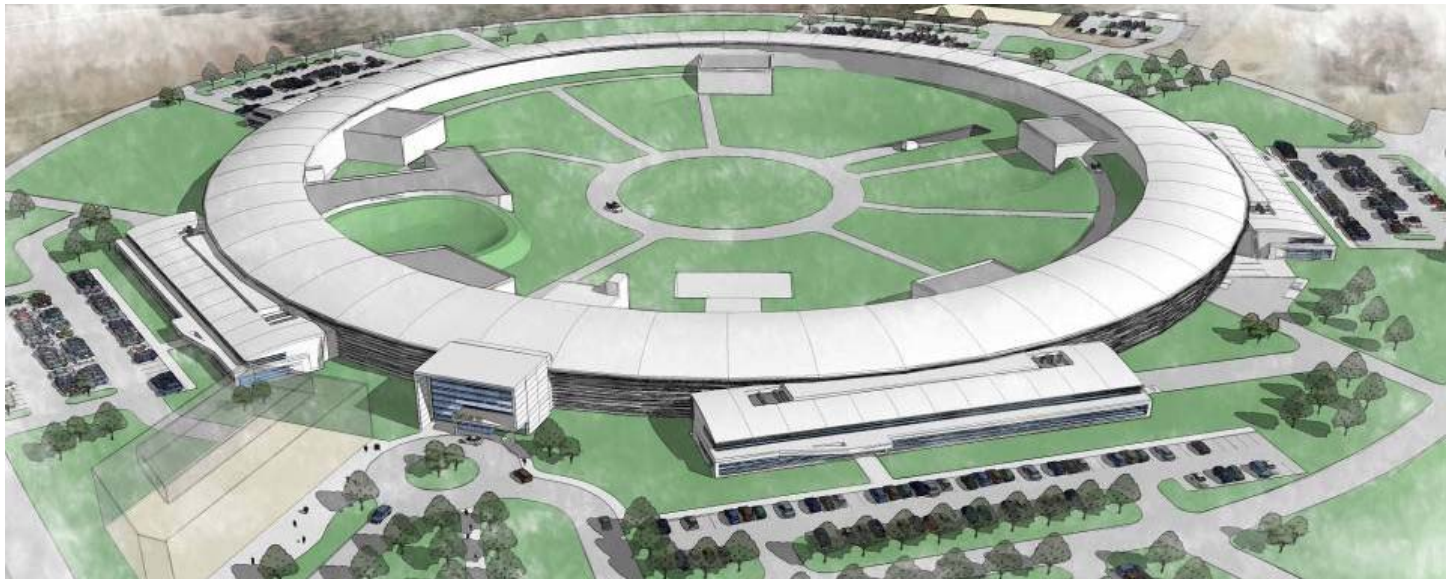
National Synchrotron Light Source II



Damping Wiggler Beamline: XAS

Paul Northrup
October 4th, 2007
EFAC Review

Office of Science
U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY
BROOKHAVEN SCIENCE ASSOCIATES

Overall Mission

- To provide a versatile and highly productive facility for applications of X-ray Absorption Spectroscopy in a wide range of scientific disciplines:
  - material science & catalysis
  - nanomaterials research
  - environmental science & geology
  - life sciences & biology
- To pursue cutting-edge capabilities and techniques appropriate to the advanced quality of the NSLS-II source

User Community Input

- Community leaders and prospective BAT members:
  - NSLS UEC and EXAFS Special Interest Group
  - NSLS PRTs and other facilities' staff
  - Scientific community representatives
- Workshops:
  - NSLS-II User Workshop July 2007, breakout sessions
    - XAS Beamline
    - Catalysis, Environmental Science, Life Sciences, High Pressure
  - Catalysis, Spring 2007
  - Environmental Science/Low-temp Geochemistry, July 2007
  - Planned XAS Beamline Workshop January 2008
- NSLS-II Technical Design Review, Sept. 12 2007

Scientific Mission -- Applications:

- High Flux:
  - Lower concentration limits:
    - Catalysts *in-situ*, real-world environmental concentrations,
    - Dispersed nanoparticles, dilute metal-organic complexes
  - Rapid, high-quality measurements:
    - Greater productivity
    - Time-resolved (minutes) studies
  - Higher energy resolution:
    - Sharp near-edge features (electronic transitions): Cr, Fe
    - Small shifts in features: Mn, As, U,
    - Resolving mixtures of known components: Cu, Hg

Scientific Mission -- Applications:

- Wide Energy Range (5-90 keV) Source:
  - Access higher-energy K edges
    - Penetrate large-volume high-pressure or catalytic cells
    - Probe buried regions or interfaces in samples
- High Brightness:
  - Focus (macro): tune spot size to sample needs
  - Microbeam XAS
  - Surface science
    - Dilute (sub-monolayer)
    - Grazing-incidence/reflectivity
    - Polarization-dependent

Beamline Requirements and Specifications

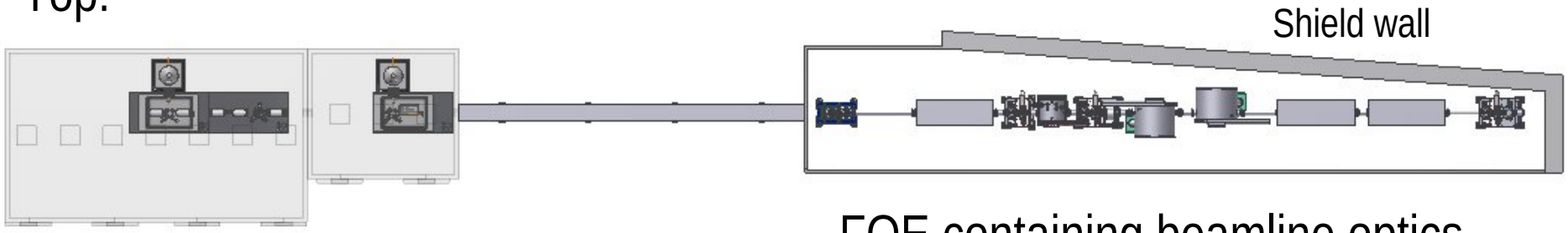
Source requirements:

- Broad spectrum, high flux
- Stability:
  - position within 10% of source size,
  - Vertical angle within 1 μrad (for monochromatic energy stability)

- Specifications:
  - Energy range: 5-50 keV, provisions to use up to 90 keV
  - Tunable spot size from 0.2 x 0.2 mm to 5 x 40 mm
  - Microbeam (1 x 1 micron) available
  - Energy resolution: standard (10^{-4}), and high (10^{-5}) modes available
  - Controlled sample environment (air-sensitive or hazardous samples)
  - Beamline stability scan-to-scan: position on sample within 5 microns, energy calibration within 0.1 eV

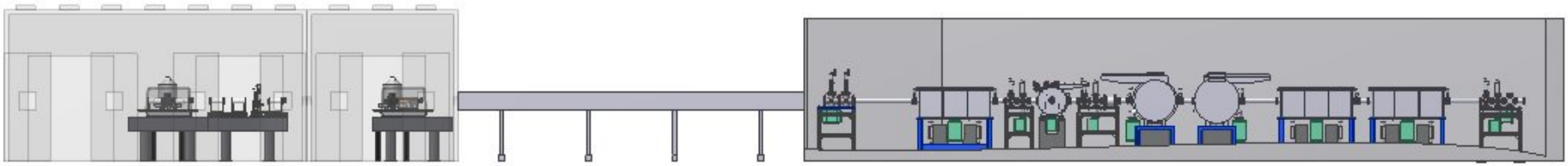
Beamline Layout -- Overview

Top:



FOE containing beamline optics and white-beam components

side:



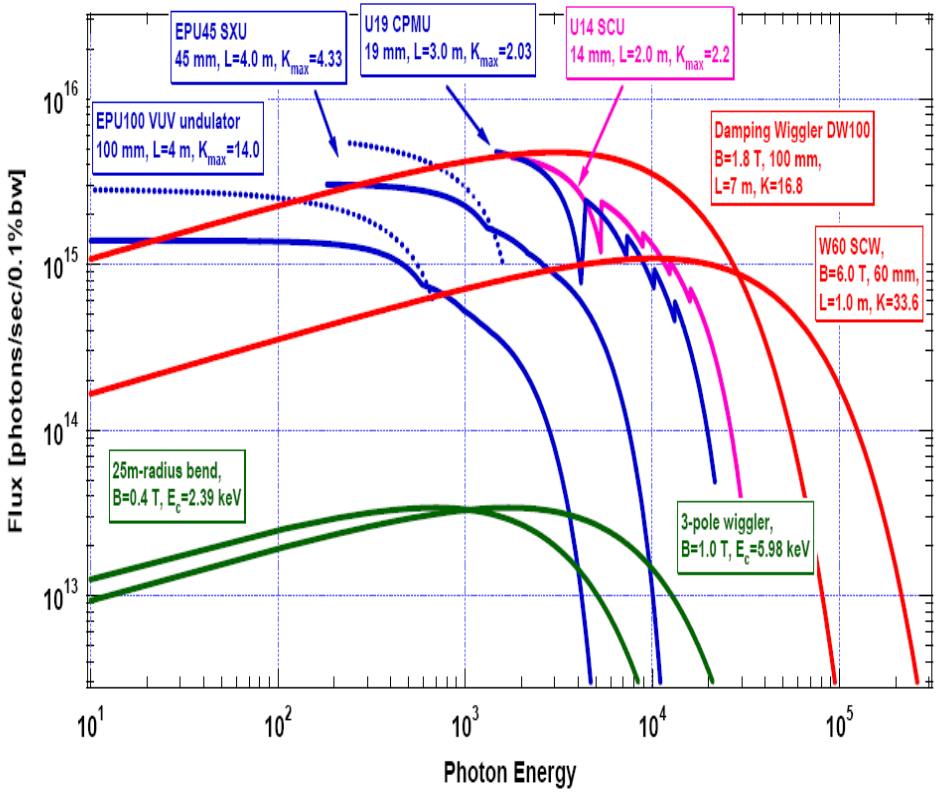
Experimental Hutches: 1- microbeam, 2- bulk (with three sample positions)

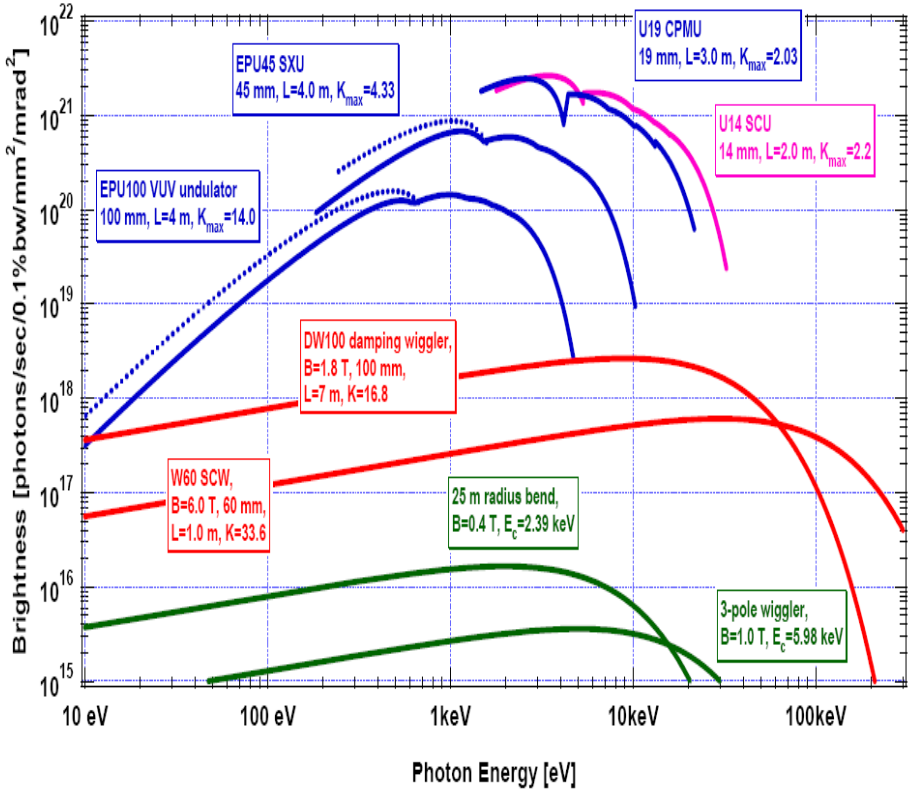
Insertion Device

- Damping Wiggler (7m or 3.5m) in high-beta straight section
- Predicted performance compared to existing facilities:
  - NSLS-II beamline will significantly outperform (in flux and brightness) any existing XAS facility worldwide
- Future upgrade: two canted 3.5m wigglers independently serving microbeam and bulk endstations

Damping Wiggler Characteristics

Flux & brightness:





Highest hard X-ray flux at NSLS-II

Highest brightness of broad-spectrum sources

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Damping Wiggler Characteristics

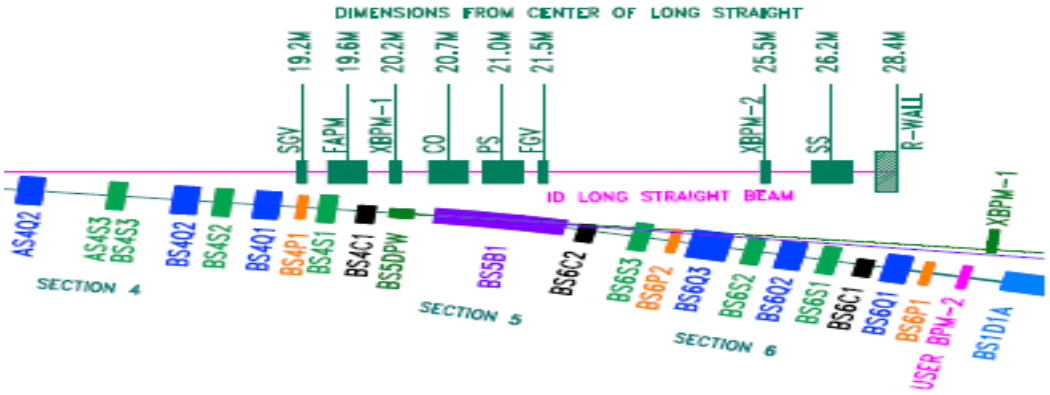
Heat load considerations

- Wiggler output 65 kW, 8 kW reaches beamline optics
- Challenging to maintain broad energy range, stability
- "Divide and conquer" approach
  - front end mask and white-beam apertures 57-65 kW (all but 8 kW)
  - filters, Be window, and attenuators 0-5 kW
  - white-beam mirror 0-7 kW
  - monochromator first crystal 0.3-2.5 kW
  - monochromator second crystal (scatter)
- Preliminary thermal analyses show that this can be done

- Heat load on sample may be significant (>100 mW)

Front End Layout

- Standard front end with white-beam apertures
  - 0 to 0.15 mrad vertical, 0 to 1.0 mrad horizontal
- Accommodations for future upgrade (canting)
  - Space for additional sets of apertures, safety shutters
  - Space for mirror to divert lower-energy beam

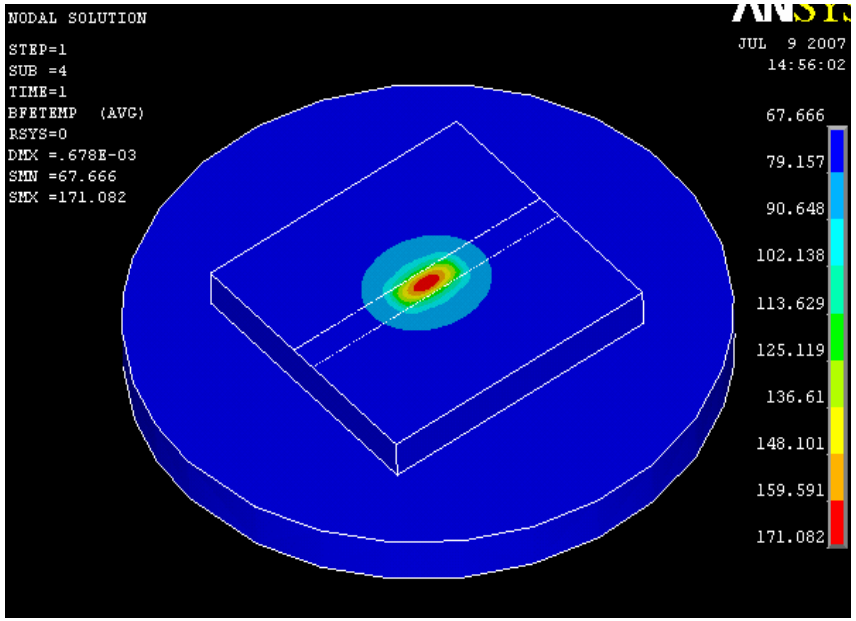


White Beam Components

- Retractable attenuators, sequentially added for higher energy experiments
- White-beam mirror (Si substrate)
  - Two “stripes” (bare Si and Pt-coated) available
  - Three positions: 2.0 or 3.15 mrad, or removed from beam
    - Cover required energy range
  - Vertical collimation and harmonics rejection
  - Cooled for heatload sharing
  - Thermal analysis: mirror can handle up to 7 kW with slope errors corrected by bend mechanism.

White Beam Components

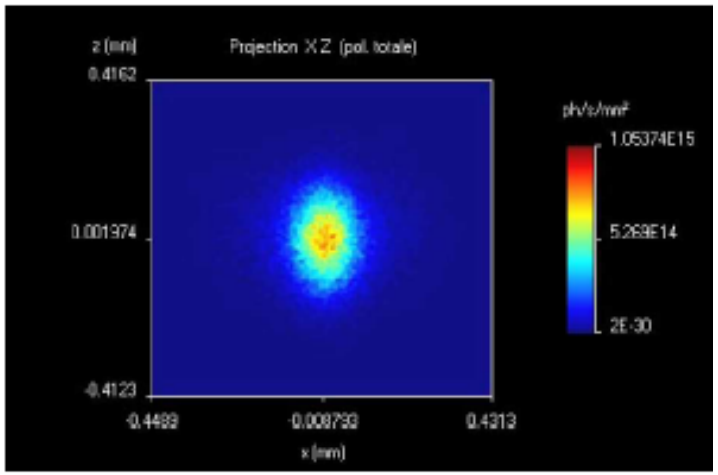
- Monochromator:
  - LN2 cooled first and second crystals
  - Side-by-side sets: Si(111) and Si(311)
  - Thermal analysis: direct-cooled crystal can handle 2.3 kW with tolerable slope error…
  - But further FEA is required
    - Full range of configurations
    - Refine crystal design and beamline configurations



Beam Conditioning Optics

- High energy resolution (10^{-5} or better) monochromator
  - In series with high-heatload monochromator (passes beam when not in use)
  - No cooling required, high precision mechanism
  - Crystals to be determined (less restrictions on material)
  - Synchronization with primary monochromator is required
- Focusing mirror (2:1 toroidal)
  - Two toroidal “stripes” match Mirror 1
  - Reflects in opposite sense

Initial ray tracing:



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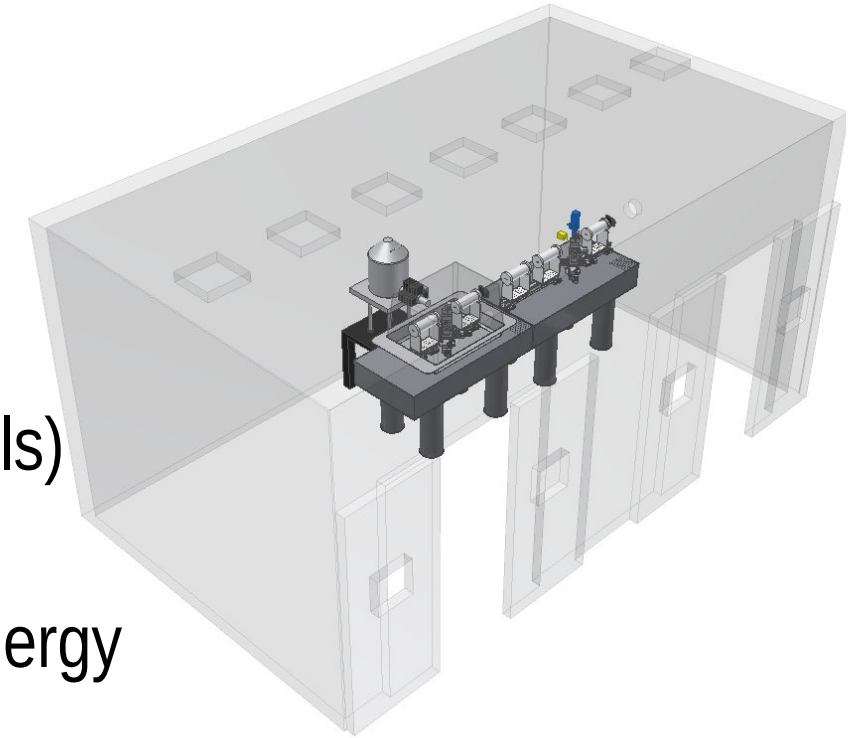
Endstation 2: Bulk XAS

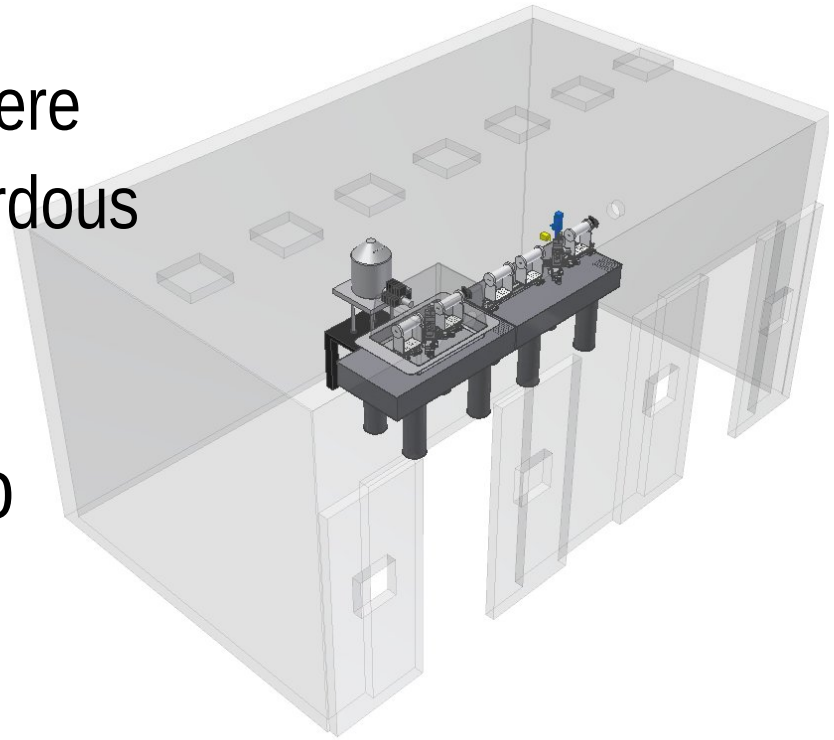
Three sample positions:

- 1) Classic benchtop XAS
  - Transmission, fluorescence and grazing-incidence geometries
  - In-situ measurements (electrochemical and solution cells)
  - Heater, cryostat and LN2 cooling
  - Standard and high-resolution (energy selective) detectors
  - Detector for powder XRD pattern, monitoring



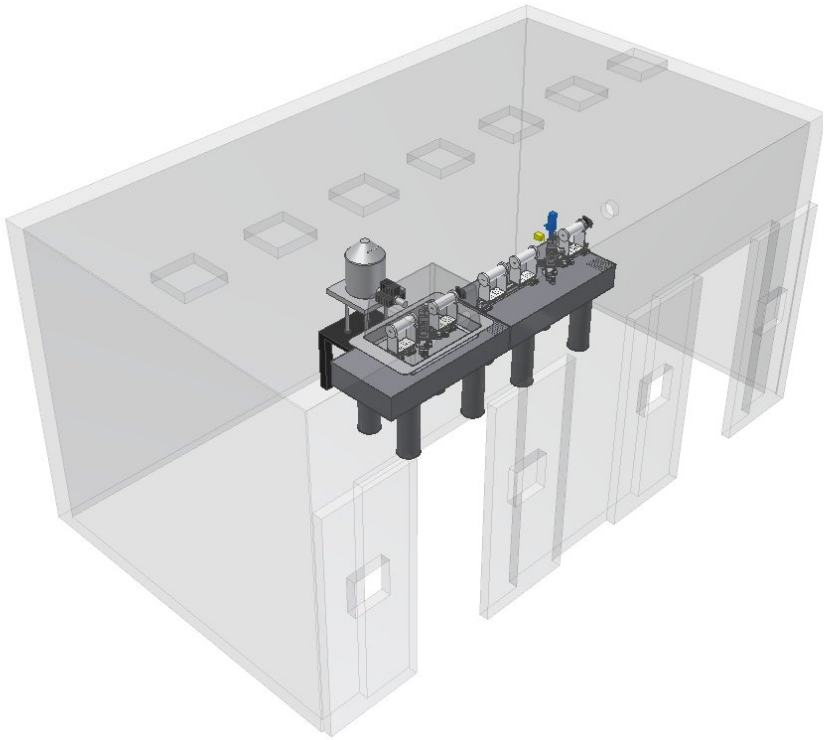
Endstation 2: Bulk XAS

- 2) Controlled environment XAS
- Multi-use enclosure:
  - Glove box for controlled atmosphere
  - Containment/fume hood for hazardous samples
  - Open-air
- Hazardous, radioactive, or nano materials
- Multi-element detector for low-concentration samples



Endstation 2: Bulk XAS

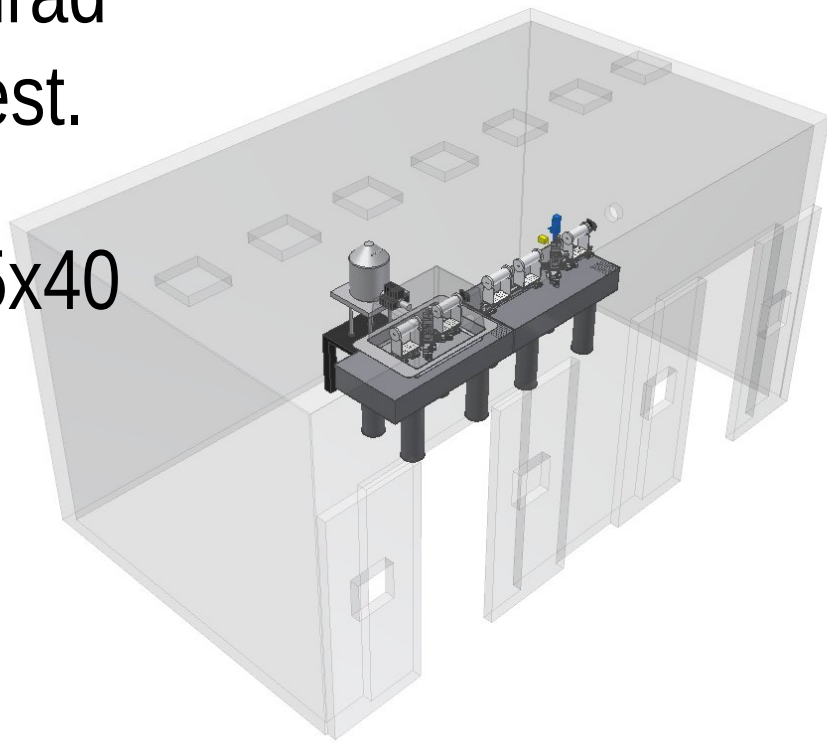
- 3) Space for move-in apparatus
  - Large-volume high-pressure or catalytic cells
  - High-field magnet
  - Available control and data channels, utilities, etc.



Endstation 2: Bulk XAS

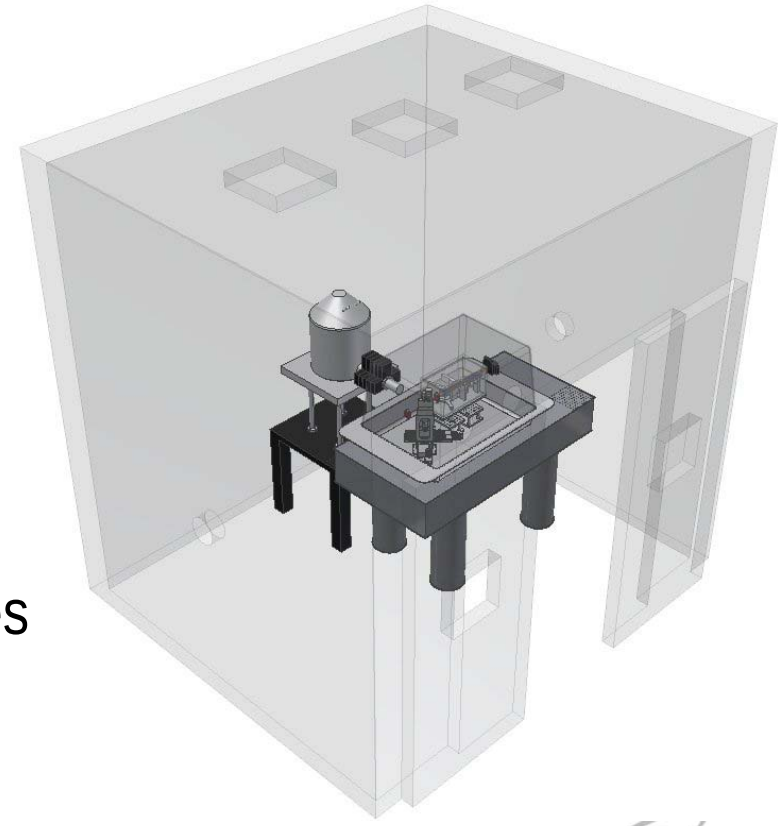
Performance:

- Acceptance up to 0.15 x 1.0 mrad
- Flux 8.3x10^{13} ph/sec (prelim. est. at 8 keV)
- Spot size ~0.2x0.2 mm up to 5x40 mm
- Continuous-scan or step-scan modes of data collection



Endstation 1: Microbeam XAS

- Microfocusing optics: conventional K-B mirrors
- Multi-element detector
- Multi-use enclosure (as described for Endstation 2)
- Acceptance:
  - up to 0.07 x 0.07 mrad on-axis
- Flux:
  - 3×10^{12} ph/sec (prelim. est. at 8 keV)
- Spot size ~1 micron
- Applications:
  - Microbeam and single-crystal XAS
  - Components of heterogeneous samples
  - Diamond anvil cell high-P XAS



Requirements Imposed:

On Conventional Facilities

- Exhaust from multi-use enclosures

On Accelerator

- Future canting
  - Current design based on at least 3.1 mrad for full separation

Outstanding Issues

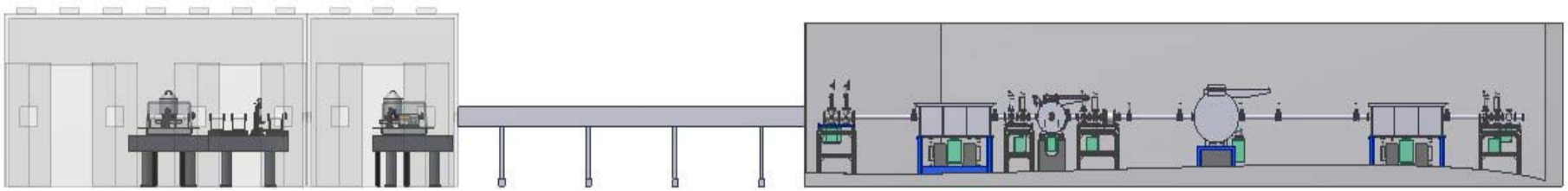
- Key design questions, and decisions still to be made:
  - More specific detector selection: to be addressed at beamline workshop in January 2008
  - Complete (and cumulative) thermal analyses of all components in several configurations
    - Power density and energy profile
  - Canting angle: to be negotiated with accelerator division
- Risks, and mitigation strategies:
  - Heat load challenge: refine component design and adjust configurations (filters, acceptance, energy range…)
  - Canting separation: if smaller angle is necessary, mirror and monochromator designs may need to be changed

Cost Estimate

1.04.05.05 Damping Wiggler Beamline 1 - XAS: Total	$10,671,923.00
1.04.05.05.01 Beamline Enclosures	$1,212,499.00
1.04.05.05.02 Beam Transport	$409,495.00
1.04.05.05.03 Utilities	$227,668.00
1.04.05.05.04 Specialized White Beam Components	$472,353.00
1.04.05.05.13 High Heatload Optics	$2,127,744.00
1.04.05.05.05 Specialized Beam Conditioning Optics	$1,583,678.00
1.04.05.05.06 Personnel Safety System	$183,352.00
1.04.05.05.07 Equipment Protection System	$86,038.00
1.04.05.05.08 Endstation 1	$752,988.00
1.04.05.05.09 Endstation 2	$1,967,186.00
1.04.05.05.10 Beamline Controls	$147,727.00
1.04.05.05.11 Beamline Control Station	$38,902.00
1.04.05.05.12 Beamline Management	$1,462,293.00

Summary: Initial Project Scope

- Both endstations included, one control station
- Single source serving both endstations
- One set of beamline optics
- Endstation 2 hutch can be accessed for set-up while Endstation 1 is in use; but not vice versa
- Includes accommodations (space, component design) for future canting of source



Potential Upgrade/Build-out Path

- Two canted wiggler sources
- Add beamline optics components to provide independent second beam for microbeam endstation
- Possible addition of mirror in front end to divert low-energy portion of overlapped fans into a third endstation for complementary 2-6 keV applications
- Net potential: 3 independent XAS endstations covering 2-90 keV energy range and microbeam capability