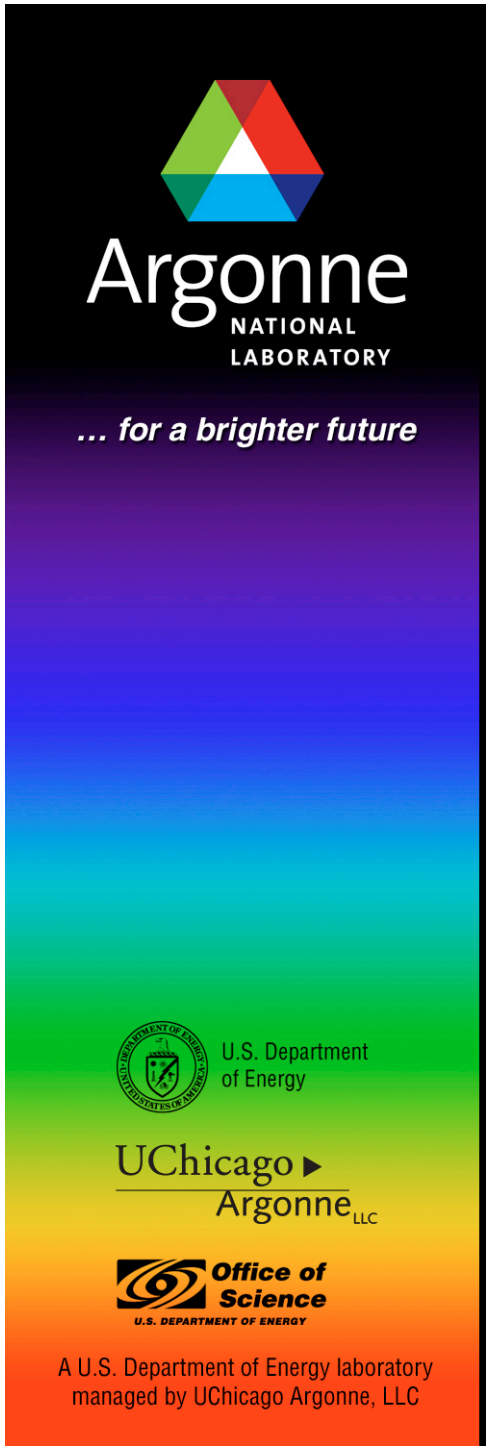

Time Resolved Tools for the APS Renewal

Klaus Attenkofer, XSD-CEP

Alec Sandy, XSD-TRR

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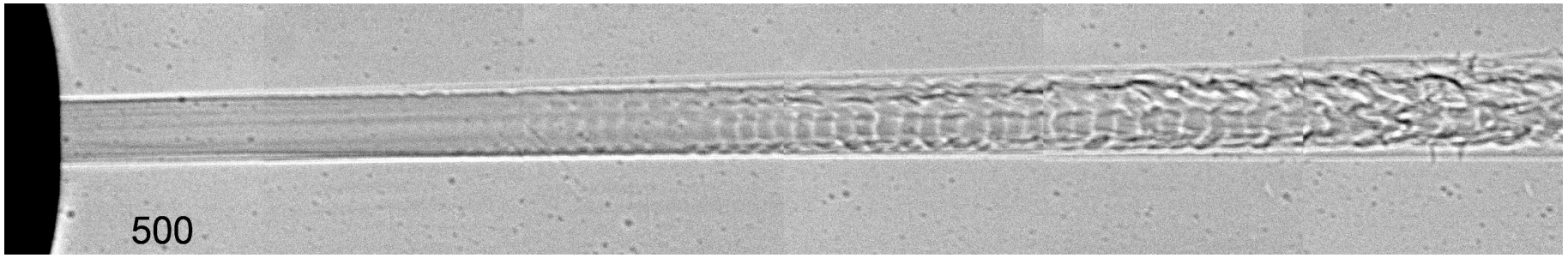
Introduction

- Time-resolved capabilities figure prominently in the “Renewal of the APS” white paper (ANL-08/38)
  - “Real Materials at Real Conditions in ***Real Time***”
- Many (7 of 10) of the October 2008 APS Renewal Workshop Science Reports include significant time-resolved components
- 3 LOI’s contain significant time resolved components (SPX, AXI and DC)
- APS strengths today
  - High peak power per pulse (large charge per bunch)
  - Special timing modes
  - High energy x-rays
  - Established and productive user communities
  - Established experimental expertise

Introduction: Classification & Overview

Instrument	Field	Time Res.	Capabilities	Existing Community
Ultrafast and single shot imaging	Engineering and life sciences	> 300 ns (hard) *> 300 ns*	APS *APS*	Academic/Industry /National Security
Short pulse x-rays	Dynamics at quantum length scales	100ps *1 ps – 100 ps*	APS *APS LCLS XFEL*	Academic
TR HEX scattering	Mechanical behavior of materials	1 s *1 μs – 1 ms*	APS ESRF *APS ESRF Petra-III*	Academic/Industry
XPCS	Dynamics in soft matter	10 ms – 1,000 s 1 μs - 1,000 s	APS ESRF *APS ESRF Petra-III LCLS XFEL*	Academic
TR MX	Macromolecular dynamics	1 ns – 100 μs *30ps – 100 μs*	APS *APS ESRF SPRING8*	Academic
TR WAXS/SAXS and spectroscopy	Chemistry and energy conversion /storage	30 ps - 100 μs 30 ps - 100 μs	APS ESRF SPRING8 SLS *APS ESRF SPRING8 SLS*	Academic

Introduction: Ultrafast and Single Shot Imaging



Field: Engineering and life sciences

Status (today):
- •Other Sources: ESRF
- •Sectors involved: 32-ID, 7-ID, 7-BM (soon)
- •Sectors dedicated: 1
- •Existing user community: yes (academic, industry)

In 5 years?
- •Potential Competitors: ESRF, Petra-III
- •Action Items: Flexible bunch structure
  High current bunches
  Efficient, fast integrating area detectors
  Long beamlines

Specific Requests: Ultrafast and Single Shot Imaging

Specific Request:

- •Sectors: 2 ID beamlines-long straight sections and long beamlines
- •End stations:
  - • Sector A: Wider field, high resolution ultrafast imaging and single shot imaging
  - • Sector B: Wider field, higher resolution, fast imaging and single shot imaging
  - •White and pink beam capable
- •ID-configuration: Narrower band tunable helical undulators

Additional Support:

- •Detectors:
  - •Fast framing, gateable, integrating area detector
  - •Ultrafast area detector for diffracted beam monitoring
- •Data Analysis and visualization:
  - •Object tracking, quantitative PCI, hydrodynamic modeling & simulation
- •Sample environment: Gases, fluids, chemicals, extreme environments
- •Lab space: Laser imaging, hydrodynamic testing
- •Experiment Apparatus: Cloneable and rapidly deployable for single shot

Required Partnerships:

- •NNSA: Extreme environments
- •EERE
- •ALCF: Simulations and modeling
- •EFRC

Summary: Ultrafast and Single Shot Imaging

Correlation with White-Paper:

- Key-Problems: Energy, environment, technology development (3/4)
- Scientific Vision: Real materials in real condition and real time

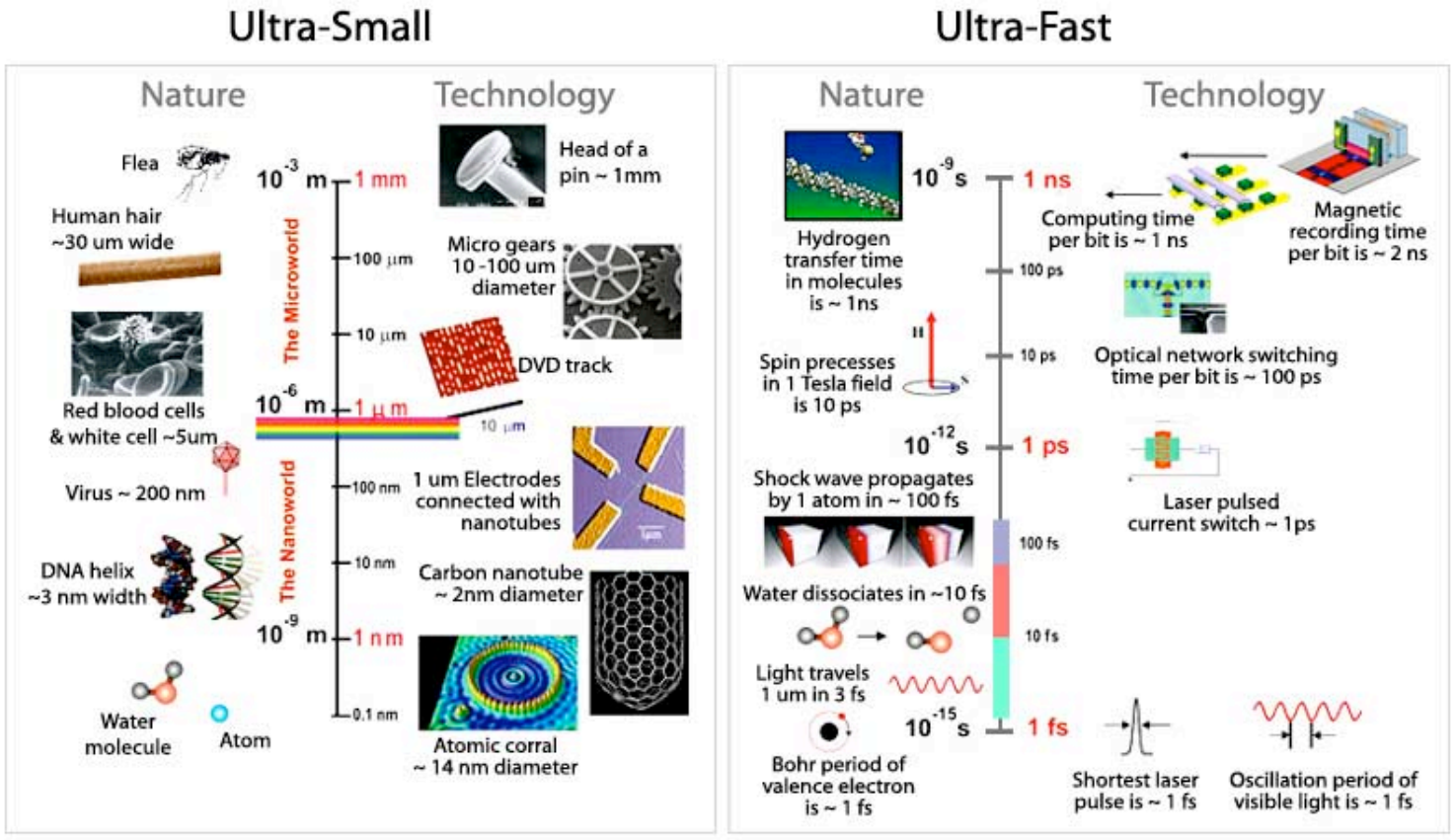
Comments:

- Key aspects already demonstrated
- Unique
- Relation to proposed DC-CDT

Introduction: Short Pulse X-Rays

Field:

- •Quantum control of atomic and molecular dynamics
- •Chemical reaction dynamics - transition state structures
- •Response of materials and devices to external fields
- •Dynamics of photo-excited materials



Introduction: Short Pulse X-Rays

Status (today):

- Other Sources: ESRF (partial), (ALS)
- Sectors involved: 7-ID, 11-ID-B
- Sectors dedicated: 1.5
- Existing user community: yes (academic)

In 5 years?

- Potential Competitors: LCLS, XFEL
- Action Items:
  * Develop and deploy CW RF cavities
  * Develop and deploy applicable high rep rate lasers
  * Integrating ultrafast area detectors

Specific Requests: Short Pulse X-Rays

Specific Request:

- •Sectors: 2 (long straight section)
  - • A: Variable polarization ID, 4-35 keV
    - •Diffraction: <≈ 50 nm spot size
    - •Spectroscopy and scattering
    - •Catalysis, geochemistry and surfaces
  - • B: Variable polarization softer x-ray ID
    - •Soft x-ray spectroscopy
- •SR/RF-configuration: CW RF cavities with variable pulse lengths (1-100 ps)

Additional Support:

- •Detectors:
  - •Integrating ultrafast area detectors with gating < pulse separation
  - •Fast, pixellated, energy resolving large area counting detectors
- •Lasers: High-rep rate lasers in shared generation and delivery facs.
- •Lab space: Co-located ultrafast laser and target development lab
- •Sample environment: Synchronized excitation sources

Required Partnerships:

- •High rep rate lasers: Argonne CSE
- •Integrating detectors: Sol Gruner, Cornell University

Summary: Short Pulse X-Rays

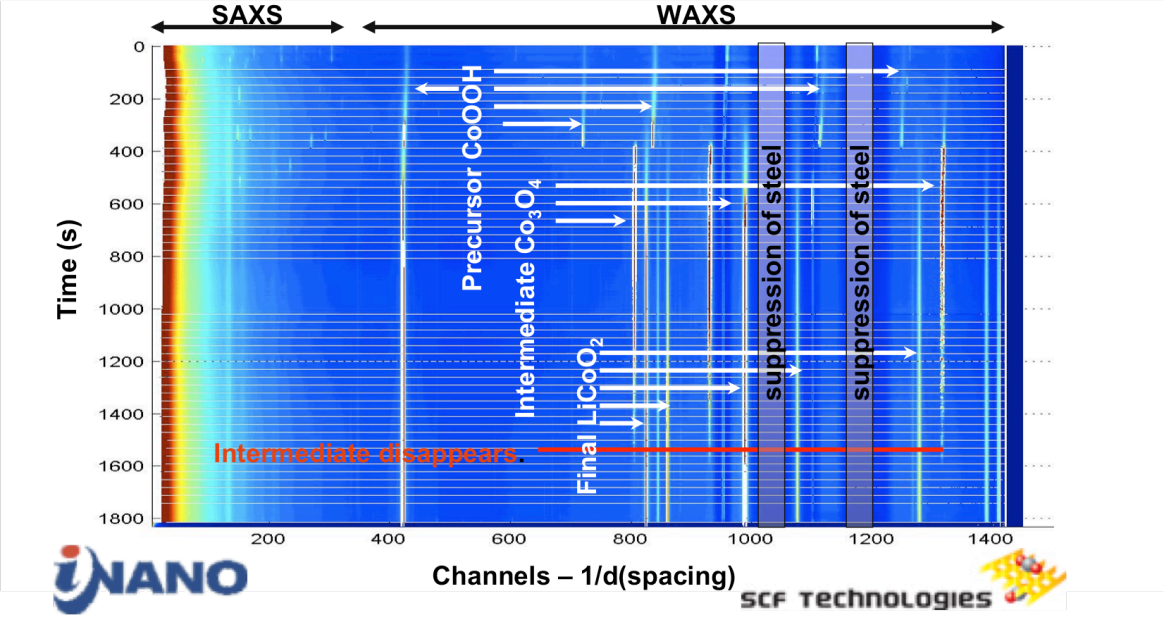
Correlation with White-Paper:

- Key-Problems: Energy, technology development (2/4)
- Scientific Vision: Real materials in real condition and real time

Comments:

- Complements FEL capabilities
- Unique
- More information required on very hard and/or softer x-ray applications

Introduction: TR HEX Scattering



Field: Time resolved studies of mechanical behavior of materials (dedicated)

Status (today):
- •Other Sources: ESRF
- •Sectors involved: 1-ID; 11-ID-C; 16-ID (?); (HP-sync ?)
- •Sectors dedicated: 0.5
- •Existing user community: yes (academic)

In 5 years?
- •Potential Competitors: ESRF, SPRING8, Petra-III
- •Action items: Optimized ID's (small gap) and FE
- •Tiled fast detectors
- •Expand user community to industry and defense

Specific Requests: TR HEX Scattering

Specific Request:

- Sectors: One (long straight section)
- Endstation: Combined SAXS/WAXS and Imaging
- ID-configuration: Multiple narrow gap ID's
  - Energy-span: 45 keV-120 keV continuously tunable
- Frontend: High heatload per narrow gap
- Optics-configuration: 2d-focusing

Additional Support:

- Detectors:
  - Tiled HEX sensitive area detector (fast readout)
  - HEX imaging detector
- Data processing: Fast and "live" data reduction and visualization
- Sample environment: Furnaces, cryogenics, dynamic compression

Required Partnerships:

- Risoe National Lab: Scintillators suitable for HEX imaging
- Perkin Elmer: Tiled, fast HEX area detectors
- NNSA: Extreme/transient environment development

Summary: TR HEX Scattering

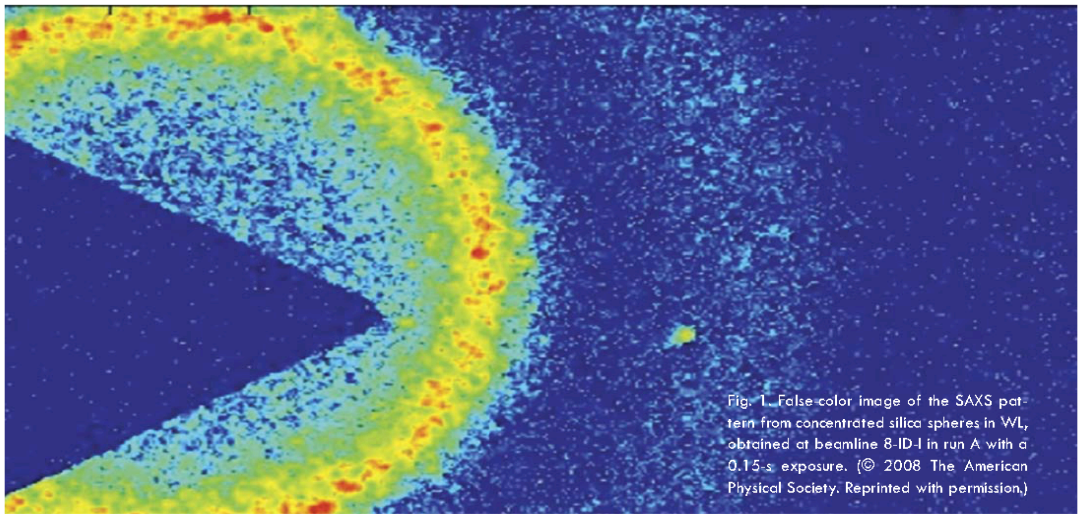
Correlation with White-Paper:

- Key-Problems: Energy, technology development (2/4)
- Scientific Vision: Real materials in real condition and real time

Comments:

- Potential for large economic and security importance
- Relation to proposed DC-CDT

Introduction: XPCS



Field: Dynamics in soft matter (dedicated)

Status (today):

- Other Sources: ESRF
- Sectors involved: 8-ID
- Sectors dedicated: 1
- Existing user community: yes (academic)

In 5 years?

- Potential competitors: ESRF, Petra-III, LCLS, XFEL
- Action items: μs-ms capable XPCS-appropriate area detectors

Specific Requests: XPCS

Specific Request:

- •Sectors: One (long straight section)
- •End station: Small (and wide angle) XPCS
  - •Long experiment station and exit flight path to resolve speckle
  - • Mechanically and thermally stable experiment environment
- •ID-configuration: Long, short period device
- •Frontend: Compatible with long, short period device
- •Optics-configuration: Virtual vertical source via diffraction-limited optics
  - •2-D focusing
  - •Brilliance and coherence preserving optics
  - •Beam deflection optics for liquid-like surfaces

Additional Support:

- •Detectors:
  - •Fast (μs), high-resolution photon counting area detector
- •Data reduction: On-the-fly compression and correlations
- •Sample environments: Ovens, cryogenics, stress rigs, troughs
- •Lab space: Light scattering characterization

Required Partnerships:

- •Peter Siddons-BNL and FNAL: μs high-res photon counting area detector

Summary: XPCS

Correlation with White-Paper:

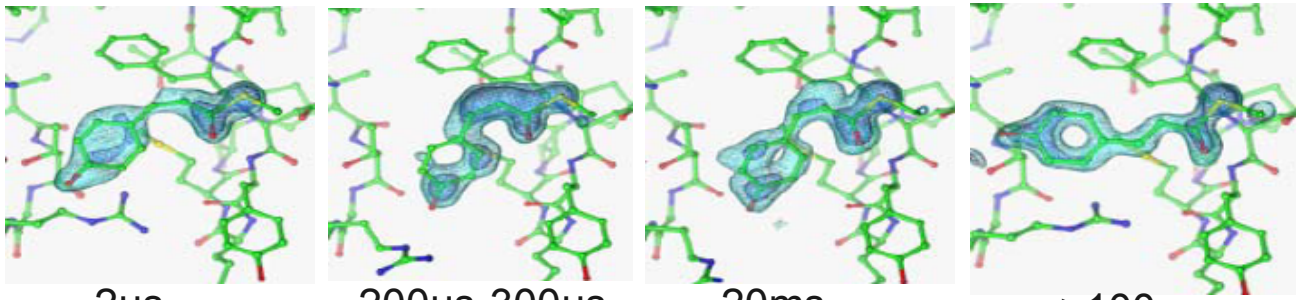
- Key-Problems: Technology development (1/4)
- Scientific Vision: Mastering hierarchical structures

Comments:

- Complements accessible times at LCLS
- High current bunches and higher energies provide unique strengths

Introduction: Macromolecular Dynamics

Vukica Srajer



2μs 200μs-300μs 20ms >100ms

Field: Time resolved studies of a reaction pathway in macromolecular systems

Status (today):

- •Other Sources: (ESRF)
- •Sectors involved: 14ID
- •Sectors dedicated: 1
- •Existing user community: yes (academic)

In 5 years?

- •Potential Competitors: ESRF, SPRING8, PETRA, (FEL's)
- •Action item: Detector development

Partners:

- •Technical : (Detectors)
- •Strategic: Phil Anfinrud

Specific Requests: Macromolecular Dynamics

Specific Request:

- •Sectors: One (existing sector)
- •Endstation: One (new optimized hutch)
  - • station1: ***crystallography***
- •ID-configuration: Energy-span: 6KeV-16KeV
  - •Frontend: High Heatload; (specific undulator)
- •Optics-configuration: 2d-focusing (30x90μm^2/ 5x10μm^2)

Additional Support:

- •Detectors:
  - ▪Fast readout
  - ▪Multiple memory-blocks per pixel
  - ▪Multi-photon mode
- •Software & IT: data reduction & visualization (significant effort done)
- •Sample environment: insitu characterization
- •Lab-availability: optical characterization; chemical treatment ….

Required Partnerships:

- •Detectors?

Summary: Macromolecular Dynamics

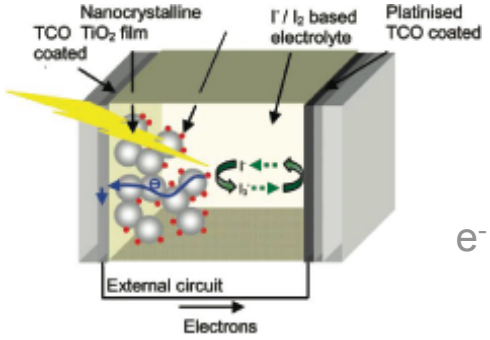
Correlation with White-Paper:

- Key-Problems: Human health, Environment, Energy (3/4)
- Scientific Vision: Real materials in real condition and real time

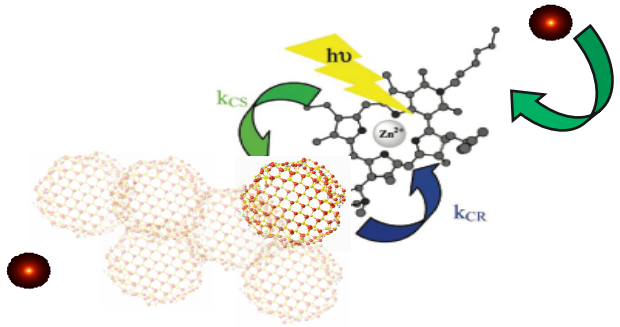
Comments:

- One of the well established programs for time dependent measurements
- Increase of productivity by collaboration with non x-ray facilities

Introduction: Chemistry & Energy Conversion/Storage



e^- (to electrode)



e^- (electrolyte)

Field: Time resolved studies of molecular system in hierarchical structures

Status (today):
- •Other Sources: ESRF (TR-WAXS), SLS (TR-XAFS)
- •Sectors involved: 11-ID-D; 7-ID; 14-ID;
- •Sectors dedicated: 1(WAXS/XAFS); 1/2(XAFS);1/4(WAXS)
- •Existing user community: yes (academic)

In 5 years?
- •Potential Competitors: ESRF, SLS, NSLSII, SPRING8, (FEL's)
- •Action item: Detector development (XAFS)

Partners:
- •Technical : Detectors ?
- •Strategic: ANL, CMM

Specific Requests:
Chemistry & Energy Conversion/Storage

Specific Request:

- Sectors: One
- Endstation: One
  - station1: ***XAFS/WAXS/SAXS (GI)***
- ID-configuration: Energy-span: 4.5KeV-35KeV
  - Frontend: High Heatload; 2 optimized undulator
- Optics-configuration: 2d-focusing (30x90μm^2/ 500x500nm^2)

Additional Support:

- Detectors:
  - Multi-photon detection system (XAFS) with energy resolution ("crystal optics")
  - Commercial 2d detector (2M Pilatus)
- Software & IT: visualization & simulation software
- Sample environment: fast sample exchange
- Lab-availability: optical characterization; chemical treatment ….

Required Partnerships:

- Technical: detectors?, excitation-mechanism
- Strategic: ANL, CMM

Summary: Chemistry & Energy Conversion/Storage

Correlation with White-Paper:

- Key-Problems: Energy, Technology Development, Environment (3/4)
- Scientific Vision:
  - Real materials in real condition and real time
  - Mastering hierachical structures through x-ray imaging

Comments:

- Good established user community
- Increase of productivity by collaboration with non x-ray facilities

Summary

- Time dependent programs covers a wide range of length and time scales
- Strong established programs
- Most of the experiments require strong user support (often collaboration effort)
- Efficiency (scientific output) can be significantly increased with link to non-x-ray user-facility (model like CNM)
- Strong points of APS:
    - Timing structure (large charge per bunch)
    - High rep-rate (in contrast to FEL's)
    - "Known experimental techniques" (in contrast to FEL's)
    - High energies available (>20KeV)
    - High through-put experiments possible (many users)

Supplementary Materials

- Proposals explicitly not considered
  - Increased time resolution to increase beamline throughput
  - IXS and NRS

- Other Existing Experiments Considered
  - Solid state TR-XAFS (20-ID, 11-ID-D)
  - Time-resolved surface scattering (11-ID-D, 33-ID)
  - Time-resolved SAXS (12-ID)
  - Polymer/materials processing (5-ID)