Report:

Instrument Execution Plan Development (IEPD) 2016

Report of the Task Force to evaluate execution plans and costs for 2016 approved NSLS-II Beamline Development Proposals.

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Acronyms and Definitions

AFM	Atomic Force Microscope
ALS	Advanced Light Source
APS	Advanced Photon Source
ARI	ARPES and RIX Nano-Imaging
ARPES	Angle Resolved Photo Electron Spectroscopy
BDP	Beamline Development Proposal
BNL	Brookhaven National Laboratory
CCD	Charge Coupled Device
CDI	Coherent Diffraction Imaging
CRL	Compound Refractive Lens
CSX	Coherent Soft X-ray
DCD	Double Crystal Deflector
DCM	Double Crystal Monochromator
EPU	Elliptically Polarized Undulator
ESH	Environmental Safety and Health
FOE	First Optical Enclosure
FWHM	Full Width Half Maximum
IEPD	Instrument Execution Plan Development
INF	Infrared Near Field nanospectroscopy
IVU	In-vacuum Undulator
NFIR	Near Field Infra Red
NSLS	National Synchrotron Light Source
PES	Photo Electron Spectroscopy
PGM	Plane Grating Monochromator
PLS	Polymer and Liquid Scattering
QIX	Quick Inelastic X-ray scattering
RIXS	Resonant Inelastic X-ray Scattering
SAC	Science Advisory Committee
SAXS	Small Angle X-ray Scattering
SMF	Soft X-ray STXM and TXM spectro-microscopy facility
SMI	Soft Matter Interfaces
STXM	Soft X-ray Transmission X-ray Microscope
TXM	Transmission X-ray Microscope
TXS	Transmission X-ray Scattering
UHV	Ultra-High Vacuum
WBS	Work Breakdown Structure
XES	X-ray Emission Spectroscopy

Report Synopsis

The Instrument Execution Plan Development (IEPD) Task Force was convened in May 2016 to develop preliminary plans for the delivery of five distinct instrument "engagements." These were derived from an extended, community-driven proposal process that included community workshops, pre-proposals, and a down-selection to solicited Beamline Development Proposals (BDPs) that were then externally reviewed and presented to our Science Advisory Committee. The beamlines were chosen based on their scientific merit, the extent to which they complemented and extended the existing capabilities at NSLS-II and utilized the unique properties of the NSLS-II source, and importantly, user community demand. This process resulted in six approved NSLS-II beamline development proposals. The taskforce was then charged to:

- clarify the scope of each instrument engagement that could be constructed
- evaluate an R&D program that might be needed to deliver the intended scope
- develop initial cost estimates (ranges) for the described scope (including R&D program)
- propose an initial technically limited schedule

The engagements were each evaluated in this context with a view to drawing high level conclusions to guide further work. The full charge, with items specific to each engagement is provided in Appendix A, with clarifications for ARI/SMF given in Appendix B.

SMF/ARI: (Soft X-ray Spectro-Microscopy Facility/ARPES and RIXS Nano-Imaging)

These instruments represent several beyond state-of-the-art soft x-ray microscopy endstations, combined in a single sector to develop complementary toolsets for nano- and meso-scale imaging. Specifically, ARI will fill a key gap in our understanding of the nanoscale origin of macroscopic (electrical, magnetic, thermodynamic and optical) properties of matter by developing spatially-resolved experimental techniques that measure near-Fermi-edge single particle and collective electronic excitations – measuring nanoRIXS and nanoARPES spectra in a unique, combined endstation. SMF will develop beyond state-of-the-art STXM and CryoSTXM imaging techniques for chemical imaging in real space. Both ARI and SMF will take advantage of the world-leading soft x-ray coherent flux of NSLS-II.

A suitable layout was needed that would accomplish the objectives of the separately-proposed SMF and ARI beamlines in a single sector. This was achieved by merging the proposed properties of the ARI beamline with those of the low energy branch of the SMF beamline, such that the same branch would meet the objectives of both. The design utilizes switchable white beam mirrors keyed to the requirements of each instrument. The proposed RIXS instrument will require R&D to establish performance limits.

CDI: (Bragg Coherent Diffraction Imaging)

The Bragg Coherent Diffraction Imaging (CDI) beamline will be a state-of-the-art beamline that takes full advantage of the world-leading coherent photon flux in the 6-15 keV energy range at NSLS-II, and will enable cutting-edge research on structural evolution in a wide-range of materials systems under *in-situ* conditions. By taking advantage of the largely empty reciprocal space at large momentum transfers, CDI has the unique capability to single out materials of interest in highly complex systems, leading to imaging of defects, dislocations, and strain fields in single grains of heterogeneous materials with relatively high signal-to-noise ratios. Additional capabilities include Bragg ptychography to allow mapping single grains in polycrystalline and extended specimens, and time-resolved measurements for both reversible and naturally occurring processes.

To realize this beamline, the Task Force team developed and evaluated an implementation that could fit inside the experimental hall and meet the CDI objectives. This was achieved through a careful layout of the required optical elements, which simulations showed could deliver the required coherent beam properties. However, the Task Force pointed out that a longer version of the CDI beamline, placing the experimental station in a satellite building outside the experimental hall, could also deliver the required beam properties, perhaps more easily but at greater cost. This issue needs further study.

PLS: (Processing and Liquid Scattering)

The Processing and Liquid Scattering beamline will be a versatile x-ray scattering facility sharing a canted straight section at 12-ID. Its science mission is to support a world-class scientific program for *operando* studies of soft matter interfaces, especially polymer thin films during processing and liquid surfaces. This facility will operate independently in parallel with the Soft Matter Interfaces (SMI) beamline at 12-ID through the use of a canted undulator. The high flux and tight focus of the NSLS-II source will enable unprecedented time-resolved studies of soft matter specimens undergoing industrially-relevant formation, processing, additive manufacturing, as well as structural transformation, weathering, degradation, and aging. These studies will encompass polymers, liquids, liquid crystals, granular materials, gels, and biomolecular materials, all of which lack the three-dimensional crystallinity characteristic of conventional hard materials. The PLS beamline will play an important role in our strategic directions in emergent behavior from complexity and in *in-situ* and operando science.

The principal challenge for this engagement was to develop a sufficiently modular endstation design to address the range of proposed experimental techniques. This was achieved through separation of the elements of the endstation into distinct, independent units in which the components could be repositioned to suit particular experimental needs.

QIX: (Quick RIXS Beamline)

The quick resonant inelastic X-ray scattering (QIX) beamline will be a soft X-ray RIXS/XES beamline with best-in-class photon flux and throughput for investigation of static and dynamic behaviors of advanced energy materials in realistic conditions. This new instrument will have a resolving power of ~10,000 at 1000 eV in an energy range of 200 – 2000 eV, with a focused beam spot of 1 μm x 10 μm. Taking advantage of the NSLS-II spectral brightness in this energy range, this soft X-ray capability will enable very fast RIXS data acquisition on the level ~1 sec for a 2D RIXS map over a few eV energy window, providing time-dependent (sec. to min.) snapshots of chemical, orbital, charge, & site-resolved electronic structures relevant to catalysis and chemical sciences and meeting the research needs of a strong and active spectroscopy user community.

For QIX, a layout was developed that would allow merging the instrument with the existing CSX-2 beamline. This was achieved by utilizing the upstream optical elements of the CSX-2 beamline for use by QIX and devising a means to pass the monochromatic beam through the existing CSX-2 endstations on to the QIX-specific optics and endstation farther downstream.

INF: (Infrared Near-Field Nanospectroscopy)

The infrared near-field nanospectroscopy (INF) beamline will be a new infrared beamline for nanospectroscopy and vibrational spectroscopy of materials central to current problems in condensed matter physics and chemical catalysis. Aperture-less near-field nanospectroscopy, based on synchrotron infrared light scattered from an atomic force microscope (AFM) tip, offers broadband spectroscopy of materials with better than 10 nm spatial resolution across the important range of wavelengths from 2 μm to 100 μm. This is the wavelength range that probes many intrinsic electronic and vibrational excitations. Applications of this novel method will include a wide range of studies in such areas as phase transitions and intrinsic inhomogeneities in Mott insulators, high T_c superconductors, magnetic and multiferroic domains in complex oxides and heterostructures, elementary excitations in low dimensional and plasmonic materials, spectroscopic and chemical catalysis of nanoparticle catalysts, and phonon vibrations in oxide nanoparticles or organic thin films.

For this beamline, a suitable layout of the INF endstations was needed that could meet the requirements of proximity to the CSX-2 beamline (one of whose endstations would also make use of a beam from INF) while satisfying ESH requirements for access and egress. This was achieved through careful placement of the INF endstations within the neighboring bending magnet sector floor space to CSX-2.

Cost and Schedule Estimates:

A common methodology was employed for developing cost and schedule estimates for each of these engagements. A shared basic WBS structure and dictionary (Appendix C) was used to capture the work anticipated for development of the engagements. Some project management and support costs were excluded from the estimates since it was assumed that they would be captured separately within the portfolio which manages the execution of the engagements. This reflects the economies of scale that come from managing engagements in groups, but is an additional cost to be factored into the completion cost of an instrument. Common resource burdens and overheads were assumed across the engagements including the application of the extraordinary project overhead rate, which has yet to be granted. Technically limited schedules (i.e. executed as fast as possible) were planned in the estimates. Other resource constraints, including staff levels and access to the storage ring for installation, as well as integration with ongoing work of the facility will likely extend these schedules.

The following table summarizes the cost and technically limited schedule estimates:

Engagement	Cost [$K]	Duration [Yrs]	Notes
SMF/ARI	30,896	4.3	Two beamlines merged in one sector. Includes R&D for the ARI spectrometers.
CDI	22,406	4.3	Costed based on endstation inside NSLS-II experimental hall. A satellite end station configuration will require separate evaluation.
PLS	10,485	3.5	Substantial infrastructure exists already at 12-ID.
QIX	9,191	3.5	Upstream portion of this beamline exists already at 23-ID-2.
INF	6,461	2.5	Two required new endstations are not commercially available yet with the necessary features.

The background for the engagements, as well as the details behind the estimates, is found in the balance of the report with the individual estimate team reports found in Appendix D.

Background

As part of the NSLS-II strategic planning and new beamlines proposal process, NSLS-II received six new beamline development proposals (BDPs) in February 2016. These new BDPs were selected from the twelve preproposals received after the 2015 NSLS-II Strategic Planning Workshop held at BNL. The six new BDPs were peer-reviewed by two Future Beamlines Review Panels consisting of well-known scientists. The panel findings and recommendations were subsequently evaluated by the NSLS-II Science Advisory Committee (SAC) at its Spring Meeting held on March 24-25, 2016.

At the SAC Meeting, NSLS-II presented the as-proposed concepts of the six new beamlines, the rankings and comments from the peer-review panels, and the preliminary prioritization order and path forward for each of the six new beamlines. In some cases, NSLS-II proposed revised beamline concepts to better take into account synergy and funding opportunities. The SAC endorsed the NSLS-II approach which envisions the development of five initial engagement plans based upon the six new BDPs. All instrument performance goals are as proposed except as noted below.

1. Soft X-ray STXM and TXM Spectro-Microscopy Facility (SMF): *proposal led by Harald Ade (NCSU), Konstanine Kaznatcheev, Juergen Thieme (NSLS-II)*

    - Focus only on proposed initial scope consisting of two independent branchlines, one in the range of 250-2000 eV and the other in 50-1200 eV, and two endstations, one conventional STXM and the other modular cryo-STXM, without the proposed TXM
    - Incorporate the nano-ARPES/nano-RIXS capabilities as proposed in the ARI BDP (see below)

2. ARPES and RIXS Nano-Imaging (ARI) Beamline: *proposal led by Peter Johnson (BNL), Elio Vescovo, Konstantine Kaznatcheev (NSLS-II)*

    - Evaluate accommodating ARI as part of the SMF beamline: potentially both the nano-ARPES and the combined nano-ARPES/RIXS endstations on the low-energy branch, with the RIXS capability predicated on successful R&D outcomes
    - Identify necessary R&D (potentially with ALS) to
        a. further develop zone-plate based RIXS spectrometer concept, and determine its feasibility
        b. explore and resolve issues related to radiation damage

3. Bragg Coherent Diffraction Imaging (CDI) Beamline: *proposal led by Ian Robinson (UCL) & Garth Williams (NSLS-II)*

   - Refine scope definition (6-15 keV), and address issues identified during the review, in particular detector positioning system and the dimensions of the endstation hutch
   - Focus only on in-situ materials applications, with laser pump-probe considered only as a potential future enhancement (i.e. consider at most only affordances in the present task force work)
   - Consider incorporation of forward-direction ptychography and Fresnel CDI capabilities in the conceptual design

4. Processing and Liquid Surfaces (PLS) – Second Branchline at 12-ID: *proposal led by Mark Schlossman (UIC) and Ben Ocko (NSLS-II)*

   - Refine the scope definition of the PLS branchline at 12-ID, with tunable 6-24 keV for liquid surfaces endstation and 13.7 keV fixed energy for the processing endstation
   - Include the capability of transmission x-ray scattering on liquid surfaces (LS-TXS) for studies of inhomogeneous horizontal liquid samples with vertically directed beam
   - Further develop the concept of the polymer processing endstation

5. Infrared Near Field Nanospectroscopy for Interface Technology and Emergence INFINITE (INF): *proposal led by Mengkun Liu (SBU) and Larry Carr (NSLS-II)*

   - Further pre-conceptual design of the INF beamline to refine scope definition and the design of the endstations
   - Consider splitting the extracted IR beam into four branches to incorporate a biology-IR program based on the existing IR microscope from former NSLS, with the other three programs as proposed – nano materials physics, nano catalysis, and combined IR and ambient pressure PES

6. Quick Resonant Inelastic X-ray Scattering (QIX): *proposal led by Jingguang Chen (Columbia) and Ignace Jarrige (NSLS-II)*

   - Evaluate the pre-conceptual design of the QIX beamline to refine scope definition and particularly the endstation
   - Consider incorporating proposed QIX capability (200-2000 eV) at the CSX-2 beamline

Overview

This section provides a summary of the work of the task force. High level attributes and issues of each of the engagements are also provided. Each engagement is summarized in the following section, with the detailed reports provided in Appendix D.

Makeup of Task Force and supporting staff

The Task Force was led by Lonny Berman. Individual teams were formed for each engagement that reported to the Task Force lead. The program managers for the specific engagements were also involved in the development of the scope and estimates that were prepared.

Engagement	BDP	Lead	Supporting	Program Manager
1	SMF	Juergen Thieme	Konstantine Kaznatcheev	Lisa Miller
	ARI	Konstantine Kaznatcheev	Juergen Thieme, Elio Vescovo	Lisa Miller
2	CDI	Garth Williams		Lisa Miller
3	PLS	Ben Ocko		Ron Pindak
4	INF	Larry Carr		Stuart Wilkins
5	QIX	Joe Dvorak	Ignace Jarrige	Stuart Wilkins

Support for various elements of preparing the engagement estimates was provided by Oleg Chubar, Mourad Idir, Greg Fries, Chris Stebbins, Zhijian Yin, and Elliott Golnar. In addition, a number of engineering and designer staff members contributed support for the Task Force effort.

Timeline of important events

May 13, 2016: Task Force charge issued
May 18, 2016: Kickoff general meeting of Task Force
June 17, 2016: Task Force charge clarification for SMF/ARI issued
June 24, 2016: Task Force general meeting with BDP PIs
August 5, 2016: Task Force general meeting with BDP PIs
September 12, 2016: Task Force general meeting with BDP PIs
September 30, 2016: Due date of Task Force deliverables, presentation of Task Force activities given at NSLS-II Strategic Retreat

October 14, 2016: PLS deliverables submitted
October 18, 2016: QIX deliverables submitted
October 20, 2016: CDI deliverables submitted
October 28, 2016: INF deliverables submitted
November 10, 2016: SMF/ARI deliverables submitted
November 29, 2016: Preliminary IEPD report submitted

It should be noted that at the time of submission of the individual engagement reports in Oct.-Nov. 2016, a number of cost and labor estimates were still at large, typically in the areas of project support or specialized labor for beamline construction such as trades labor. These omissions were noted within the individual engagement reports found in Appendix D. The composite estimates shown in this overview incorporate the estimates which were missing from the engagement reports."

Common Estimate Tools

To assist the Task Force in developing its engagement cost and labor estimates, a common work breakdown structure (WBS) was developed. Its dictionary is in Appendix C. Limited customization of this was undertaken for each engagement.

A cost/labor estimates spreadsheet tool was prepared to provide a consistent method to align estimates with the WBS, and utilize common labor rates and overheads across the engagements for consistency. Basis of estimate information was also captured for each engagement.

Engagement Specific Charges and Technical Results

(1) SMF/ARI

(a) Specific charge

Attached to the general Task Force charge of May 13 was this specific charge pertaining to SMF/ARI, separated into distinct elements pertaining to each of SMF/ARI:

SMF:

- Focus only on proposed initial scope consisting of two independent branchlines, one in the range of 250-2000 eV and the other in 50-1200 eV, and two endstations, one conventional STXM and the other modular cryo-STXM, without the proposed TXM
- Incorporate the nano-ARPES/nano-RIXS capabilities as proposed in the ARI BDP

ARI:

- Evaluate accommodating ARI as part of the SMF beamline: potentially both the nano-ARPES and the combined nano-ARPES/RIXS endstations on the low-energy branch, with the RIXS capability predicated on successful R&D outcomes
- Identify necessary R&D (potentially with ALS) to
    - further develop zone-plate based RIXS spectrometer concept, and determine its feasibility
    - explore and resolve issues related to radiation damage

Subsequently, a charge clarification pertaining to the combined SMF/ARI engagement was issued on June 17:

- Only one low-beta ID port will be developed to support this engagement
- It will have two branches based on canted undulators
    - A low energy branch will be optimized in its design around the requirements of the ARI instrument
    - A high energy branch will be optimized in its design to support the requirements of a STXM instrument
- The R&D program required for the development of a ZP RIXS spectrometer will be described and its approximate cost and required schedule evaluated
- Affordances on the low energy branch to support a STXM will be considered and estimated as separable elements of the overall engagement (i.e. clearly identified scope, activities, and costs)

(b) Summary of desired technical capabilities and key performance parameters

SMF/ARI consists of two beamlines viewing two EPU sources in a low-beta straight section. One of the beamlines (low energy) views a dedicated EPU (70 mm period) and spans an energy range of 50-1000 eV, and the other beamline (high energy) views a dedicated EPU (55 mm period) and spans an energy range of 250-3500 eV. The attributes of the two beamlines and the three endstations they serve are:

- Low energy beamline serving nano-ARPES/nano-RIXS endstation, ~10^{11}-10^{12} ph/sec with resolving power ~25,000 and spot size down to 50-100 nm, 200 mm hemispherical electron analyzer for ARPES, zone-plate-based spectrometer for RIXS having ~15,000 resolving power, coherent x-ray scattering using fast CCD delivering 5 nm spatial resolution based on ptychography
- Same low energy beamline serving STXM endstation with cryogenic capability, photon flux on sample ~10^{9}-10^{10} ph/sec with resolving power ~3,000 and spatial resolution ~20 nm

- High energy beamline serving STXM endstation with cryogenic and tomography capabilities, photon flux on sample ~10^9-10^{10} ph/sec with resolving power ~3,000 and spatial resolution ~20 nm

(c) Overview of layout and technical design

- Two canted EPU sources in a low-beta straight section with a canting angle of 1.7 mrad between them
- Horizontally-deflecting white beam mirrors located in an FOE further separate the beams radiated by the two sources
    - For the low energy beamline, there are two white beam mirrors that are swappable, a plane mirror to serve the nano-ARPES/nano-RIXS endstation and a sagittal cylindrical mirror to serve a STXM endstation
    - For the high energy beamline, there is a sagittal cylindrical mirror to serve a different STXM endstation
- The beams reflected from the white beam mirrors are delivered to dedicated PGMs (one for each beamline) in the FOE
- For each beamline, a horizontally-deflecting toroidal mirror within the FOE reflects the monochromatic beam which is then delivered to the STXM for that beamline (low energy STXM at 50 m distance from the source, high energy STXM at 60 m)
- The toroidal mirror in the low energy beamline is retractable to allow passage of the monochromatic beam on to the nano-ARPES/nano-RIXS endstation at 70 m distance from the source, which relies on a KB mirror pair to focus the beam at the sample position

(d) Special considerations (e.g. R&D, ESH)

- R&D is required for the development of a zone-plate-based spectrometer for RIXS to serve the nano-ARPES/nano-RIXS endstation
    - A staged R&D approach is proposed, beginning with the development of a low-resolution spectrometer using the CSX-1 beamline at NSLS-II
    - Later, development of a high-resolution spectrometer will be undertaken, requiring access to a beamline elsewhere (e.g. ALS) having high resolving power and sufficient space
    - Final product of the R&D will involve development of UHV RIXS spectrometers, two to serve the nano-ARPES/nano-RIXS endstations and a third to serve the STXM endstation on the low energy beamline
- Endstations will be enclosed in a large environmental cabin having provision for local curtain-covered areas around each endstation to improve ambient noise reduction and temperature stability

(2) CDI

(a) Specific charge

Attached to the general Task Force charge of May 13 was this specific charge pertaining to CDI:

- Refine scope definition (6-15 keV), and address issues identified during the review, in particular detector positioning system and the dimensions of the endstation hutch
- Focus only on in-situ materials applications, with laser pump-probe considered only as a potential future enhancement (i.e. consider at most only affordances in the present Task Force work)
- Consider incorporation of forward-direction ptychography and Fresnel CDI capabilities in the conceptual design

(b) Summary of desired technical capabilities and key performance parameters

CDI is a hard x-ray beamline viewing an IVU source (20 mm period) in a low-beta straight section and spans an energy range of 6-15 keV. The attributes of the beamline and endstation it serves are:

- Variable size highly coherent focused beam 1-7 µm FWHM
- Endstation to allow measuring three-dimensional continuous intensity distributions in forward- and Bragg-scattering geometries
- High-load multiple-circle diffractometer supporting novel sample environments
- Nanometer-scale sample positioning system having high stability
- Long-working-distance focusing optics
- Infrastructure to support time-resolved and in operando experiments

(c) Overview of layout and technical design

- 3 m long IVU source in a low-beta straight section
- Horizontally-deflecting white beam mirror located in an FOE provides beam steering and harmonic rejection, and can focus the beam horizontally at a downstream secondary source aperture
- Reflected beam is delivered to a Si(111) DCM in the FOE
- Secondary source aperture is located downstream of the FOE in a second (monochromatic beam) hutch
- Downstream of this hutch is a third (monochromatic beam) hutch which is reserved for a future optical laser and instrumentation to mix the laser and x-ray beam paths to allow later optical pump, x-ray probe experiments

- Final (monochromatic beam) hutch is large and contains the experimental endstation
    - Consists of final focusing optics based on a KB mirror pair to focus the beam at the sample position with a 1 m working distance, followed by a beam conditioning system before the experimental diffractometer
    - Multiple-circle diffractometer has a kappa axis and nano-positioning sample stage, with a circle of confusion for the primary rotation axis of under 2 µm
    - Multiple area detectors allow measurement of the intensity around multiple Bragg peaks (for ordered samples) while also allowing measurement of the forward-scattered intensity to image structure in ordered or partially-ordered samples
    - Area detector positioning system allows the Bragg peak detector to be positioned at two-theta angles beyond 90° as well as elevations of 1.5 m above the beam height
    - Forward-scattering detector works in conjunction with the sample positioner to uphold a ptychography capability
    - Temperature control of the endstation to the level of 0.1°C is required to provide the needed stability over long measuring times

(d) Special considerations (e.g. R&D, ESH)

- Conceptual beamline design has been prepared which maintains the experimental station within the main NSLS-II experimental hall, with the sample position at ~60 m from the source
    - Issues that bear upon the preferred beamline design include stability as well as optical considerations
    - Secondary source aperture is employed, in the design studied, as a coherence-defining aperture
    - Diffraction from it gives rise to structure in the final focused beam, imposing a stringent stability constraint on the relative motion between the secondary source aperture and KB mirror pair aperture; mitigation within the confines of the main NSLS-II experimental hall may be difficult
- Alternative beamline design option involves reassigning the coherence-defining function from the secondary source aperture to the upstream high-heat-load defining aperture that is in the FOE
    - This would incur lengthening the beamline to remove the endstation from the main NSLS-II experimental hall and relocate it to a distant satellite building, a consequence of the high-heat-load defining aperture being removed from the focal position and thus needing to be set wider (in the horizontal direction) as compared with the secondary source aperture employed in the shorter beamline scheme, to transmit comparable flux

    - Result is that a longer distance between the coherence-defining aperture and final focusing optics is required to preserve the same brightness as delivered using the shorter beamline scheme
    - High-heat-load beam defining aperture is followed by horizontal and vertical collimating mirrors in the FOE to prevent the beam size from enlarging further while propagating the extended distance to the final focusing optics just before the endstation in the remote satellite building
    - Final focused beam size is determined by the KB mirror pair aperture using the longer beamline scheme, not the secondary source aperture
- Further work is needed to study these design concepts

(3) PLS

(a) Specific charge

Attached to the general Task Force charge of May 13 was this specific charge pertaining to PLS:

- Refine the scope definition of the PLS branchline at 12-ID, with tunable 6-24 keV for liquid surfaces endstation and 13.7 keV fixed energy for the processing endstation
- Include the capability of transmission x-ray scattering on liquid surfaces (LS-TXS) for studies of inhomogeneous horizontal liquid samples with vertically directed beam
- Further develop the concept of the polymer processing

(b) Summary of desired technical capabilities and key performance parameters

PLS is a hard x-ray beamline viewing an IVU source (probably 20 mm period) in a high-beta straight section (shared with the SMI beamline) and spans an energy range of 6-24 keV. The attributes of the beamline and endstation it serves are:

- ~10^{13} ph/sec at 10 keV
- ~2 µm vertical focus (using secondary source aperture and CRLs) or ~10 µm vertical focus (using primary mirror), ~100 µm horizontal focus
- Three different endstation configurations using the same spectrometer and detectors
    - polymer processing, side deflecting single crystal, 200 kg sample chambers
    - liquid surfaces, single crystal deflector (SCD), large chambers, ~100 cm to detector
    - liquid surfaces, double crystal deflector (DCD), fixed sample, low vibrations, fast scanning

(c) Overview of layout and technical design

- 1.5 m long IVU source sharing a high-beta straight section with the SMI beamline at 12-ID, with a 2 mrad canting angle between the two undulator beams
- White beam is delivered through an existing front end to a Si(111) DCM in the FOE
- Following the DCM are horizontally focusing and deflecting mirrors that steer the monochromatic beam further outboard, increasing the angular separation from the neighboring SMI beam
- Following the horizontally focusing/deflecting mirrors is first a vertically focusing mirror followed by a vertically deflecting mirror to preserve a level beam trajectory in the experimental hutch
- Mirror chambers already exist in the FOE
- Secondary source aperture is located downstream of the FOE inside of an existing secondary enclosure within an existing hutch
- Just downstream of the secondary source aperture is a CRL system, followed immediately by the endstation within the same hutch
- Endstation apparatus consists of four distinct stages, each mounted on a linear translation stage supported by granite blocks
- First stage will be used in one of two modes
    - Either as single crystal deflector (SCD) (Ge(111) or Ge(220)) used for polymer processing and liquid surface studies
    - Or as double crystal deflector (DCD) (Ge(111) followed by Ge(220)) used for liquid surface studies for which the sample is maintained at a fixed position and rapid scanning of q can be undertaken
    - Deflector stage can move along the beam direction with 1.5 m travel
- Second granite supported translation stage contains the sample apparatus as well as the detector when used in conjunction with the SCD
    - Capable of supporting a 200 kg sample environment
    - Sample position can be moved laterally and in elevation to intercept the beam emerging from the SCD
    - No sample motion is required when the DCD is used
    - Detector is positioned on a two-theta arm whose vertical axis is concentric with that of the sample stage
    - On the two-theta arm, there are secondary vertical and angular motions to properly position the detector(s) for specular reflectivity or wide-angle scattering as needed
- Third granite supported translation stage contains the detector for specular reflectivity when used in conjunction with the DCD
    - Includes the necessary translation and angular motions to properly position the detector for specular reflectivity

    - Will also be used to support a flight path leading to the SAXS detector (on a fourth stage) in the polymer processing mode
- Fourth granite supported translation stage, just before the downstream wall of the hutch, contains the detector used for SAXS in conjunction with the SCD
    - Located about 3.5 m from the sample position
    - Flight path is used to deliver the beam to this stage
    - Detector is rotatable on this stage in order to orient it to be normal to the beam direction

(d) Special considerations (e.g. R&D, ESH)

- Exhaust system for processing vapors
- Under study is the possibility to implement a superconducting undulator that may be developed by the APS
    - Such an undulator, having a higher K potential than a conventional IVU, would offer brighter emission than the conventional IVU especially at higher photon energies
- For the vertical incident beam geometry, a small compact and ultra-stable 90° beam deflector, based on multiple crystal reflections, requires development effort

(4) QIX

(a) Specific charge

Attached to the general Task Force charge of May 13 was this specific charge pertaining to QIX:

- Evaluate the pre-conceptual design of the QIX beamline to refine scope definition and particularly the endstation
- Consider incorporating proposed QIX capability (200-2000 eV) at the CSX-2 beamline

(b) Summary of desired technical capabilities and key performance parameters

QIX is a soft x-ray beamline viewing an EPU source (49 mm period) in a low-beta straight section (shared with the CSX-1 and CSX-2 beamlines; QIX would be an expansion of the CSX-2 beamline) and spans an energy range of 200-2000 eV. The attributes of the beamline and endstation it serves are:

- Resolution of 100 meV at 1000 eV
- Focus size of 1.0 µm vertical x 10 µm horizontal (1σ)
- High throughput RIXS spectroscopy, full RIXS map in several minutes, single spectrum in ~ 1 sec

(c) Overview of layout and technical design

- Embraces the entire CSX-2 beamline from the EPU source all the way through to its PGM and vertical exit slit, but with replacement of one or more of the existing PGM gratings
- CSX-2 beamline is then extended from its current termination to allow the implementation of a new KB mirror system to focus the beam down to the size required by the new QIX endstation
    - Existing vertical focusing mirror is lowered from the beam path, and a beam pass-through path is implemented through the existing CSX-2 endstations
    - New KB mirror system sits just before the QIX endstation sample chamber
- Endstation sample chamber
    - Includes a sample transfer/load-lock system and various sample environment features such as manipulators, flow cells, and cryostat and heating stages
    - Also designed to be compatible with a future ambient pressure photoemission capability as well as the accommodation of an IR beam delivered from another beamline
- Centerpiece of the endstation is a RIXS spectrometer set at a fixed two-theta of 90° horizontally
    - Will be directed inboard and span across the neighboring sector floor spaces of beamlines 23-BM (whose upstream section will be developed for an IR beamline) and 24-ID (which cannot be built out due to the presence of RF cavities in the straight section)
    - Embraces a Hettrick-Underwood design, involving two horizontal collection mirrors, a vertical focusing mirror, grating system, and an area detector
    - Possible spectrometer length of up to 8 m

(d) Special considerations (e.g. R&D, ESH)

- Reaction gas delivery and handling system
- Floor layout permits the required ingress/egress to the neighboring IR beamline that would be built in sector 23-BM

(5) INF

(a) Specific charge

Attached to the general Task Force charge of May 13 was this specific charge pertaining to INF:

- Further pre-conceptual design of the INF beamline to refine scope definition and the design of the endstations
- Consider splitting the extracted IR beam into four branches to incorporate a biology-IR program based on the existing IR microscope from former NSLS, with the other three programs as proposed – nano materials physics, nano catalysis, and combined IR and ambient pressure PES

(b) Summary of desired technical capabilities and key performance parameters

INF is an IR beamline viewing a bending magnet source and delivering diffraction-limited flux/brightness over a wavenumber range of 100-7000 cm^{-1}. The attributes of the beamline and endstations it serves are:

- Extracted beam is divided and shared among four endstations, two time-shared
- One endstation is based on NFIR condensed matter and materials physics spectroscopy at ~10 nm length scale, involving an Atomic Force Microscope (AFM) optically coupled to an Asymmetric Michelson Interferometer (AMI), with cryogenic capability
- A second endstation is based on NFIR catalysis nanostructures spectroscopy at ~10 nm length scale, involving an Atomic Force Microscope (AFM) optically coupled to an Asymmetric Michelson Interferometer (AMI)
- A third endstation, time-shared with a fourth, is based on IR reflection-absorption spectroscopy (IRRAS) of surfaces in a CSX-2 endstation (the INF IR beam will be delivered to that endstation)
- A fourth endstation, time-shared with the third, is based on microspectroscopy (applications ranging from environmental, geological, planetary, biomedical, to materials systems) using an instrument repurposed from NSLS

(c) Overview of layout and technical design

- IR beam is derived via extraction from a standard gap bending magnet source using a custom vacuum/extraction chamber
    - First extraction optic is a plane mirror which collects beam radiated by the upstream half of the electron beam arc traversing this source, in all 45 mrad horizontally and 15 mrad vertically
    - Extracted beam is delivered out through the adjacent shield wall essentially horizontally transversely from the radiation source using relay optics
    - Split into three equivalent 15 mrad x 15 mrad portions that are thence delivered to the endstations (third and fourth endstations share one portion)
- First and second endstations will be commercial systems

- Third endstation will be a CSX-2 endstation, potentially the one to be developed as part of the QIX beamline
- Fourth endstation will be one repurposed from NSLS
- Endstations (except for the CSX-2 one) will be housed in experimental cabins

(d) Special considerations (e.g. R&D, ESH)

- NFIR endstations have the option to undertake single wavelength measurements using laser sources
    - Could be provided by small quantum cascade laser systems contained within the NFIR endstation cabins
    - Alternatively, by ultra-fast laser beams delivered from the nearby MET laser room
- Assuming layout of INF in the sector 23-BM floor space adjacent to CSX-2 and QIX, floor layout was prepared in a way that permits the required ingress/egress to the INF experimental cabins

Composite Cost/Labor/Schedule Estimates

- Uniform construction overhead rate of 18% has been assumed
- All costs have been properly escalated based on startup in FY17
- Discrete technical activities were identified and logical relationships between them were developed
- Design and construction efforts for the beamline endstations were scheduled to occur simultaneously with the same for the beamline photon delivery systems, rather than serially as had been the typical past practice
    - In substantial measure this shortened the construction duration as compared with the 5-6 years duration which was prevalent for previous NSLS-II beamlines.
    - This was achieved, in the resources-loaded schedules which were developed, by front-loading beamline labor resources significantly as compared with the counterpart schedules for previous beamlines, for which such resources ramped up over generally a two years period
- Suitable level-of-effort project management and support labor resources were included, with the exceptions of effort for project controls and procurement
    - Level of project controls effort will be assigned later based on sponsor expectations for project tracking
    - Level of procurement effort will be assigned later based on determination of the level of construction overhead supported labor resources

- The typical breakdown between equipment/M&S and labor was about 65% equipment/M&S and 35% labor

Engagement	Cost (K$)	Duration (Yrs)	Notes
SMF/ARI	30,896	4.3	Two beamlines merged in one sector. R&D cost estimates pertaining to ARI spectrometers were included.
CDI	22,406	4.3	Costed option based on endstation inside NSLS-II experimental hall. Will need re-evaluation if a satellite building to house the endstation is judged to be necessary.
PLS	10,485	3.5	Substantial infrastructure exists already at 12-ID. This will be the second beamline developed in that sector, viewing a canted ID source.
QIX	9,191	3.5	Upstream portion of this beamline exists already at 23-ID-2. This will be an extension of it.
INF	6,461	2.5	Two required new endstations are not commercially available yet with the necessary features. Expectation is that such features will be developed and implemented into commercially available units by when they're needed.

(a) SMF/ARI major equipment costs

- Two EPUs ($900K direct each)
- White beam mirror system including three mirrors ($740K)
- Two PGMs including their gratings and mirrors ($1.3M each)
- Two toroidal mirror systems (including the mirrors), one for each STXM ($400K each)
- Two STXMs ($1.6M each)
- KB mirror system (including the mirrors) for the nano-ARPES/nano-RIXS endstation ($450K)
- Nano-ARPES/nano-RIXS endstation exclusive of the RIXS spectrometers ($1.35M)
- RIXS spectrometers which will be products of the required R&D ($650K)
- FOE ($490K)
- Endstations cabin ($540K)

(b) CDI major equipment costs

- IVU ($1.7M direct)
- Photon delivery system ($2.7M)
- Diffractometer ($800K)
- Two area detectors ($1.96M)
- Detector positioning system ($500K)
- Four hutches ($1.52M)

(c) PLS major equipment costs

- IVU ($1.04M direct)
- DCM ($600K)
- Focusing and deflecting mirrors and the secondary source aperture and needed vacuum components all bundled together as a package ($1.5M)
- CRL system ($200K)
- Four-stage endstation spectrometer system ($850K)
- Two area detectors ($520K)

(d) QIX major equipment costs

- KB mirror system including the mirrors ($457K direct)
- Reaction gas handling system ($750K)
- Sample chamber and spectrometer optical chambers and mechanics including the gratings and mirrors ($1.04M)
- Sample cells and stages and the sample transfer/load-lock system ($341K)
- Spectrometer detector ($334K)

(e) INF major equipment costs

- UHV optical extraction chamber ($950K direct)
- Photon distribution and optical matching system ($200K)
- First NFIR endstation which includes a cryogenic capability ($800K)
- Second NFIR endstation ($500K)
- Components for the IRRAS endstation at CSX-2 ($150K)
- Endstation cabins ($290K)

APPENDIX A:

NSLS-II 2016 Taskforce on Instrument Execution Plan Development (16-IEPD)

Description:
The purpose of the taskforce is to prepare the basic elements of instrument execution plans for engagements based on the Beamline Development Proposals described below as modified by the guidance from the proposal evaluation panels, the SAC, and NSLS-II management. The work of the taskforce is to:

- clarify the scope of each instrument engagement that could be constructed
- evaluate R&D program that might be needed to deliver the intended scope
- develop initial cost estimates (ranges) for the described scope (including R&D program)
- propose an initial technically limited schedule

The information must be sufficiently well developed and documented that it could be set aside and revisited at a later time with very little loss in understanding so work on a particular engagement could resume quickly.

The work product of the taskforce is to be delivered no later than 30 September 2016, at which time the taskforce will be disbanded.

Background:
As part of the NSLS-II strategic planning and new beamlines proposal process, NSLS-II received six new beamline development proposals (BDPs) in February 2016. These new BDPs were selected from the twelve preproposals received after the 2015 NSLS-II Strategic Planning Workshop held at BNL. The six new BDPs were peer-reviewed by two Future Beamlines Review Panels consisting of well-known scientists. The panel findings and recommendations were subsequently evaluated by the NSLS-II Science Advisory Committee (SAC) at its Spring Meeting held on March 24-25, 2016.

At the SAC Meeting, NSLS-II presented the as-proposed concepts of the six new beamlines, the rankings and comments from the peer-review panels, and the preliminary prioritization order and path forward for each of the six new beamlines. In some cases, NSLS-II proposed revised beamline concepts to better take into account synergy and funding opportunities. The SAC endorsed the NSLS-II approach which envisions the development of five initial engagement plans based upon the six new BDPs. All instrument performance goals are as proposed except as noted below.

1. Soft X-ray STXM and TXM Spectro-Microscopy Facility (SMF): *proposal led by Harald Ade (NCSU), Konstanine Kaznatcheev, Juergen Thieme (NSLS-II)*
   - Focus only on proposed initial scope consisting of two independent branchlines, one in the range of 250-2000 eV and the other in 50-1200 eV, and two endstations, one conventional STXM and the other modular cryo-STXM, without the proposed TXM
   - Incorporate the nano-ARPES/nano-RIXS capabilities as proposed in the ARI BDP (see below)

2. ARPES and RIXS Nano-Imaging (ARI) Beamline: *proposal led by Peter Johnson (BNL), Elio Vescovo, Konstantine Kaznatcheev (NSLS-II)*
   - Evaluate accommodating ARI as part of the SMF beamline: potentially both the nano-ARPES and the combined nano-ARPES/RIXS endstations on the low-energy branch, with the RIXS capability predicated on successful R&D outcomes
   - Identify necessary R&D (potentially with ALS) to
     a. further develop zone-plate based RIXS spectrometer concept, and determine its feasibility
     b. explore and resolve issues related to radiation damage

3. Bragg Coherent Diffraction Imaging (CDI) Beamline: *proposal led by Ian Robinson (UCL) & Garth Williams (NSLS-II)*
   - Refine scope definition (6-15 keV), and address issues identified during the review, in particular detector positioning system and the dimensions of the endstation hutch
   - Focus only on in-situ materials applications, with laser pump-probe considered only as a potential future enhancement (i.e. consider at most only affordances in the present task force work)
   - Consider incorporation of forward-direction ptychography and Fresnel CDI capabilities in the conceptual design

4. Processing and Liquid Surfaces (PLS) – Second Branchline at 12-ID: *proposal led by Mark Schlossman (UIC) and Ben Ocko (NSLS-II)*
   - Refine the scope definition of the PLS branchline at 12-ID, with tunable 6-24 keV for liquid surfaces endstation and 13.7 keV fixed energy for the processing endstation
   - Include the capability of transmission x-ray scattering on liquid surfaces (LS-TXS) for studies of inhomogeneous horizontal liquid samples with vertically directed beam
   - Further develop the concept of the polymer processing endstation

5. Infrared Near Field Nanospectroscopy for Interface Technology and Emergence INFINITE (INF): *proposal led by Mengkun Liu (SBU) and Larry Carr (NSLS-II)*
   - Further pre-conceptual design of the INF beamline to refine scope definition and the design of the endstations
   - Consider splitting the extracted IR beam into four branches to incorporate a biology-IR program based on the existing IR microscope from former NSLS, with the other three programs as proposed – nano materials physics, nano catalysis, and combined IR and ambient pressure PES

6. Quick Resonant Inelastic X-ray Scattering (QIX): *proposal led by Jingguang Chen (Columbia) and Ignace Jarrige (NSLS-II)*
   - Evaluate the pre-conceptual design of the QIX beamline to refine scope definition and particularly the endstation
   - Consider incorporating proposed QIX capability (200-2000 eV) at the CSX-2 beamline

Task Force Initiated by: E. Johnson – NSLS-II Deputy for Construction

Schedule:

Start: Immediately after approval of the Task Force
Completion: End of September 2016

Goals & Deliverables:

The overall goal for the taskforce is to prepare documentation that can be used to provide initial scope, cost and schedule for the engagements outlined above. These documents will be used for raising funding for the engagements and provide the basis for formulating more detailed plans for the engagements and for the R&D programs that would be necessary for their construction.

For each engagement a document is to be delivered which will at a minimum include –

- Scope definition -
  - Narrative
  - WBS dictionary
- Cost estimate
  - Direct Dollars and Hours
  - A standard set of labor types (to be provided)
  - The basis of estimate (organized by WBS- template to be provided)
- Initial schedule
  - A 'cartoon' version showing major activities and anticipated technically limited durations

In addition, each engagement team should collect a record of interactions, meetings, discussions, and internal reviews associated with the development of each engagement along the way to the producing the work product.

Stakeholders:

BDP PI's, Potential user communities for the BDP's, Task force members, NSLS-II Program Managers, NSLS-II Division Directors

Taskforce Members:

Taskforce Leader: Lonny Berman

Each of the original BDP's has a lead who is responsible for developing the taskforce deliverables. For the purposes of the task force they report to the task force leader, but must also engage the identified Program Managers. SMF and ARI will be merged to a single engagement report for the purposes of the taskforce. The engagement reports are coordinated by the leads noted in **bold** in the table below.

Engagement	BDP	Lead	Supporting	Program Manager
1	SMF	**Juergen Thieme**	Konstantine Kaznatcheev	Lisa Miller
	ARI	Konstantine Kaznatcheev	Juergen Thieme, Elio Vescovo	Lisa Miller
2	CDI	**Garth Williams**		Lisa Miller
3	PLS	**Ben Ocko**		Ron Pindak
4	INF	**Larry Carr**		Stuart Wilkins
5	QIX	**Joe Dvorak**	Ignace Jarrige	Stuart Wilkins

Oleg Chubar; Insertion Device and Optics Design

Mourad Idir; Optics design/evaluation and characterization planning

Support for developing the engagements will include those specifically identified in this charge as well as others who may be requested by the task force leader on behalf of the engagement leads.

Account to be charged:

Project/Activity – 21376/21939 (Project title – BL Task Force)

Charges are to be authorized through the taskforce leader and reviewed by the Deputy for Construction.

Taskforce reviews:

Monthly status reports from the Taskforce Lead to management are expected as well as a monthly call with the BDP PI's. If needed specific Engagement reviews will be scheduled by the Deputy for Construction.

<u>Submitted by:</u>

_____ _____

Erik D. Johnson Date

Deputy Director for Construction, NSLS-II

Concurrence:

The undersigned will support the work of the proposed task force and "Do Recommend" (Yes) or "Do Not Recommend" (No) approval of the task force:

Michael Bebon Deputy Director for Operations, NSLS-II	Date	Yes _____	No _____
Qun Shen Deputy Director for Science, NSLS-II	Date	Yes _____	No _____
Ferdinand Willeke Accelerator Division Director, NSLS-II	Date	Yes _____	No _____
Paul Zschack Photon Science Division Director, NSLS-II	Date	Yes _____	No _____
Robert Lee Environmental, Safety and Health Manager, NSLS-II	Date	Yes _____	No _____
Christine Madonia Business Operations Manager, NSLS-II	Date	Yes _____	No _____

Approval:

Based on the recommendation above the NSLS-II 2016 Taskforce on Instrument Execution Plan Development (16-IEPD) is to be activated. Funds in the amount of $400k are to be released for the work of the task force. Their use is to be monitored and reported by the Deputy for Construction.

John Hill NSLS-II Facility Director, NSLS-II	Date

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managed by Brookhaven Science Associates
for the U.S. Department of Energy

Memo

date: *16 June 2016*

to: *John Hill – Director, NSLS-II*

from: *E. Johnson – Deputy Director for Construction, NSLS-II*

subject: *16* ***IEPD Taskforce Charge clarification for SMF/ARI***

In their preliminary discussions the Instrument Execution Plan Development (16-IEPD) team members working on SMF and ARI arrived at different ways to interpret the Taskforce charge to merge these two proposals into one Engagement. Following a series of e-mail exchanges a meeting was held on 15 June 2016 to discuss the matter and arrive at a uniform interpretation to allow the work of the taskforce to proceed.

Participants included Lonny Berman, Konstantine Kaznatcheev, Erik Johnson, Lisa Miller, Qun Shen, Juergen Thieme and Paul Zschack. After some discussion it was agreed that the merged engagement should be pursued under the following assumptions.

- Only one low Beta ID port will be developed to support this engagement
- It will have two branches based on canted undulators
    - A low energy branch will be optimized in its design around the requirements of the ARI instrument
    - A high energy branch will be optimized in its design to support the requirements of a STXM instrument
- The R&D program required for the development of a ZP RIXS spectrometer will be described and its approximate cost and required schedule evaluated
- Affordances on the low energy branch to support a STXM will be considered and estimated as separable elements of the overall engagement (ie clearly identified scope, activities, and costs)

I am recommending to you as the approval authority for the 16-IEPD task force that this clarification to the charge be adopted and used as the working guidance for the SMF/ARI team in completing their work.

John Hill – Director, NSLS-II	Approve	Do Not Approve	Date

APPENDIX C: Common IEPD Beamline Dictionary

(1) Management and Support
Performance of management and support activities, including labor, materials, travel, and fixed costs associated with management and support functions, consisting of construction management, reviews, administrative support, ESH, QA, configuration management, business operations, project controls, procurement, and document control.

(2) R&D Program
Equipment and effort needed to uphold a necessary R&D program pertaining to the photon delivery system or endstation.

(3) Beamline Construction
(a) Photon Delivery System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of photon delivery sub-systems and integrated system. These include the beamline optical systems upstream of the endstation (including their housings, supports, and manipulation systems), apertures and beam definition and conditioning systems, beam diagnostic/visualization systems, beam transport system, vacuum system, cooling/heating and temperature stabilization systems associated with photon delivery system components, and shielding systems (exclusive of radiological enclosures) that include collimators, masks, shutters, and beam stops.
(b) Endstation System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of endstation sub-systems and integrated system. These include sample housings, environments, visualization, and support and manipulation systems, detection systems, optical systems and beam diagnostic/visualization and conditioning/definition/deflection components just before the sample (e.g. on the same support as the sample or contiguous with it) or between the sample and detector (e.g. crystal/grating/mirror-based analyzer or spectrometer system) including their housings, supports, and manipulation systems, vacuum system, and cooling/heating and temperature stabilization systems associated with endstation components.

(4) Beamline Infrastructure
(a) Hutches
Design, specification, procurement, fabrication, assembly, installation, and testing of the required radiological enclosures, including the necessary hoist, air handling equipment, fans, labyrinths, doors, windows, and lights.
(b) Cabins and Control Station Furniture

Design, specification, procurement, fabrication, assembly, installation, and testing of required environmental cabins (not radiological enclosures) including the necessary ventilation, doors, windows, wiring, and lights, and of furniture for the beamline control station including partitions and their power and communications wiring.

(c) Mechanical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline mechanical utilities including equipment racks, DI water, process chilled water, gaseous nitrogen, compressed air, exhaust, and liquid nitrogen distribution systems.

(d) Electrical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline electrical utilities including circuit breaker panels, provisioning of power to equipment racks, and cable trays and conduits.

(e) Equipment Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Equipment Protection System (EPS) including PLC, wiring, and custom sensors.

(f) Personnel Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Personnel Protection System (PPS) including PLC, wiring, switches, locks, special interlocked personnel protective safeguards such as gates and light screens, and Human Machine Interface (HMI) panel.

(5) Accelerator Infrastructure

(a) Front End
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of front end sub-systems and integrated system. These include the front end chambers, vacuum system, supports, apertures, collimators, masks, shields, shutters, and diagnostics including flags and beam position monitors. The necessary utilities, protection systems, and controls for the front end are included.

(b) Source
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of radiation source and associated hardware. This could be an insertion device for x-rays or an extraction chamber to insert within a dipole magnet for infrared radiation. Magnetic measurements if necessary are included. The necessary utilities, protection systems, and controls for the source are included.

(c) Straight Section
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of accelerator straight section sub-systems and integrated system. These include the straight section chambers, vacuum system, supports, masks, shields, diagnostics including beam position monitors, and canting magnets with power supplies if

necessary. The necessary utilities, protection systems, and controls for the straight section are included.

(6) Beamline Controls

(a) Basic System Controls

Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation control systems. These include operator consoles for control and archive of control equipment, network routers, gateway to the machine control system, timing IOC to synchronize to the machine timing, motor controllers and associated cabling, serial to Ethernet hubs, and a soft IOC for controlling all Ethernet-based motors, serial devices, and PLCs. Ethernet and timing cables are also included.

(b) Instrument Applications

Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation instrument control applications. These include experimental control workstations, data storage and computation equipment, experimental control software and servers, and data acquisition equipment and software including for detectors.

Development plan for a soft x-ray spectromicroscopy facility at NSLS-II

Konstantine Kaznatcheev, Juergen Thieme, Elio Vescovo

The current document describes the construction of a soft X-ray spectromicroscopy suite of beamlines at NSLS-II. It is a follow-up implementation plan which, based on SAC/ NSLS-II selection, combines two approved proposals (ARI/ SMF) in a single ID-based spectromicroscopy facility occupying a single straight section sector at NSLS-II. This document specifically addresses the charge clarification of June 16, 2016 of the NSLS-II "2016 Task Force on Instrument Execution Plan Development (16-IEPD)" as it relates to the joint SMF/ARI proposals, which states:

- *One low-beta ID port will be developed with two branches based on canted undulators*
    - *A low energy branch will be optimized in its design around the requirements of the ARI instrument. Affordances on the low energy branch to support a STXM will be considered and estimated as separable elements of the overall engagement.*
    - *A high energy branch will be optimized in its design to support the requirements of a STXM instrument.*
- *The R&D program required for the development of a zone plate RIXS spectrometer will be described and its approximate cost and required schedule evaluated.*

(1) Scientific goals, experimental techniques, technical capabilities and key performance parameters.

As both original proposals (ARI and SMF) had common research focused on soft x-ray state-of-the-art microscopy techniques development, it is natural to combine them and allocate to a single ID-based sector to benefit from the development of comprehensive experimental platform of complimentary toolsets for nano- and meso-scale imaging. To the extent possible, they will share common sample (holder) environment, while providing specialized instrumentations to characterize specimen heterogeneity by x-ray absorption or electron spectroscopy or inelastic scattering detection. Following we provide the summary for end-station specific scientific goals, key performance parameters and NSLS-II world-wide unique capabilities.

(1) **ARI** should fill a key gap in our understanding of the nanoscale origin of macroscopic (electrical, magnetic, thermodynamic and optical) properties of matter by developing spatially resolved experimental techniques that measure near-Fermi-edge collective electronic excitations.

Unique Capability: (i) Low energy nano-ARPES capability is unique (ZP-based ARPES are limited to >150eV operation), (ii) High energy nano-ARPES/RIXS has ~10^3 intensity gain compared to other high energy ZP-based nano-ARPES. (iii) High NA ZP-based nano-RIXS is the first spatially resolved IXS. (iv) Simultaneous ARPES/RIXS/ptychography measurements will uniquely complement each other. Estimated on-sample flux is ~10^{11}-10^{12}ph/s at resolving power R~25,000, spot size remains below 100nm over 100-1000 eV energy range.

(a) Nano-ARPES: ~Scienta DA30 (200mm hemi) e- analyzer, working distance 34mm; angular (k range) range: ARPES DA30 lenses acceptance : +/- 15 degrees; resolution~ 0.1 degree;

(b) Nano-RIXS: one fixed angle ZP-based spectrometer placed in backreflection geometry and one variable angle (110-180°) spectrometer. RIXS collection angle reaches 0.25*0.25rad^2@300eV, energy resolving power is estimated to be 15,000.

(c) Coherent x-ray scattering: (stationary/ downstream) fast CCD covers 0-1nm^{-1} Q range and permits ~5nm spatial reconstruction (via ptychography) at 0.1s/frame rate, so 1*1um^2 field of view measurement takes ~min.

(2) **low-energy STXM** should provide analytical microscopy for studying complex materials and devices at operando conditions at high resolution, particular of Li-based energy storage material and devices.

Unique Capability: (i) cover Li (45 eV) K edge of STXM operation. Full-control polarization starts at 130 eV, low energy STXM provides high energy coverage up to Si K (1.5 keV) edge. (ii) wide temperature range (LN_2 capability).

(3) **high-energy STXM** will also focus on analytical microscopy, but compared to low energy STXM should capitalize on higher penetration depth and so shall have an emphasis on 3D tomography.

Unique Capability: (i) extended energy coverage from C K edge (250eV) to Au/Pt M (3.5keV, need special ML coated grating) edges; (ii) modular design with an ability to use environmental TEM holder; (iii) wide temperature range (LN_2 capability).

The non-invasive analytical capability of STXM microscopes provides a unique opportunity to study how nano- and meso-scale three-dimensional hierarchical structural organizations of complex systems affect their functional behavior. Both STXMs will (1) target spatial resolution of 20 nm at 100 μs/ pixel; on-sample photon flux ~10^{9-10} ph/s at resolving power R~3,000. (2) Both STXMs will have an extension to coherent x-ray scattering: fast CCD covers 0-1 nm^{-1} Q-range and enables sub-5 nm spatial reconstruction (via ptychography ~5 nm at dose 10^5 ph/nm^2). Other prominent features include:

- Measurements of system time evolution (at 1 kHz speed limited by 2D detector and extended to sub-μs for a single point FPG time correlator)
- Stroboscopic event-sorting machine for pump-probe measurements with ~100 ps time resolution

Depending on the outcome of R&D, we plan an extension of STXM operation (XAS contrast) to RIXS signal detection to improve heterogeneous phase identification (H/D) or dominant guest/ host interactions (vibrational structure).

For an extended description of scientific themes and specific research examples, refer to original proposals. Although, current document describes phased approach of beamline construction, once completed it will encompass most technical capabilities of ARI/ SMF proposals with omissions of (i) stochastic fluctuation phenomena and (ii) some inefficiency for 3D/4D(+time) volumetric (tomography) reconstruction which better be performed with full field microscopy.

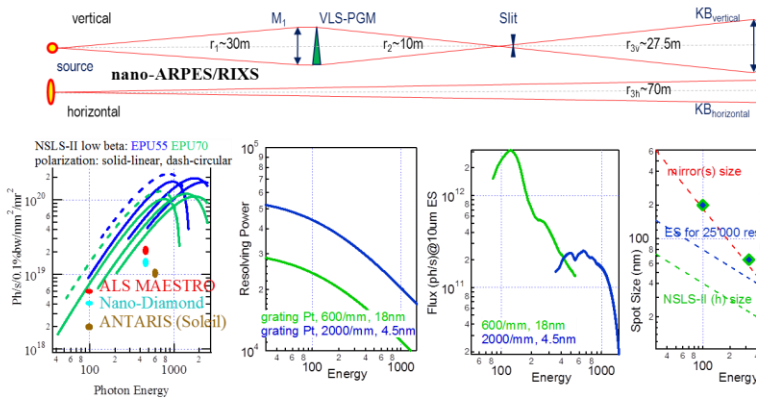


Fig.1. Optical scheme and performance of nano-ARPES/RIXS branch/ end-station.

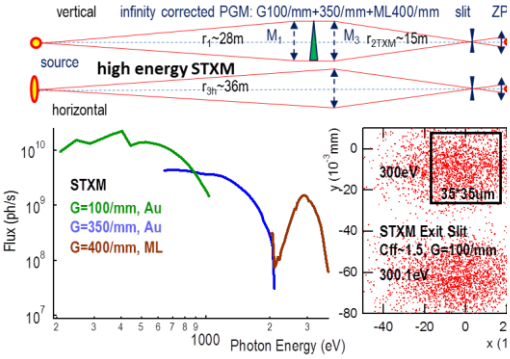


Fig.2. Optical scheme and performance of high energy STXM at nominal R=3,000 resolving power, exit slit to reach diffraction limited performance is shown as a box.

Beamline technical layout

As ARI/ SMF came as independent proposals, a team was assembled to find compromise needed for the mutual layout. We conclude that addition of first (plane) mirror to ARI (low energy branch) will provide a simple way to place both projects on the same straight section sector without compromise of each other's performance (with proper management of ID power load, see Appendix I). Fig. 3 illustrates ARI/SMF mutual layout on low-beta straight section sector (29-ID has been assumed). As one can see, the proposed layout provides adequate floor space for major beamline components, all located within existed experimental hall, while retaining optical requirements (such as ARI extra space for refocusing) outlined in the original proposals. Future extended optical analysis will be needed to detail optimized performance of high and low energy branches. It will explore different optical schemes (such as VLS PGM or use of mirror pair to improve energy purity), but for the current pricing and resource allocation exercise we chose to closely follow original optical designs. As the proposed layout fits beamline-specific goals, we do not expect substantial modifications (as of number of optical elements/vessels and their complexity) of overall layout.

The low energy branch serves ARI (located ~70m downstream) or low energy STXM (~45m) end-stations. EPU70 placed in upstream portion of straight provides an extended energy range coverage reaching energy as low as 36eV (Fig. A1). To provide low energy STXM station operation, M1 STXM mirror (stationary, sagittal cylinder) deflects the light ~2.0^o inboard and passes vertically collimated light thru common, low energy PGM. Additional retractable M1 ARI plane mirror (with the same ~2.0^o inboard deflection as M1 STXM mirror) can be inserted just upstream of M1 STXM mirror if ARI operation is required. Low energy PGM will have four interchangeable gratings for high (25,000 for ARI) and low (5,000 for STXM) energy resolving power operation. Selection of BESSY-type PGM (Bestec) would be beneficial, as one can use existing grating substrates (with sub-100nrad performance) left after ESM development. M3 STXM mirror (toroid, ~4.0^o outboard deflection placed after PGM can be inserted into the beam to deflect and focus the light to the STXM exit slit placed ~5m downstream. It is retracted for ARI operation. ARI KB focusing optics is a part of ARI end-station. It consists of two upstream/ downstream mirrors placed side-by-side (focal length 40(h)/280(v)mm, 10mm mirror-to-sample distance). With optimization of glancing angle of each KB pair, low energy KB focused beam reaches ~100nm at 60eV (optimized for 50-150eV) and high energy KB focused beam ~50nm at

600eV (150-1000eV operation). Low energy pair has an extreme curvature, which is currently beyond x-ray optic fabrication (metrology) capability, so only high energy pair is included in the initial ARI scope. Fig. 1 details the performance of ARI end-station.

The high energy branch serves high energy STXM end-station (located ~55m downstream). The downstream EPU55 provides full control over x-ray light polarization within 275-1600 eV energy range, and can reach 3.5 keV (with sufficient brightness in LH mode on third and fifth harmonics). The M1 mirror (sagittal cylinder, stationary) deflects EPU55 light outboard (~2.0^{o}) and collimates it vertically so a wide range of monochromator magnification can be used to optimize resolving power and flux. Two lower density gratings (100/mm and 350/mm) provide 250-2000 eV energy coverage at a moderate resolving power $E/\Delta E$. Third, a multilayer coated (ML) 450/mm grating, extends the beamline performance to higher energy (2.0-3.5 keV). ALS-type PGM will have adequate performance (~10,000 resolving power), slimmer footprint and should be a lesser subject of carbon contamination (as it uses high grade Al alloy for chamber fabrication). As high energy branch has minimal floor layout limitation, following the original proposal, we suggest to use moderate refocusing by M3 STXM mirror (toroid, deflecting beam outboard by ~2.0^{o}) to refocus light ~15m downstream to an exit slit, served as stationary secondary source (both vertical and horizontal foci coincide) for STXM. Ray tracing analysis suggests that resolving power as high as 7,000 (adequate for RIXS spectroscopy) can be reached (Fig. 2).

1.7 mrad chicane angle gives adequate angular separation between EPU57/ EPU70 beams (Appendix I). It also provides sufficient space, so all M1 mirrors can be placed within single vessel without any mechanical interference. Front end variable aperture opening can be adjusted to selectively expose particular set of M1 mirrors, so any branch can be taken off-line (being developed) while another branch remains fully operational (and in a common safe mode as all major optical components are retained within FOE, and there is no need for override or special operation). Aside from ARI end-station refocusing optics, low and high energy branches have similar complexity (number of optical elements, etc.) and, depending on the resources available, can be built independently. For this reasons, the following schedule does not differentiate between low and high energy branches. The only common elements are: ID chicane arrangement, front end, M1 vessel and FOE (including PPS/ EPS). ARI construction can follow low energy STXM branch development with minimum interference on low energy STXM operation.

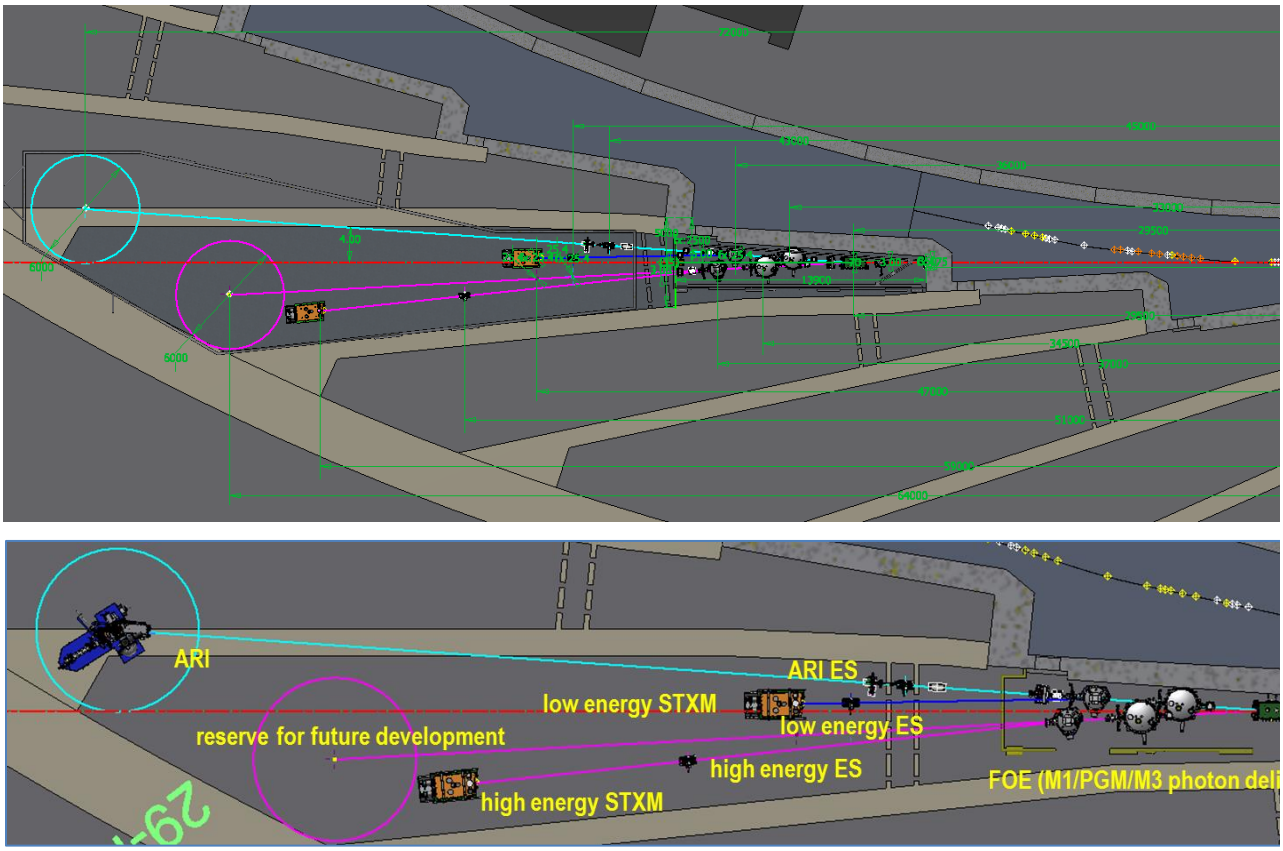


Fig.3. The ARI/SMF layout.

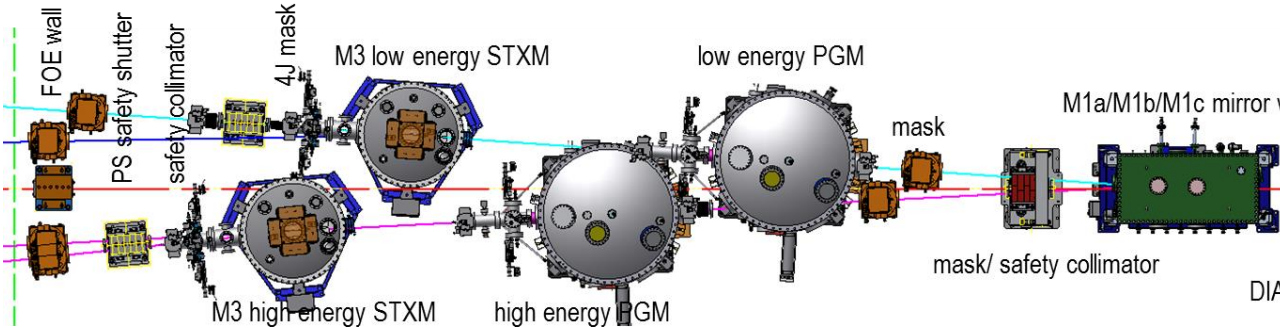


Fig.4. The layout of SR equipment inside FOE.

(2) List of major (new) equipment[1]/ construction.

(a) *Source(s)/extraction(s):* upstream ~EPU70 and downstream ~EPU57 in low-beta NSLS-II straight section in canted geometry. Canted angle of ~1.7mrad remains stationary. The straight section needs a substitution for narrow gap (outer 10.5mm) vacuum chamber to serve the EPUs. The layout of chicane magnets and central e- BPM need further discussion with ID group and engineering design. There are seems to be no major concerns with ability/cost to implement them.

[1] For complete list of SR components and their location refer to accompanying Budget Spreadsheet

(b) *Front end:* single front end with acceptance angle of 2.2mrad. As the total ID emitted power (~3kW) and large chicane angle (1.7mrad compare to 0mrad for ESM) make SMF requirements to be less critical than that of existing ESM front end, most of the components need only minor modification. Development of x-BPM is left for further investigation.

(c) *Hutches:* single ~14m long lead hutch as first optical enclosure (FOE). First mirror(s) vessel, PGM(s) and switching yard mirrors (M3) are placed inside FOE (Fig. 4). Future optical design/engineering should resolve minor layout interference. Beamline safety shutters are located within FOE. As all white/pink beam photon delivery tracks are contained within FOE, thus the PPS requirements along the rest of beamline will be minimal. High temperature stability of FOE should also benefit high-resolution PGM operation/stability.

(d) *Experimental cabins* (Fig. 5, overall perimeter shown as green line) will be essential for microscope(s) operation to warrant sub-5nm spatial resolution. The total area covered by cabins is estimated to be ~150m^2, and there will be additional (curtain-covered) areas around experimental stations to increase ambient noise reduction and temperature stability. Common cabin layout (compared to individual cabins) permits area between beamline branches to be used as a laboratory space for sample preparation and axillary analytical equipment.

(e) *Optical components on experimental floor:* see above description; detailed optical schemes and branch performances are described in original proposals.

(f) *Principal end-station components* including spectrometers and detectors: ARI station: (i) Scienta DA30 electron energy analyzer, (ii) two ZP-RIXS spectrometers (~3m long), (iii) fast CCD. Requirements of ARI sample stage, sample preparation (including ion-beam fab, sample scraping/fracture) and characterization stations will be developed at later stage. STXM station: (i) TEM environmental holder, (ii) single ZP-based RIXS spectrometer, (iii) fast CCD. Auxiliary detectors requirements (Si drift, e-, visible light spectrometer) will be developed at later stage. Time generator/sequence machine, synchronization detection scheme are the subject of separate document. List of sample preparation/characterization equipment (such as optical indexing/e-/SPM microscopes) will be developed later.

(g) *Utilities/ service lines/ rack layout requirements:* Fig. 5 shows facility utilities layout. Special accommodation includes: He purging line (STXM), vibration-free low vacuum pumping station/line, standard exhaust lines to each end-station. Cabins HVAC/chilled water (as a part of cabin contract) need to be integrated. The decision on general LN_2 line vs. local Dewar service is left for further investigation.

(h) *Control System:* EPICS and Python-based NSLS-II control will be adequate for beamline operation. PPS/EPS, diagnostic-webCCDs (~16), current amplifiers (Siddons, ~16), actuation- DeltaTau-based, ~80motors, or 3 racks*4controllers, vacuum/beamline operation- ~18 vacuum subsections: valve/ ion pump/ CCG/ TCG requirements are similar to ESM. Provisions for special (high bandwidth) channels for Scienta DA30 analyzer and fast STXM CCD (ptychography) to local data storage (expected data rate/storage capacity similar to CSX-1/ CDI/ HXN) are included in budgetary estimates.

(i) *Anticipated special ESH accommodations* (e.g. exhaust system, sample handling): pressurized gas cylinders (He) for STXM end-station purge, small lab. bottles as a gas standard (CO_2, N_2, O_2, Ne_2, Ar_2) to be used for energy calibration (small amount).

(j) *Envisioned "encroachments" into other beamline sectors or end-stations:* to accommodate high and low energy branches on a same straight section sector, the ARI original optical scheme was modified to add plane mirror (M1a) which deflects beamline inboard. ~70m long ARI branch will encroach on an adjacent BM sector, see preliminary layout (Fig. 3/ Fig. 5).

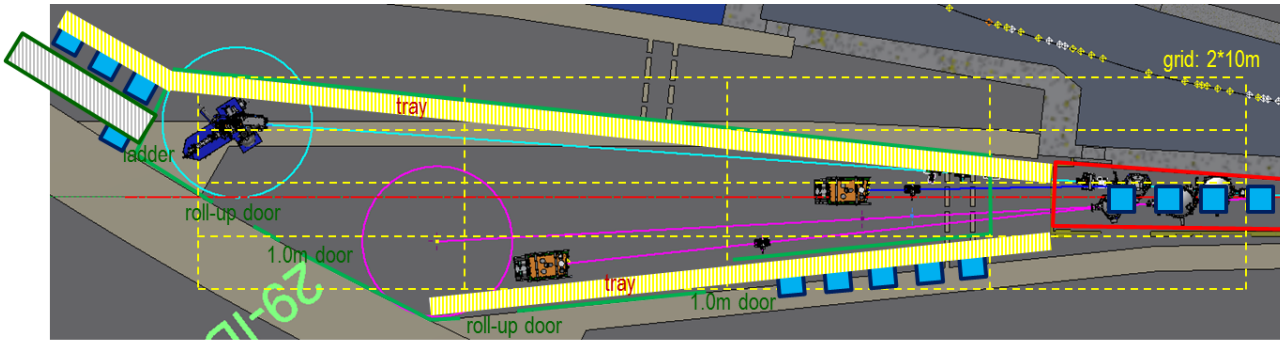


Fig.5. The utility/ cabin/racks layout. ***Cabins:*** ~30m long (total area~150m^2), ~2m wide walk up zone between FOE and cabins. Construction: similar to LOB labs, wall insulated for temp/noise control, nominal interior height ~10ft, door as indicated, location of standard 3*4' windows (with black-out shades) are not indicated Special enclosure/curtain: noise reduction areas (around exp. end-stations) are not indicated. Crane/lifting equipment. HVAC on the cabin top. Roof load ~50lb/ft^2. Fire alarm/suppression per code. Oxygen monitors at LN_2 drop-off zones.

FOE: ~14m long lead hutch to host most of beamline optical components, two sliding doors

DI water: inside FOE, three drop zones (M1, PGMs, M3/ Photon Shutters).

Chilled Water/Exhaust Line: at experimental end-station areas.

Service Tray/ Electrical- above FOE/ cabins: local drop/cabin penetration near exp. stations. 208V (high-power, bake-out) in FOE, exp. area of ARI/ high energy STXM. Compressed air/ gaseous nitrogen along beamline branches.

Racks: ~5 on the top of FOE, ~5 along outboard cabin wall, ~4 downstream end (near ARI)

(3) Required R&D:

Beamline specific R&D covers: (i) the development of high luminosity ZP-based RIXS spectrometer(s); (ii) the design of ultra-low vibration, low temperature scanning stage- to be done in cooperation with NSLS-II nano-positioning group following test/selection of commercial nano-positioning equipment, (iii) the development of KB mirror system is left outside R&D efforts, as the dialogue with JTEC (x-ray optics fabrication company, Japan) confirms that such system will be available commercially in two years time.

As ZP-based RIXS spectrometer constitutes a novel design, we propose a staged approach to bring it to a maturity/technical realization. Rather than testing a "dummy prototype", we start with the development of low resolution spectrometer for NSLS-II CSX-1 beamline. Fig. 6 shows the projected performance of ZP-spectrometer compatible with geometry of CSX-1 reflectometer. Existing ZP-stage will be used to form ~100nm spot (ZP1:160/90/90), another identical stage (with ZP2:160/90/45) will be mounted on reflectometer arm. Combination of x-ray CCD and pinhole arrays will provide different detection schemes to facilitate ZP coarse/ fine alignment. We expect that this spectrometer will help us (a) to verify ZP-spectrometer principle of operation, (b) to develop alignment scheme and to verify mechanical tolerances needed for spectrometer operation, as well as (c) to give crude flux estimates- an initial benchmark for spectrometer collection efficiency. Proposed spectrometer will have its own scientific merit as it will help to distinguish the formation of weak electronic superstructures (associated Bragg peak)

from broad-range (inelastic or diffusive) scattering and fit well into CSX-1 research program. Following initial optical design and development of software for spectrometer performance simulations (scientist*~2months), we will be ready to complete its mechanical design, parts fabrication, assembly and off-line testing. Resources needed are: $25K hardware, mech. engineer-1mnth, control engineer-1mnth, scientist-2mnth, with overall goal to get ready for CSX-1 2017-1 beamtime tests (3-6 days of beamline access thru science commissioning proposal).

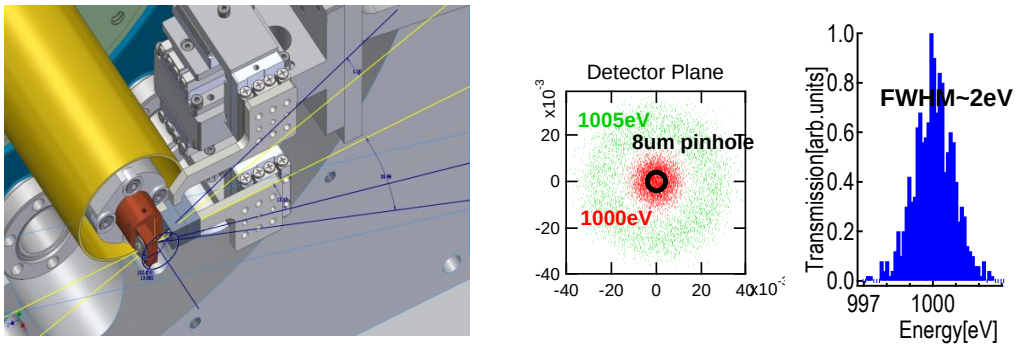


Fig.6. CSX-1 reflectometer and performance of ZP-based spectrometer.

Although stage 1 of R&D should provide sufficient answers in regard to functional performance of ZP-spectrometer, neither CSX-1 beamline resolution ($E/\Delta E$ ~1,000) nor available space (<0.5m) would be sufficient to test high resolution RIXS spectrometer and so R&D should follow to a stage 2- focused on engineering design and test of high resolution RIXS spectrometer at other SR facility (such as ALS). We estimate the resources needed as: $250K for hardware, mech. engineer-3mnth, control-1mnth, scientist- 2mnth. Stage 2 will also include optical analyses and software development for generalized case of transmission grating-based spectrometers. Final stage will include the construction of ARI UHV version of the spectrometers: one stationary in backreflected geometry, another with ability to measure angular dependence of RIXS radiation. The requested R&D budget reflects the construction of final RIXS spectrometers (3 total= 2 for ARI, 1 for STXM). We also need to stress that core of ARI scientific scope relay on ARPES nano-imaging, and although ZP-based spectrometer will expand ARI capability by adding new modality (RIXS) to its core, as a mitigation strategy in the case of failed R&D efforts, conventional spectrometer with high angular acceptance (similar to ALS) will still provide RIXS imaging capability (at reduced image quality).

(4) Budget & Schedule[2]:

Fig.7. shows main subsystem/components cost estimated based on (i) most of the vendor-supplied components, such as M1/PGM/M3 vessel and optical manipulator cost, x-ray optics (as well as beamline infrastructure: construction: FOE/ cabin cost) are based on real cost/contract POs using ESM beamline as a close prototype (Fig.7a), (ii) the NSLS-II labor is accounted in activities, such as front end/ insertion device/ mechanical/ electrical utilities construction, (iii) beamline-specific labor, such as lead scientist and his/her activity, (iv) engineering efforts (and technician jobs, where other beamline research staff, NSLS-II engineers and technicians

[2] See separate excel workbook ARI_SMF_Development _29Sep2016 for equipment/layout/cost and schedule for ARI/ SMF development

participate) are summed (conceptual to final) and shown as labor at a top level (Fig.7b). Project management group will provide its own (where labor/cost of procuring components are split in a different way with correction coefficient applied for overheads) estimate as well as WBS split. Regardless of fine details, there are few important notes to make regarding beamline cost.

- Direct costs are well understood and managed. As the optics account for large portion of beamline construction and number of vendors (negotiated power to reduce the cost by NSLS-II) are limited, further reduction is still viable if optical/engineering design will be extended to look at technical alternatives (side cooled vs. internally water cooled optics). As optics to subsystem interfaces are well understood, it will be more efficient (low price/ shorter schedule) if total integration/calibration will be done in house. There might be substantial savings if NSLS-II extended engineering (of some components) to build-to-print engineering package, so larger pool of vendors (particularly ones who specialize on ultra-high vacuum fabrication but reluctant to extend their expertise into SR engineering) can participate. That certainly comes with larger commitment of NSLS-II resources (and different style of their management), particularly engineering, but NSLS-II has in-house expertise to do it. Similar approach is suggested for ID construction. Purchasing frames/actuation and magnets separately followed by in-house shimming could reduce ID cost at least by 30%.

- Indirect cost, particularly internal labor called for different type of management. As non-expert in management but one exposed to a different beamline development environment, it will be inappropriate to comment, but certainly some facilities find a good balance between resources sharing/ direct sub-ordination to promote their efficient use. Short term well defined goals/resources allocation with direct accountability to a specific project lead seems to be the key for their efficient use.

- End-stations. Following cost analysis, have two STXM end-station estimates: using vendor supplied STXM (with LN_2 option, total $1.5M) and in-house built. Commercial option is not compliant with high resolution ptychography (coherent scattering) and lacks TEM- holder support.

- Experimental Cabins. Sub-5nm spatial resolution (which is a realistic goal for soft x-ray microscopy using ptychography) requires extreme care of ambient noise environment. To our experience, proposed cabins are the bare minimum to warrant such performance. NSLS-II IR cabins cost was used as basis for cost analysis.

- Cooperation with other facilities. US, as one of the leaders in SR instrumentation and host of four high-performance SR centers, accumulated an extended knowledge (design/drawings/etc.) and expertise (staff) in SR construction. Current project includes several system specific meetings/reviews to bring this expertise together.

Fig.7(a). The unburdened cost of major components/ sub-systems.

	Cost (K$)	Basis of Estimate
Development		
RIXS spectrometers (via R&D)	$640.00	professional judgment
Beamline Construction		
M1 vessels and optics	$790.00	ESM costs
common shields/ masks	$160.00	NSLS-II BL costs
low energy PGM and optics	$1,600.00	ESM costs
M3 (low-energy STXM) vessel and optics	$270.00	ESM costs
high energy PGM and optics	$1,700.00	ESM costs
M3 (high-energy STXM) vessel and optics	$310.00	ESM costs
low energy beamline vacuum components, shutter, diag	$420.00	ESM/SIX costs
high energy beamline vacuum components, shutter, diag	$350.00	ESM/SIX costs
Endstation Construction		
low energy beamline ARI endstation (without RIXS spect)	$1,500.00	ESM costs
ARI KB system and optics	$450.00	ESM costs and JTEC quote
low energy beamline STXM	$1,600.00	Axilon quote
high energy beamline STXM	$1,600.00	Axilon quote
Accelerator Infrastructure		
EPUs (2 m long EPU70 and 2 m long EPU55)	$1,780.00	Kyma quote
Front End	$973.00	bottom-up estimate
FOE	$490.00	NSLS-II hutches costs scaled

Fig.7(b). Beamline total cost (burden) and NSLS-II labor

WBS Area	Loaded Materials Cost (K$)	Loaded Labor Cost (K$)	Total Loaded Cost (K$)
P.01 Management	0	322	322
P.02.04 R&D	804	339	1143
P.03.01 Photon Delivery Sys	6938	1588	8526
P.03.03 Endstations	5578	3414	8992
P.04.01 Hutches and Cabins	1254	0	1254
P.04.02 Mechanical Utilities	286	158	444
P.04.03 Electrical Utilities	51	169	220
P.04.04 EPS	55	80	135
P.04.05 PPS	93	261	354
P.05.01 Front End	1185	645	1830
P.05.02 Source	2167	763	2930
P.05.03 Straight	625	474	1099
P.06 Controls	551	970	1521
Total	**19587**	**9183**	**28770**

Technically-limited schedule is shown on Fig.8. The schedule appears overly aggressive, as it assumes no limitation on resources/money constrains. The lead items are the optics delivery (which might start after optical design/spec and part of preliminary design (layout of major components) are completed), but other sub-system (FE, ID, opto-mechanical components) are not far behind. High- and low-energy branches are assumed to be developed in parallel, but there are only few sub-systems (accelerator vacuum chamber/ chicane magnets, FOE, and M1 vessel) which are common to both, and so their development (to some extent) can proceed independently, if the resources (particularly money) are constrained. Realistic analysis of procurement process, continuation of engineering resources or budget will likely substantially lengthen proposed beamline development, and call for resources-specific short term, goal oriented schedule. This is addressed in the following "2017 tasks" section.

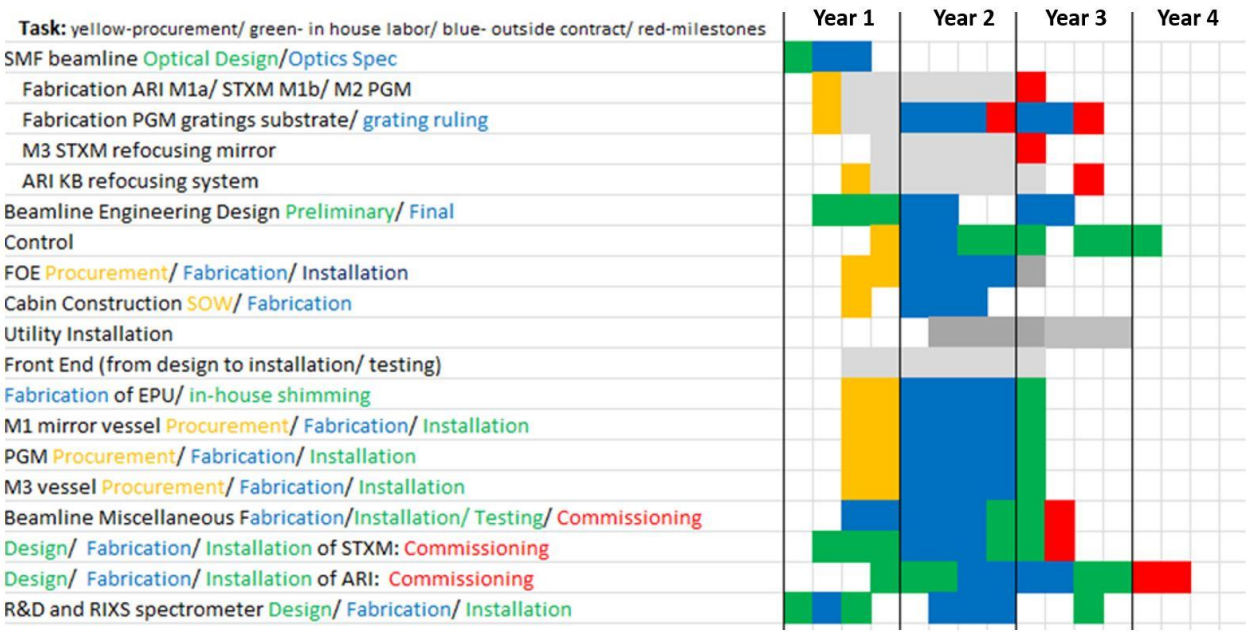


Fig.8. Schedule profile (technically-limited) for the project.

(5) Recommendations:

It's clear that in the absence of special funding for beamline construction, the development of a facility as large as SMF can only be done in phases. Such a phased approach would lead to the sequential completion of individual end-station(s), so the scientifically productive user-driven operations will start as soon as possible and permit the redeployment of resources to the development of the next end-station. It's also important to prioritize the techniques and capabilities that are unique worldwide, take advantage of NSLS-II strengths, address a wide range of user demands, and have the greatest scientific impact.

Therefore, our recommendations are to:

(1) Establish the general optical design and overall layout of the SMF facility.

(2) Proceed with the build-out of the low energy branch first, focusing on the completion of the STXM endstation but leaving affordances for the high-energy branch.

(3) *At the same time as (2), initiate the R&D program focused on the development of the zone plate-based RIXS spectrometer for the ARI endstation.*
(4) *Proceed with the construction of the ARI endstation.*
(5) *Complete the detailed design and construction of the high-energy branch for the high-energy STXM.*

Completion of the low energy STXM first will most quickly provide the unique opportunity to access low Z elements such as Li for functional *in operando* imaging of energy storage devices (such as batteries), which is a direct response to DOE's core mission. The energy range of the low energy STXM (45 – 1200 keV) will also be sufficient to develop strong and diverse programs covering polymer science, magnetic devices, complex materials, and "water-window" spectromicroscopy for environmental, geological, and biological sciences. In order to accommodate such a wide variety of samples, the in-vacuum STXM endstation will be built with high flexibility to accommodate operando and cryo environments.

The completion of the low-energy STXM will also open the road to the development of ARI end-station and enable another BNL major initiative- quantum material research. The low-energy STXM branch would be developed first (~3 years) and become operational while we are also pursuing the R&D necessary to develop the ARI/RIXS endstation, which would follow in 1-2 years. This is consistent with a phased distribution of resources (staff and materials) and procurement of long–term items (KB fabrication).

The high-energy cutoff of the low-energy branch (1.2 keV) will prevent exploration of absorption edges such as phosphorus, sulfur, and transition metals – hence the need for the high-energy STXM. Since NSLS-II currently has the capability to probe these elements with ~10 micron resolution with the TES beamline, we think some delay with the development of the high energy STXM (to reach nanoscale spatial resolution) is permissible, making the high-energy STXM the third program to be constructed in this phased approach. However, we would like to encourage NSLS-II to consider the construction of the X-ray Fluorescence Nanoprobe (XFN) beamline as an alternative to the high-energy STXM because XFN will accommodate both transmission and fluorescence experiments with a similar nanoscale spatial resolution at considerably lower cost since much of its infrastructure has already been built at sector 5.

The budgetary estimates left ambiguity as to whether the STXMs should be purchased or built in-house. We need to state that despite the perception of an "easy route" of purchasing the commercial soft x-ray STXM, such decision has a significant negative impact on soft x-ray microscopy program, as (a) there is no commercial STXM design for ptychography (coherent scattering), as an ultimate tool to reach ~2-5 nm spatial resolution, and all will rely on ZP performance (which is only good to ~20 nm), (b) commercial STXM design is not based on latest generation of ALS/CLS-build x-ray microscopes, nor utilize NSLS-II expertise (such as HXN development, Nazaretski/Lauer) or extend it, as needed to maintain NSLS-II leading position, (c) commercial STXM control is rigid and it will be difficult to upgrade/maintain in long term/ bring new capability/detectors, (d) the cost of commercial instrument ($1.5M) is similar to "in-house" development, even when the "in-house"- built will use a more advanced hardware (faster scanning stages/ more precise interferometry/ cryo-T). *Therefore, we*

recommend forming an internal team for the "in-house" development of the low energy STXM and rely on collaboration with other SR facilities (e.g. ALS, CLS) for its design.

(6) 2017 task(s):

Based on the discussion held by Task Force group, it's become clear that a dedicated scientist should be identified to lead the beamline development to ensure project success. In addition to the core managerial/technical duty, s/he should engage the user community to actively participate in the project by sharing their time/expertise and to some extent resources.

2017 priorities are:

1. Complete optical and preliminary engineering design.
2. Develop specs, SOW and launch procurements for long lead items (including for FE/EPUs).
3. Define major procurement packages scope and develop resources-loaded schedule.
4. Start STXM endstation design or define specs/SOW.
5. Pursue R&D for ARI/ STXM ZP-RIXS spectrometer.

Resources needed (at minimum): 1 FTE scientist, plus 1 FTE mech engineer, 0.5 FTE mech designer for beamline/endstation construction

(7) Meetings/Interactions Summary

(1) General Meetings
May 18, 2 PM (kickoff meeting)
June 24, 11 AM (general meeting with BDP PIs)
August 5, 2 PM (general meeting with BDP PIs)
September 7, 11 AM (beamline controls/software meeting)
September 12, 2 PM (general meeting with BDP PIs)
September 15, 2:30 PM (beamline labor/schedule profiles meeting)

(2) Meetings with SMF/ARI Team
June 7, 2 PM
June 15, 4 PM (meeting to revisit/revise SMF/ARI charge)
June 21, 3 PM
August 1, 3 PM
August 23, 1 PM
September 26, 10 AM
September 27, 9 AM
October 21, 9:30 AM
November 3, 11 AM

(8) SMF/ARI Beamline WBS Dictionary

(1) PSMF-ARI.01 Management and Support
Performance of management and support activities, including labor, materials, travel, and fixed costs associated with management and support functions, consisting of construction management, reviews, administrative support, ESH, QA, configuration management, business operations, project controls, procurement, and document control.

(2) PSMF-ARI.02.04 R&D Program
Equipment and effort needed to uphold a necessary R&D program pertaining to the endstation.

(3) PSMF-ARI.03 Beamline Construction

(a) PSMF-ARI.03.01 Photon Delivery System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of photon delivery sub-systems and integrated system. These include the beamline optical systems upstream of the endstation (including their housings, supports, and manipulation systems), apertures and beam definition and conditioning systems, beam diagnostic/visualization systems, beam transport system, vacuum system, cooling/heating and temperature stabilization systems associated with photon delivery system components, and shielding systems (exclusive of radiological enclosures) that include collimators, masks, shutters, and beam stops.

(b) PSMF-ARI.03.03 Endstation System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of endstation sub-systems and integrated system. These include sample housings, environments, visualization, and support and manipulation systems, detection systems, optical systems and beam diagnostic/visualization and conditioning/definition/deflection components just before the sample (e.g. on the same support as the sample or contiguous with it) or between the sample and detector (e.g. crystal/grating/mirror-based analyzer or spectrometer system) including their housings, supports, and manipulation systems, vacuum system, and cooling/heating and temperature stabilization systems associated with endstation components.

(4) Beamline Infrastructure

(a) PSMF-ARI.04.01 Hutches, Cabins, and Control Station Furniture
Design, specification, procurement, fabrication, assembly, installation, and testing of the required radiological enclosures, including the necessary hoist, air handling equipment, fans, labyrinths, doors, windows, and lights. Design, specification, procurement, fabrication, assembly, installation, and testing of required environmental cabins (not radiological enclosures) including the necessary ventilation, doors, windows, wiring, and lights, and of furniture for the beamline control station including partitions and their power and communications wiring.

(b) PSMF-ARI.04.02 Mechanical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline mechanical utilities including equipment racks, DI water, process chilled water, gaseous nitrogen, compressed air, exhaust, and liquid nitrogen distribution systems.

(c) PSMF-ARI.04.03 Electrical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline electrical utilities including circuit breaker panels, provisioning of power to equipment racks, and cable trays and conduits.

(d) PSMF-ARI.04.04 Equipment Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Equipment Protection System (EPS) including PLC, wiring, and custom sensors.

(e) PSMF-ARI.04.05 Personnel Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Personnel Protection System (PPS) including PLC, wiring, switches, locks, special interlocked personnel protective safeguards such as gates and light screens, and Human Machine Interface (HMI) panel.

(5) PSMF-ARI.05 Accelerator Infrastructure

(a) PSMF-ARI.05.01 Front End

Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of front end sub-systems and integrated system. These include the front end chambers, vacuum system, supports, apertures, collimators, masks, shields, shutters, and diagnostics including flags and beam position monitors. The necessary utilities, protection systems, and controls for the front end are included.

(b) PSMF-ARI.05.02 Source
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of radiation source and associated hardware. This could be an insertion device for x-rays or an extraction chamber to insert within a dipole magnet for infrared radiation. Magnetic measurements if necessary are included. The necessary utilities, protection systems, and controls for the source are included.

(c) PSMF-ARI.05.03 Straight Section
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of accelerator straight section sub-systems and integrated system. These include the straight section chambers, vacuum system, supports, masks, shields, diagnostics including beam position monitors, and canting magnets with power supplies if necessary. The necessary utilities, protection systems, and controls for the straight section are included.

(6) PSMF-ARI.06 Beamline Controls

(a) PSMF-ARI.06.01 Basic System Controls
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation control systems. These include operator consoles for control and archive of control equipment, network routers, gateway to the machine control system, timing IOC to synchronize to the machine timing, motor controllers and associated cabling, serial to Ethernet hubs, and a soft IOC for controlling all Ethernet-based motors, serial devices, and PLCs. Ethernet and timing cables are also included.

(b) PSMF-ARI.06.02 Instrument Applications
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation instrument control applications. These include experimental control workstations, data storage and computation equipment, experimental control software and servers, and data acquisition equipment and software including for detectors.

(9) Labor Estimate Summary

	Year 1	Year 2	Year 3	Year 4	Total	Basis of Estimate
beamline & endstation construction major activities:	design, procurement	design, procurement, fabrication	procurement, fabrication, assembly, installation, testing	assembly, installation, testing	person-years	
scientist / assistant sci	3	3	3	3	12	beamline project exp
mech / vac engineer	2	1.5	1.5	1	6	beamline project exp
mech designer	1	0.75	0.75	0.5	3	beamline project exp
mech / vac technician	0	0	2	2	4	beamline project exp
Total					25 pers-years or 44,000 hr	

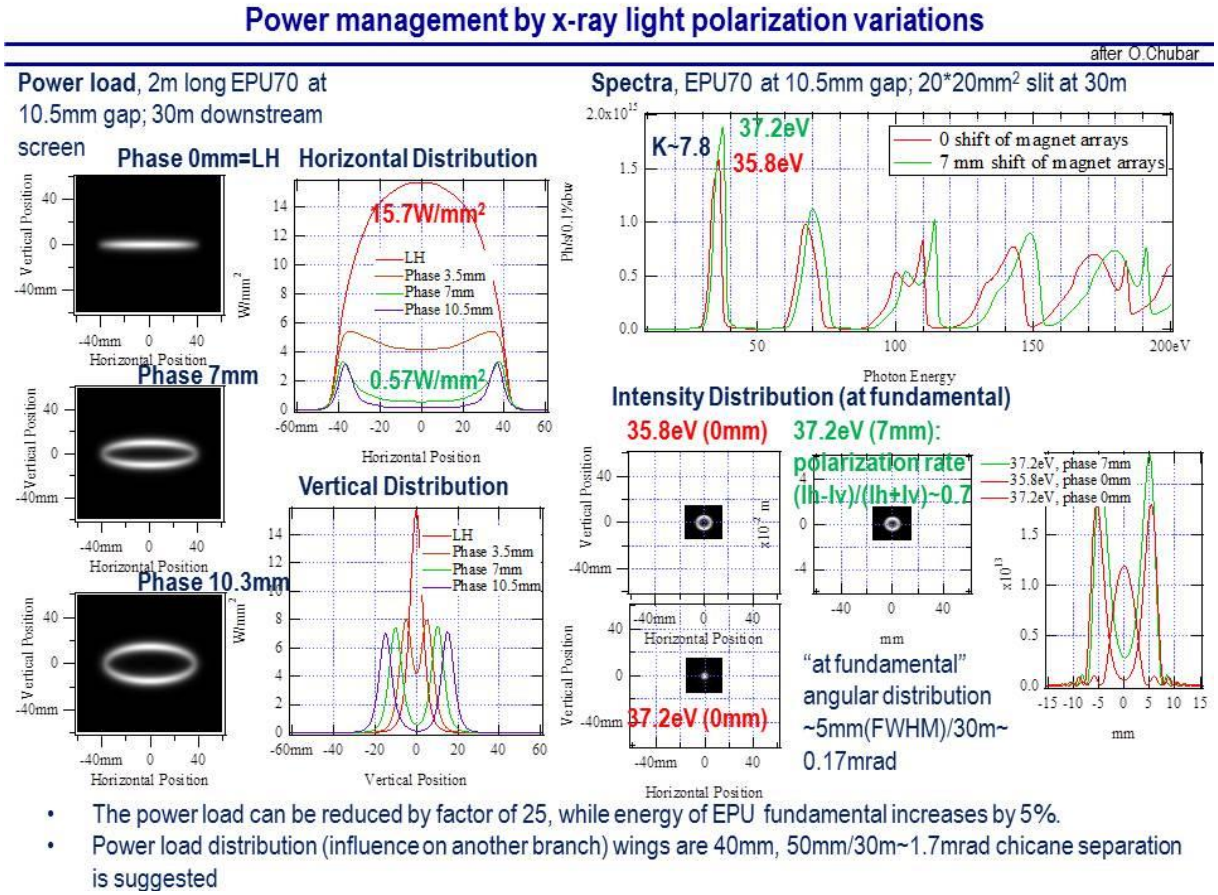
Additional Labor Required:

Project management: 2,100 hrs scientist
Project support: to be determined, requires clarification
Labor for IDs and accelerator straight: 13,100 hrs (scientist, engineer, tech, trades; bottom-up deter)
Labor for front end: 7,300 hrs (engineer, technician, trades; bottom-up determined)
Trades labor for BL construction (riggers, carpenters, masons, and surveyors): still being tallied
Labor for beamline infrastructure: 6,800 hrs (engineer, technician, trades; bottom-up determined)
Labor for beamline controls: 9,800 hrs (controls engineer, technician; bottom-up determined)
Labor for R&D: 3,200 hrs (scientist, mechanical engineer/designer, controls engineer; prof judgment)

Total Labor Required: 86,300 hrs or 49 person-years plus additional hrs still being tallied

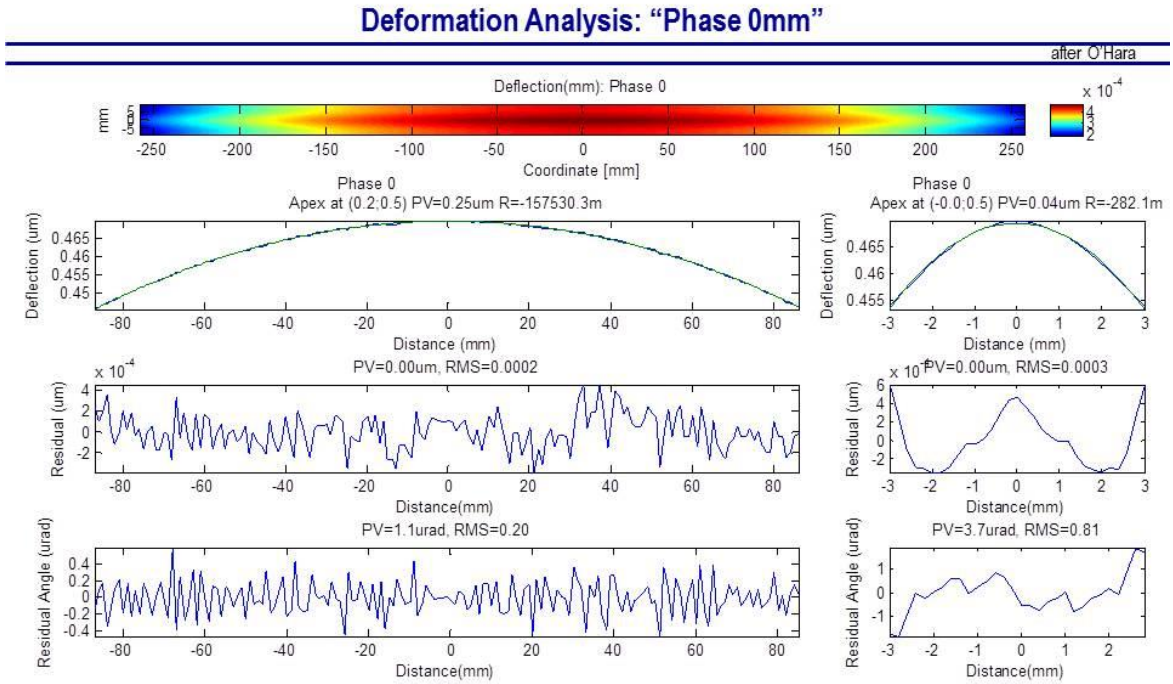
Travel Budget Required: still being determined

Appendix I.



- The power load can be reduced by factor of 25, while energy of EPU fundamental increases by 5%.
- Power load distribution (influence on another branch) wings are 40mm, 50mm/30m~1.7mrad chicane separation is suggested

Fig. A1. Spectral properties of EPU70.



EPU70 at close gap (phase 0mm, LH polarization, 36eV) emits substantial power to affect M1 optic. M1 ARI is assumed to be Si mirror with built-in water cooling channels, identical to ESM M1. Temperature rises, induced stress are not critical (see separate FEA report) but alteration of optical performance du to M1 deformation is a concern. ID light induces mirror surface deformation (within photon imprint) in a shape of cylinder with Rtang=157km (concave), Rsag= 0.28km (concave), total deformation is below ~5um.

Fig. A2. Power load and deformation of M1 (low energy branch) mirror in the most extreme case: EPU70 in LH mode at close gap operation.

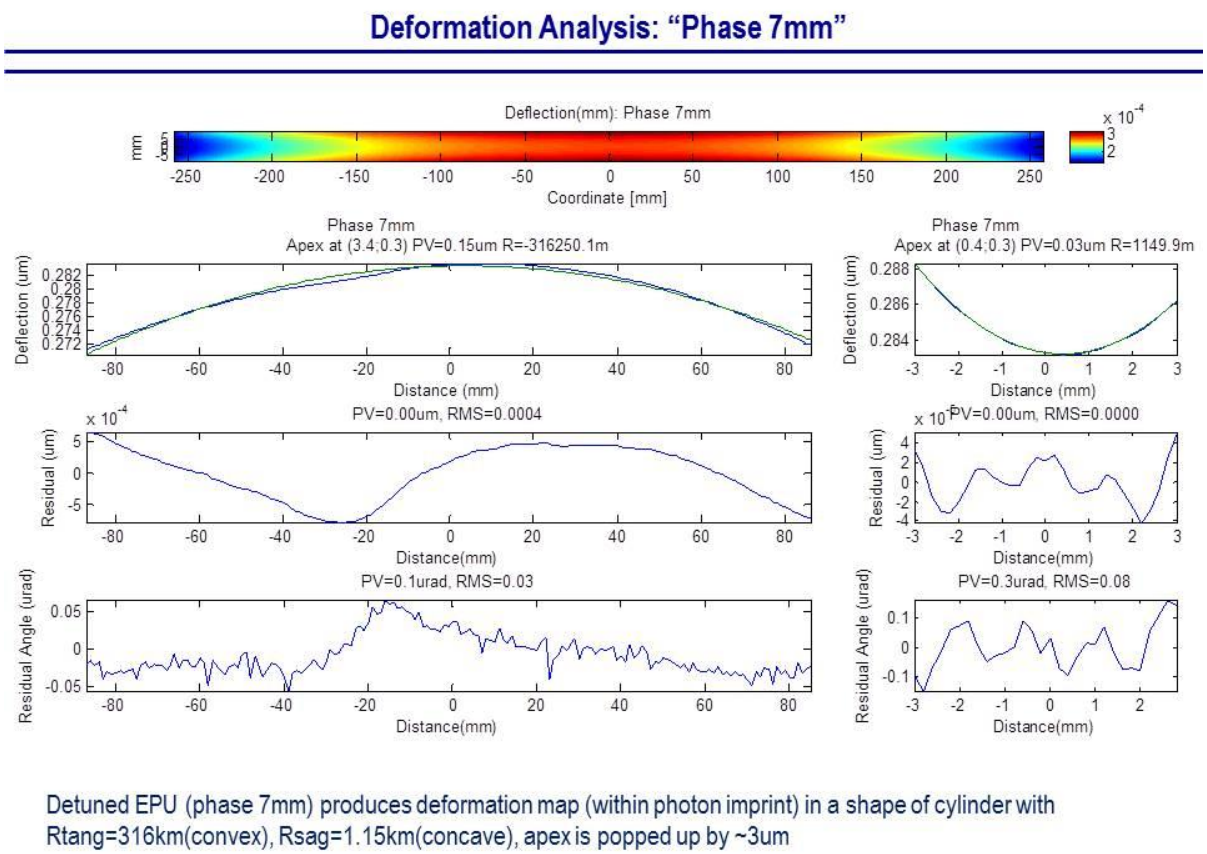
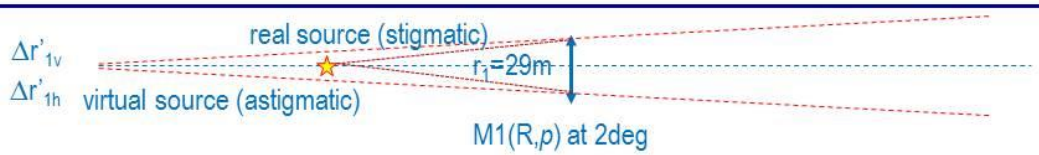


Fig. A3. Power load and deformation of M1 (low energy branch) mirror with "de-tuned" EPU70 operation: gap=10.5mm but with girders shifted to +/-7mm position to generate elliptical polarization.

Influence of M1 deformation on optical performance



Case	Power Load Total (W, 18*18mm)	Power Density Center (W/mm2)	Induced Tang Radius (km)	Induced Sag Radius (km)	Virtual Source Shift (horizontal,m)	Virtual Source Shift (vertical,m)	Depth of Focus (m, aperture: 6*6mm)	Impact
Gap 10.5mm; Phase 0mm	2.17e3	0.548	-157	-0.282	-0.303	-0.206	0.116	not acceptable
Gap 10.5mm; Phase 7mm	835	0.245	-316	1.15	-0.152	0.05	0.116	almost acceptable

Fig. A4. Summary of FEA analysis and influence of EPU power load on ARI optical performance.

Project: SMF-ARI Beamline — RESOURCE DETAIL

WBS	RESOURCE	UNITS	COST
PSMF-ARI - SMF-ARI Beamline			
PSMF-ARI.01 - SMF-ARI Management			
LABOR	Labor_Scientist_NS1	2,112.00	$ 322,016.84
	Labor_Administrative Secretary_NA3	704.00	$ 40,127.88
	Labor_ES&H Professional_NA4	1,056.00	$ 127,282.85
	Labor_QA Professional_NA5	704.00	$ 79,449.16
	Labor_Administrative_NA2	1,338.00	$ 102,600.17
	Labor_Human Resources_NB4	352.00	$ 26,991.97
	LABOR TOTAL	6,266.00	$ 698,468.87
MATERIAL	Material_Material (Purchase <$25k)_NMA	100,000.00	$ 132,323.61
	MATERIAL TOTAL	100,000.00	$ 132,323.61
PSMF-ARI.02 - SMF-ARI Design			
PSMF-ARI.02.01 - SMF-ARI Conceptual Design			
LABOR	Labor_Scientist_NS1	1,760.00	$ 250,054.24
	Labor_Mechanical Engineer_NO1	1,050.00	$ 99,444.28
	Labor_Mechanical Designer_NO2	525.00	$ 42,435.63
	LABOR TOTAL	3,335.00	$ 391,934.14
PSMF-ARI.02.02 - SMF-ARI Preliminary Design			
LABOR	Labor_Scientist_NS1	1,760.00	$ 255,179.30
	Labor_Mechanical Engineer_NO1	1,050.00	$ 100,379.84
	Labor_Mechanical Designer_NO2	525.00	$ 42,834.86
	LABOR TOTAL	3,335.00	$ 398,394.00
PSMF-ARI.02.03 - SMF-ARI Final Design			
LABOR	Labor_Scientist_NS1	1,760.00	$ 260,513.56
	Labor_Mechanical Engineer_NO1	1,050.00	$ 101,353.59
	Labor_Mechanical Designer_NO2	525.00	$ 43,250.38
	LABOR TOTAL	3,335.00	$ 405,117.53
PSMF-ARI.02.04 - SMF-ARI R&D Program			
LABOR	Labor_Scientist_NS1	440.00	$ 64,221.92
	Labor_Assistant/Associate Scientist_NS2	880.00	$ 89,529.39
	Labor_Mechanical Engineer_NO1	880.00	$ 84,650.60
	Labor_Mechanical Designer_NO2	440.00	$ 36,122.75
	Labor_Controls Engineer_NE4	587.00	$ 64,729.67
	LABOR TOTAL	3,227.00	$ 339,254.33
MATERIAL	Material_Material (Purchase >$25k)_NSM	650,000.00	$ 803,713.64
	MATERIAL TOTAL	650,000.00	$ 803,713.64
PSMF-ARI.03 - SMF-ARI Beamline Construction			
PSMF-ARI.03.01 - SMF-ARI Photon Delivery System Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	2,640.00	$ 395,675.72
	Labor_Mechanical Engineer_NO1	2,100.00	$ 205,010.05
	Labor_Mechanical Designer_NO2	1,050.00	$ 87,483.46
	Labor_Mechanical Technician_NO3	1,760.00	$ 138,015.81
	LABOR TOTAL	7,550.00	$ 826,185.04
MATERIAL	Material_Material (Purchase >$25k)_NSM	5,672,500.00	$ 7,130,140.86
	MATERIAL TOTAL	5,672,500.00	$ 7,130,140.86
PSMF-ARI.03.02 - SMF-ARI Photon Delivery System Installation and Test			
LABOR	Labor_EL - Vacuum Engineer_SE5	502.00	$ 59,491.14
	Labor_EL - Vacuum Technician_SE6	2,028.00	$ 179,968.68
	Labor_ME - Survey Engineer_MO1	156.00	$ 16,314.81
	Labor_EL - Survey Technician_SE2	374.00	$ 33,189.49
	Labor_Building Trades Unassigned_NST	62.75	$ 8,241.79
	Labor_Plant Engineering-Building Trades Carpenter_BTC	141.25	$ 17,572.17
	Labor_Plant Engineering-Building Trades Riggers_BTS	281.00	$ 35,019.71
	Labor_Scientist_NS1	1,320.00	$ 209,589.15
	Labor_Mechanical Engineer_NO1	840.00	$ 86,780.69
	Labor_Mechanical Designer_NO2	420.00	$ 37,031.72
	Labor_Mechanical Technician_NO3	1,760.00	$ 142,019.14
	LABOR TOTAL	7,885.00	$ 825,218.48
PSMF-ARI.03.03 - SMF-ARI End Station Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	7,920.00	$ 1,209,803.18
	Labor_Mechanical Engineer_NO1	3,150.00	$ 312,639.03
	Labor_Mechanical Designer_NO2	1,575.00	$ 133,411.72
	Labor_Mechanical Technician_NO3	1,760.00	$ 139,727.29
	LABOR TOTAL	14,405.00	$ 1,795,581.22
MATERIAL	Material_Material (Purchase >$25k)_NSM	4,550,000.00	$ 5,828,167.06
	MATERIAL TOTAL	4,550,000.00	$ 5,828,167.06
PSMF-ARI.03.04 - SMF-ARI End Station Installation and Test			
LABOR	Labor_Scientist_NS1	3,960.00	$ 649,235.91
	Labor_Mechanical Engineer_NO1	1,260.00	$ 134,399.75
	Labor_Mechanical Designer_NO2	630.00	$ 57,352.09
	Labor_Mechanical Technician_NO3	1,760.00	$ 146,632.75
	LABOR TOTAL	7,610.00	$ 987,620.51
PSMF-ARI.04 - SMF-ARI Beamline Infrastructure			
PSMF-ARI.04.01 - SMF-ARI Hutches			
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,060,000.00	$ 1,341,871.61
	MATERIAL TOTAL	1,060,000.00	$ 1,341,871.61
PSMF-ARI.04.02 - SMF-ARI Mechanical Utilities			
LABOR	Labor_ME - Utility Engineer_MO3	314.00	$ 31,862.69
	Labor_Mechanical Designer_NO2	264.00	$ 22,175.39
	Labor_EL - Utility Technician_SE4	908.00	$ 79,344.80

	Labor_Plant Engineering-Building Trades Plumber_BTP	202.00	$	24,995.18
	Labor_Plant Engineering-Building Trades Carpenter_BTC	32.00	$	3,884.62
	Labor_Building Trades Unassigned_NST	40.00	$	5,195.65
	LABOR TOTAL	1,760.00	$	167,458.34
MATERIAL	Material_Material (Purchase >$25k)_NSM	200,000.00	$	251,270.00
	Material_Material (Purchase <$25k)_NMA	33,200.00	$	43,463.95
	MATERIAL TOTAL	233,200.00	$	294,733.95
PSMF-ARI.04.03 - SMF-ARI Electrical Utilities				
LABOR	Labor_Electrical Engineer_NE1	103.75	$	11,995.94
	Labor_Electrical Designer_NE2	48.00	$	4,299.87
	Labor_Plant Engineering-Building Trades Electrician_BTE	1,293.00	$	159,620.06
	LABOR TOTAL	1,444.75	$	175,915.88
MATERIAL	Material_Material (Purchase <$25k)_NMA	40,000.00	$	52,366.20
	MATERIAL TOTAL	40,000.00	$	52,366.20
PSMF-ARI.04.04 - SMF-ARI EPS				
LABOR	Labor_Controls Engineer_NE4	340.00	$	39,704.85
	Labor_Electrical Technician_NE3	490.00	$	42,921.86
	Labor_Electrical Designer_NE2	40.00	$	3,677.52
	LABOR TOTAL	870.00	$	86,304.23
MATERIAL	Material_Material (Purchase <$25k)_NMA	43,000.00	$	57,532.14
	MATERIAL TOTAL	43,000.00	$	57,532.14
PSMF-ARI.04.05 - SMF-ARI PPS				
LABOR	Labor_Electrical Engineer_NE1	776.00	$	92,656.55
	Labor_Electrical Technician_NE3	1,200.00	$	108,100.56
	Labor_Electrical Designer_NE2	384.00	$	35,922.04
	Labor_Plant Engineering-Building Trades Electrician_BTE	400.00	$	49,495.42
	LABOR TOTAL	2,760.00	$	286,174.57
MATERIAL	Material_Material (Purchase >$25k)_NSM	76,000.00	$	98,800.00
	MATERIAL TOTAL	76,000.00	$	98,800.00
PSMF-ARI.05 - SMF-ARI Accelerator Infrastructure				
PSMF-ARI.05.01 - SMF-ARI Front End				
LABOR	Labor_Project Engineer_MO7	150.00	$	15,132.16
	Labor_Mechanical Engineer_NO1	1,140.00	$	112,280.44
	Labor_Mechanical Designer_NO2	600.00	$	49,452.95
	Labor_Assistant/Associate Scientist_NS2	60.00	$	6,010.04
	Labor_ME - Vacuum Engineer_MO5	220.00	$	22,109.67
	Labor_ME - D&I Engineer_NO6	260.00	$	26,004.23
	Labor_Electrical Engineer_NE1	400.00	$	46,431.04
	Labor_EL - D&I Engineer_TE1	340.00	$	39,021.87
	Labor_Controls Engineer_NE4	160.00	$	18,446.44
	Labor_Electrical Designer_NE2	160.00	$	14,639.37
	Labor_Electrical Technician_NE3	400.00	$	34,768.73
	Labor_EL - Vacuum Engineer_SE5	200.00	$	23,215.52
	Labor_ME - Utility Engineer_MO3	120.00	$	12,228.92
	Labor_Mechanical Technician_NO3	1,270.00	$	100,236.94
	Labor_ME - Survey Engineer_MO1	195.00	$	20,076.08
	Labor_EL - D&I Technician_TE2	440.00	$	38,404.62
	Labor_ME - Survey Technician_MO2	350.00	$	30,704.59
	Labor_ME - Vacuum Technician_MO6	510.00	$	41,121.73
	Labor_Plant Engineering-Building Trades Riggers_BTS	119.00	$	14,724.89
	Labor_Plant Engineering-Building Trades Electrician_BTE	48.00	$	5,939.45
	Labor_Building Trades Unassigned_NST	72.00	$	9,352.17
	Labor_ME - Utility Technician_MO4	40.00	$	3,225.23
	LABOR TOTAL	7,254.00	$	683,527.08
MATERIAL	Material_Material (Purchase >$25k)_NSM	973,000.00	$	1,283,210.48
	MATERIAL TOTAL	973,000.00	$	1,283,210.48
PSMF-ARI.05.02 - SMF-ARI Source				
LABOR	Labor_Assistant/Associate Scientist_NS2	1,220.00	$	132,604.47
	Labor_EL - Insertion Device Engineer_TE4	1,600.00	$	189,735.94
	Labor_ME - Insertion Device Engineer_NO8	840.00	$	88,504.99
	Labor_Controls Engineer_NE4	900.00	$	107,549.07
	Labor_ME - Survey Engineer_MO1	180.00	$	19,033.35
	Labor_ME - Insertion Device Technician_NO9	1,300.00	$	106,893.91
	Labor_ME - Survey Technician_MO2	360.00	$	32,446.63
	Labor_Project Engineer_MO7	80.00	$	8,504.60
	Labor_Electrical Engineer_NE1	240.00	$	29,006.66
	Labor_Mechanical Designer_NO2	160.00	$	14,435.69
	Labor_Electrical Designer_NE2	160.00	$	15,298.49
	Labor_ME - Vacuum Technician_MO6	200.00	$	16,771.21
	Labor_Electrical Technician_NE3	400.00	$	36,439.78
	Labor_Plant Engineering-Building Trades Electrician_BTE	200.00	$	25,292.16
	Labor_Plant Engineering-Building Trades Riggers_BTS	48.00	$	6,070.12
	Labor_Building Trades Unassigned_NST	80.00	$	10,619.91
	LABOR TOTAL	7,968.00	$	839,206.97
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,780,000.00	$	2,236,303.00
	MATERIAL TOTAL	1,780,000.00	$	2,236,303.00
PSMF-ARI.05.03 - SMF-ARI Straight				
LABOR	Labor_Project Engineer_MO7	60.00	$	6,029.92
	Labor_Assistant/Associate Scientist_NS2	160.00	$	16,660.28
	Labor_ME - Vacuum Engineer_MO5	520.00	$	52,163.80
	Labor_ME - Insertion Device Engineer_NO8	200.00	$	20,048.35
	Labor_ME - D&I Engineer_NO6	430.00	$	43,116.75
	Labor_Mechanical Designer_NO2	380.00	$	31,944.23

	Labor_EL - Vacuum Engineer_SE5	90.00	$	10,370.50
	Labor_Electrical Engineer_NE1	260.00	$	29,708.67
	Labor_EL - Insertion Device Engineer_TE4	180.00	$	20,800.38
	Labor_ME - Utility Engineer_MO3	160.00	$	16,229.53
	Labor_EL - D&I Engineer_TE1	430.00	$	48,665.48
	Labor_ME - Vacuum Technician_MO6	500.00	$	39,989.79
	Labor_ME - Survey Engineer_MO1	60.00	$	6,105.73
	Labor_ME - Utility Technician_MO4	40.00	$	3,225.23
	Labor_ME - Survey Technician_MO2	140.00	$	12,100.71
	Labor_Electrical Designer_NE2	380.00	$	33,714.56
	Labor_EL - D&I Technician_TE2	440.00	$	37,058.40
	Labor_Electrical Technician_NE3	720.00	$	61,242.82
	Labor_ME - Insertion Device Technician_NO9	40.00	$	3,211.59
	Labor_Plant Engineering-Building Trades Riggers_BTS	24.00	$	2,962.69
	Labor_Building Trades Unassigned_NST	24.00	$	3,110.01
	LABOR TOTAL	5,238.00	$	498,459.41
MATERIAL	Material_Material (Purchase >$25k)_NSM	513,000.00	$	644,390.68
	MATERIAL TOTAL	513,000.00	$	644,390.68
PSMF-ARI.06 - SMF-ARI Controls				
PSMF-ARI.06.01 - SMF-ARI Basic System Controls				
LABOR	Labor_Controls Engineer_NE4	2,232.00	$	254,432.91
	Labor_IT Professional (Software)_NA7	425.60	$	42,297.87
	Labor_Electrical Technician_NE3	793.60	$	69,382.48
	LABOR TOTAL	3,451.20	$	366,113.25
MATERIAL	Material_Material (Purchase <$25k)_NMA	172,300.00	$	227,479.04
	Material_Material (Purchase >$25k)_NSM	114,000.00	$	145,752.81
	MATERIAL TOTAL	286,300.00	$	373,231.85
PSMF-ARI.06.02 - SMF-ARI Instrument Applications				
LABOR	Labor_IT Professional (Software)_NA7	3,680.00	$	353,437.89
	Labor_Assistant/Associate Scientist_NS2	440.00	$	45,483.97
	Labor_Controls Engineer_NE4	2,200.00	$	247,452.30
	LABOR TOTAL	6,320.00	$	646,374.17
MATERIAL	Material_Material (Purchase >$25k)_NSM	122,400.00	$	157,810.50
	Material_Material (Purchase <$25k)_NMA	33,000.00	$	43,831.15
	MATERIAL TOTAL	155,400.00	$	201,641.65

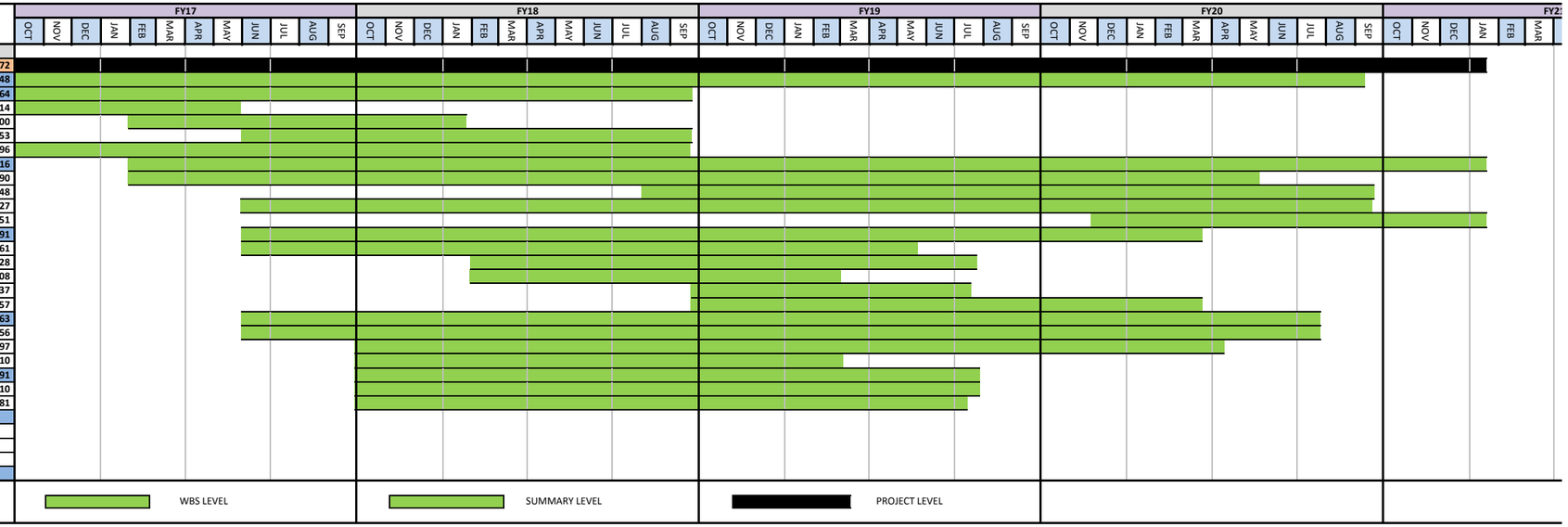
Project: SMF-ARI Beamline RESOURCE SUMMARY

WBS	RESOURCE	UNITS		COST
PSMF-ARI - SMF-ARI Beamline				
LABOR	Labor_Scientist_NS1	23,672.00	$	3,616,289.82
	Labor_Administrative Secretary_NA3	704.00	$	40,127.88
	Labor_ES&H Professional_NA4	1,056.00	$	127,282.85
	Labor_QA Professional_NA5	704.00	$	79,449.16
	Labor_Administrative_NA2	1,338.00	$	102,600.17
	Labor_Human Resources_NB4	352.00	$	26,991.97
	Labor_Mechanical Engineer_NO1	12,520.00	$	1,236,938.28
	Labor_Mechanical Designer_NO2	7,094.00	$	597,930.87
	Labor_Assistant/Associate Scientist_NS2	2,760.00	$	290,288.15
	Labor_Controls Engineer_NE4	6,419.00	$	732,315.24
	Labor_Mechanical Technician_NO3	8,310.00	$	666,631.93
	Labor_EL - Vacuum Engineer_SE5	792.00	$	93,077.16
	Labor_EL - Vacuum Technician_SE6	2,028.00	$	179,968.68
	Labor_ME - Survey Engineer_MO1	591.00	$	61,529.96
	Labor_EL - Survey Technician_SE2	374.00	$	33,189.49
	Labor_Building Trades Unassigned_NST	278.75	$	36,519.53
	Labor_Plant Engineering-Building Trades Carpenter_BTC	173.25	$	21,456.79
	Labor_Plant Engineering-Building Trades Riggers_BTS	472.00	$	58,777.41
	Labor_ME - Utility Engineer_MO3	594.00	$	60,321.14
	Labor_EL - Utility Technician_SE4	908.00	$	79,344.80
	Labor_Plant Engineering-Building Trades Plumber_BTP	202.00	$	24,995.18
	Labor_Electrical Engineer_NE1	1,779.75	$	209,798.86
	Labor_Electrical Designer_NE2	1,172.00	$	107,551.85
	Labor_Plant Engineering-Building Trades Electrician_BTE	1,941.00	$	240,347.08
	Labor_Electrical Technician_NE3	4,003.60	$	352,856.23
	Labor_Project Engineer_MO7	290.00	$	29,666.68
	Labor_ME - Vacuum Engineer_MO5	740.00	$	74,273.47
	Labor_ME - D&I Engineer_NO6	690.00	$	69,120.98
	Labor_EL - D&I Engineer_TE1	770.00	$	87,687.35
	Labor_EL - D&I Technician_TE2	880.00	$	75,463.02
	Labor_ME - Survey Technician_MO2	850.00	$	75,251.93
	Labor_ME - Vacuum Technician_MO6	1,210.00	$	97,882.73
	Labor_ME - Utility Technician_MO4	80.00	$	6,450.47
	Labor_EL - Insertion Device Engineer_TE4	1,780.00	$	210,536.32
	Labor_ME - Insertion Device Engineer_NO8	1,040.00	$	108,553.34
	Labor_ME - Insertion Device Technician_NO9	1,340.00	$	110,105.50
	Labor_IT Professional (Software)_NA7	4,105.60	$	395,735.76
	LABOR TOTAL	94,013.95	$	10,417,308.01
MATERIAL	Material_Material (Purchase <$25k)_NMA	421,500.00	$	556,996.09
	Material_Material (Purchase >$25k)_NSM	15,710,900.00	$	19,921,430.62
	MATERIAL TOTAL	16,132,400.00	$	20,478,426.71

GRAND TOTAL	**$ 30,895,734.72**

Project Name: SMF-ARI Beamline

WBS	Start	Finish	Cost
PSMF-ARI - SMF-ARI Beamline	10/1/2016	1/18/2021	$ 30,895,734.72
PSMF-ARI.01 - SMF-ARI Management	10/1/2016	9/10/2020	$ 830,792.48
PSMF-ARI.02 - SMF-ARI Design	10/1/2016	9/23/2018	$ 2,338,413.64
PSMF-ARI.02.01 - SMF-ARI Conceptual Design	10/1/2016	5/29/2017	$ 391,934.14
PSMF-ARI.02.02 - SMF-ARI Preliminary Design	1/30/2017	1/25/2018	$ 398,394.00
PSMF-ARI.02.03 - SMF-ARI Final Design	5/31/2017	9/23/2018	$ 405,117.53
PSMF-ARI.02.04 - SMF-ARI R&D Program	10/1/2016	9/21/2018	$ 1,142,967.96
PSMF-ARI.03 - SMF-ARI Beamline Construction	1/30/2017	1/18/2021	$ 17,392,913.16
PSMF-ARI.03.01 - SMF-ARI Photon Delivery System Procurement and Fabrication	1/30/2017	5/21/2020	$ 7,956,325.90
PSMF-ARI.03.02 - SMF-ARI Photon Delivery System Installation and Test	8/1/2018	9/20/2020	$ 825,218.48
PSMF-ARI.03.03 - SMF-ARI End Station Procurement and Fabrication	5/30/2017	9/18/2020	$ 7,623,748.27
PSMF-ARI.03.04 - SMF-ARI End Station Installation and Test	11/24/2019	1/18/2021	$ 987,620.51
PSMF-ARI.04 - SMF-ARI Beamline Infrastructure	5/31/2017	3/21/2020	$ 2,561,156.91
PSMF-ARI.04.01 - SMF-ARI Hutches	5/31/2017	5/22/2019	$ 1,341,871.61
PSMF-ARI.04.02 - SMF-ARI Mechanical Utilities	1/30/2018	7/24/2019	$ 462,192.28
PSMF-ARI.04.03 - SMF-ARI Electrical Utilities	1/30/2018	3/1/2019	$ 228,282.08
PSMF-ARI.04.04 - SMF-ARI EPS	9/23/2018	7/18/2019	$ 143,836.37
PSMF-ARI.04.05 - SMF-ARI PPS	9/23/2018	3/21/2020	$ 384,974.57
PSMF-ARI.05 - SMF-ARI Accelerator Infrastructure	5/31/2017	7/25/2020	$ 6,185,097.63
PSMF-ARI.05.01 - SMF-ARI Front End	5/31/2017	7/25/2020	$ 1,966,737.56
PSMF-ARI.05.02 - SMF-ARI Source	9/29/2017	4/13/2020	$ 3,075,509.97
PSMF-ARI.05.03 - SMF-ARI Straight	9/29/2017	3/3/2019	$ 1,142,850.10
PSMF-ARI.06 - SMF-ARI Controls	9/29/2017	7/27/2019	$ 1,587,360.91
PSMF-ARI.06.01 - SMF-ARI Basic System Controls	9/29/2017	7/27/2019	$ 739,345.10
PSMF-ARI.06.02 - SMF-ARI Instrument Applications	9/29/2017	7/14/2019	$ 848,015.81
PSMF-ARI.07 - SMF-ARI Conventional Facilities			$ -
PSMF-ARI.07.01 - SMF-ARI Conventional Facilities Design			$ -
PSMF-ARI.07.02 - SMF-ARI Conventional Facilities Construction			$ -
PSMF-ARI.07.03 - SMF-ARI Conventional Facilities Commissioning			$ -
PSMF-ARI.08 - SMF-ARI Special Equipment			$ -



RATE SET: Rate Set 1

16-IEPD Narrative: CDI

G. Williams, I. Robinson

This document addresses the charge of the NSLS-II 2016 Task Force on Instrument Execution Plan Development (16-IEPD) as it relates to the Bragg Coherent Diffraction Imaging (CDI) beamline proposal. The following narrative summarizes the scope definition of that proposal under the following advice:

- Refine scope definition (6-15 keV), and address issues identified during the review, in particular detector positioning system and the dimensions of the endstation hutch
- Focus only on in-situ materials applications, with laser pump-probe considered only as a potential future enhancement (i.e. consider at most only affordances in the present task force work)
- Consider incorporation of forward-direction ptychography and Fresnel CDl capabilities in the conceptual design

(1) Science and applications

The CDI beamline will provide a state-of-the-art endstation supporting coherent imaging of Materials Science samples in the Bragg and forward-scattering geometries. The instrument will be used to study materials and their structure, including their time-dependent evolution. Coherent imaging will provide 3D spatial maps of ordered and disordered materials at 10 nm resolution. In the Bragg geometry, deformation fields within ordered materials will be imaged in 3D and be sensitive to sub-Angstrom displacements. The applications span the gamut from hard condensed matter physics, for example, complex oxide investigation, to environmental applications, where the methods can be used to study the onset and evolution of deformation in geological materials.

(2) Technical capabilities and key performance parameters

The beamline shall deliver quasi-monochromatic x-rays, of photon energy spanning the range from 6 to 15 keV, to the sample in a variably sized focal spot of 1 to 7 micron full-width half-maximum. The endstation shall provide the necessary equipment to measure 3D continuous intensity distributions in the forward- and Bragg-scattering geometries, including: a high-load goniometer to support novel sample environments; a positioning system capable of stable manipulation and scanning at nanometer-scale displacements; an x-ray beam conditioning system, including the removal of stray light, attenuation, and shuttering; long-working-distance focusing optics to allow for beam conditioning and flexible sample environments; and infrastructure to support time-resolved and in operando experiments.

(3) Conceptual Design

A 3 m-long IVU20 in a low-beta straight will provide a highly coherent source of x-rays that is required for maximizing the effectiveness of the coherent imaging techniques. A high-quality horizontal-deflection mirror will provide steering and harmonic rejection from the source. A Si(111) double-crystal monochromator will provide suitable energy resolution for the measurement. The final focusing optics in the beamline will be a KB mirror pair. The beamline optical design will allow for variation in the x-ray spot size from 1 to 7 microns in size, likely by altering the size of the effective secondary source formed by the horizontal-deflection mirror. All mirror surfaces will have minimal figure error and surface roughness to avoid any perturbation in the phase of the x-ray beam.

A shielded enclosure upstream of the principle CDI endstation is reserved for future x-ray-optical laser mixing instrumentation, allowing optical pump, x-ray probe experiments to be conducted with a variety of excitation sources and high time-resolution. The final endstation is a large hutch and provides multiple large area detectors that can allow the measurement of the intensity around multiple Bragg peaks, in the case of highly ordered samples, or the forward-scattered intensity simultaneous to the intensity around a Bragg peaks, to image structure in ordered materials or materials that are partially ordered. The experiments require very high stability over long time periods, which we will accommodate by 0.1-degree-C temperature control in the endstation. A schematic of this design is presented in a plan view in Figure 1 and in an isometric view in Figure 2.

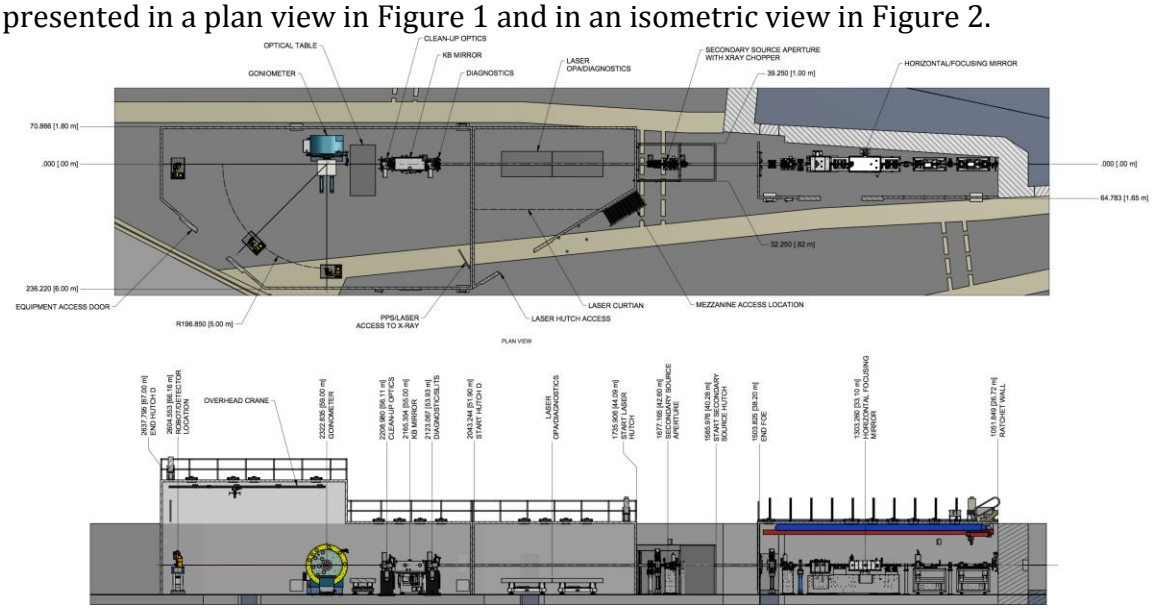


Figure 1. The overview of conceptual design for the CDI beamline if located on the experimental floor of NSLS-II.

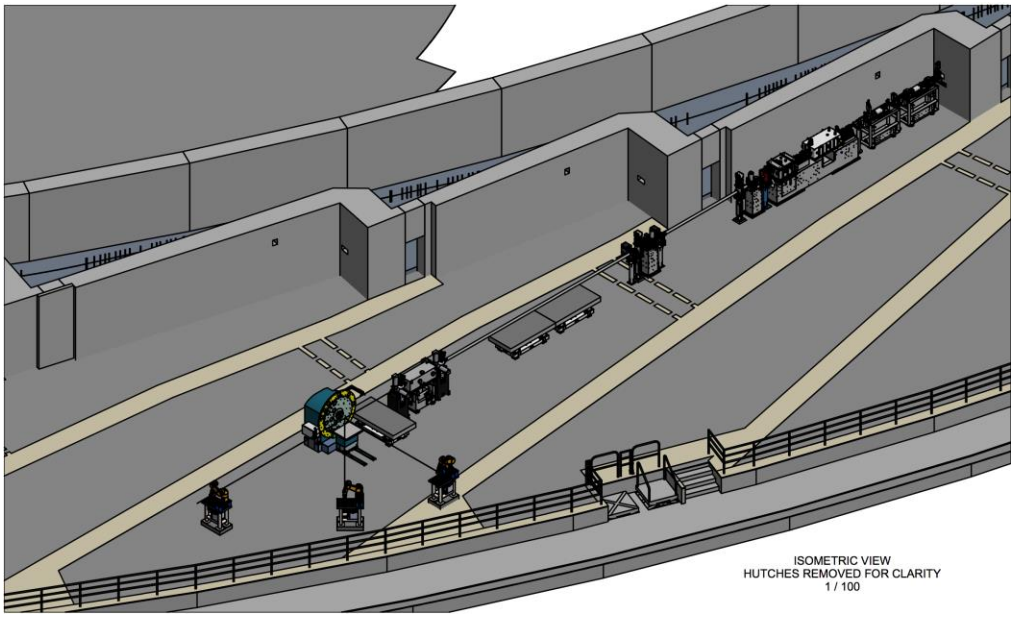


Figure 2. An isometric view of the conceptual design for the CDI beamline if located on the experimental floor of NSLS-II.

The beamline components upstream of and including the secondary source are standard items that differ negligibly from those already installed at NSLS-II. The final experimental hutch, however, is somewhat unusual due to the requirements imposed by the coherent imaging experiment. In order to achieve the desired spatial resolution in the measurement—given the availability of current x-ray detector pixel sizes—a very long and adjustable sample-to-detector distance is required. Additionally, it is desirable to change the size of the focal spot over about one order of magnitude to tailor the beam size to the typical ordered domain size in the sample. These two considerations drive the beam-sample stability requirements for the design and the former drives the floor size of the endstation.

(a) Endstation design

To fully exploit the high brightness of the source, the instrument must be designed to provide high-resolution structural information and to support novel experiments, whether these be *in situ* or time-resolved studies. To this end, full goniometric motion on a kappa diffractometer and a nano-positioning stage stack—for fine positioning and scanning—will be provided. The KB focusing optics will have a long, 1 m working distance to allow for a wide range of sample environments.

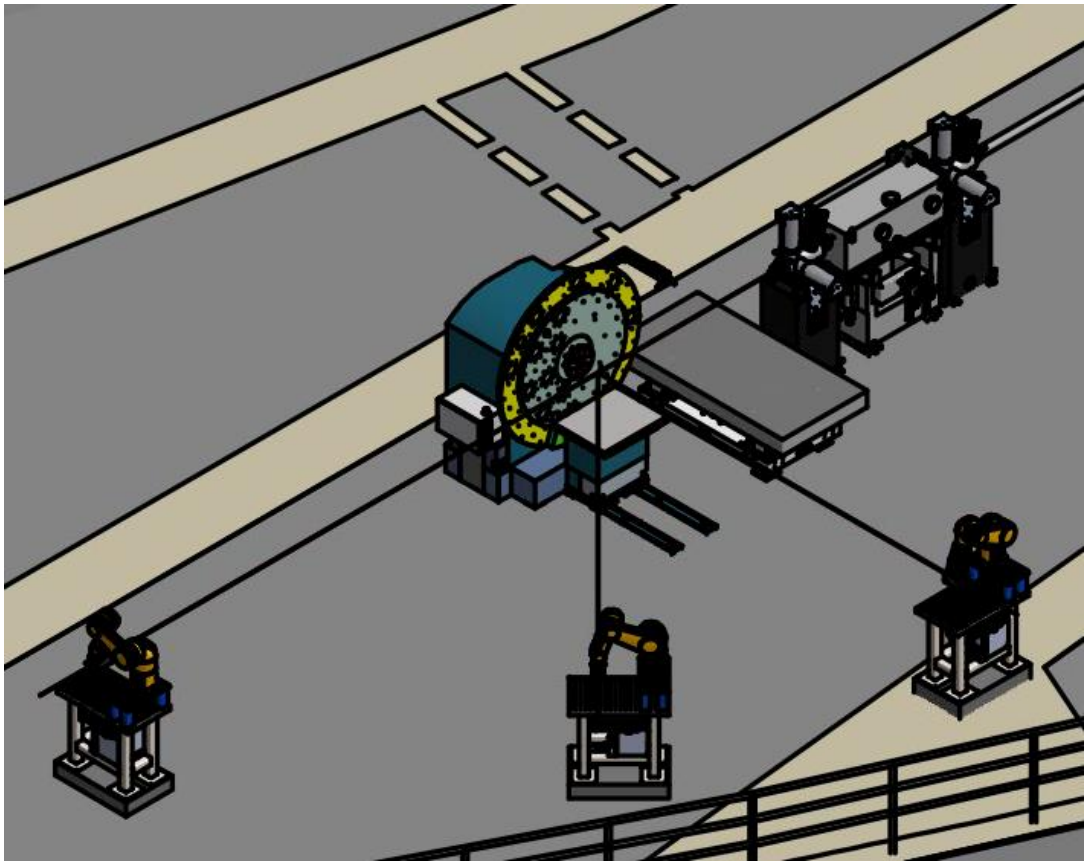


Figure 3. An expanded view of the endstation.

Standard Bragg CDI measurements are supported by goniometric sample motion and a detector positioning system that allows for beyond 90 degrees of in-plane angular and an elevation of approximately 1.5 m above the nominal beam height. Pytchographic Bragg measurements are supported by a sample nano-positioner that allows for better than 10 nm absolute XYZ precision. The circle of confusion on the primary rotation axis will be better than 2 microns. Forward-scattering experiments, including ptychography—in conjunction with the nano-positioner—and plane-wave coherent imaging, are supported by a beam clean-up system, based on passing the beam through sequential apertures, and a clear path to a large area detector at the downstream end of the hutch. Light-duty evacuated flight paths will be manually incorporated into the detector positioning system when needed.

The instrumental resolution in a CDI imaging experiment depends on the collection aperture of the detector from the point of sample-x-ray interaction. The field of view is given by the effective pixel size of the detector. Additionally, the intensity must be sampled at an appropriately high frequency in the detector plane. The relationship between the sample-to-detector distance and the wavelength is conjugate, so our requirement for this distance is a function of available technology, typical sample dimensions, desired photon energy, and the image resolution. We choose 15 keV as a convenient upper bound on the photon energy, primarily driven

by the desire to image materials such as steel, where the penetration length of the x-rays should be longer than the typical domain, which may be 20 microns or more. 15 keV is also a practical upper limit for area detectors (Pilatus, Eiger, Medipix etc) using Si sensors.

In order to provide the ability to image an approximately 10 micron object with 10 nm resolution over the range of 6 to 15 keV, we require a 4 megapixel detector located up to 5 m from the sample. While the instrument will provide the ability to position the detector out of plane, it is foreseen that some experiments, perhaps due to limitations in their *in situ* or sample environment cells will be limited to an in-plane scattering geometry; therefore, we allow in-plane scattering angles beyond 90 degrees. Our conceptual design of this system includes the lessons-learned from similar systems in place at NSLS-II. It will consist of granite or marble floor arc upon which two detector towers will travel, thus providing the in- and out-of-plane positioning required by the scientific scope. Taken together, these considerations lead to a novel, if large, experimental hutch and a complicated scenario for assessing the impact of stability of the instrument inherited from the facility.

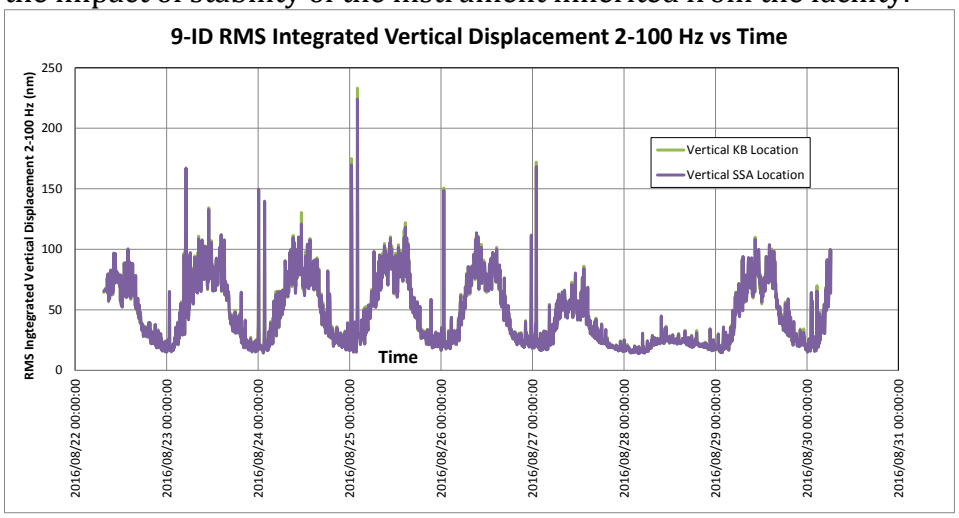


Figure 4. Total measured vertical floor motion over an 8 day period.

Figure 4 shows the typical motion of the experimental floor measured at sector 9 over an 8 day period. Figures 5 and 6 show the correlation in the motion of the floor over a 40 foot distance. We estimate that the minimum stability requirement would be 20 microns in the sample-to-detector system and 20 nm in the sample-to-focusing-optical system. It is not a straightforward exercise to estimate the vibrational transfer function of these devices, but—given the large displacements required for the detectors—the measurements of floor motion give some cause for concern. We anticipate routine data collection to occur at rates of up to 10 Hz, which increases the likelihood that the instrument would be sensitive to the uncorrelated motion seen in Figures 5 and 6.

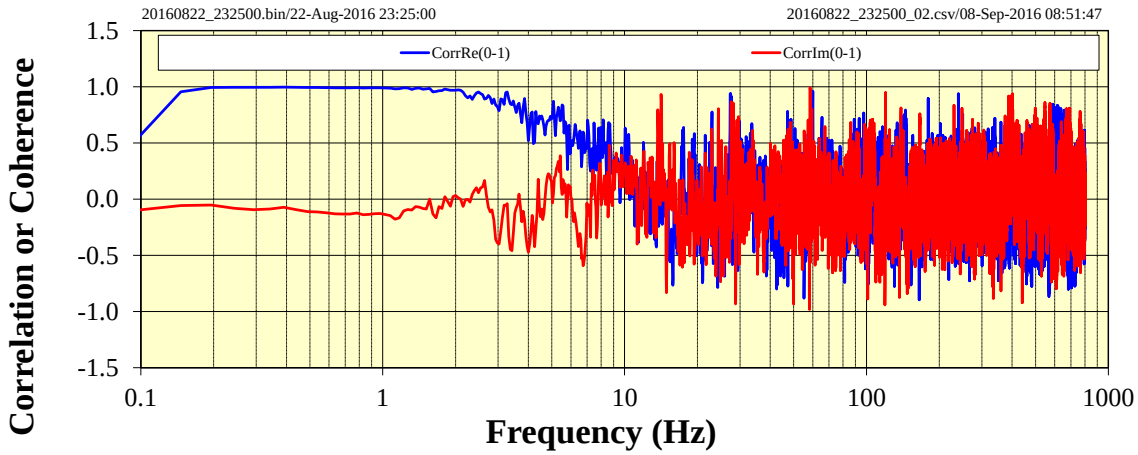


Figure 5. Vertical floor motion correlation at 40-foot (13m) separation. Motion is well-correlated at 2 Hz and below.

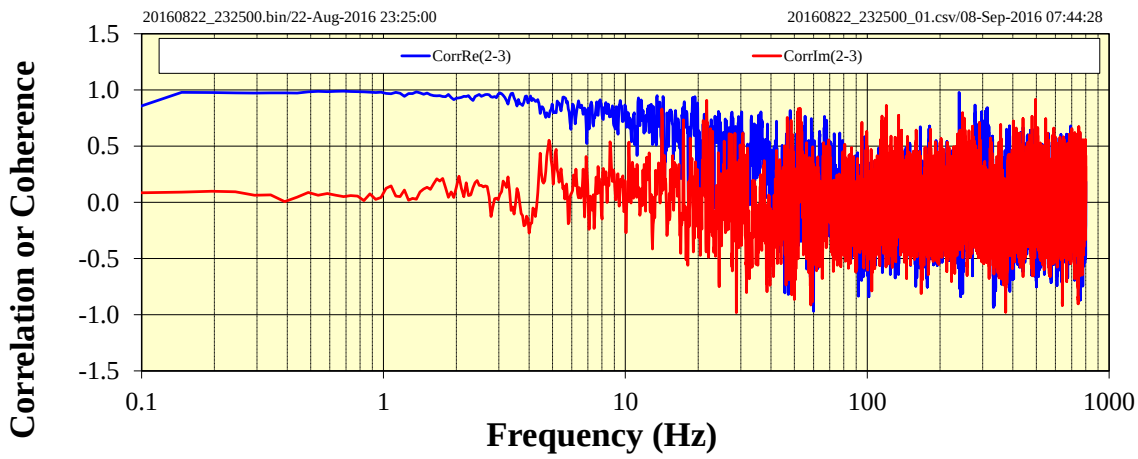


Figure 6. Horizontal floor motion correlation at 40-foot (13m) separation. Motion is well-correlated at 6 Hz and below.

A potential issue with the optical design presented in Figures 1-3 is that early simulations show that it may not be feasible to provide a clean focal spot over the desired range of 1 to 7 micron FWHM with this optical design. This arises primarily from the coherent diffraction effects of the coherence defining aperture in the horizontal and their interplay with those of the beam defining aperture controlling the secondary source, which is re-imaged to provide the final focal spot.

(b) Beamline design

As described above, the original—so-called "short"—optical design for CDI, illustrated in Figure 7, called for the central cone of radiation emerging from the undulator to be incident upon the white beam mirror. This mirror is bendable, so that it may switch between collimating the incoming radiation and providing an image of the source as a secondary source for the final focusing optics. Here, the final focal spot size is determined by the size of the secondary source, which cannot be larger than the coherent fraction of the x-ray beam incident upon it, i.e., it is also used as a coherence defining aperture. The diffraction from the secondary source

aperture imparts some structure onto the final focal spot and, depending on the wavelength of the x-rays and the desired focal spot size, can impose a strict constraint on the relative motion between the source defining aperture and the KB aperture in the horizontal. Within the bounds of the experimental floor, it may not be possible to ameliorate these concerns in the optical design, e.g., by choosing a different magnification of the undulator source or moving the secondary source aperture upstream. These issues invite the consideration of an alternate, slightly different optical design.

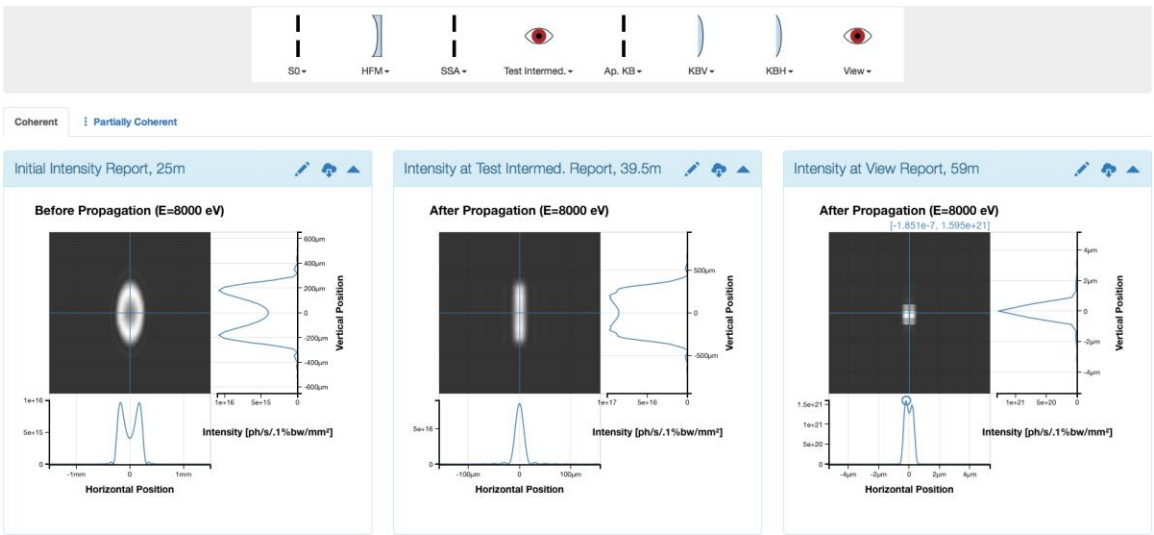


Figure 7. Indicative result of wave propagation for the "short" CDI beamline concept. Result is preliminary. Simulations were undertaken using SRW.

A design that addresses the above concerns requires either an elegant optical design or relaxing the space limitation on the beamline length. The former invites additional stability concerns and violates the common sense approach to preserving clean wave fronts by introducing a larger number of optical elements to the beam path. As such, we consider a beamline concept that would take the final experimental endstation off of the experimental floor and outside of the main NSLS-II building. Figure 8 illustrates this concept, where the x-ray beam is collimated in both the horizontal and vertical directions by fixed figure mirrors in the first optical enclosure and the secondary source aperture is used to "clean-up" the beam by removing any scattering from imperfect optical components. The first, high heat load slits are used to select the coherent fraction of the central cone of the undulator. The final x-ray spot size is then determined by controlling the aperture of the KB mirror system.

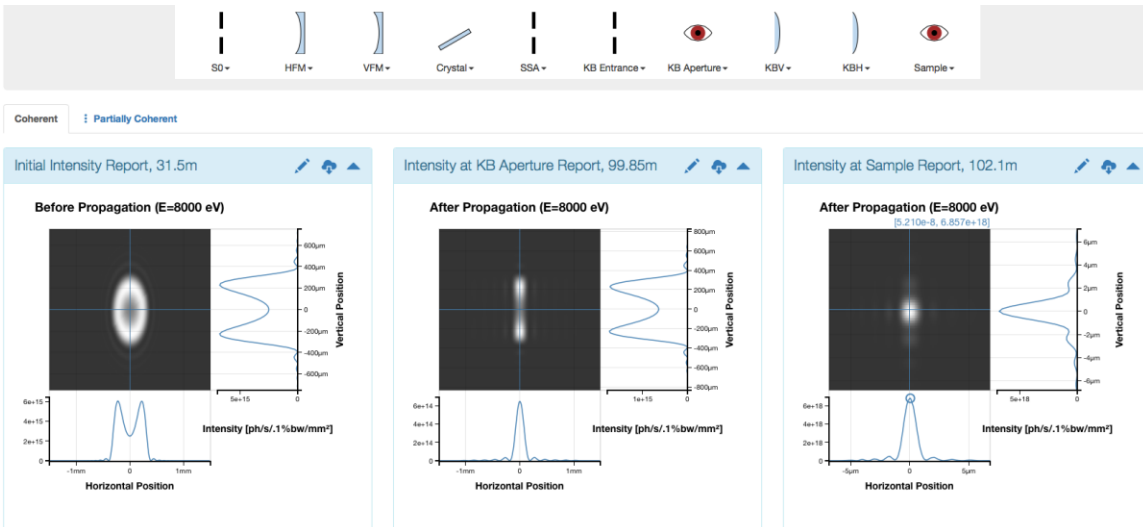


Figure 8. Indicative result of wave propagation for the "long" CDI beamline concept. Result is preliminary. Simulations were undertaken using SRW.

This second, or "long," beamline optical layout easily allows for the required variation in the focal spot size. It also addresses many of the concerns regarding vibration, since those endstations that NSLS-II has built outside the experimental building have been demonstrated to have lower amplitude vibrations and higher frequency cut-offs for the correlation of floor motion. The sole additional technical challenge is assuring the pointing stability of the vertical collimating mirror and it should be feasible to accomplish this with 10s-of-nrad-scale precision, much less than the 50-100 nrad pointing stability of the source.

(4) Summary of response to charge

We have presented the major elements of the conceptual design that underlies the cost and labor estimates that have been prepared under the 16-IEPD Task Force and the design considerations that they address. The conceptual design for the detector positioner follows from the scientific scope of the BDP and the limits of current—and foreseeable—x-ray detector technology. From this, we have demonstrated that an unusually large endstation hutch will be required for the beamline.

The layout of the beamline incorporates a laser-ready hutch—including PPS and utility systems—with a straightforward route to in-couple the optical laser to the x-ray beam path. Additionally, ample free space is provided between the KB mirror chamber and the sample location for laser in-coupling or diagnostics applications.

The addition of a clean-up aperture system and high-quality mirror specification allow the preparation of an x-ray beam suitable for conducting forward-scattering CDI experiments. The clear area on the downstream side of the diffractometer, the 8 m path to detector at the rear of the hutch, and a nanopositioning system enable these experiments.

The cost and labor estimates summarized below are based on implementation of the "short" CDI beamline concept. A final determination of the concept to be adopted, "short" vs. "long", is required and is beyond the Task Force charge pertaining to CDI; this will fall under the realm of the initial beamline design work.

Appendix 1: CDI Interactions/Meetings Summary

date	participants	summary
6/9/2016	berman	IEPD one-on-one progress meeting.
6/23/2016	mancuso	Discuss mirror design specifications for recent instruments at other facilities and vendor expectations.
6/24/2016	IEPD meeting	General meeting.
7/9/2016	robinson	Discuss options for sample positioning.
7/15/2016	tchubar	Discuss procedure for setting up SRW simulations of the proposed beamline.
7/15/2016	berman	IEPD one-on-one progress meeting.
7/20/2016	rohner	Received budgetary quotation from Dectris for Eiger 4M.
7/22/2016	apsens	Received budgetary quotation for piezo positioning system.
7/29/2016	berman	IEPD one-on-one progress meeting.
8/4/2016	robinson	Discussed beamline layout and optical design.
8/5/2016	IEPD	General meeting.
8/9/2016	robinson	Discussed detector positioning and solutions at other facilities.
8/10/2016	biermanns-foeth	First contact with RI GmbH regarding budgetary quotation.
8/10/2016	spataro	Discussed NSLS-II vibration studies.
8/12/2016	robinson	Discussed impact of vibration measurements on CDI.
8/18/2016	spataro	Discussed feasibility of vibration measurements.
8/23/2016	robinson	Discussed beamline length considerations.
8/24/2016	biermanns-foeth	Clarified scope of RI budgetary quotation regarding mirror specification and quote structure.
9/1/2016	hamill	Initial substantive contact with Huber representative regarding goniometer.
9/1/2016	berman	IEPD one-on-one progress meeting.
9/5/2016	carlucci-dayton	Discussed esimates and labor profile for detector positioning system with NSLS-II lead engineer.
9/9/2016	tchubar	Discussed optimizing SRW simulations of beamline.
9/12/2016	biermanns-foeth	Vendor query regarding slits.
9/14/2016	hamill	Clarification of need for budgetary quotation.
9/14/2016	nazaretski	Discussed vibration measures and impact on HXN and NSLS-II metrology labs.
9/15/2016	goldsborough	Received budgetary quotation on Merlin detector and advice on availability of Excalibur detector.
9/15/2016	IEPD	General meeting.
9/16/2016	biermanns-foeth	Final vendor query on vacuum systems.
9/20/2016	biermanns-foeth	Received budgetary quotation.
9/26/2016	berman	Discussed CDI slides for IEPD presentation.
9/28/2016	berman	Discussed cost estimates for CDI.
9/29/2016	hamill	Budgetary quotation received on goniometer.
9/30/2016	robinson	Discussed IEPD CDI narrative.

Appendix 2: CDI Beamline Dictionary

(1) PCDI.01 Management and Support
Performance of management and support activities, including labor, materials, travel, and fixed costs associated with management and support functions, consisting of construction management, reviews, administrative support, ESH, QA, configuration management, business operations, project controls, procurement, and document control.

(2) PCDI.03 Beamline Construction
(a) PCDI.03.01 Photon Delivery System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of photon delivery sub-systems and integrated system. These include the beamline optical systems upstream of the endstation (including their housings, supports, and manipulation systems), apertures and beam definition and conditioning systems, beam diagnostic/visualization systems, beam transport system, vacuum system, cooling/heating and temperature stabilization systems associated with photon delivery system components, and shielding systems (exclusive of radiological enclosures) that include collimators, masks, shutters, and beam stops.
(b) PCDI.03.03 Endstation System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of endstation sub-systems and integrated system. These include sample housings, environments, visualization, and support and manipulation systems, detection systems, optical systems and beam diagnostic/visualization and conditioning/definition/deflection components just before the sample (e.g. on the same support as the sample or contiguous with it) or between the sample and detector (e.g. crystal/grating/mirror-based analyzer or spectrometer system) including their housings, supports, and manipulation systems, vacuum system, and cooling/heating and temperature stabilization systems associated with endstation components.

(3) Beamline Infrastructure
(a) PCDI.04.01 Hutches and Control Station Furniture
Design, specification, procurement, fabrication, assembly, installation, and testing of the required radiological enclosures, including the necessary hoist, air handling equipment, fans, labyrinths, doors, windows, and lights. Design, specification, procurement, fabrication, assembly, installation, and testing of furniture for the beamline control station including partitions and their power and communications wiring.

(b) PCDI.04.02 Mechanical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline mechanical utilities including equipment racks, DI water, process chilled water, gaseous nitrogen, compressed air, exhaust, and liquid nitrogen distribution systems.

(c) PCDI.04.03 Electrical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline electrical utilities including circuit breaker panels, provisioning of power to equipment racks, and cable trays and conduits.

(d) PCDI.04.04 Equipment Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Equipment Protection System (EPS) including PLC, wiring, and custom sensors.

(e) PCDI.04.05 Personnel Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Personnel Protection System (PPS) including PLC, wiring, switches, locks, special interlocked personnel protective safeguards such as gates and light screens, and Human Machine Interface (HMI) panel.

(4) PCDI.05 Accelerator Infrastructure

(a) PCDI.05.01 Front End
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of front end sub-systems and integrated system. These include the front end chambers, vacuum system, supports, apertures, collimators, masks, shields, shutters, and diagnostics including flags and beam position monitors. The necessary utilities, protection systems, and controls for the front end are included.

(b) PCDI.05.02 Source
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of radiation source and associated hardware. This could be an insertion device for x-rays or an extraction chamber to insert within a dipole magnet for infrared radiation. Magnetic measurements if necessary are included. The necessary utilities, protection systems, and controls for the source are included.

(c) PCDI.05.03 Straight Section
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of accelerator straight section sub-systems and integrated system. These include the straight section chambers, vacuum system, supports, masks, shields, diagnostics including beam position monitors, and canting magnets with power supplies if necessary. The necessary utilities, protection systems, and controls for the straight section are included.

(5) PCDI.06 Beamline Controls

(a) PCDI.06.01 Basic System Controls

Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation control systems. These include operator consoles for control and archive of control equipment, network routers, gateway to the machine control system, timing IOC to synchronize to the machine timing, motor controllers and associated cabling, serial to Ethernet hubs, and a soft IOC for controlling all Ethernet-based motors, serial devices, and PLCs. Ethernet and timing cables are also included.

(b) PCDI.06.02 Instrument Applications

Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation instrument control applications. These include experimental control workstations, data storage and computation equipment, experimental control software and servers, and data acquisition equipment and software including for detectors.

Appendix 3: CDI Equipment Cost Estimate (Direct K$) and Basis of Estimate

Undulator (3 m long IVU20)	1700	Hitachi quote
Accelerator Straight Section Hardware	in progress	
Front End Hardware	730	bottom-up estimate
FOE	490	NSLS-II hutches costs scaled
Doghouse (B) Hutch	50	NSLS-II hutches costs scaled
Laser (C) Hutch	310	NSLS-II hutches costs scaled
Experimental (D) Hutch	670	NSLS-II hutches costs scaled
Beamline Construction		
RI estimate of scope of supply (shield wall to KB system)	2700	RI Research Instruments quote
photon shutter	30	NSLS-II photon shutter cost (Johnsen-Ultravac)
diagnostic beam monitors	50	catalog items
Endstation Construction		
five-circle kappa diffractometer	800	CHX diffractometer cost scaled
clean-up aperture system	25	catalog items
confocal microscope	135	Olympus quote
2 Eiger 4M detectors	1960	Dectris quote
detector positioning system	500	professional judgment
beam control/diagnostics (ion chamber, diode, attenuator, stopper)	60	catalog items
environmental control	50	catalog items
Beamline Infrastructure Hardware	415	bottom-up estimate
Beamline Control Systems Hardware	410	bottom-up estimate
Total	**11085**	

Appendix 4: CDI Labor Estimate (Person-Years and Hours), Basis of Estimate, and Schedule with Major Activities

	Year 1	Year 2	Year 3	Year 4	Total	Basis of Estimate
beamline & endstation construction major activities:	design	design, procurement, fabrication	procurement, fabrication, assembly, installation, testing	assembly, installation, testing	person-years	
scientist / assistant sci	2	2	2	2	8	beamline project exp
mech / vac engineer	1.5	1.5	1	1	5	beamline project exp
mech designer	0.75	0.75	0.5	0.5	2.5	beamline project exp
mech / vac technician	0	0	1.5	1.5	3	beamline project exp
Total					18.5 pers-years or 32,600 hrs	

Additional Labor Required:

Project management: 2,100 hrs scientist
Project support: to be determined, requires clarification
Labor for insertion device and accelerator straight section: still being tallied
Trades labor for BL constr (riggers, carpenters, masons, and surveyors): still being tallied
Labor for beamline infrastructure: 8,700 hrs (engineer, technician, trades; bot-up deter)
Labor for beamline controls: 8,000 hrs (controls engineer, technician; bot-up determine)

Total Labor Required: 51,400 hrs or 29 person-years plus additional hrs still being tallied

Travel Budget Required: still being determined

CDI Schedule Cartoon

	Year 1	Year 2	Year 3	Year 4
Design				
Procurement				
Fabrication				
Assembly				
Installation				
Testing				

Project: CDI Beamline RESOURCE DETAIL

WBS	RESOURCE	UNITS	COST
PCDI - CDI Beamline			
PCDI.01 - CDI Management			
LABOR	Labor_Scientist_NS1	2,112.00	$ 322,016.84
	Labor_Administrative Secretary_NA3	704.00	$ 40,127.88
	Labor_ES&H Professional_NA4	1,056.00	$ 127,282.85
	Labor_QA Professional_NA5	704.00	$ 79,449.16
	Labor_Administrative_NA2	1,338.00	$ 102,600.17
	Labor_Human Resources_NB4	352.00	$ 26,991.97
	LABOR TOTAL	6,266.00	$ 698,468.87
MATERIAL	Material_Material (Purchase <$25k)_NMA	100,000.00	$ 132,323.61
	MATERIAL TOTAL	100,000.00	$ 132,323.61
PCDI.02 - CDI Design			
PCDI.02.01 - CDI Conceptual Design			
LABOR	Labor_Scientist_NS1	1,173.25	$ 166,655.46
	Labor_Mechanical Engineer_NO1	880.00	$ 83,343.78
	Labor_Mechanical Designer_NO2	440.00	$ 35,565.10
	LABOR TOTAL	2,493.25	$ 285,564.34
PCDI.02.02 - CDI Preliminary Design			
LABOR	Labor_Scientist_NS1	1,173.25	$ 170,072.18
	Labor_Mechanical Engineer_NO1	880.00	$ 84,127.87
	Labor_Mechanical Designer_NO2	440.00	$ 35,899.69
	LABOR TOTAL	2,493.25	$ 290,099.73
PCDI.02.03 - CDI Final Design			
LABOR	Labor_Scientist_NS1	1,173.25	$ 173,628.35
	Labor_Mechanical Engineer_NO1	880.00	$ 84,943.96
	Labor_Mechanical Designer_NO2	440.00	$ 36,247.94
	LABOR TOTAL	2,493.25	$ 294,820.25
PCDI.03 - CDI Beamline Construction			
PCDI.03.01 - CDI Photon Delivery System Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	1,759.92	$ 263,784.13
	Labor_Mechanical Engineer_NO1	1,760.00	$ 171,817.95
	Labor_Mechanical Designer_NO2	880.00	$ 73,319.47
	Labor_Mechanical Technician_NO3	1,320.00	$ 103,511.86
	LABOR TOTAL	5,719.92	$ 612,433.40
MATERIAL	Material_Large Procurment (> $2M)_NLP	2,700,000.00	$ 3,334,194.81
	Material_Material (Purchase >$25k)_NSM	80,000.00	$ 100,476.84
	MATERIAL TOTAL	2,780,000.00	$ 3,434,671.64
PCDI.03.02 - CDI Photon Delivery System Installation and Test			
LABOR	Labor_EL - Vacuum Engineer_SE5	256.00	$ 30,928.46
	Labor_EL - Vacuum Technician_SE6	664.00	$ 60,071.26
	Labor_ME - Survey Engineer_MO1	166.00	$ 17,698.44
	Labor_EL - Survey Technician_SE2	347.50	$ 31,483.13
	Labor_Building Trades Unassigned_NST	22.00	$ 2,909.16
	Labor_Plant Engineering-Building Trades Carpenter_BTC	39.38	$ 4,912.86
	Labor_Plant Engineering-Building Trades Riggers_BTS	281.00	$ 35,397.79
	Labor_Scientist_NS1	880.00	$ 139,726.44
	Labor_Mechanical Engineer_NO1	704.00	$ 72,730.48
	Labor_Mechanical Designer_NO2	352.00	$ 31,036.11
	Labor_Mechanical Technician_NO3	1,320.00	$ 106,514.35
	LABOR TOTAL	5,031.88	$ 533,408.49
PCDI.03.03 - CDI End Station Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	5,280.00	$ 806,535.45
	Labor_Mechanical Engineer_NO1	2,640.00	$ 262,021.28
	Labor_Mechanical Designer_NO2	1,320.00	$ 111,811.73
	Labor_Mechanical Technician_NO3	1,320.00	$ 104,795.47
	LABOR TOTAL	10,560.00	$ 1,285,163.93
MATERIAL	Material_Material (Purchase >$25k)_NSM	3,530,000.00	$ 4,584,805.24
	MATERIAL TOTAL	3,530,000.00	$ 4,584,805.24
PCDI.03.04 - CDI End Station Installation and Test			
LABOR	Labor_Scientist_NS1	2,640.00	$ 432,823.94
	Labor_Mechanical Engineer_NO1	1,056.00	$ 112,639.79
	Labor_Mechanical Designer_NO2	528.00	$ 48,066.52
	Labor_Mechanical Technician_NO3	1,320.00	$ 109,974.56
	LABOR TOTAL	5,544.00	$ 703,504.81
PCDI.04 - CDI Beamline Infrastructure			
PCDI.04.01 - CDI Hutches			
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,550,000.00	$ 1,954,760.58
	MATERIAL TOTAL	1,550,000.00	$ 1,954,760.58
PCDI.04.02 - CDI Mechanical Utilities			
LABOR	Labor_ME - Utility Engineer_MO3	351.00	$ 36,102.48
	Labor_Mechanical Designer_NO2	305.00	$ 25,802.73
	Labor_EL - Utility Technician_SE4	893.00	$ 78,789.04
	Labor_Plant Engineering-Building Trades Plumber_BTP	306.00	$ 38,043.66
	Labor_Plant Engineering-Building Trades Carpenter_BTC	17.00	$ 2,103.56
	Labor_Building Trades Unassigned_NST	40.00	$ 5,284.81

	LABOR TOTAL	1,912.00	$	186,126.26
MATERIAL	Material_Material (Purchase <$25k)_NMA	130,000.00	$	170,190.15
	Material_Material (Purchase >$25k)_NSM	95,000.00	$	119,353.25
	MATERIAL TOTAL	225,000.00	$	289,543.40
PCDI.04.03 - CDI Electrical Utilities				
LABOR	Labor_Electrical Engineer_NE1	191.00	$	22,298.74
	Labor_Electrical Designer_NE2	120.00	$	10,896.78
	Labor_Plant Engineering-Building Trades Electrician_BTE	1,520.00	$	188,255.17
	LABOR TOTAL	1,831.00	$	221,450.69
MATERIAL	Material_Material (Purchase <$25k)_NMA	50,000.00	$	66,897.84
	MATERIAL TOTAL	50,000.00	$	66,897.84
PCDI.04.04 - CDI EPS				
LABOR	Labor_Controls Engineer_NE4	340.00	$	39,704.85
	Labor_Electrical Technician_NE3	490.00	$	42,921.86
	Labor_Electrical Designer_NE2	40.00	$	3,677.52
	LABOR TOTAL	870.00	$	86,304.23
MATERIAL	Material_Material (Purchase <$25k)_NMA	43,000.00	$	57,532.14
	MATERIAL TOTAL	43,000.00	$	57,532.14
PCDI.04.05 - CDI PPS				
LABOR	Labor_Electrical Engineer_NE1	1,128.00	$	134,744.10
	Labor_Electrical Technician_NE3	1,512.00	$	136,451.55
	Labor_Electrical Designer_NE2	704.00	$	66,050.36
	Labor_Plant Engineering-Building Trades Electrician_BTE	700.00	$	86,616.98
	LABOR TOTAL	4,044.00	$	423,862.98
MATERIAL	Material_Material (Purchase >$25k)_NSM	98,000.00	$	130,202.92
	MATERIAL TOTAL	98,000.00	$	130,202.92
PCDI.05 - CDI Accelerator Infrastructure				
PCDI.05.01 - CDI Front End				
LABOR	Labor_Project Engineer_MO7	150.00	$	15,132.16
	Labor_Mechanical Engineer_NO1	1,140.00	$	112,280.44
	Labor_Mechanical Designer_NO2	600.00	$	49,452.95
	Labor_Assistant/Associate Scientist_NS2	60.00	$	6,010.04
	Labor_ME - Vacuum Engineer_MO5	220.00	$	22,109.67
	Labor_ME - D&I Engineer_NO6	260.00	$	26,004.23
	Labor_Electrical Engineer_NE1	400.00	$	46,431.04
	Labor_EL - D&I Engineer_TE1	320.00	$	36,682.32
	Labor_Controls Engineer_NE4	140.00	$	16,106.90
	Labor_Electrical Designer_NE2	160.00	$	14,639.37
	Labor_Electrical Technician_NE3	380.00	$	33,016.82
	Labor_EL - Vacuum Engineer_SE5	200.00	$	23,215.52
	Labor_ME - Utility Engineer_MO3	120.00	$	12,228.92
	Labor_Mechanical Technician_NO3	1,210.00	$	95,494.00
	Labor_ME - Survey Engineer_MO1	195.00	$	20,076.08
	Labor_EL - D&I Technician_TE2	280.00	$	24,458.05
	Labor_ME - Survey Technician_MO2	350.00	$	30,704.59
	Labor_ME - Vacuum Technician_MO6	510.00	$	41,121.73
	Labor_Plant Engineering-Building Trades Riggers_BTS	119.00	$	14,724.89
	Labor_Plant Engineering-Building Trades Electrician_BTE	48.00	$	5,939.45
	Labor_Building Trades Unassigned_NST	72.00	$	9,352.17
	Labor_ME - Utility Technician_MO4	40.00	$	3,225.23
	LABOR TOTAL	6,974.00	$	658,406.55
MATERIAL	Material_Material (Purchase >$25k)_NSM	727,000.00	$	950,999.85
	MATERIAL TOTAL	727,000.00	$	950,999.85
PCDI.05.02 - CDI Source				
LABOR	Labor_Assistant/Associate Scientist_NS2	790.00	$	86,539.29
	Labor_EL - Insertion Device Engineer_TE4	1,120.00	$	134,364.94
	Labor_ME - Insertion Device Engineer_NO8	440.00	$	46,610.93
	Labor_Controls Engineer_NE4	1,150.00	$	139,343.54
	Labor_ME - Survey Engineer_MO1	90.00	$	9,560.03
	Labor_ME - Insertion Device Technician_NO9	730.00	$	60,550.53
	Labor_ME - Survey Technician_MO2	180.00	$	16,297.23
	Labor_Project Engineer_MO7	40.00	$	4,281.20
	Labor_Electrical Engineer_NE1	340.00	$	41,333.27
	Labor_ME - Vacuum Engineer_MO5	40.00	$	4,267.99
	Labor_ME - Vacuum Technician_MO6	320.00	$	26,730.74
	Labor_ME - Utility Engineer_MO3	80.00	$	8,562.40
	Labor_ME - Utility Technician_MO4	160.00	$	13,375.69
	Labor_Electrical Designer_NE2	200.00	$	19,123.12
	Labor_Electrical Technician_NE3	400.00	$	36,439.78
	Labor_Mechanical Designer_NO2	80.00	$	7,217.84
	Labor_Plant Engineering-Building Trades Electrician_BTE	160.00	$	20,233.73
	Labor_Plant Engineering-Building Trades Riggers_BTS	24.00	$	3,035.06
	Labor_Building Trades Unassigned_NST	40.00	$	5,309.95
	LABOR TOTAL	6,384.00	$	683,177.27
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,700,000.00	$	2,159,444.99
	MATERIAL TOTAL	1,700,000.00	$	2,159,444.99
PCDI.05.03 - CDI Straight				
LABOR	Labor_ME - Utility Engineer_MO3	240.00	$	23,819.52

	Labor_EL - Vacuum Engineer_SE5	90.00	$	10,120.88
	Labor_ME - Insertion Device Engineer_NO8	80.00	$	7,939.33
	Labor_EL - Insertion Device Engineer_TE4	40.00	$	4,497.40
	Labor_ME - Vacuum Technician_MO6	430.00	$	33,335.36
	Labor_Project Engineer_MO7	30.00	$	2,977.44
	Labor_ME - Survey Engineer_MO1	40.00	$	3,970.43
	Labor_Mechanical Designer_NO2	80.00	$	6,672.27
	Labor_ME - Utility Technician_MO4	40.00	$	3,101.19
	Labor_ME - Survey Technician_MO2	100.00	$	8,460.61
	Labor_ME - D&I Engineer_NO6	150.00	$	14,885.29
	Labor_EL - D&I Engineer_TE1	200.00	$	22,491.33
	Labor_Electrical Designer_NE2	200.00	$	17,676.32
	Labor_EL - D&I Technician_TE2	240.00	$	20,213.08
	Labor_Electrical Engineer_NE1	40.00	$	4,499.13
	Labor_Electrical Technician_NE3	20.00	$	1,684.53
	LABOR TOTAL	2,020.00	$	186,344.12
MATERIAL	Material_Material (Purchase >$25k)_NSM	190,000.00	$	238,632.48
	MATERIAL TOTAL	190,000.00	$	238,632.48
PCDI.06 - CDI Controls				
PCDI.06.01 - CDI Basic System Controls				
LABOR	Labor_Controls Engineer_NE4	2,172.80	$	247,654.17
	Labor_IT Professional (Software)_NA7	334.40	$	33,185.19
	Labor_Electrical Technician_NE3	894.40	$	78,182.47
	LABOR TOTAL	3,401.60	$	359,021.83
MATERIAL	Material_Material (Purchase <$25k)_NMA	139,800.00	$	184,801.90
	Material_Material (Purchase >$25k)_NSM	152,800.00	$	195,377.08
	MATERIAL TOTAL	292,600.00	$	380,178.97
PCDI.06.02 - CDI Instrument Applications				
LABOR	Labor_IT Professional (Software)_NA7	1,920.00	$	184,395.33
	Labor_Assistant/Associate Scientist_NS2	440.00	$	45,483.97
	Labor_Controls Engineer_NE4	1,200.00	$	134,973.98
	LABOR TOTAL	3,560.00	$	364,853.29
MATERIAL	Material_Material (Purchase >$25k)_NSM	76,200.00	$	97,750.50
	Material_Material (Purchase <$25k)_NMA	42,000.00	$	55,423.45
	MATERIAL TOTAL	118,200.00	$	153,173.95

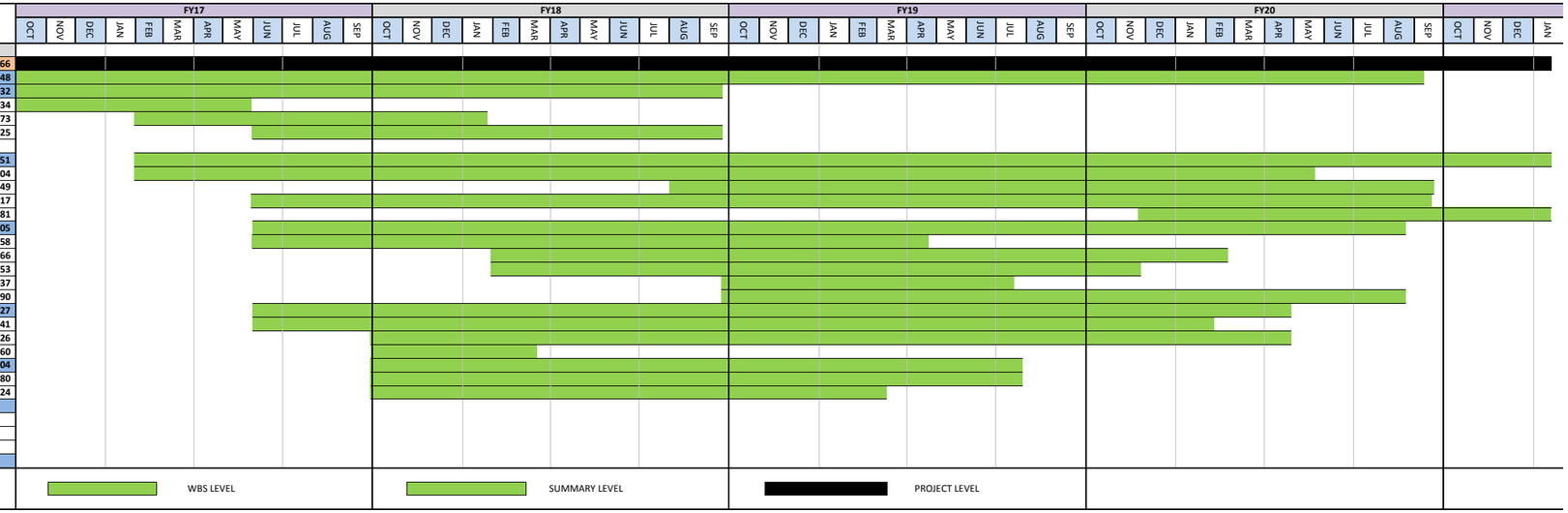
Project: CDI Beamline — RESOURCE SUMMARY

WBS	RESOURCE	UNITS		COST
PCDI - CDI Beamline				
LABOR	Labor_Scientist_NS1	16,191.67	$	2,475,242.79
	Labor_Administrative Secretary_NA3	704.00	$	40,127.88
	Labor_ES&H Professional_NA4	1,056.00	$	127,282.85
	Labor_QA Professional_NA5	704.00	$	79,449.16
	Labor_Administrative_NA2	1,338.00	$	102,600.17
	Labor_Human Resources_NB4	352.00	$	26,991.97
	Labor_Mechanical Engineer_NO1	9,940.00	$	983,905.56
	Labor_Mechanical Designer_NO2	5,465.00	$	461,092.34
	Labor_Mechanical Technician_NO3	6,490.00	$	520,290.24
	Labor_EL - Vacuum Engineer_SE5	546.00	$	64,264.86
	Labor_EL - Vacuum Technician_SE6	664.00	$	60,071.26
	Labor_ME - Survey Engineer_MO1	491.00	$	51,304.98
	Labor_EL - Survey Technician_SE2	347.50	$	31,483.13
	Labor_Building Trades Unassigned_NST	174.00	$	22,856.09
	Labor_Plant Engineering-Building Trades Carpenter_BTC	56.38	$	7,016.42
	Labor_Plant Engineering-Building Trades Riggers_BTS	424.00	$	53,157.74
	Labor_ME - Utility Engineer_MO3	791.00	$	80,713.32
	Labor_EL - Utility Technician_SE4	893.00	$	78,789.04
	Labor_Plant Engineering-Building Trades Plumber_BTP	306.00	$	38,043.66
	Labor_Electrical Engineer_NE1	2,099.00	$	249,306.27
	Labor_Electrical Designer_NE2	1,424.00	$	132,063.46
	Labor_Plant Engineering-Building Trades Electrician_BTE	2,428.00	$	301,045.32
	Labor_Controls Engineer_NE4	5,002.80	$	577,783.43
	Labor_Electrical Technician_NE3	3,696.40	$	328,697.01
	Labor_Project Engineer_MO7	220.00	$	22,390.80
	Labor_Assistant/Associate Scientist_NS2	1,290.00	$	138,033.30
	Labor_ME - Vacuum Engineer_MO5	260.00	$	26,377.66
	Labor_ME - D&I Engineer_NO6	410.00	$	40,889.52
	Labor_EL - D&I Engineer_TE1	520.00	$	59,173.65
	Labor_EL - D&I Technician_TE2	520.00	$	44,671.13
	Labor_ME - Survey Technician_MO2	630.00	$	55,462.43
	Labor_ME - Vacuum Technician_MO6	1,260.00	$	101,187.82
	Labor_ME - Utility Technician_MO4	240.00	$	19,702.11
	Labor_EL - Insertion Device Engineer_TE4	1,160.00	$	138,862.35
	Labor_ME - Insertion Device Engineer_NO8	520.00	$	54,550.26

	Labor_ME - Insertion Device Technician_NO9	730.00	$	60,550.53
	Labor_IT Professional (Software)_NA7	2,254.40	$	217,580.53
	LABOR TOTAL	71,598.14	$	7,873,011.05
MATERIAL	Material_Material (Purchase <$25k)_NMA	504,800.00	$	667,169.09
	Material_Large Procurment (> $2M)_NLP	2,700,000.00	$	3,334,194.81
	Material_Material (Purchase >$25k)_NSM	8,199,000.00	$	10,531,803.71
	MATERIAL TOTAL	11,403,800.00	$	14,533,167.61
		GRAND TOTAL	$	22,406,178.66

Project Name: CDI Beamline

WBS	Start	Finish	Cost
PCDI - CDI Beamline	10/1/2016	1/18/2021	$ 22,406,178.66
PCDI.01 - CDI Management	10/1/2016	9/10/2020	$ 830,792.48
PCDI.02 - CDI Design	10/1/2016	9/23/2018	$ 870,484.32
PCDI.02.01 - CDI Conceptual Design	10/1/2016	5/29/2017	$ 285,564.34
PCDI.02.02 - CDI Preliminary Design	1/30/2017	1/25/2018	$ 290,099.73
PCDI.02.03 - CDI Final Design	5/31/2017	9/23/2018	$ 294,820.25
PCDI.02.04 - CDI R&D Program			$ -
PCDI.03 - CDI Beamline Construction	1/30/2017	1/18/2021	$ 11,153,987.51
PCDI.03.01 - CDI Photon Delivery System Procurement and Fabrication	1/30/2017	5/21/2020	$ 4,047,105.04
PCDI.03.02 - CDI Photon Delivery System Installation and Test	8/1/2018	9/20/2020	$ 533,408.49
PCDI.03.03 - CDI End Station Procurement and Fabrication	5/30/2017	9/18/2020	$ 5,869,969.17
PCDI.03.04 - CDI End Station Installation and Test	11/24/2019	1/18/2021	$ 703,504.81
PCDI.04 - CDI Beamline Infrastructure	5/31/2017	8/22/2020	$ 3,416,681.05
PCDI.04.01 - CDI Hutches	5/31/2017	4/22/2019	$ 1,954,760.58
PCDI.04.02 - CDI Mechanical Utilities	1/30/2018	2/22/2020	$ 475,669.66
PCDI.04.03 - CDI Electrical Utilities	1/30/2018	11/25/2019	$ 288,348.53
PCDI.04.04 - CDI EPS	9/23/2018	7/18/2019	$ 143,836.37
PCDI.04.05 - CDI PPS	9/23/2018	8/22/2020	$ 554,065.90
PCDI.05 - CDI Accelerator Infrastructure	5/31/2017	4/27/2020	$ 4,877,005.27
PCDI.05.01 - CDI Front End	5/31/2017	2/8/2020	$ 1,609,406.41
PCDI.05.02 - CDI Source	9/29/2017	4/27/2020	$ 2,842,622.26
PCDI.05.03 - CDI Straight	9/29/2017	3/17/2018	$ 424,976.60
PCDI.06 - CDI Controls	9/29/2017	7/27/2019	$ 1,257,228.04
PCDI.06.01 - CDI Basic System Controls	9/29/2017	7/27/2019	$ 739,200.80
PCDI.06.02 - CDI Instrument Applications	9/29/2017	3/10/2019	$ 518,027.24
PCDI.07 - CDI Conventional Facilities			$ -
PCDI.07.01 - CDI Conventional Facilities Design			$ -
PCDI.07.02 - CDI Conventional Facilities Construction			$ -
PCDI.07.03 - CDI Conventional Facilities Commissioning			$ -
PCDI.08 - CDI Special Equipment			$ -



RATE SET: Rate Set 1

NSLS II: Processing and Liquid Surfaces (PLS)
IEPD Report, Sept 30, 2016

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APPENDIX 2: PLS Beamline Dictionary

APPENDIX 3: PLS Equipment Cost Estimate (Direct K$) and Basis of Estimate

APPENDIX 4: PLS Labor Estimate (Person-Years and Hours), Basis of Estimate, and Schedule with Major Activities

1.0 Introduction

Soft matter encompasses polymers, liquids, liquid crystals, granular materials, gels, and biomolecular materials, all of which lack the three-dimensional crystallinity characteristic of conventional hard materials [1-4]. Soft materials are increasingly called upon to address national needs in energy, health, and the environment. Although an important step towards the practical utilization of soft matter is to understand the relationship between structure and function, the ultimate aim is to replace the science of observation by the science of control of the molecular and hierarchical self-assembly process in order to create architectures with specific functional properties. High resolution, synchrotron-based scattering measurements are an essential tool for understanding structural aspects of soft matter.

Soft materials are at the frontier of material sciences and engineering. As a result of their unique properties they are displacing hard materials in an array of energy and environmental applications. For instance, energy efficient liquid crystal displays have replaced the CRT; and these in turn may soon be superseded by more efficient, emerging organic light emitting diode devices. Composite materials are significantly reducing the weight of planes and contributing to lower fuel costs. Advanced manufacturing methods such as roll-to-roll fabrication of conducting polymer thin films and the printing of mechanical parts through additive manufacturing will transform many industries over the next decade. However, the success of these and other new materials and processes demand both new synthetic materials and improved control of their structure. This requires a deeper understanding of pathway-dependent self-assembly, and non-equilibrium materials; i.e. detailed characterization of the real-time self-assembly process as well as their equilibrium structures. Here we make the case for the unique importance of synchrotron x-ray scattering and spectroscopy studies to reveal the structure of Soft Matter on length scales extending from the atomic to the meso-scale.

This effort aims to construct a versatile x-ray scattering facility at ID-12-B for operando studies of soft matter interfaces, especially polymer thin films during processing and liquid surfaces. Through the use of a canted undulator this facility will operate in parallel with the Soft Matter Interfaces (SMI) Beamline at ID-12-C. The PLS capabilities will provide new scientific opportunities at NSLS II that are not addressed by existing facilities. The high flux and tight focus of the NSLS II source will enable unprecedented time-resolved studies of materials undergoing industrially-relevant formation, processing, transformation, weathering, and aging. Whereas a Liquid Surface Spectrometer (LSS) was part of the original SMI scope (2011), running in a time-shared mode with the second SMI endstation, the LSS was de-scoped in August 2015 due to budgetary constraints. The existing SMI beamline is ideally designed and configured to enable a cost-effective build-out of a fully independent side-branch, since a canted source was envisioned in the original SMI proposal and subsequent design and construction. As a result, the PLS beamline can be completed at a fraction of the cost of a "green-field" construction.
PLS generated enormous interest in the soft-matter community; the range of potential science was too great to include in its entirety in our science case. Here we elaborate a representative subset of the diverse research programs that will benefit from the envisioned beamline. In addition to the demand from the community for the liquid surface spectrometer, as evidenced by the letters, we anticipate that the versatile, operand-optimized environment of PLS will be highly sought after by a broad range of scientific and industrial communities. This can be seen even from the range of scientists who contributed to this effort, as well as the numerous letters that support.

In the following sections (2.1 Liquid Surface and Interface Science & 2.2 Operando Polymer Processing Science) we describe how the proposed capabilities of the undulator-based PLS

beamline will help address key scientific challenges involving soft-matter interfaces. The Beam Line and End Station Designs, along with supporting information to support the design, are provided in section 3.0. Further, in this section the three PLS specific charges (in italics below), identified during the proposal review process, are addressed. These specific charges and a summary of our responses are provided below.

1. *Refine the scope definition of the PLS branchline at 12-ID, with tunable 6-24 keV for liquid surfaces endstation and 13.7 keV fixed energy for the processing endstation*
   Our endstation concept has been revised so that the liquid surface and processing configurations use the same instrumentation so that the processing studies can be carried out over the entire range of energies. The new design is presented in sections 3.2 and 3.4.

2. *Include the capability of transmission x-ray scattering on liquid surfaces (LS-TXS) for studies of inhomogeneous horizontal liquid samples with vertically directed beam.*
   To successfully include vertical scattering we have considered the requirements at various energies. This is best accomplished using a multiple bounce crystal configuration as outlined in section 3.5.

3. *Further develop the concept of the polymer processing endstation.*
   As discussed above in charge 1., the present design uses a single endstation, simplifying the design. This concept is developed in section 3.4.

2.0 Science

2.1 Liquid Surface and Interface Science

Vital societal needs require a substantially improved understanding of processes at complex heterogeneous liquid interfaces. For example, the replacement of mixtures of chemically synthesized surfactants in food, pharmaceutical, and cosmetics formulations by bio-surfactants depends upon a complex balance of interfacial interactions that are poorly understood [5]. Organic films formed on the ocean surface regulate its evaporation, and reactions at the liquid surface of sea salt aerosols influence atmospheric composition [6,7]. Liquid interfaces are used to model the complex heterogeneity of biochemical interfaces that underlie protein-lipid interactions and cell signaling, which are important for the development of functional biomaterials. In addition, dynamical processes on the molecular scale at liquid interfaces are critical to understanding ion transfer processes, such as solvent extraction, which are used to separate and purify technologically important rare earth elements and to clean up toxic and radioactive metals [8-10].

Liquid interfaces provide model systems to study the statics and dynamics of self-assembly, interfacial orientation and forces, molecular interactions, molecular recognition, and chemical reactivity. The chemical and physical environment (pH, ionic content, temperature, viscosity, interfacial electric potential) can be controlled, the interfacial density modified, and molecular species added to the neighboring bulk phases to chemically interact with the interfacial assembly in a controlled manner. Although a spectrum of complementary information is provided by the many experimental techniques that are used to study liquid interfaces, notably linear and non-linear optical spectroscopy [11], neutron scattering [12], and thermodynamic measurements [13], x-ray surface scattering has a unique role in the investigation of these complex processes on atomic and molecular length scales.

Synchrotron x-ray surface scattering is the most powerful probe of molecular and mesoscale structure at liquid-vapor and liquid-liquid interfaces. It is indispensable for understanding the fundamental science of soft interfaces, as well as interfacial model systems of natural processes important for chemical, physical, biological, and technological systems. Over the past two decades, x-ray scattering studies from liquid surfaces and interfaces have led to key discoveries of polymorphic structures of two-dimensional molecular and biomolecular films [14-38], surface ordering of organic and metallic liquids [39-46], the role of thermal fluctuations at soft interfaces [47-56], and the distribution of ions at the vapor[57] charged and electrified interfaces [33-35,58-65]. Such studies provide information that is unobtainable by any other technique and have led to a fundamentally new understanding of phenomena at liquid interfaces.

The investigation of such complex interfacial structures requires high spatial resolution and element sensitivity that can be provided by the brilliant and small x-ray beams at NSLS II. Several different surface scattering techniques are required to investigate these systems in order to span the relevant length scales (angstroms to micrometers) and to probe the varied structures of these materials, which range from crystalline to weakly ordered to amorphous or disordered. In addition to techniques that utilize scattering at or near grazing incidence, scanning transmission techniques that are under development will probe mesoscopic structures with nanoscale sensitivity. The relatively recent application of element-specific techniques to liquid interfaces has the potential to enable a broad class of new research.

Environmental Chemistry A broad area of investigation is aimed at understanding separations science for environmental applications. These include water purification, such as the separation of toxic or radioactive metals from polluted environments and nuclear waste, as well as the production of potable water from seawater or brackish waters. A range of scientific investigations into liquid interfacial structure and kinetics supports this area, including studies of interfacial distributions of metal ions, the organization of amphiphilic extractants, ion/amphiphile interactions, and the role of electrostatics at interfaces. This work addresses research needs identified by DOE BES under the topics "*Interfacial behavior under extreme environmental conditions*" and "*Mastering the behavior of actinides and fission products*" in the BES Workshop report *Basic Research Needs for Advanced Nuclear Energy Systems* [66]. In both topics, major emphasis is placed on research needs relating to "*exploiting organization to achieve selectivity at multiple length scales*", including "*fundamental understanding of phase phenomena and self-assembly in separations*".

Environmental Chemistry: Solvent extraction is the extractant-mediated transfer of metal ions from an aqueous to an immiscible organic phase (Fig 2.1) [67]. It plays a major role in the hydro-metallurgical separation of base and precious metals [68], including rare-earth metals, as well as in the separation of long-lived radionuclides from nuclear waste [69]. In spite of indirect evidence that separation occurs at the interface, the chemical species that are present at the oil-water interface, their arrangement, and the mechanism for transport across the interface are generally unknown [70]. Optimizing the selectivity and kinetics of extraction can benefit industrial processes, which currently require repetitive extraction to leverage small differences in elemental selectivity.

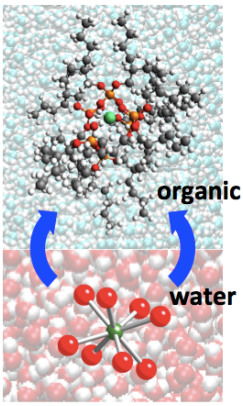


Fig. 2.1 Although the structure of hydrated metal ions in water and in reverse micelles in oil are known, the interfacial transfer mechanism represented by the blue arrows is not.

Recent x-ray reflectivity and surface fluorescence studies of model solvent extraction systems have explored the organization of extractant molecules and metal ion-extractant complexes at liquid interfaces in order to clarify the molecular-scale phenomena that control solvent extraction [71-73].

These studies uncovered non-equilibrium intermediate states in the extraction process whose character suggests that dynamical interfacial processes on the molecular scale determine the extraction kinetics.

Studies of the solvent extraction mechanism and ion transfer processes rely upon an understanding of extractant organization and the distribution of ions at oil-water, water-vapor and oil-vapor interfaces. Advances in using x-ray surface scattering and spectroscopy to probe amphiphile organization at the water-oil interface [71,72,74-83] and the distribution of monovalent ions at both water-vapor interfaces and the electrified liquid-liquid interface between two electrolyte solutions [33,34,60,84-93] have relied upon the capabilities of high brilliance synchrotron x-ray sources. The micrometer-sized beams, energy tunability, high coherence and brilliance of the NSLS II source will benefit these studies. Small beams allow for the use of smaller samples, thereby minimizing absorption and background scattering inherent in studies of buried interfaces. Facile energy tunability enables resonant reflectivity and surface-sensitive fluorescence techniques to target specific ions. High coherence will benefit the study of inhomogeneous interfacial structures of amphiphiles where the in-plane coherence lengths must be larger than interfacial inhomogeneities whose length scales may extend to 100 μm.

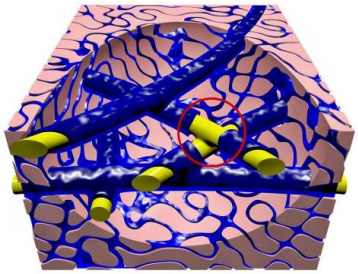


Fig. 2.2 Schematic representation of directed water channels in the nanocomposite barrier layer; the skeleton of overlapped cellulose nanofibers (yellow) guides a continuously connected system of directed water channels (blue) formed by the connected hollow cylindrical gaps between the nanofibers and the polymer matrix (pink).

Environmental Chemistry: Desalination technologies for producing fresh water from seawater and brackish water have become increasingly important. The efficiency of membrane technologies can be further improved by developing new barrier layer materials with higher permeability, while maintaining good salt rejection capability and anti-fouling characteristics. New developments in high-permeability water filtration membranes include the use of a high-flux functional nanofibrous scaffold, and the creation of a nanocomposite barrier layer, containing interconnected "directed water channels" formed between the imbedded cellulose nanofibers and cross-linked polyamide matrix (Fig. 2.2) [94-97]. The introduction of directed water channels leads to a significant increase in flux without loss of selectivity. Little is known about the evolution of the nanofibrous mesh structure during the assembly process, the subsequent interfacial polymerization process, and the anti-fouling characteristics of these new materials. X-ray reflectivity can probe aqueous protein adsorption onto these and other candidate materials, while GISAXS can characterize the structure and kinetics of directed channel formation in new membranes of highly permeable nanocomposite barrier layers.

Nanoscale and Biomolecular Materials The assembly of nano- and bio-materials with desired structure and functionality requires a significant improvement in our understanding of intermolecular interactions on the nanoscale. Liquid interfaces play a key role in this area because nanoparticles are often stabilized or synthesized as colloidal dispersions [98,99] and because the fluid and defect-free nature of liquid interfaces allows the adsorbed particles to readily attain their equilibrium configuration [100-102], including 2D crystalline order [103]. Moreover, planar liquid interfaces provide a well-controlled model system to probe the relevant interactions. Finally, the ability to form a variety of monolayer structures at liquid interfaces provides an effective means to manipulate these interactions and control the

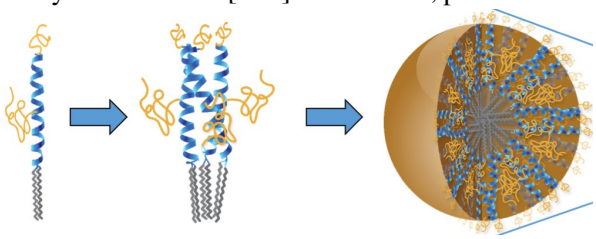


Fig. 2.3 Peptide-polymer complexes provide designed functionalized surfaces and nanoparticles.

interface-mediated assembly. Thus, the unique role of liquid interfaces extends to investigations of directed assembly.
Protein-protein and protein-lipid interactions provide fruitful examples of complex molecular interactions that are important for the development of biomolecular materials [104-108]. For instance, combining designed peptides with synthetic polymers to form peptide-polymer conjugates (2.3) shows tremendous potential in a variety of applications such as bio-implants and biosensors [109,110]. Macroscopic assembly of these conjugates into high density ordered planar arrays enhances their macroscopic response and allows them to function in a non-biological environment. An example that probes the number and quality of coiled surface groups is provided by a system based on the "1CW" peptide, which forms a 3-helical coiled-coil motif, and hexadecanoic acid (dC16) as the hydrophilic head group and hydrophobic tail respectively (Fig. 2.3). X-ray scattering from these systems at the water surface demonstrated that selective PEGylation of the 1CW-dC16 conjugate can tune the relative amount of 2-helical versus 3-helical bundles. Aligned 3-helical bundles were observed for 1CW-dC16 and 1CW-dC16-PEG2k amphiphiles whereas replacement of 1CW by a random coil peptide produced a disordered structure. These ongoing x-ray studies by Ting Xu's group provide a critical basis to design functionalized surfaces and nanoparticles with control over ligand presentation.

The organized assembly of nanoparticles at liquid and solid interfaces has been investigated for the purpose of creating interfaces with specific optical, magnetic, and electrical functionality[111-114]. Theory and simulations of these interfaces are primitive[115-117] and the connection between predictions and experimental data is limited. Although films are typically utilized in their dry state, their assembly inevitably involves liquids since these films are created from an organic solution containing solubilized NPs[112,113]. Thus, a comprehensive understanding of NP film structure requires a fundamental knowledge of NP-NP and NP-substrate interactions along with the effects of the fluids that mediate these interactions. The effect of particle type, size, capping ligands, pH, and molarity on fundamental interactions, including electrostatic repulsion, van der Waals attractions, and interface-mediated capillarity has been a major focus of theory and simulations[115-117] yet there is little experimental verification. Proposed studies at NSLS II will establish the conditions that lead to long-range order, rather than amorphous behavior, and thus provide the required underlying experimental results to permit the controlled and predictable assembly of NPs in 2D. For instance, nanoparticles can be assembled into a 2D array at the liquid-liquid interface between two immiscible electrolyte solutions. The voltage across this interface can be simply controlled with electrochemical techniques. Recent x-ray surface scattering experiments demonstrated that inter-nanoparticle distances within the 2D array can be adjusted by tuning the voltage [118]. Modifying the inter-nanoparticle distances influences the plasmon resonances of the array, which have applications in chemical and biological sensing and electro-optics [119]. The development of electrically tunable assemblies of nanoparticles has the potential to transform the use of nanoparticle arrays by providing real-time control over their properties and functionality.

Another example is provided by the DNA programmable directed assembly of nanoparticles, which exploits biomolecular interactions for the designed fabrication of complex nanoscale architectures [120-122]. The fluidity of liquid interfaces allows for regulated motion of nano-components both in- and out-of-plane [118,123,124], providing an ideal platform for nano-component assembly and manipulation. Tunable 2D nanoparticle arrays at liquid interfaces exhibit structural and mechanical

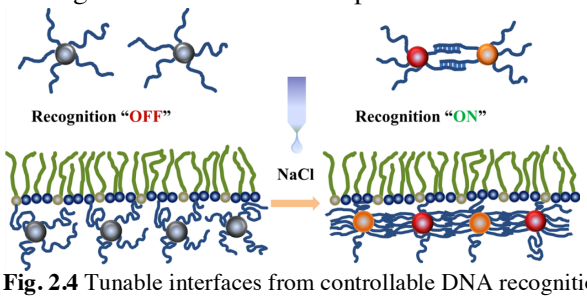


Fig. 2.4 Tunable interfaces from controllable DNA recognition.

properties that can be switched via a simple change of subphase ionic strength (Fig. 2.4) or electric potential [118,123].
The structural plasticity of DNA allows for the transformation of assembled structures by environmental factors (pH, temperature, ionic strength) [123,124] or by specific interactions with triggering strands [125]. Topological linkages between nanoparticles are regulated by the shape of multivalent DNA linkers [122], which readily permits the assembly of designed 2D interfacial arrays. Switching the interparticle connectivity on demand can dynamically alter the array structure. Entropic effects and molecular interactions provided by DNA can be exploited to optimize the ordering of binary complementary and non-complementary shaped particles [126]. Novel quasi-2D optical thin-film materials can be assembled at liquid interfaces with DNA-programmable nanoparticle methodologies. DNA-encoded nano-components added into the subphase are recognized by encoded components already assembled at the surface, promoting the formation of layered systems [127] with unique layer morphologies. Layers of quantum dots (conventional and up-converting) and plasmonic particles will be formed with precise interparticle separations, thus exhibiting finely tuned energy transfer properties and fluorescent response.

Interfacial Complexity Molecular assembly on liquid interfaces can produce both laterally homogeneous and laterally heterogeneous interfaces, depending upon the materials and the thermodynamic conditions. In the latter case, the characteristic length scale of coexisting regions can be below the resolution of optical methods. Traditional x-ray grazing or near-grazing surface scattering methods from liquids also have poor spatial resolution since the illuminated sample length is hundreds of times larger than the beam size. Characterizing these inhomogeneities at liquid interfaces requires new methods, such as the recently introduced liquid surface transmission x-ray scattering (LS-TXS) approach in which the x-ray beam strikes the liquid interface at or near normal incidence and scattered intensities are measured in transmission. Results from LS-TXS on a water meniscus in a Langmuir film raise the possibility of implementing microbeam-based scanning LS-TXS microscopy that can probe both the nanoscale structure and mesoscale inhomogeneities at liquid surfaces[128]. The liquid spectrometer, or possibly the flexible processing station should be suitable for LS-TXS studies using horizontal liquid samples with a vertically directed beam[128]. Importantly, PLS will provide the range of capabilities (high-flux, energy tunability, etc.) necessary to study the complex, inhomogeneous liquid interfaces that are actively utilized in industrial processes.

2.2 Operando Polymer Processing Science

Polymer science has had an undeniable impact on the way we live. We take for granted polymeric materials and fabrication methods that did not exist 50 years ago. There is no reason to believe that the plastics revolution will stop any time soon. Both traditional manufacturing approaches, such as roll-to-roll (R2R), and emerging technologies, such as additive manufacturing, are under active development to yield a broad range of new functional materials. Polymers form the basis for billion dollar industries that continue to grow rapidly, propelled by transformative advances in synthetic chemistry and manufacturing technology. New manufacturing processes undergo rapid deployment, often with only a poor understanding

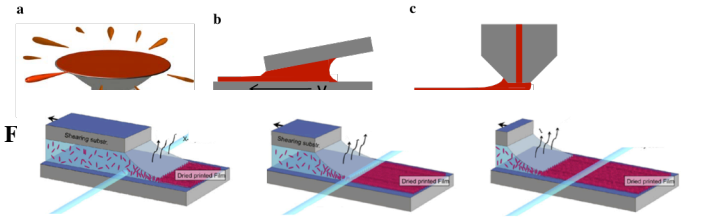


Fig. 2.6 Schematic view of different stages of the drying process. The polymer melt between the two blocks is sheared by the movement of the top block to the left. The red patch illustrates the dried, printed film. Adapted from Ref. 79.

of the underlying materials science. Nevertheless, knowledge of the structural rearrangements that take place during processing is critical for advanced manufacturing methods.

Many manufacturing processes are based upon the liquid-like flow properties of polymer melts or solutions (Fig. 2.5). Complex interactions that occur during these dynamic processing methods determine the molecular orientation, crystallinity, roughness and homogeneity, which establish the structural, optical, and electronic functionality of the finished product. Achieving a desired materials property requires a deep understanding of how processing influences structure. X-ray scattering is ideally suited to studying these problems, providing structural insights *during* processing, on time and length scales commensurate with manufacturing processes. For instance, the proposed side-station will be optimized to study the rapid liquid to gel to solid transitions that accompany deposition and solvent evaporation. During polymer film casting, order and alignment are greatly influenced by the energetics of the liquid-air interface and the drying kinetics (Fig. 2.6). The *intermediate state structure* — currently not well explored — dictates the final state and hence the materials functionality. Understanding the intermediate state structure will lead to faster and more stable processing conditions and ultimately to the development of new and improved materials.
Synchrotron x-ray scattering is the probe of choice for revealing the intermediate state structure over a wide range of length scales and with the required sub-millisecond temporal resolution [129]. A range of processing chambers and environments that mimic real processing conditions will be used to emulate industrial processes. The rich, detailed *kinetic* evolution of drying films that can be revealed by x-ray scattering tools will be used to inform and validate multi-scale physics based simulations of the structural evolution. For solution-processed films, quantitative predictions of the solvent-solid phase diagram are required. Coarse grained and molecular level simulations are then required to obtain the interphase and grain size and structure. Combining molecular-level computational methods with the new structural information of the intermediate state will lead to optimized processing conditions and methods.

The roadblocks to progress in polymer processing, and the opportunities for transformational advances in this field are well aligned with the DOE Grand Challenges "*How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?*" and "*How do we characterize and control matter away - especially very far away - from equilibrium?"* In addition, the critical need for in-situ/in-operando experiments on industry-specific tasks such as process development were identified in the report "Workshop of Industrial Research at NSLS II" (April 8-9, 2014). Studies into industrially relevant materials and processes demand flexible and versatile beamline setups. For liquid state processes, especially for spin, roll-to-roll and blade coating, the sample must remain horizontal. At present, there are no existing or planned NSLS-II beamlines that satisfy these criteria. The proposed 'open' sample environment and flexible beamline design of PLS will meet this challenge by enabling a wide range of experiments that address industrial and basic research problems, far beyond the vision described below.

Roll-to-Roll (R2R) is applied in numerous manufacturing fields such as flexible and large-area electronics devices [130], printed/flexible thin-film batteries [131,132], flexible solar panels [133], medical products [134], energy products in buildings, and membranes. Coatings are frequently made from molecular, polymeric, metallic, and oxide materials where organic/polymeric materials often serve as a binder for the latter. The EERE/DOE considers R2R processing as a key technology and has incorporated this research area as a major section in their Quadrennial Technology Review Assessment (http://energy.gov/quadrennial-technology-review-2015-omnibus#chap6sm). A better understanding of the intermediate states that occur during processing is essential. Nano-structured features develop rapidly and correspondingly fast

structural measurements on sub-millisecond time scales are essential to understand the processes. X-ray scattering can provide the crucial missing insight in these fields as shown by recent demonstration measurements at SSRL [135] using a simplified roll-to-roll processor (Fig. 2.7).

As a first example, we consider self-assembled diblock copolymer (BCP) template films. BCP thin films can enable potential applications such as substrate-supported nanodots [136-138], nanooptics [139,140], nanowires for electronic devices, nanoporous membranes for water–oil separation [141,142], and energy harvesting plasmonic devices [143,144]. Most applications require tight control over grain and micro-domain size and orientation of self-assembled blocks relative to the substrate, which may be aided by external fields such as shear [145,146], and chemical and physical patterning [142,147,148]. BCP films cast from fast evaporating solvents at room temperature typically produce films trapped in a quenched, nonequilibrium morphology, lacking long-range order due to film vitrification. Control of the subsequent annealing conditions to obtain the desired ordered BCP morphology is key to achieving functional materials [149]. Thermal annealing involves heating the BCP films above the glass transition temperature of both blocks to provide sufficient mobility to allow BCP ordering on a reasonable time scale. A variant of this, often used in processing, consists of a short exposure to elevated temperatures, but this approach can be problematic if one or more blocks can crystallize. Other conditions, such as strong electric and magnetic fields [150,151] may be applied to films to induce order, or UV cross-linking can also stabilize films. Solvent vapor annealing of BCP films, using a solvent with different properties than the deposition solvent, overcomes some of the drawbacks of thermal annealing, but can introduce new challenges [152]. The thin films swell when exposed to vapor where the extent of swelling depends on the nature and amount of solvent adsorbed. The extent of film swelling resulting from these processing conditions can affect morphology, domain orientation and crystallinity. Monitoring the development of molecular order during all of these different processing steps will greatly advance our ability to rationally design BCP thin films.

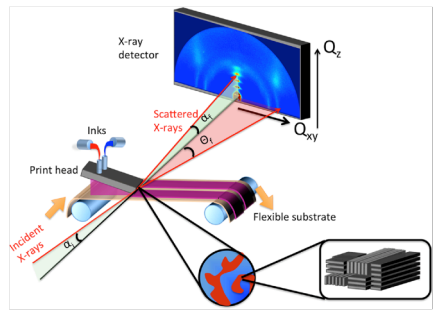


Fig. 2.7 Schematic of the in situ X-ray scattering setup for direct monitoring of the drying dynamics and morphology evolution using a mini R2R coater from Ref. 79.

As a second example, we consider R2R processing of flexible electronic devices (Fig. 2.8). Some of the potential products include flexible displays, photovoltaic devices, batteries, sensors, memories, and radio-frequency identification devices. R2R, with its low embodied energy costs and high volume production should help enable significant impact in energy production and storage technologies such as batteries, super capacitors, and photovoltaics [153]. These low-cost processes are suitable for applications where Si type performance is not required or when flexibility is a key asset. The specifics of the solvent evaporation process can significantly impact the performance of semiconducting polymers [129,154,155] and studies suggest that blade and roll-to-roll coating systems provide the best results. In the case of organic photovoltaic devices, efficiencies as high as 12% have been reported for polymer systems [156]. Rapid evaporation, such as used during spin coating, does not yield the best performing devices and this is believed to be due to a high nucleation density which gives rise to an isotropic small-grain structure. Oriented single-crystalline films appear to be desirable for achieving low

Fig. 2.8 Roll-to-roll photovoltaic.

defect density, but this normally requires a slower drying process in the so called "convective" deposition regime [129,154]. Developing strategies for controlling the grain size and orientation are required to make significant progress in the field. Operando x-ray scattering studies are essential from idealized systems in order to understand the underlying physics as well as from commercial coating equipment, too large to fit on a conventional spectrometer. The long length is required to control the drying process and to allow for multiple processing steps. Of note, with the beam constantly impinging on new areas as the roll is wound, the geometry is ideal for minimizing effects of beam damage.

Additive manufacturing (AM), often referred to as 3D printing, is an emerging technology for the rapid fabrication of objects with arbitrary shapes [157-159]. In principle, AM methods offer unique capabilities, remove much of the technical skill required to go from design to build, and greatly reduce the cost of customized manufacturing. As an example, healthcare related products need to be customized to the patient undergoing treatment and polymer AM represents a faster and significantly less expensive production method [160,161]. In the most common process for thermoplastics, Fused Deposition Molding (FDM), a thermoplastic polymer is fed though an extrusion head while the extrusion head is rastered across the surface in order to create 3 dimensional parts by repetitive and patterned deposition (Fig. 2.9). An important challenge in these manufacturing processes is that they do not always yield the same materials properties as traditional manufacturing methods. In parts prepared by this process the weld is often the point of failure. During the material extrusion process a hot layer is extruded onto the previous layer simultaneously cooling the printing layer and re-heating the substrate layer, resulting in a small window of time where the polymer-polymer interface is above the glass transition or melting temperatures. Unlike traditional processing methods where the properties of the polymer are, in general, bulk-like and formed homogeneously, weld formation in material extrusion is limited (non-bulk-like) and neighboring layers are formed in distinctly separate events (inhomogeneous). Very little is known about the interdiffusion that accompanies the weld and there are as yet no operando x-ray scattering studies of this phenomena. As the weld joint first heats, and then cools, the small and wide-angle scattering is expected to vary. Understanding these processes should lead to improved materials processing. As this field is very much in its infancy, the existing scientific literature is rather sparse.

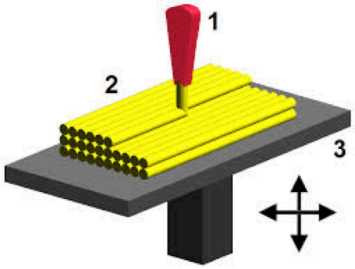


Fig. 2.9: Schematic of the Fused Deposition Molding (FDM) process.

A potential advantage of FDM prepared materials is that the molecular induced anisotropy that accompanies the processing can give rise to greatly enhanced mechanical properties. This high degree of orientation enables materials properties with "designed-in" reinforcement similar to composite construction. Here, x-ray methods can provide much needed insight, by studying the orientation, crystallinity, and microstructure (e.g. interlayer adhesion) of printed materials, especially by studying materials during deposition, drying, and fusion. Thermotropic liquid crystal polymers and polymers with nanoclay filler FDM materials are of particular interest since they exhibit varying degrees of crystallinity and orientational order which should depend on the processing conditions.

3.0 Beam Line and End Station Design

3.1 Insertion Device

During the design of at SMI (ID12) many provisions were made for the addition of a second, canted undulator, both in the accelerator, front-end and beamline optics. The electron beam scheme for ID12, shown in Fig. 3.1, maintains the standard 2 mrad canting angle between beamlines, with the center, canting magnet 1.35 m upstream of the straight center. At SMI, the undulator is a 2.8 m IVU23 with an undulator deflection parameter K_{max} = 2.05. The two undulators are asymmetrically canted with the SMI location near the straight center to allow its operation at a lower gap. Front-end design and ray tracing for all components and shielding required for both sources was completed as part of the SMI project.

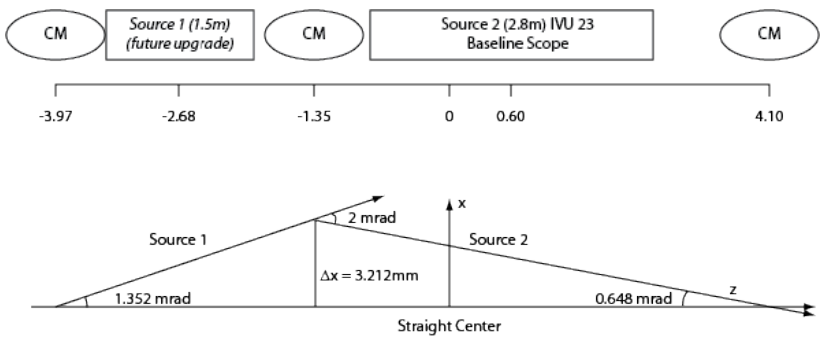


Fig. 3.1: Canting geometry (updated by Front End Group October 2013). Source 1 is where the PLS device will be located.

The undulator for PLS will be optimized in the 6-24 keV range with special consideration for providing optimal performance at the higher range of the spectrum. Due to the ~2.1 m length of the vacuum chamber, a 1.5 m magnetic length was considered for all undulator options. Based on the location of the SMI-12 ID that is at the upstream end of the High-Beta (Long) straight section, the min. "stay-clear" aperture of a constant-period undulator has to be ~7.4 mm. In the case of an APS-type SCU (G = 7.2 mm), the geometrical "stay-clear" gap value is 9.5 mm. Note that an assumption was made about the brightness calculations assumed a permanent magnet remanence in IVU/SAGU: of 1.19 T. The calculated brightness is shown in Fig. 3.2 for several different devices.

With regard to choosing the specific the type of undulator for PLS, no decision has been made but there has been consideration of using an APS/SCU type device since it would provide improved performance at the higher energy range of the spectrum over a more conventional device. At the

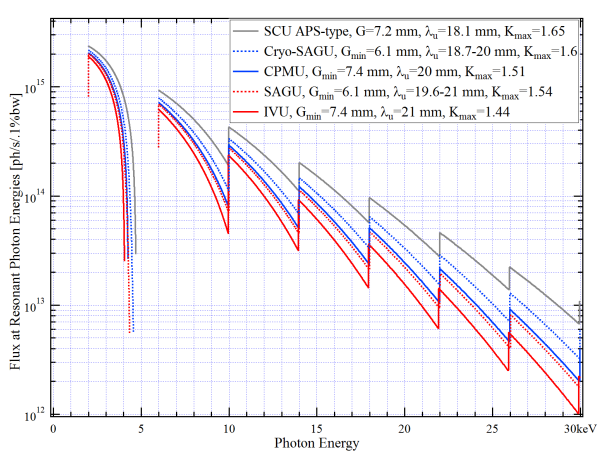


Fig. 3.2: Calculated Brightness for several different sources at PLS (courtesy of O. Chubar).

current budgeting stage (September, 2016), a conventional undulator magnet technology is being considered. If an SCU device is to be used, it would utilize the existing APS magnetic and mechanical/ cryogenic design and the SCU would be constructed at APS. The heat load (from image currents and from SR) would have to be estimated by NSLS-II and communicated to APS to allow proper scaling of the cryogenic system. Further, the effect of SCU on e-beam would have to be simulated by NSLS-II and tolerances would have to be formulated. To succeed, this would have to be a collaborative effort between APS and NSLS-II on magnetic field control and shimming. It is important to note that the NSLS-II requires higher harmonic numbers than APS, i.e. higher field quality may be required. In the long run, collaboration between APS and NSLS-II might also consider means of reducing magnetic gaps and eventually designing a SuperConducting "Segmented Adaptive-Gap Undulator" for NSLS-II.

The horizontal and vertical source sizes and angular divergences have been calculated for a 1.5 m Long SCU (related to Center of High-Beta Straight Section of NSLS-II) where single electron processes have been included. In the calculation, a 0.9 nm horizontal and 8 pm vertical e-beam emittances were used. In the Fig. 3.3, the source properties are shown over as a function of energy.

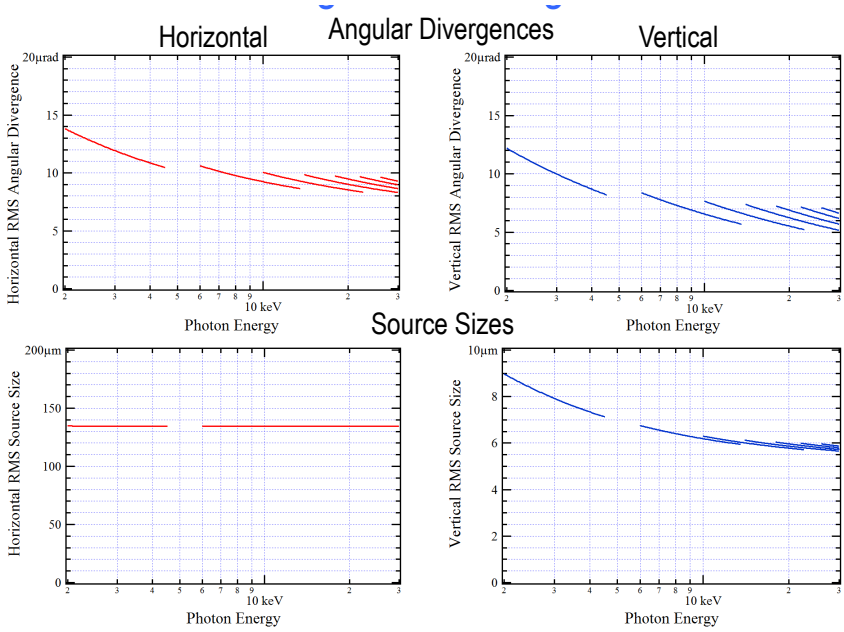


Fig. 3.3: Calculated device performance of a 1.5 m long SCU as a function of energy.

3.2 Beamline Layout

Sector 12-ID is located directly across from a laboratory/office building (LOB). This site benefits from the wet lab prep space, and is located near other Soft Matter / Materials Science beamlines. Hutches 12-ID-A, B, and C are the First Optics Enclosure, the Liquids/Polymer endstation (PLS), and the GISAXS/WAXS endstation (SMI) respectively (Fig. 3.4).

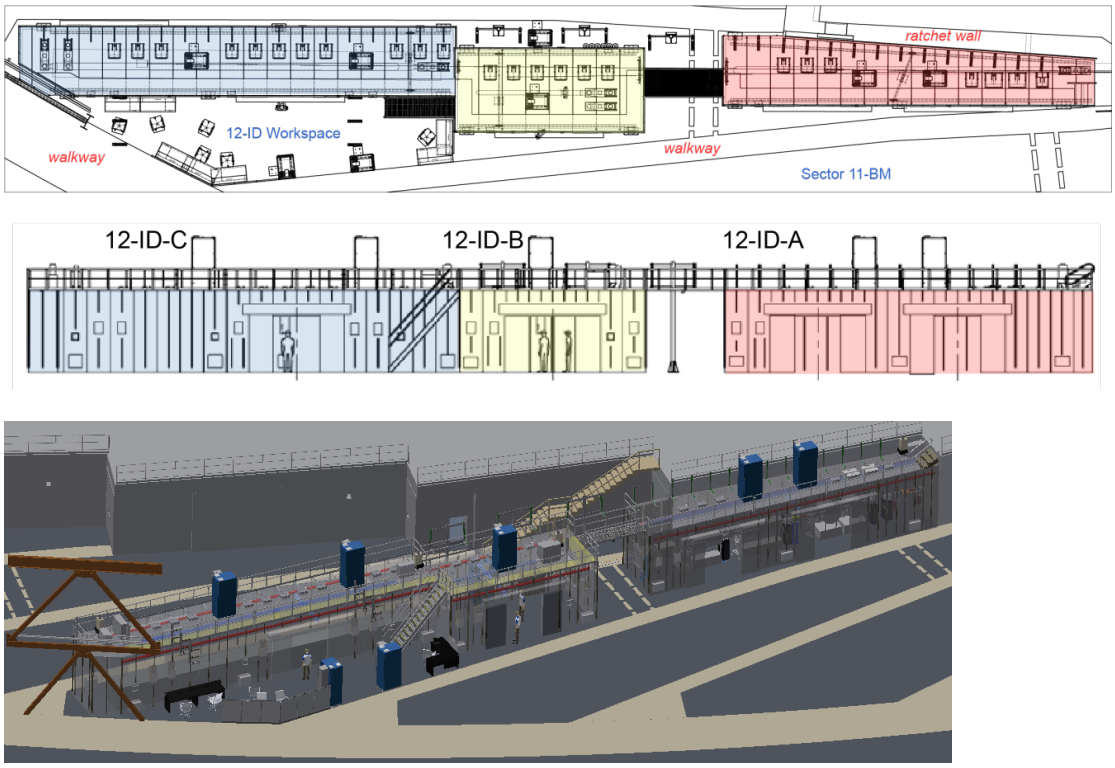


Fig. 3.4: CAD layout (top) of 12-ID and 3D rendering (bottom) of SMI hutches.

3.3 Optical Components Overview

The optical design principles for PLS include (1) separate the canted beams on the floor, (2) separate horizontal and vertical focusing, and (3) optimize beam at the sample and detector points. The SMI hardware is on the floor and their IRR is expected in mid October, 2016.

A flexible focusing scheme is needed due to beam heating effects and different focusing options. First, the PLS energy range of 6 to 24 keV varies the heat load and therefore the curvature of the DCM first crystal. Some applications require the micro-beam and others require low beam divergence. The PLS primary optics will allow focusing at either the sample or detector positions, as shown in Fig. 5. The addition of CRLs (discussed in detail below) and focusing at the SSA position will allow for a vertical microbeam at the sample position. Note that horizontal CRLs do not add much value (not included in the present design) since the increased horizontal divergence would not be well-matched to the Darwin width of the deflecting crystals

Photon delivery begins with white beam components: a fixed area mask (FAM) integrated with the bremsstrahlung collimator to create a differential pumping unit; white beam slits; DCM; white beam / bremsstrahlung stop; first x-ray beam position monitor (XBPM1). The position of these components is specified in the SMI design. Note that PLS DCM design must allow the SMI beam to pass through. The PLS mirrors will be contained in the exisitng SMI vacuum enclosures which have provisions for these additional mirrors.

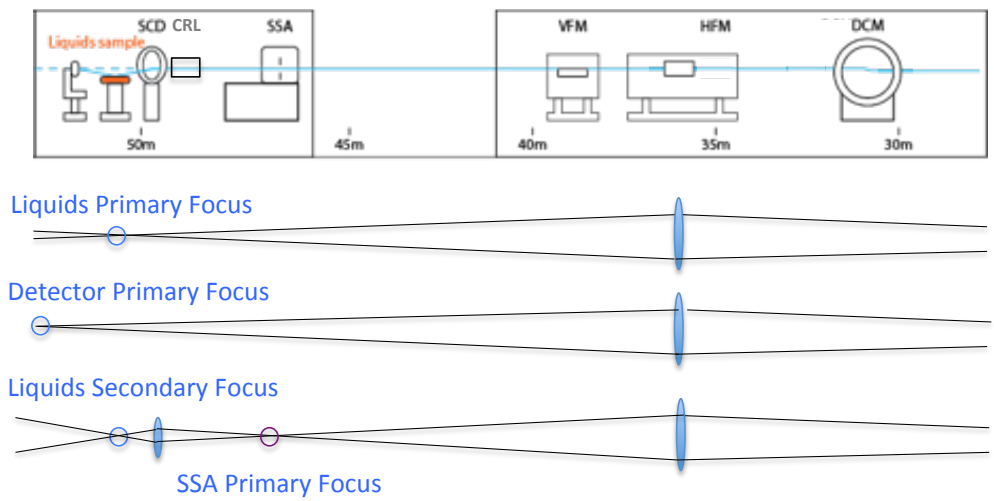


Fig. 3.5: PLS focusing schemes. Top: elevation, showing optics at right, and the end-station at left. Bottom: schematic depictions of different focusing modes.

After the XPBM1 diagnostics, a horizontally focusing and deflecting mirror sends the beam further outboard. Vertically deflecting and focusing mirrors follow, then refractive optics and a second diganostic, XBPM2. Following these, the final element in the first optical enclosure (12-ID-A) is the monochromatic x-ray shutter. A third diagnostic, XBPM3, is located in the upstream experimental hutch, and just downstream of this is the Secondary Source Aperture.

Focusing Optics

In the absence of optical aberrations, originating from crystal distortions and mirror slope error, it is straightforward to calculate the beam size at the sample position based on the source properties, from the undulator residing in the high-beta section, the optical characteristics and the location of the optical elements. The relevant parameters are provided below for PLS.

	source size(μm)	source size(μm)	divergence(μrads)	divergence(μrads)
	Gaussian	FWHM	Gaussian	FWHM
horizontal	135.0	317.25	9.0	21.15
vertical	6.0	14.1	6.5	15.275

Table 3.1: Estimated source size and divergence (Gaussian widths) based on the SCU device presented above at 10 keV. Note that the values only depend slightly on the energy. Values are given in terms of Gaussian widths and FWHM. In the following, we will use the FWHM values.

We have carried out a simple optical calculation using Gaussian beams for the specific parameters given in Tables 3.1 &. 3.2. In addition, as part of the SMI project, Shadow and SRW were used to calculate the properties of the focused beam. Since the placement of the mirrors is similar for SMI and PLS and since the source sizes and divergences are also similar, the SMI simulations provide a reasonable estimate of the focused beam properties. The secondary flat mirrors, which restore the beam to the direct beam direction, have a much smaller slope error and do not contribute significantly to the optical properties. In the modeling, slope errors based on

real mirror metrology (obtained from the NSLS-II Optics Group) were put into the SMI model. In these simulations a slope error of 0.3 μrad RMS for the vertical focusing mirror and 0.8 μrad RMS for the horizontal focusing mirror was used. The results from the SMI FDR are shown in Table 3.3.

element	distance from source (m)	distance to sample (m)
WBS (approx)	29.2	21.3
DCM (approx.)	31.1	19.4
HFM	32.3	18.2
VFM	38.7	11.8
SSA	47.0	3.5
CRL	49.5	1.0
Sample	50.5	
back wall	54.0	

Table 3.2: Position of beam line components.

In the following we will discuss our Gaussian calculations for the beam size where we take into account the positions of the PLS optical components and the source and divergence sizes where the various sources of broadening are added in quadrature. In the case of the horizontal direction, we will only consider focusing at the sample and the SSA positions although there is no particular reason to focus at the SSA position. In the horizontal, the calculation shows that the beam at the sample position is about 100 μm at the sample using the horizontal deflecting mirrors. If one were to focus further in the horizontal with CRLs, the reflectivity the deflector crystal would diminish due to the limited Darwin width acceptance of the germanium crystal(s). For instance, at 10 keV the Darwin width of Ge(111) is 62.5 μrads. This is reasonably matched to the divergence of the beam from the horizontal focusing mirror that is equal to 21.5/0.305=70.5 μrads where 0.305 is the ratio of the optical distances "f1" and "f2". However at 24 kev there will be a loss of intensity due to a smaller Darwin width (26 μrads) taking into account that the width scales inversely with the energy. Note that in the DCD configuration the smaller Darwin width of the Ge(220) crystal will further reduce the intensity throughput.

	Focusing @ Liquids Sample				Focusing at SSA with H-V mirrors			
	Mirrors, km	ES1, μm	ES1, μrad	Intensity	Mirrors, km	SSA, μm	SSA, μrad	Intensity
10778 eV	H = 7.45	143	55	1.57E+14	H = 5.99	117	70	1.74E+14
	V = 6.17	17	45		V = 4.55	12	66	
3593 eV	H = 7.68	143	39	3.77E+13	H = 6.28	113	52	2.94E+13
	V = 2.65	17	90		V = 2.04	12	130	
2101 eV	H = 7.55	149	46	3.38E+13	H = 6.01	117	68	4.23E+13
	V = 3.27	14	90		V = 2.41	11	144	

Table 3.3: SMI Calculated performance and specifications for mirrors using Shadow Ray Tracing (SMI FDR and discussions with M. Zhernenkov). Calculation for focus, beam size, divergence, and intensity at the liquids sample position (left) and SSA (right) positions. These dimensions should be ~10% smaller if the PLS mirror positions were used. With the PLS undulator, using the same technology as used at SMI, the flux will be about a factor of two smaller. However, the intensity values maybe too high (L. Berman, private comm.).

	source	sample	sample	SSA	SSA	sample	CRLs sample	CRLs (SSA=5μm) sample
		σv=0	σv=3e-7	σv=0	σv=3e-7	σv=0	σv=3e-7	σv=3e-7
Vertical	14	4.3	17.2	2.94	12.5	1.7	5.2	2.4
Horizontal	317	96.7	96.7	66.57				

Table 3.4: Vertical and horizontal focusing using both the primary mirrors and CRLs. Note that in the calculation we have either used no Gaussian mirror slope error or a value of 3e-7.

We have carried out calculations of the vertical beam size, the more critical direction for grazing incidence measurements, using a Gaussian Approximation (beam spreading factors add in quadrature). Here we find that for mirrors with no slope error, the beam size at the sample is 4.3 μm. The addition of 0.3 μrads slope error increases the beam size to 17.2 μm, consistent with the SMI calculations shown in Table 3.3. To reduce the beam size at the sample position, the beam is first focused at the SSA to 12.5 μm and is then refocused at the sample using CRLs located 2.5 m from the SSA and 1 m from the sample. This reduces the beam size to 5.2 μm at the sample position. However by using a 5 μm slits at the SSA position, the beam can be focused to about 2.4 μm at the sample position. This, of course, would reduce the intensity at the sample position by about a factor of 2. This configuration, despite the higher vertical divergence, would be ideal for liquid/liquid studies. Of course, further work is required using Shadow and SRW analysis to verify these values, but this is beyond the scope of the project at the present time.

CRL System:
Due to the short focal length, 100 cm between the sample and the CRL system, many lenses are required during the most demanding conditions. At 24 keV, 43 Be lenses are needed with a lenses curvature of 50 μm, well matched to the vertical beam size at the CRL position. Many fewer lenses are required at 6-8 keV. In calculating the transmission of such a system, taking into account the fewer lenses at the lower energies, we find that the transmission factor ranges between 65-75% over the desired energy range. Switching to Al lenses would significantly degrade the transmission performance, especially at the lower energies. However, a hybrid system, incorporating both Be and Al lenses might also be considered where only the Be lenses would be used at the lower energies. The CRL system will only require vertical translations on each of the 7 stacks of CRLs, thus simplifying the design. Further, there is no reason to use UHV as this would require additional x-ray windows. This also simplifies the design of the translators.

3.4 End-Station Conceptual Design: The technical requirements presented in the scientific case, both for liquid surfaces and processing, and the physical constraints, such as the size of the existing hutch size and the proximity to the main branch (SMI) were important considerations that were used to arrive at the proposed spectrometer configuration. These considerations include (1) compatability with the existing SMI optical configuration, (2) existing hutch layout, (3) the required 6-24 keV energy range, (4) support of large chambers which may weigh up to 200 kg and be a meter in size, (5) fixed sample height mode for liquid surface studies, (6) sufficient lateral space with respect to the beam pipe for SMI which passes through the hutch, (7) micron sized vertical beams, (8) high flux, and (9) high mechanical stability and accuracy and (10) low vibrational amplitude. We note that the proposed end-station will utilize the beam characteristics provided by the double crystal monochromator along with mirror optics which are described above.

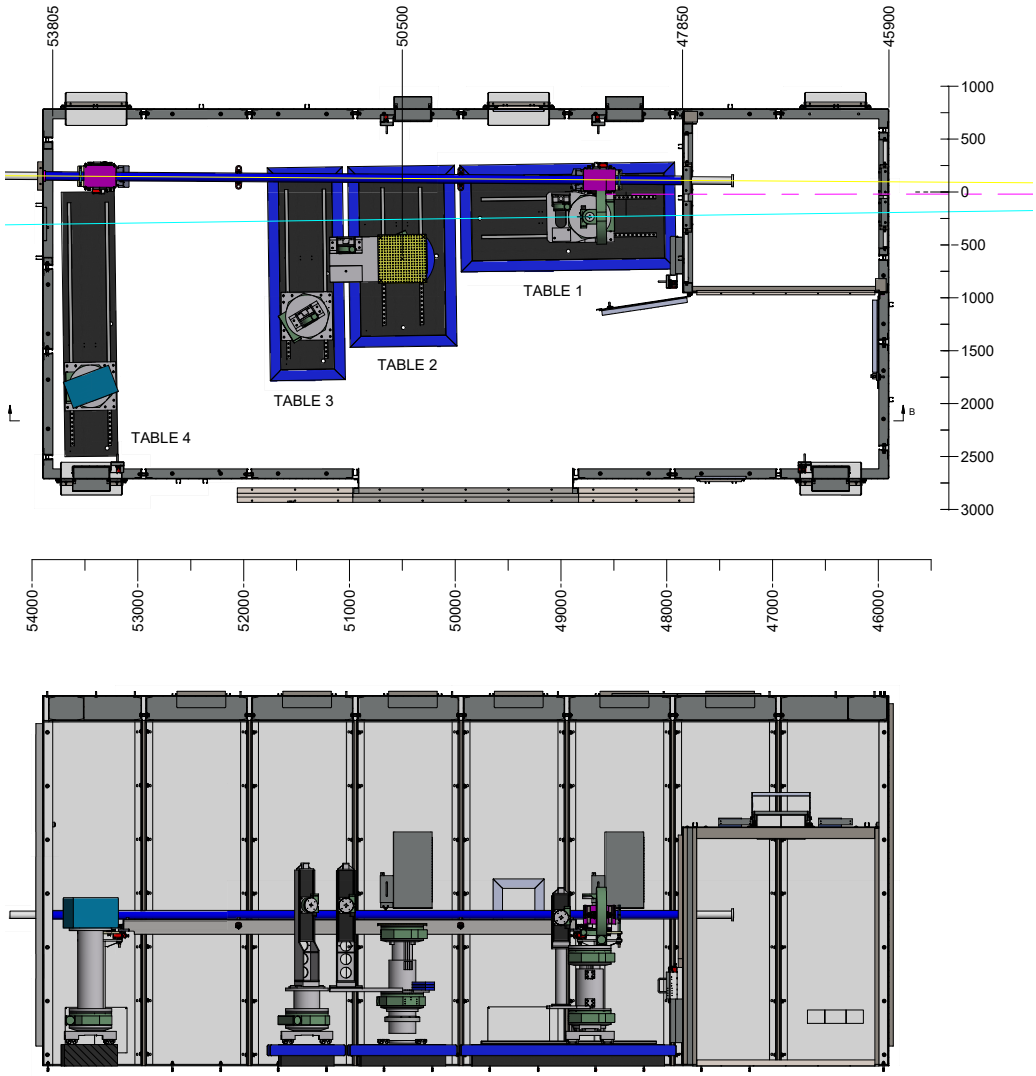


Fig. 3.6: Proposed spectrometer layout for the PLS instrument within the confines of the existing ID-12-B hutch at NSLS II. Each stage is supported by a granite table upon which mounts a long translation stage which supports each spectrometer stage.

In the initial stages of our conceptual design - proposal stage - two separate end-station scattering instruments in the PLS hutch were envisioned; one for liquid surfaces and the second for polymer processing. In the latter case, a horizontal deflecting crystal would have been located in the secondary source enclosure. While two separate instruments would likely require less set-up time to change configurations, this approach provided its own challenges due to the limited space in the hutch, the fixed energy of the polymer side-station instrument, and the duplication of instrumentation. After much consideration, we developed a single instrument plan that would satisfy the requirements of the polymer and liquid surface communities. The proposed end-station design, shown in Fig. 3.6, uses the same hardware for the polymer processing and liquids configurations.

The end-station design has four major elements, each of which is located on a linear translation stage supported by an independent granite block. These four stations (tables), shown in the Fig. 3.6, correspond to:

1. Crystal Deflection Stage (Table 1)

Purpose: To deflect the beam sideways towards the middle of the hutch and to deflect the beam downwards by a controlled angle, alpha.

- Single Crystal Deflector (SCD) mode: A single crystal, typical Ge(111) or Ge(220), will deflect the beam outboard by an angle determined by the energy and the crystal plane spacing. Chi rotation of the crystal will be used to deflect the beam downward by an angle alpha with respect to the horizontal. The SCD set-up will be used for polymer processing and liquid surfaces.
- Double Crystal Deflector (DCD): A first crystal, a Ge(111), will deflect the beam inboard. A second crystal, Ge(220), located about 25 cm from the first, will deflect the beam outboard. Chi rotation will be used to deflect the beam downward by an angle alpha with respect to the horizontal. This configuration has a special point, located about 65 cm from the first crystal, that has a fixed height, independent of alpha.
- To accommodate a variable distance between the deflector and the sample, the deflector stage is designed to move up/down stream using rails attached to a granite block. Motions will allow for the deflector to move sideways and vertically so that the centroid of the deflector stage can intercept the incident beam.

2. Sample and SCD Detector Stages (Table 2)

Purpose: To position (1) the sample stage vertically and transverse and (2) the detector arm for specular reflectivity and wide-angle scattering measurements.

- SCD mode: The sample stage position will be moved to intercept the position on the scattering cone generated by the alpha motion. This involves both a vertical and transverse motion. The sample stage should be extremely rigid to minimize motions induced by vibrations, should be able to support 200 kg as well an active vibration control stage. The detector arm theta motion should be concentric with the sample stage. The beta motion should have the ability to move vertically with an angle +/- 30 degrees by a combined rotation and vertical stage.
- DCD mode: No sample motion is required and the detector is positioned by the DCD Detector stage (described below).

3. DCD Detector Stage (Table 3)

Purpose: To position the detector arm for specular reflectivity measurements in DCD mode, especially at high energies for liquid/liquid studies.

- To minimize mechanical coupling to the sample – specifically to reduce vibrations on the liquid surface - when the detector arm is moved. This detector arm which is decoupled to the sample through separate granite bases.
- This arm will require the same vertical and rotational axis as the SCD arm for the out-of-plane motions (beta), as well as an in-plane translational and rotational stages to provide (2-theta) rotation
- This arm could also be use to help support the SAXS flight path while using the SCD.

4. SAXS Detector Stage (Table 4)

Purpose: To position the 2D SAXS detector, located about 3.5 m from the sample stage.

- The detector stage must rotate to remain normal to the beam.
- A beam stop with three degrees of motion will be place directly in front of the detector.
- Flight paths will have to be arranged by hand to suit the specific requirements.

Note that we have not included flight paths at the present, preliminary design stage.

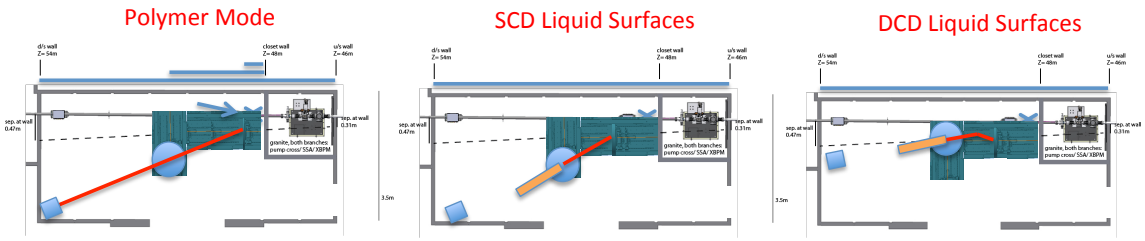


Fig. 3.7: Approximate positions of the deflector and sample stages for the three principle modes. Note that not all of the hardware is shown such as the DCD detector stage and the SAXS stage.

In Fig 3.7 we show the instrument in the three principle modes: (1) polymer processing, (2) SCD liquids mode and (3) DCD liquids mode. The considerations which affect the position of the deflector and sample stages was influenced by many factors, some of which are detailed below. In the processing configuration, the sample stage should be located as close to the center of the hutch as possible in order to maximize the amount of processing equipment that can be accommodated close to the sample. At different energies, we calculated the how far upstream the deflector must be from the sample, D_z, for a desired offset from the direct beam, D_x., where the geometry is shown in Fig. 3.8. The calculated, D_z, is shown in Table 1 for D_x =50, 75 and 100 cm at 8,16, and 24 keV, both Ge(111) and Ge(220) deflecting crystals. The total offset to the SMI direct beam is about an additional 40 cm, and the distance to the exterior of the SMI beam pipe is about 30 cm. Based on the above calculation, especially at the higher energies, the maximum D_z should be about 200 cm. For the DCD, the working distance is about 65 cm from the first crystal to the sample. To accommodate these considerations, we have chosen to locate the sample translation table at the 50.5 m position, leaving slightly more than 2.5 m to the hutch wall at 47.85 m. This will leave about 3.5-4.0 m to the position of the SAXS detector located at the rear of the hutch. For a Pilatus 1M detector, with its square 172 μm pixels, each pixel corresponds to a resolution of about 4e-4 Å at 8 keV.

Liquid Scattering Deflectors: Measurement of liquid interfaces requires a spectrometer that can tilt the incoming x-ray beam down onto a horizontal liquid sample. The PLS science case requires the capability to measure GISAXS and reflectivity, dictating that the incidence angle range from grazing incidence, with resolution comparable to the beam divergence, to at least 12°, for acceptable maximum q normal to the interface. Important technical considerations include position resolution, improving signal to noise, and increasing time resolution. The bright NSLS-II undulator beam will enable progress on all these counts, but at the increased risk of sample damage. This means that time resolution is doubly important, since fast measurements can reduce the x-ray dose.

This fact drives an important requirement for the liquids instrument: the beam deflector stage should include a two-crystal design which pivots the beam around a fixed sample height position (DCD), as illustrated at left in Fig. 3.8. However, beam diffraction through the second crystal can degrade performance through absorption losses, beam divergence mismatch to the rocking curve at high energies, and increased requirements for accuracy in alignment and tracking the beam motion. In comparison, the single crystal deflector (SCD) is sometimes preferred, at the expense of sample motion that requires a settling time in the measurement. This model deflects the beam with a single crystal as shown in the right panel of Fig. 3.8.

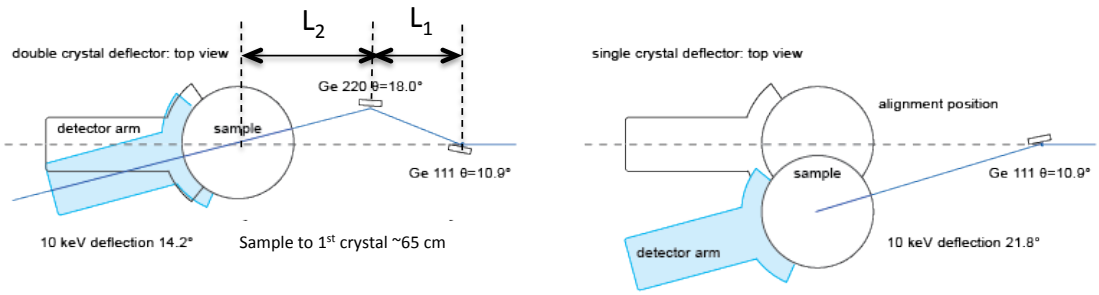


Fig. 3.8: Double (left) and single (right) crystal liquid steering stage schematics, plan view with beam level. (Prepared by E. DiMasi)

The PLS solution is to design a convertible instrument that operates in both modes, using Ge(111) and Ge(220) steering crystals. The spectrometer will have a vertical χ rotation stage equivalent to that of a standard four-circle goniometer, to rotate the assembly through an angle χ about the incident beam axis. With α the angle of incidence of the beam to the sample and Bragg scattering angles for the first and (optional) second crystals $2\theta_{111}$ and $2\theta_{220}$, the beam tilt relationships are as follows.

$$\text{DCD:} \quad \sin\alpha = \sin(2\theta_{220} - 2\theta_{111}) \times \sin(\chi)$$

$$\text{SCD:} \quad \sin\alpha = \sin(2\theta_{111}) \times \sin(\chi)$$

General specifications are:

- Mechanical range for 6 to 24 keV, 65-200 cm crystal-sample distance
- Crystal rotations based on 24 keV rocking curves
- Crystal translations as needed for tracking
- Spectrometer sphere of confusion as needed for tracking
- Distance between the 1st crystal and translation stage for 2nd crystal (L_1)

One of the important parameters in a DCD design is the distance between the two crystals (L_1) as this also gives the distance between the 1st crystal and the sample (L_1+ L_2), as shown in the left panel in Fig 3.8. If this distance is too short, then there is not enough room for the sample stage. The larger L_1 the more difficult it is to construct the instrument with high stability due to the chi dependent mechanical distortions. Further, increasing L_1 also increases the motion of the beam at the sample position due to imprecise positioning of the crystals due to the longer "lever arm". When the DCD was considered at SMI, an L_1 dimension of 40 cm was considered. At the new ESRF station ID10, an L_1 of 25 cm was used (See Fig. 3.9). Since this instrument is preforming very well and we can always increase the sample size by going to the SCD case, we have decided to specify L_1= 25 cm. This, in part, simplifies the design and the cost of the instrument.

For L_1= 25 cm, we have calculated the distance between the 1st crystal and the sample and the lateral crystal offset for the 2nd crystal (See Table 3.6). Note that there is a very slight variation in the distances and these will be accommodated for by the translation stages that are part of the instrument. With the DCD, the maximum surface normal q is determined by the reflections of the two crystals and is about 2.5 $Å^{-1}$. We note that the relationship between α and χ is shown in Fig. 3.10.

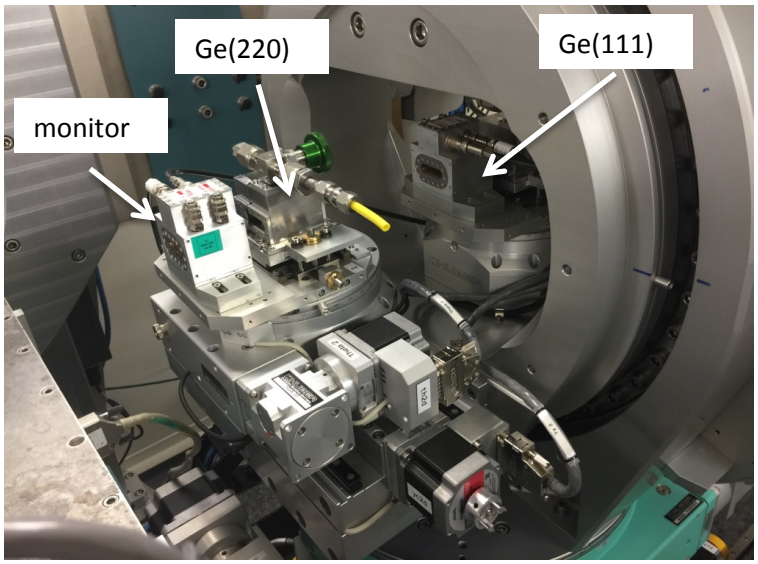


Fig. 3.9: Photo of the ID10 DCD at the ESRF. The crystals are enclosed in vacuum housings.

Energy (keV)	Dz (cm)	y1 (cm)
8.0	64.6	13.0
16.0	64.5	6.1
24.0	64.5	4.0

Table 3.6: Calculated distance D_z between the 1st crystal of the DCD and the sample using L_1=25 cm and the crystal offset of the 2nd crystal at several energies. Note that $D_z=L_1+L_2$.

To establish the DCD mechanical specifications within the SMI project (prior to de-scoping), a criterion based on intensity loss through a beam shift was used. This criterion was established for the photo delivery system specifications and adapted for the DCD. This intensity loss specification was based on the convolution of a slit acceptance with a gaussian beam characterized by a FWHM, for four different slit acceptances. The rule of thumb used for these calculations was that a beam shift of 10% if its FWHM provides no more than a 3% reduction in flux; a shift by 20% FWHM reduces flux by 10%. This requirement led to the requirement of a sphere of uncertainty (0.35μm) that was difficult (maybe impossible) for vendors to satisfy when the SMI specifications were sent for bid and only one vendor replied with an exorbitant price. At PLS, we will relax this specification by permitting more loss of intensity without mechanical corrections. We are not particularly concerned about the small loss of intensity as this can be reasonably accounted for using a beam monitor. Further, we believe that a look-up table can be established for these corrections to ensure that the beam stays in the center of the sample stage without a loss of intensity. Such a look-up table was successfully used for a mock-up DCD at the APS (ID9). In addition, it is possible to utilize active feedback to provide for the correction. These considerations will significantly reduce the cost of procurement for the DCD.

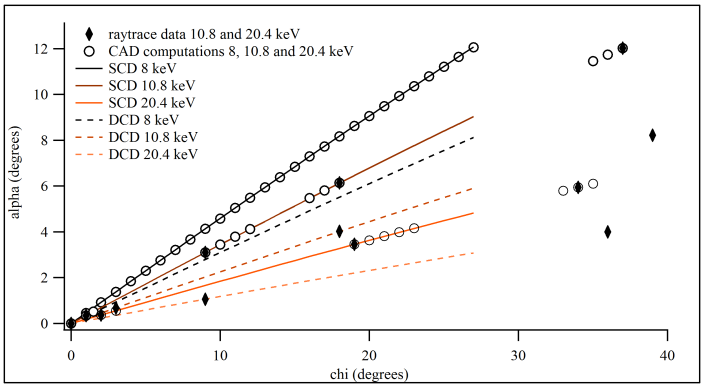


Fig. 3.10: Calculations from the tracking equations, CAD model nominal positions, and raytraced positions of the SCD and DCD, that were prepared as part of SMI (courtesy E. Di Masi)

3.5 Vertical Directed Beams

There are many scattering experiments that would benefit from transmission scattering geometry rather than the grazing incidence geometry. In the grazing incidence geometry the beam spreads out by a large numerical factor (the inverse incidence angle) and this large illuminated length makes it very difficult to carry-out microscopy studies with high spatial resolution. Further, in the grazing incidence geometry it is not possible to satisfy the Bragg condition for all azimuthal orientations and hence only a fraction of the domains scatter. This makes it virtually impossible to obtain the grain structure of thin films in the grazing incidence geometry. In contrast, the transmission geometry has virtually no surface-normal q-vector but it provides scattering information along both on-plane directions. It is this feature, along with the small beam sizes in transmission that makes this geometry ideal for scattering studies.

For thin films on solid supports, it is possible to carry out transmission x-ray scattering studies using a horizontal beam and vertical sample and this is the basis of the CD-SAXS method developed by NIST. However, for liquid surfaces, or thin polymer films in the process of drying, a vertical beam with a horizontal sample is likely required for most transmission x-ray SAXS/WAXS studies.

We have developed a concept to provide a vertical pointed beam using the single-deflector liquid spectrometer that would have lateral scanning capability with micron-sized beams.

reflection	λ(Å)	E(keV)	Structure Factor	Δθ(μrads)
Ge(333)	1.540	8.051	98	23.0
Ge(555)	0.924	13.419	60	5.1
Ge(777)	0.660	18.787	43	1.8
GE(999)	0.513	24.154	35	0.9

Table 3.7: Calculated wavelength and energy required for a 90° reflection in the beam , the structure factor and the Darwin width. The calculation was done using the CHESS Darwin width calculator, http://www.chess.cornell.edu/misc/xrclcdwn.htm .

In the simplest case, we would place a Ge(111) crystal at the sample position of the sample stage which would deflect the beam vertically and the sample (in transmission) would be located directly above the vertical deflector. To deflect vertically, we would use higher order reflections of the Ge(111) crystal (see left panel of Fig 3.11) where the energies corresponding to the reflection are shown in Table 3.7. For instance, the Ge(333) reflection could be used at 8.051 keV and the Ge(555) at 13.418 keV. This geometry suffers at the higher energies from the very small Darwin width. Without the CRLs, the vertical divergence is about 30 μrads, which is reasonably well-matched to the Ge(333) Darwin width at 8.051 keV. However, the width decreases by a factor of about 25 when the energy is increased by a factor of 3, while maintaining a reflection that allows a 90° deflection, and this would correspond to an equivalent loss of intensity close to the change in the Darwin width. In this case, it would be better to use two or three higher reflections rather than a single higher-order reflection. For the two-bounce case the deflection from each crystal is 45° degrees and in the three-bounce case the deflection from each crystal is 30°. In Table 3.8 we tabulate the energy required for several multi-bounce 90° deflectors. In these cases the Darwin width is much smaller and better suited to the angular spread of the beam.

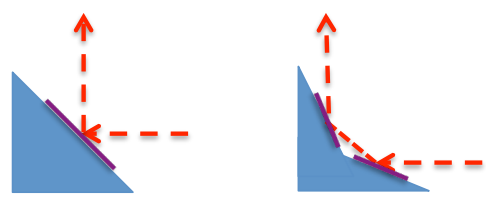


Fig. 3.11: Diagram of the single and double bounce vertical scattering crystal fixtures for the single and double bounces cases.

We have a plan to provide a simple and compact (< 6") fixture to provide the vertical deflection using multiple bounces (see right panel of Fig. 3.11) that relies on the required predefined angles along with the use of flexure or piezo stages to adjust the second and third crystals. The former should provide good long-term stability of the angles whereas the latter approach may be compromised by long-term drift. By making the second and third crystals not as wide as the previous crystal, it should be possible to translate the device laterally to adjust the earlier crystals. The proposed fixture will be much smaller and easier to install than an apparatus that provides full angular motion. To move the beam laterally, the deflector can be translated which will shift the position on the vertical deflecting fixture. In addition, the WAXS Pilatus detector would have to be mounted above the sample, pointing downwards. This could be supported by a simple modification to the detector arm.

reflection	bounces	λ(Å)	E(keV)	Structure Factor	Δθ(μrads)
Ge(111)	3	1.691	7.332	154	87.8
Ge(220)	2	1.531	8.098	190	62.5
Ge(220)	3	1.035	11.974	190	40.4
Ge(333)	2	0.833	14.877	98	9.5
Ge(333)	3	0.564	21.997	98	6.2

Table 3.8: Calculated wavelength and energy required for a 90° reflection in the beam using either two or three bounces with the same crystal. The structure factor and the Darwin width were calculated using the CHESS Darwin width calculator, http://www.chess.cornell.edu/misc/xrclcdwn.htm .

4.0 User Demand and Portfolio Impact

The proposed LSS will complement the only other US Liquid Surface Facility (Sector 15 at ANL-APS) whose operation is expected to continue after 2016. The proposed LSS instrument is essential to meet the scientific demand from the physical, chemical, materials science, and biomolecular materials communities. Without this facility researchers in the US will be left at a distinct disadvantage with respect to colleagues abroad, where several LSS instruments have been constructed recently (at the ESRF, Soleil, Diamond, PETRA III, Photon Factory, and Spring-8). The operando scattering capabilities will address the need for measuring intermediate states which occur during polymer processing and would be suited to both academic and industrial users. No existing NSLS II x-ray scattering stations provide the flexible and open scattering geometry provided by this facility. This end station would have a very strong connection to the proposed NIST/ARL/AFRL Initiative in Advanced Manufacturing. From discussions with academic and industrial partners (scientists at U. Mass and Akron U., centers for R2R processing) it is clear that there would be high demand for such a facility.

5.0 Quality of Proposers

The two co-leaders have many years of experience running beamlines and designing instruments for both NSLS and the APS. The US liquids interface x-ray scattering community has about 25 principal investigators, many of whom contributed to the successful SMI proposal and enthusiastically support this proposal. Many BNL scientists are co-PIs. In the polymer processing area there is keen interest from scientists at the University of Akron, University of Massachusetts, NIST, Henkel, and Exxon Co. Collaborators and supporters of this proposal are leaders in their field as evidenced by their curricula vita or letters of support.

6.0 Record of Interactions

<u>General Meetings</u>
May 18, 2 PM (kickoff meeting)
June 24, 11 AM (general meeting with BDP PIs)
August 5, 2 PM (general meeting with BDP PIs)
September 7, 11 AM (beamline controls/software meeting)
September 12, 2 PM (general meeting with BDP PIs)
September 15, 2:30 PM (beamline labor/schedule profiles)

<u>PLS Team Meetings (Ocko, Berman, Pindak and Coburn, not all in attendance at all meetings)</u>
June 8, 1:30 PM
June 16, 10 AM
June 21, AM
July 8, 10:30 AM
July 15, 2 PM
July 29, 11 AM
September 1, 10 AM
September 26, 2:30 PM
September 29, 10 AM

<u>Emails to Mark Schlossman</u>
Sept 30: Costing exercise
Sept 12: Costing estimate for this afternoons meeting
Sept 9: one-liner status summaries and IEPD Task Force meeting scheduled for Monday
Aug 3: Proposed slides for the presentation on Friday
Aug 1: brief presentations about IEPD Task Force engagement designs during Aug. 5 TF meeting

July 21: RFQ Follow Up: AVI Series from Herzan
July 8: SMI/PLS LSS
June 23: LSS and Polymer Processing
June 20: NSLS II Processing and Liquids Scattering (PLS) Beamline
June 10: Start of a letter to the PLS community
June 2: Phone conversations
May 4:NSLS-II BDP Letter and Report

Phone or in person conversations with Mark Schlossman
Sept 9, July 12, June 24, June 2

Discussions with Harald Reichert
Sept 9

Discussions with Cynthia Longo
June 21, July 6, Aug 16, Aug 20, Sept 22

Discussion with Ron Pindak
May 18, Jun 1, Jun 29, Jul 27, Sept 27, Sept 8, Sept 21, Oct 5

Multiple Hallway and office discussions with
Misha Zhernekov, Masa Fukuto, Elaine DiMasi, Oleg Gang, Kevin Yager, Andrei Fluearasu, Oleg Chubar, Steve Hulbert, Lutz Weigart and Ron Pindak

Roundtable discussions at the SXNS14 Conference at Stony Brook about PLS: July 12
Masa Fukuto, Jean Dalliant, Pulak Dutta, Mark Schlssoman Binhua Lin, Wenjie Wang, Tom Arnold, Philippe Fontaine, Bridget Murphy, Moshe Deutsch, Peter Pershan, Sushil Satija

NSLS Users Meeting Workshop: Characterization of Polymer Processing, May 23
Miko Cakmak, Alexander Hexemer, Tad Koga, Joseph Strzalka, Ruipeng Li, Dean DeLongchamp, Kevin Yager

Discussions and multiple emails with vendors
Riccardo Signorato (Cinel)
Norman Huber (Huber)
Chitra Venkataraman (Axilon)
Christian Mammen (JJ X-ray)

APPENDIX 1: REFERENCES

[1] de Gennes, P. G., Soft matter. Reviews of Modern Physics 1992, 64, (3), 645.

[2] Chaikin, P.; Lubensky, T. C., Introduction to Condensed Matter Physics. In Cambridge University Press, Cambridge: 1995.

[3] Kléman, M.; Laverntovich, O. D., Soft Matter Physics: An Introduction. Springer Science & Business Media: 2007.

[4] Doi, M., Soft Matter Physics. Oxford University Press: 2013.

[5] Kjell, M.; Johansson, I., Surfactants from Renewable Resources. Wiley: Chichester, 2010.

[6] Jungwirth, P.; Tobias, D. J., Molecular Structure of Salt Solutions: A New View of the Interface with Implications for Heterogeneous Atmospheric Chemistry. J. Phys. Chem. B 2001, 105, 10468-10472.

[7] Rossi, M. J., Heterogeneous reactions on salts. Chemical Reviews 2003, 103, (1), 4823-4882.

[8] Rydberg, J.; Choppin, M. C.; Choppin, G. R., Principles and Practices of Solvent Extraction. Marcel Dekker: New York, NY, 1992.

[9] Guyon, F.; Parthasarathy, N.; Buffle, J., Permeation Liquid Membrane Metal Transport: Studies of Complex Stoichiometries and Reactions in Cu(II) Extraction with the Mixture 22DD-Laurate in Toluene/Phenylhexane. Anal. Chem 2000, 72, 1328-1333.

[10] Stevens, G. W.; Perera, J. M.; Grieser, F., Metal ion extraction. Curr. Opin. Colloid Interface Sci. 1997, 2, 629.

[11] McFearin, C. L.; Beaman, D. K.; Moore, F. G.; Richmond, G. L., From Franklin to Today: Toward a Molecular Level Understanding of Bonding and Adsorption at the Oil-Water Interface. Journal of Physical Chemistry C 2009, 113, (4), 1171-1188.

[12] Taylor, D. J. F.; Thomas, R. K.; Penfold, J., Polymer/surfactant interactions at the air/water interface. Adv. Coll. Int. Sci. 2007, 132, 69-110.

[13] Adamson, A. W.; Gast, A. P., Physical Chemistry of Surfaces. 6th ed.; Wiley: New York, 1997.

[14] Dutta, P.; Peng, J. B.; Lin, B.; Ketterson, J. B.; Prakash, M.; Georgopoulos, P.; Ehrlich, S., X-ray diffraction study of an organic monolayer on the surface of water. Phys. Rev. Lett. 1987, 58, 2228.

[15] Wolf, S. G.; Deutsch, M.; Landau, E. M.; Lahav, M.; Leiserowitz, L.; Kjaer, K.; Als-Nielsen, J., A Synchrotron X-ray Study of a Solid-Solid Phase Transition in a Two-Dimensional Crystal. Science 1988, 242, 1286.

[16] Daillant, J.; Bosio, L.; Benattar, J. J.; Meunier, J., Capillary waves and bending elasticity of monolayers on water studied by X-ray reflectivity as a function of surface pressure. Europhys. Lett. 1989, 8, 453.

[17] Lin, B.; Shih, M. C.; Bohanon, T. M.; Ice, G. E.; Dutta, P., Phase diagram of a lipid monolayer on the surface of water. Phys. Rev. Lett. 1990, 65, 191.

[18] Daillant, J.; Bosio, L.; Benattar, J. J., X-ray reflectivity study of the liquid-expanded liquid-condensed phase transition. Europhys. Lett. 1990, 12, 715.

[19] Leveiller, F.; Jacquemain, D.; Lahav, M.; Leiserowitz, L.; Deutsch, M.; Kjaer, K.; Als-Nielsen, J., Crystallinity of the double layer of cadmium arachidate films at the water surface. Science 1991, 252, 1532.

[20] Weissbuch, I.; Addadi, L.; Lahav, M.; Leiserowitz, L., Molecular recognition at crystal interfaces. Science 1991, 253, 637.

[21] Jacquemain, D.; Leveiller, F.; Weinbach, S.; Lahav, M.; Leiserowitz, L.; Kjaer, K.; Als-Nielsen, J., Crystal structure of self-aggregates of insoluble aliphatic amphiphilic molecules at the air-water interface. An x-ray synchrotron study. J. Am. Chem. Soc. 1991, 113, 7684.

[22] Jacquemain, D.; Wolf, S. G.; Leveiller, F.; Lahav, M.; Leiserowitz, L.; Deutsch, J.; Kjaer, K.; Als-Nielsen, J., Dynamics of two-dimensional self-aggregation: Pressure and pH-induced structural changes in a fluorocarbon amphiphile at liquid-air interfaces. An x-ray synchrotron study. J. Am. Chem. Soc. 1990, 112, 7724.
[23] Wang, J.-L.; Leveiller, F.; Jacquemain, D.; Kjaer, K.; Als-Nielsen, J.; Lahav, M.; Leiserowitz, L., Two-dimensional structures of crytalline self-aggregates of amphiphilic alcohols at the air-water interface as studied by grazing incidence synchrotron x-ray diffraction and lattice energy calculations. J. Am. Chem. Soc. 1994, 116, 1192.
[24] Kuzmenko, I.; Buller, R.; Bouwman, W. G.; Kjaer, K.; AlsNielsen, J.; Lahav, M.; Leiserowitz, L., Formation of chiral interdigitated multilayers at the air-liquid interface through acid-base interactions. Science 1996, 274, (5295), 2046-2049.
[25] Lipp, M. M.; Lee, K. Y. C.; Takamoto, D. Y.; Zasadzinski, J. A.; Waring, A. J., Coexistence of buckled and flat monolayers. Physical Review Letters 1998, 81, (8), 1650-1653.
[26] Kaganer, V. M.; Mohwald, H.; Dutta, P., Structure and phase transitions in Langmuir monolayers. Rev. Mod. Phys. 1999, 71, 779.
[27] Kuhl, T. L.; Majewski, J.; Howes, P. B.; Kjaer, K.; Nahmen, A. v.; Lee, K. Y. C.; Ocko, B.; Israelachvili, J. N.; Smith, G. S., Packing Stress Relaxation in Polymer-Lipid Monolayers at the Air-Water Interface: An X-ray Grazing Incidence Diffraction and Reflectivity Study. J. Am. Chem. Soc. 1999, 121, 7682.
[28] Zheng, S.; Strzalka, J.; Jones, D. H.; Opella, S. J.; Blasie, J. K., Comparative structural studies of Vpu peptides in phospholipid monolayers by x-ray scattering. Biophysical Journal 2003, 84, 2393-2415.
[29] Wu, G. H.; Majewski, J.; Ege, C.; Kjaer, K.; Weygand, M. J.; Lee, K. Y. C., Lipid corralling and poloxamer squeeze-out in membranes. Physical Review Letters 2004, 93, (2), -.
[30] Ye, S. X.; Discher, B. M.; Strzalka, J.; Xu, T.; Wu, S. P.; Noy, D.; Kuzmenko, I.; Gog, T.; Therien, M. J.; Dutton, P. L.; Blasie, J. K., Amphiphilic four-helix bundle peptides designed for light-induced electron transfer across a soft interface. Nano Letters 2005, 5, (9), 1658-1667.
[31] Strzalka, J.; Xu, T.; Tronin, A.; Wu, S. P.; Miloradovic, I.; Kuzmenko, I.; Gog, T.; Therien, M. J.; Blasie, J. K., Structural studies of amphiphilic 4-helix bundle peptides incorporating designed extended chromophores for nonlinear optical biomolecular materials. Nano Letters 2006, 6, (11), 2395-2405.
[32] Xu, T.; Wu, S. P.; Miloradovic, I.; Therien, M. J.; Blasie, J. K., Incorporation of designed extended chromophores into amphiphilic 4-helix bundle peptides for nonlinear optical biomolecular materials. Nano Letters 2006, 6, (11), 2387-2394.
[33] Travesset, A.; Vaknin, D., Bjerrum pairing correlations at charged interfaces. Europhys. Lett. 2006, 74, (1), 181-187.
[34] Bu, W.; Vaknin, D.; Travesset, A., How Accurate is Poisson-Boltzmann Theory for Monovalent Ions near Highly Charged Interfaces? Langmuir 2006, 22, (13), 5673-5681.
[35] Pittler, J.; Bu, W.; Vaknin, D.; Travesset, A.; McGillivray, D. J.; Losche, M., Charge inversion at minute electrolyte concentrations. Phys. Rev. Lett. 2006, 97, 046102.
[36] Magnussen, O. M.; Ocko, B. M.; Deutsch, M.; Regan, M. J.; Pershan, P. S.; Abernathy, D.; Grubel, G.; Legrand, J. F., Self-assembly of organic films on a liquid metal. Nature 1996, 384, (6606), 250-252.
[37] Ocko, B. M.; Kraack, H.; Pershan, P. S.; Sloutskin, E.; Tamam, L.; Deutsch, M., Crystalline phases of alkyl-thiol monolayers on liquid mercury. Physical Review Letters 2005, 94, (1), -.

[38] Kraack, H.; Ocko, B. M.; Pershan, P. S.; Sloutskin, E.; Deutsch, M., Structure of a Langmuir film on a liquid metal surface. Science 2002, 298, (5597), 1404-1407.
[39] Regan, M. J.; Kawamoto, E. H.; Lee, S.; Pershan, P. S.; Maskil, N.; Deutsch, M.; Magnussen, O. M.; Ocko, B. M., Surface layering in liquid Gallium: X-ray reflectivity study. Phys. Rev. Lett. 1995, 75, 2498.
[40] Magnussen, O. M.; Ocko, B. M.; Regan, M. J.; Penanen, K.; Pershan, P. S.; Deutsch, M., X-ray reflectivity measurements of surface layering in liquid mercury. Phys. Rev. Lett. 1995, 74, 4444.
[41] Shpyrko, O. G.; Grigoriev, A. Y.; Streitel, R.; Pontoni, D.; Pershan, P. S.; Deutsch, M.; Ocko, B.; Meron, M.; Lin, B. H., Atomic-scale surface demixing in a eutectic liquid BiSn alloy. Physical Review Letters 2005, 95, (10).
[42] Shpyrko, O. G.; Streitel, R.; Balagurusamy, V. S. K.; Grigoriev, A. Y.; Deutsch, M.; Ocko, B. M.; Meron, M.; Lin, B. H.; Pershan, P. S., Surface crystallization in a liquid AuSi alloy. Science 2006, 313, (5783), 77-80.
[43] Ratajczak, M. K.; Chi, E. Y.; Frey, S. L.; Cao, K. D.; Luther, L. M.; Lee, K. Y. C.; Majewski, J.; Kjaer, K., Ordered Nanoclusters in Lipid-Cholesterol Membranes. Physical Review Letters 2009, 103, (2), 028103.
[44] Mechler, S.; Pershan, P. S.; Yahel, E.; Stoltz, S. E.; Shpyrko, O. G.; Lin, B.; Meron, M.; Sellner, S., Self-Consistent Interpretation of the 2D Structure of the Liquid $Au_{82}Si_{18}$ Surface: Bending Rigidity and the Debye-Waller Effect. Physical Review Letters 2010, 105, (186101).
[45] Elsen, A.; Festersen, S.; Runge, B.; Koops, C. T.; Ocko, B. M.; Deutsch, M.; Seeck, O. H.; Murphy, B. M.; Magnussen, O. M., In situ X-ray studies of adlayer-induced crystal nucleation at the liquid–liquid interface. Proceedings of the National Academy of Sciences 2013, 110, (17), 6663-6668
[46] Elsen, A.; Murphy, B. M.; Ocko, B. M.; Tamam, L.; Deutsch, M.; Kuzmenko, I.; Magnussen, O. M., Surface layering at the mercury-electrolyte interface. Physical review letters 2010, 104, (10), 105501.
[47] Schwartz, D. K.; Schlossman, M. L.; Kawamoto, E. H.; Kellogg, G. J.; Pershan, P. S.; Ocko, B. M., Thermal diffuse x-ray scattering studies of the water-vapor interface. Phys. Rev. A 1990, 41, 5687-5690.
[48] Sanyal, M. K.; Sinha, S. K.; Huang, K. G.; Ocko, B. M., X-ray scattering study of capillary wave fluctuations at a liquid surface. Phys. Rev. Lett. 1991, 66, 628-631.
[49] Tidswell, I. M.; Rabedeau, T. A.; Pershan, P. S.; Kosowsky, S. D., Complete wetting of a rough surface: An x-ray study. Phys. Rev. Lett. 1991, 66, 2108.
[50] Napiórkowski, M.; Dietrich, S., Structure of the effective Hamiltonian for liquid-vapor interface. Phys. Rev. E 1993, 47, 1836.
[51] Ocko, B. M.; Wu, X. Z.; Sirota, E. B.; Sinha, S. K.; Deutsch, M., X-ray reflectivity study of thermal capillary waves on liquid surfaces. Phys. Rev. Lett. 1994, 72, 242.
[52] McClain, B. R.; Lee, D. D.; Carvalho, B. L.; Mochrie, S. G. J.; Chen, S. H.; Litster, J. D., X-ray reflectivity study of an oil-water interface in equilibrium with a middle-phase microemulsion. Phys. Rev. Lett. 1994, 72, 246.
[53] Tolan, M.; Seeck, O. H.; Schlomka, J. P.; Press, W.; Wang, J.; Sinha, S. K.; Li, Z.; Rafailovich, M. H.; Sokolov, J., Evidence for capillary waves on dewetted polymer film surfaces: A combined x-ray and atomic force microscopy study. Phys. Rev. Lett. 1998, 81, 2731.
[54] McClain, B. R.; Yoon, M.; Litster, J. D.; Mochrie, S. G. J., Interfacial roughness in a near-critical binary fluid mixture: X-ray reflectivity and near-specular diffuse scattering. Eur. Phys. J. B 1999, 10, 45.

[55] Fradin, C.; Braslau, A.; Luzet, D.; Smilgies, D.; Alba, M.; Boudet, N.; Mecke, K.; Daillant, J., Reduction in the surface energy of liquid interfaces at short length scales. Nature 2000, 403, 871.
[56] Mora, S.; Daillant, J.; Mecke, K.; Luzet, D.; Braslau, A.; Alba, M.; Struth, B., X-ray synchrotron stud of liquid-vapor interfaces at short length scales: Effect of long-range forces and bending energies. Phys. Rev. Lett. 2003, 90, 216101-1 - 216101-4.
[57] Sloutskin, E.; Baumert, J.; Ocko, B. M.; Kuzmenko, I.; Checco, A.; Tamam, L.; Ofer, E.; Gog, T.; Gang, O.; Deutsch, M., The surface structure of concentrated aqueous salt solutions. Journal of Chemical Physics 2007, 126, (5), 54704-54704.
[58] Bloch, J. M.; Yun, W. B.; Yang, X.; Ramanathan, M.; Montano, P. A.; Capasso, C., Adsorption of counterions to a stearate monolayer spread at the water-air interface: a synchrotron x-ray study. Phys. Rev. Lett. 1988, 61, 2941-2944.
[59] Bloch, J. M.; Sansone, M.; Rondelez, F.; Peiffer, D. G.; Pincus, P.; Kim, M. W.; Eisenberger, P. M., Concentration profile of a dissolved polymer near the air- liquid interface: x-ray fluorescence study. Phys. Rev. Lett. 1985, 54, 1039.
[60] Luo, G.; Malkova, S.; Yoon, J.; Schultz, D. G.; Lin, B.; Meron, M.; Benjamin, I.; Vanysek, P.; Schlossman, M. L., Ion Distributions Near a Liquid-Liquid Interface. Science 2006, 311, 216-218.
[61] Vaknin, D.; Kruger, P.; Losche, M., Anomalous X-Ray Reflectivity Characterization of Ion Distribution at Biomimetic Membranes. Phys. Rev. Lett. 2003, 90, (17), 178102.
[62] Shapovalov, V. L.; Brezesinski, G., Breakdown of the Gouy-Chapman Model for Highly Charged Langmuir Monolayers: Counterion Size Effect. J. Phys. Chem. B 2006, 110, 10032-10040.
[63] Shapovalov, V. L.; Ryskin, M. E.; Konovalov, O. V.; Hermelink, A.; Brezesinski, G., Elemental Analysis within the Electrical Double Layer Using Total Reflection X-Ray Fluorescence Technique. J. Phys. Chem. B 2007, 111, 3927-3934.
[64] Mezger, M.; Schroder, H.; Reichert, H.; Schramm, S.; Okasinski, J. S.; Schoder, S.; Honkimaki, V.; Deutsch, M.; Ocko, B. M.; Ralston, J.; Rohwerder, M.; Stratmann, M.; Dosch, H., Molecular Layering of Fluorinated Ionic Liquids at a Charged Sapphire (0001) Surface. Science 2008, 322, (5900), 424-428.
[65] Pershan, P. S.; Schlossman, M. L., Liquid Surfaces and Interfaces: Synchrotron X-ray Methods. Cambridge University Press: Cambridge, 2012.
[66]
[67] Rydberg, J.; Cox, M.; Musikas, C.; Choppin, G. R., Solvent Extraction Principles and Practice. Marcel Dekker: New York, NY, 2004.
[68] Tasker, P. A.; Plieger, P. G.; West, L. C., Metal Complexes for Hydrometallurgy and Extraction. In Comprehensive Coordination Chemistry II: From Biology to Nanotechnology, McCleverty, J. A.; Meyer, T. J., Eds. Elsevier: Oxford, 2004; Vol. 9, pp 759-808.
[69] Nash, K. L., Twenty-First Century Approaches to Actinide Partitioning. In Separations for the Nuclear Fuel Cycle in the 21st Century, ACS Symposium Series 933, Lumetta, G. J.; Nash, K. L.; Clark, S. B.; Friese, J. I., Eds. American Chemical Society: Washington, D. C., 2006; pp 21-40.
[70] Danesi, P. R.; Chiarizia, R., The Kinetics of Metal Solvent Extraction. Crit. Rev. Anal. Chem. 1980, 10, 1-126.
[71] Bu, W.; Yu, H.; Luo, G.; Bera, M. K.; Hou, B.; Schuman, A. W.; Lin, B.; Meron, M.; Kuzmenko, I.; Antonio, M. R.; Soderholm, L.; Schlossman, M. L., Observation of a Rare Earth Ion-Extractant Complex Arrested at the Oil-Water Interface During Solvent Extraction. J. Phys. Chem. B 2014, 118, 10662-10674.

[72] Bu, W.; Mihaylov, M.; Amoanu, D.; Lin, B.; Meron, M.; Kuzmenko, I.; Soderholm, L.; Schlossman, M. L., X-ray Studies of Interfacial Strontium-Extractant Complexes in a Model Solvent Extraction System. J. Phys. Chem. B 2014, 118, 12486-12500.
[73] Scoppola, E.; Watkins, E.; Destri, G. L.; Porcar, L.; Campbell, R. A.; Konovalov, O.; Fragnetoa, G.; Diat, O., Structure of a liquid/liquid interface during solvent extraction combining X-ray and neutron reflectivity measurements†. Phys. Chem. Chem. Phys. 2015, 17, 15093-15097.
[74] Schlossman, M. L.; Tikhonov, A. M., Molecular ordering and phase behavior of surfactants at water-oil interfaces as probed by X-ray surface scattering. Annu. Rev. Phys. Chem. 2008, 59, 153-177.
[75] Zhang, Z.; Mitrinovic, D. M.; Williams, S. M.; Huang, Z.; Schlossman, M. L., X-ray Scattering from Monolayers of $F(CF_2)_{10}(CH_2)_2OH$ at the Water-(Hexane Solution) and Water-Vapor Interfaces. J. Chem. Phys. 1999, 110, 7421-7432.
[76] Li, M.; Tikhonov, A.; Schlossman, M. L., An x-ray diffuse scattering study of domains in $F(CF_2)_{10}(CH_2)_2OH$ monolayers at the hexane-water interface. Europhys. Lett. 2002, 58, 80-86.
[77] Tikhonov, A. M.; Li, M.; Schlossman, M. L., Phase transition behavior of fluorinated monolayers at the water-hexane interface. J. Phys. Chem. B 2001, 105, 8065.
[78] Tikhonov, A. M.; Patel, H.; Garde, S.; Schlossman, M. L., Tail ordering due to headgrup hydrogen bonding interactions in surfactant monolayers at the water-oil interface. J. Phys. Chem. B 2006, 110, 19093-19096.
[79] Tikhonov, A. M.; Schlossman, M. L., Surfactant and Water Ordering in Triacontanol Monolayers at the Water-Hexane Interface. J. Phys. Chem. B 2003, 107, 3344-3347.
[80] Tikhonov, A. M.; Pingali, S. V.; Schlossman, M. L., Molecular ordering and phase transitions in alkanol monolayers at the water-hexane interface. J. Chem. Phys. 2004, 120, 11822-11838.
[81] Tikhonov, A. M.; Schlossman, M. L., Vaporization and layering of alkanols at the oil/water interface. J. Phys. Condens. Matter 2007, 19, 375101.
[82] Pingali, S. V.; Takiue, T.; Luo, G.; Tikhonov, A. M.; Ikeda, N.; Aratono, M.; Schlossman, M. L., X-ray Reflectivity and Interfacial Tension Study of the Structure and Phase Behavior of the Interface between Water and Mixed Surfactant Solutions of $CH_3(CH_2)_{19}OH$ and $CF_3(CF_2)_7(CH_2)_2OH$ in Hexane. J. Phys. Chem. B 2005, 109, 1210-1225.
[83] Tamam, L.; Pontoni, D.; Sapir, Z.; Yefe, S.; Sloutskin, E.; Ocko, B. M.; Reichert, H.; Deutsch, M., Modification of deeply buried hydrophobic interfaces by ionic surfactants. Proc. Natl. Acad. Sci. USA 2011, 108, (14), 5522-5525.
[84] Bu, W.; Ryan, P. J.; Vaknin, D., Ion distributions at chargd aqueous surfaces by near-resonance x-ray spectroscopy. J. Synchrotron Rad. 2006, 13, 459-463.
[85] Bu, W.; Vaknin, D.; Travesset, A., Monovalent Counterion Distributions at Highly Charged Water Interfaces: Proton-Transfer and Poisson-Boltzmann Theory. Phys. Rev. E 2005, 72, 060501.
[86] Luo, G.; Malkova, S.; Yoon, J.; Schultz, D. G.; Lin, B.; Meron, M.; Benjamin, I.; Vanysek, P.; Schlossman, M. L., Ion Distributions at the Nitrobenzene-Water Interface Electrified by a Common Ion. J. Electroanal. Chem. 2006, 593, 142-158.
[87] Laanait, N.; Yoon, J.; Hou, B.; Vanysek, P.; Meron, M.; Lin, B.; Luo, G.; Benjamin, I.; Schlossman, M. L., Communications: Monovalent Ion Condensation at the Electrified Liquid/Liquid Interface. J. Chem. Phys. 2010, 132, 171101-1 - 171101-4.

[88] Laanait, N.; Mihaylov, M.; Hou, B.; Yu, H.; Vanysek, P.; Meron, M.; Lin, B.; Benjamin, I.; Schlossman, M. L., Tuning Ion Correlations at an Electrified Soft Interface. Proc. Nat. Acad. Sci. (USA) 2012, 109, 20326-20331.
[89] Luo, G.; Bu, W.; Mihaylov, M.; Kuzmenko, I.; Schlossman, M. L.; Soderholm, L., X-ray reflectivity reveals a non-monotonic ion-density profile perpendicular to the surface of $ErCl_3$ aqueous solutions. J. Phys. Chem. C 2013, 117, 19082–19090.
[90] Hou, B.; Laanait, N.; Yu, H.; Bu, W.; Chen, C.-H.; Yoon, J.; Lin, B.; Luo, G.; Vanysek, P.; Schlossman, M. L., Ion distributions at the water/1,2-dichloroethane interface: Potential of mean force approach to analyzing X-ray reflectivity and interfacial tension measurements J. Phys. Chem. B 2013, 117, 5365-5378.
[91] Hou, B.; Bu, W.; Luo, G.; Vanysek, P.; Schlossman, M. L., Ion Distributions at ElectrifiedWater-Organic Interfaces: PB-PMF Calculations and Impedance Spectroscopy Measurements. J. Electrochem. Soc. 2015, 162, H890-H897.
[92] Bera, M. K.; Luo, G.; Schlossman, M. L.; Soderholm, L.; Lee, S.; Antonio, M. R., Erbium(III) Coordination at the Surface of an Aqueous Electrolyte. J. Phys. Chem. B 2015, 119, 8734−8745.
[93] Miller, M.; Chu, M.; Lin, B.; Meron, M.; Dutta, P., Observation of Ordered Structures in Counterion Layers near Wet Charged Surfaces: A Potential Mechanism for Charge Inversion. Langmuir 2016, 32, 73-77.
[94] Ma, H.; Burger, C.; Hsiao, B. S.; Chu, B., Ultrafine Polysaccharide Nanofibrous Membranes for Water Purification. Biomacromolecules 2011, 12, 970-976.
[95] Ma, H.; Burger, C.; Hsiao, B. S.; Chu, B., Nanofibrous Microfiltration Membrane Based on Cellulose Nanowhiskers. Biomacromolecules 2012, 13, 180-186.
[96] Ma, H.; Burger, C.; Hsiao, B. S.; Chu, B., Highly Permeable Polymer Membranes Containing Directed Channels for Water Purification. ACS Macro Letters 2012, 1, 723-726.
[97] Wang, Z.; Ma, H.; Hsiao, B. S.; Chu, B., Nanofibrous ultrafiltration membranes containing cross-linked poly(ethylene glycol) and cellulose nanofiber composite barrier layer. Polymer 2014, 55, 366-372.
[98] Kinge, S.; Crego-Calama, M.; Reinhoudt, D. N., Self-assembling nanoparticles at surfaces and interfaces. ChemPhysChem 2008, 9, 20–42.
[99] Shipway, A. N.; Katz, E.; Wilner, I., Nanoparticle arrays on surfaces for electronic, optical, and sensor applications. ChemPhysChem 2000, 1, 18–52.
[100] Lin, Y.; Skaff, H.; Emrick, T.; Dinsmore, A. D.; Russell, T. P., Nanoparticle assembly and transport at liquid-liquid interfaces. Science 2003, 299, 226-229.
[101] Bresme, F.; Oettel, M., Nanoparticles at fluid interfaces. J. Phys.: Condens. Matter 2007, 19, 413101.
[102] Russell, J. T.; Lin, Y.; Boker, A.; Su, L.; Carl, P.; Zettl, H.; He, J. B.; Sill, K.; Tangirala, R.; Emrick, T.; Littrell, K.; Thiyagarajan, P.; Cookson, D.; Fery, A.; Wang, Q.; Russell, T. P., Self-Assembly and Cross-Linking of Bionanoparticles at Liquid–Liquid Interfaces. Angew. Chem., Int. Ed. 2005, 44, 2420–2426.
[103] Jiang, Z.; Lin, X.-M.; Sprung, M.; Narayanan, S.; Wang, J., Nano Lett. 2010, 10, 799–803.
[104] Kooijman, E. E.; Vaknin, D.; Bu, W.; Joshi, L.; Kang, S. W.; Gericke, A.; Mann, E. K.; Kumar, S., Structure of Ceramide-1-Phosphate at the Air-Water Solution Interface in the Absence and Presence of Ca2+. Biophysical Journal 2009, 96, (6), 2204-2215.
[105] Chi, E. Y.; Frey, S. L.; Winans, A.; Lam, K. L. H.; Kjaer, K.; Majewski, J.; Lee, K. Y. C., Amyloid-beta Fibrillogenesis Seeded by Interface-Induced Peptide Misfolding and Self-Assembly. Biophysical Journal 2010, 98, (10), 2299-2308.
[106] Stenger, P. C.; Wu, G. H.; Miller, C. E.; Chi, E. Y.; Frey, S. L.; Lee, K. Y. C.; Majewski, J.; Kjaer, K.; Zasadzinski, J. A., X-Ray Diffraction and Reflectivity Validation of

the Depletion Attraction in the Competitive Adsorption of Lung Surfactant and Albumin. Biophysical Journal 2009, 97, (3), 777-786.
[107] Neville, F.; Ishitsuka, Y.; Hodges, C. S.; Konovalov, O.; Waring, A. J.; Lehrer, R.; Lee, K. Y. C.; Gidalevitz, D., Protegrin interaction with lipid monolayers: grazing incidence X-ray diffraction and X-ray reflectivity study. Soft Matter 2008, 4, (8), 1665-1674.
[108] Kent, M. S.; Yim, H.; Sasaki, D. Y.; Satija, S.; Seo, Y. S.; Majewski, J., Adsorption of myoglobin to Cu(II)-IDA and Ni(II)-IDA functionalized Langmuir monolayers: Study of the protein layer structure during the adsorption process by neutron and X-ray reflectivity. Langmuir 2005, 21, (15), 6815-6824.
[109] Börner, H. G.; Schlaad, H., Bioinspired functional block copolymers. Soft Matter 2007, (3), 394–408.
[110] Xu, T.; Shu, J., Coiled-coil helix bundle, a peptide tertiary structural motif toward hybrid functional materials. Soft Matter 2010, 6, (2), 212-217.
[111] Bigioni, T. P.; Lin, X.-M.; Nguyen, T. T.; Corwin, E. I.; Witten, T. A.; Jaeger, H. M., Kinetically driven self assembly of highly ordered nanoparticle monolayers. Nature materials 2006, 5, (4), 265-270
[112] Garbin, V.; Jenkins, I.; Sinno, T.; Crocker, J. C.; Stebe, K. J., Interactions and Stress Relaxation in Monolayers of Soft Nanoparticles at Fluid-Fluid Interfaces. Physical review letters 2015, 114, (10), 108301.
[113] Lu, A. H.; Salabas, E. e. L.; Schüth, F., Magnetic nanoparticles: synthesis, protection, functionalization, and application. Angewandte Chemie International Edition 2007, 46, (8), 1222-1244.
[114] Shipway, A. N.; Katz, E.; Willner, I., Nanoparticle arrays on surfaces for electronic, optical, and sensor applications. ChemPhysChem 2000, 1, (1), 18-52.
[115] Botto, L.; Lewandowski, E. P.; Cavallaro, M.; Stebe, K. J., Capillary interactions between anisotropic particles. Soft Matter 2012, 8, (39), 9957-9971.
[116] Bresme, F.; Oettel, M., Nanoparticles at fluid interfaces. Journal of Physics: Condensed Matter 2007, 19, (41), 413101.
[117] Oettel, M.; Dietrich, S., Colloidal interactions at fluid interfaces. Langmuir 2008, 24, (4), 1425-1441.
[118] Bera, M. K.; Chan, H.; Moyano, D. F.; Yu, H.; Tatur, S.; Amoanu, D.; Bu, W.; Rotello, V. M.; Meron, M.; Kral, P.; Lin, B.; Schlossman, M. L., Interfacial transport and voltage-tunable arrays of charged nanoparticles. Nano Letters 2014, 14, 6816-6822.
[119] Halas, N. J.; Lal, S.; Chang, W.-S.; Link, S.; Nordlander, P., Plasmons in Strongly Coupled Metallic Nanostructures. Chem. Rev. 2011, 111, 3913-3961.
[120] Nykypanchuk, D.; Maye, M. M.; Lelie, D. v. d.; Gang, O., DNA-guided crystallization of colloidal nanoparticles. Nature 2008, 451, 549-552.
[121] Vial, S.; Nykypancuk, D.; Yager, D. G.; Tkachenko, A. V.; Gang, O., Linear mesostructures in DNA-nanorod self-assembly. ACS Nano 2013, 7, 5437.
[122] Tian, Y.; Wang, T.; Liu, W.; Xin, H. L.; Li, H.; Ke, Y.; Shih, W. M.; Gang, O., Prescribed nanoparticle cluster architectures and low-dimensional arrays built using octahedral DNA origami frames. Nature Nanotechnology 2015, 10, 637–644.
[123] Srivastava, S.; Nykypanchuk, D.; Fukuto, M.; Gang, O., Tunable nanoparticle arrays at charged interfaces. ACS Nano 2014, 10, 9857-9866.
[124] Srivastava, S.; Nykypanchuk, D.; Fukuto, M.; Halverson, J. D.; Tkachenko, A. V.; Yager, K. G.; Gang, O., Two-Dimensional DNA-Programmable Assembly of Nanoparticles at Liquid Interfaces. J. Am. Chem. Soc. 2014, 136, 8323
[125] Zhang, Y.; Srinivasan, B.; Vo, T.; Pal, S.; Kumar, S.; Gang, O., Selective Re-Programming Transforms Nanoparticle Superlattices. Nature Materials 2015, 14, 840-847.

[126] Lu, F.; Yager, K. G.; Zhang, Y.; Xin, H.; Gang, O., Superlattices assembled through shape-induced directional binding. Nature Communications 2015, 6, 6912.
[127] Maye, M. M.; Nykypanchuk, D.; Cusiner, M.; Lelie, D. v. d.; Gang, O., Stepwise surface encoding for high-throughput assembly of nanoclusters. Nature Materials 2009, 8, 388.
[128] Fukuto, M., Yang, L., Nykypanchuk, D. & Kuzmenko, I. , Transmission X-ray scattering as a probe for complex liquid-surface structures. J. Synchrotron Rad. (in press) 2016, 23.
[129] Wan, J.; Li, Y.; Ulbrandt, J. G.; Smilgies, D.-M.; Hollin, J.; Whalley, A. C.; Headrick, R. L., Transient phases during fast crystallization of organic thin films from solution. APL Materials 2016, 4, (1), 016103.
[130] Bae, S.; Kim, H.; Lee, Y.; Xu, X.; Park, J.-S.; Zheng, Y.; Balakrishnan, J.; Lei, T.; Kim, H. R.; Song, Y. I., Roll-to-roll production of 30-inch graphene films for transparent electrodes. Nature nanotechnology 2010, 5, (8), 574-578.
[131] Carlson, S. Innovative Manufacturing and Materials 1314 for Low-Cost Lithium-Ion Batteries, 1315; Optodot Corporation, 2012.
[132] Oakes, L.; Hanken, T.; Carter, R.; Yates, W.; Pint, C. L., Roll-to-Roll Nanomanufacturing of Hybrid Nanostructures for Energy Storage Device Design. ACS Applied Materials & Interfaces 2015, 7, (26), 14201-14210.
[133] Søndergaard, R.; Hösel, M.; Angmo, D.; Larsen-Olsen, T. T.; Krebs, F. C., Roll-to-roll fabrication of polymer solar cells. Materials Today 2012, 15, (1), 36-49
[134] Vig, A. L.; Mäkelä, T.; Majander, P.; Lambertini, V.; Ahopelto, J.; Kristensen, A., Roll-to-roll fabricated lab-on-a-chip devices. Journal of Micromechanics and Microengineering 2011, 21, (3), 035006
[135] Gu, X.; Reinspach, J. A.; Worfolk, B. J.; Diao, Y.; Zhou, Y.; Yan, H.; Gu, K.; Mannsfeld, S.; Toney, M. F.; Bao, Z., A compact roll-to-roll coater for in situ X-ray diffraction characterization of organic electronics printing. ACS Applied Materials & Interfaces 2015, 1944-8244.
[136] Chai, J.; Wang, D.; Fan, X.; Buriak, J. M., Assembly of aligned linear metallic patterns on silicon. Nat Nanotechnol 2007, 2, (8), 500-6.
[137] Varghese, J.; Ghoshal, T.; Deepak, N.; O'Regan, C.; Whatmore, R. W.; Morris, M. A.; Holmes, J. D., Fabrication of Arrays of Lead Zirconate Titanate (PZT) Nanodots via Block Copolymer Self-Assembly. Chemistry of Materials 2013, 25, (8), 1458-1463.
[138] Xu, J.; Hong, S. W.; Gu, W.; Lee, K. Y.; Kuo, D. S.; Xiao, S.; Russell, T. P., Fabrication of silicon oxide nanodots with an areal density beyond 1 teradots inch^{-2}. Advanced Materials 2011, 23, (48), 5755-5761.
[139] Thurn-Albrecht, T.; Schotter, J.; Kästle, G. A.; Emley, N.; Shibauchi, T.; Krusin-Elbaum, L.; Guarini, K.; Black, C. T.; Tuominen, M. T.; Russell, T. P., Ultrahigh-density nanowire arrays grown in self-assembled diblock copolymer templates. Science 2000, 290, (5499), 2126-2129.
[140] Xiao, S.; Yang, X.; Lee, K. Y.; Ver der Veerdonk, R. J. M.; Kuo, D.; Russell, T. P., Aligned nanowires and nanodots by directed block copolymer assembly. Nanotechnology 2011, 22, (30), 305302
[141] Hahn, J.; Filiz, V.; Rangou, S.; Clodt, J.; Jung, A.; Buhr, K.; Abetz, C.; Abetz, V., Structure formation of integral-asymmetric membranes of polystyrene-block-Poly (ethylene oxide). Journal of Polymer Science Part B: Polymer Physics 2013, 51, (4), 281-290.
[142] Lei, L.; Xia, Y.; Chen, X.; Shi, S., Long-range-ordered, hexagonally packed nanoporous membranes from degradable-block-containing diblock copolymer film templates. Journal of Applied Polymer Science 2014, 131, 1097-4628.

[143] Fang, Z.; Zhu, X., Plasmonics in nanostructures. Advanced Materials 2013, 25, (28), 3840-3856
[144] Naik, G. V.; Shalaev, V. M.; Boltasseva, A., Alternative plasmonic materials: beyond gold and silver. Advanced Materials 2013, 25, (24), 3264-3294.
[145] Wang, H.; Newstein, M. C.; Krishnan, A.; Balsara, N. P.; Garetz, B. A.; Hammouda, B.; Krishnamoorti, R., Ordering kinetics and alignment of block copolymer lamellae under shear flow. Macromolecules 1999, 32, (11), 3695-3711.
[146] Zhang, R.; Lee, B.; Bockstaller, M. R.; Al-Enizi, A. M.; Elzatahry, A.; Berry, B.; Karim, A., Soft-Shear Induced Phase-Separated Nanoparticle String-Structures in Polymer Thin Films. Faraday Discussions 2015.
[147] Bita, I.; Yang, J. K. W.; Jung, Y. S.; Ross, C. A.; Thomas, E. L.; Berggren, K. K., Graphoepitaxy of self-assembled block copolymers on two-dimensional periodic patterned templates. Science 2008, 321, (5891), 939-943
[148] Xu, J.; Park, S.; Wang, S.; Russell, T. P.; Ocko, B. M.; Checco, A., Directed Self-Assembly of Block Copolymers on Two-Dimensional Chemical Patterns Fabricated by Electro-Oxidation Nanolithography. Advanced Materials 2010, 22, (20), 2268-2272
[149] Modi, A.; Bhaway, S. M.; Vogt, B. D.; Douglas, J. F.; Al-Enizi, A.; Elzatahry, A.; Sharma, A.; Karim, A., Direct Immersion Annealing of Thin Block Copolymer Films. ACS Appl Mater Interfaces 2015, 7, (39), 21639-45.
[150] Cakmak, M.; Batra, S.; Yalcin, B., Field assisted self-assembly for preferential through thickness ("z-direction") alignment of particles and phases by electric, magnetic, and thermal fields using a novel roll-to-roll processing line. Polymer Engineering & Science 2015, 55, (1), 34-46
[151] Singh, G.; Batra, S.; Zhang, R.; Yuan, H.; Yager, K. G.; Cakmak, M.; Berry, B.; Karim, A., Large-scale roll-to-roll fabrication of vertically oriented block copolymer thin films. ACS Nano 2013, 7, (6), 5291-5299
[152] Park, S.; Lee, D. H.; Xu, J.; Kim, B.; Hong, S. W.; Jeong, U.; Xu, T.; Russell, T. P., Macroscopic 10-terabit–per–square-inch arrays from block copolymers with lateral order. Science 2009, 323, (5917), 1030-1033.
[153] Hösel, M.; Dam, H. F.; Krebs, F. C., Development of Lab-to-Fab Production Equipment Across Several Length Scales for Printed Energy Technologies, Including Solar Cells. Energy Technology 2015, 3, (4), 293-304.
[154] Wo, S.; Headrick, R. L.; Anthony, J. E., Fabrication and characterization of controllable grain boundary arrays in solution-processed small molecule organic semiconductor films. Journal of Applied Physics 2012, 111, (7), 073716
[155] Ro, H. W.; Downing, J.; Engmann, S.; Herzing, A. A.; DeLongchamp, D. M.; Richter, L. J.; Mukherjee, S.; Ade, H.; Abdelsamie, M.; Jagadamma, L. K.; Amassiana, A.; Liu, Y.; Yanr, H., 2016 (manuscript in preparation).
[156] Xiong Gong, private communication.
[157] Huang, S. H.; Liu, P.; Mokasdar, A.; Hou, L., Additive manufacturing and its societal impact: a literature review. The International Journal of Advanced Manufacturing Technology 2013, 67, (5-8), 1191-1203.
[158] Gibson, I.; Rosen, D. W.; Stucker, B., Additive Manufacturing Technologies. Springer: 2010.
[159] Kruth, J. P.; Leu, M.-C.; Nakagawa, T., Progress in additive manufacturing and rapid prototyping. CIRP Annals-Manufacturing Technology 1998, 47, (2), 525-540
[160] Giannatsis, J.; Dedoussis, V., Additive fabrication technologies applied to medicine and health care: a review. The International Journal of Advanced Manufacturing Technology 2009, 40, (1-2), 116-127

[161] Studart, A. R., Additive manufacturing of biologically-inspired materials. Chem Soc Rev 2016, 45, (2), 359-76.

Appendix 2: PLS Beamline Dictionary

(1) PPLS.01 Management and Support
Performance of management and support activities, including labor, materials, travel, and fixed costs associated with management and support functions, consisting of construction management, reviews, administrative support, ESH, QA, configuration management, business operations, project controls, procurement, and document control.

(2) PPLS.03 Beamline Construction
   (a) PPLS.03.01 Photon Delivery System
   Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of photon delivery sub-systems and integrated system. These include the beamline optical systems upstream of the endstation (including their housings, supports, and manipulation systems), apertures and beam definition and conditioning systems, beam diagnostic/visualization systems, beam transport system, vacuum system, cooling/heating and temperature stabilization systems associated with photon delivery system components, and shielding systems (exclusive of radiological enclosures) that include collimators, masks, shutters, and beam stops.
   (b) PPLS.03.03 Endstation System
   Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of endstation sub-systems and integrated system. These include sample housings, environments, visualization, and support and manipulation systems, detection systems, optical systems and beam diagnostic/visualization and conditioning/definition/deflection components just before the sample (e.g. on the same support as the sample or contiguous with it) or between the sample and detector (e.g. crystal/grating/mirror-based analyzer or spectrometer system) including their housings, supports, and manipulation systems, vacuum system, and cooling/heating and temperature stabilization systems associated with endstation components.

(3) PPLS.04 Beamline Infrastructure
   (a) PPLS.04.02 Mechanical Utilities
   Design, specification, procurement, fabrication, assembly, installation, and testing of beamline mechanical utilities including equipment racks, DI water, process chilled water, gaseous nitrogen, compressed air, exhaust, and liquid nitrogen distribution systems.
   (b) PPLS.04.03 Electrical Utilities
   Design, specification, procurement, fabrication, assembly, installation, and testing of beamline electrical utilities including circuit breaker panels, provisioning of power to equipment racks, and cable trays and conduits.
   (c) PPLS.04.04 Equipment Protection System

Design, specification, procurement, fabrication, assembly, installation, and testing of Equipment Protection System (EPS) including PLC, wiring, and custom sensors.

(d) PPLS.04.05 Personnel Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Personnel Protection System (PPS) including PLC, wiring, switches, locks, special interlocked personnel protective safeguards such as gates and light screens, and Human Machine Interface (HMI) panel.

(4) PPLS.05 Accelerator Infrastructure

(a) PPLS.05.02 Source
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of radiation source and associated hardware. Magnetic measurements are included. The necessary utilities, protection systems, and controls for the source are included.

(5) PPLS.06 Beamline Controls

(a) PPLS.06.01 Basic System Controls
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation control systems. These include operator consoles for control and archive of control equipment, network routers, gateway to the machine control system, timing IOC to synchronize to the machine timing, motor controllers and associated cabling, serial to Ethernet hubs, and a soft IOC for controlling all Ethernet-based motors, serial devices, and PLCs. Ethernet and timing cables are also included.

(b) PPLS.06.02 Instrument Applications
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation instrument control applications. These include experimental control workstations, data storage and computation equipment, experimental control software and servers, and data acquisition equipment and software including for detectors.

Appendix 3: PLS Equipment Cost Estimate (Direct K$) and Basis of Estimate

Undulator (1.5 m long IVU21)		1040	Hitachi quote
Beamline Construction			
	white beam slits	100	SMI cost / prof judg
	monochromator plus cryocooling system	600	Cinel quote
	mirrors and SSA and vacuum items	1500	Cinel quote
	beam monitors	50	cat items
Endstation Construction			
	CRL system	200	JJ X-Ray quote
	four-stage spectrometer system	850	Huber quote
	flight path systems and vibration isolation	50	prof judg
	2 PILATUS 1M detectors	520	Dectris quote
	silicon drift detector system	25	cat item
	ancillary items	25	prof judg
Beamline Infrastructure Hardware		60	bot-up est
Beamline Control Systems Hardware		160	bot-up est
Total		**5180**	

Appendix 4: PLS Labor Estimate (Person-Years and Hours), Basis of Estimate, and Schedule with Major Activities

	Year 1	Year 2	Year 3	Total	Basis of Estimate
beamline and endstation construction major activities:	design	design, procurement, fabrication	procurement, fabrication, assembly, installation, testing	person-years	
scientist / assistant sci	1.25	1.25	1.5	4	beamline project exp
mech / vac engineer	1	0.75	0.75	2.5	beamline project exp
mech designer	0.5	0.375	0.375	1.25	beamline project exp
mech / vac technician	0	0	1	1	beamline project exp
Total				8.75 person-years or 15,400 hrs	

Additional Labor Required:

Project management: 1,600 hrs scientist
Project support: to be determined, requires clarification
Labor for insertion device: still being tallied
Trades labor for BL constr (riggers, carpenters, masons, and surveyors): still being tallied
Labor for beamline infrastructure: 1,400 hrs (engineer, technician, trades; bot-up deter)
Labor for beamline controls: 4,400 hrs (controls engineer, technician; bot-up determine)

Total Labor Required: 22,800 hrs or 13 person-years plus additional hrs still being tallied

Travel Budget Required: still being determined

Schedule Cartoon

	Year 1	Year 2	Year 3
Design			
Procurement			
Fabrication			
Assembly			
Installation			
Testing			

Project: PLS Beamline — RESOURCE DETAIL

WBS	RESOURCE	UNITS	COST
P_PLS - PLS Beamline			
P_PLS.01 - PLS Management			
LABOR	Labor_Scientist_NS1	1,584.00	$ 236,470.72
	Labor_Administrative Secretary_NA3	528.00	$ 29,527.25
	Labor_ES&H Professional_NA4	792.00	$ 93,658.39
	Labor_QA Professional_NA5	528.00	$ 58,460.98
	Labor_Administrative_NA2	1,004.00	$ 75,533.78
	Labor_Human Resources_NB4	264.00	$ 19,861.47
	LABOR TOTAL	4,700.00	$ 513,512.60
MATERIAL	Material_Material (Purchase <$25k)_NMA	75,000.00	$ 98,172.35
	MATERIAL TOTAL	75,000.00	$ 98,172.35
P_PLS.02 - PLS Design			
P_PLS.02.01 - PLS Conceptual Design			
LABOR	Labor_Scientist_NS1	586.75	$ 83,398.77
	Labor_Mechanical Engineer_NO1	440.00	$ 41,671.89
	Labor_Mechanical Designer_NO2	220.00	$ 17,782.55
	LABOR TOTAL	1,246.75	$ 142,853.21
P_PLS.02.02 - PLS Preliminary Design			
LABOR	Labor_Scientist_NS1	586.75	$ 85,107.13
	Labor_Mechanical Engineer_NO1	440.00	$ 42,063.93
	Labor_Mechanical Designer_NO2	220.00	$ 17,949.84
	LABOR TOTAL	1,246.75	$ 145,120.90
P_PLS.02.03 - PLS Final Design			
LABOR	Labor_Scientist_NS1	586.75	$ 86,885.21
	Labor_Mechanical Engineer_NO1	440.00	$ 42,471.98
	Labor_Mechanical Designer_NO2	220.00	$ 18,123.97
	LABOR TOTAL	1,246.75	$ 147,481.16
P_PLS.03 - PLS Beamline Construction			
P_PLS.03.01 - PLS Photon Delivery System Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	879.75	$ 131,736.63
	Labor_Mechanical Engineer_NO1	880.00	$ 85,787.05
	Labor_Mechanical Designer_NO2	440.00	$ 36,607.71
	Labor_Mechanical Technician_NO3	440.00	$ 34,384.91
	LABOR TOTAL	2,639.75	$ 288,516.30
MATERIAL	Material_Material (Purchase >$25k)_NSM	2,280,000.00	$ 2,854,707.86
	MATERIAL TOTAL	2,280,000.00	$ 2,854,707.86
P_PLS.03.02 - PLS Photon Delivery System Installation and Test			
LABOR	Labor_EL - Vacuum Engineer_SE5	40.00	$ 4,705.30
	Labor_EL - Vacuum Technician_SE6	100.00	$ 8,808.62
	Labor_ME - Survey Engineer_MO1	50.00	$ 5,190.46
	Labor_EL - Survey Technician_SE2	125.00	$ 11,010.77
	Labor_Building Trades Unassigned_NST	18.00	$ 2,345.24
	Labor_Plant Engineering-Building Trades Carpenter_BTC	40.00	$ 4,964.79
	Labor_Plant Engineering-Building Trades Riggers_BTS	100.00	$ 12,411.97
	Labor_Scientist_NS1	440.00	$ 69,051.52
	Labor_Mechanical Engineer_NO1	352.00	$ 35,980.84
	Labor_Mechanical Designer_NO2	176.00	$ 15,354.02
	Labor_Mechanical Technician_NO3	440.00	$ 35,129.48
	LABOR TOTAL	1,881.00	$ 204,953.01
P_PLS.03.03 - PLS End Station Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	2,640.00	$ 402,778.16
	Labor_Mechanical Engineer_NO1	1,320.00	$ 130,819.30
	Labor_Mechanical Designer_NO2	660.00	$ 55,824.21
	Labor_Mechanical Technician_NO3	440.00	$ 34,807.28
	LABOR TOTAL	5,060.00	$ 624,228.96
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,670,000.00	$ 2,163,424.11
	MATERIAL TOTAL	1,670,000.00	$ 2,163,424.11
P_PLS.03.04 - PLS End Station Installation and Test			
LABOR	Labor_Scientist_NS1	1,320.00	$ 209,956.18
	Labor_Mechanical Engineer_NO1	528.00	$ 54,701.19
	Labor_Mechanical Designer_NO2	264.00	$ 23,342.51
	Labor_Mechanical Technician_NO3	440.00	$ 35,604.58
	LABOR TOTAL	2,552.00	$ 323,604.46
P_PLS.04 - PLS Beamline Infrastructure			
P_PLS.04.01 - PLS Hutches			
MATERIAL	Material_Material (Purchase >$25k)_NSM	30,000.00	$ 39,858.04
	MATERIAL TOTAL	30,000.00	$ 39,858.04
P_PLS.04.02 - PLS Mechanical Utilities			
LABOR	Labor_EL - Utility Engineer_SE3	60.00	$ 6,748.70
	Labor_Mechanical Designer_NO2	52.00	$ 4,337.65
	Labor_EL - Utility Technician_SE4	210.00	$ 17,687.58
	Labor_Plant Engineering-Building Trades Carpenter_BTC	4.00	$ 484.30
	Labor_Building Trades Unassigned_NST	16.00	$ 2,033.52
	LABOR TOTAL	342.00	$ 31,291.75
MATERIAL	Material_Material (Purchase <$25k)_NMA	10,000.00	$ 13,091.55
	Material_Material (Purchase >$25k)_NSM	10,000.00	$ 12,563.50

	MATERIAL TOTAL	20,000.00	$ 25,655.05
P_PLS.04.03 - PLS Electrical Utilities			
LABOR	Labor_Electrical Engineer_NE1	36.00	$ 4,049.22
	Labor_Electrical Designer_NE2	24.00	$ 2,121.65
	Labor_Plant Engineering-Building Trades Electrician_BTE	273.00	$ 33,053.44
	LABOR TOTAL	333.00	$ 39,224.31
MATERIAL	Material_Material (Purchase <$25k)_NMA	5,000.00	$ 6,545.78
	MATERIAL TOTAL	5,000.00	$ 6,545.78
P_PLS.04.04 - PLS EPS			
LABOR	Labor_Controls Engineer_NE4	310.00	$ 36,218.02
	Labor_Electrical Technician_NE3	340.00	$ 29,782.52
	Labor_Electrical Designer_NE2	40.00	$ 3,677.52
	LABOR TOTAL	690.00	$ 69,678.06
MATERIAL	Material_Material (Purchase <$25k)_NMA	32,000.00	$ 42,814.62
	MATERIAL TOTAL	32,000.00	$ 42,814.62
P_PLS.05 - PLS Accelerator Infrastructure			
P_PLS.05.02 - PLS Source			
LABOR	Labor_Assistant/Associate Scientist_NS2	630.00	$ 67,777.93
	Labor_EL - Insertion Device Engineer_TE4	950.00	$ 111,699.40
	Labor_ME - Insertion Device Engineer_NO8	360.00	$ 37,576.14
	Labor_Controls Engineer_NE4	1,150.00	$ 135,544.11
	Labor_ME - Survey Engineer_MO1	90.00	$ 9,455.97
	Labor_ME - Insertion Device Technician_NO9	700.00	$ 56,961.49
	Labor_ME - Survey Technician_MO2	170.00	$ 15,239.94
	Labor_Project Engineer_MO7	40.00	$ 4,211.83
	Labor_Electrical Engineer_NE1	340.00	$ 40,290.77
	Labor_ME - Vacuum Engineer_MO5	40.00	$ 4,129.25
	Labor_ME - Vacuum Technician_MO6	320.00	$ 26,188.90
	Labor_ME - Utility Engineer_MO3	80.00	$ 8,423.66
	Labor_ME - Utility Technician_MO4	160.00	$ 13,158.95
	Labor_Electrical Designer_NE2	200.00	$ 18,743.60
	Labor_Electrical Technician_NE3	380.00	$ 34,015.14
	Labor_Mechanical Designer_NO2	80.00	$ 7,217.84
	Labor_Plant Engineering-Building Trades Electrician_BTE	80.00	$ 10,116.86
	Labor_Plant Engineering-Building Trades Riggers_BTS	18.00	$ 2,276.29
	Labor_Building Trades Unassigned_NST	30.00	$ 3,982.47
	LABOR TOTAL	5,818.00	$ 607,010.54
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,040,000.00	$ 1,301,800.18
	MATERIAL TOTAL	1,040,000.00	$ 1,301,800.18
P_PLS.05.03 - PLS Straight			
LABOR	Labor_ME - Vacuum Engineer_MO5	120.00	$ 11,694.44
	Labor_EL - Vacuum Engineer_SE5	90.00	$ 9,870.40
	Labor_EL - Insertion Device Engineer_TE4	40.00	$ 4,326.09
	Labor_ME - Insertion Device Engineer_NO8	60.00	$ 5,786.90
	Labor_ME - Utility Engineer_MO3	80.00	$ 7,756.08
	Labor_ME - Vacuum Technician_MO6	430.00	$ 32,880.03
	Labor_Project Engineer_MO7	10.00	$ 984.59
	Labor_ME - Survey Engineer_MO1	20.00	$ 1,969.18
	Labor_Mechanical Designer_NO2	40.00	$ 3,314.92
	Labor_ME - Utility Technician_MO4	40.00	$ 3,076.14
	Labor_ME - Survey Technician_MO2	40.00	$ 3,356.91
	LABOR TOTAL	970.00	$ 85,015.68
MATERIAL	Material_Material (Purchase >$25k)_NSM	95,000.00	$ 115,652.44
	MATERIAL TOTAL	95,000.00	$ 115,652.44
P_PLS.06 - PLS Controls			
P_PLS.06.01 - PLS Basic System Controls			
LABOR	Labor_Controls Engineer_NE4	1,373.00	$ 155,002.25
	Labor_Electrical Technician_NE3	516.00	$ 43,460.91
	Labor_IT Professional (Software)_NA7	223.00	$ 21,417.86
	LABOR TOTAL	2,112.00	$ 219,881.02
MATERIAL	Material_Material (Purchase <$25k)_NMA	129,800.00	$ 170,538.45
	MATERIAL TOTAL	129,800.00	$ 170,538.45
P_PLS.06.02 - PLS Instrument Applications			
LABOR	Labor_IT Professional (Software)_NA7	1,160.00	$ 111,401.74
	Labor_Assistant/Associate Scientist_NS2	440.00	$ 45,483.97
	Labor_Controls Engineer_NE4	240.00	$ 26,994.80
	Labor_Electrical Technician_NE3	-	$ -
	LABOR TOTAL	1,840.00	$ 183,880.51
MATERIAL	Material_Material (Purchase <$25k)_NMA	30,000.00	$ 39,274.65
	MATERIAL TOTAL	30,000.00	$ 39,274.65

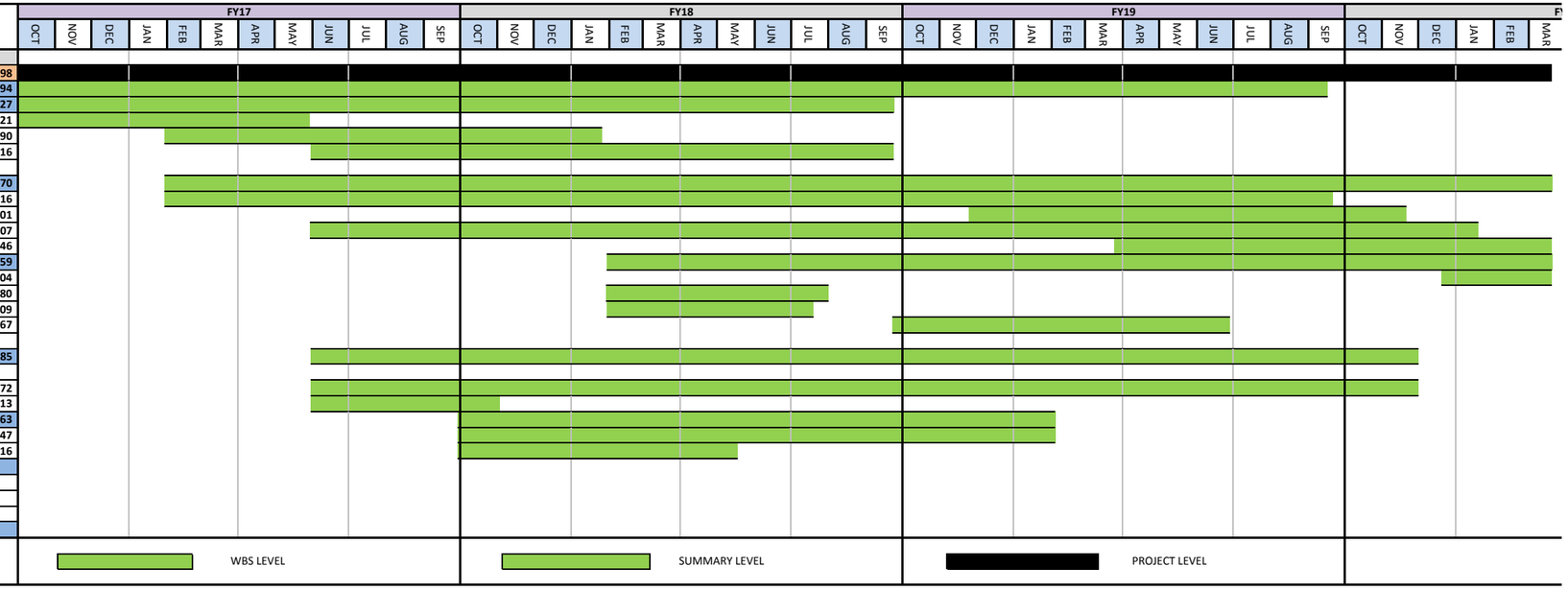
Project: PLS Beamline — RESOURCE SUMMARY

WBS	RESOURCE	UNITS	COST
P_PLS - PLS Beamline			
LABOR	Labor_Scientist_NS1	8,624.00	$ 1,305,384.32
	Labor_Administrative Secretary_NA3	528.00	$ 29,527.25

	Labor_ES&H Professional_NA4	792.00	$	93,658.39
	Labor_QA Professional_NA5	528.00	$	58,460.98
	Labor_Administrative_NA2	1,004.00	$	75,533.78
	Labor_Human Resources_NB4	264.00	$	19,861.47
	Labor_Mechanical Engineer_NO1	4,400.00	$	433,496.18
	Labor_Mechanical Designer_NO2	2,372.00	$	199,855.23
	Labor_Mechanical Technician_NO3	1,760.00	$	139,926.26
	Labor_EL - Vacuum Engineer_SE5	130.00	$	14,575.70
	Labor_EL - Vacuum Technician_SE6	100.00	$	8,808.62
	Labor_ME - Survey Engineer_MO1	160.00	$	16,615.62
	Labor_EL - Survey Technician_SE2	125.00	$	11,010.77
	Labor_Building Trades Unassigned_NST	64.00	$	8,361.23
	Labor_Plant Engineering-Building Trades Carpenter_BTC	44.00	$	5,449.09
	Labor_Plant Engineering-Building Trades Riggers_BTS	118.00	$	14,688.26
	Labor_EL - Utility Engineer_SE3	60.00	$	6,748.70
	Labor_EL - Utility Technician_SE4	210.00	$	17,687.58
	Labor_Electrical Engineer_NE1	376.00	$	44,339.99
	Labor_Electrical Designer_NE2	264.00	$	24,542.77
	Labor_Plant Engineering-Building Trades Electrician_BTE	353.00	$	43,170.31
	Labor_Controls Engineer_NE4	3,073.00	$	353,759.18
	Labor_Electrical Technician_NE3	1,236.00	$	107,258.56
	Labor_Assistant/Associate Scientist_NS2	1,070.00	$	113,261.90
	Labor_EL - Insertion Device Engineer_TE4	990.00	$	116,025.49
	Labor_ME - Insertion Device Engineer_NO8	420.00	$	43,363.04
	Labor_ME - Insertion Device Technician_NO9	700.00	$	56,961.49
	Labor_ME - Survey Technician_MO2	210.00	$	18,596.85
	Labor_Project Engineer_MO7	50.00	$	5,196.42
	Labor_ME - Vacuum Engineer_MO5	160.00	$	15,823.69
	Labor_ME - Vacuum Technician_MO6	750.00	$	59,068.92
	Labor_ME - Utility Engineer_MO3	160.00	$	16,179.74
	Labor_ME - Utility Technician_MO4	200.00	$	16,235.09
	Labor_IT Professional (Software)_NA7	1,383.00	$	132,819.60
	LABOR TOTAL	32,678.00	$	3,626,252.45
MATERIAL	Material_Material (Purchase <$25k)_NMA	281,800.00	$	370,437.39
	Material_Material (Purchase >$25k)_NSM	5,125,000.00	$	6,488,006.14
	MATERIAL TOTAL	5,406,800.00	$	6,858,443.52
		GRAND TOTAL	$	10,484,695.98

Project Name: PLS Beamline

WBS	Start	Finish	Cost
P_PLS - PLS Beamline	10/1/2016	3/19/2020	$ 10,484,695.98
P_PLS.01 - PLS Management	10/1/2016	9/16/2019	$ 611,684.94
P_PLS.02 - PLS Design	10/1/2016	9/23/2018	$ 435,455.27
P_PLS.02.01 - PLS Conceptual Design	10/1/2016	5/29/2017	$ 142,853.21
P_PLS.02.02 - PLS Preliminary Design	1/30/2017	1/25/2018	$ 145,120.90
P_PLS.02.03 - PLS Final Design	5/31/2017	9/23/2018	$ 147,481.16
P_PLS.02.04 - PLS R&D Program			$ -
P_PLS.03 - PLS Beamline Construction	1/30/2017	3/19/2020	$ 6,459,434.70
P_PLS.03.01 - PLS Photon Delivery System Procurement and Fabrication	1/30/2017	9/20/2019	$ 3,143,224.16
P_PLS.03.02 - PLS Photon Delivery System Installation and Test	11/25/2018	11/20/2019	$ 204,953.01
P_PLS.03.03 - PLS End Station Procurement and Fabrication	5/30/2017	1/18/2020	$ 2,787,653.07
P_PLS.03.04 - PLS End Station Installation and Test	3/25/2019	3/19/2020	$ 323,604.46
P_PLS.04 - PLS Beamline Infrastructure	1/30/2018	3/19/2020	$ 255,067.59
P_PLS.04.01 - PLS Hutches	12/20/2019	3/19/2020	$ 39,858.04
P_PLS.04.02 - PLS Mechanical Utilities	1/30/2018	7/31/2018	$ 56,946.80
P_PLS.04.03 - PLS Electrical Utilities	1/30/2018	7/18/2018	$ 45,770.09
P_PLS.04.04 - PLS EPS	9/23/2018	6/27/2019	$ 112,492.67
P_PLS.04.05 - PLS PPS			$ -
P_PLS.05 - PLS Accelerator Infrastructure	5/31/2017	11/30/2019	$ 2,109,478.85
P_PLS.05.01 - PLS Front End			$ -
P_PLS.05.02 - PLS Source	5/31/2017	11/30/2019	$ 1,908,810.72
P_PLS.05.03 - PLS Straight	5/31/2017	11/2/2017	$ 200,668.13
P_PLS.06 - PLS Controls	9/29/2017	2/3/2019	$ 613,574.63
P_PLS.06.01 - PLS Basic System Controls	9/29/2017	2/3/2019	$ 390,419.47
P_PLS.06.02 - PLS Instrument Applications	9/29/2017	5/17/2018	$ 223,155.16
P_PLS.07 - PLS Conventional Facilities			$ -
P_PLS.07.01 - PLS Conventional Facilities Design			$ -
P_PLS.07.02 - PLS Conventional Facilities Construction			$ -
P_PLS.07.03 - PLS Conventional Facilities Commissioning			$ -
P_PLS.08 - PLS Special Equipment			$ -



RATE SET: Rate Set 1

Conceptual design of QIX, V2

J. Dvorak, I. Jarrige, W. Leonhardt, I. Waluyo, A. Hunt, S. Sananayake, S. Wilkins

October 9, 2016

Summary

A conceptual optical design for a RIXS spectrometer to be implemented on the CSX2 beamline is presented. The goal is to provide RIXS capabilities for the study of ambient pressure heterogenous and homogeneous reactive / in operando systems, as well as more conventional solid state samples. The goal is to reach ~10,000 resolving power at 1000 eV along with fast RIXS data acquisition, ~ 1 sec for a 2-dimensional RIXS map over a several eV energy window. This will require an ~8 m long spectrometer.

We propose to extend the current CSX2 beamline in a straight line 13.5 m past the existing first beamline focus, introducing a refocusing KB mirror pair to provide the required focus. We have evaluated a Hettrick-Underwood RIXS spectrometer design, and ascertained that it can meet the resolution goals. The details of the current beamline performance, the conceptual design of the spectrometer, and the costing details related to the beamline and spectrometer hardware are presented.

Although not part of the original scope, the QIX team has identified an opportunity to enhance the ambient pressure photoemission (AP-PES) capabilites at CSX2. In short, the tighter focus provided by the new refocusing mirrors will allow the AP-PES analyzer to operate at higher pressures. We have done a conceptual engineering study and ascertained that it is possible to implement both PES and RIXS capabilites on the same endstation in a time-sharing manner.

Overview

This document is prepared to address the charge of the NSLS-II 2016 Taskforce on Instrument Execution Plan Development (16-IEPD) as it relates to the QIX proposal. The two QIX specific charges to be addressed are:

1. Evaluate the pre-conceptual design of the QIX beamline to refine scope definition and particularly the endstation.
2. Consider incorporating proposed QIX capability (200-2000 eV) at the CSX-2 beamline.

This document will present the overall rational for the proposed buildout of CSX2 to incorporate the QIX spectrometer and an initial conceptual design of the branch line/endstation/spectrometer.

Note: To keep consistent with historical nomenclature, features belonging to CSX1 (coherent branch) are labeled with the letter 'A', features belonging to the existing CSX2 branch (polarization branch) are labeled with the letter 'B'.

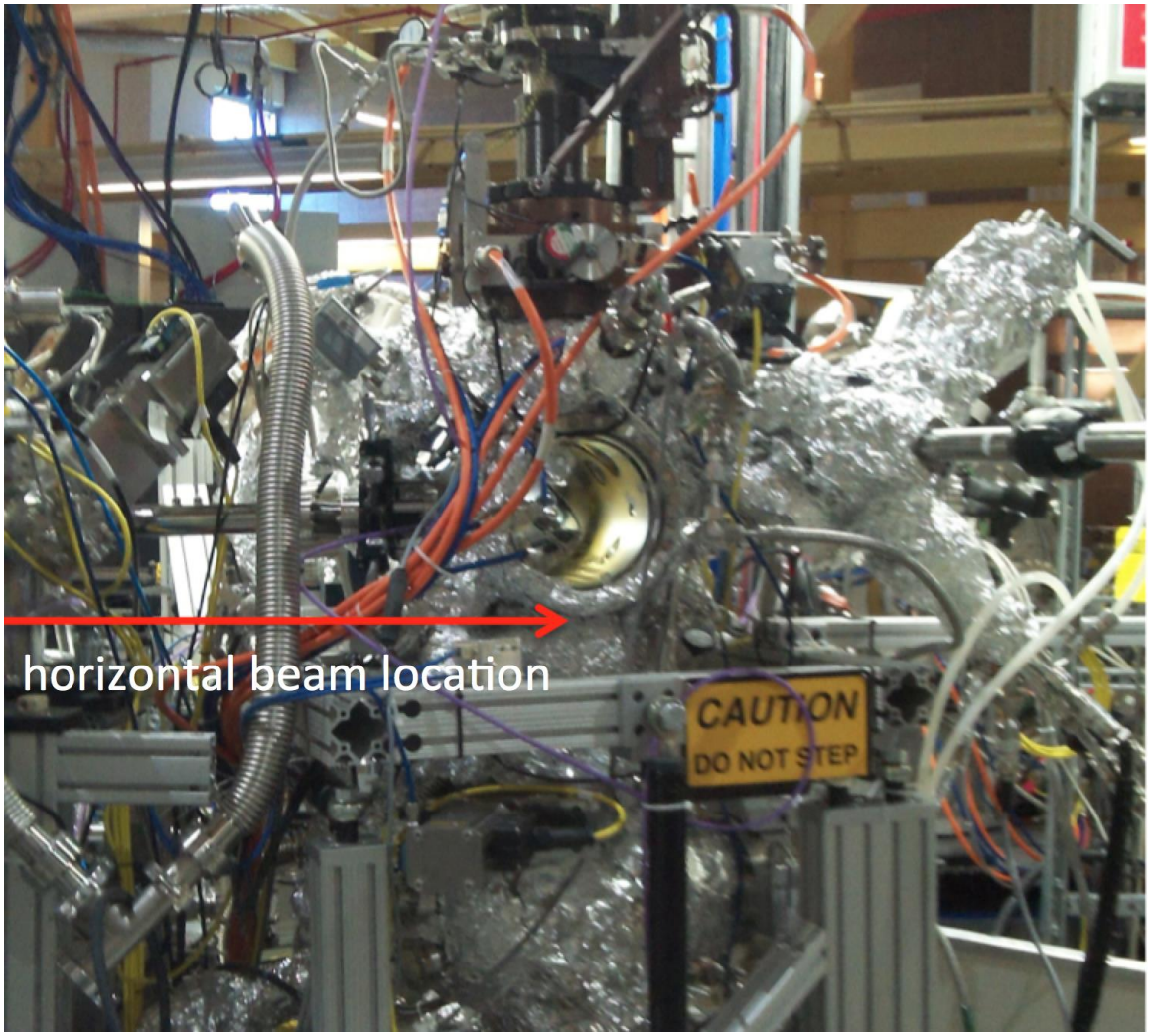
We propose (as required by the charge) to utilize the existing CSX2 optics and mechanics up to and including the monochromator and vertical exit slit, with the possibility of replacing some or all of the current gratings. The current CSX2 beamline will be extended in the same direction to allow a new KB refocusing stage to refocus the beam down to the size required for the QIX endstation. This will be accomplished by lowering the current vertical refocusing mirror, M3B, which provides the focus at the first sample position (currently a NEXAFS chamber and an elevated pressure photoemission endstation), out of the beam path allowing the beam to pass under these endstations undeflected. In this way, from the point of view of the QIX endstation, the first vertical focus of the beam is at the vertical exit slit of the monochromator, and the first horizontal focus is at the first sample focus SF-B1, due to the action of the M1-B1 toroidal mirror. The refocusing KB pair will be designed to work off of these astigmatic foci.

Several factors not mentioned directly in the charge but implied must be considered. Any changes to the monochromator gratings must not limit the operation of the existing CSX2-B branch. The effects of the buildout on the existing CSX2 program as well as the effects of the proposed buildout on the development of the INFINITE beamline must be considered. The possibility of coupling the IR beam from the INFINITE beamline into the QIX endstation is also addressed.

Global considerations: The current optical design of CSX2 allows for the beam from both undulators to be fed to the first sample focus, SF-B1. The two beams follow similar but independent paths through the optical system, eventually overlapping at the sample location SF-B1. In practice, however, this mode is not currently used. A single undulator (the upstream undulator) reflecting off of a single toroid (the upstream toroid, M1-B1) is used so that both CSX1 and 2 can run simultaneously and independently, each using a single undulator. We will design the beamline extension under the assumption that the single undulator mode will be used. Implementing a dual beam capability at the QIX endstation will require the horizontal refocusing mirror to be twice as long and the vertical refocusing mirror to be twice as wide. Furthermore, it will place additional experimental overhead on operations as the two beams must overlap closely in the vertical (within ~5 um) for this mode of operation to work with a RIXS spectrometer without degrading the energy resolution. The need for dual, fast switchable polarization capabilities was not expressed in the science case for the QIX endstation, and due to the extra cost and complications this entails it is not implemented in this conceptual design. This mode of operation will remain possible for the first beamline focus.

The next question that must be addressed is how much to alter the current beamline optical scheme. Currently, the first toroid (M1-B1) collimates the beam in the vertical and focuses the beam in the horizontal at the sample position SF-B1. The grating disperses and focuses the light vertically at the exit slit, and a 1:1 sphere (M3-B) transfers an image of the exit slit to the sample position SFB1 in the vertical. This mirror deflects the beam upwards at 2.5°. This results in a focused beam size of 30 um H x 4.0 um V 1σ (70.5 H x 9.4 V FWHM) as determined by raytracing (see the NSLS-II Project PDR). There is currently no diagnostic located directly at the SFB1 position for verification.

By lowering the vertical refocusing mirror (M3-B) out of the way, the beam can propagate horizontally under the first sample focus. There is then 130 mm clearance between the two beams at the first sample position. A horizontal exit slit would need to be placed at or near this position to allow control of the horizontal source size and stability for the new refocusing stage. This would require the chamber at the first sample position to have a pass through port for the beam, which would require modification of this chamber. We note however that the current location of the ambient pressure photoemission analyzer is not ideal, as the focus at SFB1 position is relatively large and was not initially intended for the location of the ambient pressure photoemission endstation. We have made provisions to incorporate an AP-PES analyzer on the new RIXS spectrometer endstation. If the analyzer is moved to the new location, the difficulty of modifying the existing chamber is eliminated.



The alternative would be to place a horizontal deflection mirror somewhere upstream of the vertical exit slit to allow the beam to be deflected horizontally for a new branch line for the QIX endstation. This is feasible. A 1.5° incident angle off of a plane mirror placed close to the downstream end of the monchromator would allow a 3° beam deflection, which would give ~500 mm horizontal clearance between the SFB1 focus and the branch line. An additional vertical exit slit would be required. This would result in additional reflectivity losses, an additional optical element 'inside' the monochromator which is a potential source of resolution degradation and instabilities, would be more expensive to implement, and would result in a shorter spectrometer to fit in the floor space. We do not recommend this.

These considerations lead to the following assumptions for the incorporation of QIX at CSX2.

1. The single undulator operating mode will be assumed to be the only operating mode. Reason: the QIX proposal has not called for the polarization control afforded by a dual chopped beam operating mode. Implementing this mode would require the refocusing horizontal KB mirror to be longer by a factor of two, and would put additional alignment overhead on the experimental setup.
2. The current mechanics CSX2 optics and mechanics up to the vertical exit slit will be used, with the possibility that some or all of the gratings may need to be replaced. Reason: the

mechanics and optics currently are working and are commissioned, and replacing any of these does not eliminate the need for additional refocusing optics.

3. The beamline will extend directly behind the existing CSX2 branch, enabled by lowering the existing M3-B out of the beampath.

The proposed floor layout is shown in the following figures. The top panel shows an overview of the entire beamline, and how the proposed spectrometer sits in relationship to the adjacent beamline areas and the ratchet wall. There is > 2 m between the detector chamber and the ratchet wall. The lower panel shows a close-up view of the QIX endstation/spectrometer.

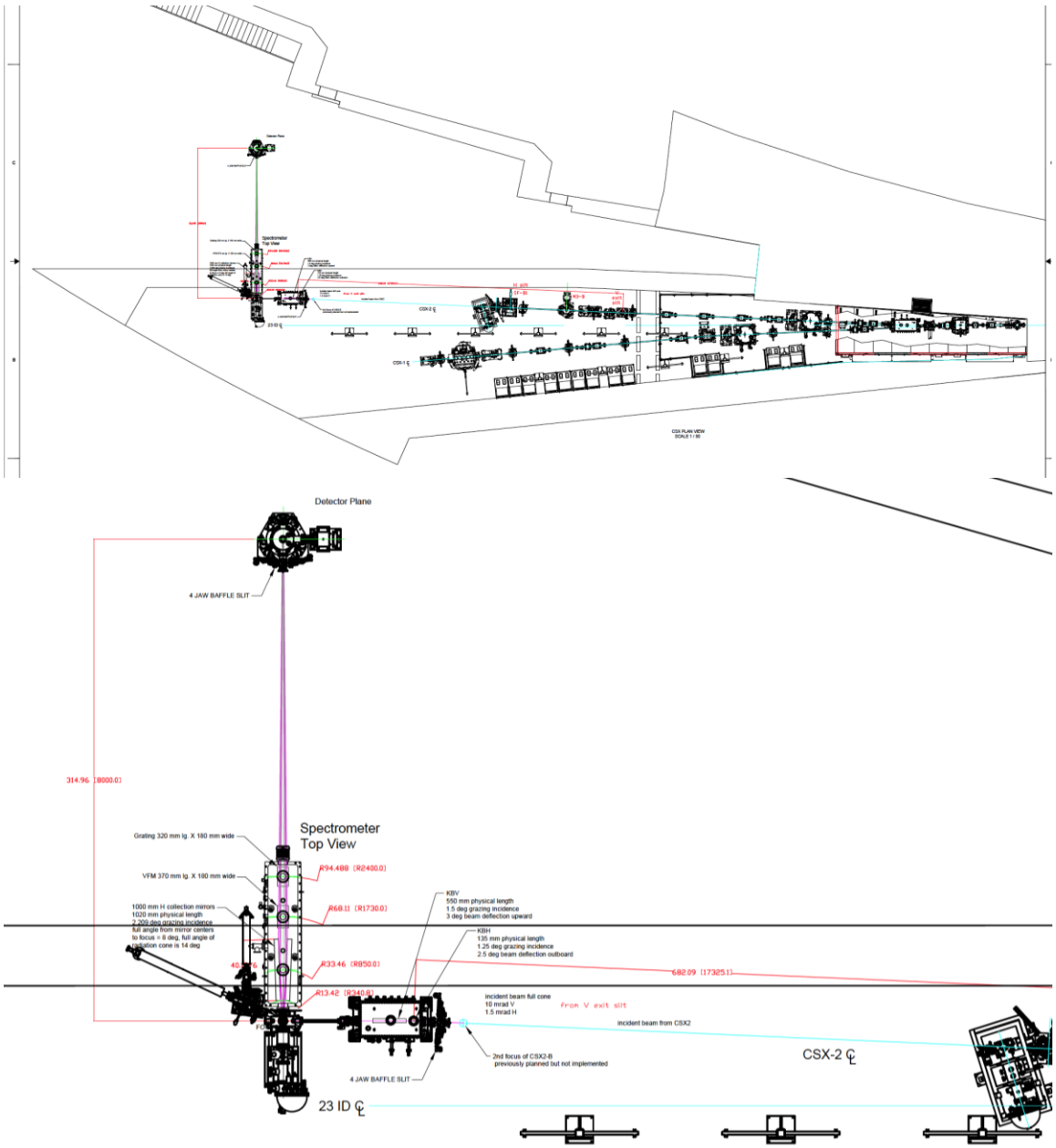


Figure: Floor plan of the QIX conceptual design. The current beamline utilizes M1-B1, the PGM, the vertical exit slit, and M3-B to create a stigmatic focus at the sample location SF-B1. To implement the beamline extension for QIX, the mirror M3-B would be lowered out of the beam path, and the beam would pass underneath the current focus position. An additional horizontal slit, and a KB mirror pair would refocus the beam at SF-B2 location, which would be at the center of the QIX endstation, and act as the source for the spectrometer.

Incorporation of ambient pressure photoemission (AP-PES) capabilities into RIXS endstation: Although this is not part of the original scope of the QIX proposal, the QIX team has identified the potential for an enhancement of the AP-PES capabilities at CSX-2. The current AP-PES spectrometer underperforms in terms of maximum achievable pressure, as it is located at the first sample focus which is larger than ideal. The original plan was to provide a second focus via a KB mirror pair for the AP-PES endstation. This was eliminated at some point during the CSX buildout due to lack of funds. With the implementation of RIXS, the KB mirrors will now exist, and the proposed idea is to combine the two capabilities in the same endstation. It is envisioned that the AP-PES and RIXS experimental modes will operate on a time sharing basis, not concurrently.

In order to ascertain whether this idea is workable, the help of William Leonhardt was enlisted to do a conceptual design of the chamber, to make sure that there is physical space to fit the desired equipment in the crowded area near the sample, and identify any likely geometric constraints. The design goals are listed in the section entitled *RIXS spectrometer.* The following figures illustrate the conceptual design. The main conclusion is that it will be possible to incorporate both RIX and AP-PES capabilities into the same experimental chamber. In addition, we have verified that the required ports for insertion and extraction of the IR beam can be provided in the chamber design.

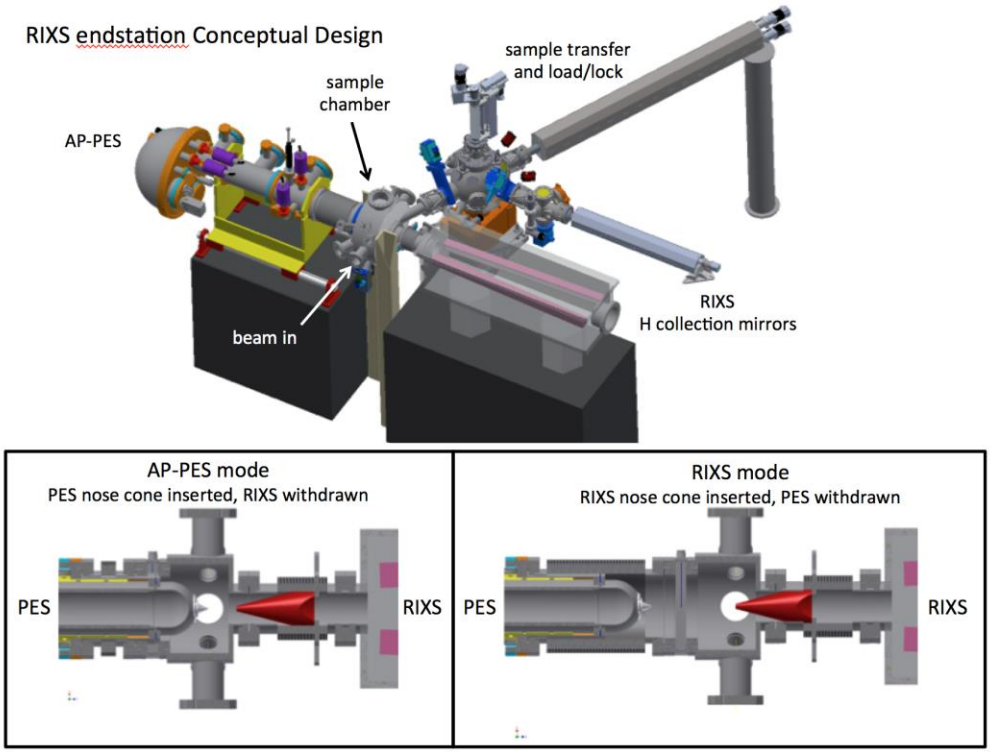


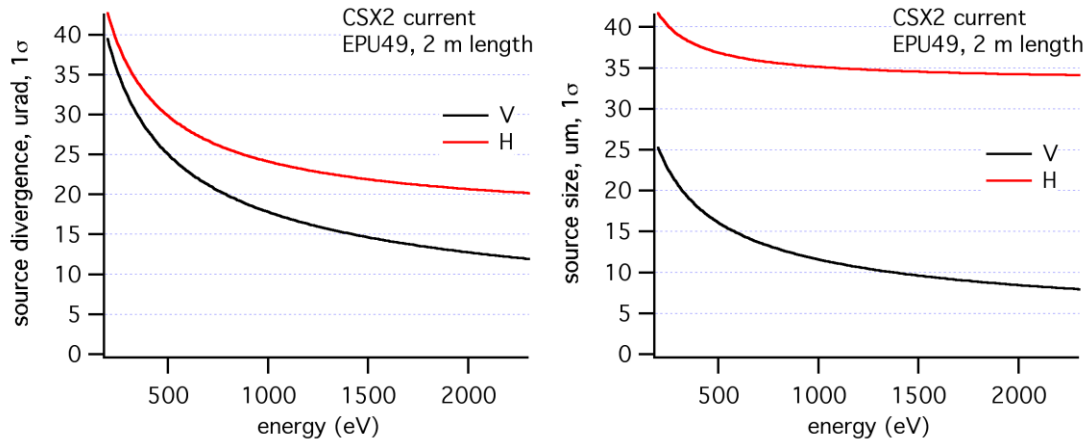
Figure: The conceptual design of the RIXS endstation, incorporating an AP-PES analyzer. The top panel shows a large scale view of the overall endstation. The bottom panels show a cutaway view of the sample chamber showing the two envisioned operating modes. The left panel shows the chamber with the PES nosecone extended close to the sample and the RIXS nosecone withdrawn, and the right panel shows the opposite configuration.

Current (June 2016) CSX2 Optical Design and Performance

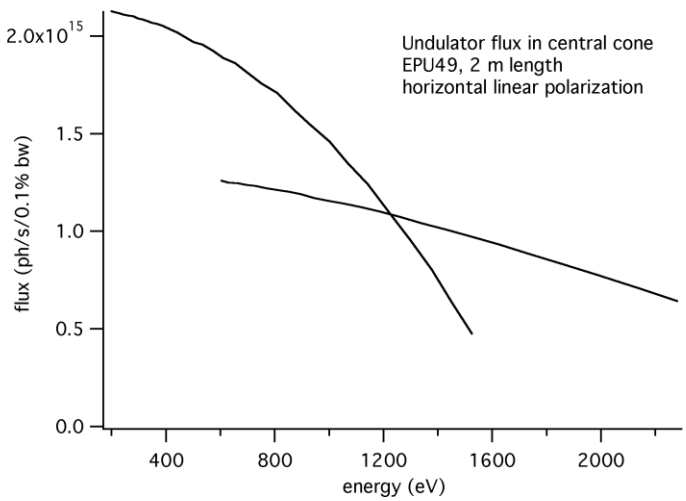
Current CSX2 optical layout				
		nominal distance from center of straight section[1]		
		mm		
upstream undulator	EPU49	-1195		upstream undulator currently used by CSX2 2 m nominal length
downstream undulator	EPU49	+2485		downstream undulator currently used by CSX1 2 m nominal length
M1-B1	toroid	32000	horizontal, inboard deflection θ_{inc} = 88.751° R = 1.173 km ρ = 1.442 m o_V, i_V, f_V = 33077 mm, ∞, 33077 mm o_H, i_H, f_H = 32385 mm, 21122 mm, 12784 mm optical dims: 240 mm x 10 mm tan slope err < 1 urad (0.5 urad preferred) sag slope err < 5 urad	upstream mirror currently used by CSX2 internal water cooled collimates the beam in the vertical focuses the beam at SF-B1 in horizontal actual distance from center of straight = 31878 mm actual distance to source = 33073 mm actual distance to horizontal focus = 21122 mm
M1-B2	toroid	32000	horizontal, inboard deflection θ_{inc} = 88.749° grazing R = 1.151 km ρ = 1.346 m o_V, i_V, f_V = 30826 mm, ∞, 30826 mm o_H, i_H, f_H = 31536 mm, 20887 mm, 12565 mm optical dims: 240 mm x 10 mm tan slope err < 1 urad (0.5 urad preferred) sag slope err < 5 urad	downstream mirror not currently used by CSX2 internal water cooled collimates the beam in the vertical focuses the beam at SF-B1 in horizontal actual distance from center of straight = 32113 mm actual distance to source = 29628 mm actual distance to horizontal focus = 20887 mm
M2-B	plane	~36500	θ_{inc} = varies optical dims: 350 x 30 mm tan slope err <0.2 urad rms sag slope err <2 urad rms	internal water cooled physical size: 400 x 50 x 70 mm
CSX2 gratings	plane VLS	37000	$r_1 = \infty$ r_2 = 10000 mm <u>LEG-P, c=1.5, 140 mm x 20 mm optical</u> a_0 = 150 mm^{-1} a_1 = 0.0540 mm^{-2} a_2 = 8.09x10^{-6} mm^{-3} a_3 = <|1x10^{-8}| mm^{-4} tan slope error < 0.2 urad rms <u>MEG-P, c=1.5, 100 mm x 20 mm optical</u> a_0 = 400 mm^{-1} a_1 = 0.144 mm^{-2} a_2 = 2.2x10^{-5} mm^{-3} a_3 = <|5x10^{-8}| mm^{-4} tan slope error < 0.2 urad rms <u>HEG-P, c=2.2, 100 mm x 20 mm optical</u> a_0 = 1200 mm^{-1} a_1 = 0.3020 mm^{-2} a_2 = 4.5x10^{-5} mm^{-3} a_3 = <|2x10^{-8}| mm^{-4} tan slope error < 0.1 urad rms	beam exits gratings -15 mm relative to beam height in the machine physical dim: 150 mm (l) x 30 mm (w) x 23 mm (h) sag slope err: <0.4 urad rms the VLS parameters were determined at 1000 eV
V exit slit	---	47000		gratings focus in the vertical at this point
M3-B	sphere	50000	vertical, upward deflection θ_{inc} = 88.75 R = 137.5 m o, i , f= 3000 mm, 3000 mm, 1500 mm optical dims: 250 x 20 mm tan slope err: 0.3 urad rms sag slope err: 2 urad rms	1:1 sphere images the exit slit onto the first beamline focus in the vertical.
SF-B1	sample focus	53000	---	beam is focused both horizontally and vertically at this location

[1] PD-CSX-1010 Beamline layout drawing
detailed information on the optics is obtained from the associated procurement documents
values in green are derived from the mirror figure; there is some discrepency between the object distances as determined by the tangential and sagittal figures and those determined from the specifications and drawings.

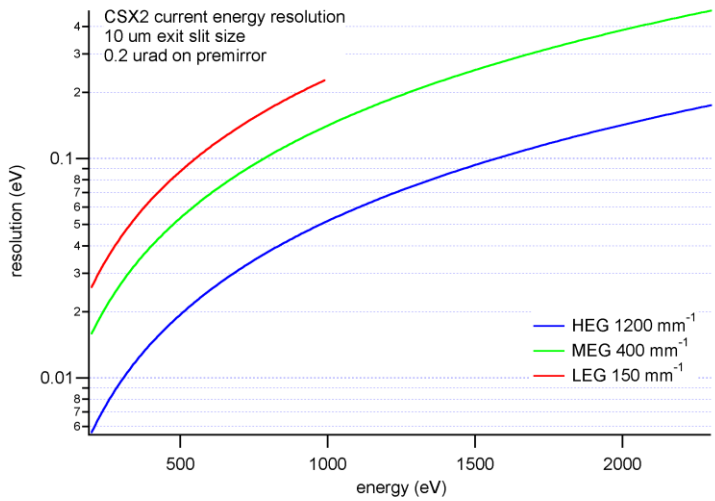
Source: the current source for the CSX2 branch is the upstream undulator. The CSX undulators are 49 mm period EPUs with a nominal length of 2 m. The source size and divergences as a function of energy are shown in the following graph.



The undulator output per 0.1% bandwidth for the flux in the central radiation cone is shown in the following graph.

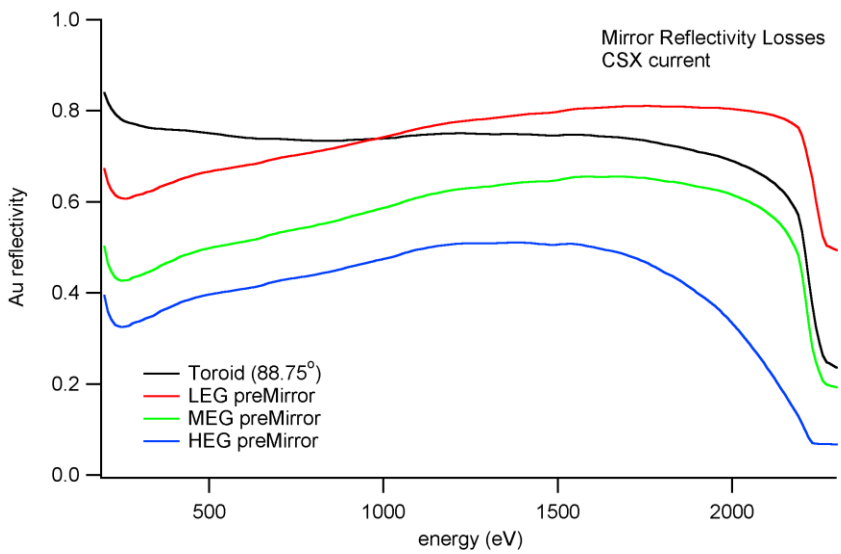


Resolution: the resolution of the beamline has been calculated, including the relevant grating parameters, and including slope error on the premirror and the gratings. The slope error on the premirror is 0.2 urad. The slope error on the toroid has been ignored, as the effective slope error in the vertical direction is less than the premirror. The results are shown in the following plot. The focusing of the monochromator in the vertical is such that the monochromatic spot size at the exit slit is ~10 um FWHM at 200 eV and decreases with increasing energy. The current HEG (1200 mm^{-1}) gives a resolution of 50 meV at 1000 eV, which is reasonably well matched to the target resolution for the beamline (70 meV at 1000 eV).

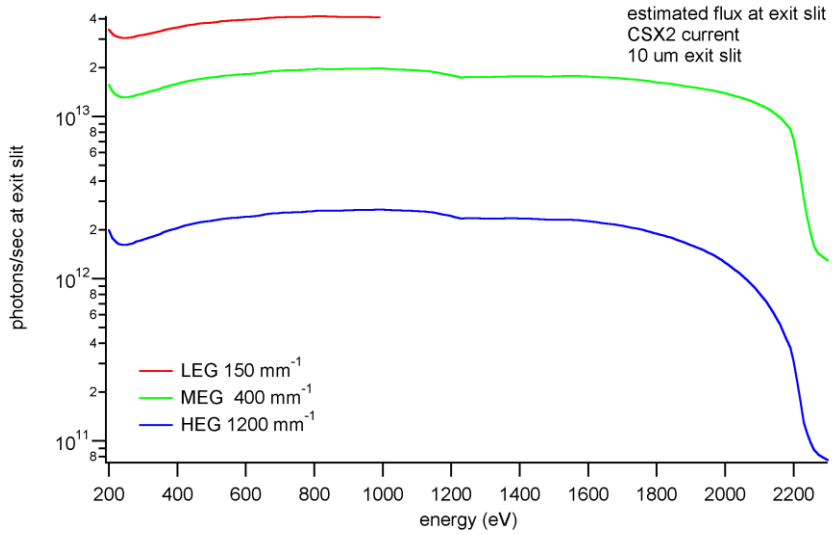


<u>Flux at the exit slit</u>: The estimated flux right after the exit slit is determined by taking the calculated undulator flux, and multiplying it by the reflectivity of the toroid, the premirror, the first order grating efficiency, and correcting for the monochromator bandwidth at 10 um slits. At this level, the grating efficiency is treated very simply, and is taken as independent of angle for a laminar grating (LEG 0.22, MEG 0.22, HEG 0.10). The reflectivity of the mirrors is shown in the following plot.

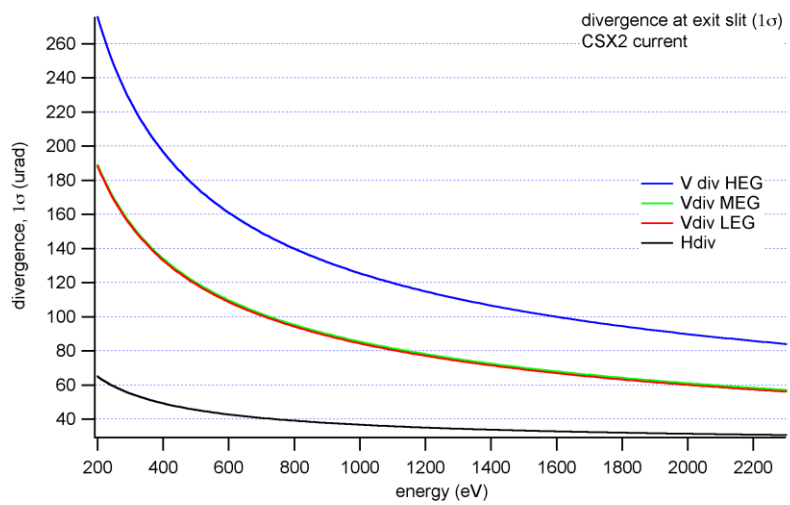
The estimated flux right after the exit slit is shown in the following plot. The flux using the HEG, which has roughly the desired resolution, is approximately 5 times less than for the SIX beamline run at a similar resolution. The reasons are CSX2 has a shorter undulator, and a laminar grating. A



blazed grating with increased efficiency should be considered.



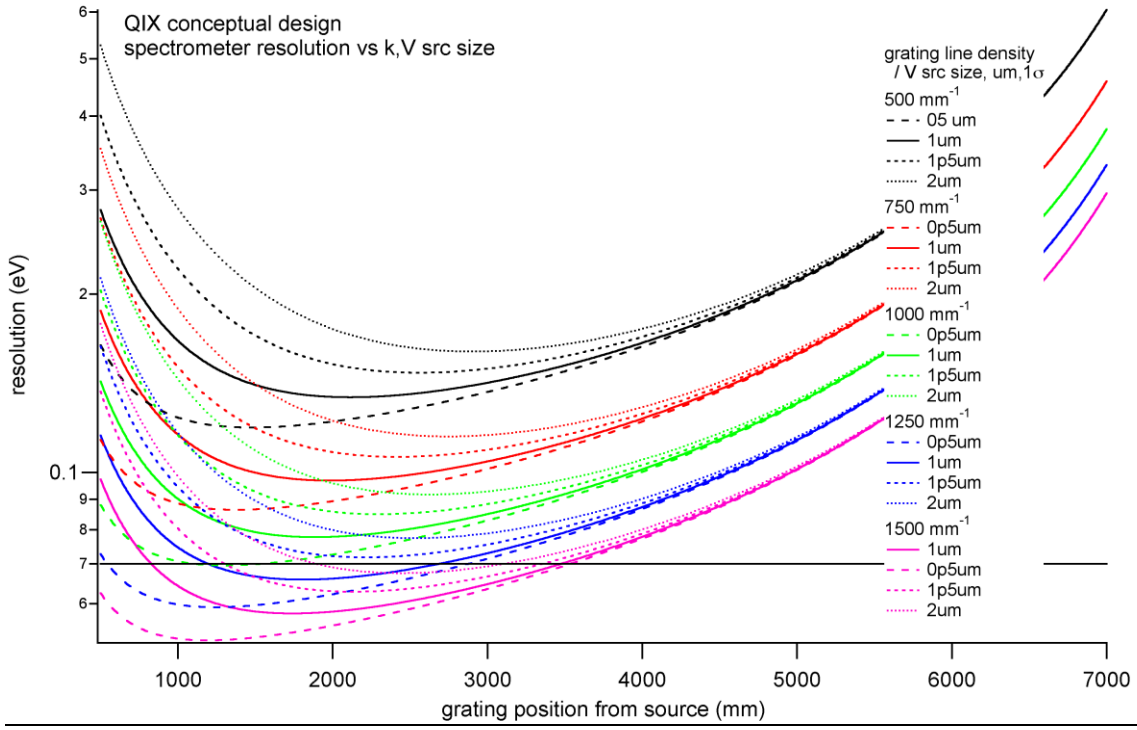
<u>Divergence after the exit slit</u>: To design the KB refocuing mirror pair, it is necessary to know the divergence after the exit slit. This is shown in the following graph.



Conceptual Design of the QIX Beamline

General considerations: To determine what an appropriate focus size for the beamline is, it is necessary to consider how this affects the energy resolution and throughput of the spectrometer. A conceptual layout is shown in Figure 1, showing that at least 8 m is available for the spectrometer. Thus, one can calculate the spectrometer resolution for a given line density on the grating as a function of the spot size. For this calculation, several assumptions are made. It is assumed there is one optic before the grating with a slope error of 0.2 urad rms in the dispersion direction. The slope error on the grating is taken as 0.2 urad rms. The energy is set at 1000 eV. The incident angle on the grating, α, is 88.3°, which represents a reasonable compromise between acceptance and efficiency. The diffraction order is taken as +1, so $c > 1$. The detector is assumed to operate with the incident beam along the normal. A reasonable tradeoff must be found between the focus size, the line density on the grating, and the acceptance and position of the grating. We will assume a detector spatial resolution of 3 um 1σ at 1000 eV.

The following figure shows the results of this analysis. Keeping in mind that sufficient space must be kept for the horizontal collection mirrors (~ 1m in length, extending from ~750 to 1750 mm from the sample) and a possible premirror, the closest the gratings can get to the source is ~2500 mm. The plot contains a fair amount of information. First, as the gratings will be operated in positive first order, and it is easier to make the focus size smaller than the detector resolution, the ideal placement for the grating is closer to the source. What follows from this is that there is little advantage to pushing the vertical focus size to very small, as to take advantage of this the grating must be placed too close to the source. A 1250 mm^{-1} grating placed 2500 mm from the source, with a 1 um 1σ V source size fulfills the resolution criteria of 70 meV at 1000 eV. Keeping the vertical focus size reasonable has other advantages. It is easier to align the mirrors, and it may be possible with a carefully designed visible light optical system to adjust the focus with a YAG screen visually. This analysis gives a basis for the main parameter choices for the beamline refocusing stage and the spectrometer.



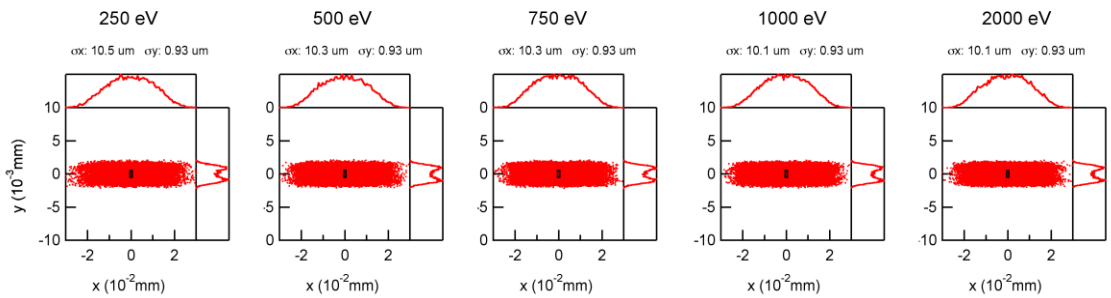
Beamline KB refocusing stage:

In its proposed location, the QIX focus position, SFB2, is 19,500 mm past the V exit slit, and 13,500 mm past the H exit slit.

KBV mirror: This mirror provides the critical vertical focus at the QIX endstation. The effective variance of a square wave is 0.34*full width. The geometric demagnification needed for a 10 um exit slit width (3.4 um variance) is then x3.4 to reach a focus variance of 1 um. However, this puts the mirror ~4.4 m away from the focus, requiring a slope error of 34 nrad on a highly curved ellipse. This is not possible. The solution is to increase the demagnification of the mirror, which puts it closer to the focus, and allows a greater tolerance for the slope error. A reasonable compromise is a demagnification of 10 (o=17730, i=1770 mm) and a slope error of 0.25 urad rms. With these values, the focus size is dominated by the slope error. If we design the mirror to accept 3σ of the radiation at 300 eV, the following results are obtained. The mirror must accept a vertical divergence of 798 urad, which requires a mirror optical length of 648 mm if the incident angle is 88.75°, or 540 mm if the incident angle is 88.5°. The good news is the horizontal divergence of the beam after the H slit is small, and a 5 mm wide mirror will accept more than 4σ of the beam at 250 eV.

KBH mirror: The horizontal beam size at SFB1 is 50 um 1σ at 250 eV, assuming a slope error of 1 urad rms on the toroidal mirror. The horizontal focus is not critical for the energy resolution. The horizontal beam divergence after SFB1 is much less, only 60 urad 1σ at 250 eV. It can be made to accept 4σ of the beam at 250 eV. This can be accomplished with a mirror with a 125 mm long optical length at an incident angle of 88.75°. The mirror optical height should be 20 mm to accept 4σ of the beam at 250 eV. Allowing 10 mm extra on the end of each KB mirror, and 50 mm free space between the two mirrors, means the center of the mirror can be placed 2175 mm from the focus (o=11325, i=2175). The geometric demagnification is 5.2, for a geometric spot size of 9.61 um at 250 eV. A 1 urad slope error would broaden this to 10.5 um 1σ.

The raytracing for the beamline is shown in the following plot. It confirms the expected performance, and shows the energy independent nature of the focus. All slope errors are included on the optics.



Focus at the SF-B2 position. The spot size is 10.3 H x 0.93 V um 1σ and is independent of energy. The double peaked feature in the vertical is an artifact of the way SHADOW treats slope errors. This is not real, and the resulting beam profile will be Gaussian.

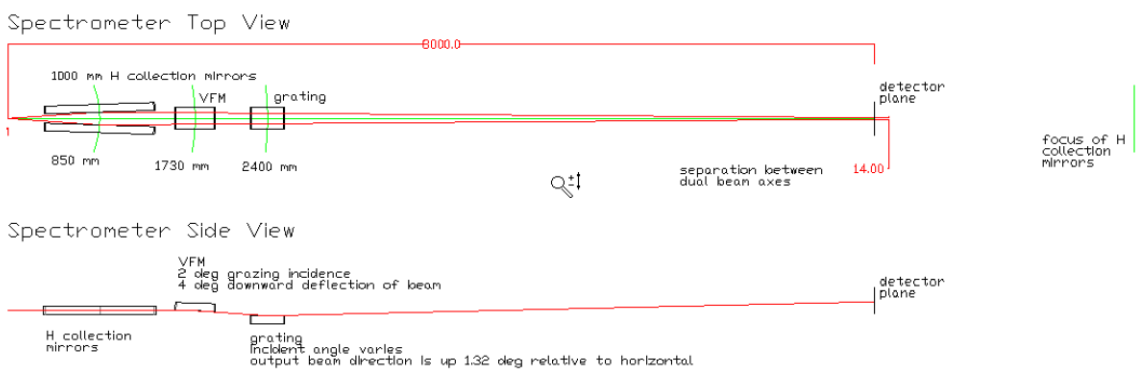
Beamline SHADOW model

	dist from src mm	input/output plane mm	details	notes
source	0	NA	250 eV: 22.6V x 40.1H um 1σ 35.3V x 38.9H urad 1σ 500 eV: 16.1V x 36.9H um 1σ 25.0V x 29.9H urad 1σ 750 eV: 13.3V x 35.7H um 1σ 20.5V x 26.1H urad 1σ 1000 eV: 11.6V x 35.1H um 1σ 17.8V x 24.1H urad 1σ 1500 eV: 9.6V x 34.5H um 1σ 14.6V x 21.9H urad 1σ 2000 eV: 8.4V x 34.2H um 1σ 12.7V x 20.7H urad 1σ	EPU49, 2m length upstream undulator
toroid	33073	input = 33073 output = 4000	horizontal, inboard deflection, orientation=270° θ_{inc} = 88.751° R = 1,182,700 mm ρ = 1442 mm o_V, i_V = 33073 mm, ∞ o_H, i_H = 33073 mm, 21122 mm optical dims: 240 mm x 10 mm tan slope err < 1 urad (0.5 urad preferred) [2.25e-8] sag slope err < 5 urad [1.125e-7]	M1-B1 upstream mirror currently used by CSX2 collimates the beam in the vertical focuses the beam at SF-B1 in horizontal actual distance to source = 33073 mm actual distance to horizontal focus = 21122 mm
plane premirror	37695	input = 622 output = 250	downward deflection, orientation = 270° θ_{inc} = varies @250 eV = 84.8821 @500 eV = 86.3894 @750 eV = 87.0542 @1000 eV = 87.4499 @1500 eV = 87.9186 @2000 eV = 88.1978 optical dims: set to infinite tan slope err <0.2 urad rms [4.5e-9] sag slope err <2 urad rms [4.5e-8]	
VLS gratings	38195	input = 250 output = 10000	upward deflection, orientation = 180° $r_1 = \infty$ r_2 = 10000 mm HEG-P, c=2.2, 100 mm x 20 mm optical a_0 = 1200 mm^{-1} a_1 = 0.3020 mm^{-2} $a_2 = 4.5\times10^{-5}$ mm^{-3} $a_3 = <\|2\times10^{-8}\|$ mm^{-4} tan slope error < 0.1 urad rms [2.25e-9] @250 eV α=86.7936 , β= -82.9705 @500 eV α=87.7432, β= -85.0357 @750 eV α=88.1602, β= -85.9483 @1000 eV α=88.4079, β= -86.4919 @1500 eV α=88.701, β= -87.1362 @2000 eV α=88.8755, β= -87.5202	beam exits gratings -15 mm relative to beam height in the machine sag slope err: <0.4 urad rms [9.0e-9] the VLS parameters were determined at 1000 eV
V exit slit	48195	NA	10 um height nominal	
H exit slit	54195			implemented as a screen on KBH
KBH	65520	input = 17325 output = 205	horizontal, inboard deflection, orientation=90° θ_{inc} = 88.750° R_c = 167278 mm o_H = 11325 mm i_H = 2175 mm optical dims: 125 mm x 20 mm tan slope err < 1 urad [2.25e-8] sag slope err < 2 urad [4.5e-8]	
KBV	65925	input = 200 output = 1770	vertical upward deflection, orientation=90° θ_{inc} = 88.50° R_c = 122959 mm o_V = 17730 mm i_V = 1770 mm optical dims: 540 mm x 5 mm tan slope err < 0.25 urad [5.63e-9] sag slope err < 5 urad [1.125e-7]	
SFB2	67695			

Conceptual Design of QIX Spectrometer

General consideration: The emphasis of this spectrometer is on speed of data acquisition, to enable either fast data acquisition on a large number of samples, or to be able to explore a wide area of parameter space (e.g. temperature, concentration, pressure) for kinetic studies on catalytic or energy conversion systems. The target resolution is 70 meV at 1000 eV, to allow a net resolution of 100 meV at 1000 eV. Within this resolution target, the goal is to maximize throughput. An additional goal is to minimize to mechanical complexity, to allow for quick and reproducible alignment. This can be accomplished with a Hettrick-Underwood optical scheme working in fixed included angle. This scheme is similar, but simpler than the optical design adopted for the SIX spectrometer. However, the SIX spectrometer operates with a variable included angle. This allows the coma to be cancelled at all energies, which is required to obtain the ultrahigh resolution over an extended energy range. However, it requires the detector height to vary over several meters, or an additional plane redirection mirror. Since the target resolution of the QIX spectrometer is a factor of 10 lower, it is possible to operate the spectrometer in fixed included angle, which then fixes the output beam direction and eliminates the need to change the detector height. It is not possible to cancel coma at all energies then, but with a suitable set of gratings the entire energy range can be covered with adequate resolution.

Schematic view of the spectrometer optical scheme.



Horizontal collection mirror: I have allowed for a working distance of 350 mm from the edge of the mirror to the sample position. For a 1000 mm mirror, this puts the center at 850 mm. This mirror will not be exactly collimating. The width of the beam coming off the mirror is ~40 mm wide. If the beam is collimated, the spectrometer will need two 1" wide detectors just to catch the beam from one branch, for a total of 4 detectors. However, if the collection mirror is made to slightly condense the beam, then beam from both branches can illuminate a single detector, and not overlap. Assuming the detector is 8 m from the source, an elliptical mirror with o=850 mm, i=9533 mm will work. The horizontal focus point is then past the detector.

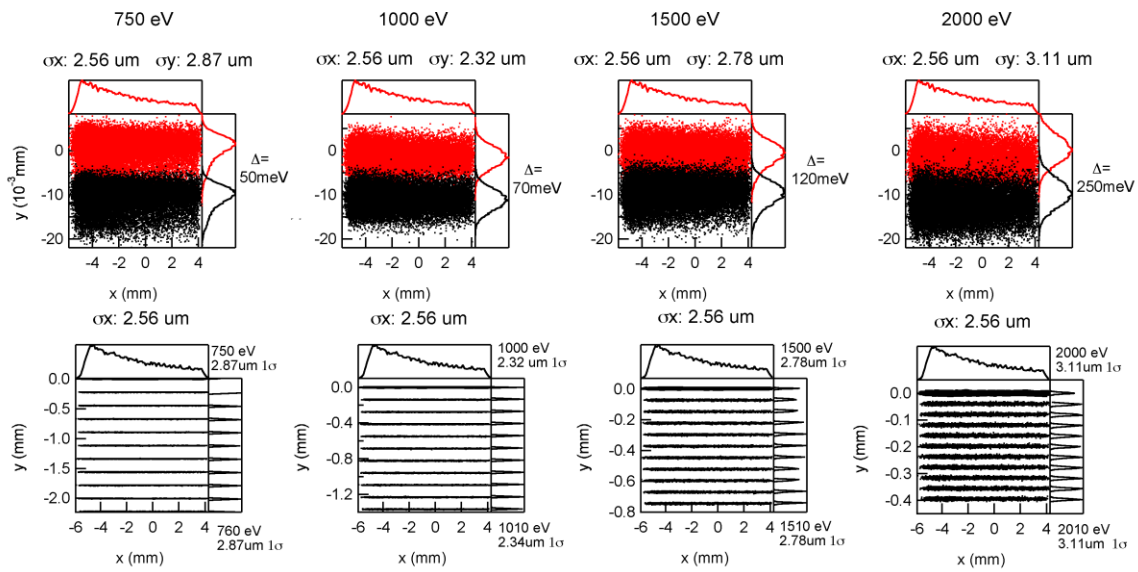
Vertical focusing mirror: The center of this mirror is placed at 1730 mm from the source. For an 8 m long spectrometer, and the grating placed at 2400 mm from the source, the image distance such that |r1|=r2=5600 mm is i=6270.

The spectrometer can accept ~10 mrad in the vertical while keeping the aberrations tolerable. That means this mirror must intercept 17.3 mm of the beam in the vertical. At 88 degrees incident angle, this requires a 500 mm long mirror. This is a long mirror, and would require a similar length grating for the spectrometer to accept all the light. A more reasonable length for the grating is 300 mm. A 300 mm long grating at 88° can accept a 10.5 mm high beam. If the grating is placed at 2400 mm from the source, the VFM must accept 10.5*(6270/5600) = 11.8 mm high beam. At an incident angle

of 88°, the VFM must be 340 mm long. The optical surface must be 160 mm wide to accept the dual beams from the H collection mirrors.

To have the minimum aberrations in the virtual source for the grating, this mirror is taken as an elliptical cylinder. In the final design stage it can be investigated whether a sphercial cylinder will perform adequately.

Gratings: The gratings will be VLS-plane gratings. Because the grating will be working in fixed included angle, it will have a finite range over which it can operate with tolerable aberrations. We have investigated this for a high energy spectrometer grating (HESG), 1250 mm^{-1}, designed to give ~70 meV resolution at 1000 eV. There are two things to consider. The first is how the grating images when the energy is change from the optimal energy, and how the image changes over a 10 eV energy window at a fixed central energy. The results are shown in the following plot.



Imaging properties of a 1250 mm^{-1} grating. The grating parameters are optimized at 1000 eV. The spectrometer vertical acceptance is 10 mrad and the source (sample focus) is 0.93 um 1s in the vertical. The top panels show the image for two closely spaced energies, demonstrating the energy resolution at a given central energy. The bottom panels show the imaging over a 10 eV window at a given central energy. Each panel shows ten 'spots' separated by 1 eV each. Slope errors are included on all the optics.

The HESG grating parameters are optimized at 1000 eV. It performs well from ~1000-2000 eV. As you go lower than 1000 eV, aberrations begin to increase. By 750 eV, the coma is becoming very apparent, indicated by the tails in the vertical image. Thus a single grating can cover about an octave in energy. Three gratings would be required to cover the entire energy range. The resolution of each spectrometer grating should be matched to that of the corresponding beamline grating. The following parameters are chosen:

1. HESG: High energy spectrometer grating, 1250 mm^{-1}, for the 1000-2000 eV energy range with a target resolution of 70 meV at 1000 eV, to be used with the HEG beamline grating (1200 mm-1, ~50 meV at 1000 eV).
2. MESG: Medium energy spectrometer grating, 450 mm^{-1}, for the 500-1000 eV energy range with a target resolution of 70 meV at 500 eV, to be used with the MEG beamline grating (400 mm^{-1}, ~54 meV at 500 eV).
3. LESG: Low energy spectrometer grating, 200 mm^{-1}, for the 200-500 eV energy range with a target resolution of 35 meV at 250 eV, to be used with the LEG beamline grating (150 mm^{-1}, ~35 meV at 250 eV).

The current design calls for a grating that is 300 mm long, operating at 88.3° at the design energy. The gratings must be 160 mm wide to accept the dual beam from the H collection mirrors. In principle, the spectrometer can accept up to 10 mrad in the vertical while keeping aberrations tolerable; thus, up to a 500 mm long grating can be used if one is available, and there is money to purchase it. The length of the vertical focusing mirror must increase proportionately as well.

Spectrometer SHADOW model

	dist from src mm	input/output plane mm	details	notes
source	0	NA	10.3 H x 0.93 V um 1σ spectrometer acceptance to be determined	focus of beamline KB mirrors
H collection mirrors	850	input = 850 output = 500	horizontal, outboard deflection, orientation=90° θ_{inc} = 88.0° R_c = 44730.1 mm o_H, i_H = 850 mm, 9550 mm optical dims: 1000 mm x 15 mm (will need to be wider if multiple stripes) tan slope err < 5 urad [1.125e-7] sag slope err < 1 urad [2.25e-8]	elliptical cylinder, but weakly focusing. purpose is to condense the beam to ~10 mm size at the detector distance between center of dual beams at the detector plane should be 2*6+2 = 14 mm.
vertical focusing mirror	1730	input = 380 output = 335	downward deflection, orientation = 90° elliptical cylinder θ_{inc} = 88° (check SHADOW model) R_c = 77703 mm o_H, i_H = 1730 mm, 6270 mm optical dims: 350 mm long x 160 mm wide tan slope err <0.2 urad rms [4.5e-9] sag slope err <5 urad rms [1.125e-7]	mirror mag = 3.6243
plane-VLS gratings	2400	input = 335 output = 5600	upward deflection, orientation = 180° r_1 = 5600 mm r_2 = 5600 mm substrate optical dims: 300 mm x 160 mm wide <u>HESG (High Energy Spectrometer Grating)</u> a_0 = 1250 mm^{-1} a_1 = 0.445885 mm^{-2} a_2 = 1.19144e-4 mm^{-3} a_3 = 2.8264e-08 mm^{-4} @1000 eV α=88.300, β= -86.3849 @1500 eV α=87.981, β= -86.7041 @2000 eV α=87.821, β= -86.8637 <u>MESG (Medium Energy Spectrometer Grating)</u> a_0 = 450 mm^{-1} @500 eV α=88.300, β= -86.3849 <u>LESG (Low Energy Spectrometer Grating)</u> a_0 = 200 mm^{-1} @250 eV α=88.300, β= -86.3849	tan slope err: <0.1 urad rms [2.25e-9] sag slope err: <0.4 urad rms [9.0e-9] nominal energy range of each grating HESG: 1000-2000 eV MESG: 500-1000 eV LESG: 250-500 eV
detector	8000			

Hardware Cost Estimates

Photon delivery section

The beamline will use the current CSX2 beamline optics and mechanics from the front end up to and including the vertical exit slit of the monochromator, with the following exception:

> The beamline gratings do not provide the highest flux possible. At the time of procurement, the only available gratings were laminar. Currently, blazed gratings are available. During the preliminary design phase, an estimate of the gain in throughput, taking into account harmonic rejection efficiency, should be done to evaluate the advantages of replacing one or several of the beamline gratings. The cost for the ESM gratings was $87,000 per grating, and the cost for the final three gratings for the SIX beamline/spectrometer was $81,000 per grating. Inprentus has quoted $65,000 for the beamline grating. We therefore estimate the cost as $85,000 per grating for the CSX2 monochromator. The estimated delivery is 18 mos. based on ESM delivery time.

After the beamline V exit slit, the proposed scheme is to lower the M3B mirror out of the way and allow the beam to propagate (parallel to the floor) to the endstation. Apart from the usual vacuum hardware (pumps, controllers, beam tube, supports, EPS, ect) the following major items are required.

1. Gas absorption cell for resolution diagnostics for the monochromator. There is already one on the beamline to serve this purpose.
2. High precision horizontal slit. The opening should be controlled by a single drive, and the position by another drive. The nominal H beam size at this location is 71.5 um FWHM. The slit should be motorized and encoded, and the slits themselves isolated with electrical connections for drain current measurement. The slits will go after the monochromator, so heat load should not be an issue. The system should have a retractable fluorescence screen and a viewport for a camera. A chamber for the slit, and a manually adjustable base. The slit itself will be at a nominal height of 1400 mm from the floor. The system does not need to have any travel along the beam direction. FMB Berlin provided a quotation of $57,500, and a delivery time of 22 weeks via email.
3. Beam diagnostics and associated mechanics (Yag crystal, Au wire grid …). Cost is $7000 based on ESM costs.
4. KB mirror mechanics. This item is very similar to the KB mirror mechanics required for the ESM photoemission branch. This contract was awarded to Chinel for $576,800 during April 2014 and completed in 21 months. The contract included the cost of two state of the art optics from JTec (KBH and KBV). These optics were priced separately through JTec at $200,000 for combined. That leaves an estimated $376,800 for the KB mirror mechanics.
5. KB optics (see Optics).
6. Grating substrate and ruling (see Optics).
7. Potential modification to the monochromator sine bar. According to Jochen Deiwiks, FMB Berlin, the following is required. The current plungers in the CSX monochromator (connecting parts between pitch drive unit head and sine arm) can be replaced with an integrated piezo stack of approximately 180 mm unit length. 200 mm maximum may be possible. A strain gauge based measuring system could be added to the piezo units. Tw modified plungers are required. In addition, one or two electrical feedthroughs for connection of the piezo units, the piezo drivers, power supplies, DeltaTau macro interface unit, connectors. This box could be connected to the CSX PGM control box via macro connection (fiber optics). Software is also required, FMB can provide this, providing that the FMB supplied monochromator software has not been modified. The implementation of the voltage applied to the monochromator requires care. It the piezo stack is driven too hard/fast, it will drive considerable vibrations into the monochromator itself. FMB Berlin responded with a budgetary estimate on September 30 quoting $13,750 for just the hardware, excluding the piezo controller, software and

any installation costs. I am using a cost of $50,000 as my professional judgement for the total cost.

Note: A quick survey of commercial stacks shows that approximately 100 um of linear travel is possible with a 100 mm long piezo stack. The sine bar on the CSX monos is ~14'' (355 mm) long, which gives an angular range of 281 urad for 100 um travel. The table shows the achievable energy ranges for a 100 um travel range of the piezo stack. It shows that above 500 eV, a useful energy range can be achieved by scanning a piezo.

eV	disp (eV/rad)	scan range (eV)
250	-5133.64	1.4
500	-14536.5	4.1
1000	-41138.9	11.5
1500	-75590.9	21.2

8. Modifications to existing beamline to allow the beam to pass directly under the current SF-B1 position. The cost for this depends upon the final fate of the photoemission endstation. I use professional judgement to estimate a cost of $20,000 for the construction of a relatively complex new chamber (interior mu-metal shielding is required) if the photoemission capabilities are not transferred to the new RIXS endstation.
9. Required vacuum pumps and associated hardware. These costs are included in the RIXS endstation cost.
10. Beampipes, supports, ect. This is estimated to cost $20,000 based on costs for SIX and ESM.

RIXS spectrometer

A set of preliminary specifications for the RIXS spectrometer and mechanics was written and sent to two companies for evaluation. The specifications, and description of what was to be included in the quotation are listed below. In order to minimize the work for the companies, a basic system was specified. All the additional ancillary equipment required was costed separately by the QIX team and is listed in the next section.

Contacts for pricing:

RI Research Instruments GmBH

Christian Piel: Christian.Piel@research-instruments.de

did a lot of work for the ABBIX beamlines

PreVac

Adam Dziwoki at Prevac: a.dziwoki@prevac.pl

recently did the PEAXIS spectrometer at BESSY

As of September 23, RI has responded with a budgetary quotation for the RIXS endstation/spectrometer. The pricing includes the sample chamber, required chambers and mechanics for the motions of the RIXS optics, the photoemission analyzer, the detector, as well as granite stands. The details were laid out in a specifications document sent to the companies. It does not include 'peripherals', e.g. sample manipulators, reaction cells, load lock system, vacuum pumps, etc. These items have been costed out separately and are listed below. The RI quotation came in at $537,600 (480,000 Eu) with a delivery time of 18 mos.

A disclaimer on the specifications: In order to obtain price quotes on some of the items, a preliminary set of specifications for mechanical motions was listed. These values were based on experience designing similar instruments. In no way are they to be considered final. To determine exact values for these specifications, a detailed analysis of the sensitivity of the performance to the various mechanical motions must be undertaken, and a detailed engineering design must be completed. This is outside the scope of this project.

1. The chamber should be as small as possible on RIXS spectrometer side, to allow the horizontal collection mirrors to be placed as close to the sample as is reasonable, with the constraint that they need to be located outside of the sample chamber. Currently, the conceptual design allows for 340 mm working distance between the upstream end of the mirrors and the sample focus. The requirement that the mirrors be placed outside of the chamber is due to the fact that the inside of the experimental chamber will be exposed to 'dirty' conditions, eg. ambient pressures of reactive gasses and the potential rupture of liquid and gaseous flow cells. There is no requirement that the chamber be symmetrical.
2. A vacuum tight retractable nose cone with two selectable x-ray windows on the spectrometer side is required. One way to achieve this would be to have two windows placed permanently on the nose cone with a small translation selecting either one. This nose cone must be fully removable out of the beam path for experiments on solid state samples under UHV conditions. The spectrometer accepts beam over a 14° (250 mrad) emission cone. A 1 mm window would need placed within 4 mm of the sample to satisfy this criteria. We envision using thin (~100 nm thick), small silicon nitride, diamond, or similar windows. Due to their small size, these windows are capable of withstanding 1 atmosphere pressure differential without breaking. The windows themselves would be provided by BNL. The nose cone would have to allow for convenient replacement of the windows in the case of breakage, and the retraction range must be sufficient to allow for convenient servicing of the windows.
3. A vacuum tight retractable nose cone, with at least two selectable windows, on the beam entrance port. The windows must allow a 10 mrad cone of radiation to propagate to the sample. A 0.5 mm window located up to 50 mm from the sample satisfies this criterion. The requirements are similar to item 2. The nose cone must be retractable from the experimental chamber, completely removable from the beam path when not required, and allow for easy exchange of the windows.
4. Base, mechanics, and chamber for horizontal collection mirrors: The base should be stable granite. An optics baseplate, outside of vacuum, coupled to the granite block, with typical coarse, lockable adjustments for initial survey positioning of the optics baseplate should be provided. This is envisioned to be standard threaded rod/push screws type of arrangement or equivalent. A vacuum chamber, isolated via edge welded bellows from the optics base plate and optics is needed. The following fine motions are required.

fine motions	range	resolution	repeatability	actuation
height	25 mm	0.010	0.1 mm	motorized, encoded required if mirrors are striped
lateral	±2 mm	2 um	10 um	manual, encoded required independent for both mirrors
longitudinal	---	---	---	not required, survey in place
pitch	±15 mrad	5 urad	1 urad	motorized, encoded required independent for both mirrors
roll	±15 mrad	2 urad	---	manual required independent for both mirrors
yaw	±20 mrad	100 urad	---	manual required independent for both mirrors

5. Base, mechanics, and chamber for vertical focusing mirror: The base should be stable granite. An optics baseplate, outside of vacuum, coupled to the granite block, with typical coarse, lockable adjustments for initial survey positioning of the optics baseplate should be provided. This is envisioned to be standard threaded rod/push screws type of arrangement or equivalent. A vacuum chamber, isolated via edge welded bellows from the optics base plate and optics is needed. The following fine motions to move the mirror are required.

fine motions	range	resolution	repeatability	
height	±2 mm	0.1 um	0.4 um	motorized, encoded
lateral	---	---	---	not required, survey in place

longitudinal	±5 mm	10 um	50 um	motorized, encoded
pitch	±5 mrad	0.1 um	0.4 um	motorized, encoded
roll	±15 mrad	5 urad	---	manual, encoded
yaw	±15 mrad	25 urad	---	manual, encoded

6. Base, mechanics, and chamber for gratings: The base should be stable granite. An optics baseplate, outside of vacuum, coupled to the granite block, with typical coarse, lockable adjustments for initial survey positioning of the optics baseplate should be provided. This is envisioned to be standard threaded rod/push screws type of arrangement or equivalent. A vacuum chamber, isolated via edge-welded bellows from the optics base plate and optics is needed.

   A mechanism for exchanging the gratings in vacuum is needed. This is typically accomplished with a laterally translating grating cradle, as in a modern soft x-ray plane grating monochromator, with the whole grating cradle then attached to a single high precision pitch rotation mechanism. Fine adjustments for the height, roll, and yaw of the individual gratings are typically implemented via manual screw type adjustments accessible in vacuum via a wobble stick.

In vacuum individual adjustments for each grating				
fine motions	range	resolution	repeatability	
height	±1 mm	10 um	---	manual, accessible in vacuum
roll	±10 mrad	10 urad	---	manual, accessible in vacuum
yaw	±10 mrad	50 urad	---	manual, accessible in vacuum

   In addition, a high precision pitch axis for the entire grating is critical. The full angular range will be determined during the design phase, but will be ~10°. It needs to have a resolution better than 0.1 urad and a repeatability better than 0.5 urad. It requires a high precision angular encoder with a resolution better than 50 nrad.
7. Vacuum pumps for all chambers, beam flight tube, supports, and other associated vacuum equipment (pump controllers, vacuum gauges and controllers, gate valves, ect.) should be provided.
8. Slits and apertures: A vertically translatable set of fixed apertures, with a translation range of ~200 mm and a translation accuracy/repeatability of ~10 um should be provided either directly upstream or downstream of the parabolic mirrors, the vertical focusing mirror, and the gratings. An adjustable four jaw slit in front of the detector is also needed.
9. Base, mechanics and chamber for detector: The required long range stability of the detector is ~1 um. The base should therefore be granite. The base should be provided with typical coarse, lockable adjustments for initial survey positioning for position and angular adjustment. This is envisioned to be standard threaded rod/push screws type of arrangement or equivalent.

   In principle, the spectrometer is designed to have an energy independent focus. In practice, it is difficult to rule a grating to give exactly the required focus distance, and to match these exactly between different gratings. The detector must be translatable in both the vertical. Either a translation of the detector within the chamber, or translation of the entire chamber is in principle satisfactory. If translation of the entire chamber is chosen, bellows of sufficient length and diameter are needed as well. The following table lists the required motorized fine motions.

fine motions	range	resolution	repeatability	
height	±10 mm	5 um	25 um	motorized, encoded
longitudinal	±250 mm	10 um	50 um	motorized, encoded

10. The following is a list of the required ports for the chamber. (Ports indicated with a ** need to "see" the sample)
    - Mini flange for leak valve (x1)
    - Mini flange for gas feed line (x1)

- Mini flange for TFY photodiode, with a view of the sample on the QIX side. It need not be in the horizontal plane** (x1)
- Small viewports for cameras** (x3)
- 2¾'' conflat port for SDD Vortex, with a view of the sample on the photoemission side. It need not be in the horizontal plane ** (1x)
- 4.5" conflat port for reaction cell manipulator (XYZ theta); this port currently should come from the from the bottom** (x1)
- 4.5" conflat port for the sample transfer system that brings sample from load loack, through sample prep chamber, to the sample chamber** (x1)
- 4.5" conflat port (or 2¾'' (x2)) for turbo pump(s); currently CSX-2 uses one 700L/s turbo (vacuum ~$2x10^{-9}$ mbar) (x1)
- 6" conflat port for vertical sample manipulator coming from top** (x1)
- Need ports for a burst disk and a PPS vacuum switch, but this does not require line of sight to the sample position, and can be a tee off at some point.
- Mini flanges for high-pressure gas nozzles, one for the AP-PES side, and one on the QIX side.** These would be for dosing gas during operation of either the AP-PES or RIX. The gas jet would need to be able to hit the surface of the sample regardless of where it is in theta. It would be optimal if the feedline for the gas jet can come down along the sample manipulator, and thus have the gas jet mounted on the sample holder, which would ensure that it would face that sample regardless of where the sample is in (X,Y,Z,theta). (x2)

RIXS Endstation and Spectrometer – additional equipment

The following lists all the additional equipment that must be incoorporated into the basic chamber / optical system quoted in the previous section to make a working endstation.

1. Manipulator for top flange: x,y,z, theta and limited 'tilt' for single crystal work, 2.5'' central bore, with the required sample insertions: A low temperature cryostat, and a high temperature heating stage.

Manipulator				
motions	range	resolution	repeatability	
x	± 5 mm	1 um	5 um	motorized, encoded
y	± 5 mm	1 um	5 um	motorized, encoded
z	100 mm	1 um	2 um	motorized, encoded
theta	360°			motorized, encoded

The cost, from catalogue prices, is $22,260 including the motors and encoders.

2. A second (x,y,z, theta) manipulator, for an additional port, optimized for flow cells is required. The requirements would be similar to item 4. Central bore TBD. The specifications will be similar to the manipulator listed above. The price is $22,260.
3. Cryostat: Open cycle flow cryostat, $10,050, cryostat transfer line, $9,870, UHV temperature instrumentation (Si diodes, heater cartridge, feedthroughs, ect.), $7650, Lakeshore temperature controller, $11,430, for a total of $39,000. The design should have a sample holder compatibly with the chosen load lock system.
4. Heating sample stage: a sample holder rod, with a sample holder compatible with the load lock system, and capable to be heated to ~ 1000 K is required. The sample holder, rod, vacuum feedthroughs, UHV heater, T sensors, power supply and control electronics would be required. I estimate $15,000 cost using professional judgement.
5. A gas flow cell and liquid flow cell should be provided. A CAD model for the reaction cell from the ALS should be available. The cost is $110,000 for two cells, from a recent purchase order placed with ALS.

6. A high resolution camera with a spatial resolution of ~1 um is required. A Questar offers long working distance and superior spatial resolution due to the high acceptance of its reflective lens. Cost is $11,440 from a 2014 purchase order.
7. Sample load lock and transfer system. Total $132,000.
    a. Vacuum envelope (load lock and garage chamber chambers, two dual axis power probes, pumps): $82K, as per quote from Kurt J Lesker.
    b. nner mechanics (sample puck receptacles in load lock and garage, power probes claws, sample transfer system interlock system, sample puck holders for two manipulators in sample chamber): Estimate from Stephen Antonelli, based on previous experiences dealing with the central shop, for $50K.
8. Auxillary cameras and ports. Costs for the cameras and lenses are included in the controls section.
9. Vacuum hardware (pumps, pump controllers, vacuum gauges, etc.) for the extension of the CSX2 beamline and the endstation/spectrometer. Total $120,000.
    a. Pnematic gate valves: total of 20 (13 for beamline section of QIX and spectrometer, 7 for vacuum manifold), unit cost $2350 (as per quote from Kurt J Lesker), total cost $47K
    b. PPS vacuum switches: 2 needed, unit cost $1.8K (as per quote), total cost $3.6K
    c. 12 ion pumps, $40K (based on previous Gamma Vacuum ion pump purchases for NEXT beamlines)
    d. 2 700L/s turbo pumps, $30K (as per "HiPace Set 700M" + "OPS400" + "Protection screen" in Pfeiffer quote)
    e. 2 roughing multi-stage root pumps, $24K (as per "Dry Pump A100L" in Pfeiffer quote)
    f. 1 NEG pump, $18K (as per SAES quote)
10. Water cooled electronic racks. 7 are required, 4 are available for use already as CSX, for a total of 3 racks needing to be purchased. Chris Stebbins states the cost at $4000 per rack, plus ~$1000 for additional hardware needed to mount to the floor and hook up to the cooling water and electrical power. The costs are included in the common beamline systems section.
    a. 2 vacuum racks (11 vacuum sections)
    b. 4 motion racks (110 axes)
    c. 1 server rack
11. Detector: The price of a soft x-ray detector based on an e2v electron multiplying detector (single detector) is 278,000 EU. This is similar to the detector purchased for the SIX beamline. A cryocooler is also required ($19,549.00, PO). A computer ($2,500) and a frame grabber board ($1,000) are also required. The total cost then via a current XCAM quotation for a single detector unit is $334,409. The award for the SIX detector was granted on May 30, 2015, and it was delivered in September 2016, but still has some testing to go before acceptance. I therefore estimate 18 mos. for delivery. The detector most suitable for the project, a 1000 Hz frame rate soft X-ray detector from PNDetector was quoted at 227,000 Eu, or $254,240. This quotation was received late.

Endstation- Specific Equipment for IR capabilities

1. Infrared interferometer, and transfer and focusing optics, and detector. The proper ports for IR beam input and extraction must be provided. The cost for beam transfer line, steering mirrors, mirror mechanics, focusing mirrors, interferometer, and detectors is estimated at $150,000 from Larry Carr. These items may be included in the scope for INF, however, we note that the same optics can be used productively at QIX with a conventional IR source, in which case an IR system could be implemented at QIX prior to the implementation of INF.

Endstation- Specific Equipment for the Near Ambient Pressure Photoemission

1. Photoemission analyzer: The analyzer should have ~50 um diameter aperture to allow

pressures up to 100 torr to be reached. The ideal working distance of the aperture from the sample is 2x the aperture size. The desired spectrometer is a Specs PHOIBOS 150 NAP. It accepts an electron emission angle of ±22°. The price is $342K according to a recent quote that someone else got (not including the turbo pumps). The nose cone should be fully retractable behind gate valve. The standard cone that comes with the analyzer has an aperture of 300 um. The weight, without turbo pumps, is ~200 kg. The electron photoemission cone divergence of ±22° gives a cross section of 40 um diameter at 50 um from the sample. The analyzer itself costs $301.611,60. The required turbo and scroll pumps for differential pumping cost $90.436,50.

Photoemission analyzer requirements: The aperture on the nose cone with be ~ 50 um in diameter, and needs to be placed to within ~ 100 um of the sample surface. It also must be aligned laterally and up and down with a sample focus that is 24 um H x 2.2 um V FWHM. The analyzer plus nose cone is 254 mm long, with a weight of 200 kg, not including the turbo pumps. The whole analyzer/nose cone ideally needs to be retracted outside of the chamber, which requires a longitudinal travel of >254 mm, allowing for clearance of a gate valve. This may not be doable with bellows and gate valve mounted outside of the chamber. I will put in a nominal longitudinal travel of 50 mm for some retraction ability for safety. The main mounting flange is DN200CF. The weight, without turbo pumps, is ~200 kg. The recommended first stage turbo pump speed is 500 l/sec on a DN160 port. There are two more DN100 ports for differential pumping, suitable for Pfeiffer Hi-Pace 400 turbo pumps.

Photoemission Analyzer motion requirements				
fine motions	range	resolution	repeatability	actuation
height	+/- 1 mm	1 um	5 um	motorized, encoded
lateral	+/- 2 mm	2 um	10 um	motorized, encoded
longitudinal	50 mm	1 um	5 um	motorized, encoded

In addition to the fine motions, coarse manual lockable adjustments on a baseplate need to be provided to initially survey the spectrometer into place. This is envisioned to be standard threaded rod/push screws type of arrangement.

2 Laser sample heating system. $88,087.50 from Specs quotation.

3 Vortex detector Hitachi, Oxford Instruments. The required specifications were discussed with a company representative, but they have not responded with a quote yet, despite several followups. A quotation from 2014 for a similar detector came in at $44,625.

4 Preparation chamber and associated equipment

a.	LEED package	30,889.35
b.	IQE 11/35 3kV ion source package	10,453.05
c.	Gas Inlet System	2,466.45
d.	Multi-Pocket E-beam evaporator EBE-4-2L2F package	40,990.05
e.	SPECS 5-axes Sample Manipulator (XYZPAz)	62,248.50
f.	UVS 300 UV NAP Source Package with ETC capillary	60,486.75
g.	Differential Pumping Package for UVLS/UVS 300	17,269.50
h.	Z-manipulator	2,818.80
i.	DN40CF Hexapod for source alignment	3,288.60
j.	Gas Inlet System GI-1	2,466.45
k.	chamber and stand (est)	20,000.00
l.	Shipping	9,000.00
m.	Installation	22,680.00
n.	TOTAL	$285,058

Reaction gas handling system

Total $750,000.

1. System for 10 gases, no hutch: $700K, based on comparison with quotes received for the ISS, ISR and XPD2 systems
2. Interface with fire alarm and fire shutdown systems: $50K, from cost at ISS and ISR

Optics

It has been my experience that while vendors can subcontract out the optics, they prefer not to. For gratings, they strongly resist taking responsibility for these as the lead times are very long and there are few grating suppliers. The mechanical interface between the optic and the mechanics is simple and straightforward for BNL to manage. A single official drawing of the optical substrate is all that is required, at least for non-bendable optics, and the optics contracts are quite clear and straightforward to manage as well. For VLS gratings, the number of parameters to get straight is larger and there is less risk in miscommunication if the contract is handled directly by BNL rather than going through a middleman, especially if the design changes during the engineering phase and the VLS parameters need to be modified. I therefore price all optics out separately. The following table is a summary of information collected from various vendors.

optic	optics suppliers						grating rulings[2]	
beamline	Zygo	JTec	SESO	Winlight	Zeiss	---	Inprentus	DIOS
grating substrate		No Bid		21,000 Eu ea 42,000 Eu tot ($47,040 tot) T0+6 mos	$8,721 ea $17,442 tot 6 mos ARO			
grating ruling	---	---	---	---	---		$65,000 ea 6 mos ARO	no response yet
KBH <1 urad tan se		$30,000		18,000 Eu (~$19,980) T0+6 mos (5 urad sag se)	$26,790 6 mos ARO			
KBV <0.25 urad tan se		$50,000		91,000 Eu (~$101,000) T0+12 mos	$52,380 8 mos ARO			
spectrometer	---	---	---	---	---	---	---	---
H collimating mirrors (x2)		No Bid too long		90,000 Eu ea 180,000 Eu tot (~$199,800) T0+10 mos (10 urad sag se)	$73,530 ea $147, 060 tot 8 mos ARO			
VFM		$100,000 ea 2 required[1] $200,000 tot		No Bid	$51,980 8 mos ARO			
grating blanks		$40,000 ea 9 required[1] $360,000 tot		No Bid	$12,825 ea $76,950 tot 6 mos ARO			
grating ruling	---	---	---	---	---	---	$70,000 ea 6 mos ARO	no response yet

[1]JTec cannot polish an optic 160 mm wide. They would polish two narrower substrates. This also would be acceptable, with proper mechnics design
[2]Inprentus quote is low based on actual costs at SIX and ESM. Based on ac†ual costs for ESM and SIX, grating ruling to be $85,000 per grating, with a delivery time of 18 mos based on the experience with the ESM gratings.

Additional Notes:

As this is a conceptual design, it is not optimized. Here is a list of some of the things that should be optimized for the preliminary design. The spectrometer geometry (mirror positions and sizes) should be optimized to maximize throughput, and take into account the actual length of the spectrometer at design time. The benefits of double striped mirrors, with Ni for low energy, should be looked at. To simplify the design, the throughput of a simpler plane grating spectrometer in fixed included angle should be investigated, keeping in mind the focal plane is near grazing, so the angle of operation of the detector, as well as any energy resolution degredation across the detector needs to be looked at. The grating angle and efficiency needs to be optimized as well. For more exotic design changes, the performance of a spectrometer with a single reflection zone plate optic for each edge could be investigated.

The beamline should be ray-traced to verify the energy resolution, and the entire design should be analyzed to quantify the throughput.

It would also be desirable to analyze any alternative optical schemes for throughput, such as one based on total external reflection blazed transmission gratings, or reflective zone plates, and also on single multilayer gratings optimized for each elemental edge.

The following exchange rates were used:

pounds to dollars x1.31

euros to dollars x 1.12

Appendix 1: Summary of QIX task force meetings

General Meetings: 7 general meetings, involving all of the teams involved in the IEPD task force were organized by Lonny Berman to discuss the overall progress of the individual team efforts and serve as reminders for the remaining tasks to be completed. During September, the meetings began to focus in greater detail on cost, schedule, and preparing the WBS for each team. In particular, during the September meetings, several things with direct impact to the costs were discussed. One, it was decided to explicitly include software/controls effort beyond basic motor control, but still necessary for a properly functioning beamline (data acquisition, display, analysis, as well as any advanced control – e.g. coordination of mono scans with undulator gap control). Also, during one of these meetings the historical labor profiles from the ABBIX project were compiled and presented by Lonny Berman as guides for the development of the individual team labor profiles.

(1) General Meetings
May 18, 2 PM (kickoff meeting)
June 24, 11 AM (general meeting with BDP PIs)
August 5, 2 PM (general meeting with BDP PIs)
September 7, 11 AM (beamline controls/software meeting)
September 12, 2 PM (general meeting with BDP PIs)
September 15, 2:30 PM (beamline labor/schedule profiles)

QIX team meetings with the IEPD task force chair: In addition to the general meetings, 8 meetings were held between the QIX team lead and co-lead with Lonny Berman. The earlier meetings focused on discussion of the general progress of the QIX team regarding primarily costing of the equipment and floor layout. The meeting in September concentrated on developing a labor and schedule profile for the QIX endstation. With this, and knowledge of the required major pieces of equipment for QIX, a WBS was developed for QIX. The results of the later meetings are captured in the QIX WBS.

(2) Meetings with QIX Team
June 7, 4 PM
July 15, 3 PM
July 29, 10 AM
August 16, 3 PM
August 23, 2 PM (together with INF)
September 1, 3 PM (together with INF)
September 26, 11 AM
September 27, 10 AM

Additional meetings: The QIX team, including Joseph Dvorak, Ignace Jarrige, Adrian Hunt, Iradwikanari Waluyo, William Leonhardt, and occasionally Larry Carr and Stuart Wilkins, met on numerous occasions throughout the duration of the IEPD work.

In one of the early meetings, the potential advantages of combining the current ambient pressure photoemission capabilities at CSX-2 within the new QIX endstation were realized, and it was decided to determine the feasibility of this.

The QIX team met on a nearly weekly basis throughout the summer and into the second week of September. These meeting concentrated on the efforts to combine both ambient pressure photoemission capabilities and RIXS capabilities in the same endstation. The requirements for both of these experimental modes were compiled, and served as input

to William Leonhardt, to prepare a conceptual engineering design for the endstation that could satisfy these requirements.

Also discussed during these meetings were the requirements for the major pieces of equipment, and the costing of these items.

The results of these discussions are captured in the previous scope narrative for QIX.

Appendix 2: QIX Beamline Dictionary

(1) PQIX.01 Management and Support
Performance of management and support activities, including labor, materials, travel, and fixed costs associated with management and support functions, consisting of construction management, reviews, administrative support, ESH, QA, configuration management, business operations, project controls, procurement, and document control.

(2) PQIX.03 Beamline Construction
(a) PQIX.03.01 Photon Delivery System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of photon delivery sub-systems and integrated system. These include the beamline optical systems upstream of the endstation (including their housings, supports, and manipulation systems), apertures and beam definition and conditioning systems, beam diagnostic/visualization systems, beam transport system, vacuum system, cooling/heating and temperature stabilization systems associated with photon delivery system components, and shielding systems (exclusive of radiological enclosures) that include collimators, masks, shutters, and beam stops.
(b) PQIX.03.03 Endstation System
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of endstation sub-systems and integrated system. These include sample housings, environments, visualization, and support and manipulation systems, detection systems, optical systems and beam diagnostic/visualization and conditioning/definition/deflection components just before the sample (e.g. on the same support as the sample or contiguous with it) or between the sample and detector (e.g. crystal/grating/mirror-based analyzer or spectrometer system) including their housings, supports, and manipulation systems, vacuum system, and cooling/heating and temperature stabilization systems associated with endstation components.

(3) PQIX.04 Beamline Infrastructure
(a) PQIX.04.01 Control Station Furniture
Design, specification, procurement, fabrication, assembly, installation, and testing of furniture for the beamline control station including partitions and their power and communications wiring.
(b) PQIX.04.02 Mechanical Utilities
Design, specification, procurement, fabrication, assembly, installation, and testing of beamline mechanical utilities including equipment racks, DI water, process chilled water, gaseous nitrogen, compressed air, exhaust, and liquid nitrogen distribution systems.
(c) PQIX.04.03 Electrical Utilities

Design, specification, procurement, fabrication, assembly, installation, and testing of beamline electrical utilities including circuit breaker panels, provisioning of power to equipment racks, and cable trays and conduits.

(d) PQIX.04.04 Equipment Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Equipment Protection System (EPS) including PLC, wiring, and custom sensors.

(e) PQIX.04.05 Personnel Protection System
Design, specification, procurement, fabrication, assembly, installation, and testing of Personnel Protection System (PPS) including PLC, wiring, switches, locks, special interlocked personnel protective safeguards such as gates and light screens, and Human Machine Interface (HMI) panel.

(4) PQIX.06 Beamline Controls

(a) PQIX.06.01 Basic System Controls
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation control systems. These include operator consoles for control and archive of control equipment, network routers, gateway to the machine control system, timing IOC to synchronize to the machine timing, motor controllers and associated cabling, serial to Ethernet hubs, and a soft IOC for controlling all Ethernet-based motors, serial devices, and PLCs. Ethernet and timing cables are also included.

(b) PQIX.06.02 Instrument Applications
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation instrument control applications. These include experimental control workstations, data storage and computation equipment, experimental control software and servers, and data acquisition equipment and software including for detectors.

Appendix 3: QIX Equipment Cost Estimate (Direct K$) and Basis of Estimate

Beamline Construction			
	optics	182	quotes from optics and grating vendors
	KB mirror chamber and mechanics	377	ESM costs
	horizontal slit	58	FMB Berlin quote
	vacuum components, diagnostics, and misc	97	quotes, ESM and SIX costs, and prof judgment
Endstation Construction			
	sample chamber and spectrometer optical chambers/mechanics	538	RI Research Instruments quote
	optics	501	quotes from optics and grating vendors
	area detector	334	XCAM and PN Detector quotes
	sample transfer and load-lock system	132	based on quotations
	sample cells and stages	220	quotations and catalogue items
	vacuum components and miscellaneous	120	based on quotations
Reaction Gas Handling System		750	hardware based on quotes for ISR and ISS installation based on costs for ISR and ISS
Beamline Infrastructure Hardware		126	bottom-up estimate
Beamline Control Systems Hardware		223	bottom-up estimate
Total		**3658**	

Appendix 4: QIX Labor Estimate (Person-Years and Hours), Basis of Estimate, and Schedule with Major Activities

	Year 1	Year 2	Year 3	Total	Basis of Estimate
beamline and endstation construction major activities:	design	design, procurement, fabrication	procurement, fabrication, assembly, installation, testing	person-years	
scientist / assistant sci	1.5	1.75	1.75	5	beamline project exp
mech / vac engineer	1.5	1.5	1	4	beamline project exp
mech designer	0.75	0.75	0.5	2	beamline project exp
mech / vac technician	0	0	2	2	beamline project exp
Total				13 person-years or 22,900 hrs	

Additional Labor Required:

Project management: 1,600 hrs scientist
Project support: to be determined, requires clarification
Trades labor for BL constr (riggers, carpenters, masons, and surveyors): still being tallied
Labor for beamline infrastructure: 2,300 hrs (engineer, technician, trades; bot-up deter)
Labor for beamline controls: 8,000 hrs (controls engineer, technician; bot-up determine)

Total Labor Required: 34,800 hrs or 20 person-years plus additional hrs still being tallied

Travel Budget Required: still being determined

QIX Schedule Cartoon

	Year 1	Year 2	Year 3
Design			
Procurement			
Fabrication			
Assembly			
Installation			
Testing			

Project: QIX Beamline — RESOURCE DETAIL

WBS	RESOURCE	UNITS	COST
P_QIX - QIX Beamline			
P_QIX.01 - QIX Management			
LABOR	Labor_Scientist_NS1	1,584.00	$ 236,470.72
	Labor_Administrative Secretary_NA3	528.00	$ 29,527.25
	Labor_ES&H Professional_NA4	792.00	$ 93,658.39
	Labor_QA Professional_NA5	528.00	$ 58,460.98
	Labor_Administrative_NA2	1,004.00	$ 75,533.78
	Labor_Human Resources_NB4	264.00	$ 19,861.47
	LABOR TOTAL	4,700.00	$ 513,512.60
MATERIAL	Material_Material (Purchase <$25k)_NMA	75,000.00	$ 98,172.35
	MATERIAL TOTAL	75,000.00	$ 98,172.35
P_QIX.02 - QIX Design			
P_QIX.02.01 - QIX Conceptual Design			
LABOR	Labor_Scientist_NS1	750.00	$ 106,557.20
	Labor_Mechanical Engineer_NO1	700.00	$ 66,296.18
	Labor_Mechanical Designer_NO2	350.00	$ 28,290.42
	LABOR TOTAL	1,800.00	$ 201,143.80
P_QIX.02.02 - QIX Preliminary Design			
LABOR	Labor_Scientist_NS1	750.00	$ 108,886.78
	Labor_Mechanical Engineer_NO1	700.00	$ 67,127.80
	Labor_Mechanical Designer_NO2	350.00	$ 28,645.29
	LABOR TOTAL	1,800.00	$ 204,659.87
P_QIX.02.03 - QIX Final Design			
LABOR	Labor_Scientist_NS1	750.00	$ 108,886.78
	Labor_Mechanical Engineer_NO1	700.00	$ 67,127.80
	Labor_Mechanical Designer_NO2	350.00	$ 28,645.29
	LABOR TOTAL	1,800.00	$ 204,659.87
P_QIX.03 - QIX Beamline Construction			
P_QIX.03.01 - QIX Photon Delivery System Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	900.00	$ 130,198.22
	Labor_Mechanical Engineer_NO1	700.00	$ 66,711.99
	Labor_Mechanical Designer_NO2	350.00	$ 28,467.85
	Labor_Mechanical Technician_NO3	350.00	$ 26,093.99
	LABOR TOTAL	2,300.00	$ 251,472.05
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,463,300.00	$ 1,799,016.27
	MATERIAL TOTAL	1,463,300.00	$ 1,799,016.27
P_QIX.03.02 - QIX Photon Delivery System Installation and Test			
LABOR	Labor_EL - Vacuum Engineer_SE5	251.00	$ 27,146.20
	Labor_EL - Vacuum Technician_SE6	1,014.00	$ 82,120.91
	Labor_ME - Survey Engineer_MO1	78.00	$ 7,444.55
	Labor_EL - Survey Technician_SE2	187.00	$ 15,144.59
	Labor_Building Trades Unassigned_NST	31.00	$ 3,855.14
	Labor_Plant Engineering-Building Trades Carpenter_BTC	71.00	$ 8,411.27
	Labor_Plant Engineering-Building Trades Riggers_BTS	141.00	$ 16,704.07
	Labor_Scientist_NS1	450.00	$ 63,934.32
	Labor_Mechanical Engineer_NO1	280.00	$ 26,518.47
	Labor_Mechanical Designer_NO2	140.00	$ 11,316.17
	Labor_Mechanical Technician_NO3	350.00	$ 25,891.01
	LABOR TOTAL	2,993.00	$ 288,486.69
P_QIX.03.03 - QIX End Station Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	3,600.00	$ 521,933.90
	Labor_Mechanical Engineer_NO1	2,800.00	$ 267,662.61
	Labor_Mechanical Designer_NO2	1,400.00	$ 114,219.04
	Labor_Mechanical Technician_NO3	1,400.00	$ 104,375.96
	LABOR TOTAL	9,200.00	$ 1,008,191.50
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,833,519.00	$ 2,249,089.09
	MATERIAL TOTAL	1,833,519.00	$ 2,249,089.09
P_QIX.03.04 - QIX End Station Installation and Test			
LABOR	Labor_Scientist_NS1	1,800.00	$ 255,737.29
	Labor_Mechanical Engineer_NO1	1,120.00	$ 106,073.90
	Labor_Mechanical Designer_NO2	560.00	$ 45,264.67
	Labor_Mechanical Technician_NO3	1,400.00	$ 103,564.03
	LABOR TOTAL	4,880.00	$ 510,639.88
P_QIX.04 - QIX Beamline Infrastructure			
P_QIX.04.01 - QIX Hutches			
MATERIAL	Material_Material (Purchase >$25k)_NSM	30,000.00	$ 36,521.82
	MATERIAL TOTAL	30,000.00	$ 36,521.82
P_QIX.04.02 - QIX Mechanical Utilities			
LABOR	Labor_EL - Utility Engineer_SE3	184.00	$ 19,900.00
	Labor_Mechanical Designer_NO2	162.00	$ 13,094.42
	Labor_EL - Utility Technician_SE4	445.00	$ 36,039.25
	Labor_Plant Engineering-Building Trades Plumber_BTP	101.00	$ 11,965.33
	Labor_Plant Engineering-Building Trades Carpenter_BTC	9.00	$ 1,066.22
	Labor_Building Trades Unassigned_NST	40.00	$ 4,974.37
	LABOR TOTAL	941.00	$ 87,039.59
MATERIAL	Material_Material (Purchase <$25k)_NMA	44,000.00	$ 56,362.80
	Material_Material (Purchase >$25k)_NSM	35,000.00	$ 42,608.80
	MATERIAL TOTAL	79,000.00	$ 98,971.60
P_QIX.04.03 - QIX Electrical Utilities			
LABOR	Labor_Electrical Engineer_NE1	54.00	$ 5,840.22
	Labor_Electrical Designer_NE2	24.00	$ 2,040.05
	Labor_Plant Engineering-Building Trades Electrician_BTE	607.00	$ 71,910.43
	LABOR TOTAL	685.00	$ 79,790.69
MATERIAL	Material_Material (Purchase <$25k)_NMA	20,000.00	$ 25,619.46
	MATERIAL TOTAL	20,000.00	$ 25,619.46
P_QIX.04.04 - QIX EPS			
LABOR	Labor_Controls Engineer_NE4	310.00	$ 33,527.19
	Labor_Electrical Technician_NE3	340.00	$ 27,535.61
	Labor_Electrical Designer_NE2	40.00	$ 3,400.08
	LABOR TOTAL	690.00	$ 64,462.88
MATERIAL	Material_Material (Purchase <$25k)_NMA	27,000.00	$ 34,586.27
	MATERIAL TOTAL	27,000.00	$ 34,586.27
P_QIX.06 - QIX Controls			
P_QIX.06.01 - QIX Basic System Controls			
LABOR	Labor_Controls Engineer_NE4	2,966.00	$ 338,125.61
	Labor_Electrical Technician_NE3	898.00	$ 75,635.46

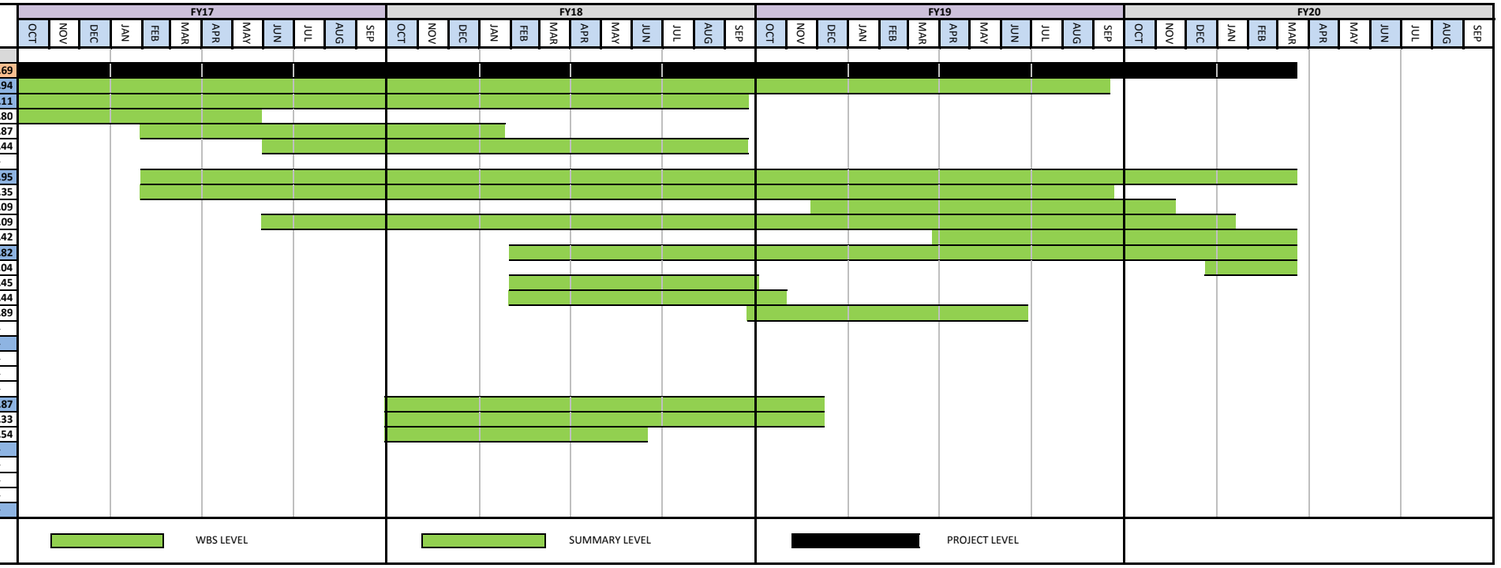
	Labor_IT Professional (Software)_NA7	408.00	$	39,186.03
	LABOR TOTAL	4,272.00	$	452,947.10
MATERIAL	Material_Material (Purchase <$25k)_NMA	56,700.00	$	74,224.35
	Material_Material (Purchase >$25k)_NSM	142,500.00	$	179,029.88
	MATERIAL TOTAL	199,200.00	$	253,254.23
P_QIX.06.02 - QIX Instrument Applications				
LABOR	Labor_IT Professional (Software)_NA7	1,920.00	$	184,395.33
	Labor_Assistant/Associate Scientist_NS2	440.00	$	45,483.97
	Labor_Controls Engineer_NE4	1,360.00	$	152,970.52
	LABOR TOTAL	3,720.00	$	382,849.82
MATERIAL	Material_Material (Purchase <$25k)_NMA	24,000.00	$	31,419.72
	MATERIAL TOTAL	24,000.00	$	31,419.72

Project: QIX Beamline — RESOURCE SUMMARY

WBS	RESOURCE	UNITS		COST
P_QIX - QIX Beamline				
LABOR	Labor_Scientist_NS1	10,584.00	$	1,532,605.21
	Labor_Administrative Secretary_NA3	528.00	$	29,527.25
	Labor_ES&H Professional_NA4	792.00	$	93,658.39
	Labor_QA Professional_NA5	528.00	$	58,460.98
	Labor_Administrative_NA2	1,004.00	$	75,533.78
	Labor_Human Resources_NB4	264.00	$	19,861.47
	Labor_Mechanical Engineer_NO1	7,000.00	$	667,518.75
	Labor_Mechanical Designer_NO2	3,662.00	$	297,943.14
	Labor_Mechanical Technician_NO3	3,500.00	$	259,924.98
	Labor_EL - Vacuum Engineer_SE5	251.00	$	27,146.20
	Labor_EL - Vacuum Technician_SE6	1,014.00	$	82,120.91
	Labor_ME - Survey Engineer_MO1	78.00	$	7,444.55
	Labor_EL - Survey Technician_SE2	187.00	$	15,144.59
	Labor_Building Trades Unassigned_NST	71.00	$	8,829.51
	Labor_Plant Engineering-Building Trades Carpenter_BTC	80.00	$	9,477.49
	Labor_Plant Engineering-Building Trades Riggers_BTS	141.00	$	16,704.07
	Labor_EL - Utility Engineer_SE3	184.00	$	19,900.00
	Labor_EL - Utility Technician_SE4	445.00	$	36,039.25
	Labor_Plant Engineering-Building Trades Plumber_BTP	101.00	$	11,965.33
	Labor_Electrical Engineer_NE1	54.00	$	5,840.22
	Labor_Electrical Designer_NE2	64.00	$	5,440.12
	Labor_Plant Engineering-Building Trades Electrician_BTE	607.00	$	71,910.43
	Labor_Controls Engineer_NE4	4,636.00	$	524,623.31
	Labor_Electrical Technician_NE3	1,238.00	$	103,171.07
	Labor_IT Professional (Software)_NA7	2,328.00	$	223,581.37
	Labor_Assistant/Associate Scientist_NS2	440.00	$	45,483.97
	LABOR TOTAL	39,781.00	$	4,249,856.35
MATERIAL	Material_Material (Purchase <$25k)_NMA	246,700.00	$	320,384.94
	Material_Material (Purchase >$25k)_NSM	3,504,319.00	$	4,306,265.86
	MATERIAL TOTAL	3,751,019.00	$	4,626,650.80
		GRAND TOTAL	$	8,876,507.15

Project Name: QIX Beamline

WBS	Start	Finish	Cost
P_QIX - QIX Beamline	10/1/2016	3/19/2020	$ 9,191,111.69
P_QIX.01 - QIX Management	10/1/2016	9/16/2019	$ 611,684.94
P_QIX.02 - QIX Design	10/1/2016	9/23/2018	$ 614,123.11
P_QIX.02.01 - QIX Conceptual Design	10/1/2016	5/29/2017	$ 201,143.80
P_QIX.02.02 - QIX Preliminary Design	1/30/2017	1/25/2018	$ 204,659.87
P_QIX.02.03 - QIX Final Design	5/31/2017	9/23/2018	$ 208,319.44
P_QIX.02.04 - QIX R&D Program			$ -
P_QIX.03 - QIX Beamline Construction	1/30/2017	3/19/2020	$ 6,399,535.95
P_QIX.03.01 - QIX Photon Delivery System Procurement and Fabrication	1/30/2017	9/20/2019	$ 2,119,085.35
P_QIX.03.02 - QIX Photon Delivery System Installation and Test	11/25/2018	11/20/2019	$ 313,166.09
P_QIX.03.03 - QIX End Station Procurement and Fabrication	5/30/2017	1/18/2020	$ 3,402,146.09
P_QIX.03.04 - QIX End Station Installation and Test	3/25/2019	3/19/2020	$ 565,138.42
P_QIX.04 - QIX Beamline Infrastructure	1/30/2018	3/19/2020	$ 445,296.82
P_QIX.04.01 - QIX Hutches	12/20/2019	3/19/2020	$ 39,858.04
P_QIX.04.02 - QIX Mechanical Utilities	1/30/2018	10/3/2018	$ 191,734.45
P_QIX.04.03 - QIX Electrical Utilities	1/30/2018	10/31/2018	$ 107,901.44
P_QIX.04.04 - QIX EPS	9/23/2018	6/27/2019	$ 105,802.89
P_QIX.04.05 - QIX PPS			$ -
P_QIX.05 - QIX Accelerator Infrastructure			$ -
P_QIX.05.01 - QIX Front End			$ -
P_QIX.05.02 - QIX Source			$ -
P_QIX.05.03 - QIX Straight			$ -
P_QIX.06 - QIX Controls	9/29/2017	12/7/2018	$ 1,120,470.87
P_QIX.06.01 - QIX Basic System Controls	9/29/2017	12/7/2018	$ 706,201.33
P_QIX.06.02 - QIX Instrument Applications	9/29/2017	6/15/2018	$ 414,269.54
P_QIX.07 - QIX Conventional Facilities			$ -
P_QIX.07.01 - QIX Conventional Facilities Design			$ -
P_QIX.07.02 - QIX Conventional Facilities Construction			$ -
P_QIX.07.03 - QIX Conventional Facilities Commissioning			$ -
P_QIX.08 - QIX Special Equipment			$ -



RATE SET: Rate Set 1

Narrative for INFINITE
October 2016

This document addresses the charge of the NSLS-II "2016 Taskforce on Instrument Execution Plan Development (16-IEPD)" as it relates to the proposed INFINITE multiple infrared beamline programs:

Tasks

- *Use SRW to determine source extraction limitations*
- *Determine whether a 4th horizontal source segment can be utilized effectively*
- *Identify necessary R&D*

Introduction

This document presents the initial design idea for the INFINITE beamlines for infrared nanospectroscopy and microspectroscopy, with three independently operated branchlines and endstations, utilizing a standard gap dipole bend magnet as source. The proposed location would be the 24BM-B dipole bending magnet as source and the 23BM and 24ID experimental floor space. The three endstation programs would be 1) Near-field Infrared spectroscopy for condensed matter and materials physics, 2) Near-field Infrared spectroscopy of nanomaterials for catalysis and 3) Infrared Reflection-Absorption Spectroscopy of catalytic systems under ambient pressure. The latter is in combination with the CSX-2 branch program. Endstation 3 would also provide conventional mid-IR microspectroscopy of materials (shared time, most likely well over 50%).

A candidate floor plan for these endstations is shown in Figure 1 (below) with the storage ring and ratchet shield wall at the very bottom.

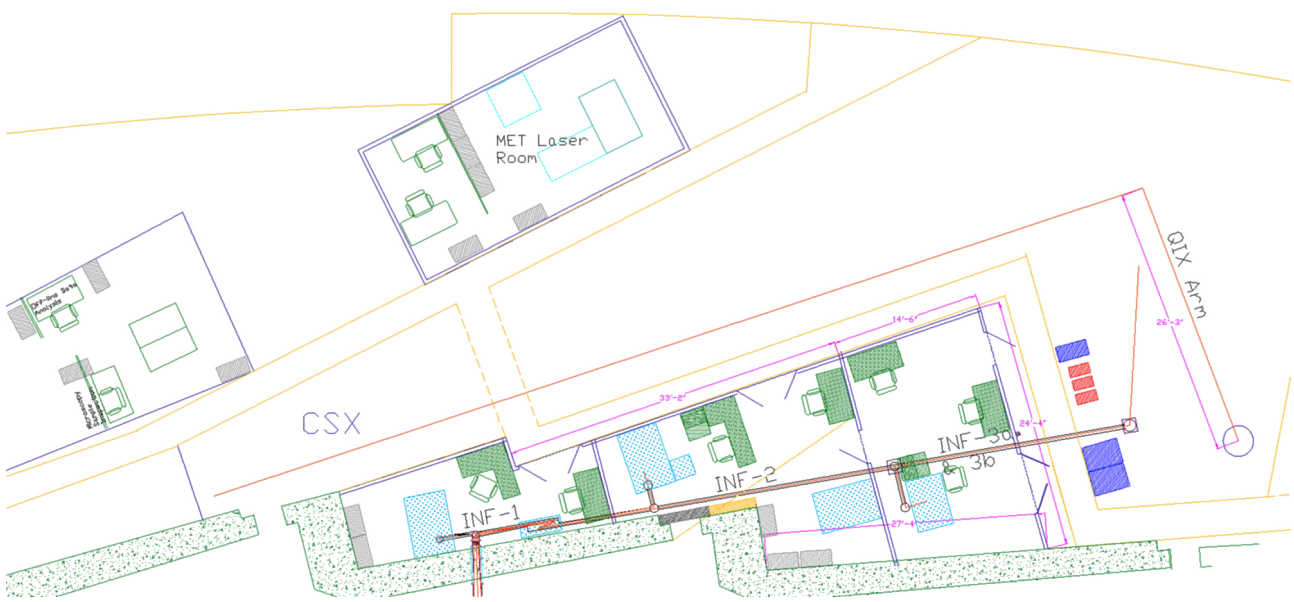


Figure 1: Schematic of a candidate floor layout in the 23BM and 24ID floor areas, showing the cabins and a possible beam pipe routing. Just above this is the CSX (23ID) floor area. A portion of the MET cabins are also shown in 22BM. This is to illustrate the close proximity of the MET laser room that can offer a source for near-field imaging at specific wavelengths during non-operational periods of the synchrotron storage ring.

The proposed location is the upstream portion of the 24ID space, plus some of the 23BM space near the ratchet. The area above these is occupied by the existing CSX-1 and CSX-2 beamlines. Three laboratory cabins will be located here to accommodate each of the branchlines, with the exception of the IRRAS branch that will end near the CSX-2 sample chamber. The cabins are necessary as an additional buffer to changes in humidity and CO_2, as well as to control draft and acoustic noise that affect the AFM nanoscope systems. The beam transport pipe will emerge through the shield side wall and then run along it at a level above the plug door and other obstacles. It then passes through the outer cabins at a level that does not restrict egress, eventually reaching the planned location of the CSX-2 endstation. An insertable mirror will extract a portion of the beam for the middle cabin. A 2nd insertable/removable mirror will serve to direct beam down into the last cabin for microspectroscopy. Stable pylons will be needed to support mirror optics and avoid vibrations.

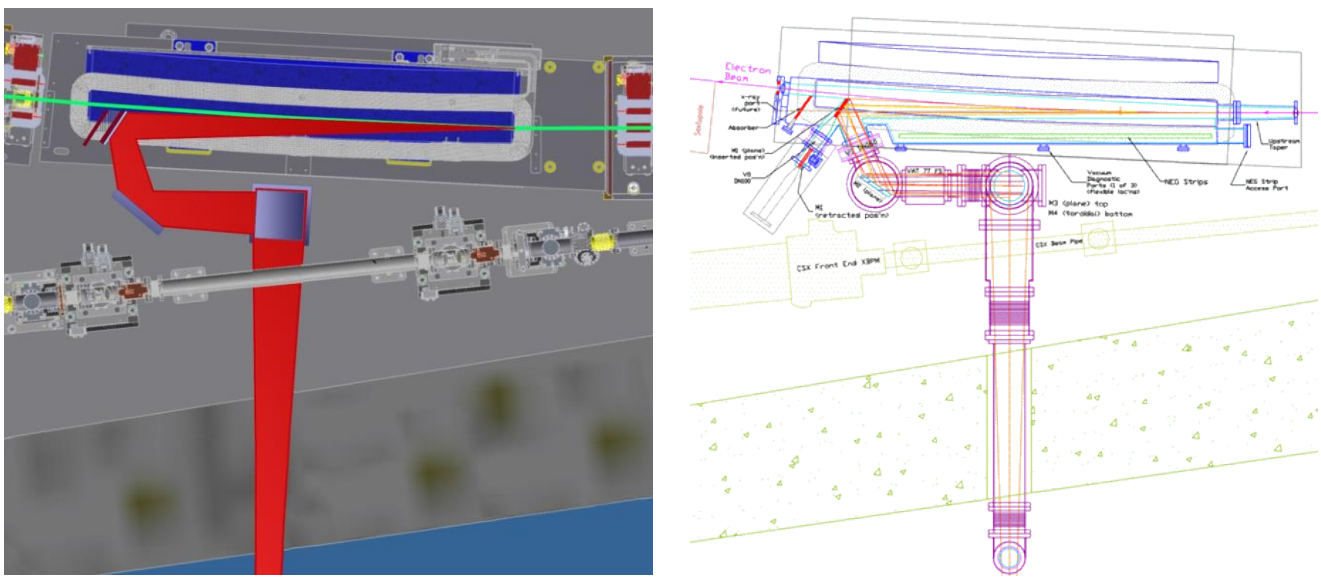


Figure 2: Optical extraction of the dipole synchrotron radiation and delivery through the shield wall onto the experimental floor. The extraction closely follows the extraction design already being developed for the MET and FIS infrared beamlines at cell 23BM-B.

An important component of the optical extraction is the dipole vacuum chamber design and footprint of the dipole bend radiation as it lands on the 1st extraction optic (the M1 plane mirror) (Figure 2). For this purpose, a preliminary design for a dipole chamber cross section has been developed. The proposed cross section is shown in Figure 3a along with the dipole magnet pole faces above and below the electron beam orbit. Initial checks using ANSYS for mechanical integrity indicate the design is feasible based on aluminum alloy material. Such a chamber allows infrared from the 1st half of the electron beam arc (0 mrad out to 45 mrad) to be extracted by a mirror located approximately 2.2 meters from where the electron beam enters the dipole field. The distance from the mirror edge to the electron beam at this location is just over 30 mm. The vertical collection is a constant 15 mrad across this horizontal swath. The geometric extent of the infrared beam profile at various positions through the chamber is shown for various locations in Figure 3b.

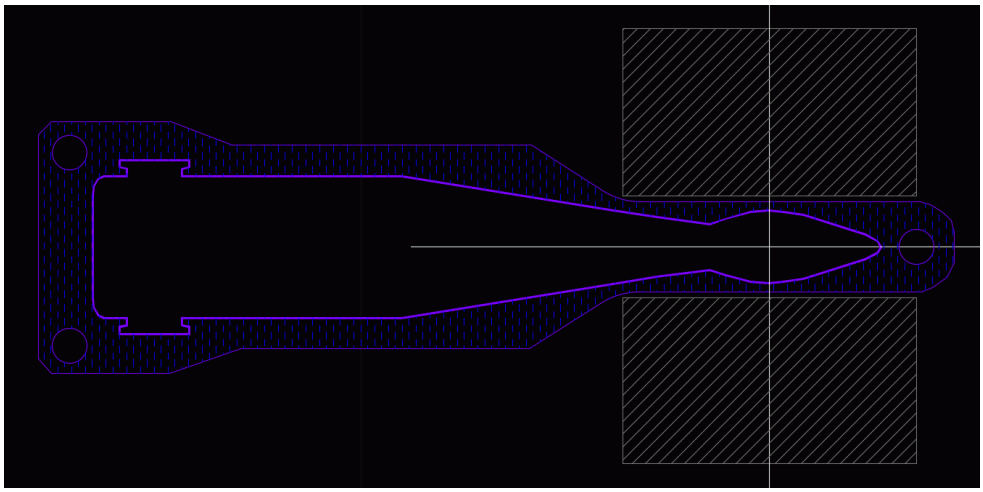


Figure 3a: Candidate dipole vacuum chamber design for allowing 15 mrad vertical extraction across the full 45 mrad horizontal collection.

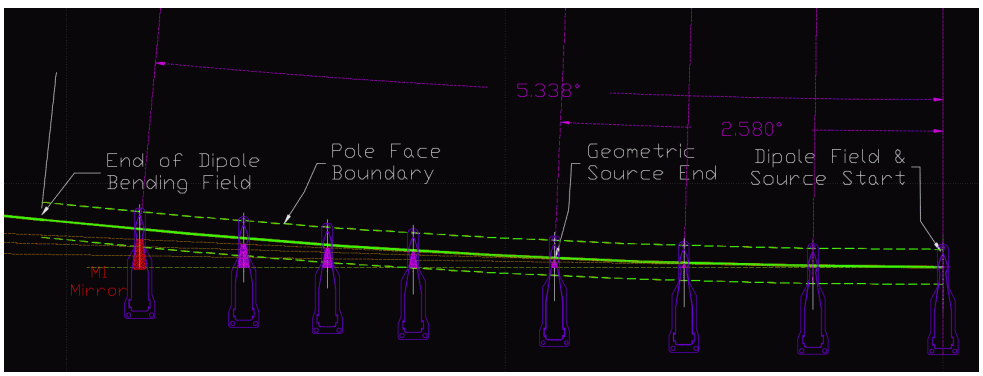


Figure 3b: Collection geometry through the cell 24 dipole bend, showing the 15mrad by 45mrad infrared beam profile (magenta) along with chamber cross sections.

The M1 mirror will have a horizontal slot to allow the x-ray components of the beam to pass through to a downstream absorber.

The SRW calculations for the beam footprint at the M1 location are shown in Figure 4 where the overall shape of the beam footprint is from the dipole bending magnet radiation. The expected extent of the M1 mirror is outlined by violet lines above and below the beam footprint. The yellow vertical dashed lines indicate the source portion that would be available for 3 independently operating endstations, where each segment contains 15 mrad by 15 mrad (HxV) angular collection. Note that the collection is not quite ideal at the lowest frequency (100 cm^{-1}) planned for the science program. Dividing the source into 4 segments would result in more significant degradation for most of the critical spectral range planned for near-field infrared. Therefore, it is recommended to have a maximum of 3 horizontal source segments.

It should be noted that SRW does not include any aspect of the metal vacuum chamber (shadowing or long wavelength cutoff). As a result, the SRW output indicates intensity "fringes" due to the interference between light generated at the end of the upstream dipole (24BM-A in this case) and where the electron beam enters this relevant dipole. These fringes - due to edge radiation - are not expected to be present, especially for the long wavelength portion of the spectrum. Existing beamlines throughout the world have not reported any issues with the extracted infrared.

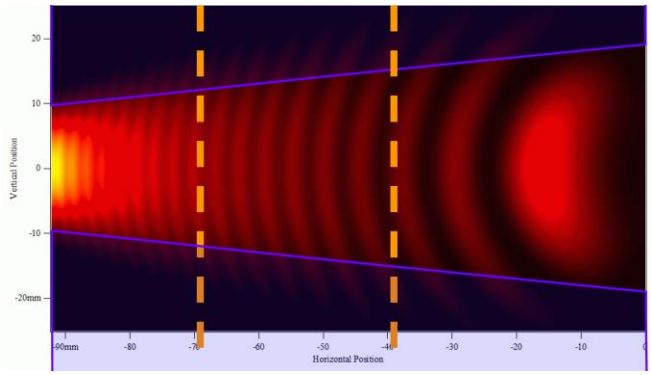


Figure 4a: SRW output (red/orange) for a frequency of 100 cm^{-1} (100 μm wavelength) along with the boundaries for expected extraction as determined by the dipole vacuum chamber geometry.

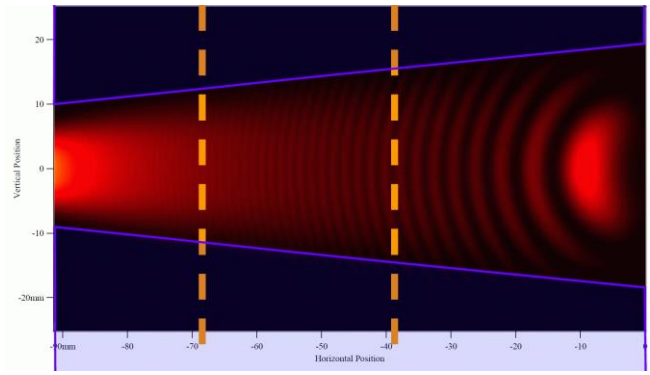


Figure 4b: same as 4a but for a frequency of 300 cm^{-1} (33 μm wavelength). The source collection is effectively ideal for this frequency and above.

Scientific goals and experimental techniques

Note that the beamline programs are labeled 1, 2 and 3. The actual source segment to be used will depend on the physical requirements for endstation instruments and may not directly match the order of the horizontal source segments.

INFINITE 1: Condensed Matter and Materials Physics: The scientific goal is to spectroscopically and spatially resolve structures, modulations, domains and inhomogeneities on a ~10 nm length scale in order to understand their role in the electronic behavior of materials. These include complex oxides with competing orders and emergence, multi-ferroics, topological insulators with surface/edge states, metamaterials and 2D electronic systems and inhomogeneous metal-insulators and superconductors.

The principal instrument would be an Atomic Force Microscope (AFM) optically coupled to an Asymmetric Michelson Interferometer (AMI). The AFM would offer additional scanning modalities (e.g. magnetic force, thermal/electrical conductivity, dielectric) to assist in locating and mapping relevant nanoscale objects. A cold sample stage will be crucial for conducting measurements across low-temperature phase boundaries. The AMI provides the spectroscopic sensitivity (both magnitude and phase of the infrared scattered at the tip/sample interface) in combination with an appropriate infrared detector.

INFINITE 2: Nanostructures for Catalysis: The scientific goal is to spectroscopically and spatially resolve vibrational modes for small collections of molecules adhered to various nanostructures on surfaces. The principal instrument would be an Atomic Force Microscope (AFM) optically coupled to an Asymmetric Michelson Interferometer (AMI), the same as for INFINITE 1. The differences would be in the AFM modalities, e.g. capable of sensing catalysis relevant features.

INFINITE 3: Infrared Microspectroscopy and Infrared Reflection-Absorption Spectroscopy of Surfaces: The scientific goal is to perform chemical/vibrational surface spectroscopy of molecular adsorbates (CSX-2) and for microspectroscopy in a wide range of scientific systems ranging from environmental, geological, planetary, biomedical and materials systems.

The principal instruments would be a conventional FTIR spectrometer combined with an ambient pressure chamber for catalysis (CSX-2) or a scanning infrared microspectrometer.

Technical capabilities and key performance parameters

The NFIR endstations will offer a spatial resolution approaching 10 nm. All spectrometers should be capable of 0.1 cm^{-1} resolution. The beamline optics can be capable of delivering a minimum 50% diffraction-limited flux and brightness to the relevant spectrometer system from 7000 cm^{-1} down to 100 cm^{-1}.

List of major equipment and construction activities

Source: Custom dipole vacuum chamber and UHV optical extraction system for bringing beam through tunnel side wall. Approximately 20 months from contract award to delivery and installation. Coordinated with storage ring operation schedule for construction and installation.
Hutches: None
Experimental cabins: Conventional construction with cost scaled using MET and FIS construction. Approximately 12 months from design specification to delivery.
Endstation components: Mostly commercial systems (e.g. Anasys, NeaSpec, MDT), including spectrometers (Bruker) and detectors (IR Labs, QMC Instruments, Komar Tech). Up to 18 months from specification to delivery for the cryogenic version.

Utility, service line, and rack layout requirements:

We do not anticipate any special or unusual requirements for managing these items. Utility needs will be similar to what is presently installed in the 1L L10 infrared laboratory. Each endstation cabin will benefit from a single rack, with up to two additional racks located outside of the 3rd cabin to manage network and other control systems.

Control System:

There is not much history for control systems at infrared beamlines, other than for monitoring vacuum and valve status in the UHV section. The operation of infrared endstations has been managed by commercial software packages provided by the instrument vendor. Few, if any, have been readily adaptable to EPICS or other software environments commonly used at x-ray beamlines. We expect that a control system serving INFINITE would have a structure suitable for FIS and MET, given that a Fourier Transform Interferometer serves as the core spectrometer in all cases. We propose that the development of a control system be managed on behalf of all infrared activities (including off-line instruments using internal sources).

ES&H:

Requirements for ES&H will be similar to those for the infrared beamline activities at NSLS beamlines U10 and U4IR.

Samples: Except for a cryogenic AFM/NFIR system, samples are measured under ambient conditions, i.e. in the open air. Therefore all specimens will need to be fixed to a flat substrate. The exception is the infrared reflection absorption spectroscopy at the CSX-2 endstation. All ES&H requirements for that will be managed at CSX-2.

Visible Synchrotron Beam: The visible portion of the synchrotron radiation constitutes an eye hazard near a beam waist. For normal measurement conditions, this visible beam is contained within the metal beampipe and spectrometer system. When alignment by beamline staff is required without these protections, the cabin room provides an enclosure for containing the beam.

Laser Systems: The near-field infrared (NFIR) systems have the option to perform measurements at single-wavelengths using laser sources. This could be from small quantum cascade laser systems (QCLs) where the few milliwatt beam can be contained within the NFIR system enclosure, or from mixing of two near-IR ultra-fast laser beams. This mixing could be performed in the MET laser room and brought into one of the INFINITE cabins. Power levels would be below 100 mW and the beam can be controlled inside the NFIR enclosure, with the cabin serving as an additional boundary for alignment needs.

Sector floor space:

The proposed location at the cell 23BM and 24ID space was chosen for the following reasons:

1) Proximity to MET and its infrared work area for managing detectors (cryogenic and vacuum preparation).
2) Proximity to the MET laser cabin for future access to laser-generated mid-infrared.
3) Adjacent to the CSX-2 endstation for the INF-3 IRRAS program.
4) 23BM floor space has no potential x-ray source other than a soft bend (the taper upstream of 23BM-B prevents a 3PW source). Additionally, a 23BM soft x-ray beamline would need to pass by the two RF cavities and systems (possible space issue).
5) 24ID floor space has no potential x-ray source since the 24ID long straight is occupied by the two RF cavities (C and D).

R&D considerations:

The beamline itself involves no new technology. For the endstations , AFM-based near-field microscope systems are now commercially available, although a custom system -- based on mostly commercial components -- may be desired for one of the endstations to expand the available AFM techniques. The community, in general, will require some more advanced detectors based on modifications of existing technology, but this is outside the scope of this particular beamline project. Therefore, it can be stated that no particular R&D is required as part of this beamline project.

Appendix 1: INF Interactions/Meetings Summary

(1) General Task Force Meetings
May 18, 2 PM (kickoff meeting)
June 24, 11 AM (general meeting with BDP PIs)
August 5, 2 PM (general meeting with BDP PIs)
September 7, 11 AM (beamline controls/software meeting)
September 12, 2 PM (general meeting with BDP PIs)
September 15, 2:30 PM (beamline labor/schedule profiles meeting)

(2) INF-Specific Meetings
June 10, 1:30 PM
August 23, 2 PM (together with QIX)
September 1, 3 PM (together with QIX)
September 23, 3 PM
October 6, 2 PM

Appendix 2: INF Beamline Dictionary

(1) PINF.01 Management and Support
Performance of management and support activities, including labor, materials, travel, and fixed costs associated with management and support functions, consisting of construction management, reviews, administrative support, ESH, QA, configuration management, business operations, project controls, procurement, and document control.

(2) PINF.03 Beamline Construction
   (a) PINF.03.01 Photon Delivery System
   Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of photon delivery sub-systems and integrated system. These include the beamline optical systems upstream of the endstation (including their housings, supports, and manipulation systems), apertures and beam definition and conditioning systems, beam diagnostic/visualization systems, beam transport system, vacuum system, cooling/heating and temperature stabilization systems associated with photon delivery system components, and shielding systems (exclusive of radiological enclosures) that include collimators, masks, shutters, and beam stops.
   (b) PINF.03.03 Endstation System
   Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of endstation sub-systems and integrated system. These include sample housings, environments, visualization, and support and manipulation systems, detection systems, optical systems and beam diagnostic/visualization and conditioning/definition/deflection components just before the sample (e.g. on the same support as the sample or contiguous with it) or between the sample and detector (e.g. crystal/grating/mirror-based analyzer or spectrometer system) including their housings, supports, and manipulation systems, vacuum system, and cooling/heating and temperature stabilization systems associated with endstation components.

(3) PINF.04 Beamline Infrastructure
   (a) PINF.04.01 Cabins and Control Station Furniture
   Design, specification, procurement, fabrication, assembly, installation, and testing of required environmental cabins (not radiological enclosures) including the necessary ventilation, doors, windows, wiring, and lights, and of furniture for the beamline control station including partitions and their power and communications wiring.
   (b) PINF.04.02 Mechanical Utilities
   Design, specification, procurement, fabrication, assembly, installation, and testing of beamline mechanical utilities including equipment racks, DI water, process chilled water, gaseous nitrogen, compressed air, exhaust, and liquid nitrogen distribution systems.
   (c) PINF.04.03 Electrical Utilities
   Design, specification, procurement, fabrication, assembly, installation, and testing of beamline electrical utilities including circuit breaker panels, provisioning of power to equipment racks, and cable trays and conduits.
   (d) PINF.04.04 Equipment Protection System
   Design, specification, procurement, fabrication, assembly, installation, and testing of Equipment Protection System (EPS) including PLC, wiring, and custom sensors.

(4) PINF.05 Accelerator Infrastructure

(a) PINF.05.02 Source
Design (including simulations and radiological ray tracing), specification, procurement, fabrication, assembly, installation, and testing of radiation source and associated hardware. This includes an extraction chamber to insert within a dipole magnet for infrared radiation. The necessary utilities, protection systems, and controls for the source are included.

(5) PINF.06 Beamline Controls
(a) PINF.06.01 Basic System Controls
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation control systems. These include operator consoles for control and archive of control equipment, network routers, gateway to the machine control system, timing IOC to synchronize to the machine timing, motor controllers and associated cabling, serial to Ethernet hubs, and a soft IOC for controlling all Ethernet-based motors, serial devices, and PLCs. Ethernet and timing cables are also included.
(b) PINF.06.02 Instrument Applications
Design, specification, procurement, fabrication, assembly, installation, and testing of photon delivery system and endstation instrument control applications. These include experimental control workstations, data storage and computation equipment, experimental control software and servers, and data acquisition equipment and software including for detectors.

Appendix 3: INF Equipment Cost Estimate (Direct K$) and Basis of Estimate

UHV Optical Extraction and Miscellaneous Materials		980	FIS/MET cost scaled
Cabins for Endstations (3)		290	FIS/MET cost scaled
Beamline Construction			
	photon distribution and optical matching	200	FIS/MET cost scaled
Endstation Construction			
	NFIR endstation no. 1 w/ cryo	800	prof judgment
	NFIR endstation no. 2	500	prof judgment
	IRRAS FTIR endstation (CSX-2)	150	prof judgment
	IR detectors (5)	50	catalog items
Beamline Infrastructure Hardware		110	bot-up est
Beamline Control Systems Hardware		in prog	
Total		**3080**	

Appendix 4: INF Labor Estimate (Person-Years and Hours), Basis of Estimate, and Schedule with Major Activities

	Year 1	Year 2	Year 3 (half-year)	Total	Basis of Estimate
beamline and endstation construction major activities:	design, procurement	procurement, fabrication, assembly, installation, testing	procurement, fabrication, assembly, installation, testing	person-years	
scientist	0.75	0.75	0.5	2	beamline project exp
scientific associate	0.375	0.375	0.25	1	beamline project exp
mech / vac engineer	0.5	0.35	0.15	1	beamline project exp
mech designer	0.25	0.175	0.075	0.5	beamline project exp
mech / vac technician	0	0.375	0.375	0.75	beamline project exp
Total				5.25 person-years or 9,200 hrs	

Additional Labor Required:

Project management: 1,300 hrs scientist
Project support: to be determined, requires clarification
Labor for source-related work: still being tallied
Trades labor for BL constr (riggers, carpenters, masons, and surveyors): still being tallied
Labor for beamline infrastructure: 2,000 hrs (engineer, technician, trades; bot-up deter)
Labor for beamline controls: still being tallied

Total Labor Required: 12,500 hrs or 7 person-years plus additional hrs still being tallied

Travel Budget Required: still being determined

Schedule Cartoon

	Year 1	Year 2	Year 3 (half-year)
Design			
Procurement			
Fabrication			
Assembly			
Installation			
Testing			

Project: INF Beamline — RESOURCE DETAIL

WBS	RESOURCE	UNITS	COST
PINF - INF Beamline			
PINF.01 - INF Management			
LABOR	Labor_Scientist_NS1	1,320.00	$ 195,272.51
	Labor_Administrative Secretary_NA3	440.00	$ 24,422.06
	Labor_ES&H Professional_NA4	660.00	$ 77,465.10
	Labor_QA Professional_NA5	440.00	$ 48,353.23
	Labor_Administrative_NA2	836.00	$ 62,424.41
	Labor_Human Resources_NB4	220.00	$ 16,427.48
	LABOR TOTAL	3,916.00	$ 424,364.79
MATERIAL	Material_Material (Purchase <$25k)_NMA	62,500.00	$ 81,448.29
	MATERIAL TOTAL	62,500.00	$ 81,448.29
PINF.02 - INF Design			
PINF.02.01 - INF Conceptual Design			
LABOR	Labor_Scientist_NS1	293.25	$ 41,628.35
	Labor_Mechanical Engineer_NO1	176.00	$ 16,668.76
	Labor_Mechanical Designer_NO2	88.00	$ 7,113.02
	Labor_Scientific Associate_NS3	176.00	$ 14,007.49
	LABOR TOTAL	733.25	$ 79,417.61
PINF.02.02 - INF Preliminary Design			
LABOR	Labor_Scientist_NS1	293.25	$ 41,628.35
	Labor_Mechanical Engineer_NO1	176.00	$ 16,668.76
	Labor_Mechanical Designer_NO2	88.00	$ 7,113.02
	Labor_Scientific Associate_NS3	176.00	$ 14,007.49
	LABOR TOTAL	733.25	$ 79,417.61
PINF.02.03 - INF Final Design			
LABOR	Labor_Scientist_NS1	293.25	$ 41,628.35
	Labor_Mechanical Engineer_NO1	176.00	$ 16,668.76
	Labor_Mechanical Designer_NO2	88.00	$ 7,113.02
	Labor_Scientific Associate_NS3	176.00	$ 14,007.49
	LABOR TOTAL	733.25	$ 79,417.61
PINF.03 - INF Beamline Construction			
PINF.03.01 - INF Photon Delivery System Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	440.25	$ 65,507.00
	Labor_Mechanical Engineer_NO1	350.80	$ 33,979.31
	Labor_Mechanical Designer_NO2	175.40	$ 14,459.50
	Labor_Scientific Associate_NS3	158.25	$ 12,909.53
	Labor_Mechanical Technician_NO3	198.00	$ 15,254.67
	LABOR TOTAL	1,322.70	$ 142,110.01
MATERIAL	Material_Material (Purchase <$25k)_NMA	200,000.00	$ 261,774.64
	MATERIAL TOTAL	200,000.00	$ 261,774.64
PINF.03.02 - INF Photon Delivery System Installation and Test			
LABOR	Labor_EL - Vacuum Engineer_SE5	40.00	$ 4,540.52
	Labor_EL - Vacuum Technician_SE6	100.00	$ 8,500.15
	Labor_ME - Survey Engineer_MO1	50.00	$ 5,008.70
	Labor_EL - Survey Technician_SE2	125.00	$ 10,625.18
	Labor_Building Trades Unassigned_NST	8.00	$ 1,021.91
	Labor_Plant Engineering-Building Trades Carpenter_BTC	40.00	$ 4,867.50
	Labor_Plant Engineering-Building Trades Riggers_BTS	140.00	$ 17,036.25
	Labor_Scientist_NS1	220.00	$ 33,306.70
	Labor_Mechanical Engineer_NO1	140.00	$ 13,809.42
	Labor_Mechanical Designer_NO2	70.00	$ 5,892.86
	Labor_Mechanical Technician_NO3	198.00	$ 15,254.67
	Labor_Scientific Associate_NS3	88.00	$ 7,281.06
	LABOR TOTAL	1,219.00	$ 127,144.92
PINF.03.03 - INF End Station Procurement and Fabrication			
LABOR	Labor_Scientist_NS1	1,320.00	$ 193,293.30
	Labor_Mechanical Engineer_NO1	529.20	$ 50,791.66
	Labor_Mechanical Designer_NO2	229.40	$ 18,804.75
	Labor_Scientific Associate_NS3	633.75	$ 51,318.22
	Labor_Mechanical Technician_NO3	462.00	$ 35,083.84
	LABOR TOTAL	3,174.35	$ 349,291.77
MATERIAL	Material_Material (Purchase >$25k)_NSM	1,500,000.00	$ 1,883,882.23
	MATERIAL TOTAL	1,500,000.00	$ 1,883,882.23
PINF.03.04 - INF End Station Installation and Test			
LABOR	Labor_Scientist_NS1	660.00	$ 100,066.80
	Labor_Mechanical Engineer_NO1	212.00	$ 20,919.69
	Labor_Mechanical Designer_NO2	106.00	$ 8,927.01
	Labor_Mechanical Technician_NO3	462.00	$ 35,608.34
	Labor_Scientific Associate_NS3	352.00	$ 29,148.21
	LABOR TOTAL	1,792.00	$ 194,670.06
PINF.04 - INF Beamline Infrastructure			
PINF.04.01 - INF Hutches			
MATERIAL	Material_Material (Purchase >$25k)_NSM	320,000.00	$ 397,400.15
	MATERIAL TOTAL	320,000.00	$ 397,400.15
PINF.04.02 - INF Mechanical Utilities			
LABOR	Labor_ME - Utility Engineer_MO3	137.00	$ 13,381.11
	Labor_Mechanical Designer_NO2	110.00	$ 8,948.18
	Labor_EL - Utility Technician_SE4	343.00	$ 28,799.01
	Labor_Plant Engineering-Building Trades Carpenter_BTC	8.00	$ 968.60
	Labor_Building Trades Unassigned_NST	32.00	$ 4,067.04
	Labor_Plant Engineering-Building Trades Plumber_BTP	17.00	$ 2,058.27
	LABOR TOTAL	647.00	$ 58,222.21
MATERIAL	Material_Material (Purchase <$25k)_NMA	20,000.00	$ 25,619.46
	Material_Material (Purchase >$25k)_NSM	10,000.00	$ 12,173.94
	MATERIAL TOTAL	30,000.00	$ 37,793.40
PINF.04.03 - INF Electrical Utilities			
LABOR	Labor_Electrical Engineer_NE1	73.00	$ 8,198.69
	Labor_Electrical Designer_NE2	48.00	$ 4,191.07
	Labor_Plant Engineering-Building Trades Electrician_BTE	571.00	$ 69,353.57
	LABOR TOTAL	692.00	$ 81,743.33
MATERIAL	Material_Material (Purchase <$25k)_NMA	40,000.00	$ 52,366.20
	MATERIAL TOTAL	40,000.00	$ 52,366.20
PINF.04.04 - INF EPS			
LABOR	Labor_Controls Engineer_NE4	310.00	$ 34,856.17
	Labor_Electrical Technician_NE3	340.00	$ 28,637.03
	Labor_Electrical Designer_NE2	40.00	$ 3,536.08

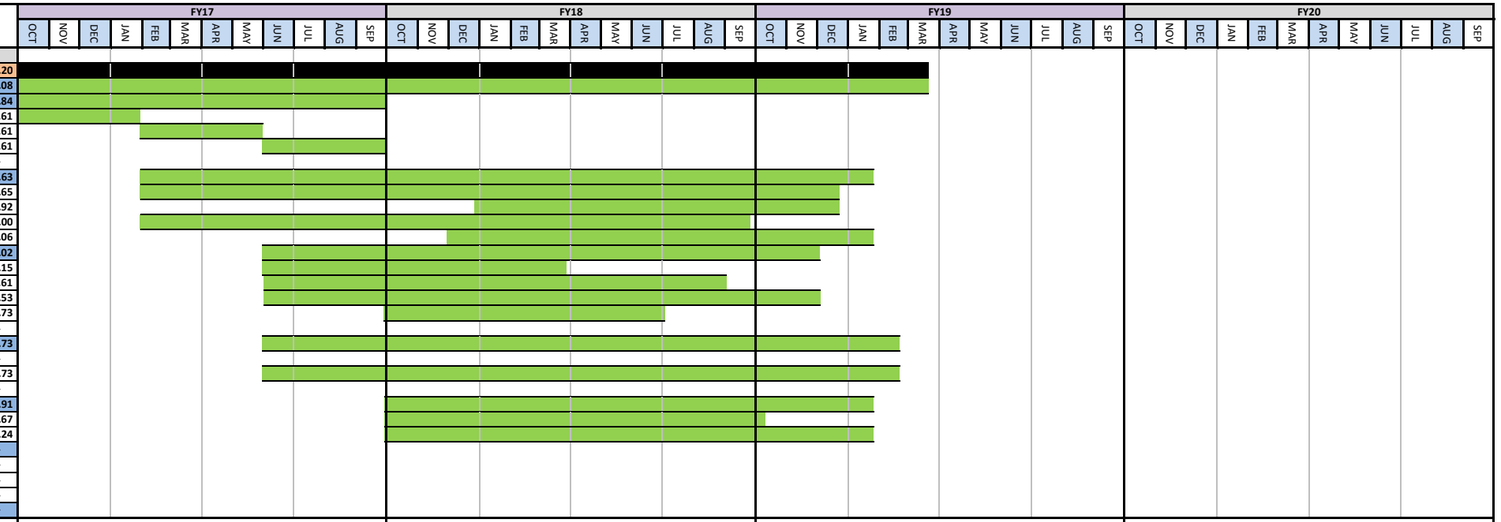
	LABOR TOTAL	690.00	$	67,029.28
MATERIAL	Material_Material (Purchase >$25k)_NSM	27,000.00	$	33,921.45
	MATERIAL TOTAL	27,000.00	$	33,921.45
PINF.05 - INF Accelerator Infrastructure				
PINF.05.02 - INF Source				
MATERIAL	Material_Material (Purchase >$25k)_NSM	980,000.00	$	1,234,416.73
	MATERIAL TOTAL	980,000.00	$	1,234,416.73
PINF.06 - INF Controls				
PINF.06.01 - INF Basic System Controls				
LABOR	Labor_Controls Engineer_NE4	1,132.00	$	127,517.05
	Labor_Electrical Technician_NE3	234.00	$	19,709.02
	Labor_IT Professional (Software)_NA7	194.00	$	18,632.57
	LABOR TOTAL	1,560.00	$	165,858.64
MATERIAL	Material_Material (Purchase <$25k)_NMA	97,000.00	$	127,019.03
	MATERIAL TOTAL	97,000.00	$	127,019.03
PINF.06.02 - INF Instrument Applications				
LABOR	Labor_Controls Engineer_NE4	2,000.00	$	224,956.64
	Labor_IT Professional (Software)_NA7	1,920.00	$	184,404.86
	Labor_Assistant/Associate Scientist_NS2	440.00	$	45,483.97
	Labor_Electrical Technician_NE3	-	$	-
	LABOR TOTAL	4,360.00	$	454,845.47
MATERIAL	Material_Material (Purchase <$25k)_NMA	36,000.00	$	47,254.77
	MATERIAL TOTAL	36,000.00	$	47,254.77

Project: INF Beamline — RESOURCE SUMMARY

WBS	RESOURCE	UNITS		COST
PINF - INF Beamline				
LABOR	Labor_Scientist_NS1	4,840.00	$	712,331.36
	Labor_Administrative Secretary_NA3	440.00	$	24,422.06
	Labor_ES&H Professional_NA4	660.00	$	77,465.10
	Labor_QA Professional_NA5	440.00	$	48,353.23
	Labor_Administrative_NA2	836.00	$	62,424.41
	Labor_Human Resources_NB4	220.00	$	16,427.48
	Labor_Mechanical Engineer_NO1	1,760.00	$	169,506.35
	Labor_Mechanical Designer_NO2	954.80	$	78,371.36
	Labor_Scientific Associate_NS3	1,760.00	$	142,679.49
	Labor_Mechanical Technician_NO3	1,320.00	$	101,201.53
	Labor_EL - Vacuum Engineer_SE5	40.00	$	4,540.52
	Labor_EL - Vacuum Technician_SE6	100.00	$	8,500.15
	Labor_ME - Survey Engineer_MO1	50.00	$	5,008.70
	Labor_EL - Survey Technician_SE2	125.00	$	10,625.18
	Labor_Building Trades Unassigned_NST	40.00	$	5,088.95
	Labor_Plant Engineering-Building Trades Carpenter_BTC	48.00	$	5,836.10
	Labor_Plant Engineering-Building Trades Riggers_BTS	140.00	$	17,036.25
	Labor_ME - Utility Engineer_MO3	137.00	$	13,381.11
	Labor_EL - Utility Technician_SE4	343.00	$	28,799.01
	Labor_Plant Engineering-Building Trades Plumber_BTP	17.00	$	2,058.27
	Labor_Electrical Engineer_NE1	73.00	$	8,198.69
	Labor_Electrical Designer_NE2	88.00	$	7,727.15
	Labor_Plant Engineering-Building Trades Electrician_BTE	571.00	$	69,353.57
	Labor_Controls Engineer_NE4	3,442.00	$	387,329.86

Project Name: INF Beamline

WBS	Start	Finish	Cost
PINF - INF Beamline	10/1/2016	3/20/2019	$ 6,460,810.20
PINF.01 - INF Management	10/1/2016	3/20/2019	$ 505,813.08
PINF.02 - INF Design	10/1/2016	9/28/2017	$ 238,252.84
PINF.02.01 - INF Conceptual Design	10/1/2016	1/29/2017	$ 79,417.61
PINF.02.02 - INF Preliminary Design	1/30/2017	5/30/2017	$ 79,417.61
PINF.02.03 - INF Final Design	5/31/2017	9/28/2017	$ 79,417.61
PINF.02.04 - INF R&D Program			$ -
PINF.03 - INF Beamline Construction	1/30/2017	1/25/2019	$ 2,958,873.63
PINF.03.01 - INF Photon Delivery System Procurement and Fabrication	1/30/2017	12/22/2018	$ 403,884.65
PINF.03.02 - INF Photon Delivery System Installation and Test	12/27/2017	12/22/2018	$ 127,144.92
PINF.03.03 - INF End Station Procurement and Fabrication	1/30/2017	9/25/2018	$ 2,233,174.00
PINF.03.04 - INF End Station Installation and Test	11/30/2017	1/25/2019	$ 194,670.06
PINF.04 - INF Beamline Infrastructure	5/31/2017	12/3/2018	$ 728,476.02
PINF.04.01 - INF Hutches	5/31/2017	3/27/2018	$ 397,400.15
PINF.04.02 - INF Mechanical Utilities	6/1/2017	9/1/2018	$ 96,015.61
PINF.04.03 - INF Electrical Utilities	6/1/2017	12/3/2018	$ 134,109.53
PINF.04.04 - INF EPS	9/28/2017	7/2/2018	$ 100,950.73
PINF.04.05 - INF PPS			$ -
PINF.05 - INF Accelerator Infrastructure	5/31/2017	2/20/2019	$ 1,234,416.73
PINF.05.01 - INF Front End			$ -
PINF.05.02 - INF Source	5/31/2017	2/20/2019	$ 1,234,416.73
PINF.05.03 - INF Straight			$ -
PINF.06 - INF Controls	9/29/2017	1/25/2019	$ 794,977.91
PINF.06.01 - INF Basic System Controls	9/29/2017	10/10/2018	$ 292,877.67
PINF.06.02 - INF Instrument Applications	9/29/2017	1/25/2019	$ 502,100.24
PINF.07 - INF Conventional Facilities			$ -
PINF.07.01 - INF Conventional Facilities Design			$ -
PINF.07.02 - INF Conventional Facilities Construction			$ -
PINF.07.03 - INF Conventional Facilities Commissioning			$ -
PINF.08 - INF Special Equipment			$ -



RATE SET: Rate Set 1