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Strategic Planning for Science at the Advanced Photon Source

George Srajer

X-ray Science Division - APS

3-Way Meeting

March 18, 2008

Outline

1. Introduction
   - Beamlines at the APS

2. Planning Process
   - Midterm
   - Long Term
   - New Beamlines

3. Summary

1. Beamlines at the APS

Two flavors:

- **Facility-operated** $\Rightarrow$ *X-ray Operations and Research (XOR)*

  30 beamlines (out of 55 beamlines total)

- **Independently-operated** $\Rightarrow$ *Collaborative Access Teams (CAT)*

  DuPont-Northwestern-Dow (DND) CAT

  Materials Research (MR) CAT

  GeoScience Environmental Science (GSECARS) CAT

  Chemistry/Materials (ChemMatCARS) CAT

  High Pressure (HP) CAT

  Biophysics (Bio) CAT

1. Independently-Operated Beamlines, Continued

- **Independently-operated** $\Rightarrow$ *Macromolecular Crystallography*

  Biological Sciences (BioCARS) CAT

  Industrial Macromolecular Crystallography Association (IMCA) CAT

  Structural Biology Center (SBC) CAT

  Life Sciences (LS) CAT

  Southeast Regional (SER) CAT

  General Medicine/Cancer Institute (GM/CA) CAT

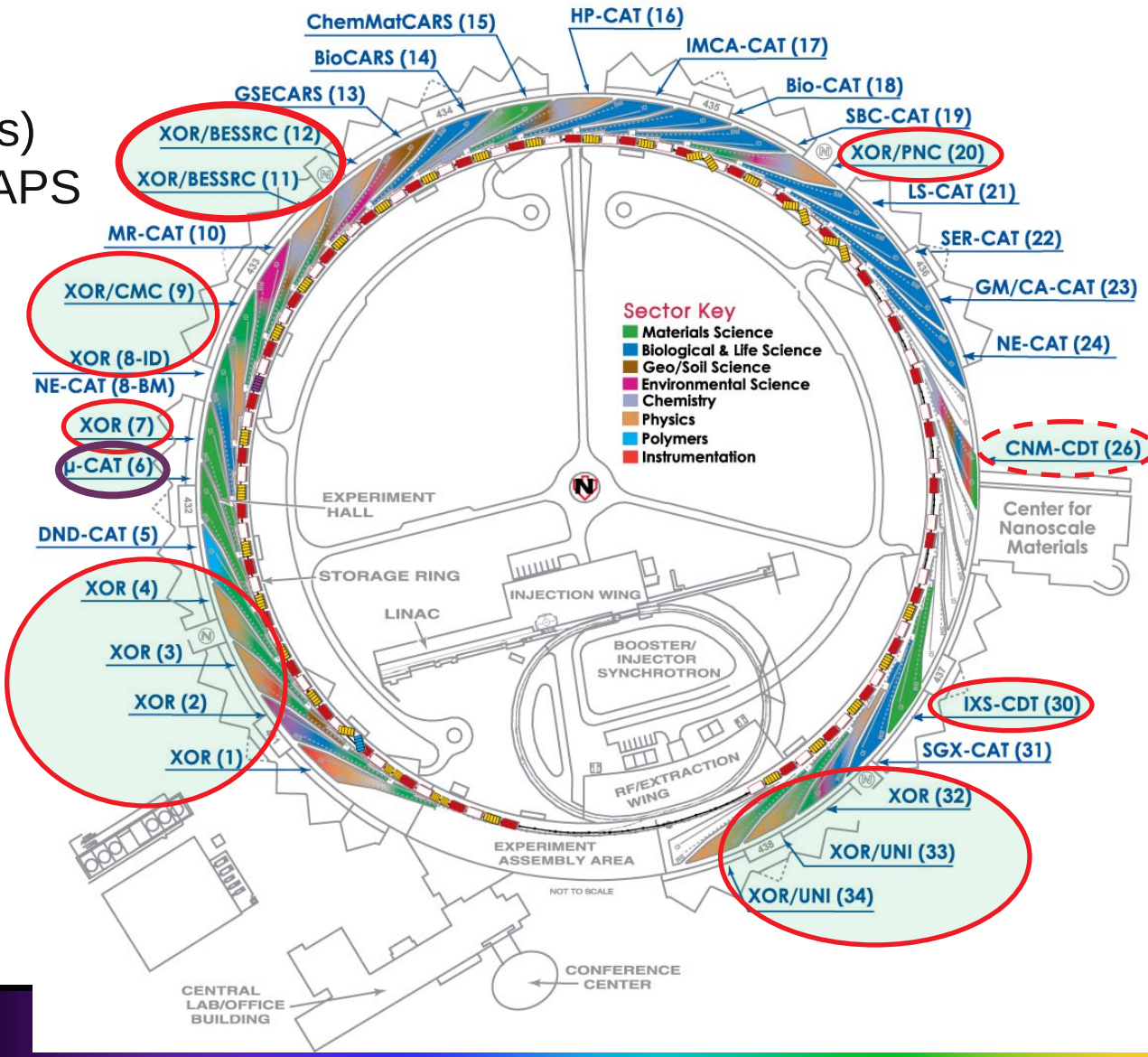
  Northeastern (NE) CAT

  Structural Genomix (SGX) CAT

XOR Today:

16 Sectors
(30 beamlines)
operated by APS

MU-CAT (sector 6) transition to XOR begun in Oct. 2007



Joint operation with CNM

2. Planning Process

Two parts:

Midterm (next 5 years) ⇒ Facility and beamlines enhancements

(1) Beamlines upgrades

- **detectors**
- **instrumentation and infrastructure**
- **software**
- **optics**

(2) X-ray source enhancements

- **specialized undulators**
- **customized timing structures**
- **higher current (~ 200 mA)**
- **extended (8m or 12m) straight sections**

Long term (beyond 5 years) ⇒ Possibly a new source

Midterm Enhancement Proposal

Ground rules:

- **Proposals have to be *science driven***
- **Input by Advisory Committees critical**
- **Time frame (all dates in 2008)**

  - March 28: deadline for written proposals

  - May 5: preliminary plan to be discussed at the Users Meeting

  - May-October: proposal to be refined

Long Term Enhancement Proposal

Discussions have been on-going in the last 1.5 years

Possible ERL and scientific implications using

- **Imaging**
- **Coherence**
- **Timing**

The plan is to discuss enhancement proposals at the:

***Future of the APS* Planning Workshop on October 20-21, 2008**

Final document to follow

Contributors in the Enhancements Planning

- Originate from individual beamlines

- Discussions with Advisory Committees

- APS users organizations getting involved

⇒ *APS Users Organization Steering Committee*

⇒ *Partner Users Council (i.e. Contributing Users)*

⇒ Science Interest Groups, Round Tables, etc.

- APS Science Advisory Committee

XOR User Advisory Committees

Surface/Interface Scattering *(Peter Eng - Chair)*

Structural Characterization *(Angus Wilkinson - Chair)*

Microstructure/Mechanical Properties *(Matt Miller - Chair)*

Time-Resolved Spectroscopy and Scattering *(R. Schoenlein - Chair)*

Sector 8 *(Simon Mochrie - Chair)*

Sector 3 *(Brent Fultz - Chair)*

Sector 9 *(Kent Blasie - Chair)*

Sector 30 *(John Hill - Chair)*

Sector 4 *(Dario Arena - Chair)*

Sector 6 *(Alan Goldman - Chair)*

High Energy Wide Angle Scattering-PDF *(Angus Wilkinson-Chair)*

Small Angle X-Ray Scattering *(David Cookson - Chair)*

Spectroscopy *(Ed Stern - Chair)*

X-Ray Microscopy and Imaging *(Gayle Woloschak)*

Timeline Summary

(1) Midterm first draft to be completed by March 28, 2008

(2) Preliminary document completed by May 5 $\Rightarrow$ APS Users Meeting

(3) Document refinement from May to October, 2008

(4) APS Future (Midterm+Long Term) Plans at the October 20-21 Workshop

(5) Document to be finalized after the October Workshop

Looking into the Future Started in Summer 2004

Strategic planning for most compelling opportunities for the scientific growth areas in the next 5 - 10 years at the Advanced Photon Source

Proposed New Beamlines After 2004

Uncommitted sectors:

- **Intermediate Energy X-ray (NSF awarded; DOE funds promised)**
- **Advanced X-ray Imaging**
- **X-Ray Interfacial Science**
- **BioNanoprobe**
- **High Magnetic Field**

Existing beamlines:

- **Fuel Spray Radiography and Tomography (DOE funds)**
- **High Throughput Fluorescence Microscopy**

Intermediate Energy Beamline

Juan Carlos Campuzano (University of Illinois Chicago)

Peter Abbamonte (University of Illinois Urbana Champaign)

James Allen (University of Michigan)

Physics of materials with competing interactions

Similar energy scales for:

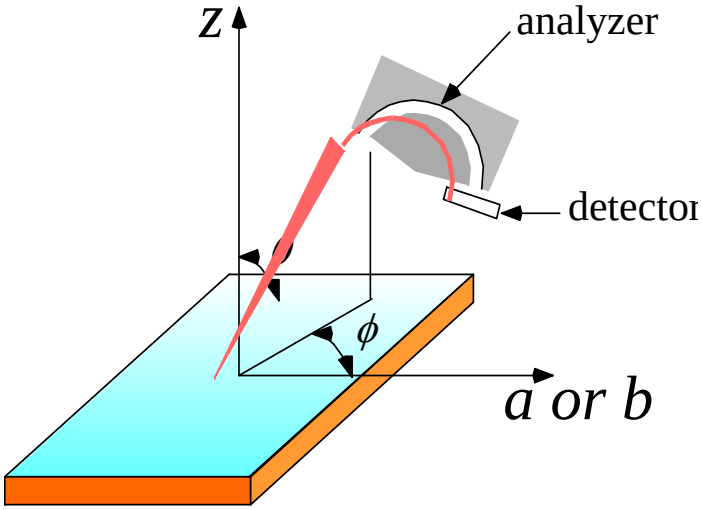
- Valence bonding
- Coulomb repulsion
- Kinetic energy of electrons

Examples:

- Manganese oxides $\Rightarrow$ *T or H* $\Rightarrow$ colossal magneto-resistance
- Copper oxides $\Rightarrow$ *Carrier density* $\Rightarrow$ AF, spin-glass, SC, metal
- Spin ladders $\Rightarrow$ *P* $\Rightarrow$ charge order, SC

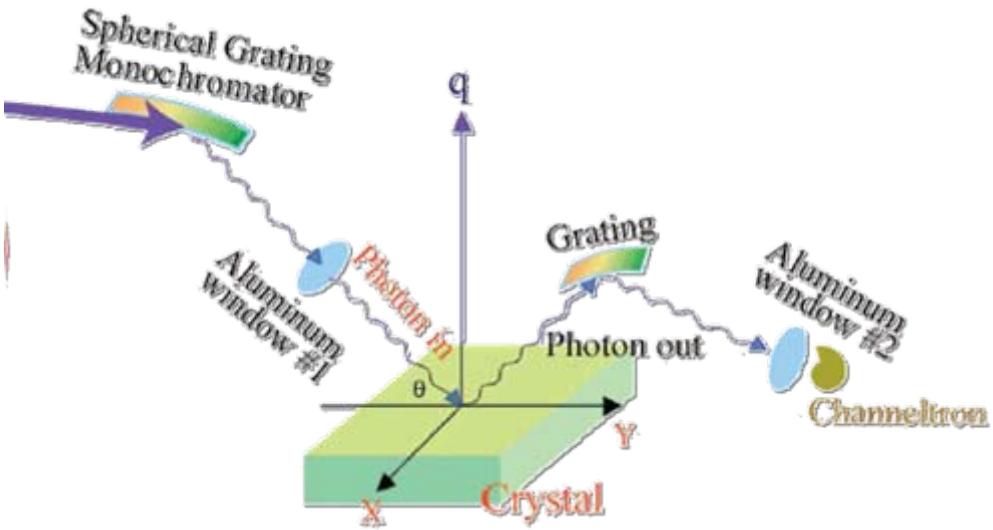
Techniques on the Intermediate Energy Beamline

Angle-Resolved Photoemission



$$\vec{k}^{f}_{//} = \vec{k}^{i}_{//} = \sqrt{\frac{2mE}{\hbar^2}} sin\theta$$

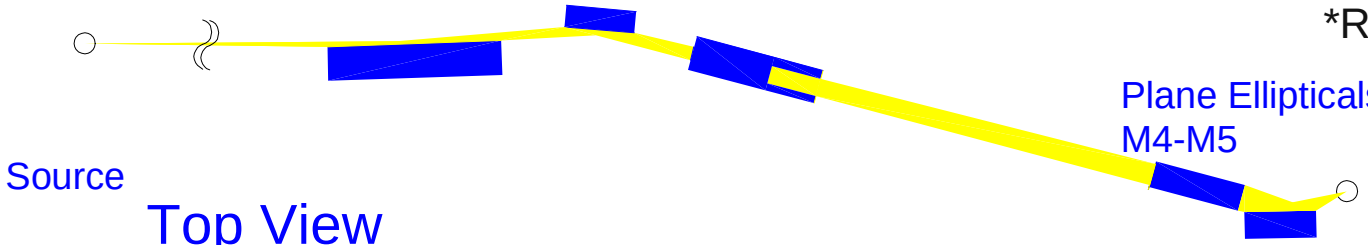
Resonant Scattering



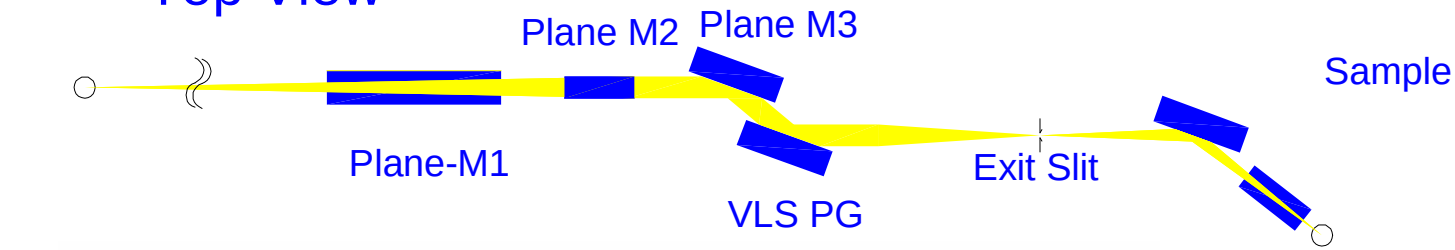
*Intermediate Energy Beamline: Layout**

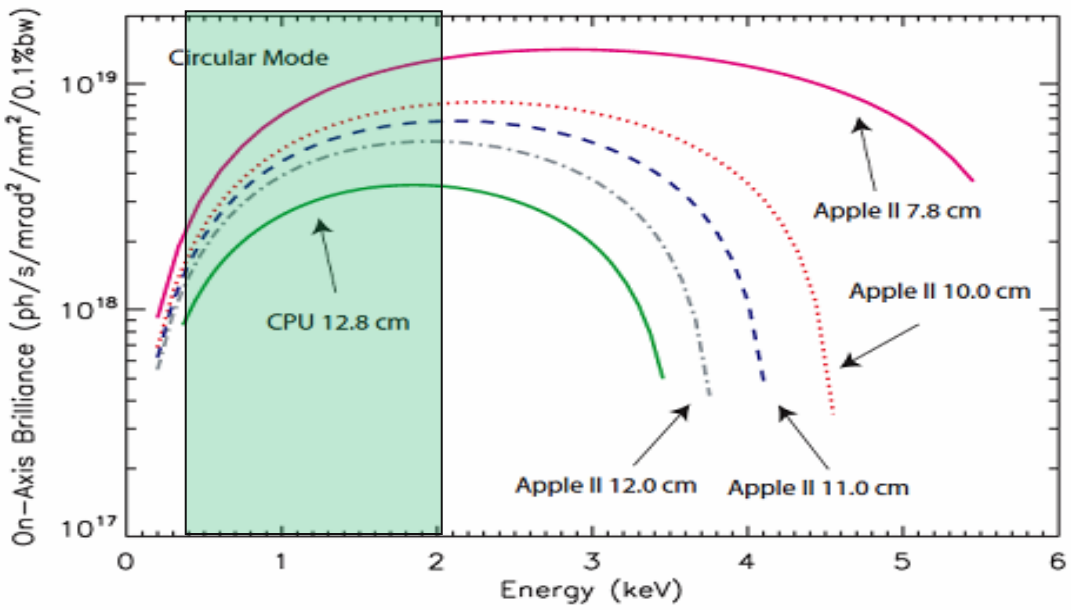
Side View

*R. Reininger



Top View





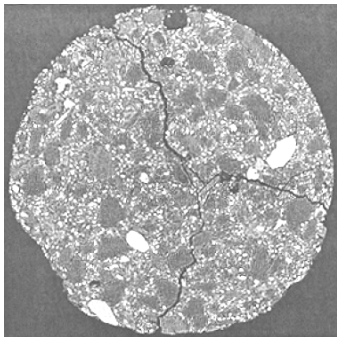
R. Dejus

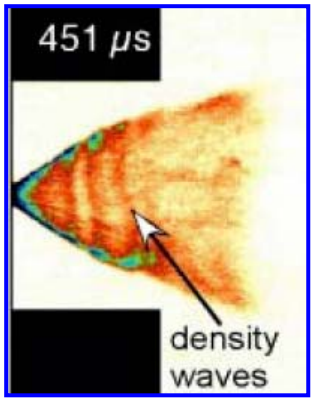
Advanced X-Ray Imaging

Jon Harrison (Arizona State University)
John Miao (UCLA)
Ian McNuty (APS)

Materials Science:

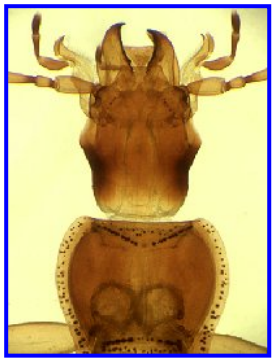
- ➔ Materials deformation, fatigue and fracture
- ➔ Failure mechanism in engineered structures
- ➔ Dynamic processes in extreme environments
- ➔ High-resolution imaging of nonperiodic structures





Biological Science:

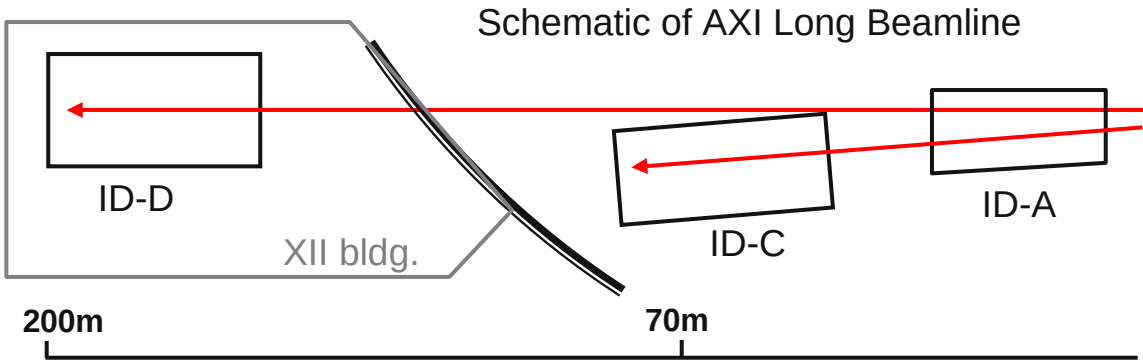
- ➔ Imaging of gene expression for discovery of gene function
- ➔ Real-time imaging of physiological processes
- ➔ Comparative biology on evolutionary transitions
- ➔ Discovery & description of early life in micro-fossils
- ➔ Medical imaging of weak-absorbing features



Proposed Long Beamline

X-ray Imaging Institute (XII) proposed by APS; Building may be funded by State of Illinois

Could enclose a 150-200m long imaging beamline, and provide office & lab (optics, detectors, etc.) spaces to staff and visitors

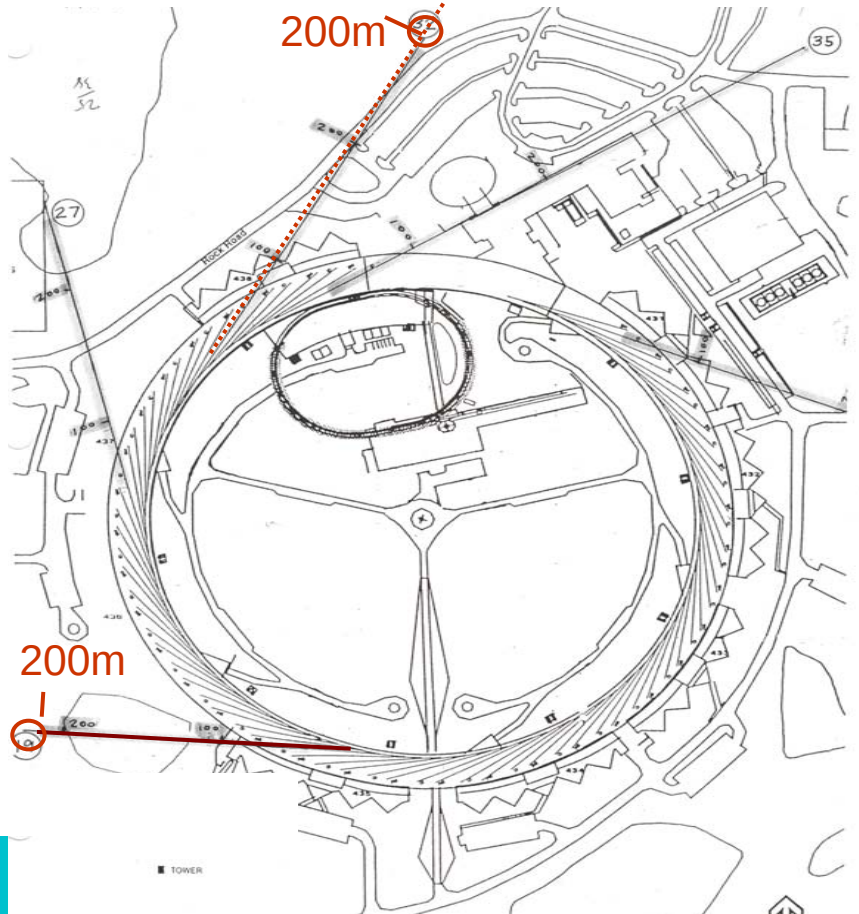


New Imaging Capabilities at Long BL

- High phase sensitivity:
  → internal defect & crack propagations in low-Z materials e.g. polymer foams & nanocomposites

- 100x field of view:
  → opens up comparative biology to larger animals – essential for understanding of evolutionary transitions
  → biomedical imaging and physiological studies on small animals such as mouse, critical for medical applications

- 20m-long CDI hutch:
  → unique at APS, allows the use of high-dynamic-range area detectors such as Pilatus pixel arrays for CDI → crucial in reaching <10nm resolution



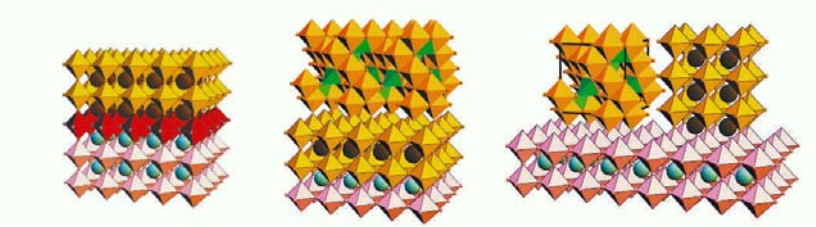
X-Ray Interfacial Science

Michael Bedzyk (Northwestern University)
Paul Fenter (Argonne National Laboratory)
Paul Fuoss (Argonne National Laboratory)

Materials Growth and Processing

New materials with novel properties and exciting new science

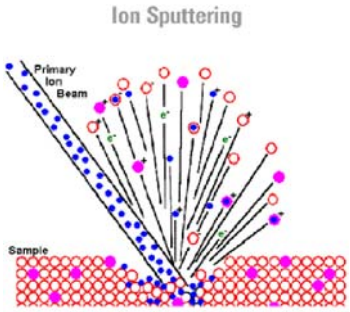
Molecular Beam Epitaxy
Atomic Layer Deposition
Chemical Vapor Deposition
Metal-organic CVD
Pulsed Laser Deposition



Multi-ferroic thin-film architectures: Single phase epitaxy, multi-phase epitaxy (horizontal), multi-phase nano-dots (vertical)

Ramesh & Spaldin, Nature Materials (2007)

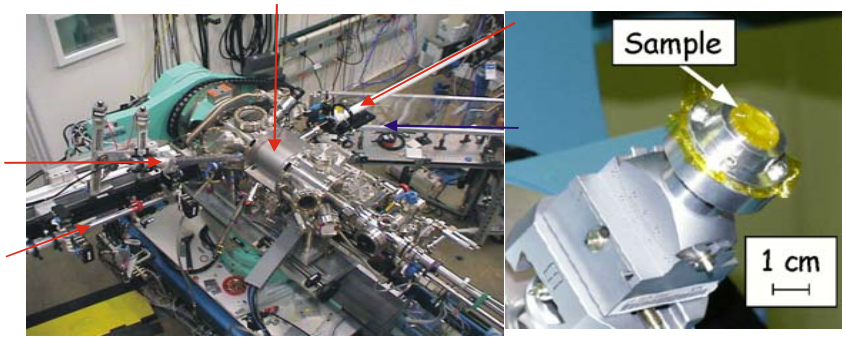
- Lithographic techniques
  e- beam, nano-imprint, …
- Focused Ion Beam Sputtering
- Dry etching – plasma etching
- Reactive ion etching (RIE)
- Magnetically enhanced RIE (MERIE)
- Reactive ion beam etching
- High-density plasma etching
- Wet chemical etching
- Oxidation



Structure, Strain, Composition ⇒ properties

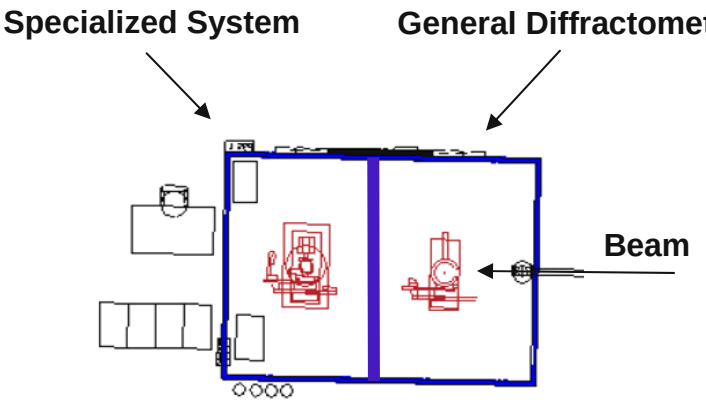
Proposed Sector for Interface Science

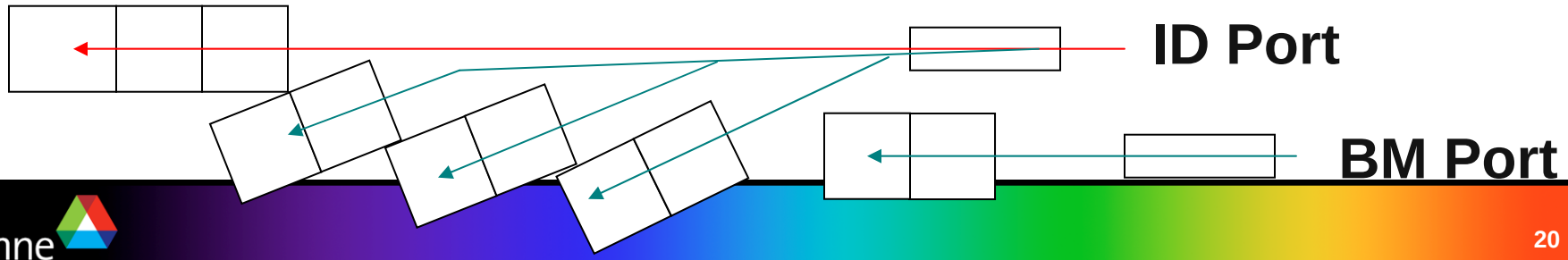
- Exploit APS X-ray Source brilliance & stability
- Required Energy Range well matched to APS ID spectrum
- Highly Efficient Beam Line Designs
- End-stations developed by Partner Groups



Facilities Include:

- Dual-canted Undulator ID Beam Line
  - One fully tunable branch Beam Line
  - One branch with fixed-energy Beam Lines
- One BM line (diffraction)
- 11 experimental stations with 5 simultaneous x-ray experiments
- Specialized end-stations available off-line
- Environmental Cells attach to General Diffractometers
- Lab Facilities & Infrastructure supporting Interface Science





BioNanoprobe

Gayle Woloschak (Northwestern University)
Peter A. Lay (University of Sydney, Australia)
James E. Penner-Hahn (University of Michigan)
Thomas V. O'Halloran (Northwestern University)
Stefan Vogt (APS)

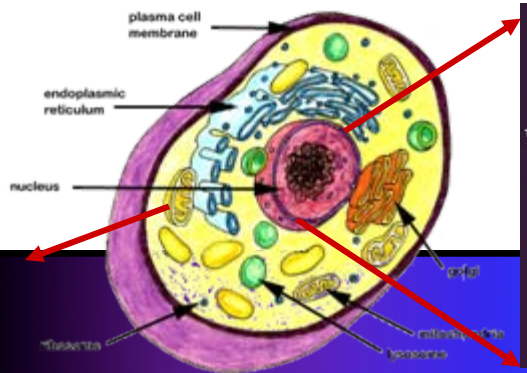
Trace **metals** play **critical role** in many cellular processes, e.g., 1/3 of all proteins contain a metal co-factor

Better understanding their action will enable critical advancements in:

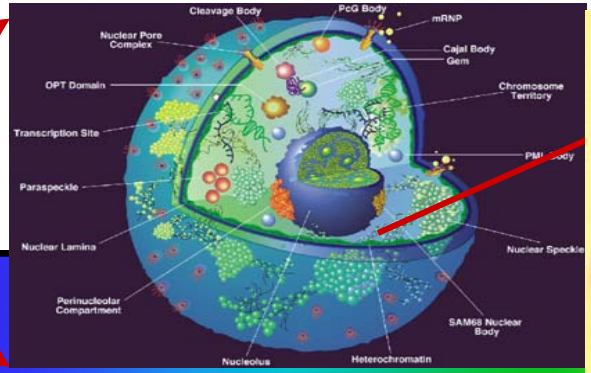
- Basic understanding of metals' **essential role** as cofactors in proteins
- Understanding **metal-linked diseases** (e.g., Alzheimer's)
- Developing **novel therapeutic drugs** and **functional contrast agents** (nano)

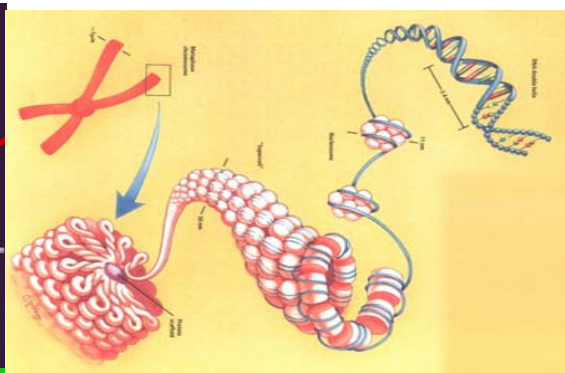
S. Vogt

Cell: ~10 μm



Nucleus: ~5 μm, with many substructures <100nm





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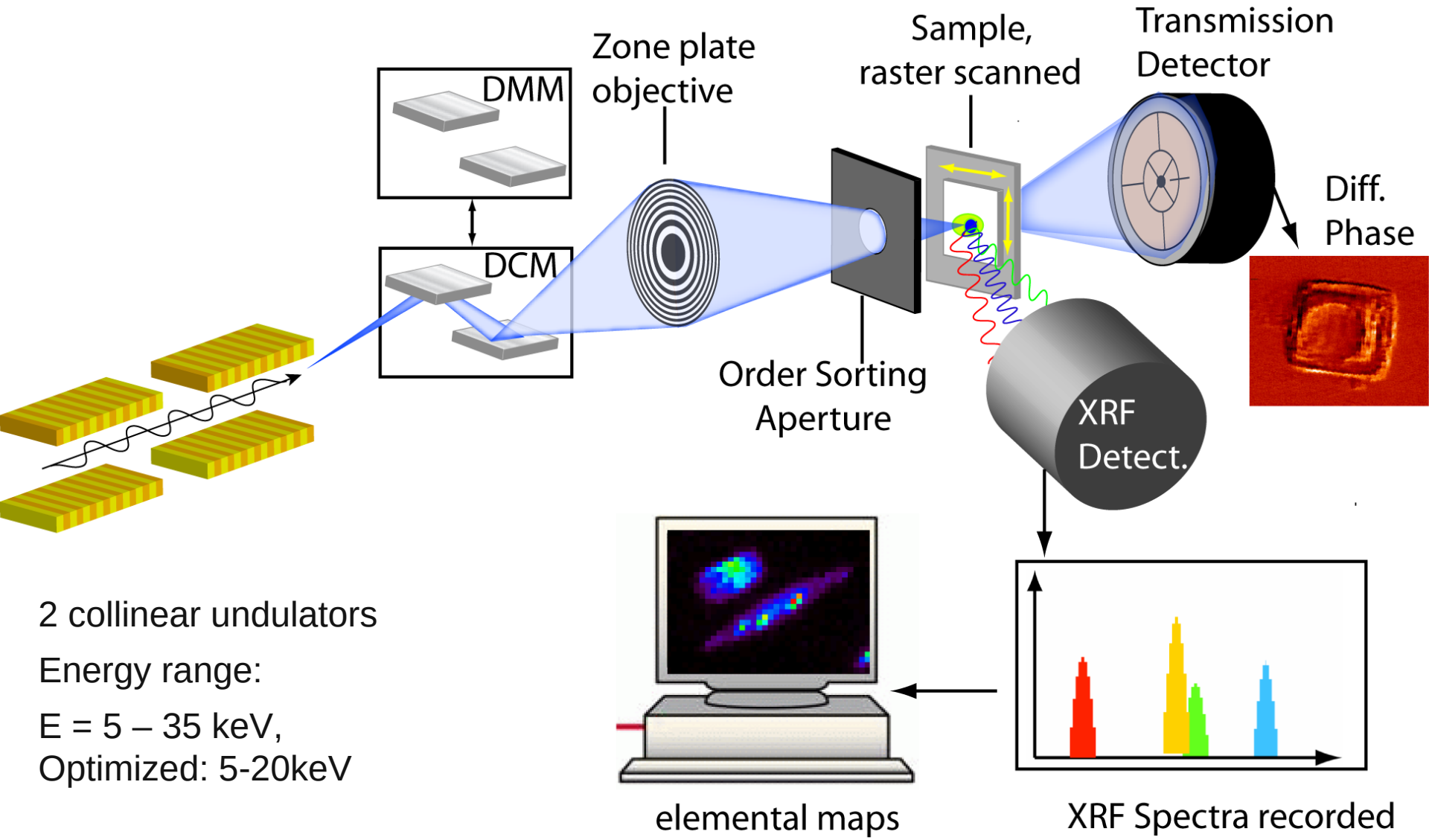
Proposed BioNanoprobe Beamline



2 collinear undulators

Energy range:

E = 5 – 35 keV,
Optimized: 5-20keV

Spatial resolution: Mapping: **δ=20 nm**; Spectroscopy: δ=50 nm; In vacuum, cryo-system

High Field Diffraction

Valery Kiryukhin (Rutgers University)

Young S. Lee (Massachusetts Institute of Technology)

Mark Bird (National High Magnetic Field Laboratory)

Zahirul Islam (APS)

Application of magnetic field effects:

magnetic properties

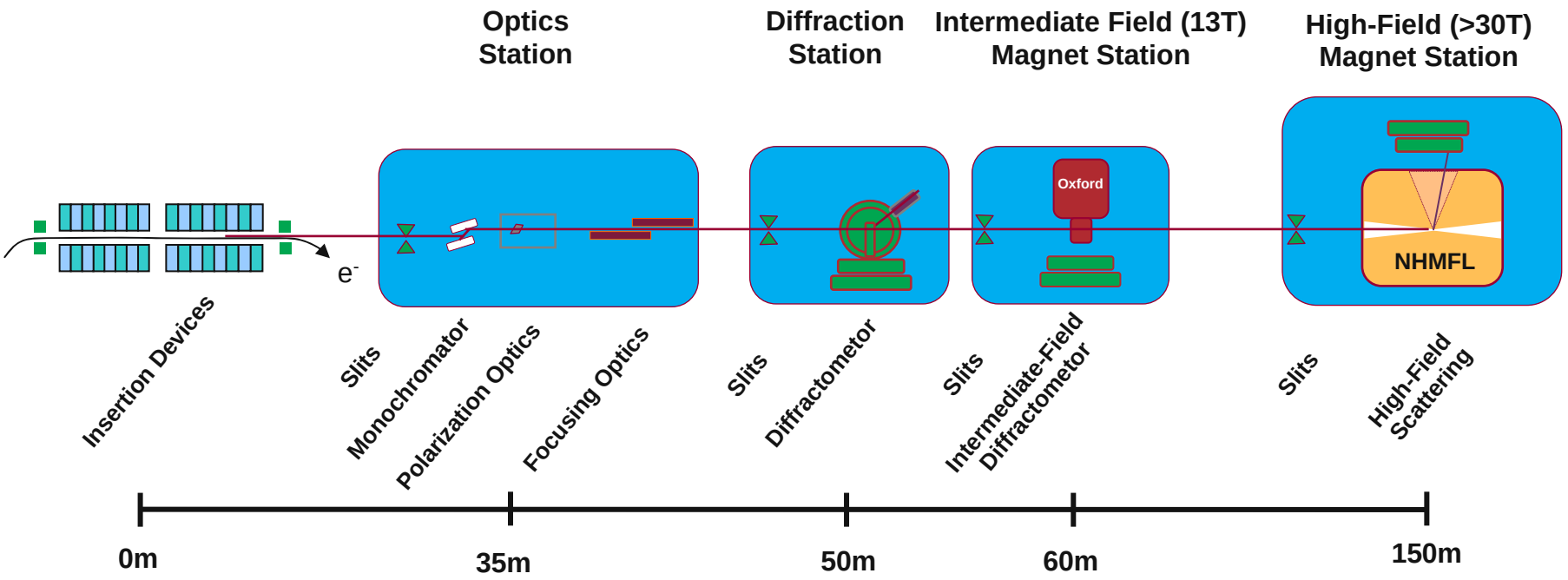
orbital

charge

structural degrees of freedom

X-rays can study all these effects simultaneously

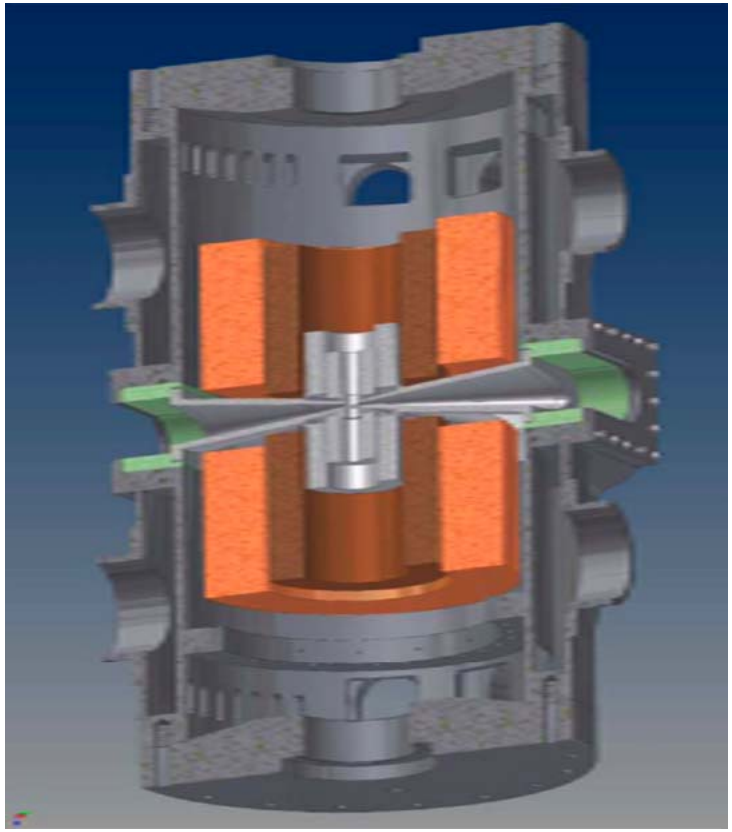
Proposed High Field Beamline

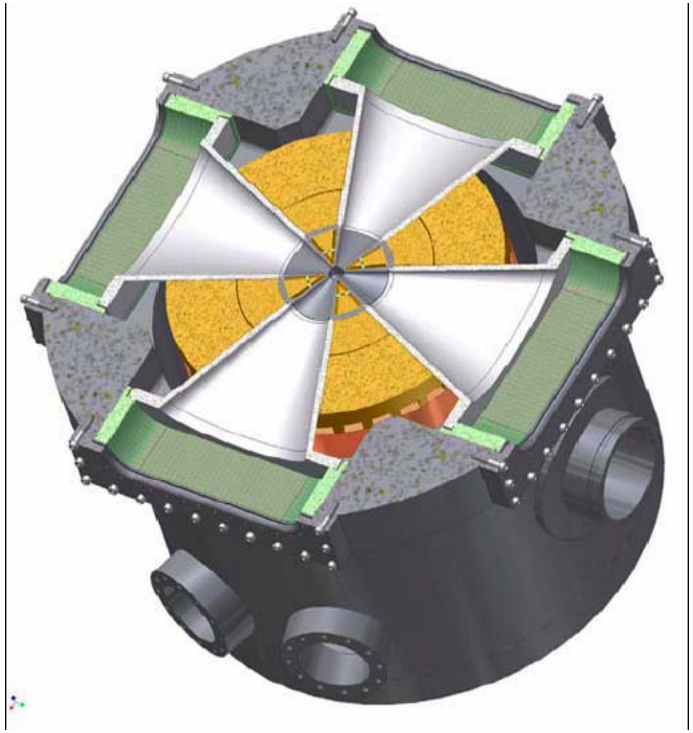


Due to physical size and required utilities high-field magnet would have reside outside the current experimental hall

High-Field 30T Split-Gap Magnet

- Split-gap absolutely required for single crystal work
- Ground breaking science



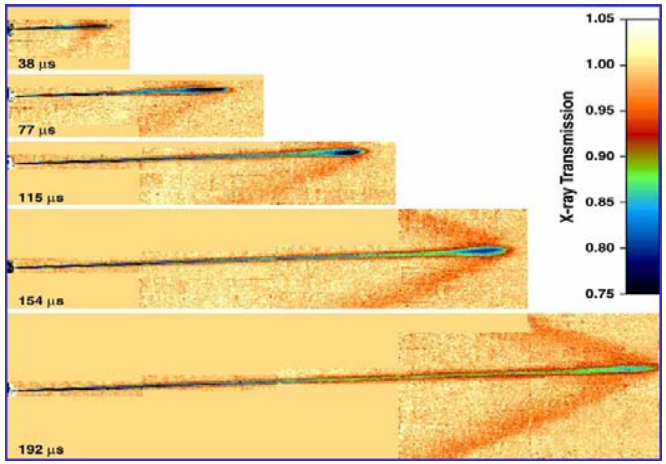


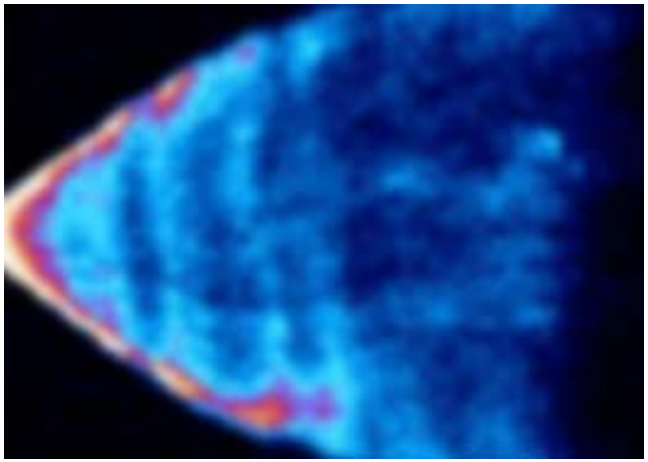
NHMFL confident to build

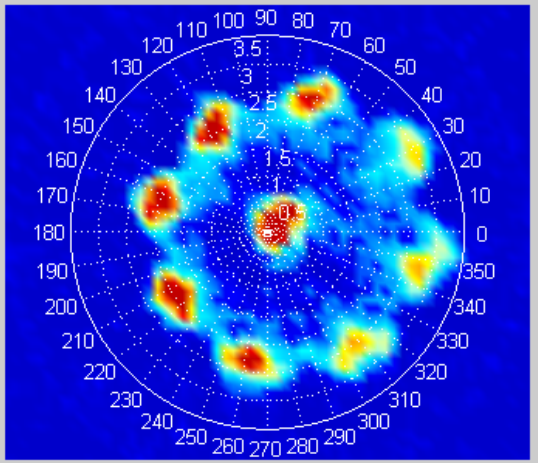
NSF proposal submitted to do design work
V. Kiryukhin, M. Bird, Z. Islam

Fuel Sprays Radiography: 7-BM

- Absorption-based µs-radiography of highly transient fuel sprays
- Ultrafast µs-tomography of sprays
- Building a large user community from both research institutes and industrial partners:
- A test bed for x-ray-based engine-related research facility at the APS
- Sector 7-BM is the site such a facility:
  - Multilayer mono beam for high intensity
  - Adjustable beamsize to match object size
  - Cornell Pixel Array Detector for ultrafast framing imaging

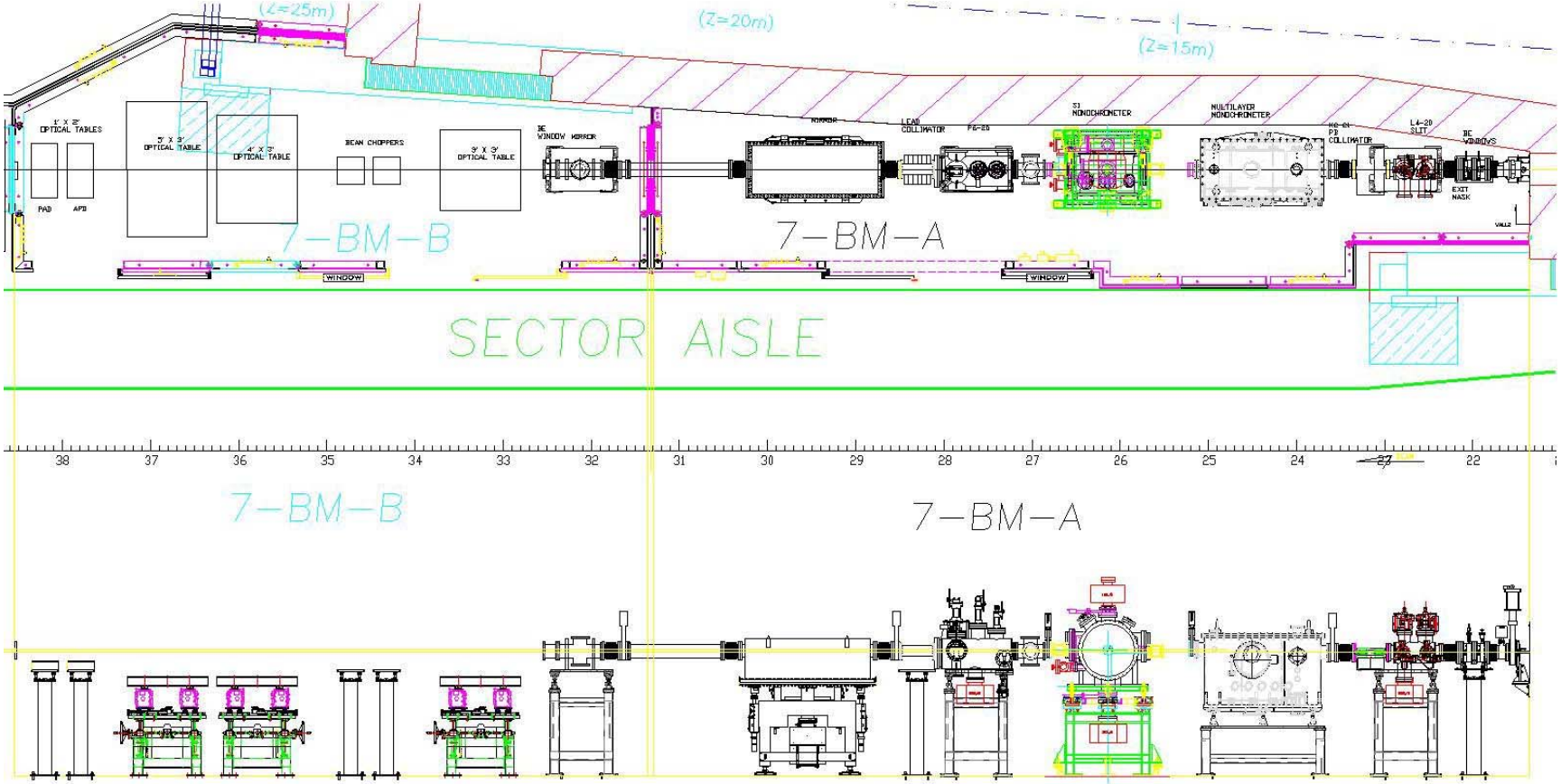






Proposed Beamline Layout: 7-BM

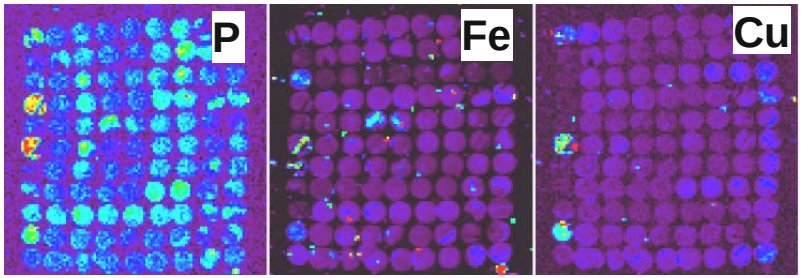
- Partnership between two areas of DoE: applied and basic science
- Collaboration between Energy Systems Division (L. Johnson) and APS (J. Wang)
- Scheduled to be commissioned in 2009



High Throughput Trace Element Analysis: 8-BM

Stefan Vogt (XSD)

Lydia Finney (XSD/Biophysics)



- Metals play critical role in life, disease, and the environment
  - Bioremediation: Knowing the fates of metals in bacteria can significantly aid in cleaning up contaminated sites.
  - Life: Metals are required for nearly every metabolic process in the cell, also in cancer
  - Disease: in the US alone, more than five million people suffer from metal-related diseases
- X-ray microprobes are highly successful, but slow
- High throughput is needed:
  - for statistically relevant measurements
  - to solve problems that cannot be addressed with conventional techniques

Tissue Zn concentration and cancer risk

- Zinc is an important co-factor in the esophageal-carcinogenic action of nitrosamines in animal studies, but zinc status is difficult to assess in humans.
- XRF allows direct analysis on thin section of biopsy tissues. XRF showed significantly increased risk for esophageal cancer for fraction of population with low Zn (Abnet *et. al*., J. Nat. Cancer. Inst., 2005)

Proposed Beamline Layout: 8-BM

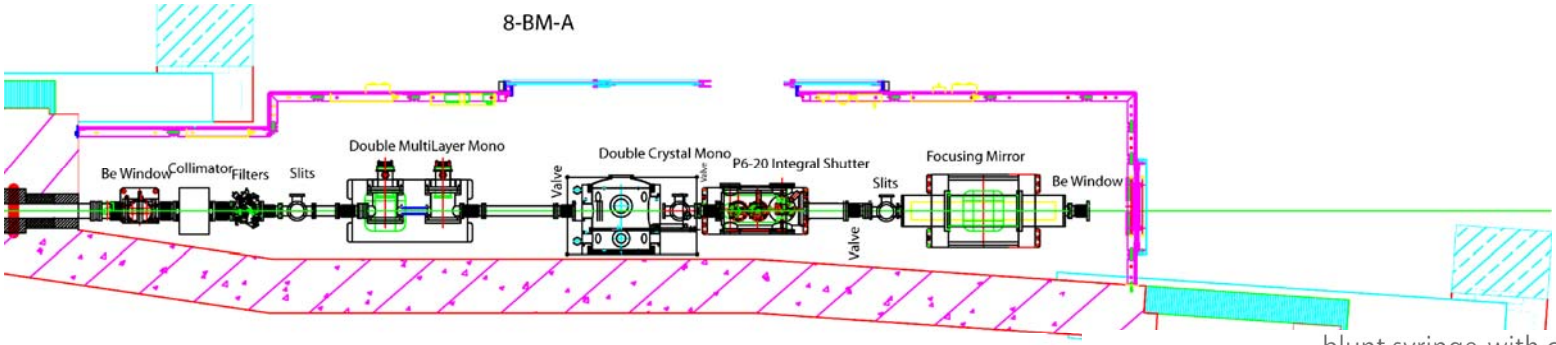


Fig.3: Layout of the optics hutch 8-BM-A, top view

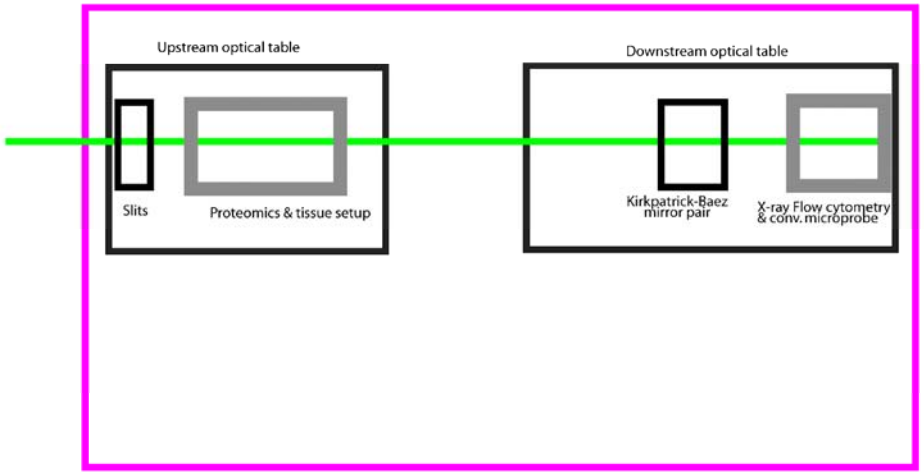
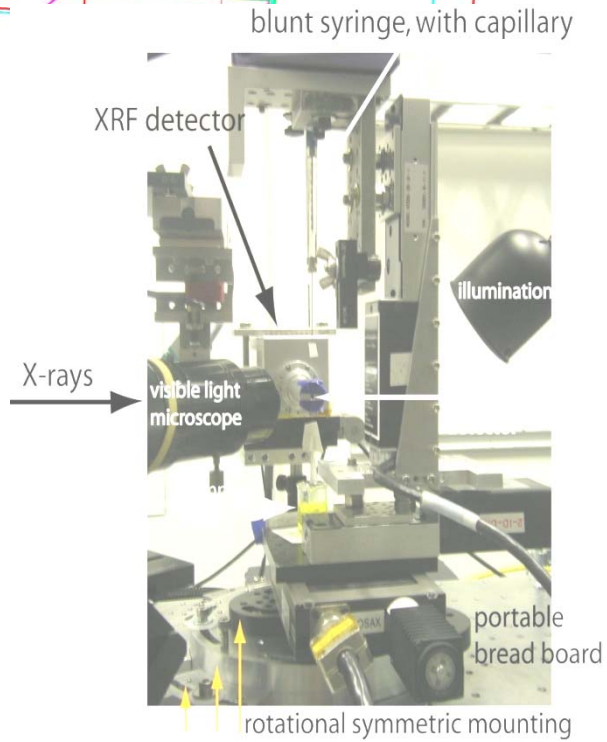


Fig.4: Schematic of the hutch 8-BM-B, top view



Prototype end-station instrument

Summary

- Strategic planning started in Summer 2004 - Lake Geneva
  - Focus on four “free” sectors
- Future facility - Summer 2006
  - Energy recovery linac
- Midterm (next five years) facility enhancements - Winter 2008
  - Beamlines, detectors, optics, software
  - X-ray source
  - Infrastructure - laboratories, offices,
- Scientific cases put forward for new beamlines
  - Motivated by Lake Geneva Strategic Planning
- Discuss midterm and long term plans at October 20-21, 2008 Workshop