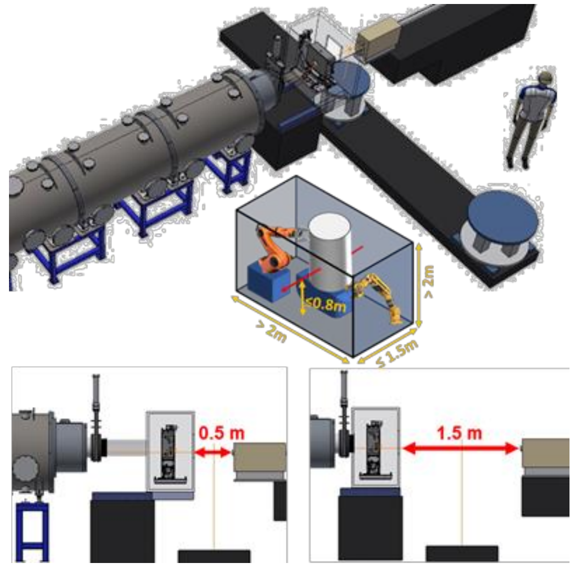
Beamline Proposal 3-letter acronyms

Acronym	Full title
AMP	Advanced Materials Processes Beamline
ANI	Advanced Nanoscale Imaging Beamline
ATM	Advanced Tender Microscopy Beamline
CST	Coherent Soft and Tender Scattering Beamline for Spectro-nano--imaging
HRD	High Resolution Diffraction Beamline
HRS	High Resolution Spectroscopy Beamline
HTS	High Throughput Soft X-ray Scattering and sSectroscopy Beamline
MAX	Massively Automated Crystallography Beamline
MCT	Micro-Computed Tomography Beamline
QCT	Quantitative Cellular Tomography Beamline
RAX	Rapid Access X-ray Diffraction Beamline
SID	Simultaneous Imaging and Diffraction Beamline
STX	Automated Scanning Transimission X-ray Microscope Beamline
TXN	Tender X-ray Nanoprobe Beamline

Advanced Materials Processes (AMP)

Technique(s): coherent and incoherent time-resolved small angle X-ray scattering ([c]-(GI)SAXS), X-ray photon correlation spectroscopy (XPCS), wide-angle X-ray scattering ((GI)WAXS), full-field imaging (radiography)
Energy range / Source: 7 to 30 keV / undulator
Beam Size: 2 – 400 µm, with variable coherence
Number of hutches: 2, FOE and large Endstation
Photon delivery system: White-beam mirror, DCM/DMM, horz. and vert. refractive focusing (transfocator)
Endstation: in-vacuum SAXS detector, ≥270º WAXS detector, positioning capabilities for ultra-large sample environments (≈3×2×1.5 m^3)



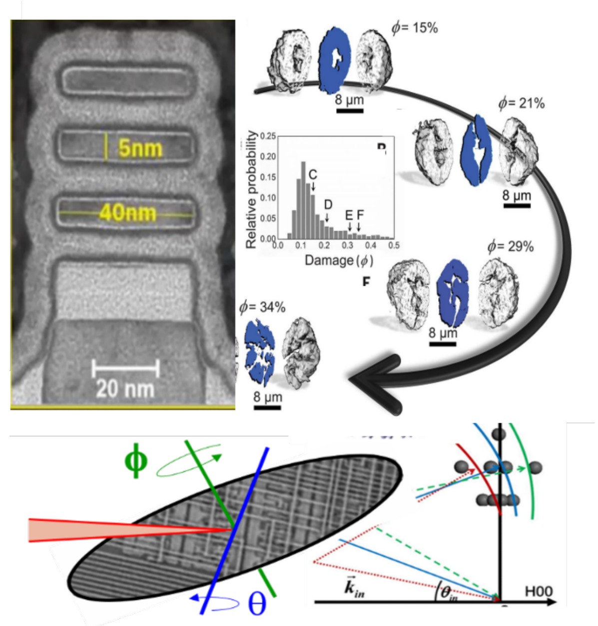
Beamline Concept
The AMP beamline is a coherent and incoherent small- and wide-angle scattering ((c)-SAXS/WAXS) beamline for time-resolved, microbeam in-situ/operando studies of materials undergoing processing or in operation under real-world conditions. AMP will be designed to measure structure and dynamics in materials, spanning length scales from Angstrom to micrometer, with micrometer spatial and tens of microsecond temporal resolution. A key feature is an ability to accommodate large sample platforms up to 3×2×1.5 m^3 and ancillary characterization techniques. This large sample area can also be used for multi-setups of medium-scale sample environments with the ability to switch automatically between different setups and accompanying X-ray beam settings.

AMP will provide a utility infrastructure commensurate with the materials processing and other sample platforms it will host. This includes power from 115V to 400V 3-phase, gas handling for hazardous gases, exhaust, utility gases (nitrogen, high-capacity compressed air), chilled water, trigger system for synchronization of sample environments and data acquisition, PLD laser, flammable cabinets and vapor delivery for metalorganic precursors.

Examples of Science Areas
The scientific mission of AMP is to provide researchers with a holistic understanding of modern materials, and the ability to delineate the foundational processes that govern their nano- to mesoscale dynamics and structure from composition through processing to device performance. To achieve this goal, AMP will provide unique multimodal scattering capabilities to unravel out-of-equilibrium, time and spatially heterogeneous processes under relevant *in-situ*/*operando* conditions, where 'relevant' might refer to industrial processing conditions or extreme operating conditions, for instance, in automotive or aerospace applications. Novel materials that can be integrated into functional structures/devices with unprecedented performance promise solutions to many of today's most critical challenges in energy harnessing and storage, sustainability and recycling, quantum information, microelectronics, transformative manufacturing and bio-preparedness with topics ranging from precision materials synthesis and processing to thin-film growth of quantum materials and 3D printed bio-scaffolds for organ growth. The selection of targeted science areas includes:

- **Transformative Manufacturing:** temporospatial material transformations and structure formation in 3D printing of soft matter, nanocomposites, and ceramics, continuous compression molding and induction welding of thermoplastics
- **High-Performance Polymers and Nanocomposites:** crosslinking, polymerization, and mechanical performance in conjunction with upcycling under real-world, industry-relevant processing conditions
- **Quantum Materials and Microelectronics:** out-of-equilibrium interfacial processes during thin film growth and ion beam nanopatterning
- **Material Discovery and Design:** *in-situ*/autonomous synthesis and assembly of novel functional nanomaterials based on robotic sample environments and auxiliary multimodal characterization

ANI: Advanced Nanoscale Imaging



Technique(s): Scanning and full-field nanoscale imaging

Source: IVU-18

Energy range/resolution:

- Monochromatic: 6-25 keV Using DCM (dE/E ~10^{-4})
- Wide bandpass: 6-25 keV using DMM (dE/E ~$3x10^{-2}$)

Spatial resolution: sub-5 nm via transmission/Bragg ptychography

Focus size: variable focus size from ~30 to ~300 nm

Focus flux: ~$5x10^{11}$ (DCM) and ~10^{13} (DMM) for 45 nm beam size

Photon delivery system: filters, water-cooled horizontal collimating mirror, cryo-cooled Horizontal DCM, water-cooled horizontal DMM, horizontal focusing mirror, vertical focusing mirror. secondary source aperture, beam diagnostics for active beam feedback.

Endstation:
One small pink-beam hutch housing SSA and beam diagnostics
One large pink-beam experiment hutch (~25 m x ~6 m)

Satellite Building: Similar to HXN (vibration isolated)

Rationale and synergies for ANI at NSLS-II:

- Offering new imaging capabilities, taking advantage of fast switching between scanning and full-field imaging for exploiting high-measurement sensitivity and large imaging volume.
- Enabling more efficient in-situ imaging with zooming capability and with diverse imaging modalities (XRF, XAS, XRD, and ptychography).
- Rapid imaging using a mono and pink beam, providing competitive capabilities against the imaging beamlines at the diffraction-limited light sources.
- Ptychographic imaging in both transmission and diffraction channels for sub-5 nm resolution with an imaging field of view up to 100 um x 100 um with about 100X faster speed than HXN.
- Full-field imaging with flexible imaging field of view up to 200 um x 200 um, using either fast projection imaging or quantitative holographic tomography.
- Laminographic tomography ideal for investigating samples on a substrate covering a wide range of classes of materials (i.e. novel processing of thin films, as fabricated semiconductor samples) with no or minimal sample preparation.
- Compressive diffraction imaging capabilities using two angular degrees of freedom for the sample, energy-scanning for zero circle-of-confusion error for rocking curve, and pink beam capability.
- Correlative imaging using XRF, XANES, and EXAFS, co-registered with ptychographic/full-field imaging
- Automatic sample exchanger through a load-lock
- Capable of taking full advantage of the future enhancement of the NSLS-II emittance

Examples of Science Areas & Impact:

- Comprehensive nanoscale 3D imaging for microelectronics material systems, processing, and device integration, detecting physical, chemical, and strain defects.
- Energy materials (batteries, fuel cells, solar cells) and novel synthesis (DNA origami, additive manufacturing, non-equilibrium growth, etc), providing fundamental knowledge on nanometer-scale interfaces with a meaningful statistical analysis over a large volume.
- Investigation of material deformation in single crystalline and polycrystalline materials system.
- Biological and environmental sciences, visualizing sub-cellular organelles, neural connections in the brain, microbes, and plants.

New Beamline – Advanced Tender Microscopy (ATM) - *Best Value for your $cience*

Technique(s): High-throughput X-ray spectroscopy/imaging

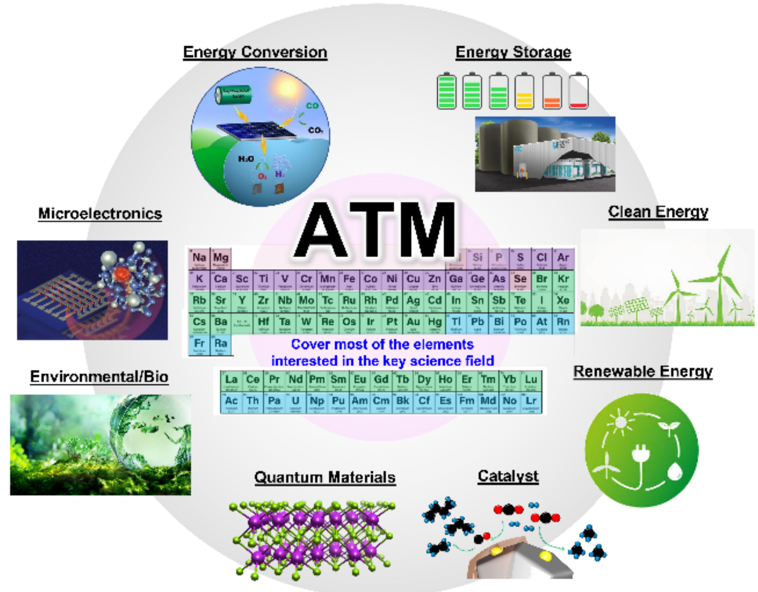
Source: 5 poles Wiggler optimized for tender x-ray

Energy range/resolution power: 1.7 – 13 keV / ~5000 InSb(111) and Si(111) From Si k-edge to Pt L-edge EXAFS

Spatial resolution: 1 um – 500 um

Photon delivery system: White-beam vertical collimating mirror, re-direction mirror, vertical DCM, pre-focusing mirrors, redirection mirror, secondary source aperture, in situ BPMs

Endstation: Include two sections: a high-throughput XAS section upstream of the SSA; a micro-beam (KB-focusing) autonomous section to provide comprehensive x-ray imaging, XAS, and laser micro-Raman techniques.



Rationale and synergies for ATM at NSLS-II:

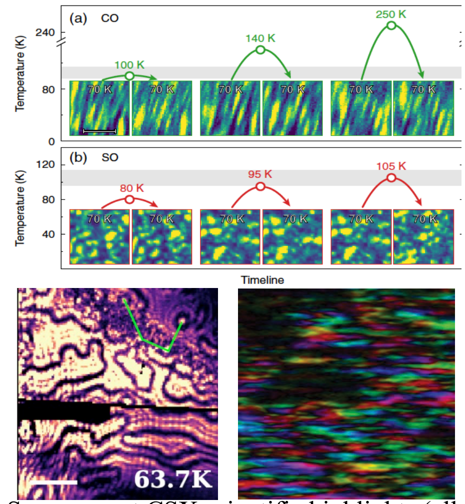
- Covers nearly all elements above Si, including >90% elements of interest in energy, catalysis, and environment fields
- There is an urgent need to increase the tender X-ray capacity of NSLS-II to meet the growing interest of the user community. Tender X-ray capabilities are in great demand with few existing beamlines in the DOE user facility complex and worldwide, and with only one tender X-ray beamline at NSLS-II (TES).
- Support diverse and productive scientific community, including hydrogen generation/storage, CO_2 capture, energy storage, biomass, molten salt materials, quantum material, high-entropy materials, biology, environmental science, etc.
- Unique combined X-ray/Raman imaging capability is greatly attractive to energy storage, biology, and environmental science
- Synergy with existing NSLS-II beamlines for energy research by linking and filling in the gap of photon energy spectrum between soft (IOS) and hard (SRX, HXN, ISS, QAS) X-ray energy range.

Examples of Science Areas & Impact:

- Energy storage: a comprehensive beamline for the all majority of next-generation battery systems, including advanced Li-ion batteries (e.g., disordered-rocksalt, high-entropy materials, Si anode), beyond-Li batteries (e.g., Na/Ca/Al/Mg/K/Zn-ion batteries), Li-S, and all-solid-state batteries (e.g., sulfide/halide-based system) that are required a wide range of elements covering Si, S, P, and 3d metals at the same beamline. The combined X-ray imaging, XAS, and laser Raman techniques can identify materials invisible to a single technique, such as the polysulfide in Li-S batteries, and significantly improve reliability of the data.
- Clean and renewable energy: provide insight into the structure-function relationship and improve design for catalytic materials important in fuel cells, biomass conversion, CO_2 capture, and H_2 production/storage, many of which contain Si, S, P, Cl (e.g., zeolites, metal sulfides, Cl-doped carbon nanostructures), which can only be studied with tender X-rays.
- Quantum information science: investigate how the structural, chemical, and electronic properties of materials in superconducting transmon qubits, e.g., Nb and Ta (L-edge), affect device coherence times.
- Energy conversion: a comprehensive beamline for developing better perovskite solar cells (e.g., ABX_3, B = Pb/Sn, X = Cl/Br/I) with higher efficiency and lower cost; developing advanced molten salt materials (e.g., Cl, K, Ca, Zn, etc.) for the next generation nuclear power plant.

New Beamline – CST (Coherent Soft and Tender x-ray scattering for spectro-nano-imaging)

Technique(s): Resonant Elastic X-ray Scattering (REXS), X-ray Photon Correlation Spectroscopy (XPCS), Nanodiffraction (NanoD)
Source: 2x Elliptically Polarizing Undulator (EPU) with Phaser
Energy range / resolution: 450-5000 eV; $E/\Delta E \sim 5*10^3$
Spatial resolution: ~ 50 nm
Photon delivery system: Horizontally bouncing mirror for power management, Variable-Line-Spacing (VLS) monochromator (vertical focusing) with multiple gratings, horizontal bouncing mirror (horizontal focusing and harmonic rejection), exit slits/pinhole for resolution management and coherence extraction.
Endstation: Horizontal diffractometer (including azimuth and UHV belt/triple rotating flange), zone plate optics, fast 2D detector (out of vacuum), polarization analyzer, energy filter, UHV SDD detector for nano multimodality, full cryogenic sample capability incl. cryo-transfer and electrical contacts via load lock, fast chopper for time resolved measurements.



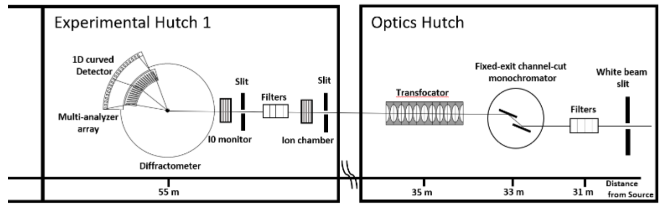
Some recent CSX scientific highlights (all coherence limited), paving the way for even greater achievements at CST.

Rationale and synergies for CST at NSLS-II:
CST will build upon important coherence-based achievements at CSX, by expanding previous capabilities with a dedicated and optimized configuration for fast XPCS, high resolution nanoD, and advanced imaging at Q>0. Additionally, for these techniques CST will extend the photon energy range from the soft to the rich tender X-ray regime, thereby accessing several absorption edges relevant for DOE mission need areas. This will include Rare Earths, 4d and 5d ions, lanthanides, and the lighter actinides. Within strongly correlated electron systems, CST main programmatic targets are microelectronics, QIS, and energy related materials. As such, CST will form a synergistic partnership with other NSLS-II beamlines including: CSX (dedicated to slow orderings by soft REXS, surface scattering/reflectivity, and advanced imaging-mode coherent spectroscopies), SXN (STXM and ptychography in transmission only), ISR (hard X-ray REXS), and HXN (hard X-ray structural imaging).
Overall, CST will be a unique instrument worldwide, a world-class beamline and instrument for fast and stable imaging of electronic orderings and investigation of collective, interacting dynamics. In tandem with the future upgrade of our accelerator (NSLS-II U), CST will allow NSLS-II to lead in coherence-based techniques over the years, by providing full spatial coherence through the tender X-ray range. In particular, it will excel in performing fast and highly entangled time-space measurements, it will implement Orbital Angular Momentum control of the impinging beam from day-1, it will provide in-situ and in-operando capabilities with load lock access. It will also allow proof-of-principle demonstration of coherent-RIXS techniques.

Examples of Science Areas & Impact:
- Strongly correlated electron systems: CST will provide another significant jump in the field, just as CSX did starting in 2015. CST will push for even faster time scale measurements using fast, in-air, flange mounted detectors and will optimize time/space resolution based on newly developed approaches to more photon hungry techniques;
- QIS: CST will provide in-situ and in-operando capabilities for proxy measurements down to mild cryogenic conditions. Together with the use of high photon energies, this will enable crucial measurements to disentangle the role of strain from electronic defects and inhomogeneities (microscopic self-organization);
- Spin-orbit phenomena: the capability of accessing resonances in high Z materials will provide the opportunity of investigating spin-orbit driven phenomena directly, and study the effect of spin injectors and valves with spatial and temporal resolution under in-operando conditions;
- Exotic electronic orderings (nuclear waste oriented): CST will enable studies of the electronic structures of radioactive materials, to understand their role in interacting with the environment and their unique characteristics in terms of electronic orderings and dynamics.

High Resolution X-Ray Powder Diffraction (HRD)

Techniques: powder diffraction; diffraction mapping; thin film diffraction



Source: IVU (Ve divergence of the photon beam ~10µrad matches monochromator and analyzer crystal acceptances)

Energy range / resolution: 6-25keV / ~1.2×10^{-4} $\Delta E/E$

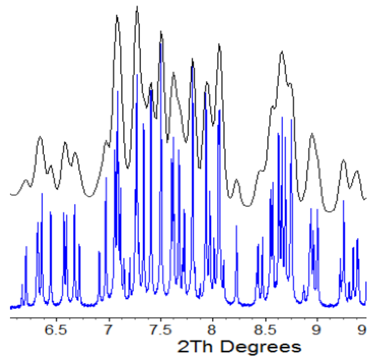
Spatial resolution: variable, 10µm up to 0.5mm

Photon flux: ~1.2×10^{12} photons/s in a $(0.5mm)^2$ spot at 20keV

Time resolution: seconds

Photon delivery system: LN_2-cooled Double-Crystal Mono, CRLs, no mirror. Mininal cost and technical risks.

Endstation 1: 3-circle servo diffractometer; array of analyzers in fly-scanning mode; pixelated area, photon counting detector with time-stamping (ms) and energy discrimination (harmonic rejection) (in house R&D); robot; shared in situ capabilities.



Gadolinium and Uranium based Salt Inclusion Materials (SIMs) for nuclear waste handling. Courtesy of S. Gill (BNL), G. Morrison (U. of South Carolina). Top: 28ID data. Bottom: high resolution (APS).

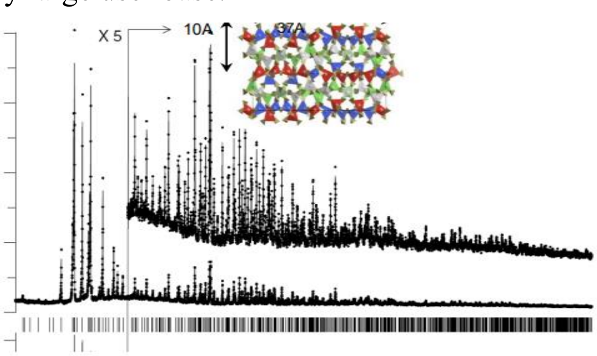
Rationale and synergies for HRD at NSLS-II:

- Cutting edge fast operando/in situ experiments with super high resolution (at the moment, time scales below minutes in the high-resolution mode are not achievable in the US)
- Beam focusing for combining spatial resolution and high Q-space resolution (novel in the US)
- Highly automated high throughput (materials discovery, standardized environments)
- Intuitive user ops (minimum set of adjustable start-up parameters, fast acquisition, rapid turn-over)
- Merges core information technologies, robotics and AI/ML (data quality sweep, autonomation and on-the-fly data analysis) in an "internet of things" approach
- A long-due solution to the source-performance limitations and the oversubscription of the only dedicated high-resolution instrument in the US
- Powerful addition to existing beamlines tailored to higher energy, fast diffraction with modest resolution

	High acquisition rate and S/N	High data quality and resolution	Qualification
APS 11BM-B		X	slow and clean
NSLS-II 28ID	X		fast and dirty
This proposal	X	X	fast and clean

Examples of Science Areas & Impact:

- Predictable high impact in such fields as: chemistry, structural physics, pharmaceuticals & drug design, environmental, earth & planetary, engineering, energy storage and conversion, nuclear, advanced manufacturing, and quantum sciences.
- Very large user base.



Low Temperature diffraction pattern of the candidate H_2 storage material $Mg(BH_4)_2$. The aim is to solve the structure operando under high gradients (H_2 pressure, T) rather than on recovered samples. High peak separation power, in situ and seconds time resolution are needed to see intermediate states during decomposition without compromising data quality.

Transient phases can be missed at 11-BM-B because they appear and disappear too fast. They also can be missed at 28ID because the diffraction patterns do not show enough details.

New Beamline – High Resolution X-Ray Spectroscopy (HRS)

Techniques: High resolution X-ray emission spectroscopy with pink and monochromatic beam for bulk measurements and microscale emission imaging, elastic and inelastic X-ray scattering.

Source: IVU (U20)

Energy range: 3-24keV

Spatial resolution: variable, 1µm up to 0.5 mm

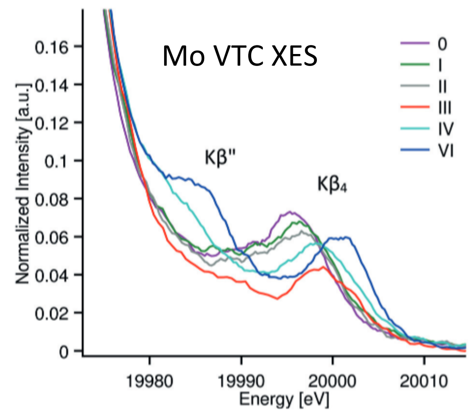
Energy resolution: incident beam < 5×10^{-5} ΔE/E (monochromatic) + ~1×10^{-2} ΔE/E (pink),

Photon flux at sample: 5×10^{13} monochromatic, 5×10^{15} pink

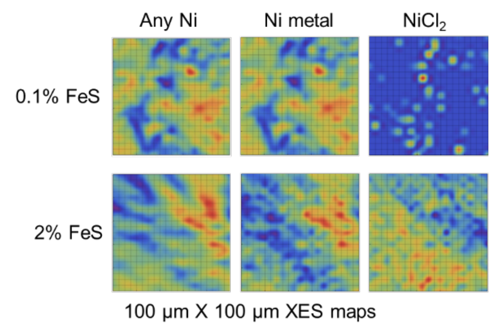
Time resolution: 1 ms, down to 100 ps for time-resolved studies

Photon delivery system: High heat load mirror, LN_2-cooled multilayer monochromator, Si(311) high resolution monochromator, focusing mirror pair, a variable focus CRL assembly.

Endstation: high efficiency multi-crystal dispersive spectrometer and backscattering analyzer, combined with heavy duty sample environment positioning system.



Valence-to-core XES with pink beam opens up new opportunities for understanding the electronic structure of TMs (from 10.1002/anie.202003621)



XES mapping is capable of producing chemical information on multiple elements on a time scale of a conventional XRF experiment

Rationale and synergies for HRS at NSLS-II:

We propose an instrument that will allow to probe materials properties in operando, from a millimeter to micron-sized features, zooming in and out like a photographer's lens. Imaging using emission spectroscopy adds chemical information and using the pink beam accelerates the mapping speed by orders of magnitude. This unique instrument will bridge the existing imaging and spectroscopy capabilities available at NSLS-II. With the help of dedicated crystal spectrometers, comprehensive information on the chemical structure and dynamics will be obtained. Leveraging these spectrometers combined with the ability to readily switch between pink and monochromatic beams, HRS will deliver speed, throughput, and high energy and spatial resolution. Driven by an expert user, and/or artificial intelligence, HRS will provide the overall picture of the system and then home onto the regions of interest, critical to the system performance.

Examples of Science Areas & Impact:

- Heterogeneous, electro- and photocatalysts, battery and fuel cell materials where overall performance is determined by processes at multiple length scales
- Nuclear materials, molten salts and related corrosion processes
- Carbon sequestration and storage, materials for environmental remediation
- Hydrogen production and storage

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New Beamline – HTS (High Throughput Soft X-ray Spectroscopy and Scattering)

Technique(s): X-ray Photoemission Spectroscopy (XPS), X-ray Absorption (XAS), Near Edge X-ray Absorption Fine Structure (NEXAFS), X-ray Magnetic Circular Dichroism (XMCD) and soft X-Ray Reflectivity and Magnetic Scattering (XR&MS).

Source: Bending Magnet or 3PW

Energy range / resolution: 40-2000 eV E/ΔE ~1E4

Spatial resolution: < 10µm

Photon delivery system: Collection optics, Focusing Variable-Line-Spacing Plane Grating Monochromator with three gratings, and exit optics to refocus the X-ray Beam.

Endstation: XPS, XAS, and XR&MS capabilities. Sample preparation chamber with full surface treatment capabilities. Fully automated acquisition, preparation, transfer, and data processing for high-throughput material studies.

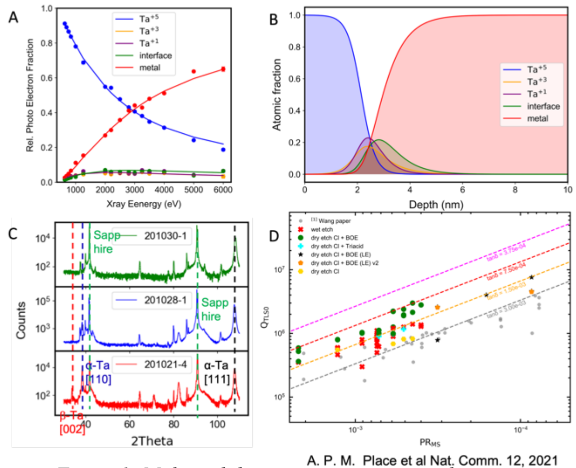


Figure 1: Multimodal investigation into correlation between material properties and qubit performance using: photon energy dependent XPS (A), Conversion of A to a depth profile (B), X-ray diffraction (C) and microwave loss measurements (D.)

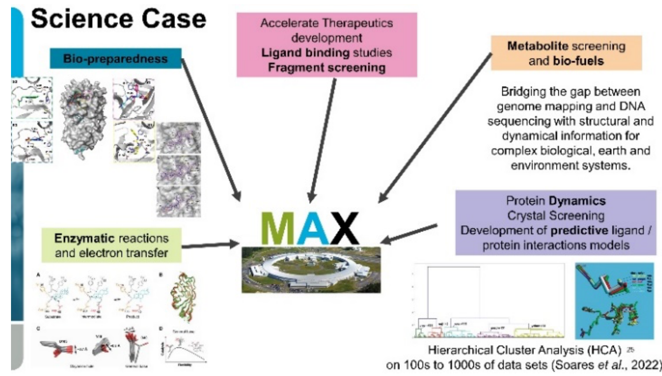
Rationale and synergies for NSLS-II:

- Allows high throughput material characterization to understand chemical, structural, and magnetic variation to aid in improving performance of technologically relevant materials by providing enterprise soft X-ray spectroscopy and scattering techniques quickly and effectively, providing complementary capabilities to IOS (ambient pressure) and SST (tender energy range).
- Energy range from 40 eV to 2000 eV will allow for a wide range of applications, and a highly versatile instrument including reaching the highly sought-after Li edge (not currently possible for XAS at NSLS-II) and the edges from all other battery materials at thee one beamline.

Examples of Science Areas & Impact:

- Quantum Materials: Insight into mechanisms for performance losses in quantum devices.
- Energy Materials: Insight into the relationship between chemical state and performance of energy materials.
- Magnetic Materials: Insight into Multiferroics, topological magnetism and spintronic properties and how these can be utilized in devices.
- Real-time interfacial roughness, film density and thickness for processing conditions to complement spectroscopy results – bridging the gap between surface and bulk.

New Beamline – Massively Automated Crystallography (MAX)



Technique(s): Macromolecular Crystallography (MX)
Source: 3 m IVU (short straight low β section: 15-ID)
Energy range / resolution: Fixed energy: 18.5 keV (3-5 eV)
Spatial resolution: 2-10-20 µm; discrete and selectable
Number of hutches: Two, including FOE
Photon delivery system: IVU**:** cryocooled Si(111) DCM (V-bounce), CRLs (pre-focusing): > 2 10^{12} ph.s^{-1}
Endstation: cryo-stream, microDiffractometer, 2D CRLs focusing lenses, two high capacity sample changers, 1 six-axis robot and high DQE area detector (> 2000 Hz), beam conditioning and diagnostics
Estimated Size of User Community: >150 unique users/year

Rationale and Synergies for MAX at NSLS-II

- Provides a dedicated instrument available to the community studying these science cases:
  - . bio-preparedness
  - . metabolite screening and bio-fuels
  - . accelerate therapeutics development using ligand binding studies and fragment screening
  - . enzymatic reactions and electron transfer
  - . protein dynamics
  - . development of predictive ligand / protein interactions models
- Provide a unique high-throughput dedicated instrument for crystal screening
- Complement the highly automated high-throughput AMX beamline.
- Complementing FMX by releasing it from such studies so it can focus on the most advanced and challenging experiments down to 1 micron.
- Instrument optimized for samples > 2 µm with adequate capability to perform automated rasters
- Will provide world-class highest throughput for ligand-binding studies: ~ 3000 data sets / day (extreme case)
- Support a diverse and productive scientific community.
- Using expertise from building AMX/FMX for automated operation, with complete data-base recording of the experiment, and pipe-lined data analysis, we will produce a robust, stable, reduced complexity, fully automated beamline. Support will be one technical staff, one Science Associate, and 2 Scientists.

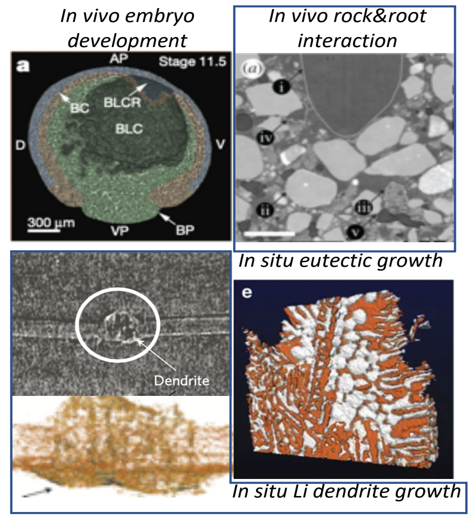
Examples of Science Areas & Impact

- Rapid development/optimization of drug candidates for upcoming pandemics
- Metabolite screening for bio-fuels research and BER topics
- Drug development: rapid screening of cancer-drug targets & next generation drugs
- Therapeutics including viral recombinant proteins
- Vaccine design
- Fragment screening for accelerated therapeutics development
- Protein dynamics from many crystals (1000s) and Hierarchical Cluster Analysis
- In partnership with a BNL lab: screening of up to 5000 samples per day (~ 5 crystals per mount)
- Improving protein/ligand prediction models

Additional Remarks (optional)

- Key aspect of MAX proposal is that advanced data analysis will be provided for every samples with optimized workflows and pipelines developed for each of the science cases.
- Unattended operation of the beamline with no local users, no remote user.
- For the bio-fuels and metabolite projects: will be associated with an extensive chemical library for high throughput screening at the NSLS-II crystallization facility
- End-Station will be temperature/humidity controlled to further increase throughput.
- Optimized for samples: < 400 Å cell and ~ 1.4 Å resolution.
- Area detector optimized for 18.5 keV and with framing rate greater than 2000 Frames Per Second (FPS)
- Dedicated software for autonomous operation (automation, decision making and self-recovery)
- Dedicated long term storage (5 years) and computing (1200 cores) for automated real time processing and post processing.
- Advanced data processing and analysis software tools for automated structure solution including ligand recognition and fully refined structure. For fragment screening studies, structure ensembles will be further refined and upgraded ligand with increased binding will be extrapolated.
- Double gripper with 2 high-capacity sample Dewar (up to 80 pucks).
- Protein dynamics studies necessitating data collection at ambient temperature will also access FMX beamline.
- Metallo-enzyme studies necessitating access to flexible energy will access AMX and FMX resources.

New Beamline – Micro-Computed Tomography (MCT)



Technique(s): X-ray absorption and phase CT
Source: High-field (>1.8T) 3PW@end of a high-β section
Energy range / resolution: 5 to 50 keV / ~2%BW
Spatial resolution: 1 – 20 μm variable/50x10mm^2 max FOV
Number of hutches: 3, including FOE
Photon delivery system: Bendable white-beam mirror, double multilayer mono, white beam filter box
Endstation: μ-CT setup with fast detector, various in situ environment controls including furnace and loading devices
Estimated Size of User Community: ~150 unique users/year

Rationale and Synergies for MCT at NSLS-II
- Provides large-volume, high throughput, and fast morphological characterization capability that is a popular and productive routine technique at almost all other synchrotron facilities but currently not available at NSLS-II.
- Improve multi-modal and multi-scale imaging capabilities of NSLS-II, complementary to nano-imaging beamlines FXI and HXN and other NSLS-II microprobes in studying complex systems that have hierarchical structures under real conditions in real time.
- Supports diverse and productive scientific community.
- Provides key techniques required for multidimensional studies at NSLS-II.

Examples of Science Areas & Impact
- *in situ* tests of structural materials (including additive materials) fatigue behavior under cyclic loading and corrosive environments
- *in situ* observation of alloy solidification processes
- *in situ* high-resolution imaging of water generation and transportation in fuel cells
- *in situ characterization of solid-state electrolyte morphological structure evolution in Li-battery cycling*
- high resolution morphological structure characterizations of novel biomimetic materials
- noninvasive internal structure imaging of precious paleontology materials
- complex geo-materials' chemo-physical structural change under high temperature and pressure
- structural imaging of biological and environmental systems in complementary to elemental imaging at NSLS-II
- *in vivo* physiological imaging of living organs/animals

Additional Remarks (optional)
- Every major synchrotron facility in the world has at least one dedicated micro-imaging beamline. For instance, the beamline 2-BM at APS regularly welcomes about 50 user groups and generates more than 40 journal papers every year, including quite few high-impact papers on journals Nature/Science/Acta Materialia etc. every year. The demands to such a beamline were well echoed in the NSLS-II Science Strategic Workshops on November 2019.

Quantitative Cellular Tomography - QCT

Technique(s): Soft x-ray tomography (SXT)
Source: Bending Magnet
Energy range/resolution: 200-1000eV
Spatial Resolution: 20-50nm
Hutches: 1 including FOE
Photon delivery system: Mirror zone-plate
Endstation: transmission soft x-ray microscope with correlated fluorescence microscope.
User Community: > 100 unique users/year

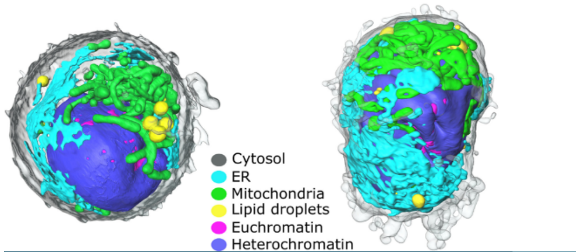


***Figure 1**. 3D renderings of native and fixed human B lymphocytes of cell line GM12878. Valentina Loconte et-al, https://doi.org/10.1016/j.crmeth.2021.100117*

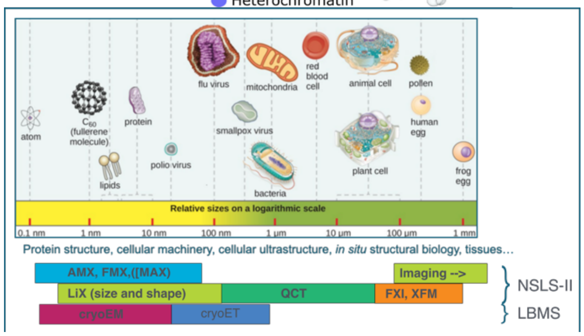


***Figure 2**. The interplay and overlap of instruments available at NSLS-II and the LBMS for the study of biosciences. The QCT beamline fills an essential niche in the length scales to be covered to enable coverage across the biological scales.*

Introduction

A formidable challenge amongst biologists, is the ability to design an imaging experiment in near-native conditions. This is difficult to achieve because many imaging techniques involve manipulation, such sectioning for TEM, which can **disrupt** the cellular ultrastructure, or fluorescent labelling, which can bias one's measurements to labelled components, thus **excluding** observation of other cellular compartments. Furthermore, few methods capture the entire cellular volume at once, and therefore lack a comprehensive snapshot of the dynamics and changes to the cell resulting from the experiment. Incorporating Quantitative Cellular Tomography (QCT) within the biologist's toolkit produces 3D renderings of the cellular ultrastructure as shown in Figure 1 above. Importantly, preparing samples for QCT measurements **circumvent mechanical manipulation of the sample**, **and the bias created from other imaging techniques**, since it requires no labels. This is accomplished because the soft x-ray energies proposed at QCT are within the "water window:" an X-ray energy range above the absorption edge of Carbon, but below that of Oxygen, that creates contrast between the carbon rich organelles of the cell (the ultrastructure) and water, producing reconstructions like that in Figure 1.

Examples of Science Areas & Impact

Scientific applications include **quantification** of both **temporal and spatial** ultrastructural modifications resulting from infection, drug treatment, or genetic modification. Only such experiments can map the progression of infections in all cell types (prokaryotes to eukaryotic cells) and are important for evaluating effective treatments of both present and future stressors on biological systems; this aligns with national science priorities. Moreover, the QCT beamline can image all biological cell types, opening the beamline to a community of scientists outside human health. For example, plant models genetically modified to improve resilience in the face of climate change can be imaged and assessed on a whole-cell level to understand the ultrastructural changes that contribute to their resilience, and one might exploit this to improve food reliability to the nation. Numerous examples of these scientific applications exist in the literature to support the use of soft-x-ray tomography, and for NSLS-II to be a world-class facility for biological research, it needs QCT as part of its portfolio to continue to lead the world in providing cutting edge science tools for the user community.

Community, Rationale and Synergies for QCT at NSLS-II

NSLS-II is optimally situated to accept all members of the proposed QCT community, from plant and cellular biologists to microbiologists, and structural biologists. It already provides a suite of structural biology under one roof at NSLS-II, obtaining results spanning the biological scales (Figure 2). One can combine results from QCT to perform large scale science with MX, cryoEM, and XFP, already in place at NSLS-II. Additionally, NSLS-II contains laboratories situated across from the proposed QCT beamline that can accommodate preparation for nearly all the cell types that can be studied at QCT. Furthermore, the HXN and hard X-ray nano-imaging beamline at NSLS-II will complement the Soft X-ray cellular imaging with resolution down to 20-30nm. Within the United States, there is only **one** badly oversubscribed SXT beamline (NCXT at ALS), and a few more in Europe; a severe deficit for the demand. Importantly, NSLS-II lies in the void of SXT facilities between the West Coast of the United States and Europe. Once it's built, one expects that the beamline will be rapidly oversubscribed.

New Beamline – Rapid Access X-Ray Diffraction (RAX)

Technique(s): X-ray diffraction (XRD), X-ray Reflectivity (XRR) and Pole figures, with robot enabled sample exchange on one endstation for high throughput, and a second endstation of a standard 6 circle diffractometer for rapid access.

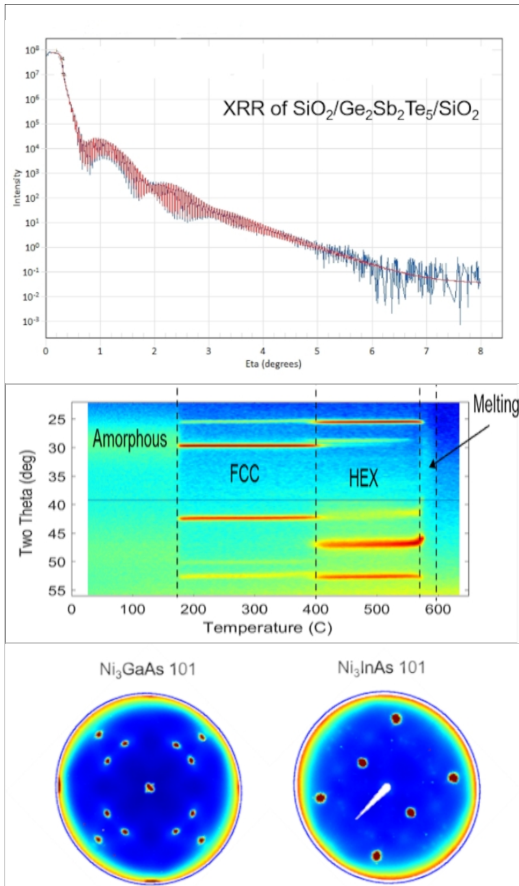


Figure 1: Top: X-Ray Reflectivity, Middle: X-Ray Diffraction (Rapid Thermal Anneal) Bottom: Pole Figure

Source: 3-Pole Wiggler

Energy range/resolution: DCM; 5-30 keV / 1E-4,
DMM; 8-15 keV / 1E-2

Beam size: 50µm (v) x 300µm (h)

Two Hutches: 1 FOE and 1 large hutch for endstations

Photon delivery system: White-beam collimating mirror, Multi-bandpass DCM/DMM mono, 2nd matching mirror.

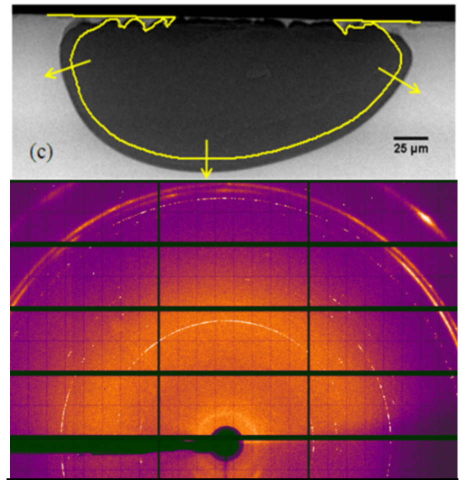
Endstations: 1) Robotic sample changer/automated remote operation and Area detector, with built in diffractometer and dedicated chamber for XRD, including static measurements and in-situ RTA up to 1100C and 50°C/s.
2) Standard 6-circle diffractometer, area detector.

Estimated Size of User Community: >50 unique users/year. Potential pool includes all thin film growth in Albany and other industrial and academic growers around the country.

Rationale and Synergies at NSLS-II: RAX is a high through-put, rapid access, diffraction-centered beamline. We anticipate switching between two access modes; 1) an overnight, highly automated mode based on a robotic sample changer and diffractometer with an option for running remotely and 2) a daytime, rapid access to a 6 circle diffractometer. The x-ray techniques here will be mostly reciprocal space mapping (XRD), x-ray reflectivity (XRR) and Pole Figures, all well established methods for materials characterization. Primary silicon monochromator enables reflectivity on thick films. Flux hungry experiments (e.g. time resolved) might use the multilayer monochromator.
Endstation 1 is optimized for thin film characterization, and is based on the IBM rapid thermal anneal (RTA) chamber, with a standard sample puck, a proven design, extensively tested, that can be mass produced and sent to users. The endstation has been used for studying phase transformations, kinetics, alloy formation, and other industrially important processes. Endstation 2 enables rapid access and enhanced experimental versatility. In the same way that the 3PW beamlines QAS, CMS and XFM all serve their respective communities, RAX could serve the diffraction community. By providing **rapid** access to reciprocal space measurements, RAX is complementary to ISR and other beamlines that study crystalline materials. RAX is also complementary to BMM, because RAX will have an offset chi circle that will enable in-situ environments like displexes, and ovens. Integration of IBM sample automation needs DSSI support.

Examples of Science Areas & Impact: Growth of **QIS relevant materials**, such as **Ta superconducting thin film Qubits**, can be studied by C2QA university collaborators, even remotely. **Microelectronics and other industries** characterizing thin film blanket or nano-patterned materials and devices can also benefit. **Materials for clean energy**, such as **CIGS** alloys (Copper Indium Gallium Selenide) or **CZTS**, have a large composition space to be explored, and the high throughput can play a key role. The 6 circle rapid access mode will allow any user project or beamline to incorporate diffraction measurements into a user science project, enabling **multi-modal** measurements that could improve the overall quality of a scientific result.

New Beamline – SID: Synchronous Imaging and Diffraction



Corrosion dynamics and chemistry observed ex-situ in two different experiments [Majid Ghahari et al., Corrosion Science 100, 25 (2015)]. At SID, this study can be done simultaneously and in-situ.

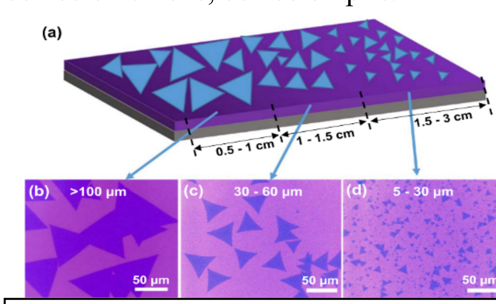
Technique(s): Time multiplexed, dual beam, imaging and micro-diffraction in harsh sample environments.
Source: in-vacuum undulator.
Energy range/resolution: 10 to 30 keV, both beams independently.
Spatial resolution:
<u>Spot size for Diffraction:</u> 1 µm size with full beamline flux and 0.5m working distance (WD). A smaller 0.1 µm size option, with reduced flux and a shorter 0.05 m WD.
<u>Imaging Resolution:</u> 1 µm with a 2 mm Field of View.
Photon delivery system: 2 monos, 2 flat mirror systems, slits, beam switch, diagnostics, micro-KB on scanning stage
Endstation 1: Two slots: 1) In-situ tomography, with high-resolution imaging camera. 2) An open slot for custom in-situ instrumentation, for example a mechanical test-rig for tomography.
Endstation 2: For large in-situ instrumentation, for instance a precision sample orientation/positioning device in growth chamber.
Both endstations use a high-resolution imaging camera and a robotically positioned 2D-detector for micro-diffraction.

<u>Rationale and synergies for NSLS-II:</u> The Strategic Planning Workshop in October 2019 expressed a pressing need for multi-modal approaches to enable the study of complex material behaviors. Emphasis was given to in-operando X-ray diffraction and imaging. We present a novel beamline design which combines these two powerful techniques into one experimental tool, and the two techniques can be applied synchronously on the same sample during an in-operando process. Two independent X-ray beams pass through separate optical systems, and are combined on the sample, where one beam is focused to a spot for spatially resolved diffraction, and the other beam is unfocused for phase contrast imaging of the sample. With a fast shutter one can quickly alternate between the phase-contrast enhanced radiography imaging and the focused micro-diffraction beam. Latter can be positioned and scanned anywhere inside the area covered by the imaging beam.

This novel tool, that allows observation of the atomic structure via diffraction, and the sample morphology through PER-imaging, in a time-multiplexed way, gives researchers a powerful in-situ probe of materials dynamics. SID is like an Electron Microscope, in that one can use imaging to locate ROIs, and then use the micro-diffraction beam interactively to obtain local structural information. Another type of experiment that SID enables, is to constantly switch beams and record changes in morphology and atomic structure, during an in-situ process, for example the charging and discharging cycles of batteries. Depending on the experiment, one may choose to use either mode exclusively.

<u>Examples of Science Areas & Impact:</u> In-situ tomography in Endstation 1 will serve applied sciences such as: Biomaterials and tissues (bone structure and implants from nano to macro length scales). Soil-Plant Interactions: interface between soil and roots (rhizosphere). Geology: simultaneous measurement of strain accommodation and evolution of fractures and pores. Planetary Science: Mineral phases/inclusions. Material science: Stress heterogeneities, defect nucleation, crack growth, fatigue. Corrosion: Stress corrosion cracks, corrosion pits.

The second endstation could accommodate bespoke large-scale instrumentation, for example experiments that need extremes in sample temperatures; either very cold, (dilution refrigerator) or very hot (ovens); both extremes drive large endstations. More common examples of large endstations are vacuum/growth chambers, which are necessary to create advanced functional materials like 2D semiconductors, magnetic layers and other materials that are of interest. Vacuum systems also allow one to preserve samples during study, for example monolayer flakes of Transition Metal Dichalcogenides (TMD) that are exfoliated, which degrade much slower under vacuum. SID could have a significant impact in the study of TMD flakes, because the SID beam size matches to typical TMD flakes sizes. Furthermore, the small beam size allows one to interrogate the structure of individual flakes, and to correlate with other physical properties such as Raman, for example as shown in the figure where one can have different polymorphs of the material at different locations in the chamber.



Growth of Transition Metal Di-Chalcogenide monolayer flakes

New Beamline – Automated Scanning Transmission X-ray Microscope (STX)

Technique(s): Cryogenic Soft X-ray Scanning Transmission X-ray Microscope (STXM).

Scientific Objective: Compositional analysis and functional performance of soft matter compounds in cryogenic and *in operando* conditions

Source: side lobe of a 3-pole wiggler

Energy range / resolution: 200-3000 eV (1/5000 resolution)

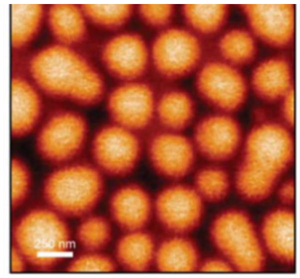
Spatial resolution: 25 nm (~10 nm with Ptychography)

Number of hutches: Two: FOE (shared with main branch) and one endstation environmental hutch.

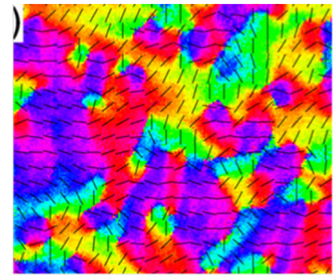
Photon delivery system: kicker mirror/vertical cylinder mirror, horizontal spherical grating monochromator with entrance and exit slits.

Endstation: direct nano-focusing/imaging and ptychography. Main components: zone plate/order sorting aperture sample stage, avalanche diode /PMT for fast scanning and CMOS for imaging, also electron yield, and fluorescence modes.

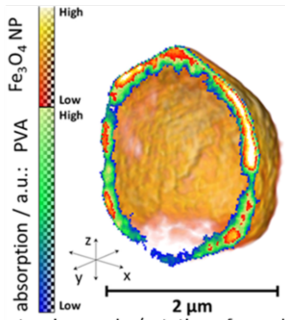
Estimated Size of User Community: ~100 unique users/year



Chemical compositional map of two OPV polymer components



Molecular orientaional domain morphology from linear dichroism



Laminography (rotation of sample) 3D structure of PVA nanospheres

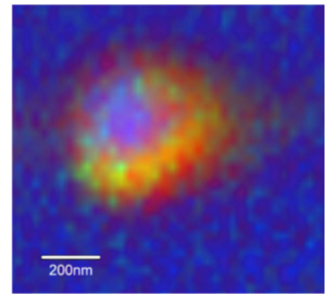


Image of nanoparticle encapsulated chemo-drug delivery to cancer cell

Rationale and Synergies for STX at NSLS-II

- Optimized for nano-focused spatially resolved quantification of chemical concentration and structure with high throughput Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy; from 100 to 3000 eV, covering all relevant edges for soft materials.
- Variable focus scanning ~25 nm to many microns. Ptychography using an area detector will enable lower resolution to ~10 nm.
- Primary focus of design will be to control and minimize beam damage to soft matter, a necessity for current NSLS-II soft matter community. Cryogenic capability and automation central to this design aspect
- Cryogenic transfer and measurement of 25-100 samples at a time will allow highly automated measurement of grid samples in addition to unlocking new classes of vitrified samples for STXMs
- Complements SXN and other potential microscopes with high throughput versatile system, automated, cryogenic sample transfer, storage, and measurement, rapid highly automated imaging capabilities.
- Complements user communities of resonant soft and tender scattering at SST-1 and SMI beamlines with a high level of multimodality: unified sample stages and convergent analysis pipelines.
- Multimodality will drive productivity between SST-1, SMI (also CMS, CHX, LIX), spectroscopy and microscopy at TES, SST-2, SRX, HXN as well as electron microscopy at the CFN and LBMS cryo EM facilities.
- Strategic potential to leverage NSLS-II's three pole wiggler side lobes sources

Examples of Science Areas & Impact

- **Polymer/ nanocomposite blends**: phase separation, swelling and *in situ* processing for in organic photovoltaics, transistors, OECTs.
- **Fuel cell and battery membranes**: understanding structure permeability relationship.
- **Catalysis** and **Electrochemistry** imaging and in operando monitoring of membrane structure
- **Biological** membrane/thin film imaging, DNA-guided rational mesoscale self-assembly.
- **Environmental**, atmospheric, geo-chemical microstructure characterization.
- Organic based **Hydrogen** storage and water filtration, water splitting membrane structure

New Beamline – Tender X-ray Nanoprobe (TXN)

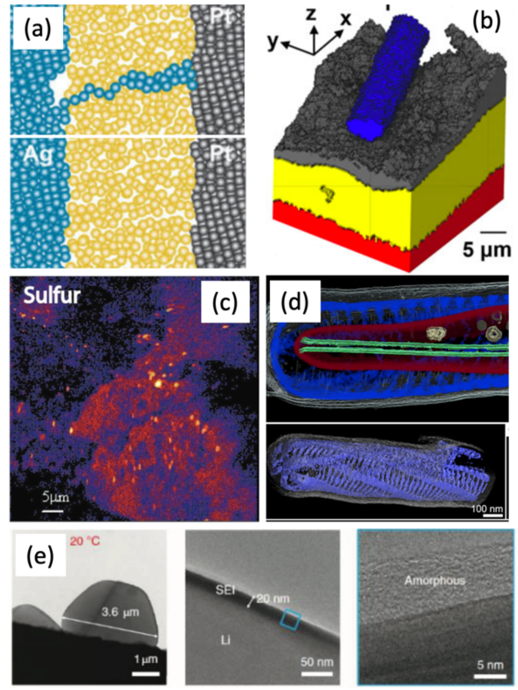


Figure 1 (a) The on and off states of an Ag/Ag-Ge-Se/Pt electrochemical metallization cells. (b) Multiphase structure in a polymer electrolyte fuel cell. (c) Chemical and structural distribution of a Stardust sample. (d) 3D view of the silica cell wall and membrane of a diatom. (e) The nano-scale hierarchical structure at the cathode and electrolyte interface.

Technique(s):
Multimodal scanning x-ray imaging using fluorescence, scattering, spectroscopy, and ptychography, fluorescence(using ~50 nm x-ray beam).
Source: in-vacuum undulator
Energy range / resolution:
~1.7 to 9 keV / ~$2x10^{-4}$ $\Delta E/E$ (Si K-edge to Ni K-edge).
Spatial resolution:
5 – 200 nm. Minimum beam size of ~50 nm. Sub-50 nm using ptychography.
Photon delivery system:
White-beam horizontal collimating mirror, cryo-cooled vertical monochromator, horizontal and vertical pre-focusing mirrors, secondary source aperture. At least 2 fast in-situ beam position monitors.
Endstation:
A, B, and C hutches. B is a small hutch housing in-situ beam diagnostics, and C is in the satellite building, similar to HXN. C-hutch houses an in-vacuum XAS endstation and scanning x-ray microscope at the end of the beamline.

Rationale and Synergies for TXN at NSLS-II
- The NSLS-II source provides high brightness for tender X-ray imaging.
- Provide nanoscale chemical and structural imaging for broad scientific areas, filling NSLS-II beamline portfolio between the soft x-ray (SXN) and hard x-ray (HXN) nanoprobes.
- Meet the high demand from the user community for spectroscopic microscopy with tender X-rays.
- TXN will be the only tender X-ray beamline around the world using KB mirrors to deliver a sub-100 nm focus.

Examples of Science Areas & Impact
- In-situ nano-scale morphological and chemical evolution of electrode/electrolyte interface/interphases of batteries using elements for tender energy range, especially for Li-S, Li-Si batteries, all solid-state batteries.
- Multimodal imaging characterization of microelectronics, capable of accessing K and L edges of elements used in next generation neuromorphic devices.
- Hierarchically porous catalysts: meso- to nano-scale morphological and chemical heterogeneity.
- Chemical and mineral characterization of interplanetary dust and NASA-return samples, emphasizing the spectroscopic microscopy capability with nano-scale resolution.
- High-entropy alloys in energy storage and catalysis applications with functional low-Z elements.