. Woicik et al., Phys. Rev. B 75, Rapid Communications, 140103 (2007).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

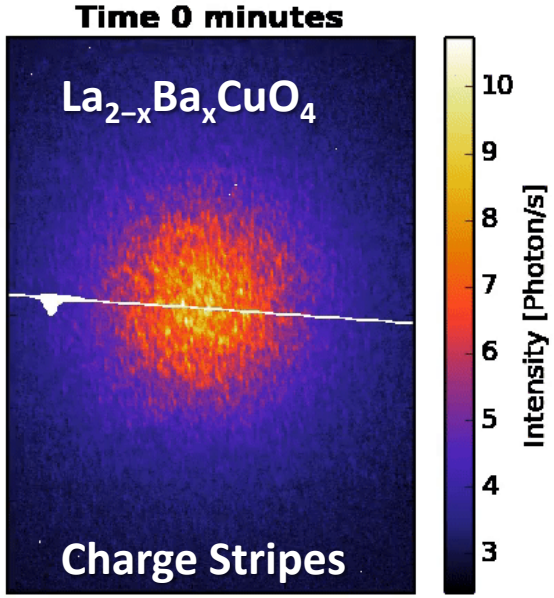
Soft X-ray Scattering & Spectroscopy BLs (1)

SIX – Soft Inelastic X-ray Scattering

- Resonant Inelastic X-ray Scattering with between world-leading energy resolution (100,000 resolving power) 165-2300 eV
- Continuous momentum transfer tunability
- Medium energy resolution available
- Optimized for measurements of low-energy excitations (charge, spin, orbital, lattice) in correlated electron systems, ultrathin films and heterostructures, heavy fermion quantum criticality, and topological phases of f electron systems

CSX-1 – Coherent Soft X-ray Scattering

- World leading soft coherent capabilities:
  - $5x10^{13}$ ph.s^{-1} coherent flux
  - Soft x-ray nanodiffraction.
  - Soft x-ray XPCS
  - Soft x-ray Coherent Diffraction Imaging
- Spatially and time resolved measurements of electronic textures in quantum materials.



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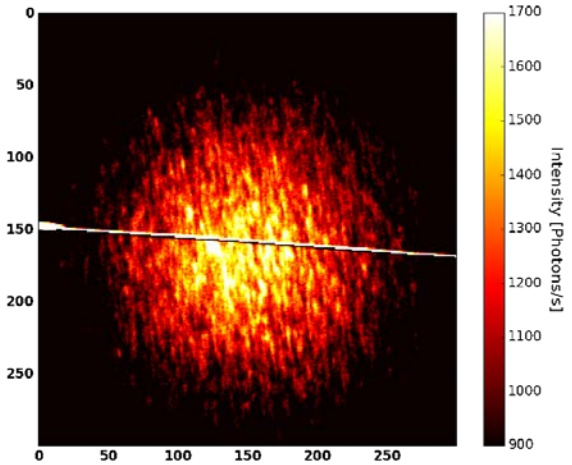
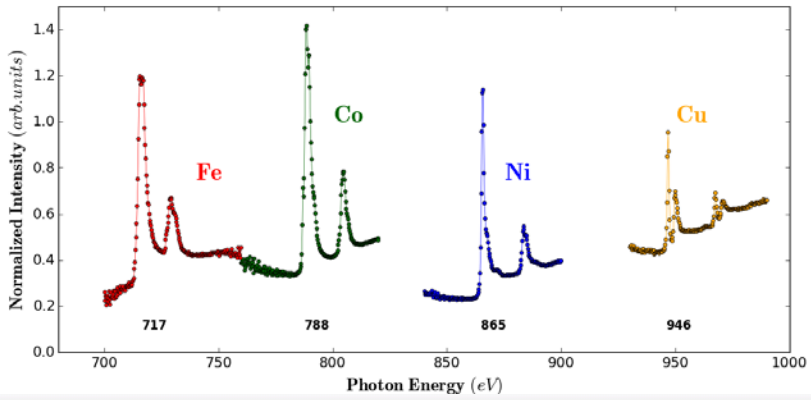
Sample translation (10 μm)



Soft X-ray Scattering & Spectroscopy BLs (2)

ESM – Electron Spectro-Microscopy

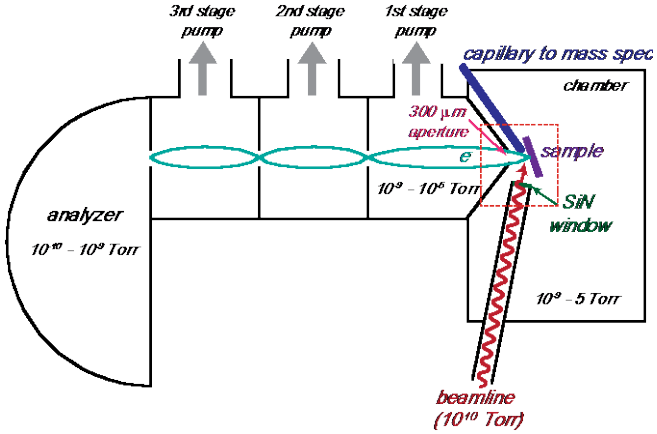
- Wide range of spectroscopies: ARPES, SP-ARPES-XPS-XAS-MLD-XMCD
- High flux over wide photon energy range: 15 to 1500 eV
- High energy and spatial resolution - scanning microscopy with 1μ lateral resolution & AC-PEEM with 10 nm lateral resolution
- Sub-meV nano-ARPES; LEEM/PEEM
- Photoemission to characterize electronic structure of functional materials w/ high spatial resolution



CSX-2 – Soft X-ray Spectroscopy

Ambient pressure XPS; probe of core levels and valance bands; sensitivity to chemical environment and oxidation state; solid-gas interfaces up to 10 torr.

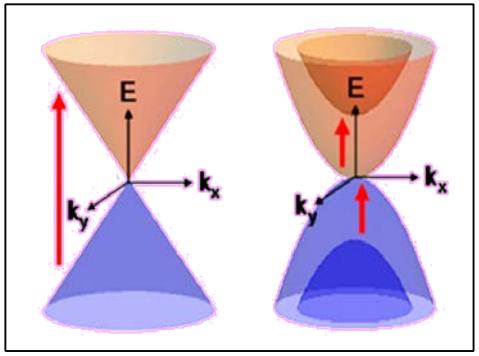
- In situ/operando XAS; probe of unoccupied states, Sensitive to: oxidation state, chemical bonding, Solid-gas (>1 atm) and solid-liquid interfaces.
- 250-2000 eV energy range with high flux (3 x 10^{13} ph.s^{-1}) and high resolution – E/ΔE up to 10^4



Soft X-ray Scattering & Spectroscopy BLs (3)

MET – Magneto, Ellipsometry, Time res. IR

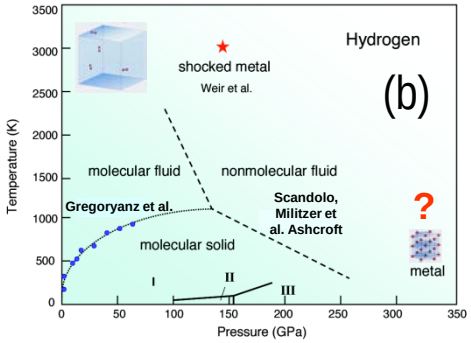
- Full infrared spectroscopic coverage for collective excitations, vibrations, and electronic transitions (0.25 – 4 eV)
- Ellipsometry for direct extraction of optical constants. Dielectric (□) and magnetic (□) response functions.
- High-field magnet (sense orbital and spin degrees) and photo-excited time-resolved for dynamics.



Electronic structure of Few Layer Graphene (FLG) can have both massless (linear) and massive (parabolic) bands

FIS – Frontier synchrotron Infrared Spectros.

- In-situ optical studies of a wide variety of materials by spectroscopic techniques at extreme P-T conditions (to several hundred GPa and 4~6000 K)
- Far-infrared to visible spectra with diffraction-limited spatial resolution
- The combination of the high brightness and low noise of NSLS-II with dedicated high-pressure facilities will be unique and world leading

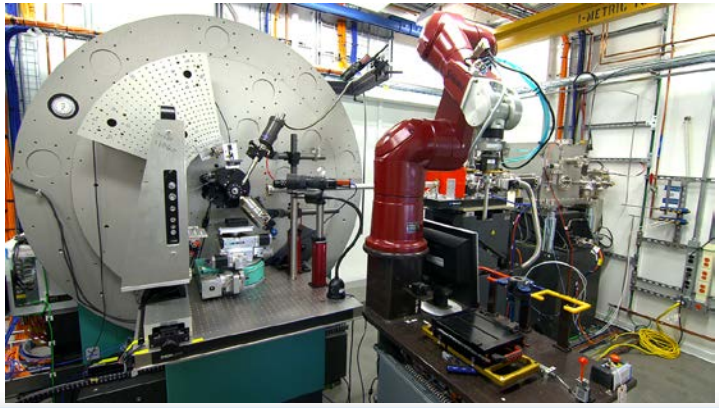


In situ high P-T optical studies of various hydrous minerals as well as hydrogen metallization at extreme high P-T conditions

In-situ Scattering & Diffraction Program Beamlines (1)

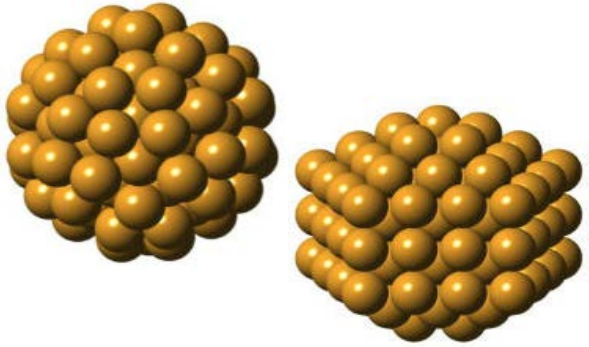
XPD – X-ray Powder Diffraction

- *in situ* or *in operando* diffraction studies with varying temperature, pressure, magnetic/electric/stress field, chemical environment, etc… from 30 – 70 keV
- Focus on areas such as materials processing, advanced structural ceramics, catalysis, hydrogen storage, and CO2 sequestration.
- High throughput powder diffraction, total scattering, and tomography with high energy resolution and sub-second time resolution.



PDF – Pair Distribution Function Scattering

- Pair Distribution Function (PDF) approach can be used to study the crystal structure of complex materials on different length-scales
- Studies of nanoscale structural fluctuations in complex materials, such as, superconductors, multiferroics, thermoelectrics, catalysts, and functional nanomaterials
- in-situ operando studies of materials at 4 different X-ray energies, 39 keV, 64 keV, 75 keV and 117 keV



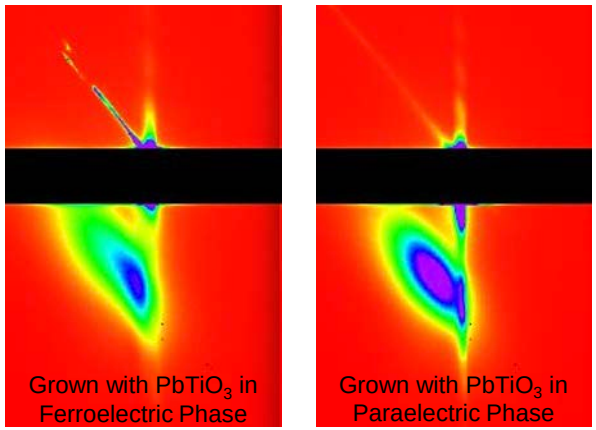
Distinct structural forms found in $Au_{144}(SH)_{60}$ – icosahedral (top) and decahedral (bottom).

K. M. Jensen and P. Juhas, M. A. Tofanelli, C. L. Heinecke, G. Vaughan, C. J. Ackerson, and S. J. Billinge, *Nature Communications*, **7** 11859 (2016).

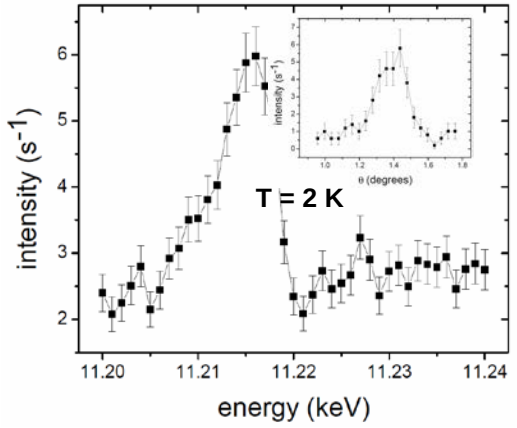
In-situ Scattering & Diffraction Program Beamlines (2)

ISR – In-Situ and Resonant x-ray studies

- Resonant diffraction at wide-range of atomic absorption edges important for advanced electronic and magnetic materials
- Tunable beam size for study of µm-sized individual domains over E = 2.4 – 24 KeV
- Full polarization control/analysis for charge/magnetic/orbital ordering studies under in-situ conditions
- Diffractometers to accommodate both portable and heavy-load in-situ chambers



Reciprocal Space Maps of 20 nm $BaTiO_3$ on Ultrathin $PbTiO_3$, Dawber Group (Stony Brook University)



Resonant Magnetic X-ray Scattering from an Iridate, Kim Group (University of Toronto)

Structural Biology Program Beamlines (1)

FMX – Frontier Macromol. Xtal.

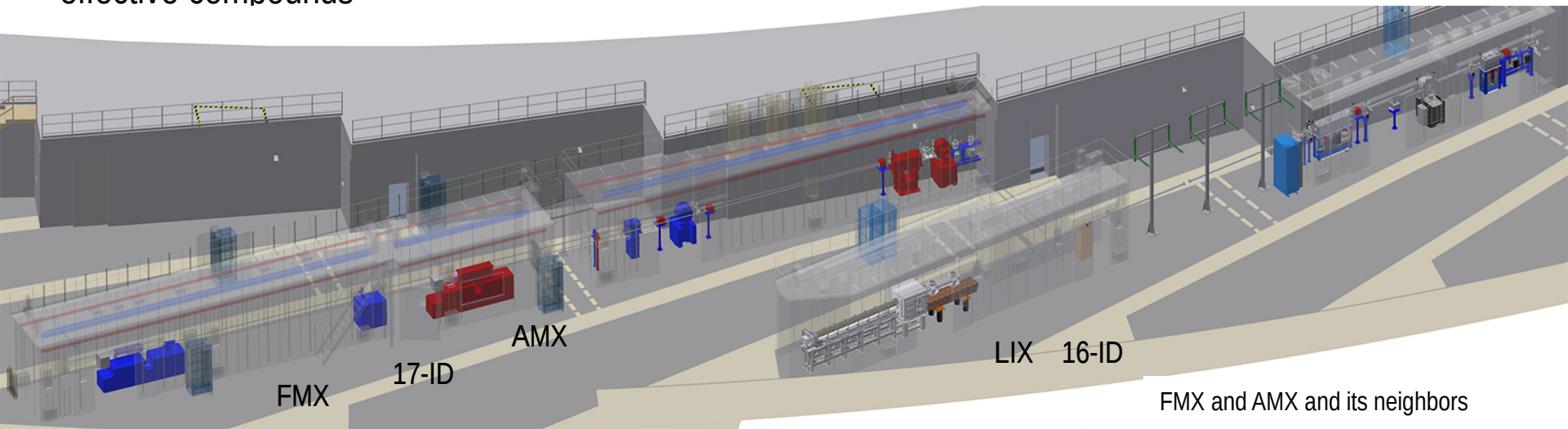
- Tunable 1µm beam of high intensity for micro-crystallographic studies of small crystals and large unit cells
- Studies of enzymatic pathways of cellular and microbiological processes
- Studies of drug-target interactions of new and improved pharmacologically effective compounds

AMX – Automated Macromol. Xtal

- Precise structure determinations with unprecedented throughput
- Atomic structure of large protein and nucleic acid complexes, including membrane proteins
- Highly automated to support remote access and extensive experimental searches

LIX – Life Science X-ray Scat.

- Time-resolved solution scattering down to 10µs
- Grazing incidence scattering from 2D solutions of proteins embedded in near-native membranes
- 1µm beam scanning probe imaging and tomography of biological tissues

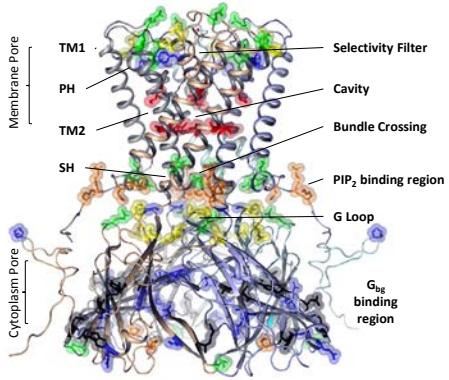


FMX and AMX and its neighbors

Structural Biology Program Beamlines (2)

X-ray Footprinting (XFP) - CWRU

- X-ray mediated hydroxyl-radical footprinting (XFP) will provide a local probe of solvent-accessibility for *in-vivo* and *in-vitro* structural studies of biomolecular complexes and their interactions.
- Time-resolved XFP studies to elucidate local structural dynamics from microsecond to millisecond time scales.



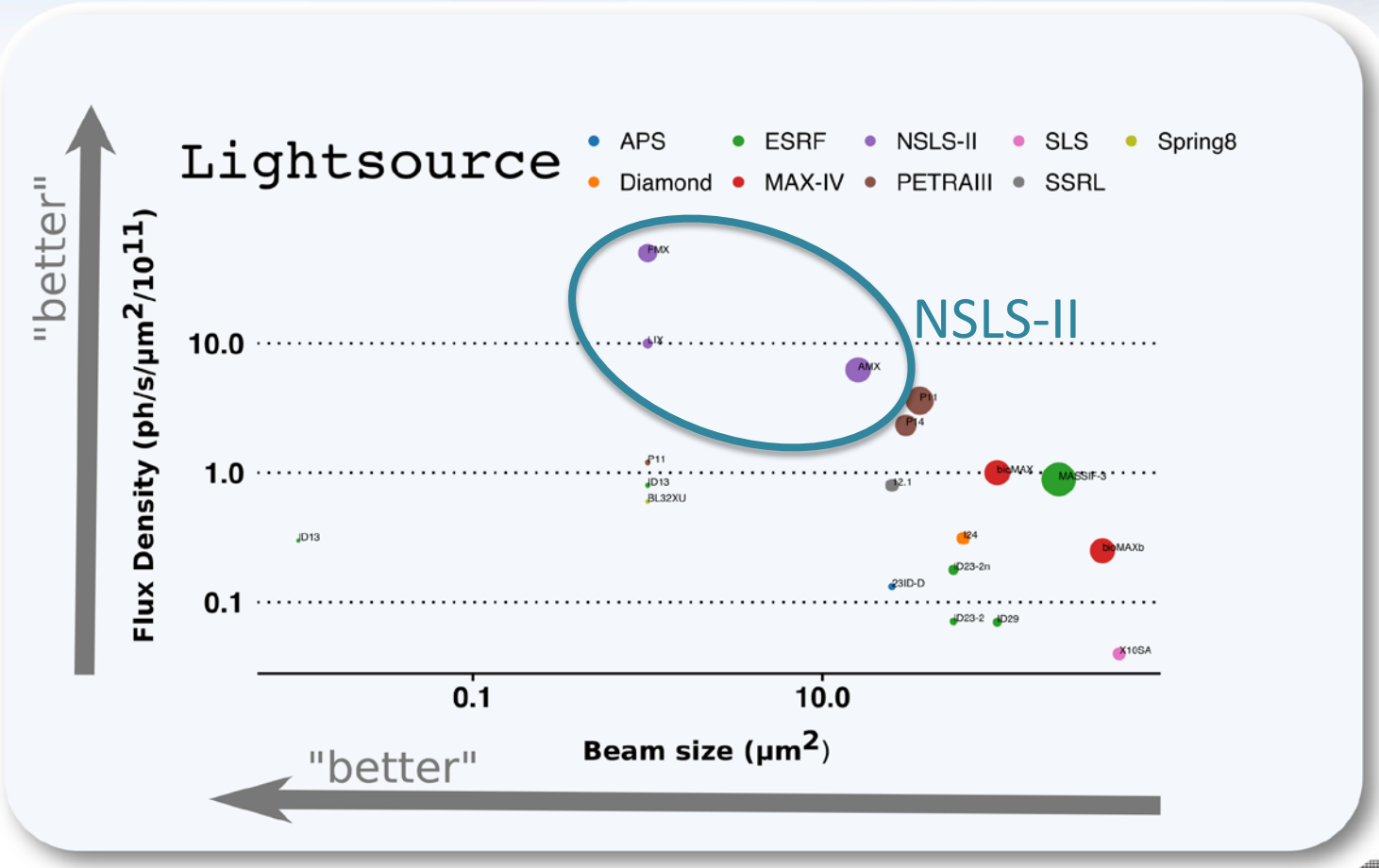
Steady state and time-resolved X-ray hydroxyl-radical mediated Protein and Nucleic Acid Footprinting

NYSBC Microdiffraction Beamline (NYX) - NYSBC

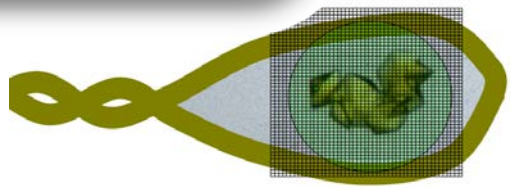
- Diffraction from micron-sized crystals and rastered scans for optimized diffraction from macromolecules and complexes
- Access to a broad range of resonant edges for anomalous diffraction (MAD and SAD) phasing, (3.5 – 17 KeV)
- Optimization of anomalous scattering at resonant edges and lower energy for increased f '‘ with light elements (sulfur)

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

NSLS-II: Brightest MX beamlines

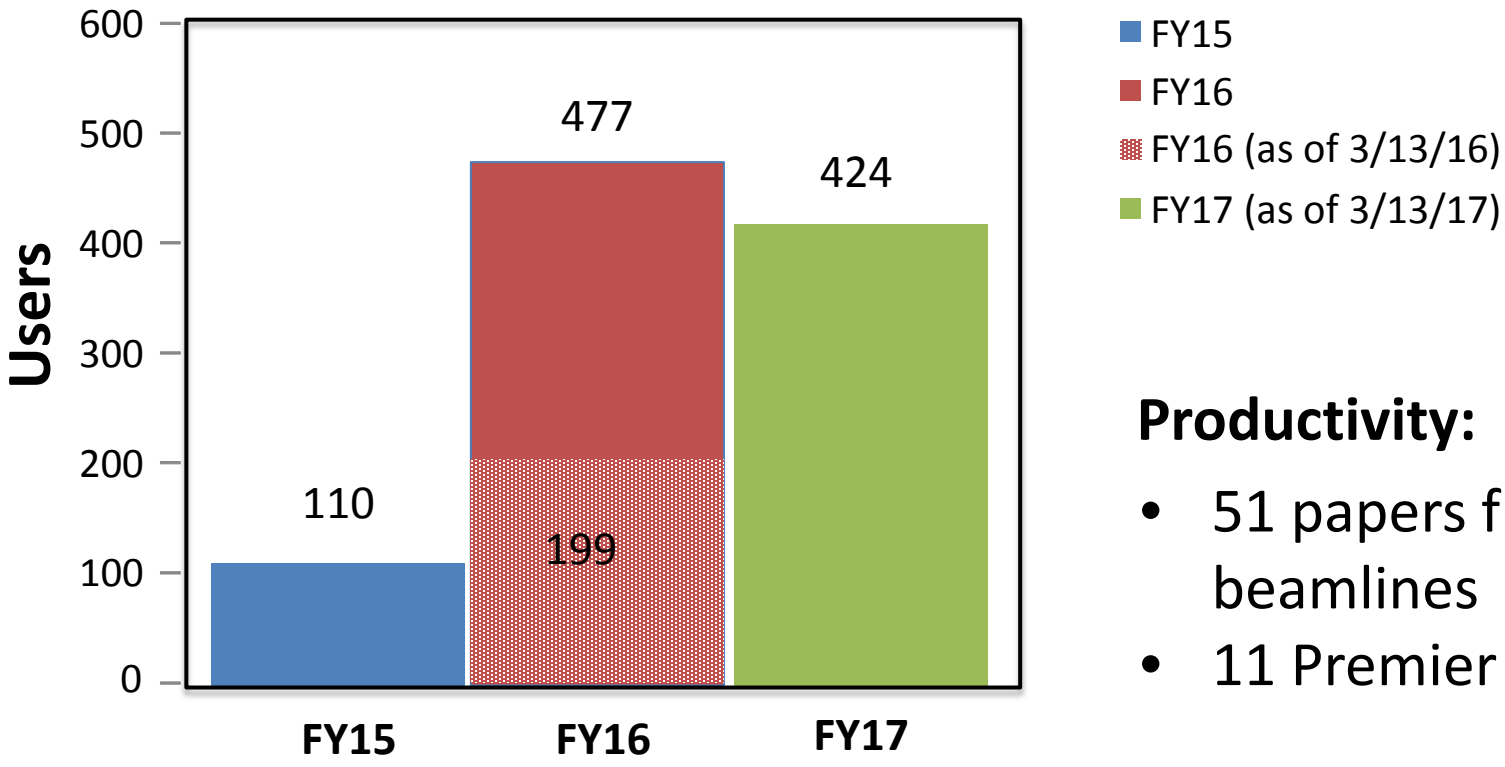


NSLS-II can change the way structural biology is done



NSLS-II Facility Users by FY

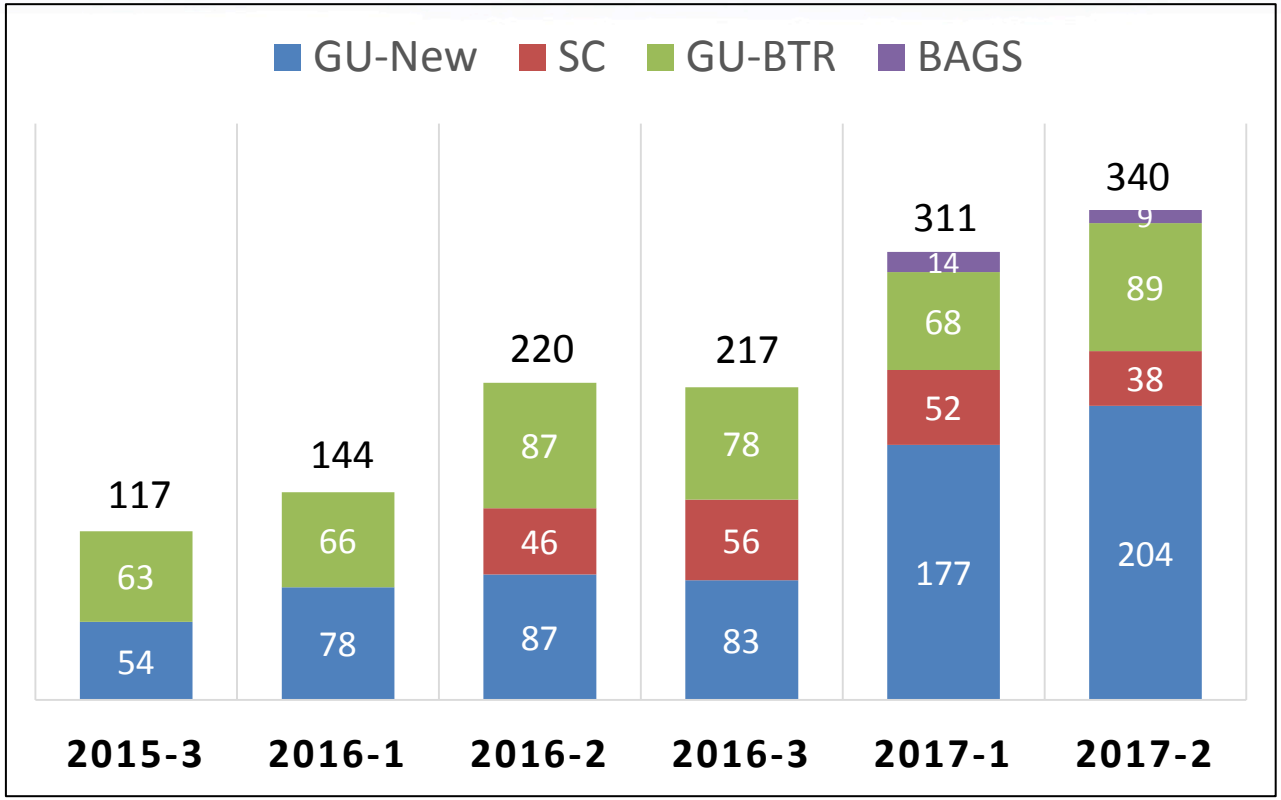
(as of March 13, 2017)



Productivity:

- 51 papers from NSLS-II beamlines
- 11 Premier

Beam Time Proposals

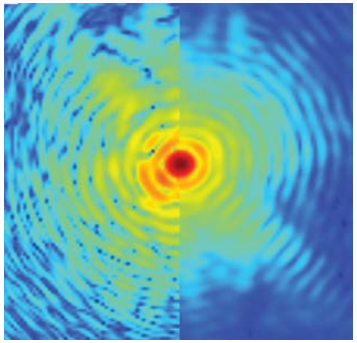


BTR: Beam Time Request (against existing proposal)
GU = General User
SC = Science Commissioning
BAGs = Block Allocation Groups

2016-1: Jan-Apr 2016
2016-2: May-Aug 2016
2016-3: Sept-Dec 2016
2017-1: Jan-Apr 2017
2017-2: May-Aug 2017

New Beamlines Planned

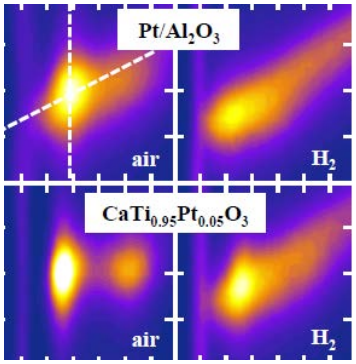
1) Hard x-ray imaging
World-leading lensless imaging down to 5nm



2) Soft x-ray imaging-1
Chemical and electronic structure down to 5 nm resolution

3) Soft x-ray imaging-2
State-of-the-art transmission x-ray microscope

4) Chemical reactions
Time-resolved snapshots of chemical reactions in-operando



5) Polymer processing and liquids
Liquid interfaces and thin film processing studied in-situ

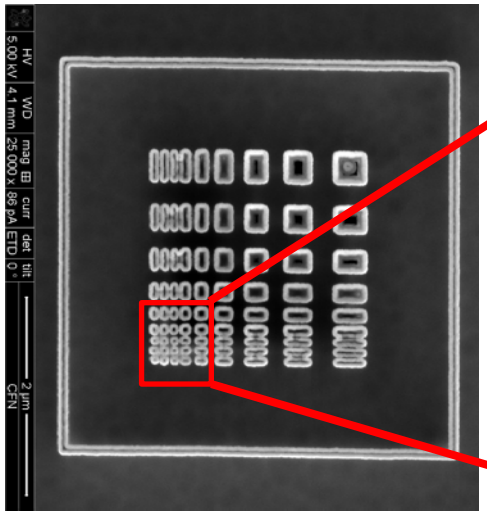
6) Infra-red spectroscopic imaging
Nano-IR spectroscopy on heterogeneous solid state systems

These beamlines will provide world-leading capabilities that will significantly enhance NSLS-II. We are working with BES and others to seek additional funds to develop and operate them.

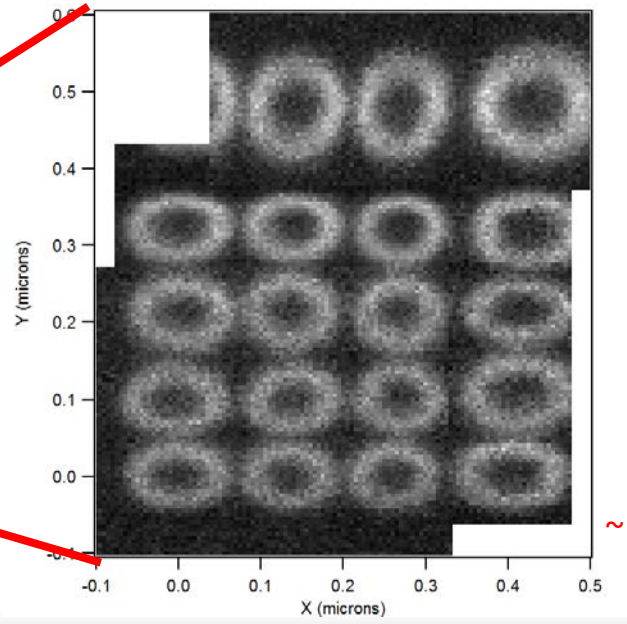
Summary

- Accelerator & beamline operations have been excellent
- The User program is rapidly ramping up
- Aggressive beamline construction and commissioning program underway for 28 beamlines by FY2019
- Advanced planning for the next round of beamline construction.

SEM image of test pattern



First benchmark X-ray image from HXN



~ 11 x 13 nm resolution