The Materials Imaging and Dynamics Instrument at the European X-Ray Free-Electron Laser Facility (XFEL.EU)

May 25, 2012

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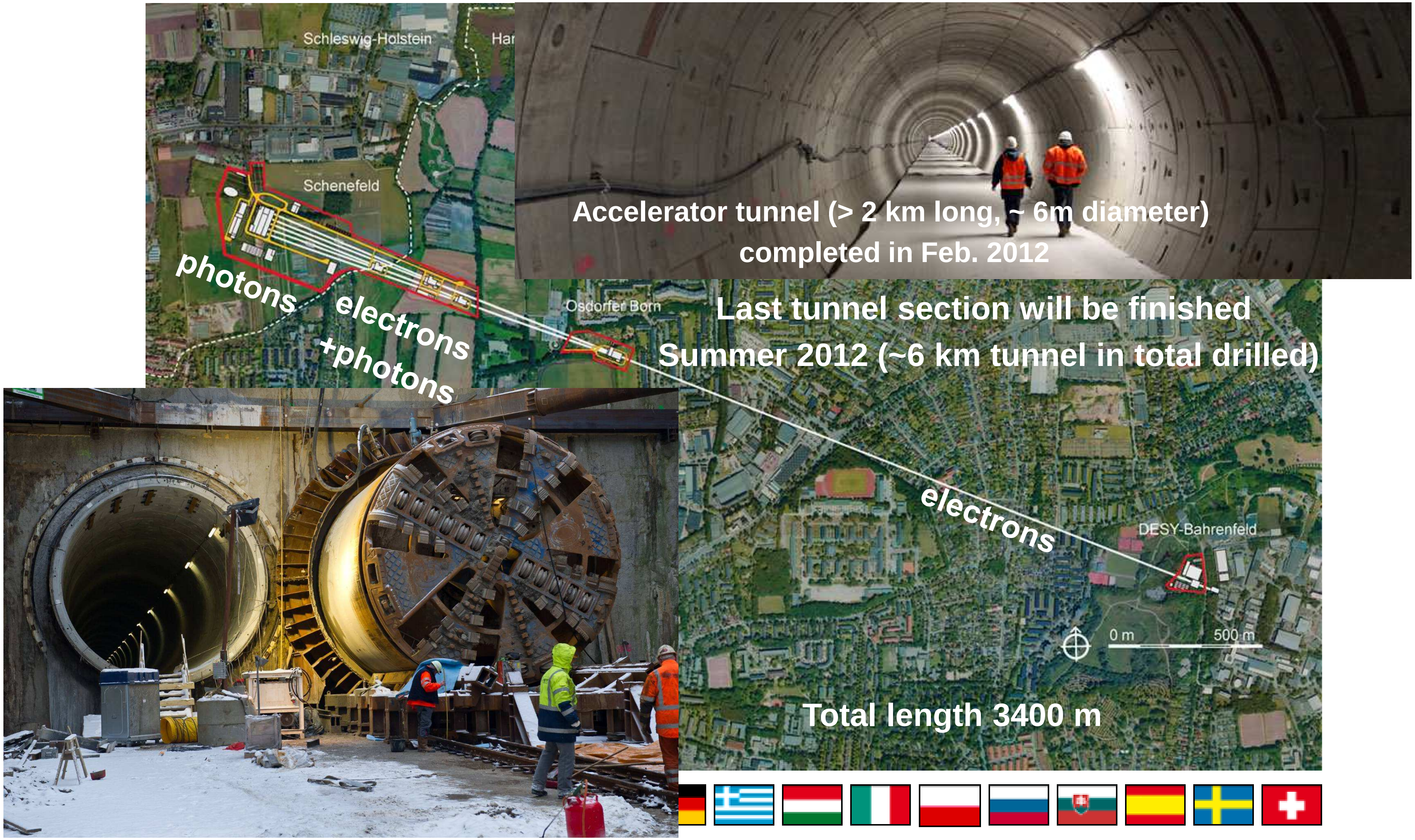
The European XFEL. An underground facility



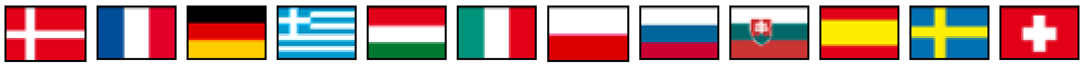
The European XFEL. Also visible overground…

The XFEL.EU HQ

The Experimental Hall

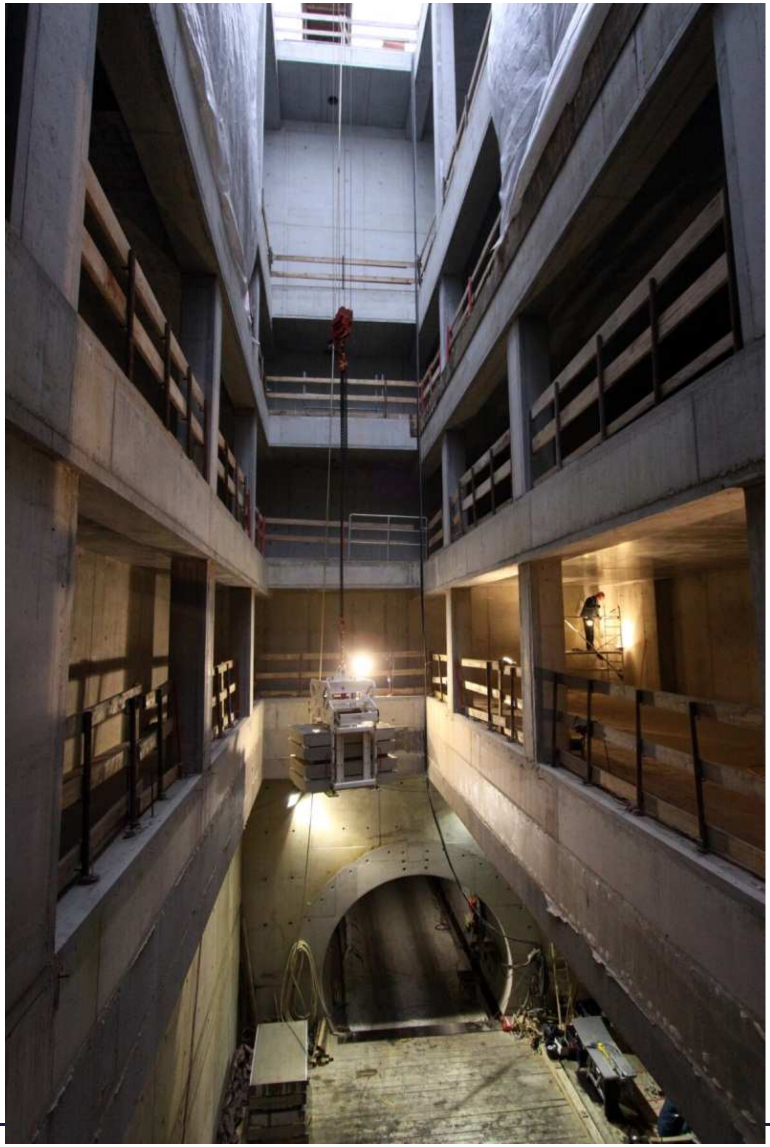
MID Tunnel (SASE 2), May 14

The XFEL.EU HQ



XFEL.EU at the DESY-Bahrenfeld Site

XFEL.EU at the DESY-Bahrenfeld Site



XTL linac tunnel

entrance shaft

30m under ground

The European XFEL

Facts and figures:

timeline

Construction phase (2009 - 2015)

Operation phase (from 2015, users from 2016)

money

Construction cost: ~1.1 billion EUR (2005 prices)

accelerator

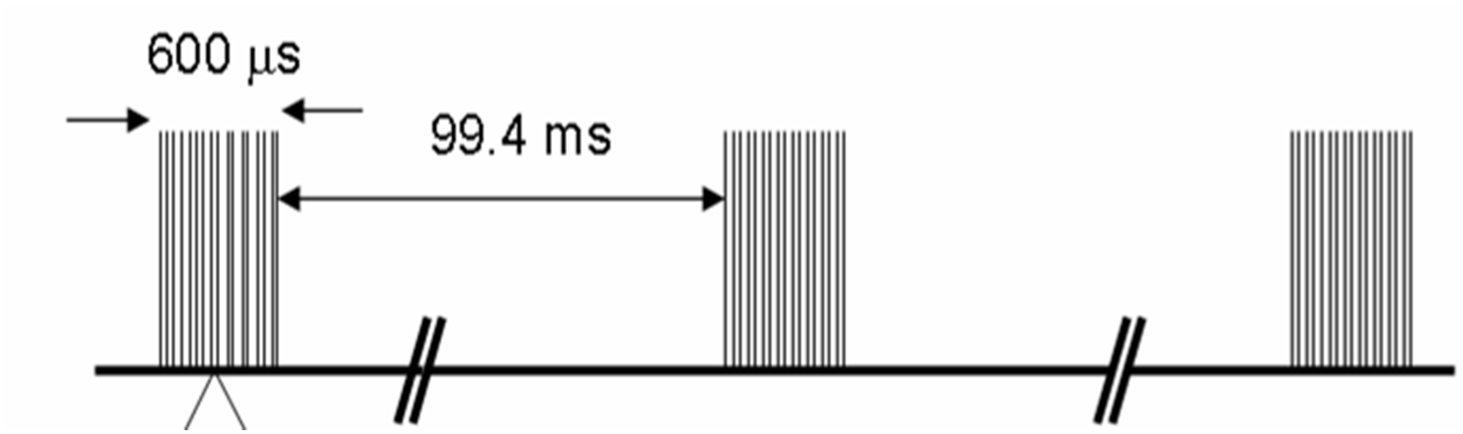
Superconducting 2.1 km long linac (-271^{o}C)

101 accelerator cavities in Nb

Electron energy: Up to 17.5 GeV

27000 pulses/s, >1nC per pulse (>1e10 e^{-})

Beam Properties



2700 pulses in each train, 220 ns between pulses, 10 trains/sec

Pulse length <100 fs

Photon flux ~ 10^{13} ph/pulse (>10^{17} ph/s)

Photon Energy: SASE up to 25 keV

Almost fully transverse coherent (optical laser like)

ΔE/E envelope ~ 1e-3 + fine structure → temp. coherence not optical laser like)

Seeding offers the potential to get rid of the SASE noise

Science at the European XFEL

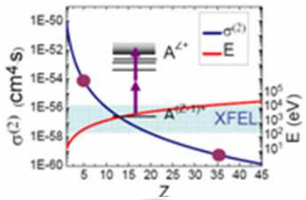
Keywords: Ultra-Fast , Ultra-Bright, and Ultra-Coherent

- Time-resolved X-ray scattering and pump – probe experiments
- Time-resolved ultrafast spectroscopies
- Single-particle scattering and nano-crystallography
- Coherent diffraction imaging and speckle correlation spectroscopy
- Extreme states of matter

… all possible combinations + the things we can’t imagine today

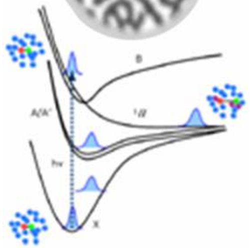
The Suite of Experimental Stations

SQS Small Quantum Systems

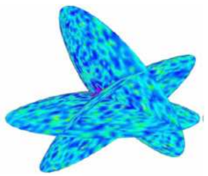


SCS Spectroscopy & Coherent Scattering

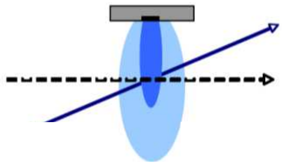
FXE Femtosecond X-ray Experiments



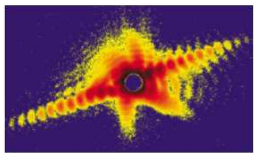
SPB Single Particle & Biomolecules

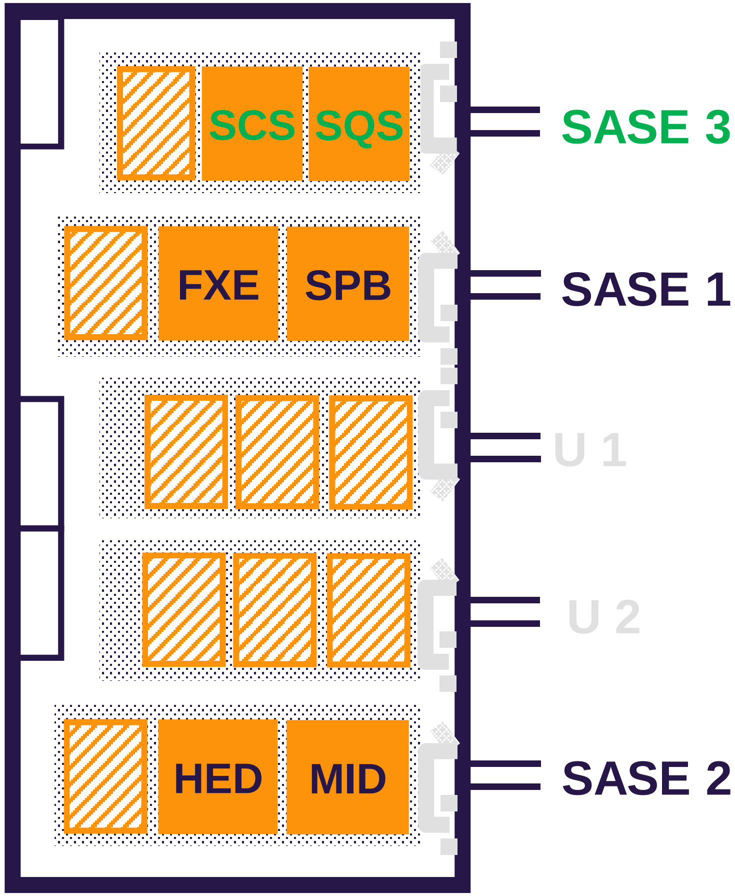


HED High Energy Density Science



MID Materials Imaging & Dynamics





More info:
European XFEL Technical Design Report (TDR)
www.xfel.eu

Materials Imaging and Dynamics Instrument

XFEL.EU TN-2011-008

CONCEPTUAL DESIGN REPORT

Scientific Instrument MID

November 2011

A. Madsen
for Scientific Instrument MID (WP83)
at the European XFEL

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Albert-Einstein-Ring 19
22761 Hamburg
Germany

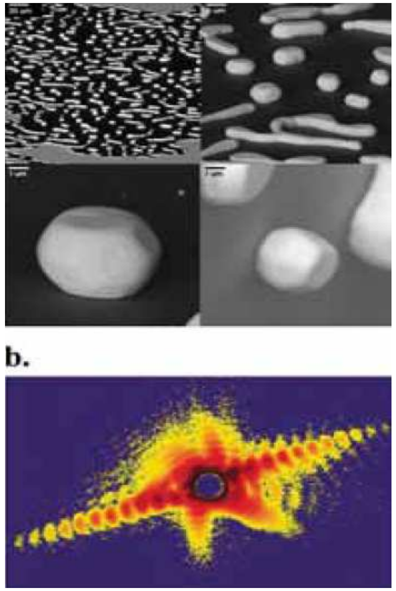
European XFEL

CDR online

MID Advisory and Review Team (ART):

G. Grübel, J. Hastings, H. F. Poulsen,
I. K. Robinson, G. Ruocco, and T. Salditt

Materials Imaging and Dynamics Instrument



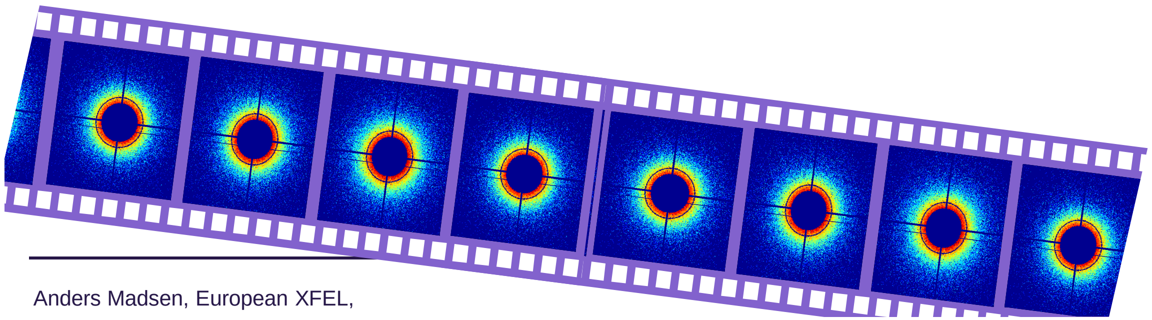
Full burst mode (4.5 MHz) for high rep. rate experiments

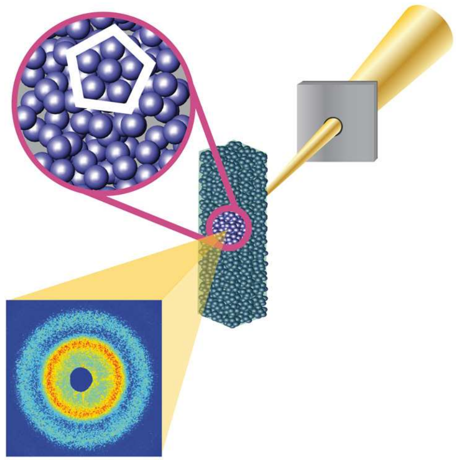
Special XPCS modes

- **every nth pulse**
- **logarithmic pulse pattern**
- **two pulses spaced by t, 220 ns > t > 1 ns**

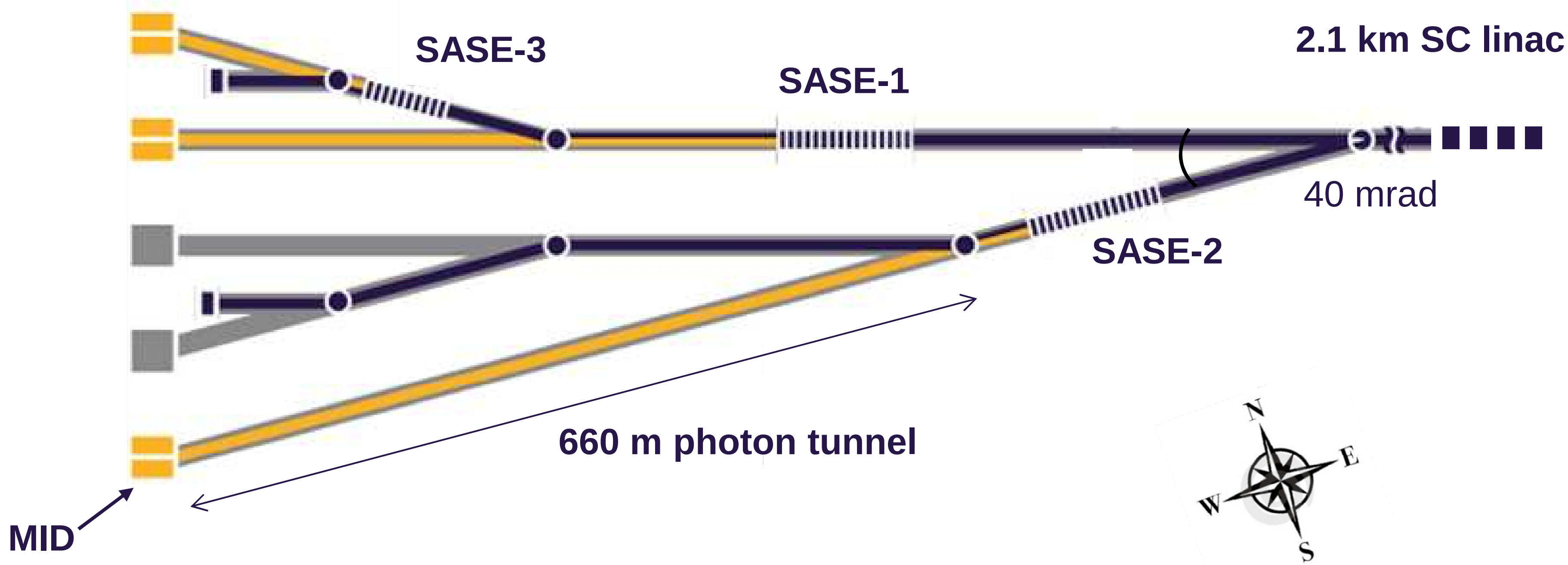
1 bunch/train (10 Hz) mode for alignment and special experiments

Bunch charge: 1 pC – 1 nC
Photon energy: 5 – 25 keV, possibly > 25 keV
Bandwidth: 1e-3, 1e-4, 1e-5,…
Seeding: YES
Beam spot on sample: 1 μm, 10 μm, 100 μm or more



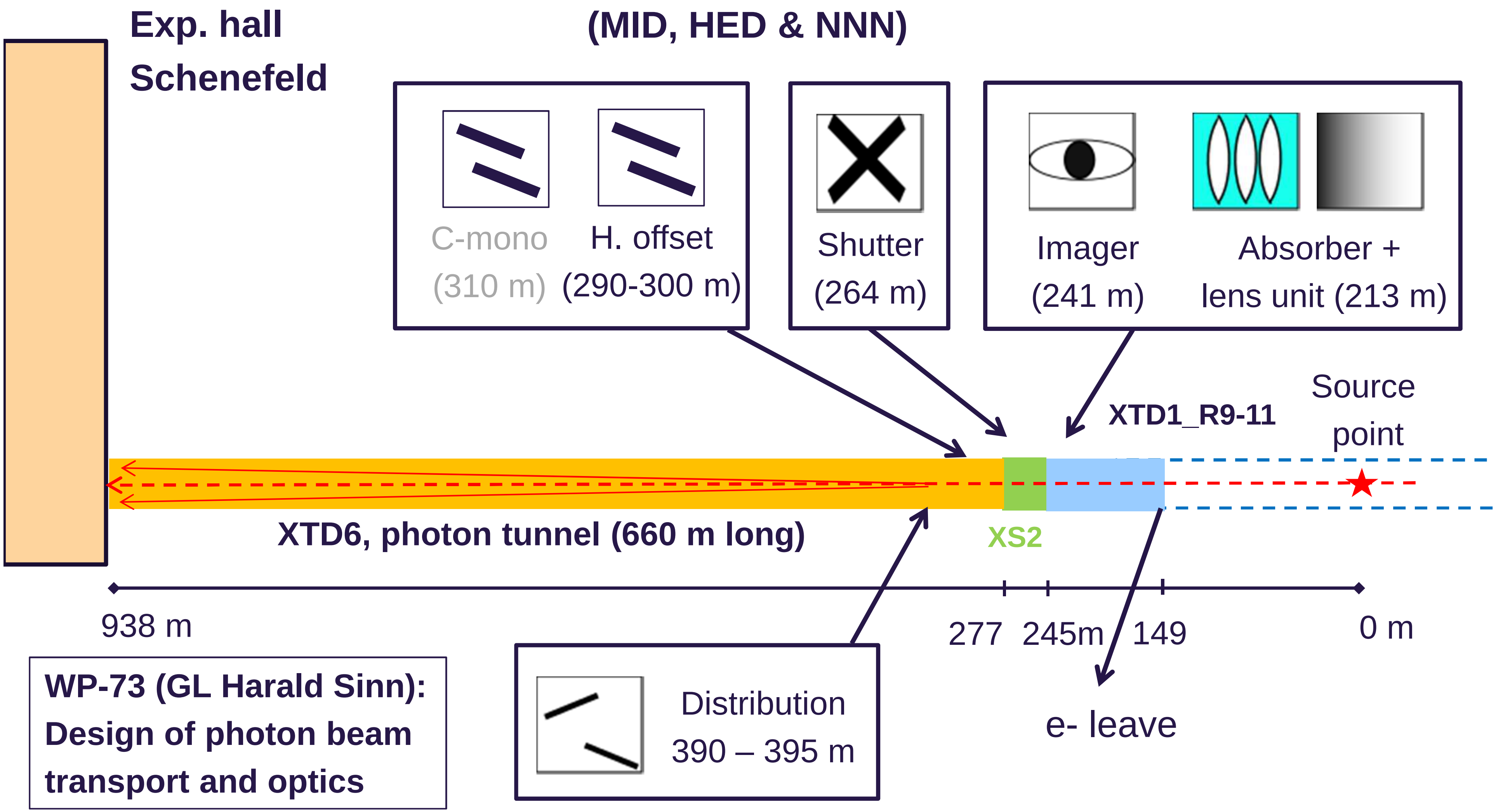


Outline of the European XFEL Facility



SASE-2 Overview

Common to all SASE-2 beamlines (MID, HED & NNN)

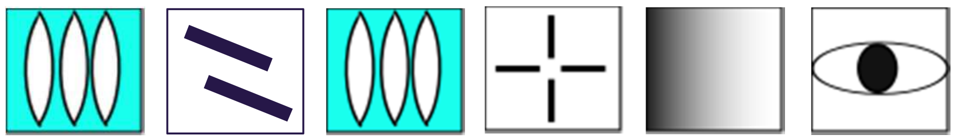


MID Specific Tunnel Optics

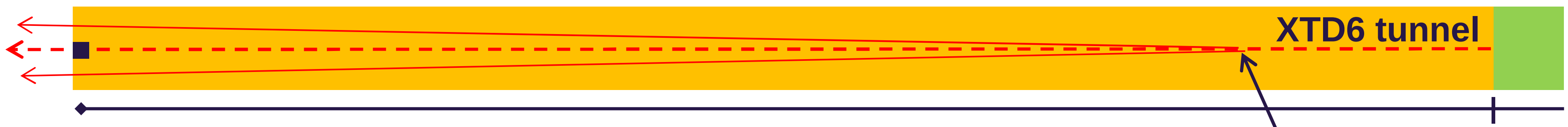
The MID station occupies the central branch of the SASE-2 beamline

~1.4 m beam separation at tunnel exit

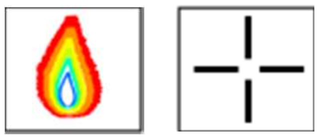
MID end-of-tunnel optics



Lens (936 m) | Si(111) mono | Lens (high E) | Slit | ATT | Imager



938 m | 726 m | 277 m

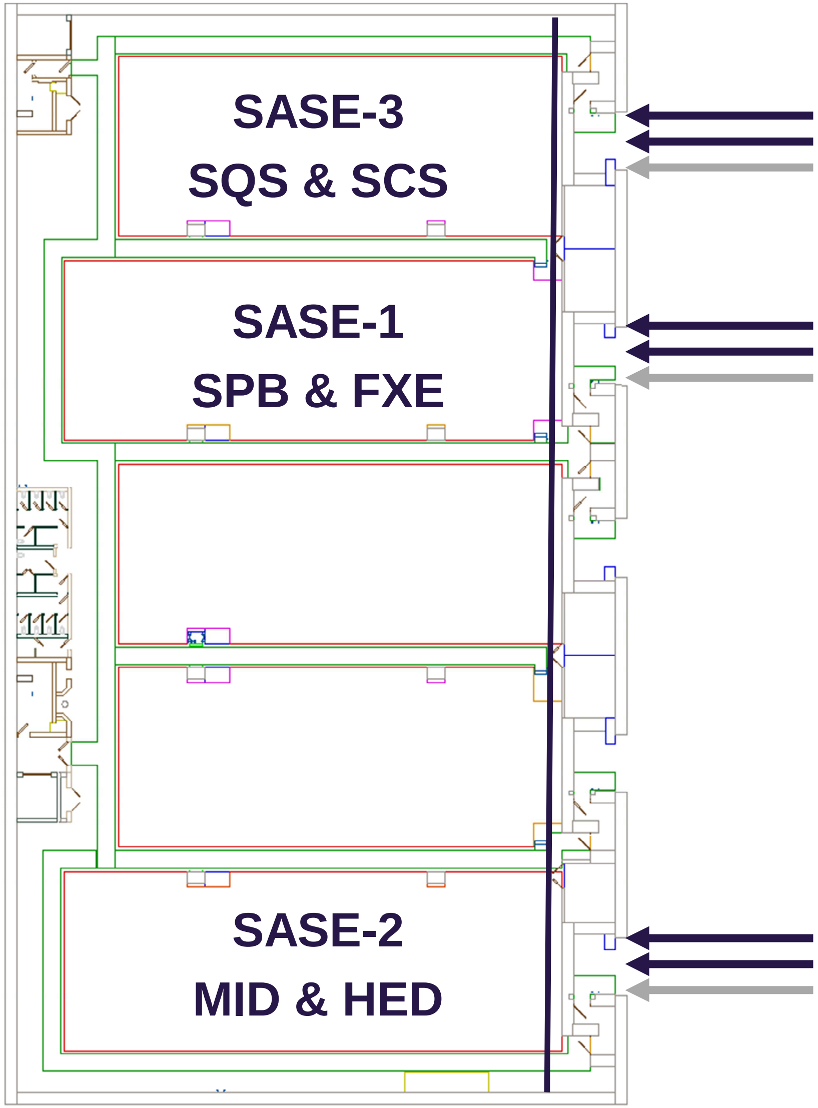


Intermediate focus option. Beamsize: 50 - 100 μm

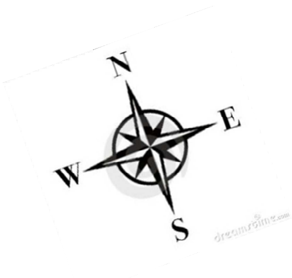
Distribution 390 – 395 m

Experimental Floor

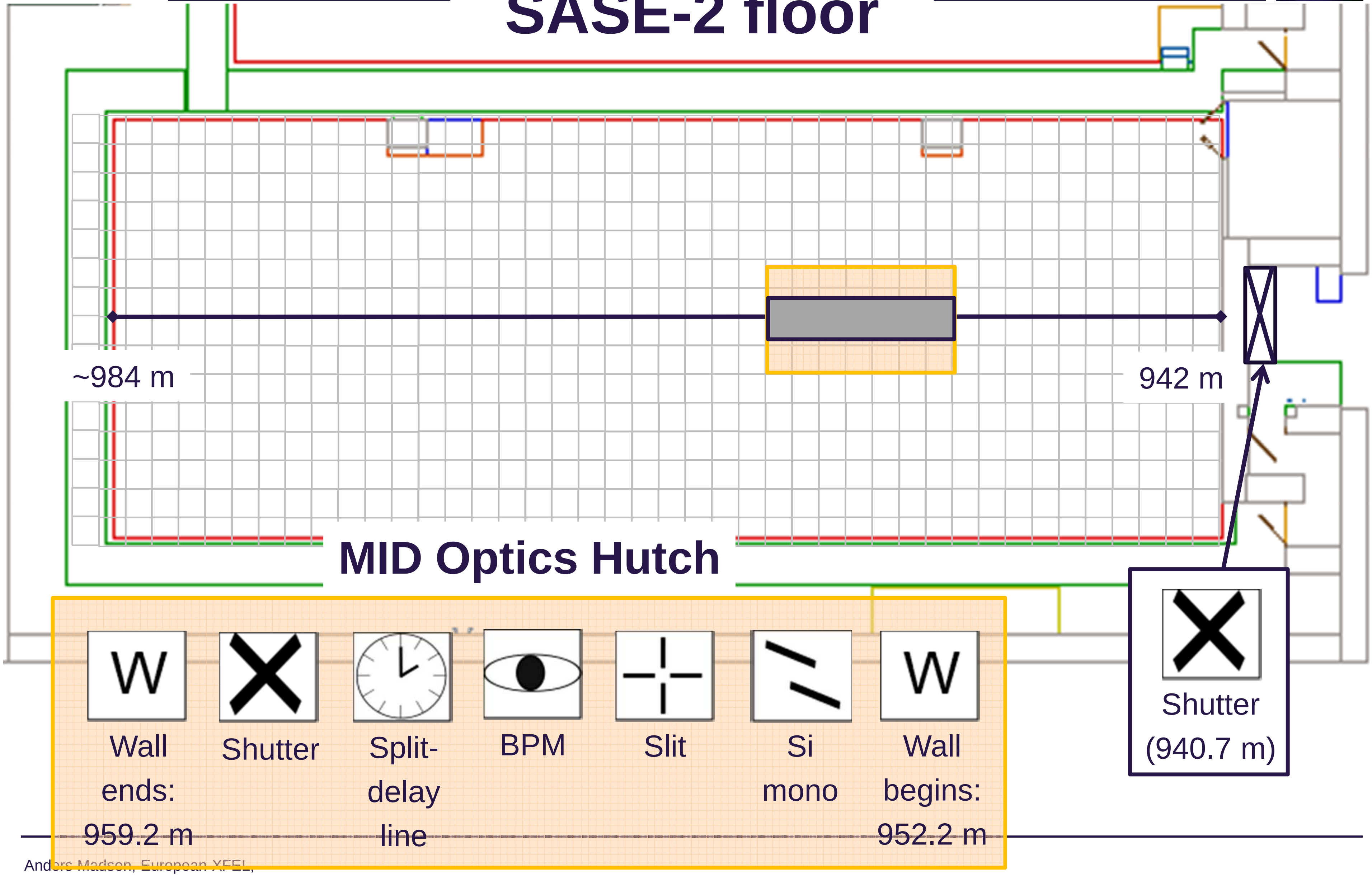
Experimental floor
~ 90 x 46 m



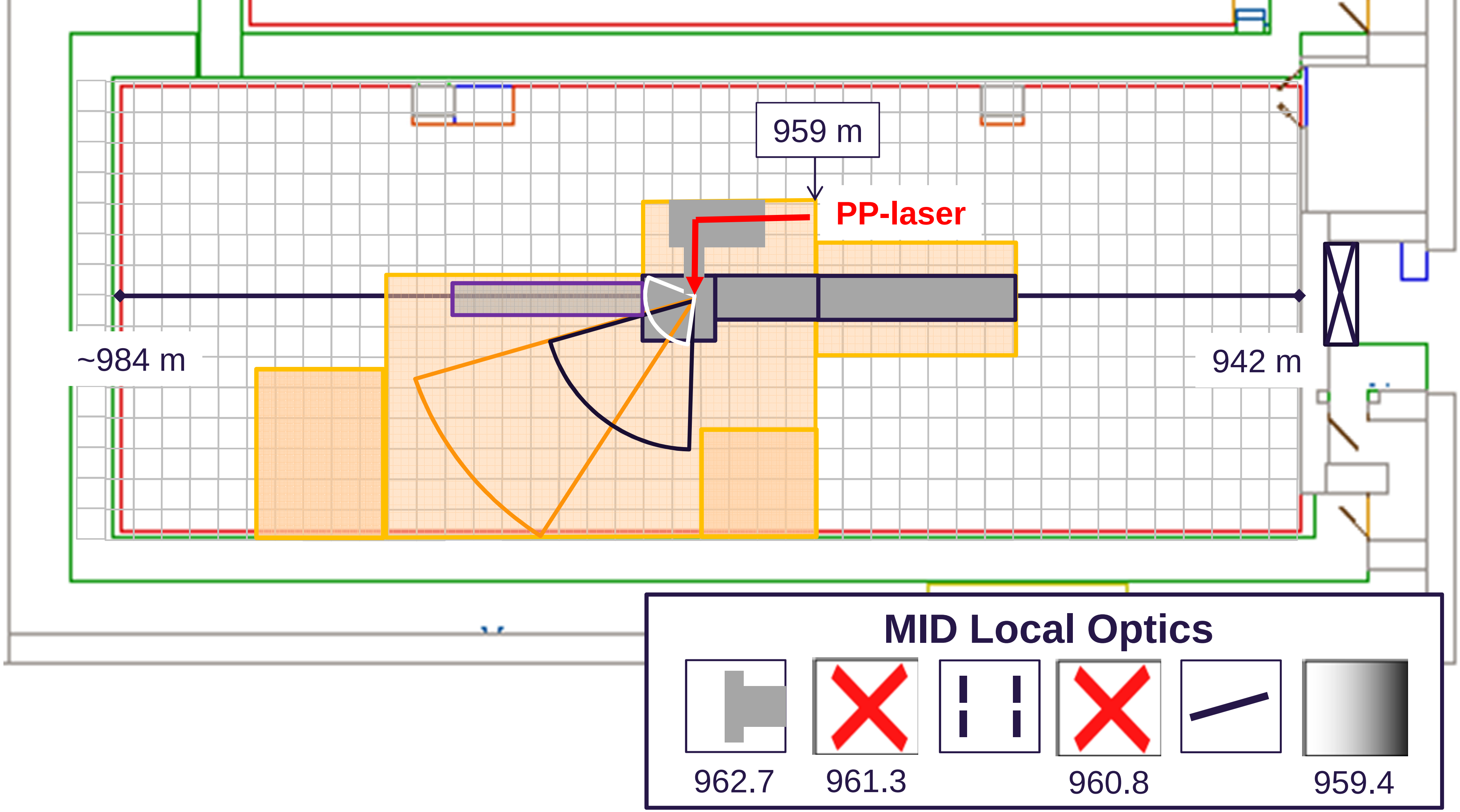
Football field size:
105 x 68m



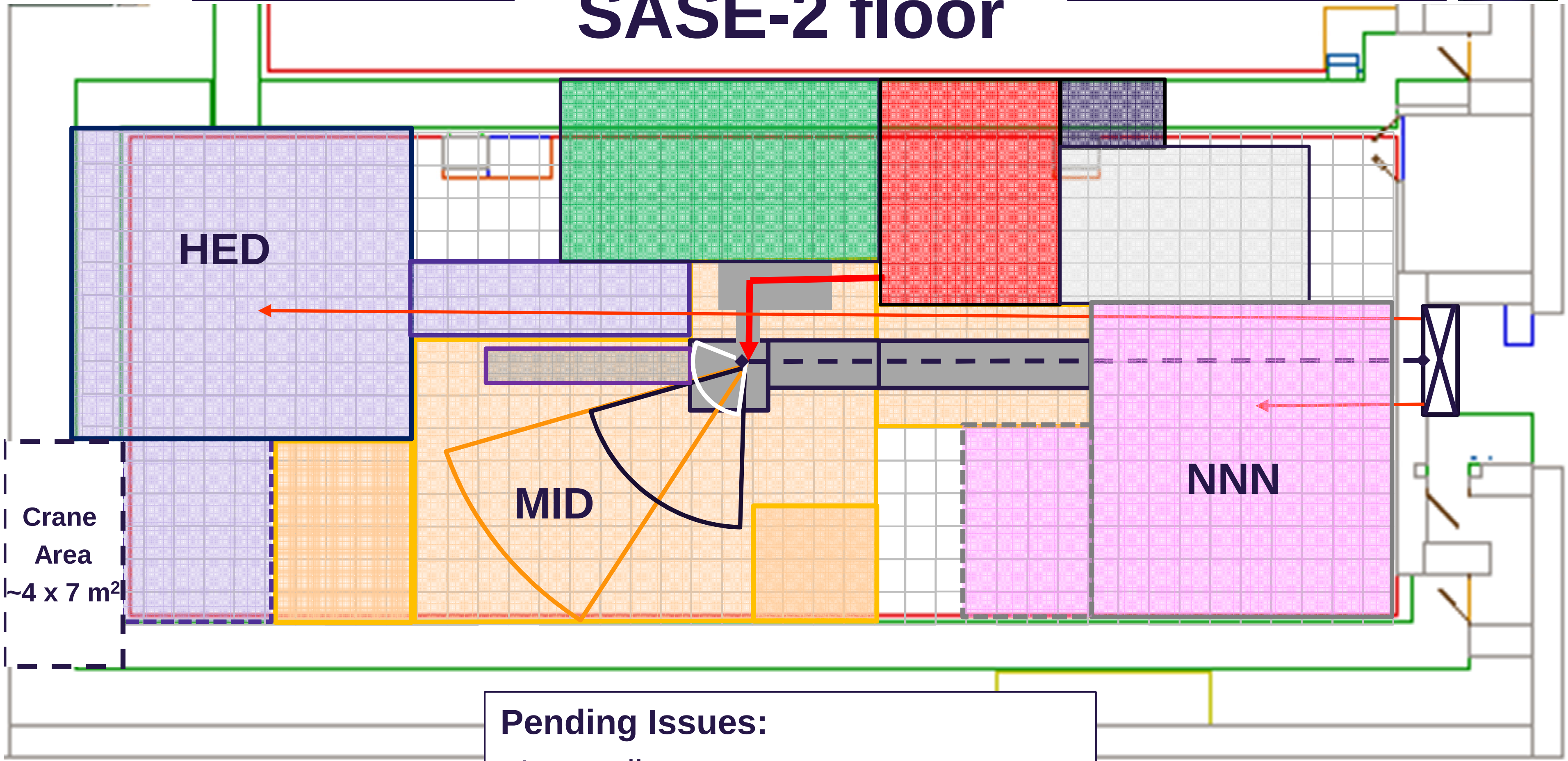
SASE-2 floor


~984 m
942 m
MID Optics Hutch
W
Wall
ends:
959.2 m
Shutter
Split-
delay
line
BPM
Slit
Si
mono
W
Wall
begins:
952.2 m
Shutter
(940.7 m)

SASE-2 floor



SASE-2 floor



Pending Issues:

- Last adjustments
- Radiation safety requirements
- Position and shape of laser hutches
- Requirements of NNN experiment?

MID Instrument Ingredients (work in progress…)

Long SAXS tube, preferably with detector movable in-vacuum

WAXS setup with up to 10 m detector-sample distance

Windowless operation preferred

Sample environment and positioning system (stationary targets, injector)

Optical microscopes, photon, electron, ion(?) detectors

Laser pump with tunable wavelength

Large 2D X-ray detector with small pixels and 4.5 MHz operation

SASE up to 25 keV, >25 keV an option (E_c ~ 160 keV, higher harmonic lasing)

Flexible bandwidth: 1e-3, 1e-4, 1e-5. Self seeding much wanted!

BPMs, spectral monitor, coherence monitor

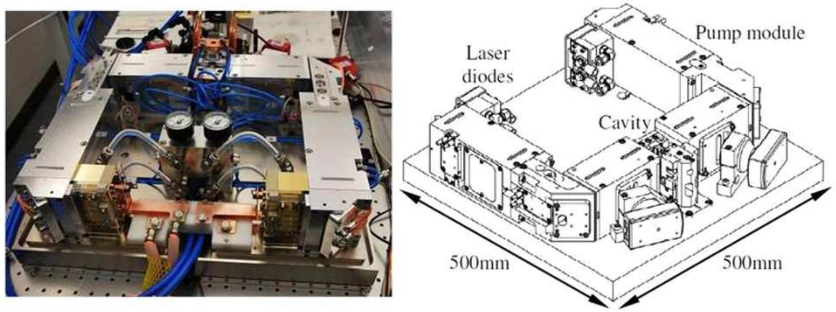
Focusing and beam tailoring by Be refractive lenses (CRL)

X-ray split-delay line for time correlation experiments and pump-probe studies

MID Interfaces to other groups

Optical lasers

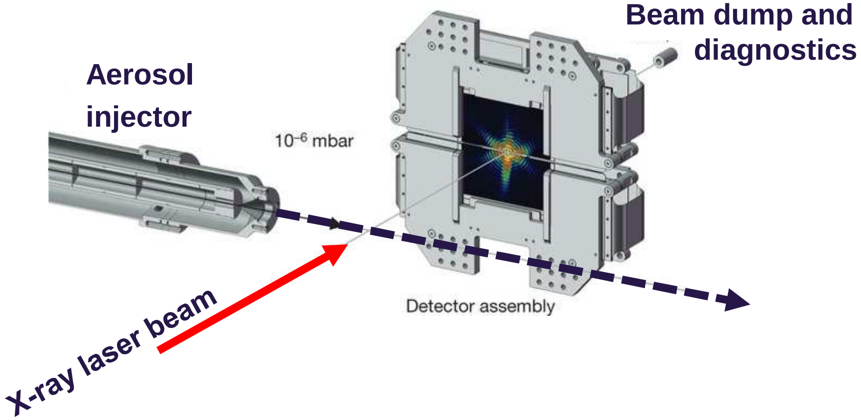
- several energy levels (µJ – 100 mJ),
- pulse durations (10-20 fs, 100 fs, ps),
- frequency conversion
- synchronization (<10 fs)



InnoSlab Design, ILT Aachen/Ampheos

Sample environments & diagnostics

- fast exchange
- precision positioning and motion
- pulse-resolved diagnostics



Detectors

- 2D pixel detectors
- high rep. rate and small pixels

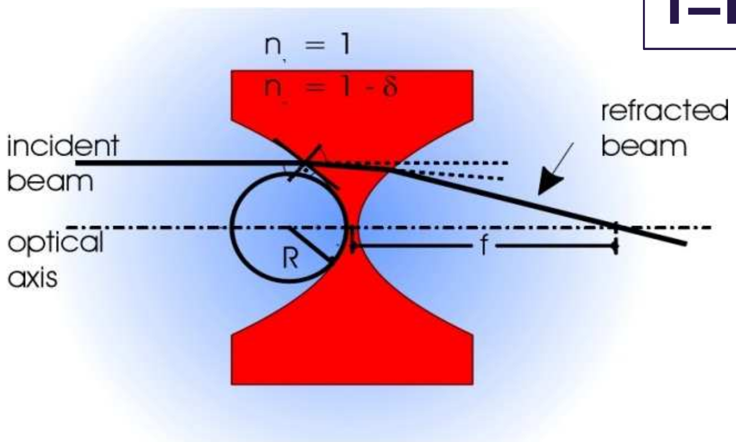
DAQ & data handling

- user-friendly, flexible environment
- data stream, storage, software and remote access

AGIPD

Adaptive Gain Integrating Pixel Detector

Refractive Beryllium lenses for X-Ray focusing

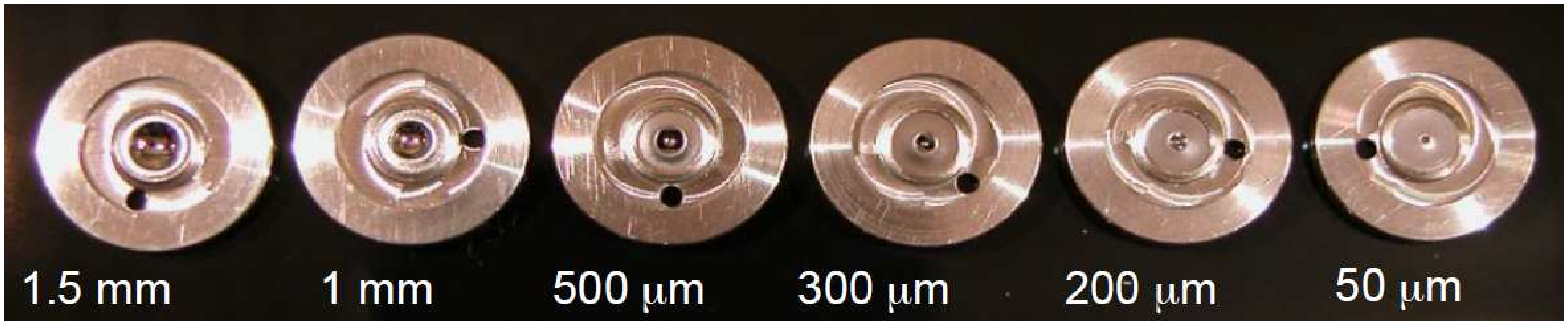


$$f=R/2\delta$$

Refractive in-line optics (CRL)

- Good choice for high energies
- Stability
- Easy alignment

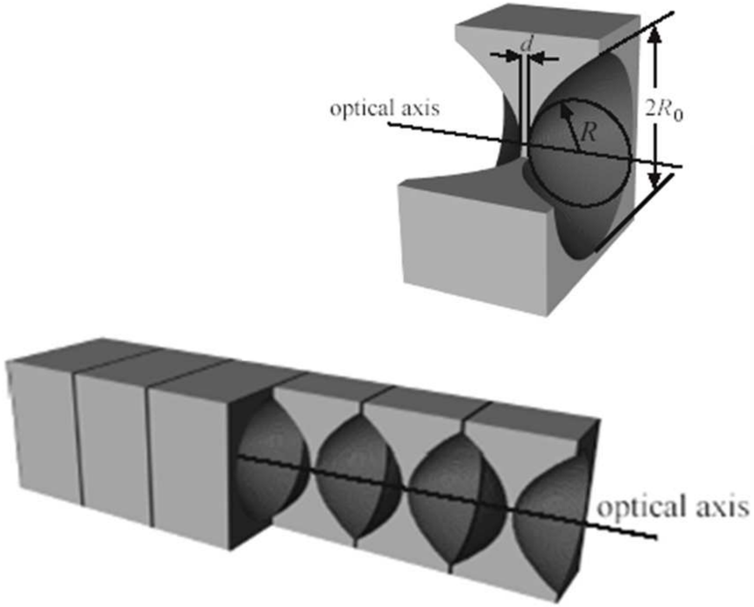
Downsides:
- Chromatic focusing
- Small angle scattering (?)
- Efficiency at low energies



B. LENGELER, RXOPTICS and RWTH AACHEN UNIVERSITY

The CRL chamber at ID10 (ESRF)

1e-8 mbar
Water cooled
One rod w/ vertical movement
4 slots for lens stacks

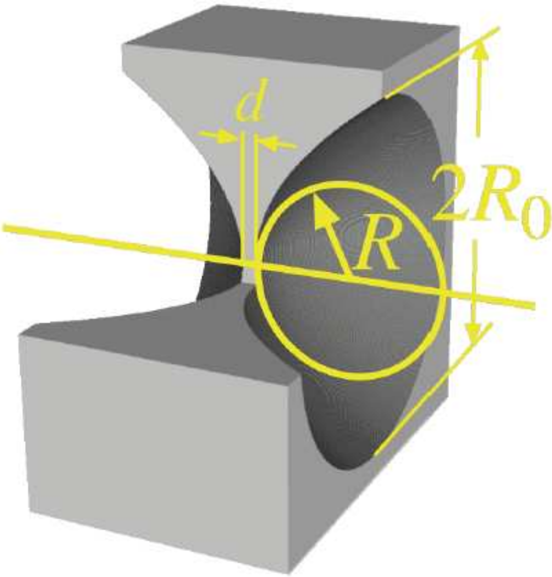


$$f = R/2N\delta$$

B. Lengeler *et al*

Numerical aperture

B. Lengeler



Parabola cut-off defines physical aperture R_0 (depends on R and Be thickness)

Absorption correction:

$$D_{eff} = 2R_0\sqrt{\left[1-\exp\left(-a_p\right)\right]/a_p}$$

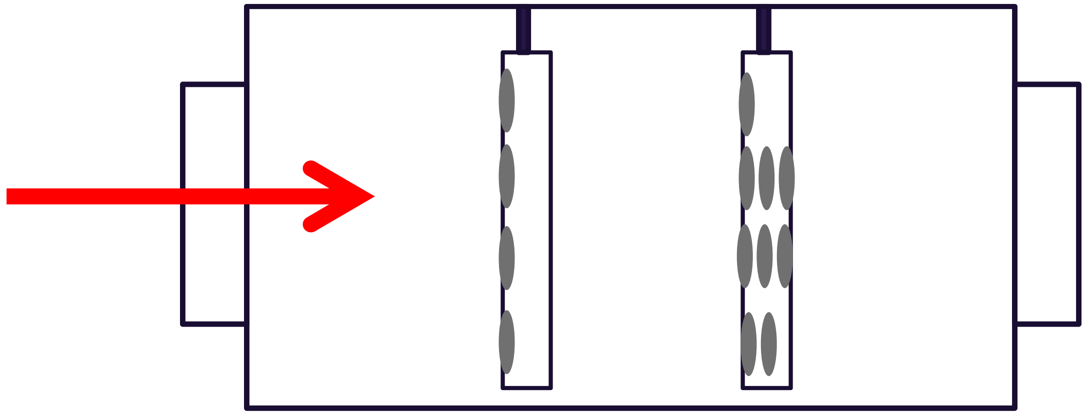
$$a_p = \mu N z_0 = \frac{1}{2}\mu L_{st}$$

Currently best quality Be (minimum FeO impurities) is only available in 0.5 mm thick slabs

Be parabolas up to R > 5 mm can now be fabricated with small abberations

CRL1 Chamber (213 m from the source)

CRL1 rod 1 CRL1 rod 2



Parallel beam option

IF1 quality Beryllium

0.5 mm thick, f = 213m

CRL1 rod 1

name	R (μm)	N	$2R_0$ (μm)	E(keV)	D_{eff} (μm)
CRL1_11	5800	1	3406	**5.0**	3245
CRL1_12	4000	1	2820	**6.0**	2743
CRL1_13	2800	1	2366	**7.2**	2325
CRL1_14	2000	1	2000	**8.5**	1980

13 lenses needed
Mounted in 2 x 4 slots this gives 25 possible combinations (incl. rod 1 and/or rod 2 OUT)

CRL1 rod 2

name	R (μm)	N	$2R_0$ (μm)	E(keV)	D_{eff} (μm)
CRL1_21	2300	1	2145	**8.0**	2120
CRL1_22	2800	3	2366	**12.5**	2338
CRL1_23	2000	3	2000	**14.8**	1982
CRL1_24	500	2	1000	**24.1**	996

European XFEL

CRL1 Chamber (213 m from the source)

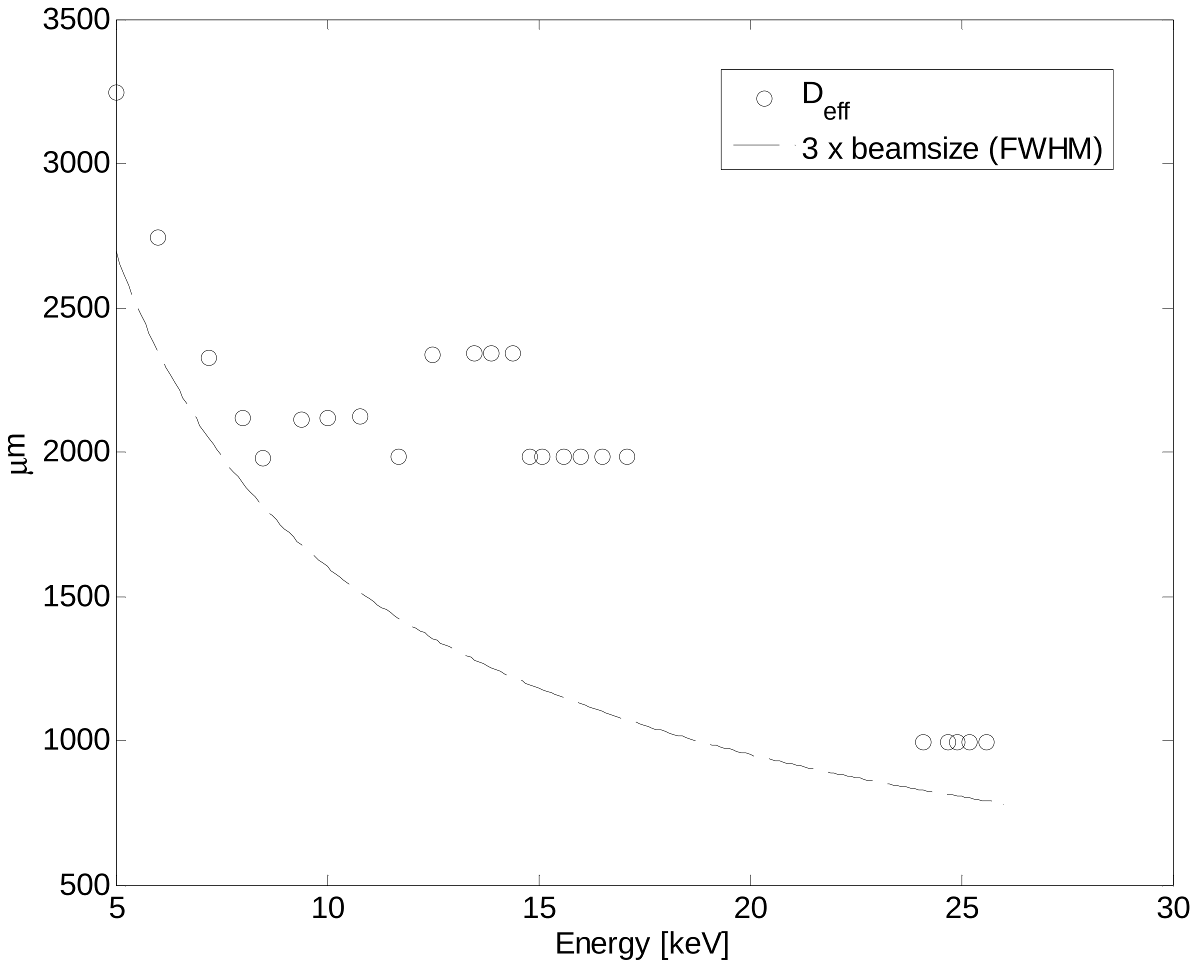
Parallel beam energies by combinations of the two rods

(Energy and effective diameter)

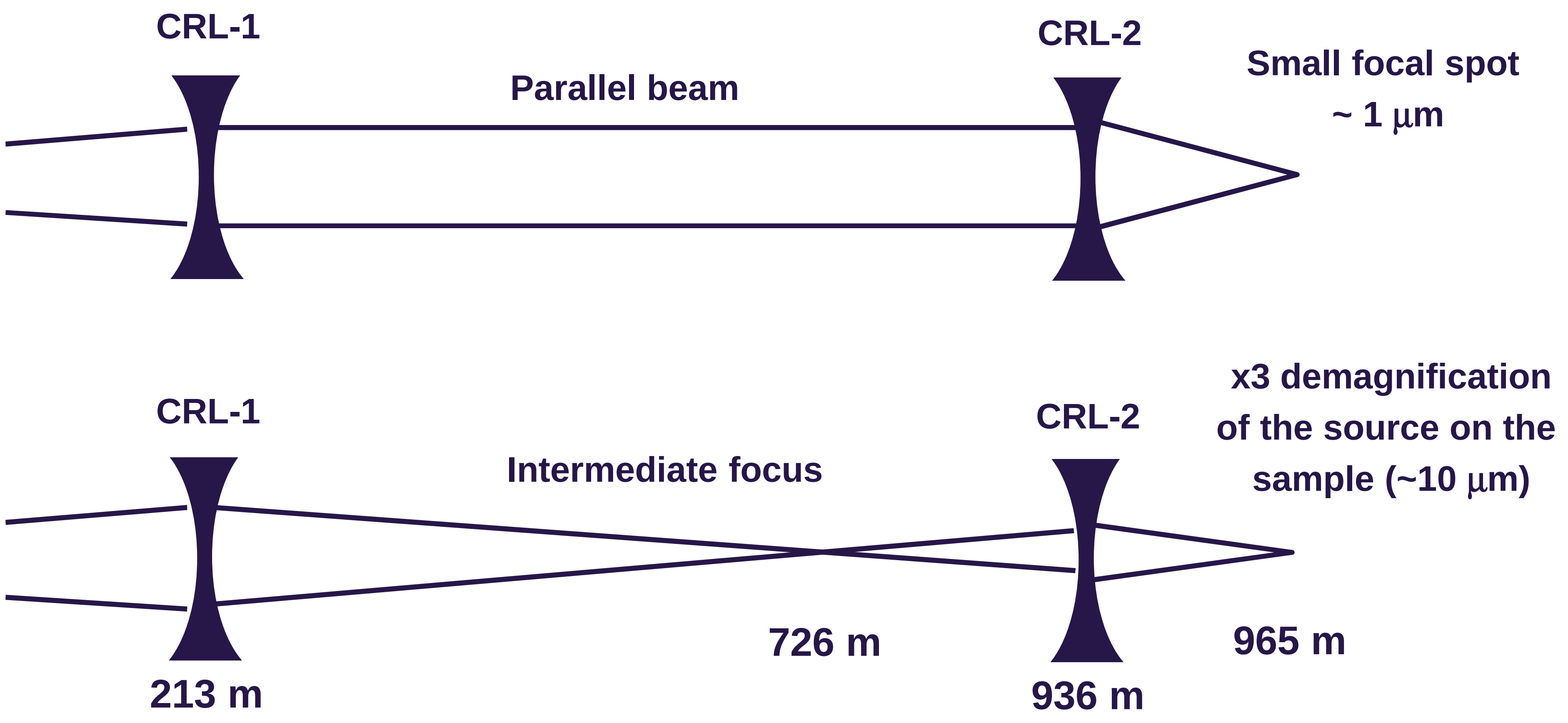
	CRL1_21	CRL1_22	CRL1_23	CRL1_24
CRL1_11	**9.4** keV 2113 µm	**13.5** keV 2341 µm	**15.6** keV 1983 µm	**24.7** keV 996 µm
CRL1_12	**10.0** keV 2117 µm	**13.9** keV 2343 µm	**16.0** keV 1984 µm	**24.9** keV 996 µm
CRL1_13	**10.8** keV 2121 µm	**14.4** keV 2344 µm	**16.5** keV 1984 µm	**25.2** keV 996 µm
CRL1_14	**11.7** keV 1982 µm	**15.1** keV 1983 µm	**17.1** keV 1985 µm	**25.6** keV 996 µm

CRL1 Chamber (213 m from the source)

Comparison of beam size at 213 m (3 x FWHM, worst-case estimate from WP-73 CDR) and the effective lens diameter D_{eff}



Sketch of two re-focusing schemes at MID



Refocusing geometry (~ 10 μm beam size)

Focus at the 726 m point, i.e. 513 m downstream of the CRL1 lens

$$1 / f = 1 / 213 + 1 / 513 \rightarrow f = 150.5 \text{ m}$$

CRL1 rod 1

name	R (μm)	N	$2R_0$ (μm)	E(keV)	D_{eff} (μm)
CRL1_11	5800	1	3406	4.2	3245
CRL1_12	4000	1	2820	5.0	2743
CRL1_13	2800	1	2366	6.0	2325
CRL1_14	2000	1	2000	7.1	1980

CRL1 rod 2

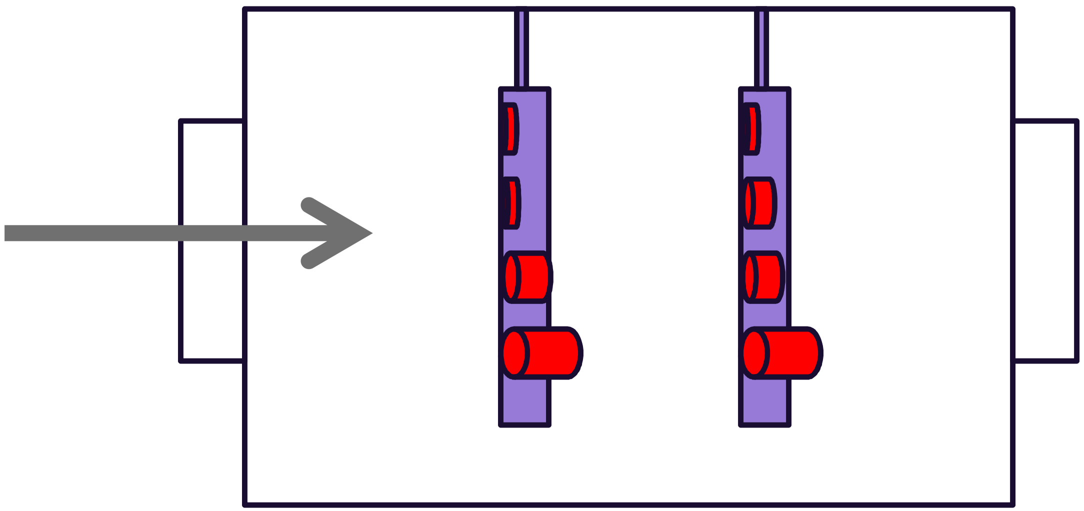
name	R (μm)	N	$2R_0$ (μm)	E(keV)	D_{eff} (μm)
CRL1_21	2300	1	2145	6.7	2120
CRL1_22	2800	3	2366	10.4	2338
CRL1_23	2000	3	2000	12.4	1982
CRL1_24	500	2	1000	20.2	996

Refocusing geometry (~ 10 µm beam size)

	CRL1_21	CRL1_22	CRL1_23	CRL1_24
CRL1_11	**7.9 keV** 2113 µm	**11.3 keV** 2341 µm	**13.0 keV** 1983 µm	**20.6 keV** 996 µm
CRL1_12	**8.4 keV** 2117 µm	**11.6 keV** 2343 µm	**13.3 keV** 1984 µm	**20.8 keV** 996 µm
CRL1_13	**9.0 keV** 2121 µm	**12.1 keV** 2344 µm	**13.8 keV** 1984 µm	**21.1 keV** 996 µm
CRL1_14	**9.8 keV** 1982 µm	**12.6 keV** 1983 µm	**14.3 keV** 1985 µm	**21.4 keV** 996 µm

Second CRL chamber

CRL2 rod 1 CRL2 rod 2



Similar to 1st CRL chamber

f = 25.5, 28, or 29 m depending on the status of CRL1 (refocusing, out, parallel beam)

27 lenses needed
Mounted in 2 x 4 slots this gives the possibility to focus/refocus 5-14 keV

Refocusing > 15 keV requires additional lenses (3rd chamber)

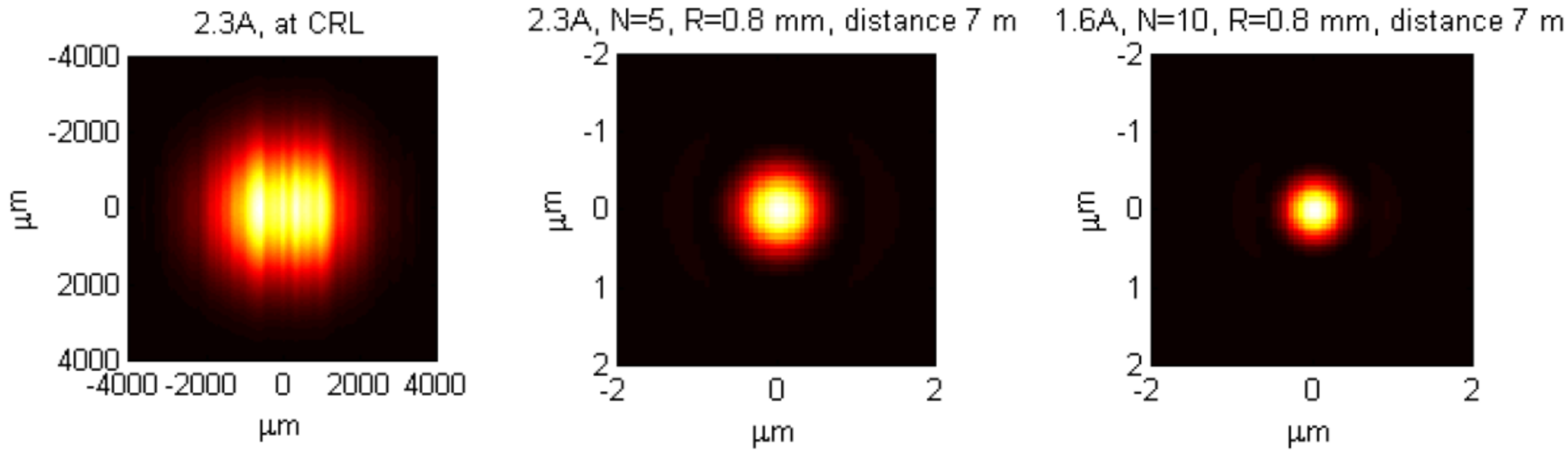
CRL2 rod 1

name	R (µm)	N	$2R_0$ (µm)
CRL2_11	2300	1	2145
CRL2_12	2000	1	2000
CRL2_13	2000	4	2000
CRL2_14	1000	7	1414

CRL2 rod 2

name	R (µm)	N	$2R_0$ (µm)
CRL2_21	2000	1	2000
CRL2_22	2000	2	2000
CRL2_23	2300	3	2145
CRL2_24	2000	8	2000

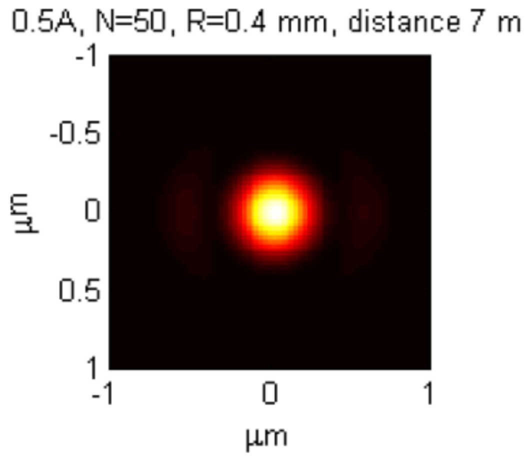
Wavefront analysis (work in progress…)



Advanced simulations of CRLs and the effect on the beam shape and wave front (in progress..)

L. Samoylova (XFEL.EU)

Thermal modeling in progress…

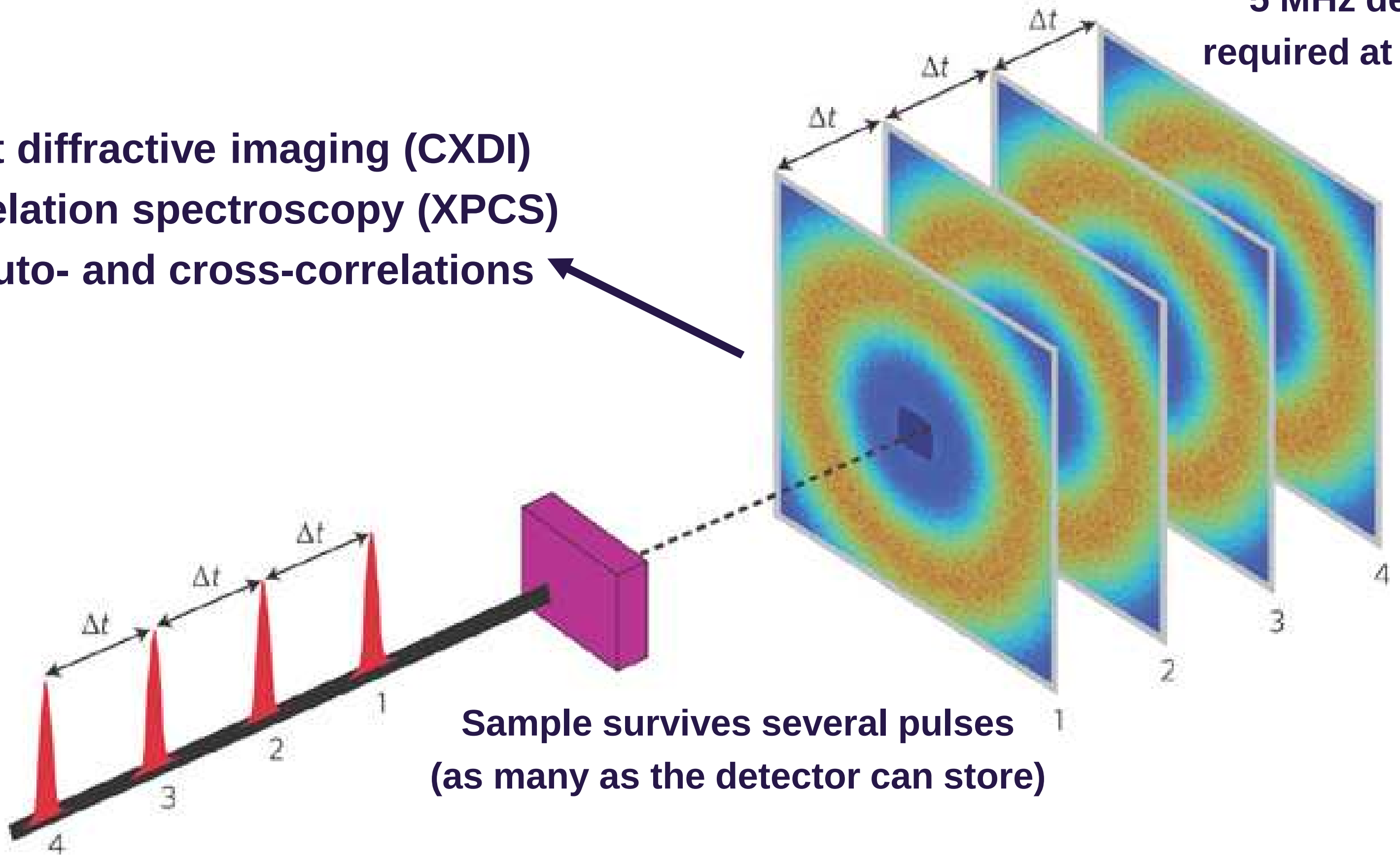


Fast Acquisition of Diffraction Patterns

sequential mode for coherent scattering

5 MHz detector required at XFEL.EU

Coherent diffractive imaging (CXDI)
Time correlation spectroscopy (XPCS)
Spatial auto- and cross-correlations

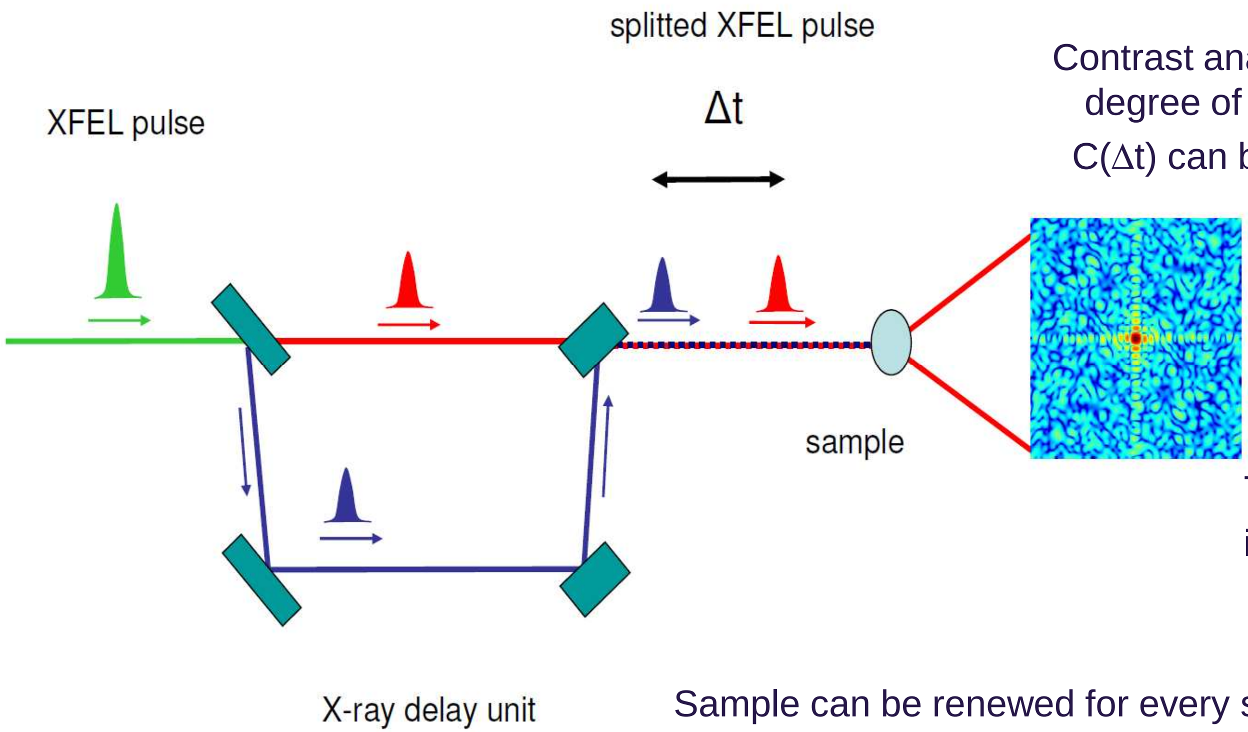


Sample survives several pulses (as many as the detector can store)

From Nature News and Views
G. B. Stephenson et al, Nature Materials 8, 702 - 703 (2009)

Time resolution in XPCS or XPXP beyond 220 ns

Double pulse from split-delay or special machine mode (1.3 GHz RF frequency)
ps and fs only available with split-delay of the photon pulses



Contrast analysis yields the degree of correlation C.
C(Δt) can be mapped out

Time-resolution independent of detector speed

Sample can be renewed for every shot
(injector, new solid target,..)

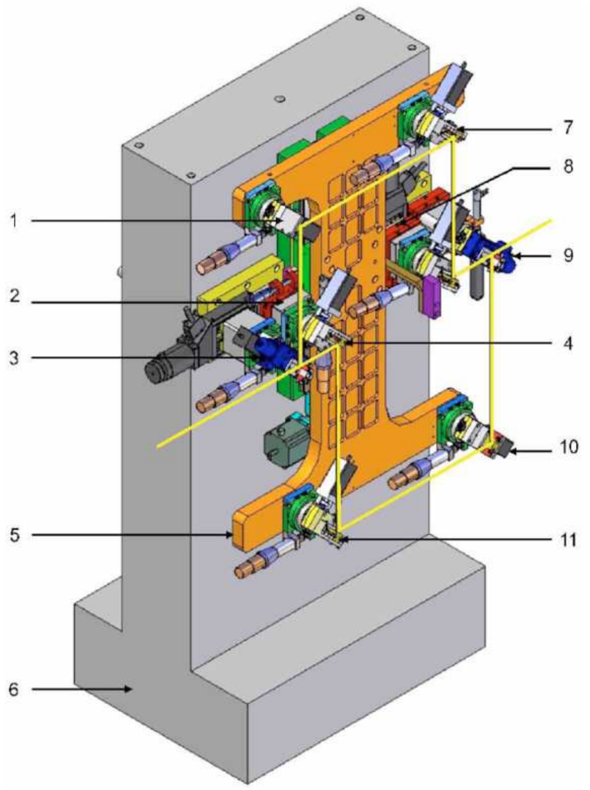
C. Gutt et al, Optics Express 17, 55 (2009)

Experiments with Coherent X-Rays

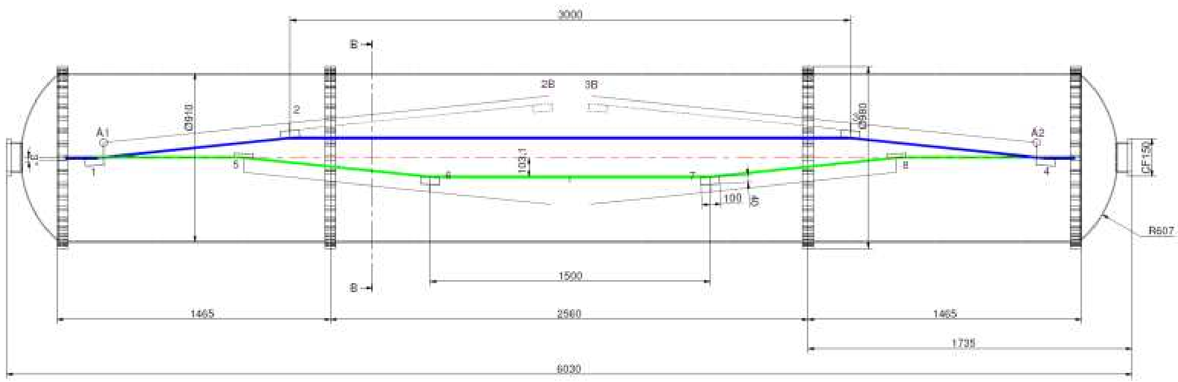
Faster than 220 ns in XPCS or XPXP experiments ?

Possible by split-delay or by custom mode operation of the linac

Bragg crystals:
Split-delay line (W. Roseker, Grübel group, DESY)



Grazing incidence mirrors:
Split-delay line, FLASH style auto-correlator
(Prof. Zacharias group, Uni. Münster)

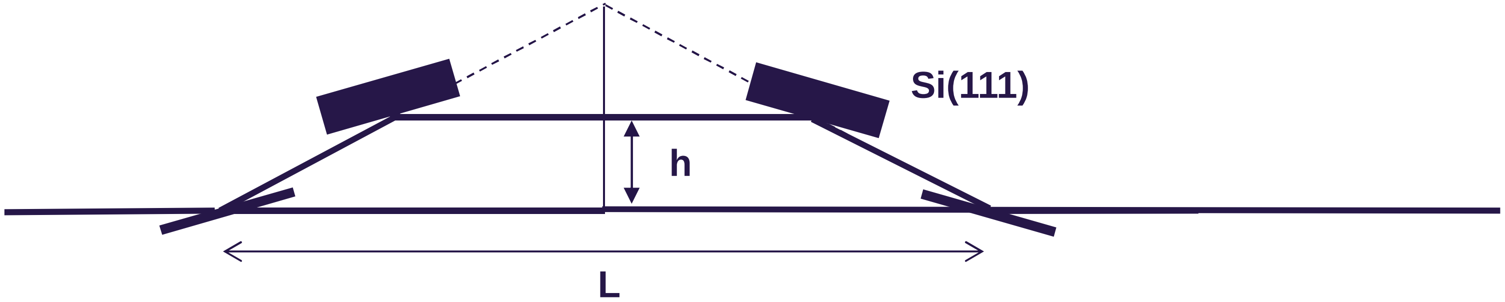


fs – ps range within reach using split-delay techniques

MID X-Ray Split-Delay Line (draft, in progress…)

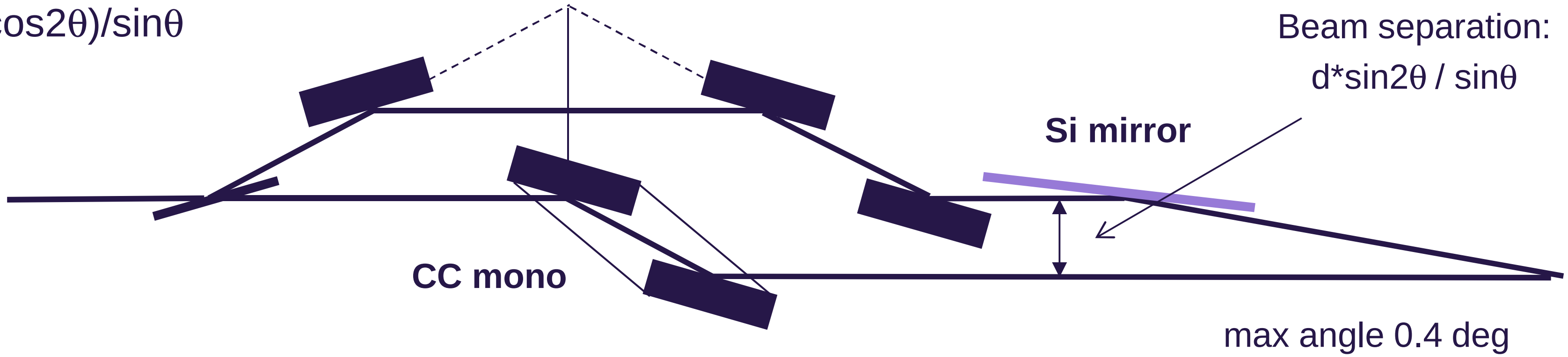
Delay of simple pyramid (base L, height H) split-delay line

PLD (up-down) = $2h/\tan 2\theta \times (1-\cos 2\theta) / \cos 2\theta$; $h \in [h_{min}; H]$ with $H = L/2 * \tan 2\theta$



Extra path length by lower CC mono (d: channel width)

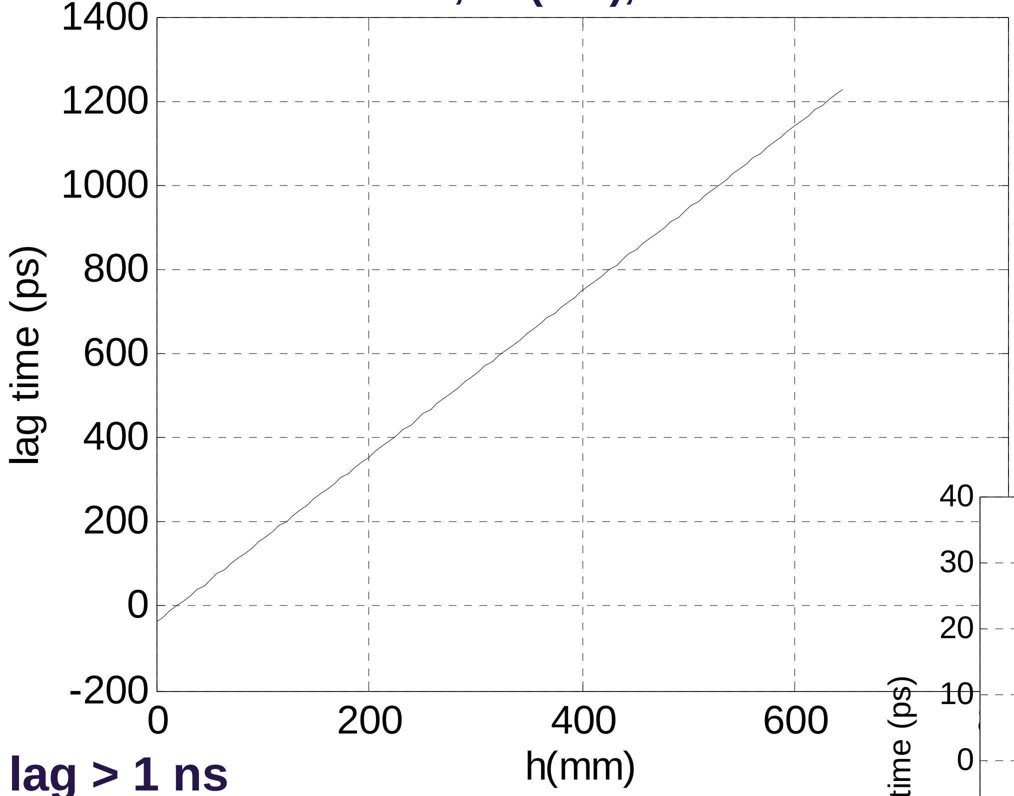
$d(1-\cos 2\theta)/\sin\theta$



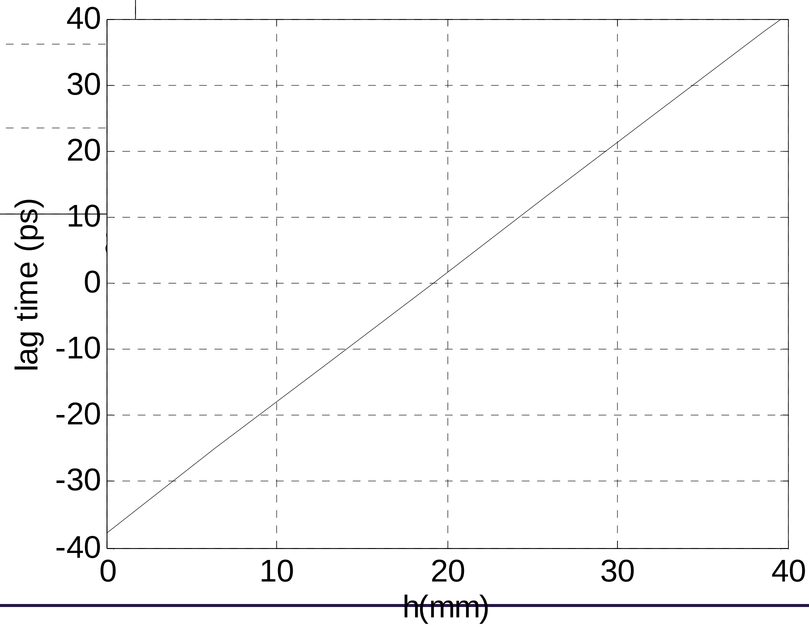
Split-delay line 8 m upstream of the sample i.e. max beam separation 56 mm

X-Ray Split-Delay Line (in progress…)

E= 7 keV, Si (111), L =2000 mm



CC lower mono with d = 20 mm offsets the lag time 0 point to h = 20 mm



max lag > 1 ns

Resolution: 2 ps/mm or 2 fs/µm

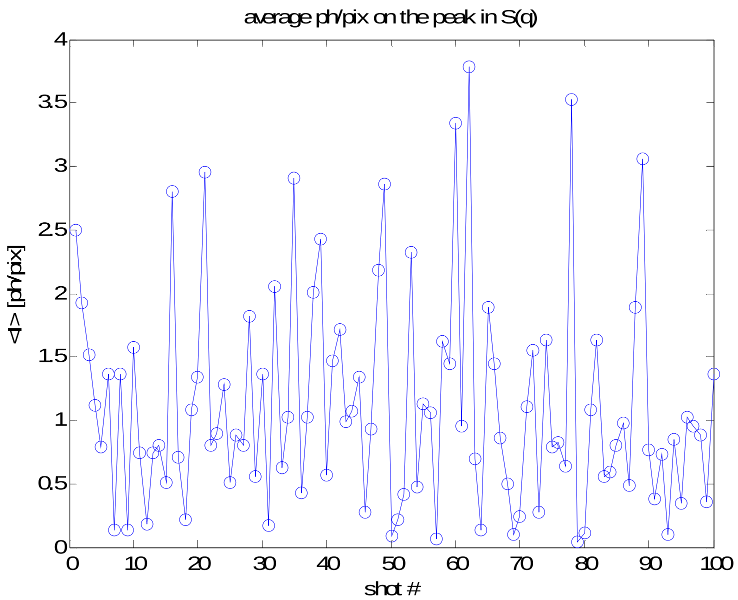
Very compact device (20 cm) if max lag required is ~100 ps.

Challenges and First Experience from LCLS

Particular challenges:

SASE fluctuations (temporal fine-structure) are problematic:

- Intensity fluctuations behind a mono (needed for high-q experiments)
- Fluctuations in spectral properties lead to fluctuations in longitudinal coherence length



Sorry, no picture

High-q scattering from an amorphous material

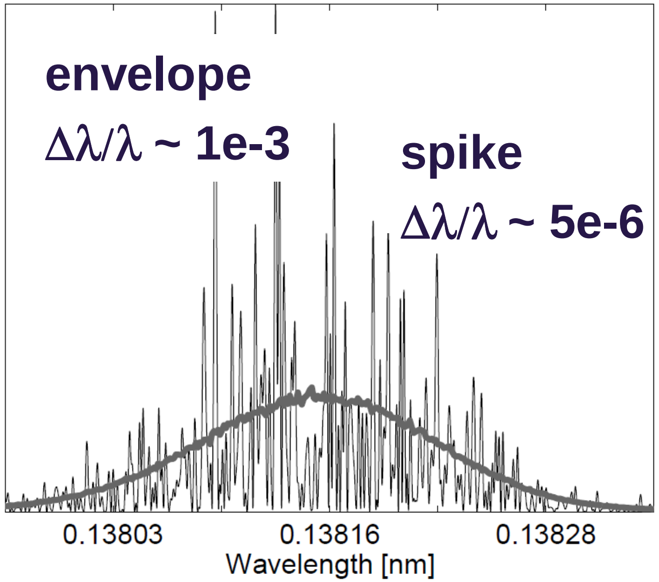
LCLS experiment L-467, Jan. 2012

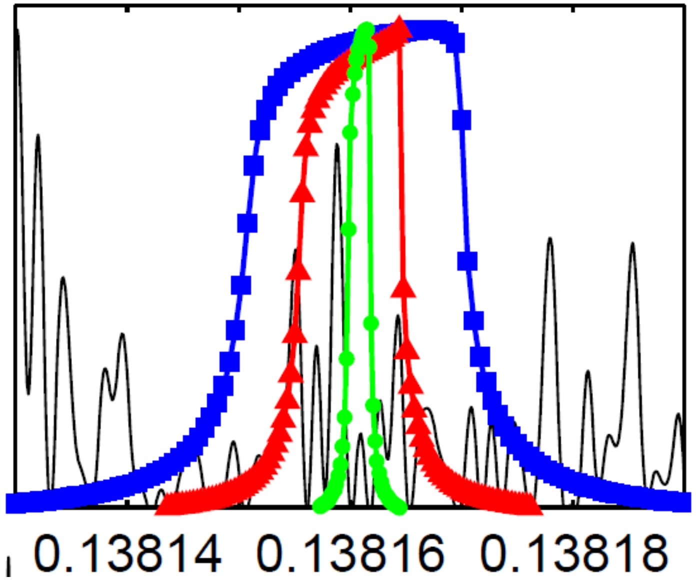
Sorry, no picture

Seeding of the SASE process and single-shot diagnostics (intensity, spectrum, coherence) required

Shot-to-Shot Intensity Fluctuations

LCLS simulations, S. Lee *et al*., Optics Express <u>20</u>, 9790 (2012)





Si(111) Δλ/λ ~ 1.4e-4

Si(220) Δλ/λ ~ 6.1e-5

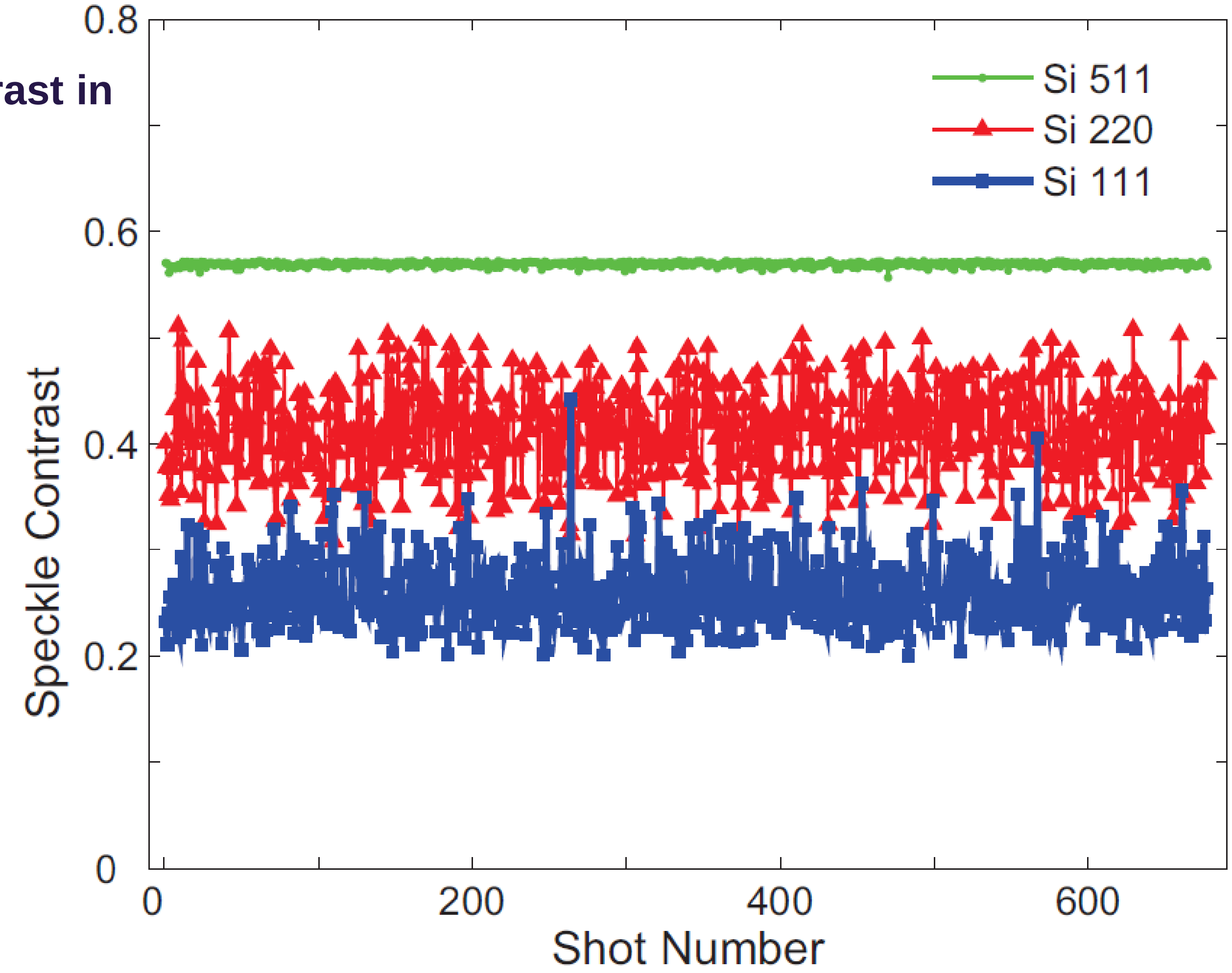
Si(511) Δλ/λ ~ 1.1e-5

About 15 spikes will pass through the Si(111) mono

Coherence time (and hence longitudinal coherence length) not well defined for Si(111) and Si(220)

Shot-to-Shot Contrast Fluctuations in WAXS

Simulated contrast in X-ray speckle at q=2.6 Å $^{-1}$



LCLS simulations, S. Lee *et al*., Optics Express 20, 9790 (2012)

Seeding Workshop

Science with Seeded FEL beams

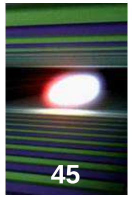
July 19-20 @ DESY

Organizers:

A. Madsen, M. Meyer, S. Molodtsov, T. Tschentscher

https://indico.desy.de/conferenceDisplay.py?ovw=True&confId=5665

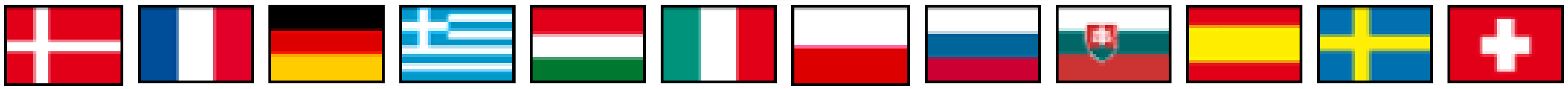
Conclusion



- Lots of work ahead, we must be at the forefront scientifically and technically
- The MID instrument will offer plenty of new experimental possibilities (e.g. time-resolved scattering, speckle, pump-probe) that we only got a glimpse of so far
- Challenging development of enabling technologies (detectors, optics, diagnostics, lasers, data management and storage)
- First materials science experiments with hard X-ray lasers have taken place at LCLS. SACLA (Japan) also on-line now. XFEL.EU probably next in line (Dec. 2015)

Next MID milestone: Technical Design Report due in spring 2013

www.xfel.eu



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Experiment L467 @ LCLS

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