FXE Instrument

Femtosecond X-Ray Experiments

Christian Bressler

January 25, 2011

XAS/XES/XRD at the FXE instrument

- Dynamics of Solids and Liquids
- Combine versatile structural tools into one single setup
  - x-ray absorption (XANES, EXAFS)
  - x-ray emission (XES, RXES, …)
  - x-ray scattering (XRD, diffuse scattering)

→ Obtain new information during the dynamics

- Maintain both ambient and vacuum options
  - ambient conditions for liquids, solids, …
  - vacuum chamber for surfaces, cryogenic samples, …

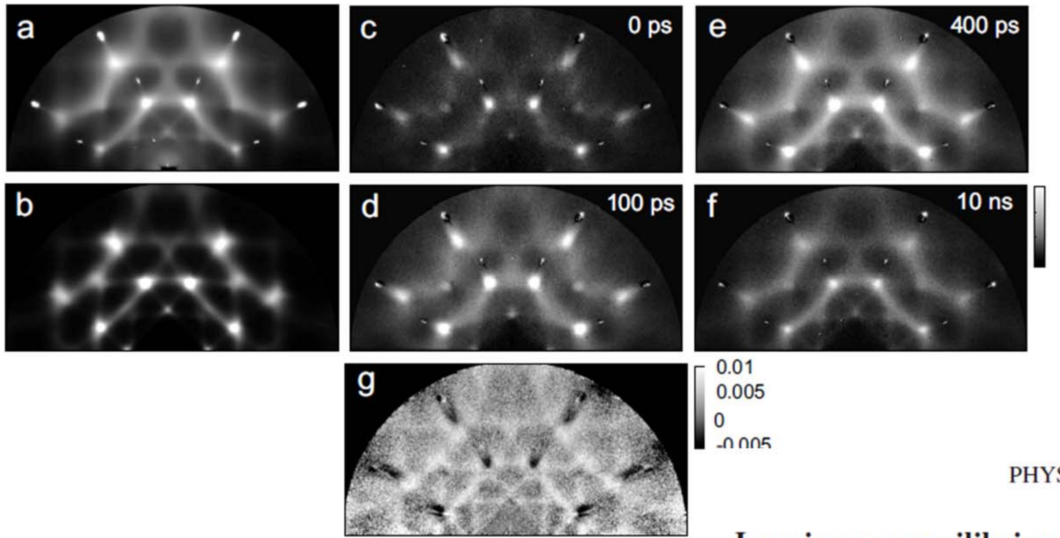
- Exploit the highest possible time resolution (≤25 fs)

  …include as much flux as possible (≥ 120 pulses)

Science Case

Solid state phenomena

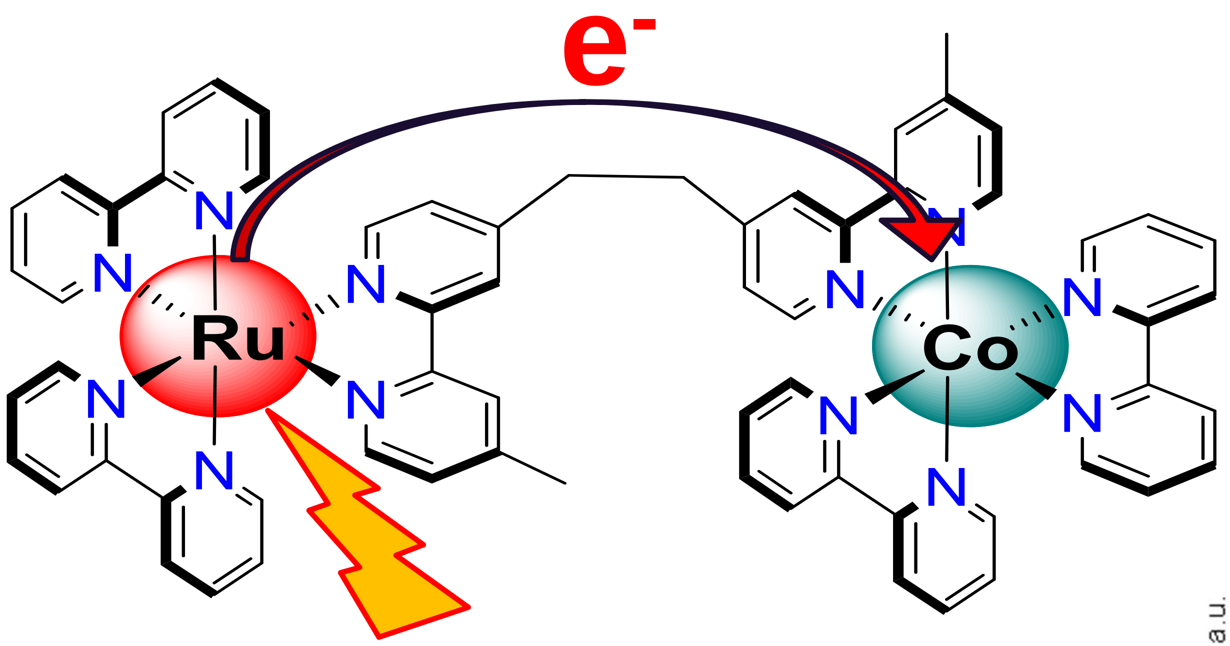
FXE offers new opportunities to study mechanisms that create or destroy long and short range symmetries of the lattice, charge, orbital, and spin degrees of freedom in a solid. These mechanisms are a key factor in understanding many cooperative phenomena in complex solids. The tools to study this include XRD, RXRD, and GID.



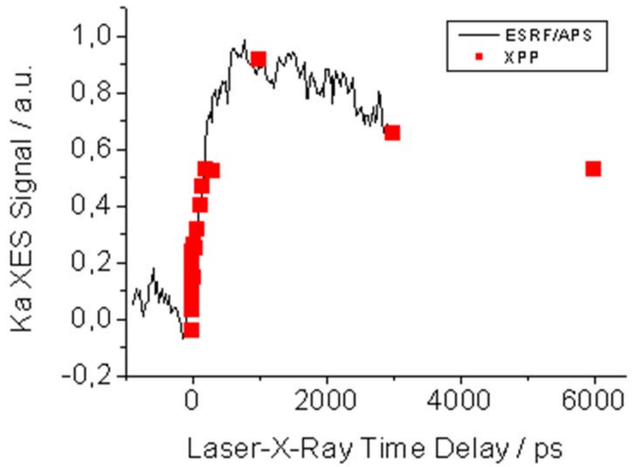
PHYSICAL REVIEW B 82, 235205 (2010)

Imaging nonequilibrium atomic vibrations with x-ray diffuse scattering

Chemistry: Complementary Tools Desired

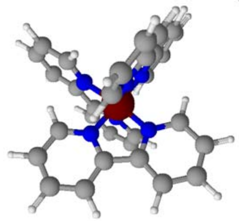


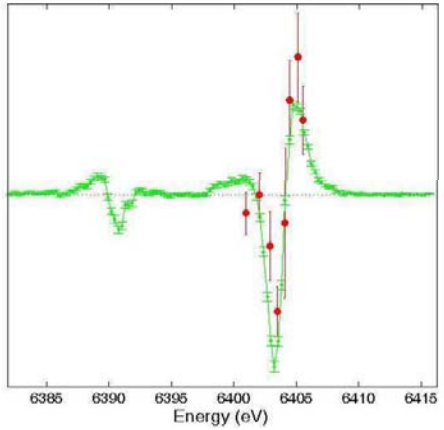
XES: occupied DOS (spin)
XAS: empty DOS (orbitals)
XRD: geometric structures



1) Ru(II) → Ru(III) (**XAS**, XES, optical)
2) IVR + e-transport (**XRD, optical**)
3) Co(III) → Co(II) (**XAS**, XES, optical)
4) Co(II) LS→HS (XAS, **XES**)

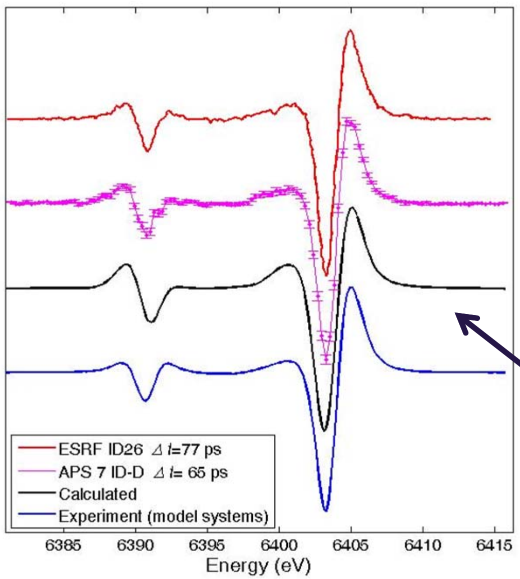
Chemical Dynamics Applications (at MHz rep-rates!)

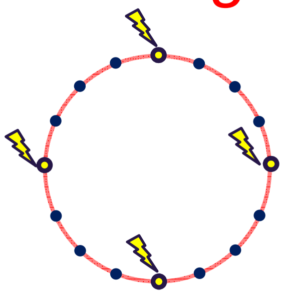


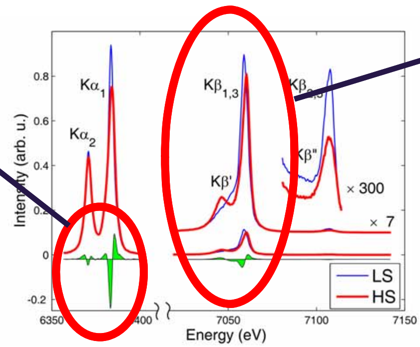


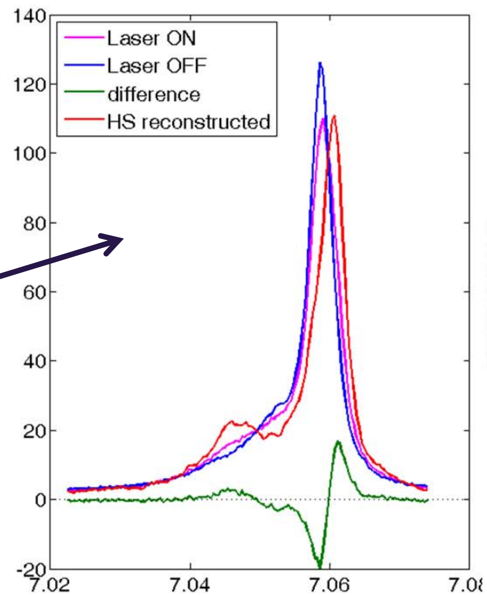
March1-15, 2011, ESRF, Grenoble FRANCE

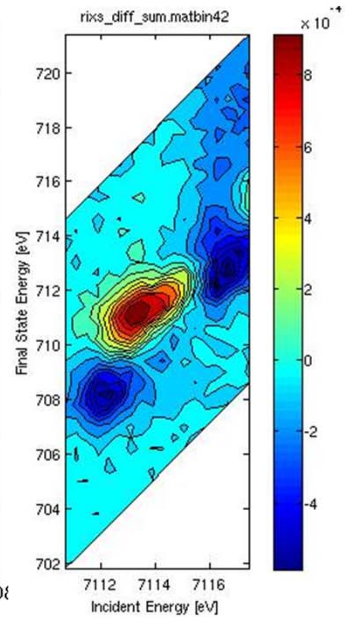
March 9-24, 2011; APS Argonne USA





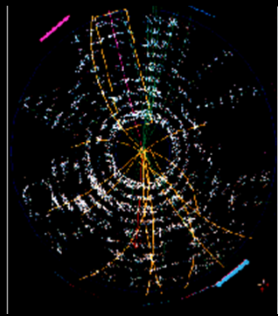


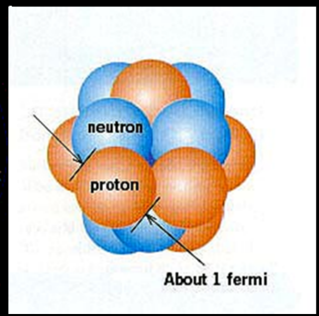




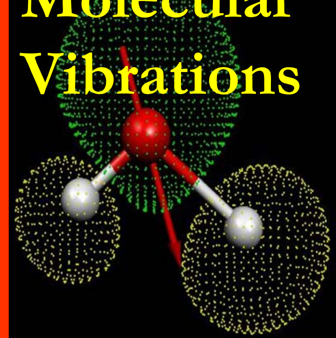
What are the fundamental timescales?

Chemistry and Biochemistry
Solid State Dynamics

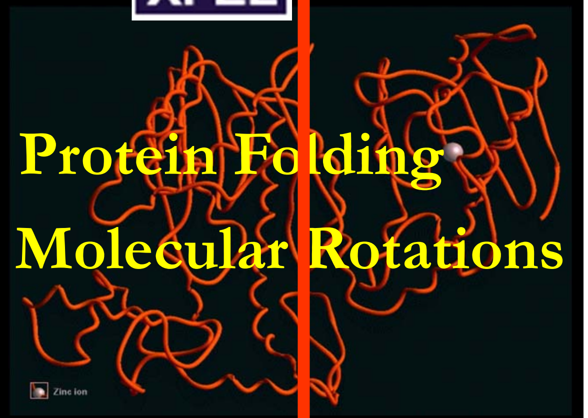




Photosynthesis
Vision
Molecular
Vibrations



European XFEL



Protein Folding
Molecular Rotations

Strings,
Cosmology

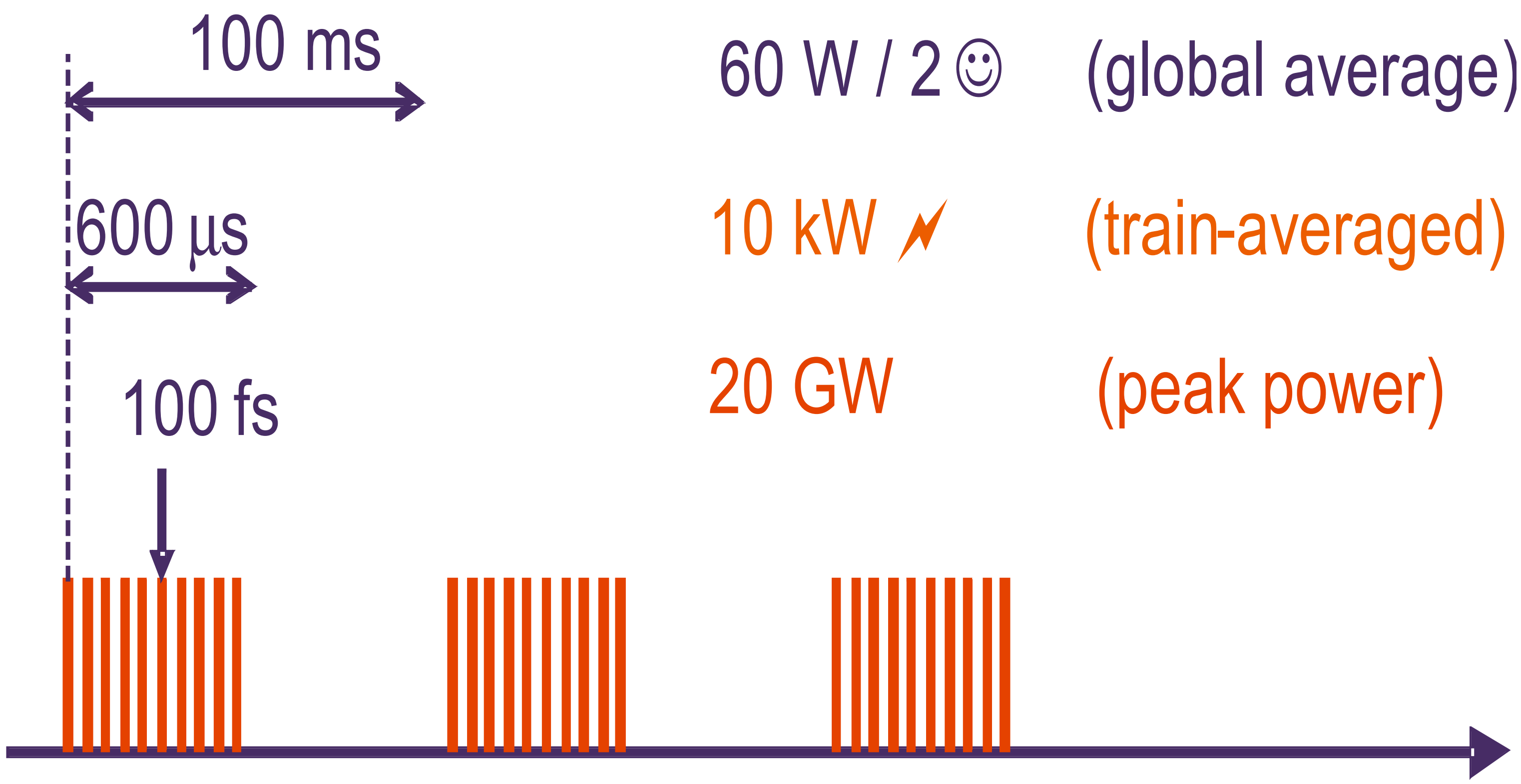
Particle
Collisions

Electron dynamics

harpo	yacto	zepto	atto	femto	pico	nano	micro	milli
10^{-27}	10^{-24}	10^{-21}	10^{-18}	10^{-15}	10^{-12}	10^{-9}	10^{-6}	10^{-3}

Time /seconds

Time and Power Scales



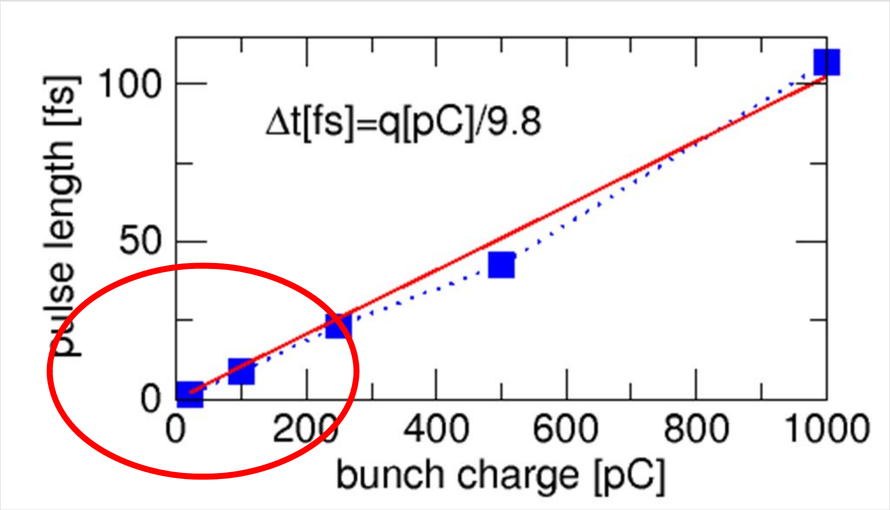
2700 pulses
(2 mJ/pulse)

FXE Overview Specifications

- 5 – 20 keV (24), 0.1 % bw
  → > 10 A-1 q-range possible (WAXS)
- 1e-4 (Si-111) – XANES, XES, XRD
- 1e-5 (Si-311, 333) – RIXS

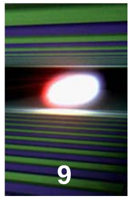
(primary monochromator)

- Low-Charge Mode (< 250 pC)!
  < 25 fs pulse width !
- 120 pulses/burst, up to 2700
- Flexible Spot Size (< 1 mm)
  (line, spot)



European XFEL

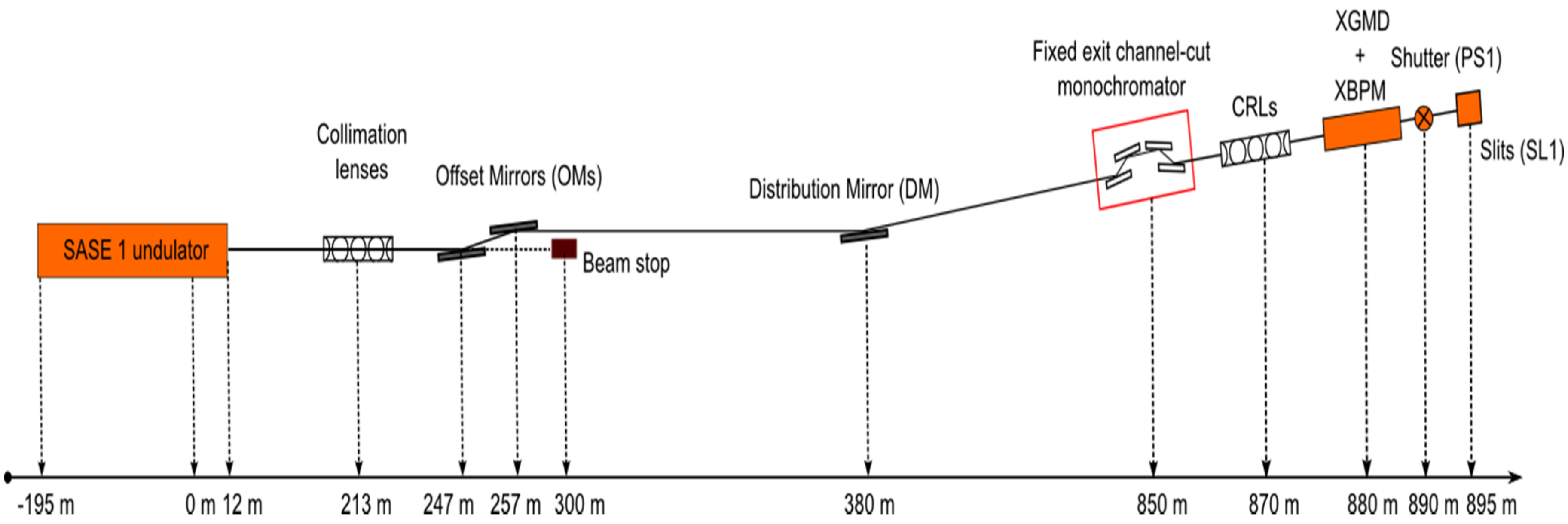
Overview



- From/since FXE Workshop (12/2009)
  - Emphasis on secondary spectrometers
  - Diffraction capability
  - Ultrahigh time Resolution (1st goal: <30 fs cc)

- Users want
  - variable pulse patterns (1-10 Hz, 1-1000 pulses/burst)
  - small foci (SAXS nano, Protein XRD)
  - large spots (solid PT, Protein XRD, surface refl, …)
  - < 0.5 mrad divergence
  - < 1e-3 energy bw (down to e-5)
  - usual laser conditions (<25 fs, UV-vis/NIR, THz, …)

X-Ray Beam Transport (5-20 keV), top view



European XFEL

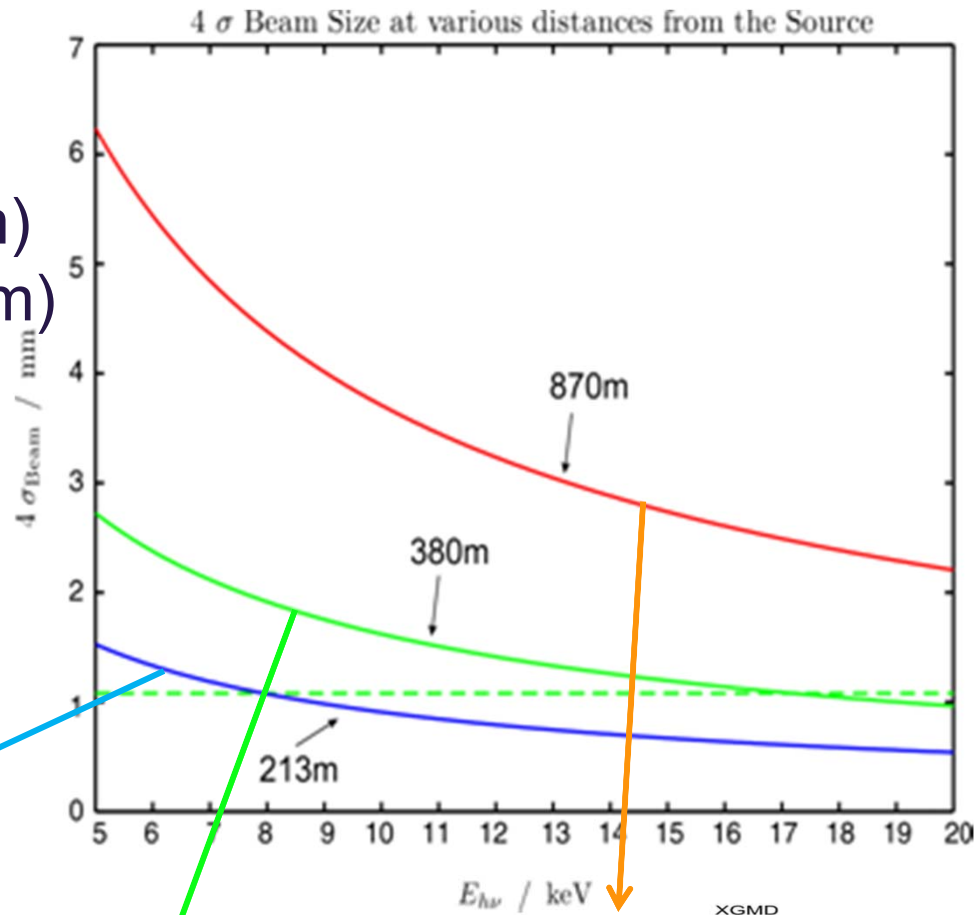
Natural Divergence (urad) and spot sizes

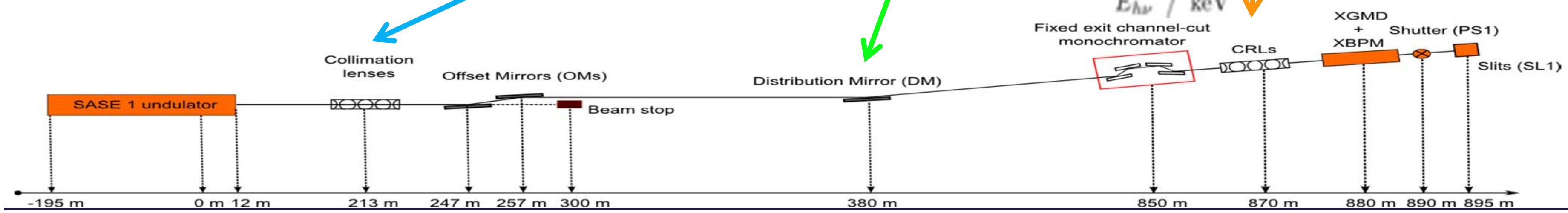
- Beam on DM (380 m):

- horizontally bend OM (250 m) (intermediate focus near 600 m)

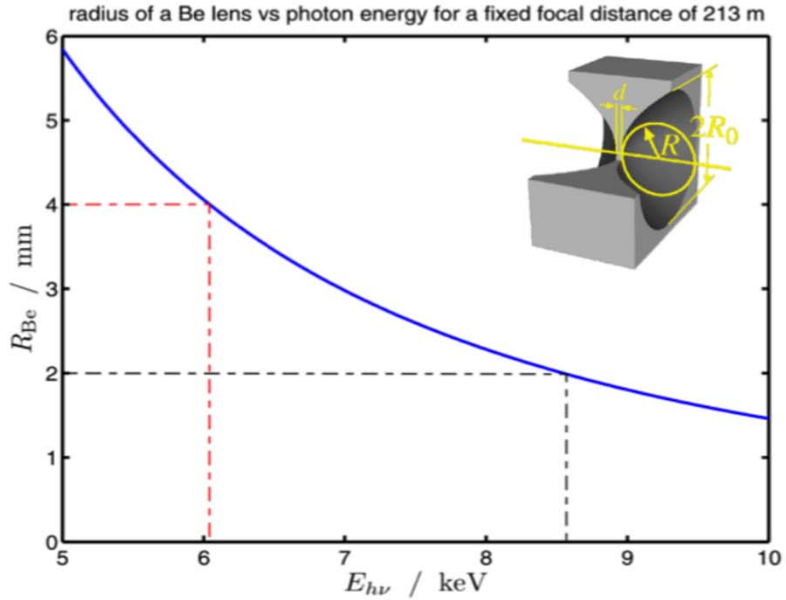
- collimate beam at 213 m (CRL collection)

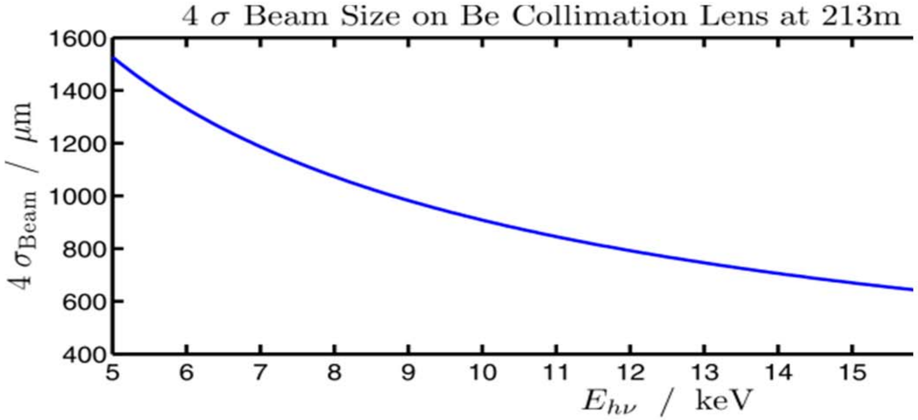
- combination of both

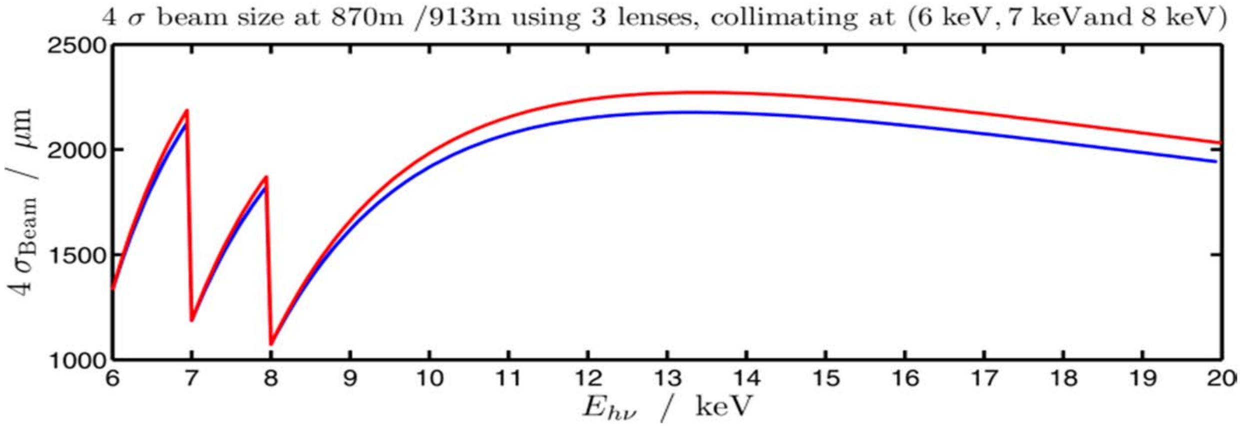




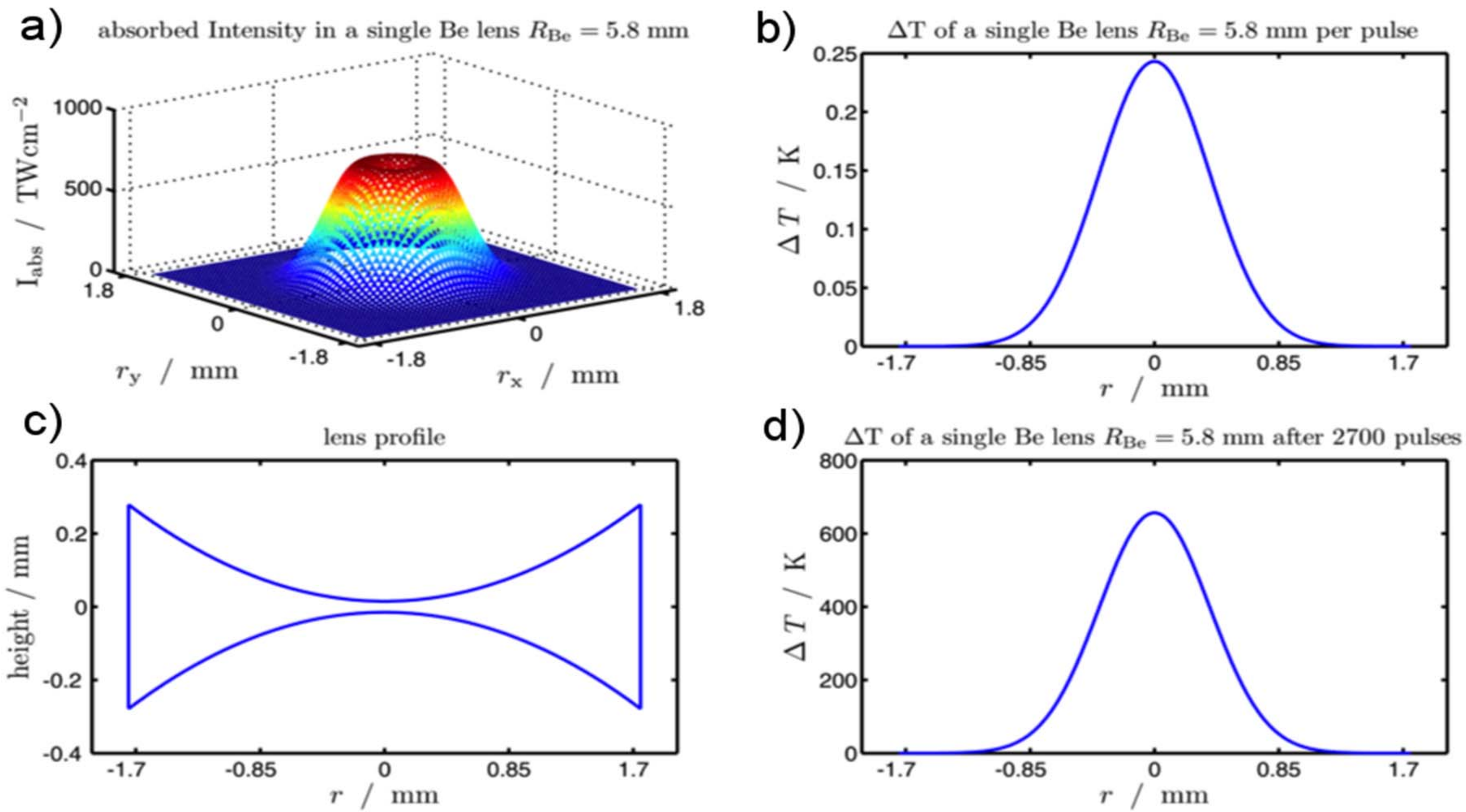
Be lenses (CRL) at 213 m: Spot Sizes



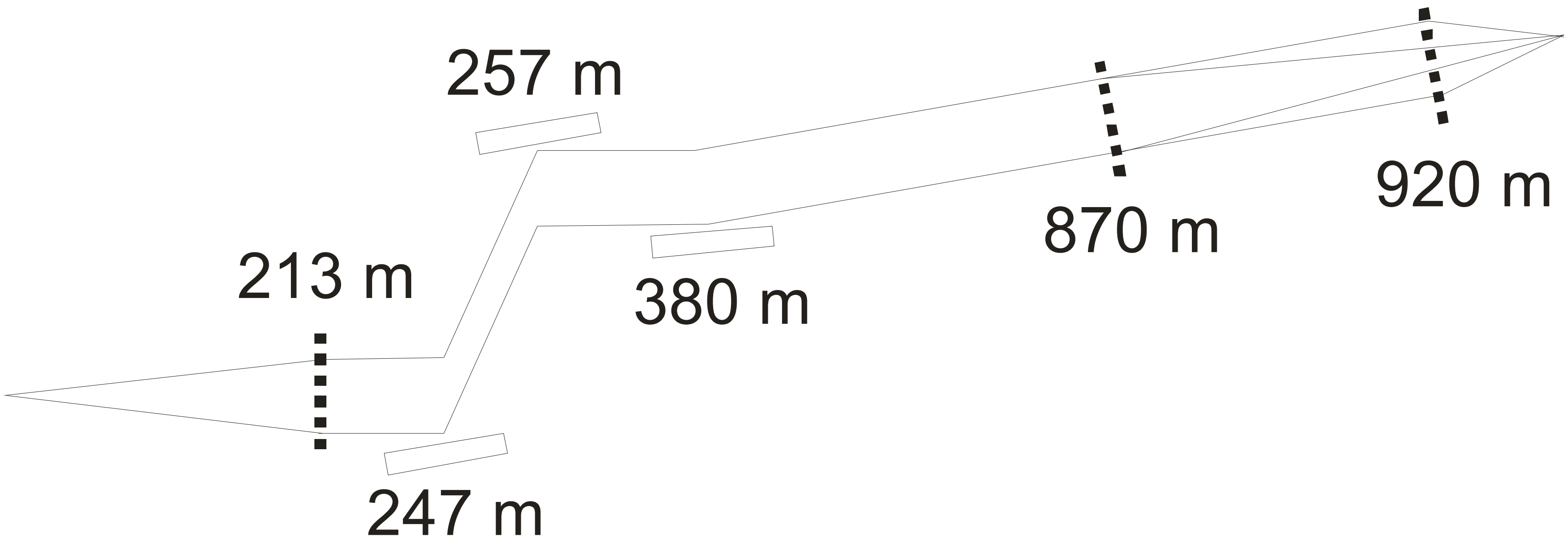


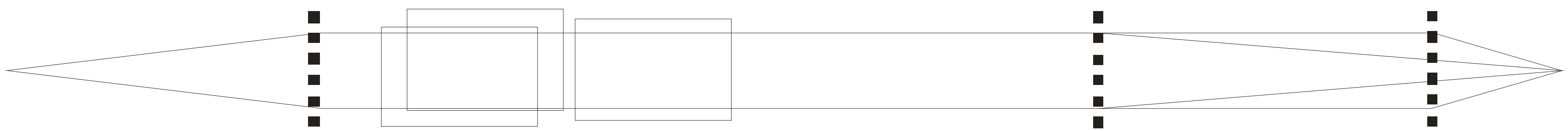


Heat Load on Be lens (213 m), 5 keV/0.25 nC



Beam Transport Concept: < 250 pC CRLs ok





European XFEL

Refocussing lenses: 870 m, 913 m

Table 1: *Relevant beam parameters (divergences, focal sizes, etc.) for selected x-ray energies at the FXE instrument using CRL stacks for focusing and beam collimation*

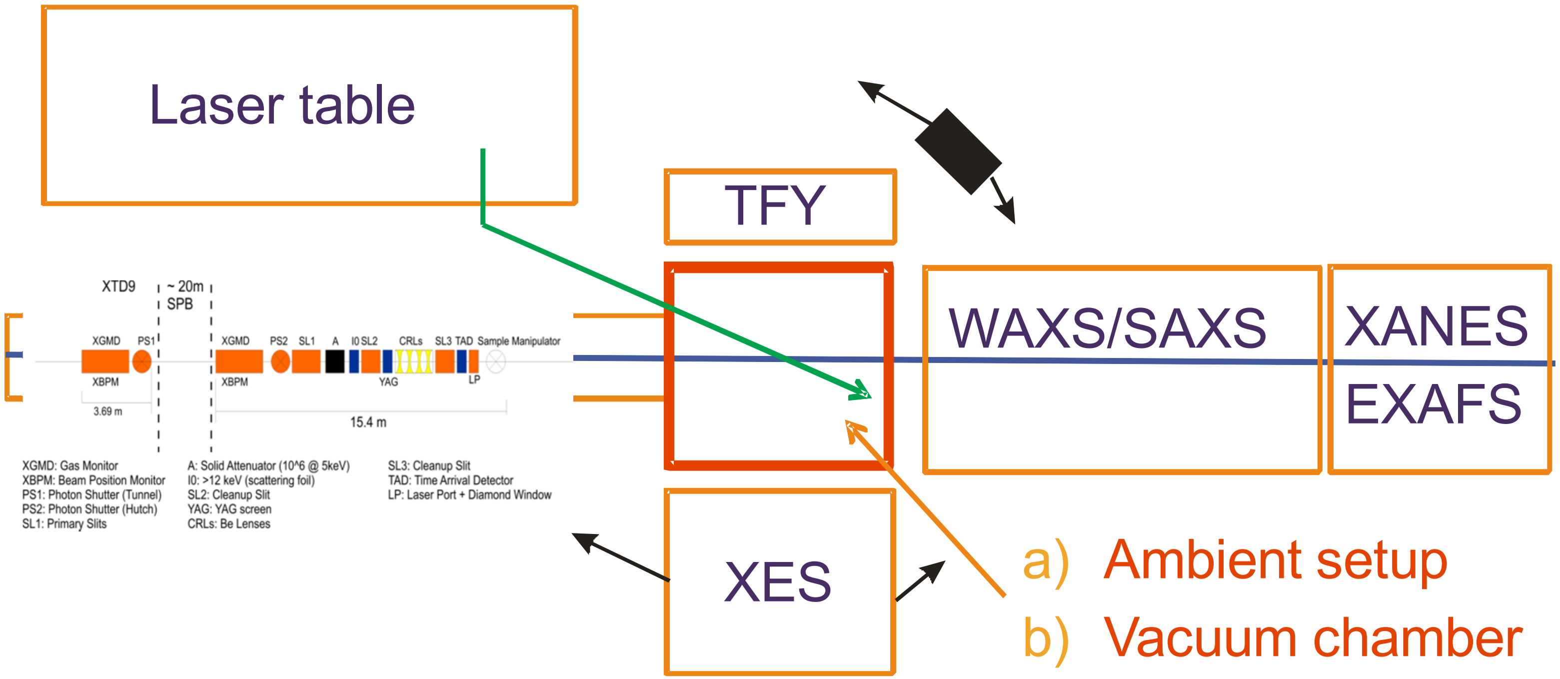
X-ray energy /keV	Source divergence *4σ* / rad	Spot size (213 m) *4σ* /mm	Divergence at 870 m / rad	Focal spot Size FWHM / m (Be stack at 870m)	Focal spot Size FWHM / m (Be stack at 913 m)
6	6.25	1.33	0	5.6 (f = 48m, N = 2)	0.6 (f = 5m, N = 16)
7	5.57	1.19	0	5.4 (f = 48m, N = 2)	0.6 (f = 5m, N = 21)
8	5.04	1.07	0	5.2 (f = 48m, N = 3)	0.5 (f = 5m, N = 28)
9	4.61	0.98	0.57	5.1 (f = 46.3m, N = 4)	0.5 (f = 5m, N = 35)
12.4	3.63	0.77	1.25	4.7 (f = 42.5m, N = 8)	0.5 (f = 5m, N = 67)
18	2.74	0.58	1.30	4.3 (f = 41.8m, N = 17)	0.5 (f = 5m, N = 142)

870 m: 5 um focus

913 m: 0.6 um focus

- Additional Option: smaller KB system (913 m)

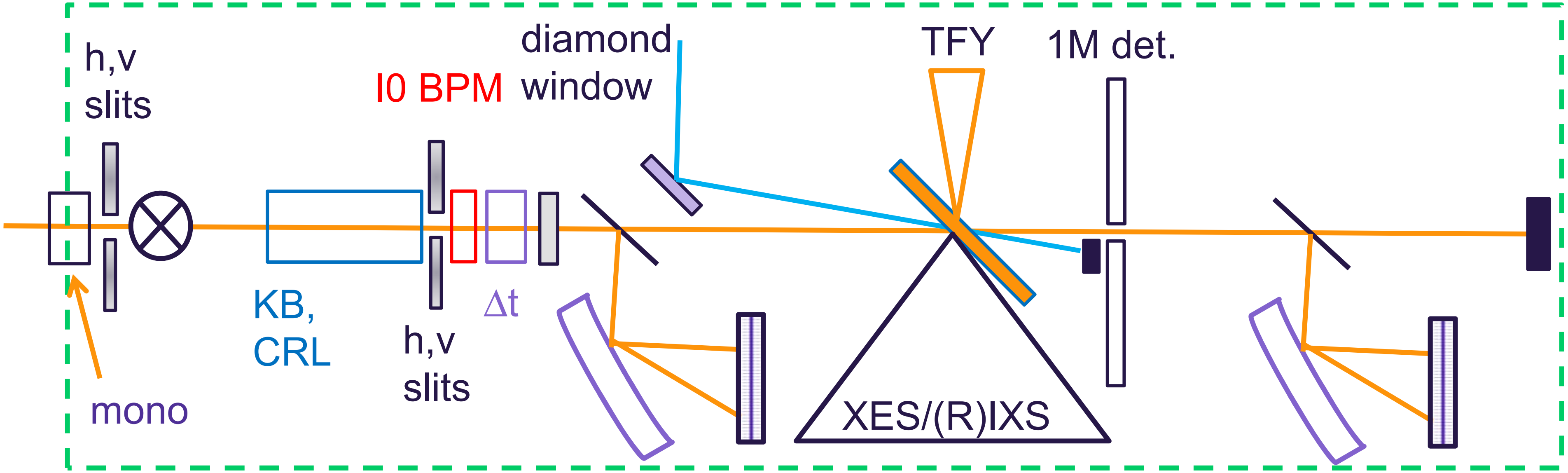
FXE basic design



Maintaining Options for 5 – 600 um Spots Sizes

- Ambient Experimental Station
  - 50 – 600 um spot sizes (line, spot)
  - **flexible He environment**
  - → rotatable XES/RIXS spectrometer
  - divergence adjustable (0 – 70 urad)
  - samples can survive beam in low-charge mode
- Add-on Equipment: Vacuum Chamber
  - small foci possibility
  - **vacuum chamber compatible**
  - may even exploit 4.5 MHz (e.g. 10 um/us)
  - divergence ca 120 urad (no hi-res xtallography)

Dispersive I0 / I1 Spectrometer



- Scatter off foil before sample
- disperse radiation behind sample
→ XANES without primary mono!

single shot spectrum, normalizable

European XFEL

Laser Parameters

- Burst Mode Laser
  - 800 nm, 15 fs
  - 0.2 mJ (or more), depending on rep-rate
  - OPA for wavelength tuning (UV-NIR), ca 1-10 uJ

Work horse for pp studies

- 4.5 MHz laser system (Tangerine)
  - 1030 nm, 285 fs, 20 W (4 uJ)
  - 515 nm, <220 fs, 10 W (2 uJ)
  - NOPA for short pulses and UV-NIR

„tickle and probe“

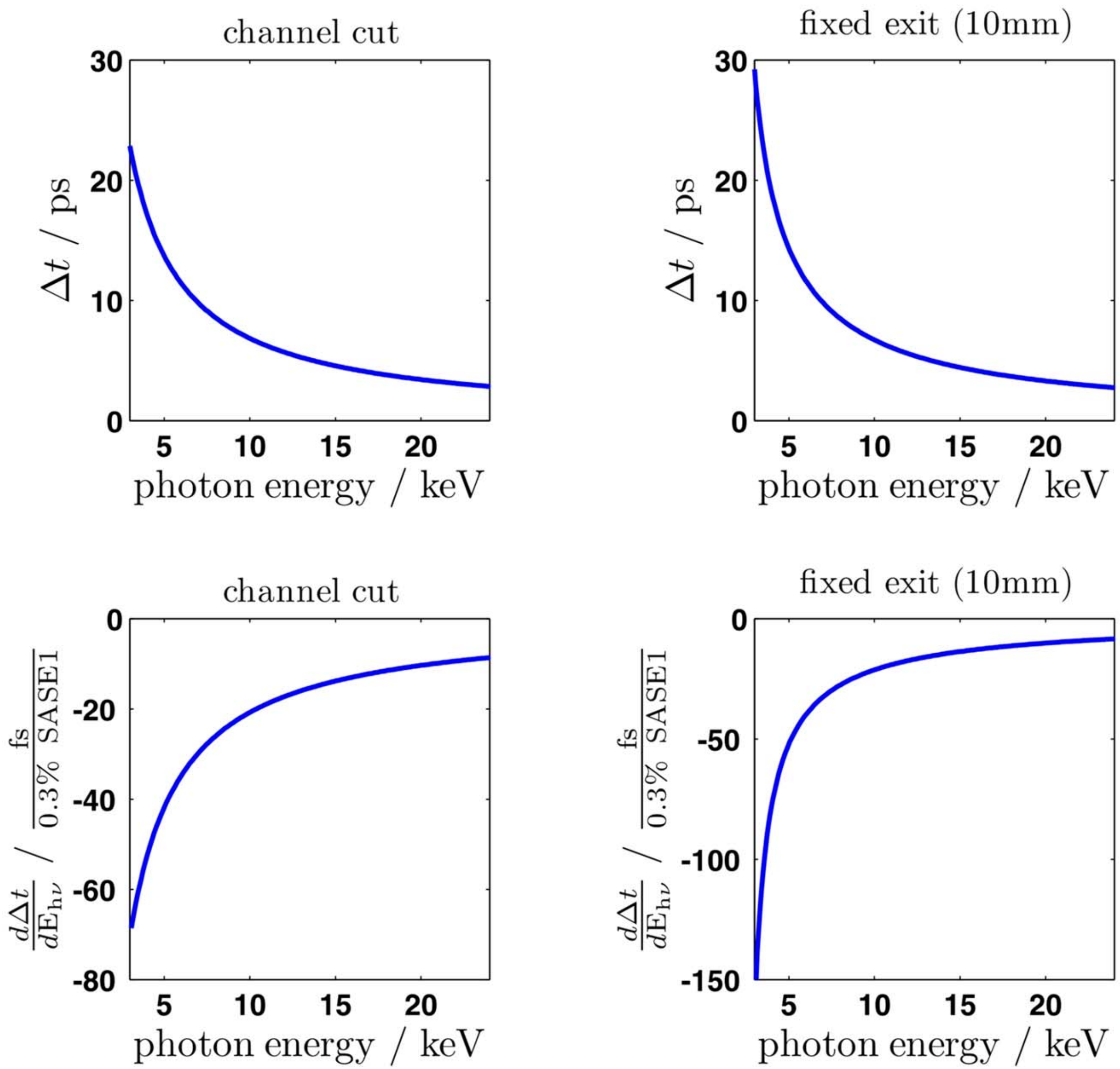
Veto laser (interpulse optical pp)

Laser fluence conditions (rep-rate dependent)

- Solids (e.g., GID)
  - 1-20 mJ/cm2
- Liquids (diffuse scattering, XAS, XES
  - 10-100 mJ/cm2 (10-15 mJ/cm2)
- Molecular Xtals,
  - <5 mJ/cm2 (30 pulses)

- Burst mode strategies
  - small spots/lines (5-20 um) → move to new sample
  - very large spots (500 um) → sample survives

Si(111): Time arrival shifts (channel-cut)

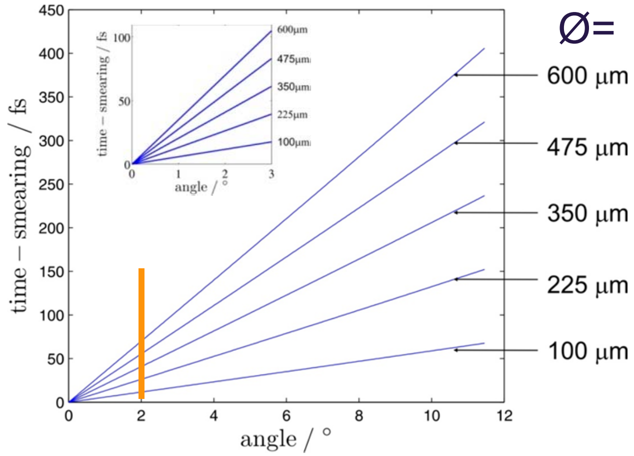


- on-axis mono (4-bounce): x 2

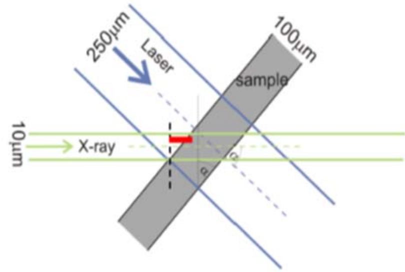
European XFEL

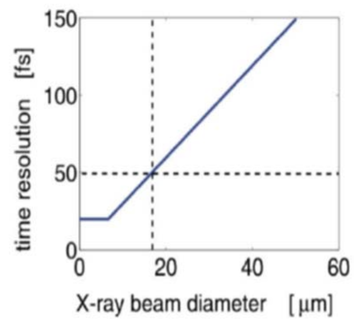
Femtoseconds: Laser-XFEL Interfacing Issues

- Time smearing (avoid via wave-front tilt)



- Refractive Index (100 um ←→ 10 um) (167 fs 17fs) can be improved



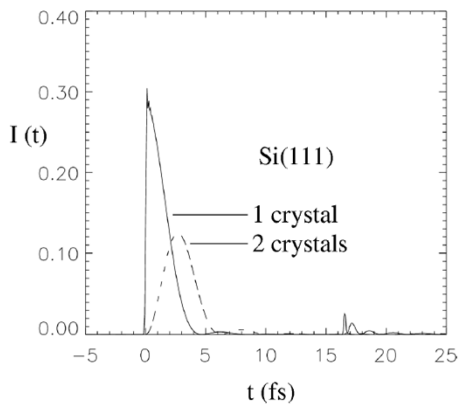


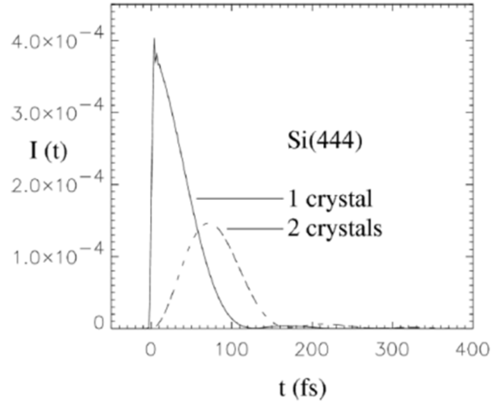
- xray mono effects:

Si(111): ca 3 fs (2e-4)

Si(444): 80 fs (5e-6)

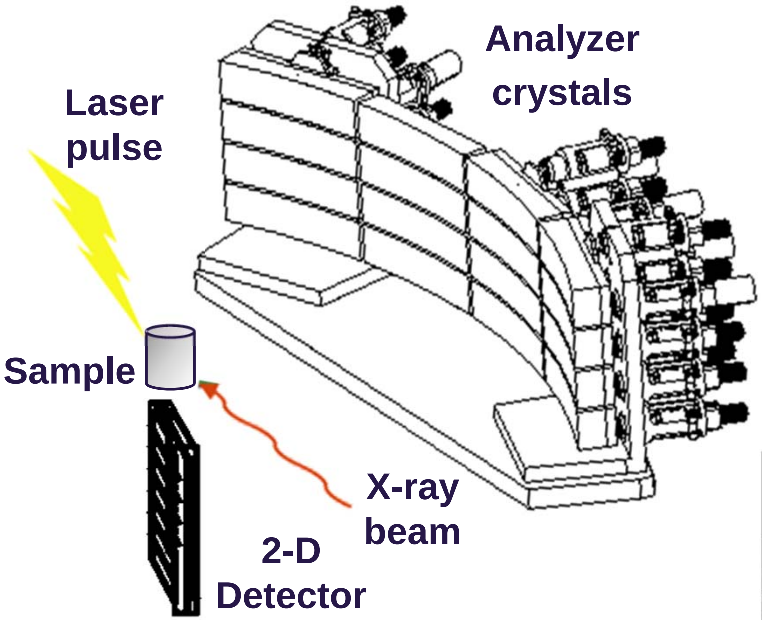
$$\Delta E \Delta t/(2.35)^2 > \hbar/2$$

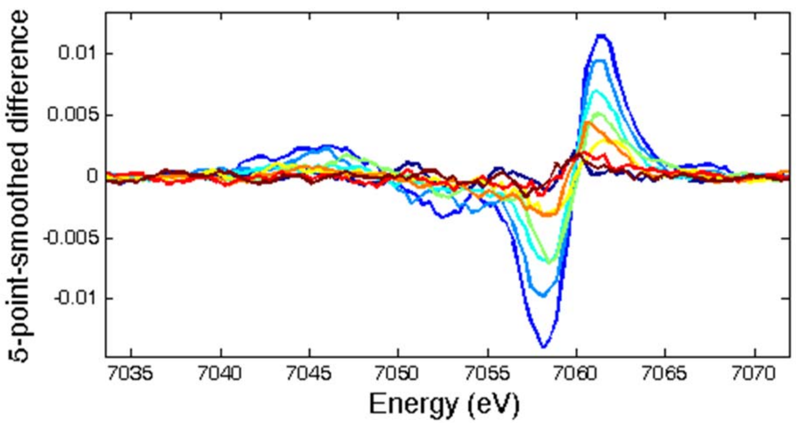


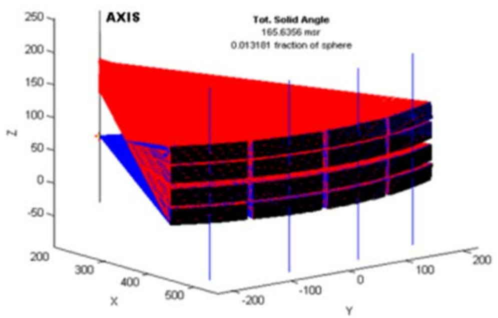


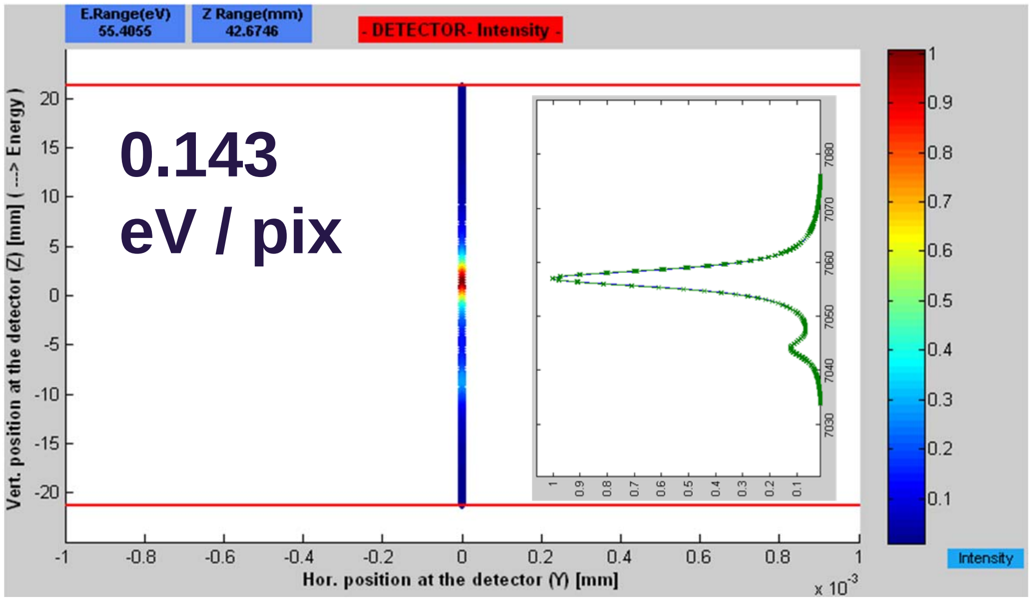
J. Synchrotron Rad. (2001). **8**, 1131–1135

XES spectrometer: von Hamos (R. Alonso Mori)

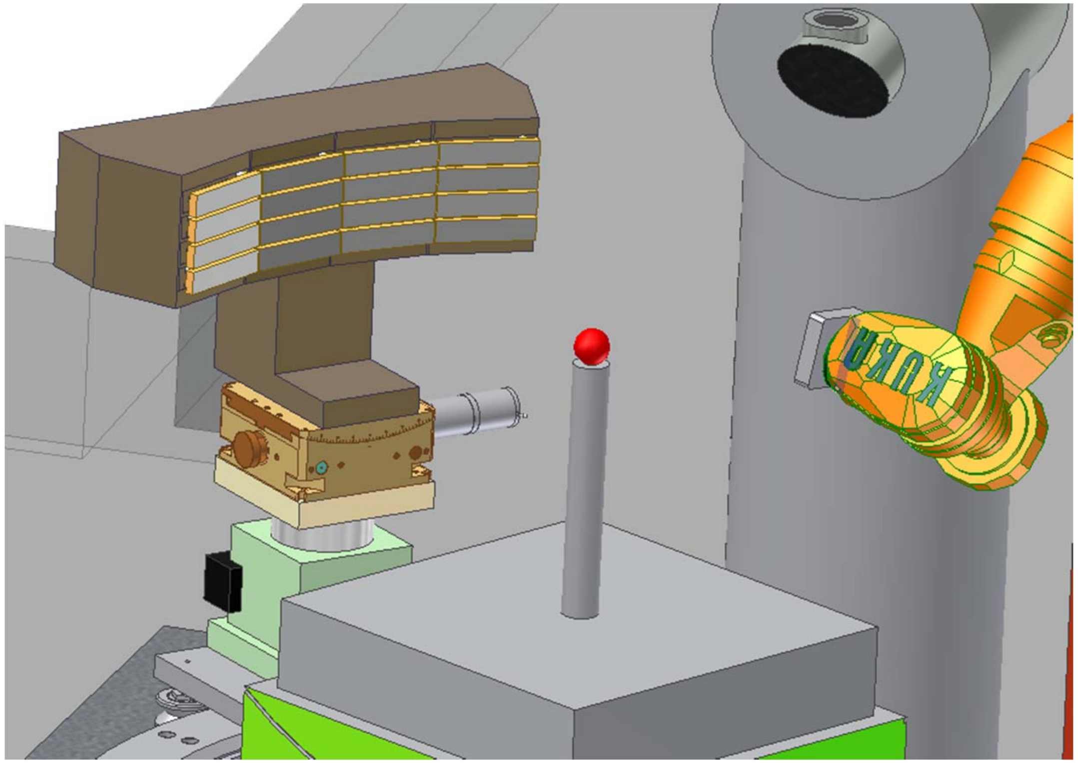








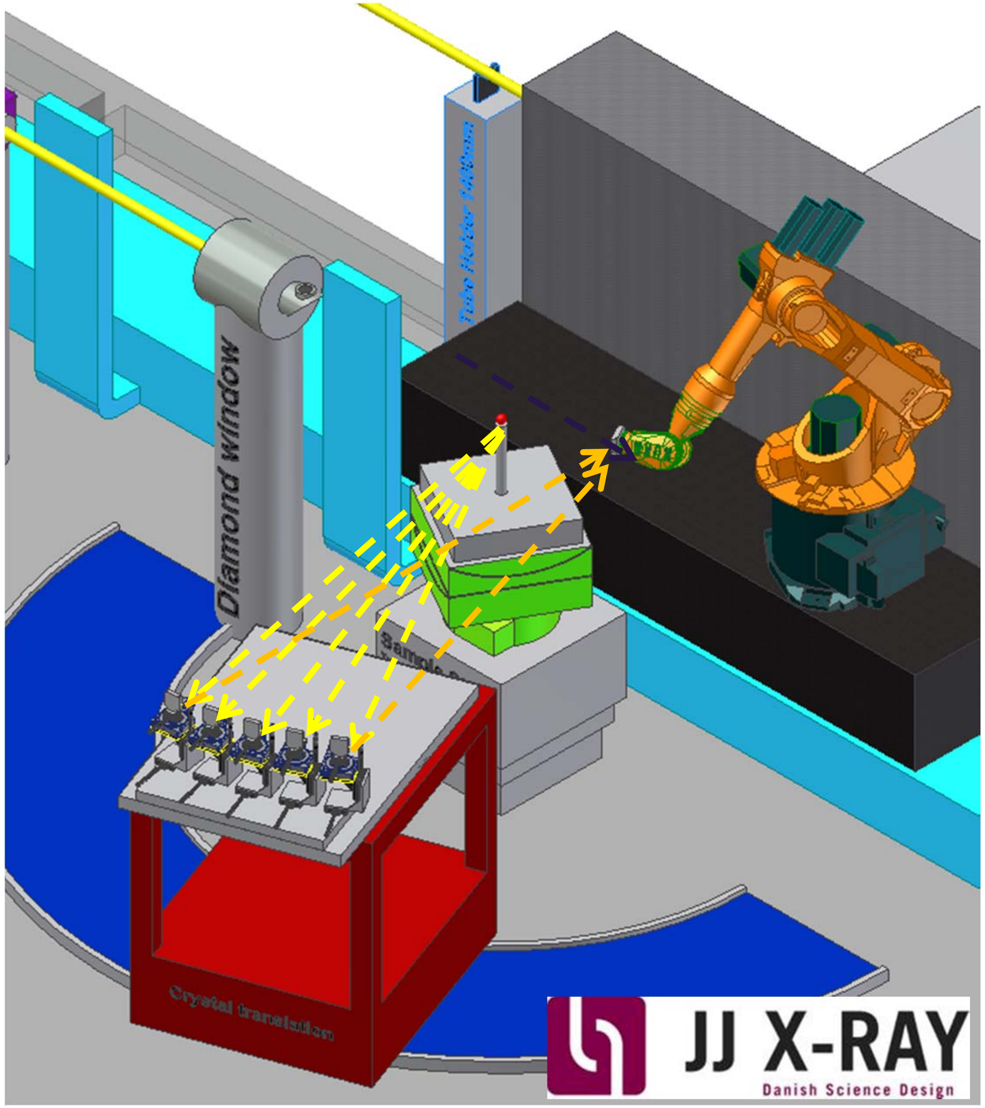
Von Hamos spectrometer setup



- Each crystal motorized by 3 actuators. Crystal fixture box is also motorized: 2 rotations and 1 translation.

JJ X-RAY
Danish Science Design

Five Element Johann Setup

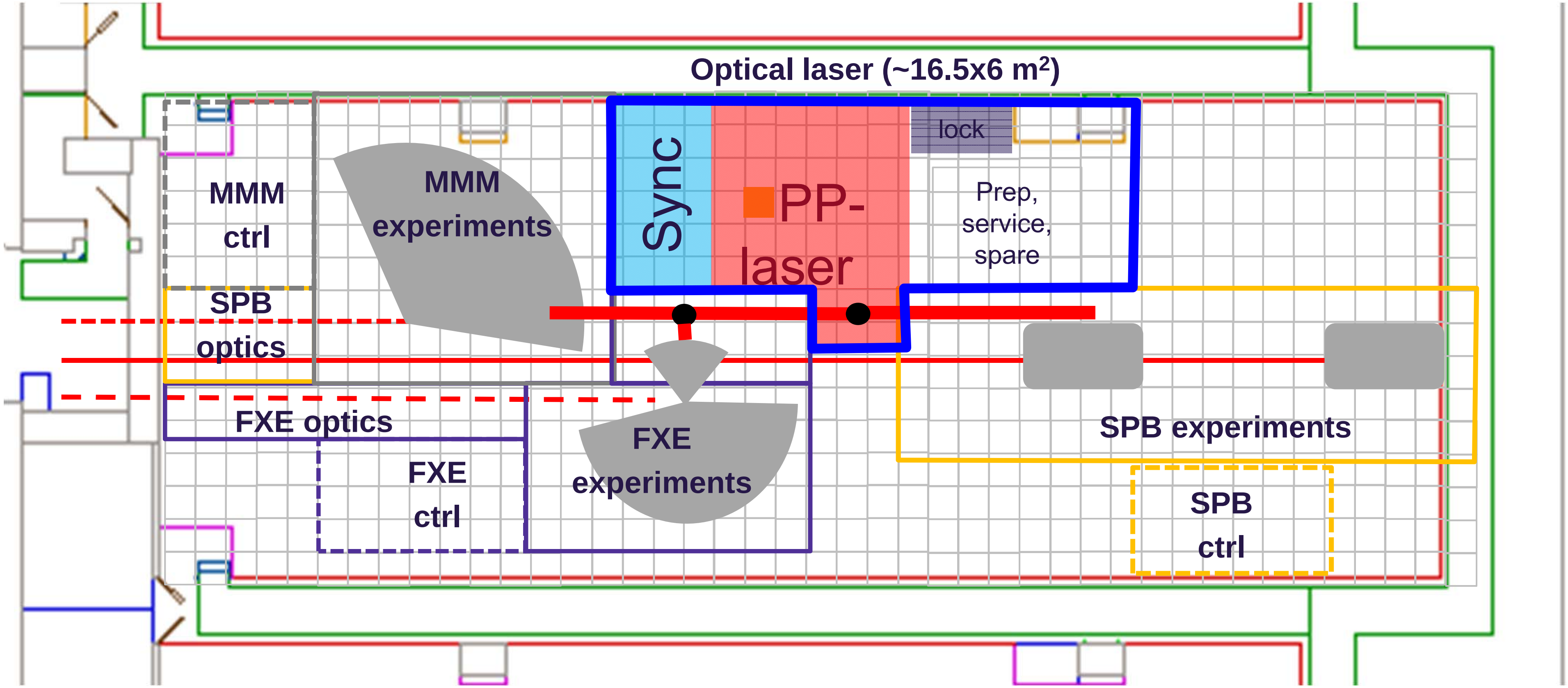


Diamond window:
- 120 pulses/burst
- 0.3 mm ok
  (5 keV)

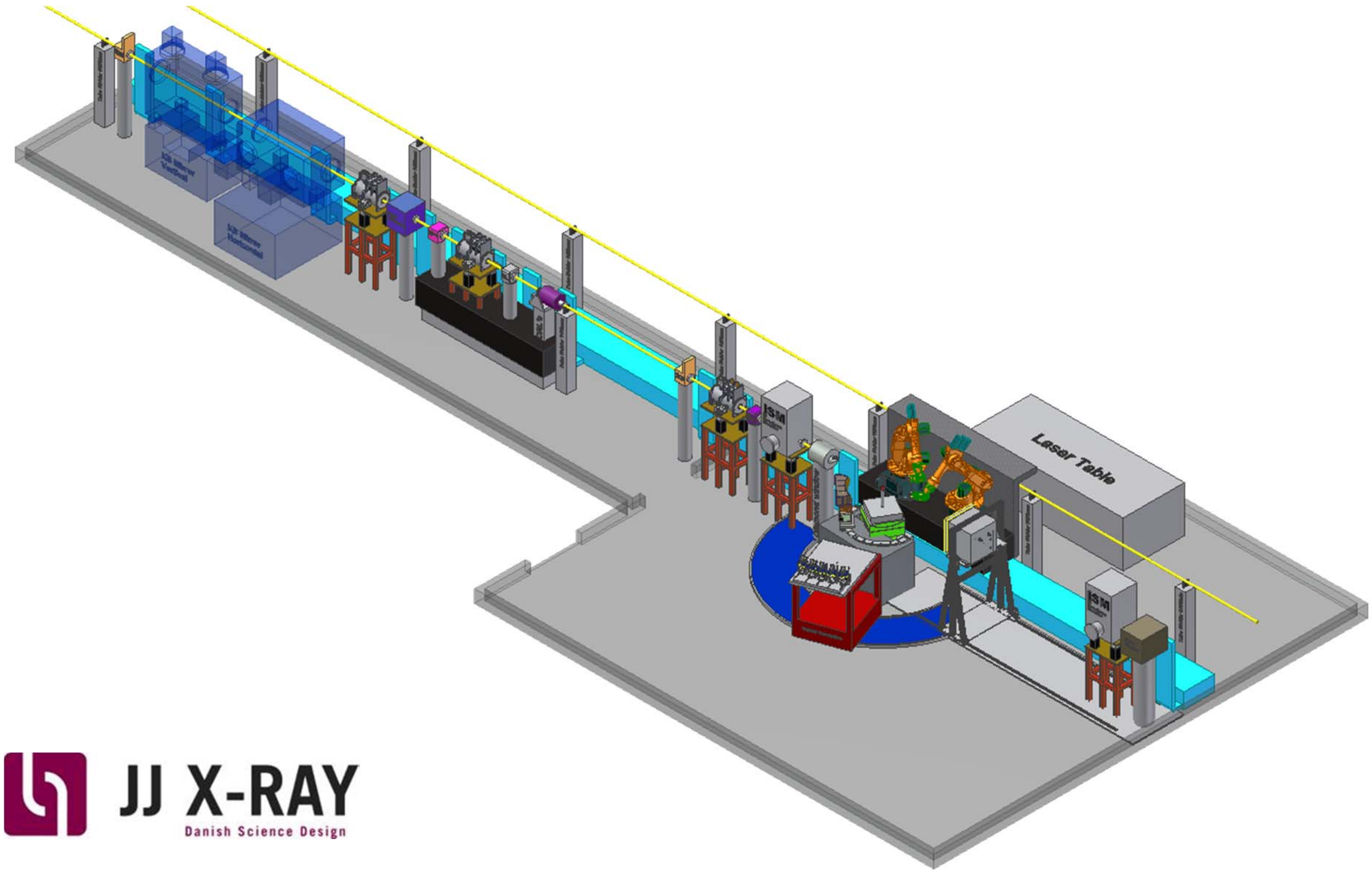
Baseline Detectors

	Diffuse Scattering	XES Analyzer	Versatile	Time Domain Monitor
Detector Type	2D Pixel	1D Strip/2D	2D	2D
Energy Range	3-20 keV	3-20 keV	3-20 keV	UV-vis
Energy Resolution	No	No (or < 200 eV@7 keV)	No	No
Frame Rate	4.5 MHz	4.5 MHz	4.5 MHz	4.5 MHz
Pixel/Strip Size	< 500 x 500 μm^2	100 x 100 μm^2	100 x 100 μm^2	< 100 x 100 μm^2
Sensitive Area	22 x 22 cm^2	2 x 6 cm^2	up to 10 x 10 cm^2 (2 x 6)	ca. 1 x 1 cm^2
# Pixels	1M	200 x 600	≥200 x 600	100 x 100
Sensor Material	Si	Si	Si	Si
Sensor Thickness	500 μm	500 μm	500 μm	-

Basic layout (work in progress)



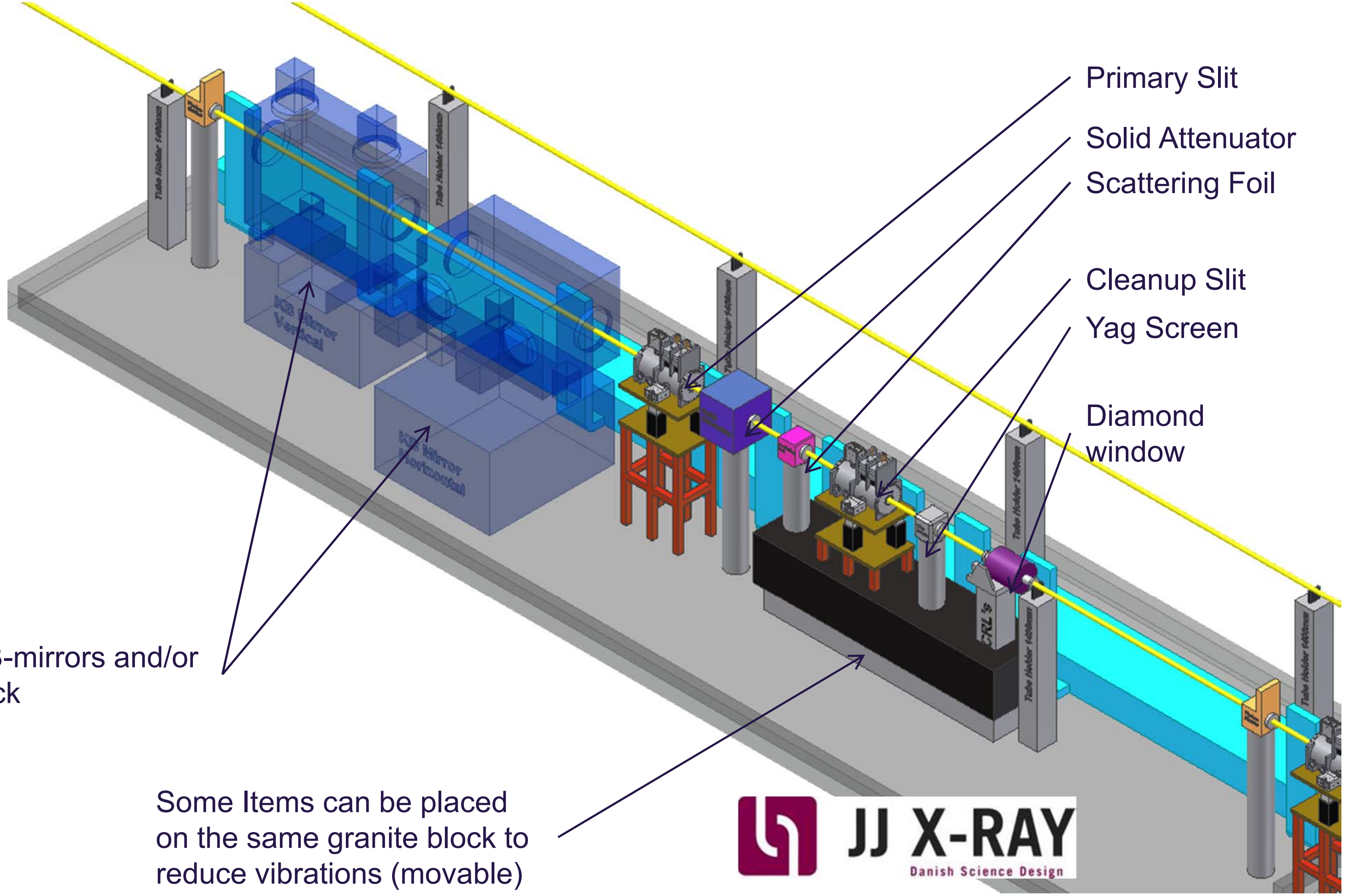
FXE Layout concept



JJ X-RAY
Danish Science Design

European XFEL

FXE Optics and Diagnostics Branch



Summary

FXE Instrument

- **Dynamics of Solids and Liquids (nuclear-lattice, electronic, spin,..)**
- **Focus on ultrafast time resolution (< 25 fs c.c.)**
- **Suitable laser conditions (pulse energy, wavelength, pulse width)**
- **flexible spot size (refresh, damage,…)**
- **versatile secondary spectrometer instrumentation**
- **ambient-He environment, + vacuum add-on**
- **1M (< 0.5 mm), 100k (0.1 mm), possibly strip (0.05 mm), 0D, …**

Time Line

- April 2011: CDR out
- 2012: TDR
- 2013+: commence ordering of components
- 2014+: Installation in exp. Hall
- Late 2014/2015: ready for beam

- Tomorrow (Thursday) 14:00: Building 48b, room 110
  FXE Workshop: Status and **User Input** (+coffee)
- Tomorrow (Thursday) 12:00: Wojciech Gawelda
  „Molecular Dynamic Processes in Spin Transition Compounds“
- Friday: FXE CDR Poster

Awcknowledgments

- FXE Team

- Andreas Galler
- Wojciech Gawelda

- European XFEL Team Members

- FXE Instrument Advisory Review Team

- Martin Meedom Nielsen (chair)
- Rafael Abela (SAC representative)
- Pieter Glatzel (ESRF)
- Alke Meents (DESY)
- Simone Techert (MPI)
- Steven Johnson (ETHZ)
- David Fritz (SLAC)
- Aymeric Robert (SLAC)