New Science at Materials Imaging and Dynamics (MID) End-Station at European XFEL Facility

Chan Kim
Materials Imaging and Dynamics (MID),
European XFEL GmbH

Technische Universität München in Garching
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chan.kim@xfel.eu

Outlines

- Introduction
  - What is x-ray free-electron laser (XFEL)?
  - New technologies at European XFEL
- Materials imaging and dynamics (MID) end station
  - Details of materials imaging dynamics (MID) instrument
  - Possible new science at MID
  - Scheduled experiments in the first half of 2019
- Result from other instrument (SPB/SFX) at European XFEL
- Discussion
  - Summary and future works

XFEL Facilities in Worldwide

Brief Comparison between Worldwide XFELs

Going great guns

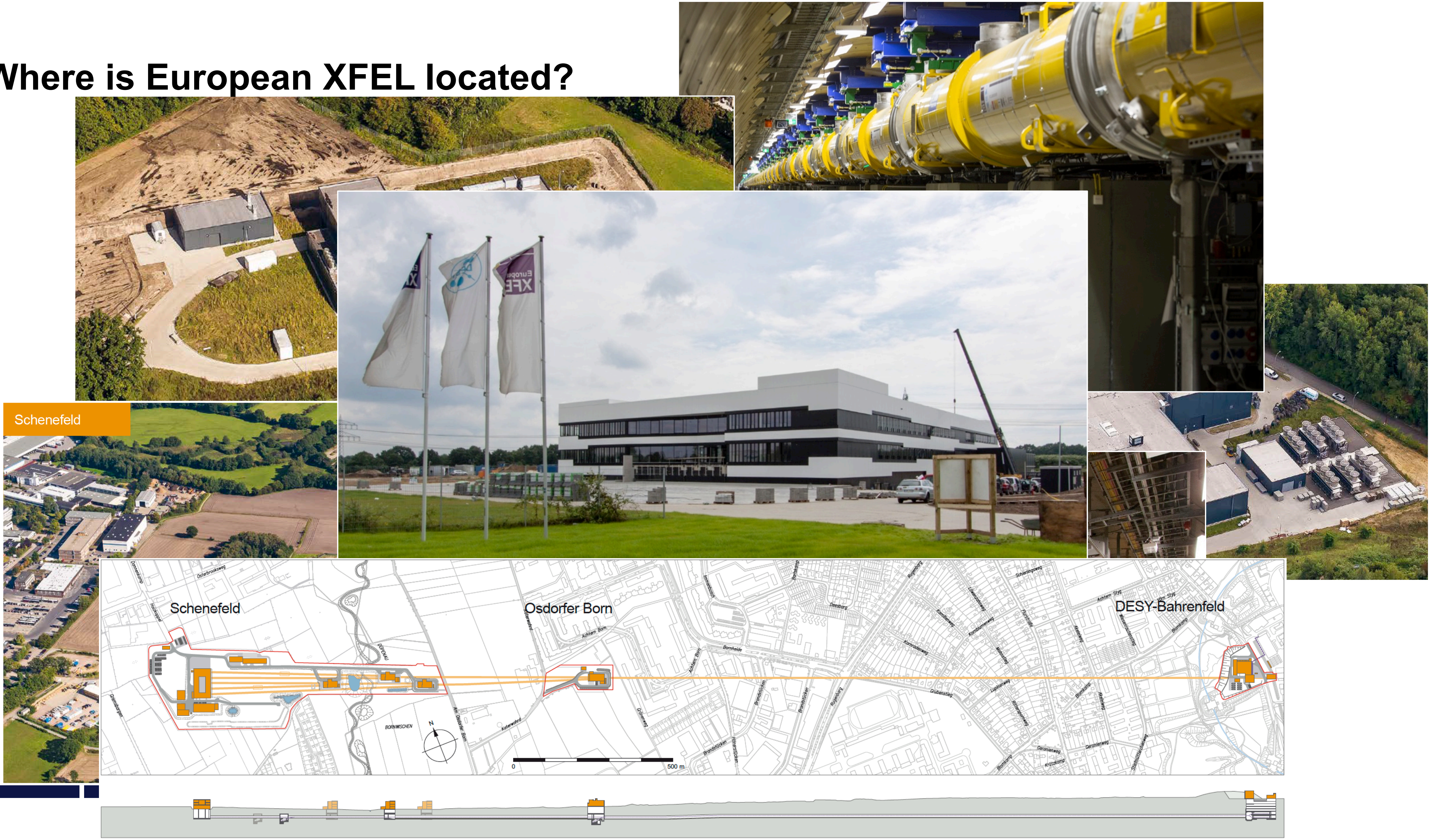
Three new free electron lasers (FELs) are set to open up in the next year. The European XFEL gets its high repetition rate from the superconducting cavities that drive its electron beam.

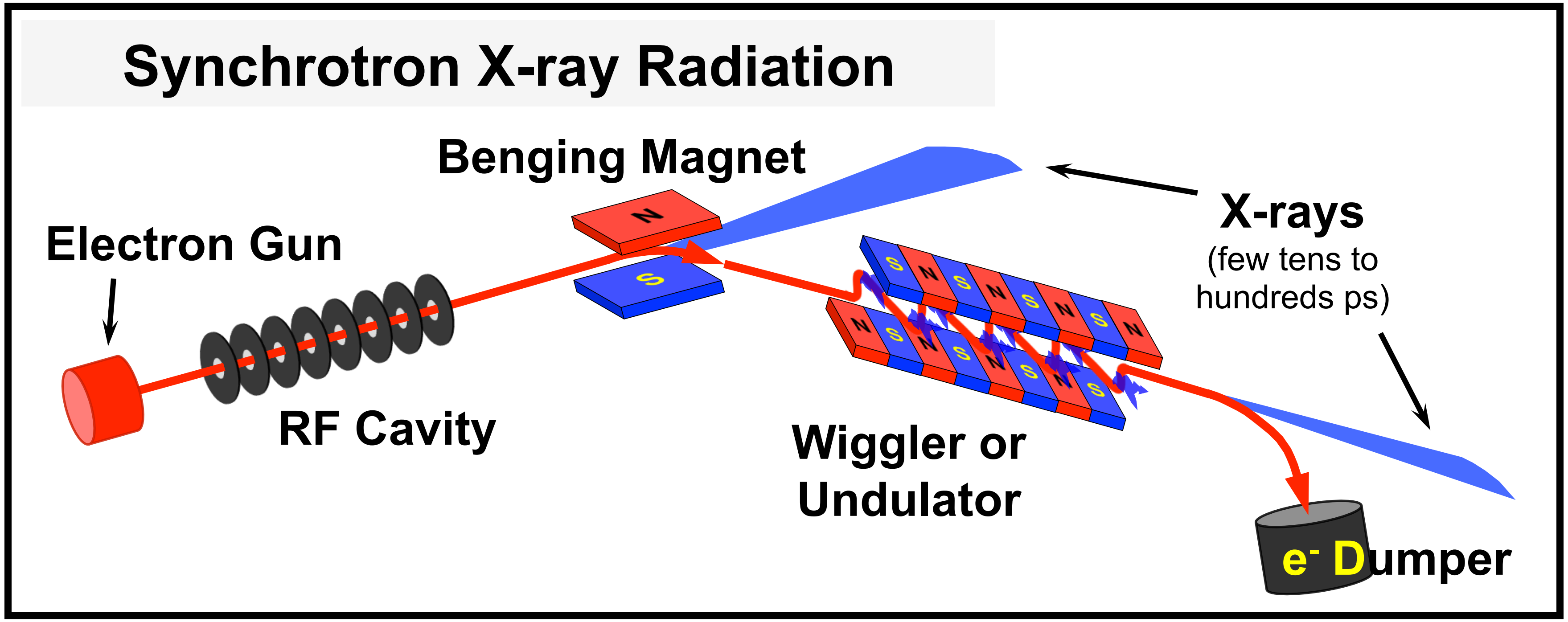
NAME/COUNTRY	LCLS/ UNITED STATES	LCLS-II/ UNITED STATES	SACLA*/ JAPAN	EUROPEAN XFEL/ GERMANY	SWISSFEL/ SWITZERLAND	PAL-XFEL*/ SOUTH KOREA	SHINE/ CHINA
Date of first x-rays	2009	2020	2011	2017	2017	2016	2025
Cost (in U.S. millions)	$415	$1000	$370	$1600	$280	$400	$1400
Number of instruments	7	9	8	6	3	4	3
Max. electron energy (GeV)	14.3	4.5	8.5	17.5	5.8	10	8
Min. pulse duration (femtoseconds)	15	15	10	5	2	30	~10
Pulses per second	120	1,000,000	60	27,000	100	60	1,000,000

**SACLA is the Spring-8 Angstrom Compact free electron Laser and PAL-XFEL is the Pohang Accelerator Laboratory X-ray Free Electron Laser*

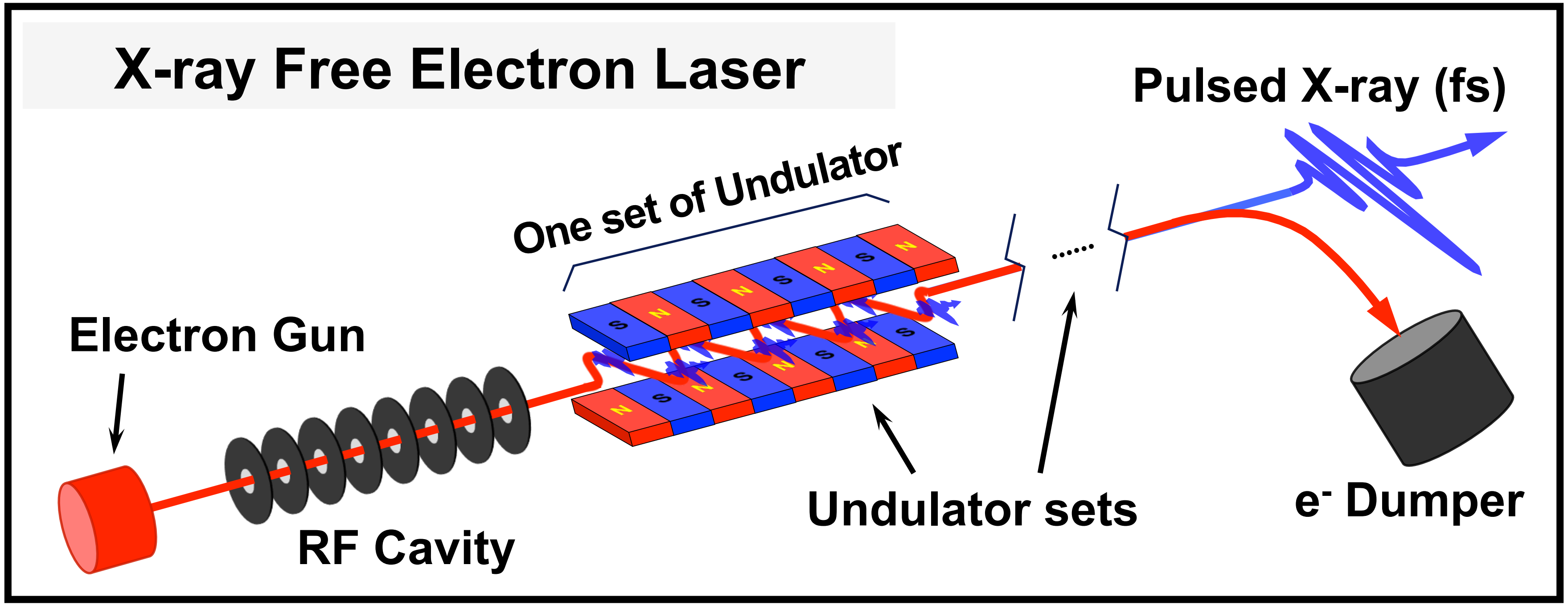
Edwin Cartlidge, "European XFEL to shine as brightest, fastest x-ray source" Science 354(6308), 22-23 (2016)

Where is European XFEL located?



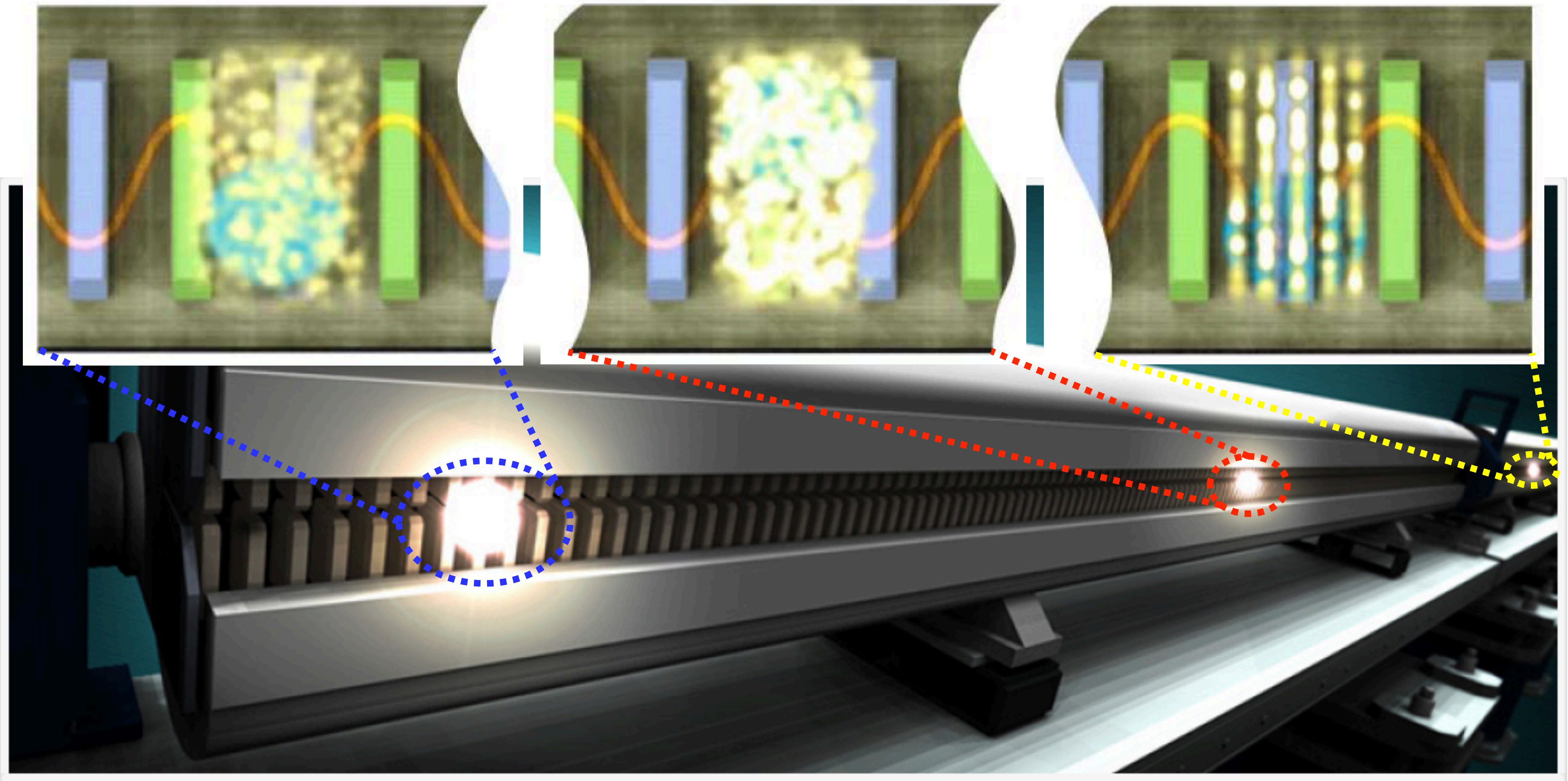


Synchrotron X-ray Radiation
Benging Magnet
Electron Gun
RF Cavity
Wiggler or Undulator
X-rays
(few tens to hundreds ps)
e- Dumper



X-ray Free Electron Laser
Pulsed X-ray (fs)
One set of Undulator
Electron Gun
RF Cavity
Undulator sets
e- Dumper

Self-Assembly Spontaneous Emission (SASE)



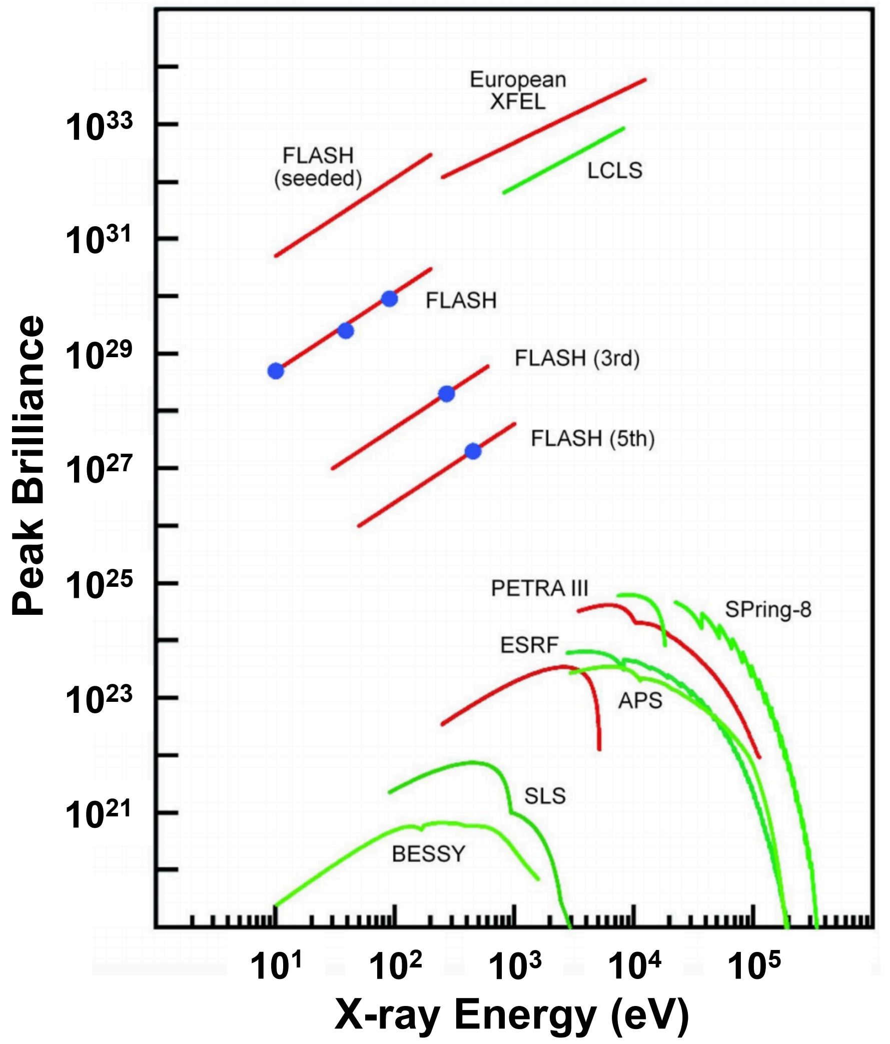
Electron pulse travelling through an undulator, emitting radiation
Generation of electron microbunches in SASE undulator
Images drawed by Greg Stewart (SLAC)

New Technology & Science at European XFEL

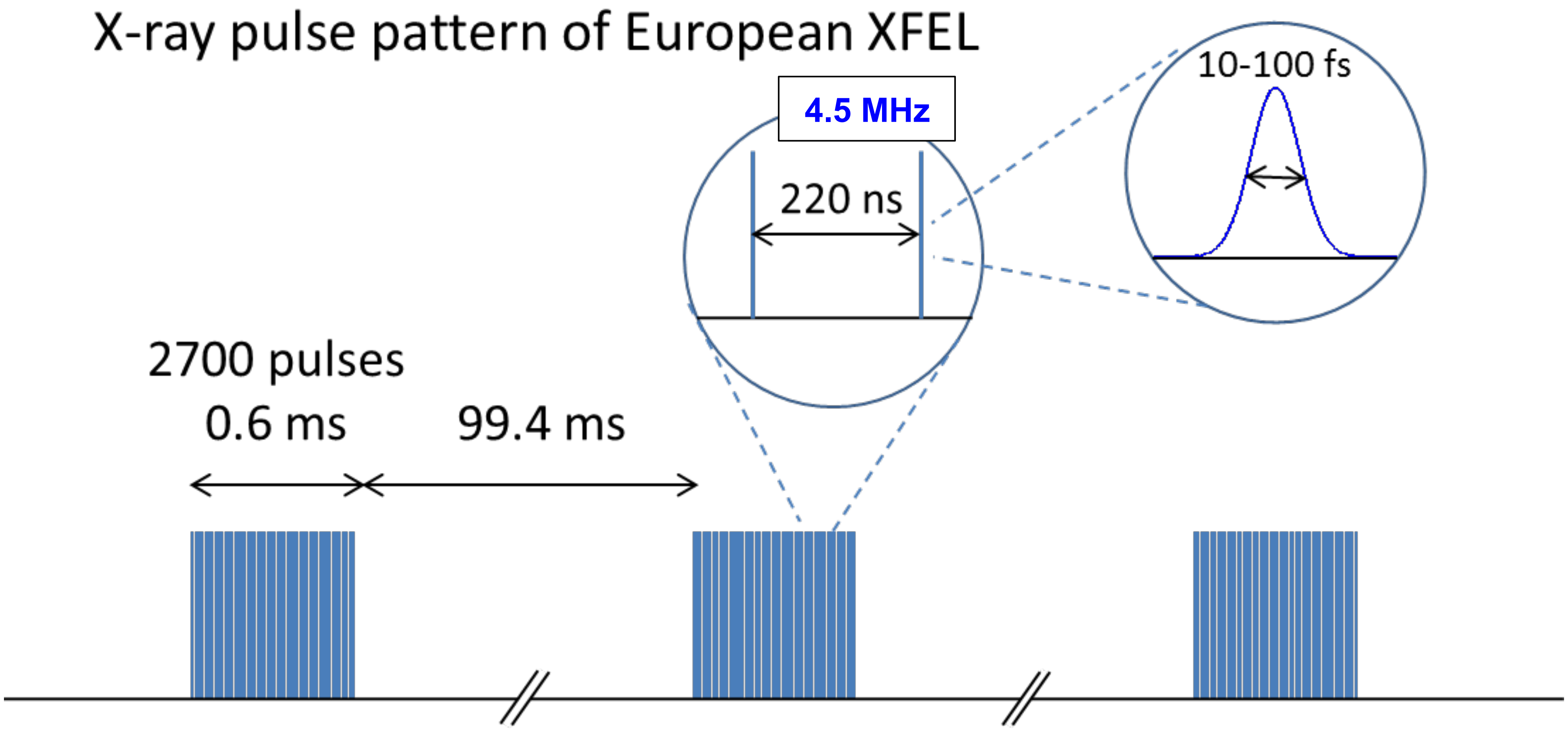
- Superconducting accelerator -271°C (High repetition rate)
- Ultrashort pulse width (5 femtosecond)

- The most brilliance x-ray source in the world
  - Peak brilliance: 5 x 10^{33} Photons/sec/mrad^2/mm^2/0.1%BW
  - Average brilliance: 1.6 x 10^{25} Photons/sec/mrad^2/mm^2/0.1%BW

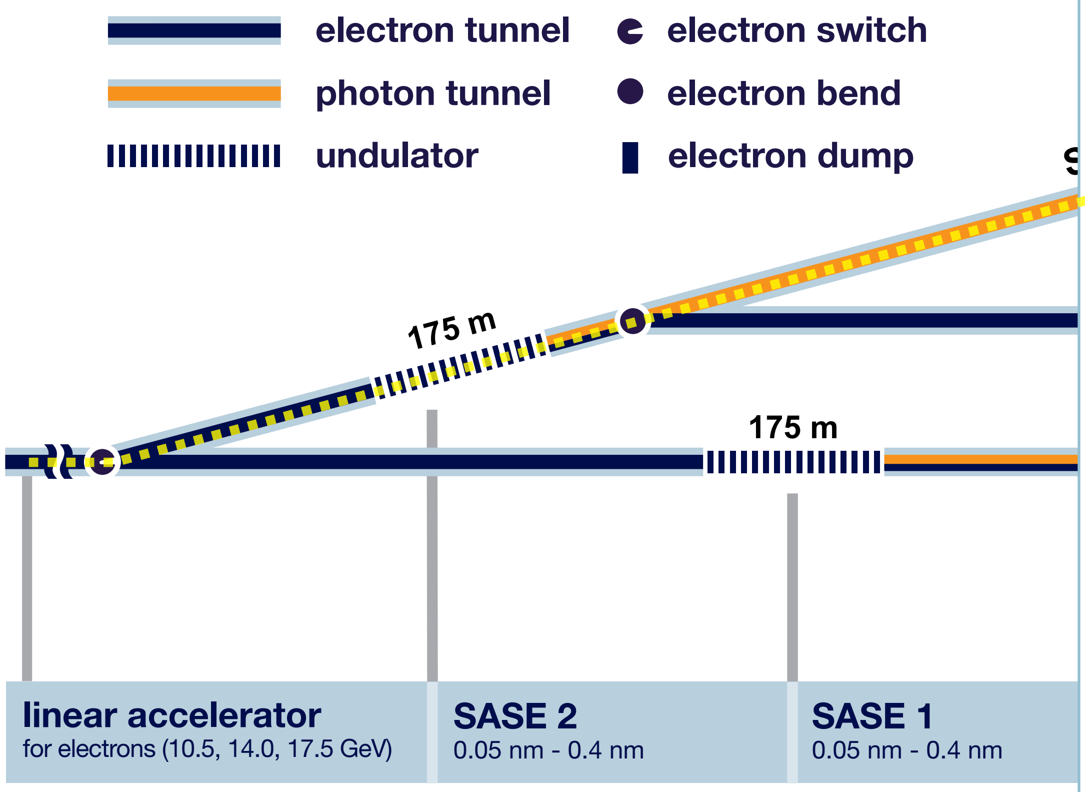
- Various pumping sources
  - High power (100J) and high brilliance (100TW) laser
  - Pulsed magnet (15T)

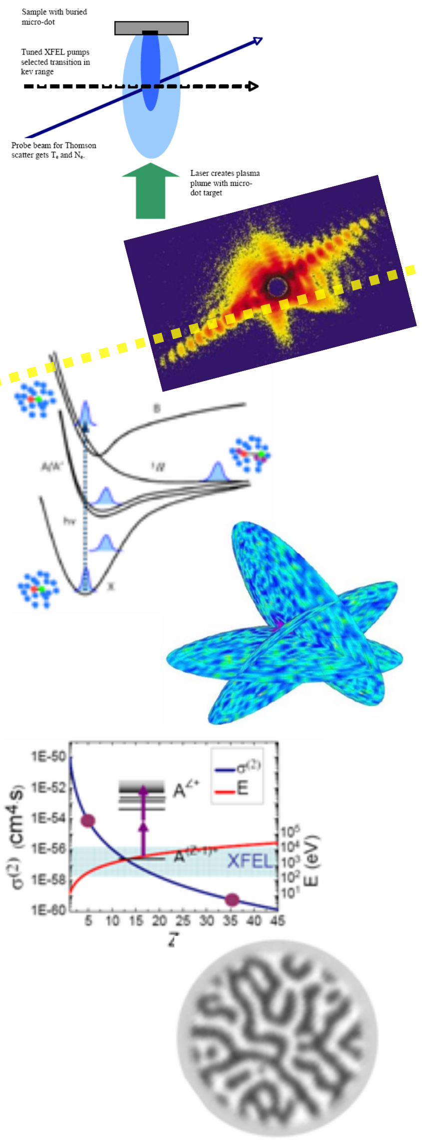


Time Structure of European XFEL



Six Instruments in European XFEL





HED (High Energy Density Science)

: Investigation of matter under extreme conditions using hard x-ray FEL radiation, e.g. probing dense plasmas

MID (Materials Imaging & Dynamics)

: Structure determination of nanodevices and dynamics at the nanoscale

The MID experiment station aims at structural investigations of crystalline, nanostructured, or less well-ordered materials, such as glasses, liquids, and biological substances. Applications comprise the exploration of visco-elastic properties in liquids and glasses, polymer dynamics, phase transitions, protein folding, or switches in magnetic orientation.

FXE (Femtosecond X-ray Experiments)

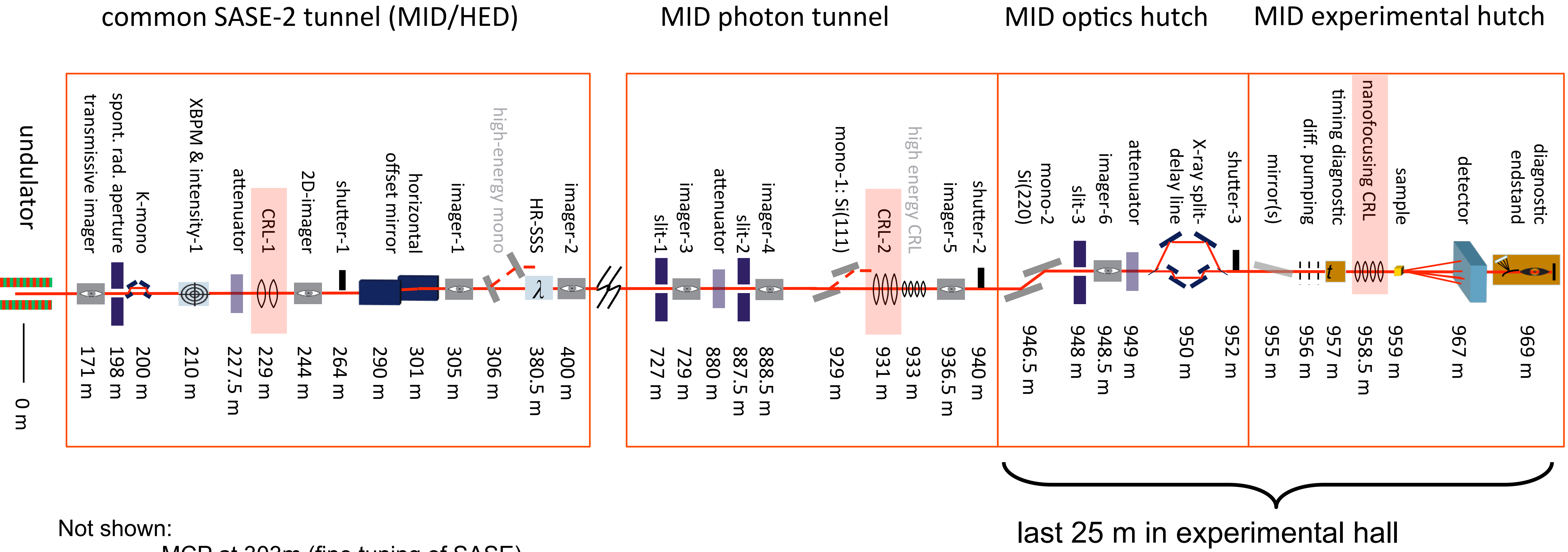
SPB/SFX (Single Particle & Biomolecules)

SOS (Small Quantum Systems)

SCS (Spectroscopy & Coherent Scattering)

: Electronic and atomic structure and dynamics of nanosystems and of non-reproducible biological objects using soft x-rays

MID Beamline Overview



Not shown:

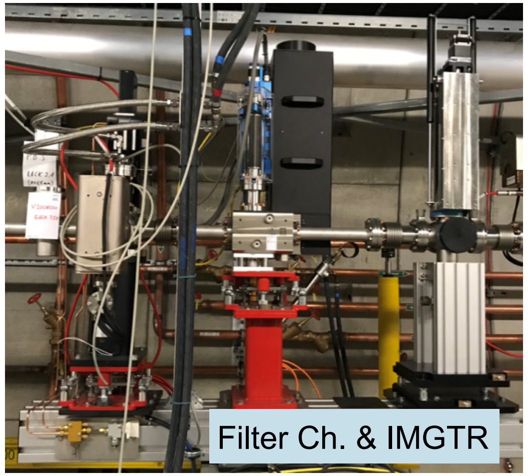
MCP at 303m (fine tuning of SASE)
Distribution mirror(s) at 390m and 395m (MID on central branch)
Beam loss monitors, PES (photo-emission spectroscopy)

Tunnel Diagnostics

- all SASE2 diagnostics vacuum systems are in the tunnel

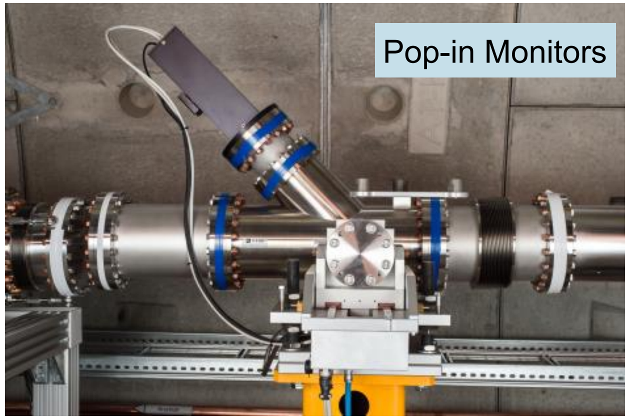

XGM

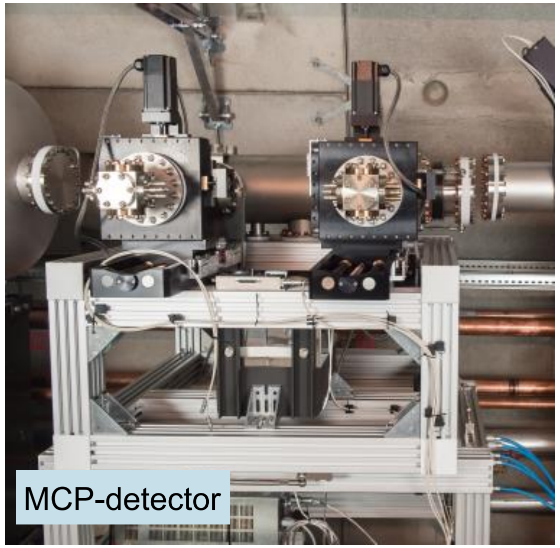

Gas supply


Filter Ch. & IMGTR


IMGFEL


K-mono


Pop-in Monitors


MCP-detector

General layout of MID scientific instrument @ SASE-2

Materials Imaging and Dynamics

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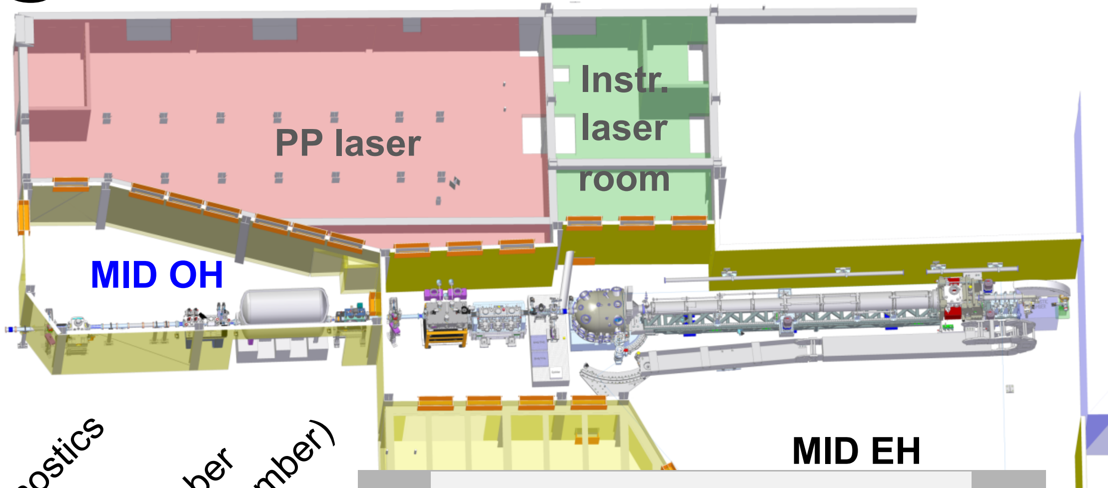
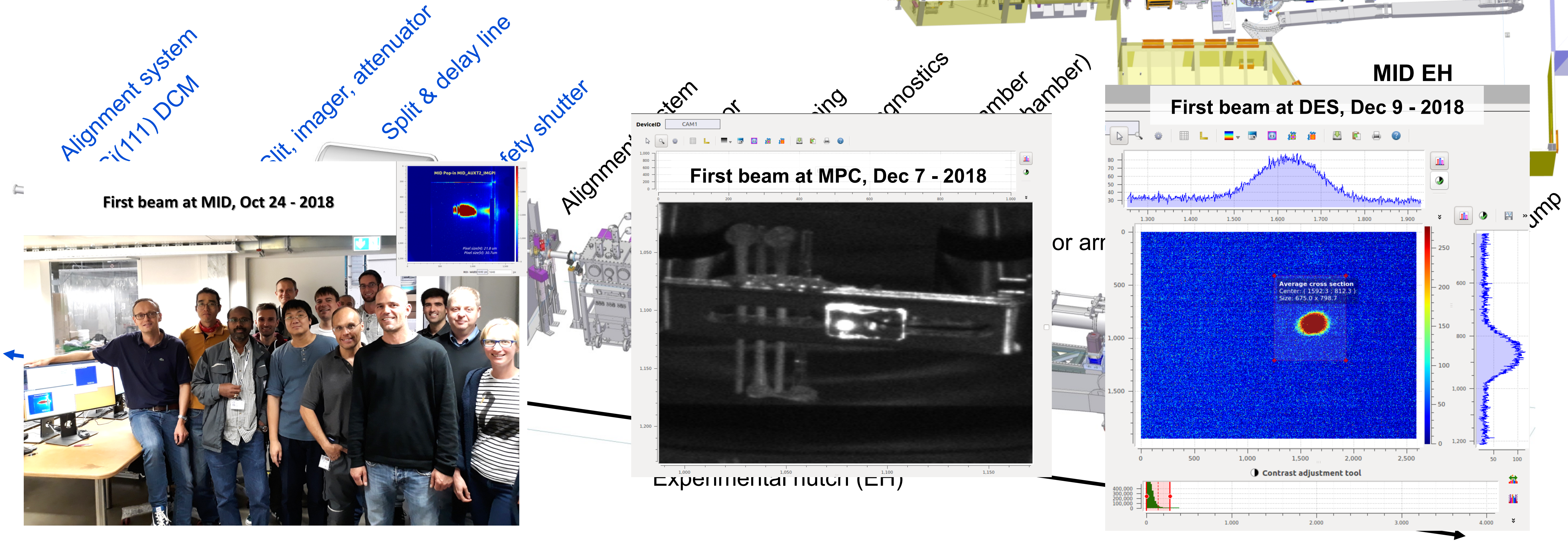
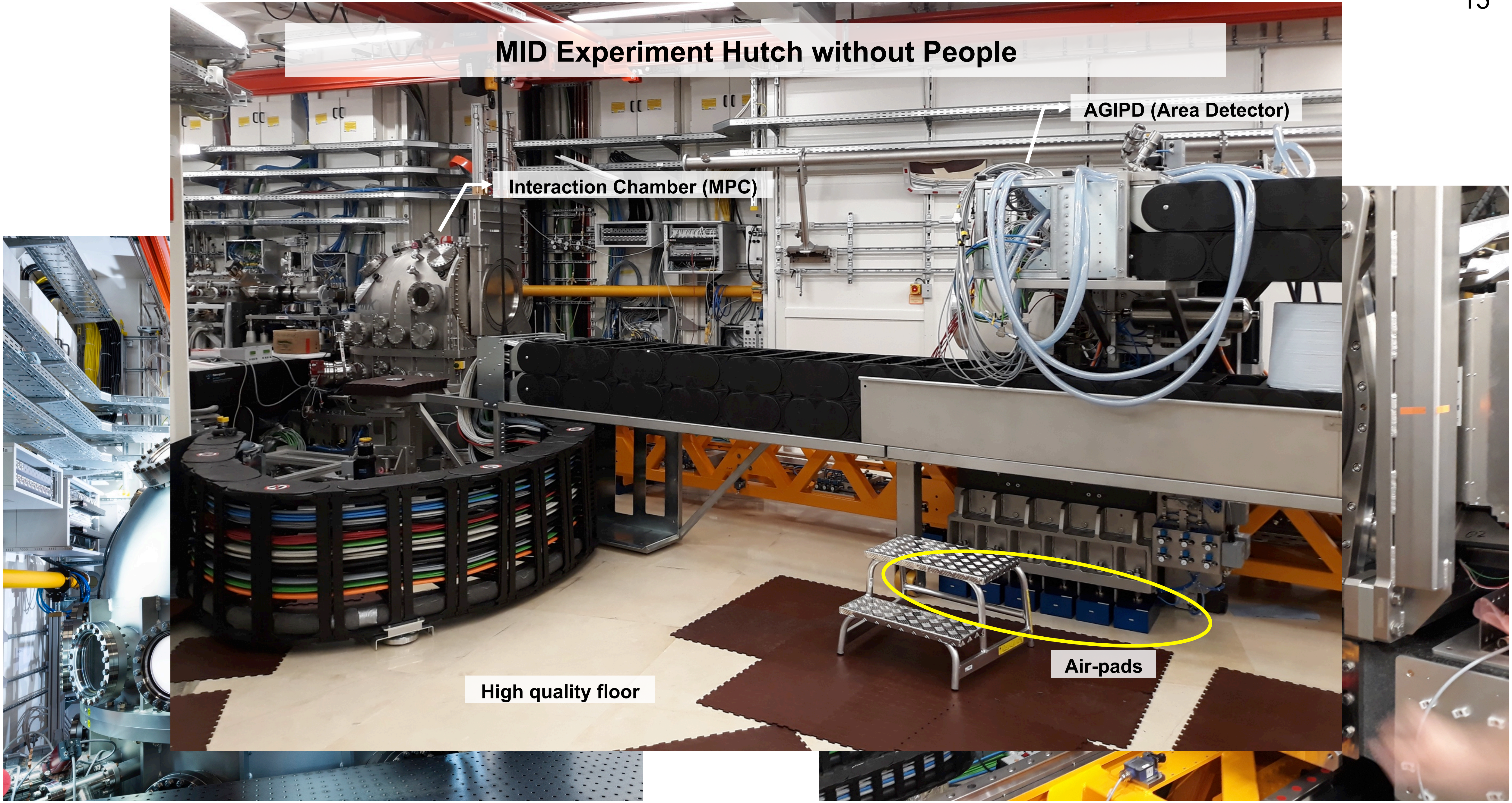
ultrafast scattering and imaging
nano-focusing, coherent diffractive imaging
pump-probe, speckle techniques
absorption spectroscopy



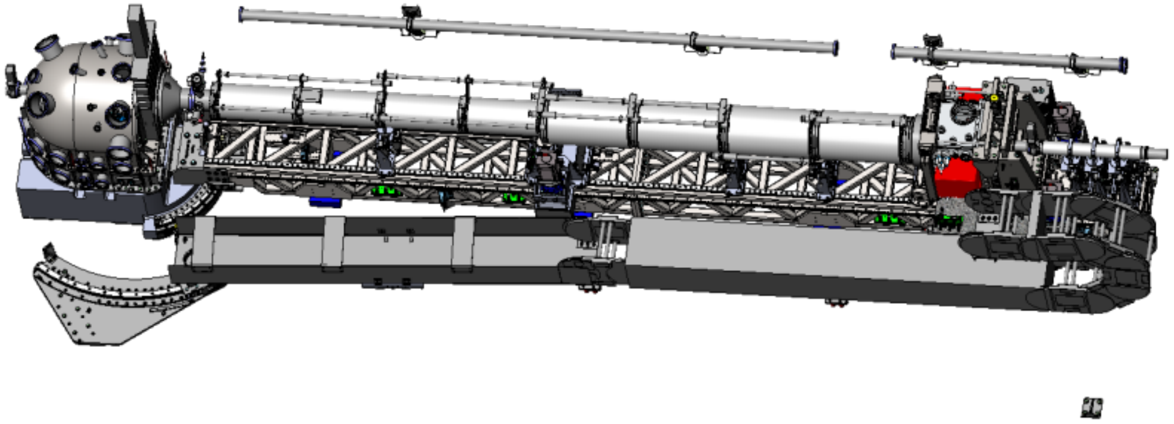


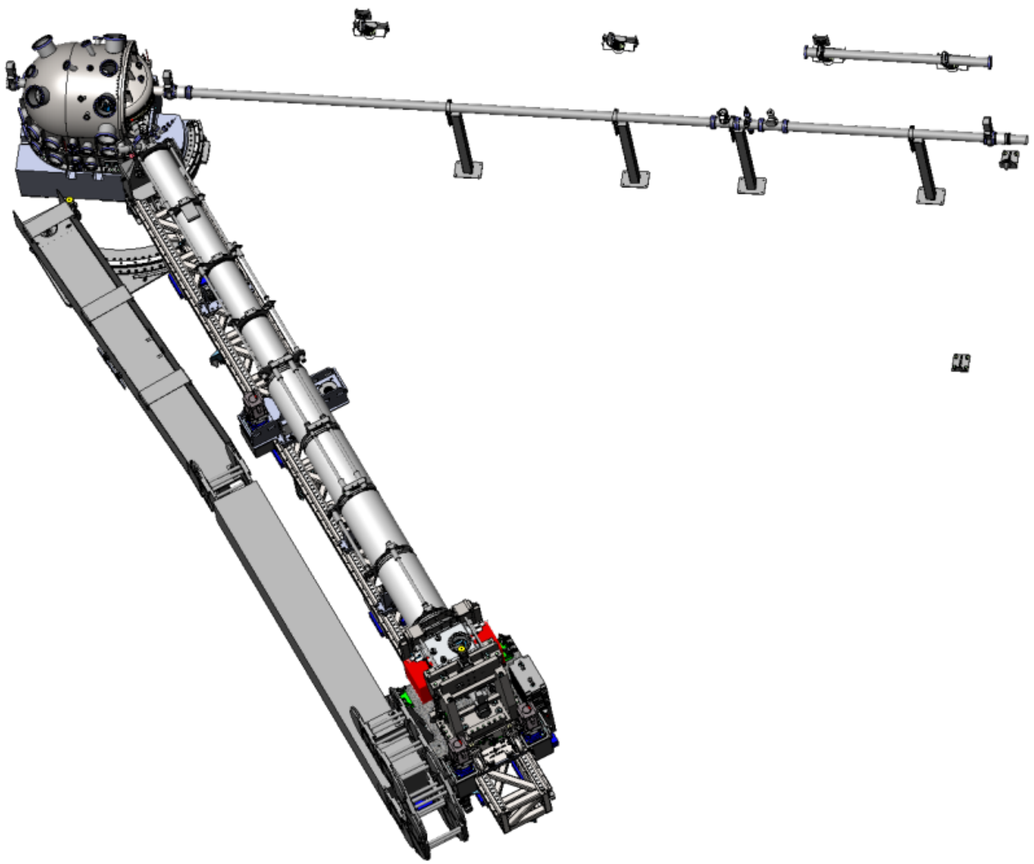

MID Group Photo after Successful X-ray Commissioning at EH
Anders Madsen (GL)
Robert Rosca (CAS)
Jolanta S.-Dambietz (DET)
Nicole Elleuche (MB)
Robert Fiedenhans'l (MB)
PHYSICS
XFEL


MID Experiment Hutch without People
AGIPD (Area Detector)
Interaction Chamber (MPC)
Air-pads
High quality floor

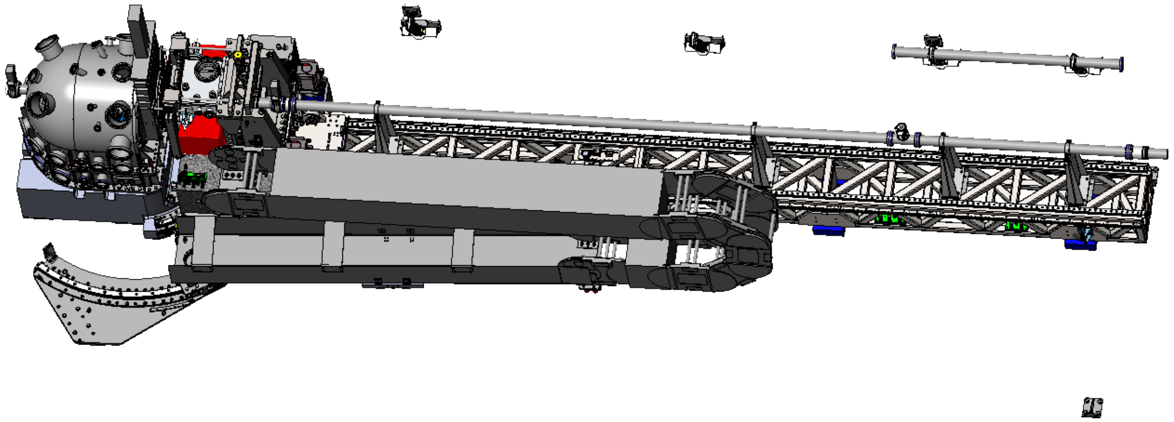
Scattering Geometry

Long SAXS configuration
(max sample-detector dist. ~ 8 m)



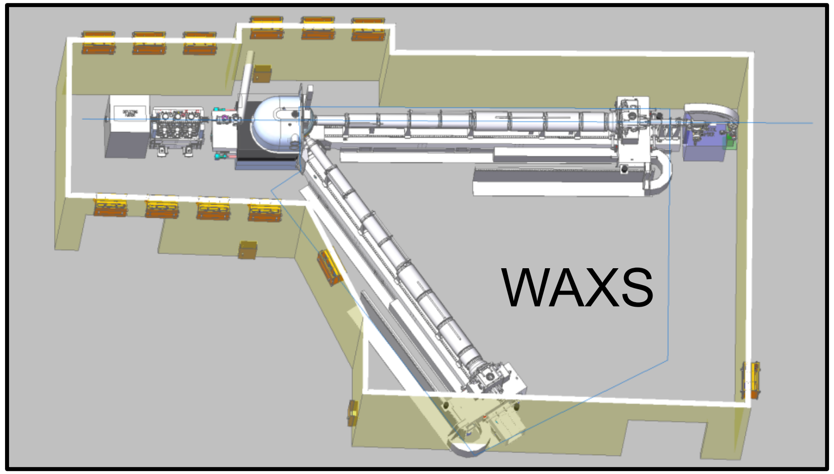


WAXS configuration
(max 2θ ~ 50º)

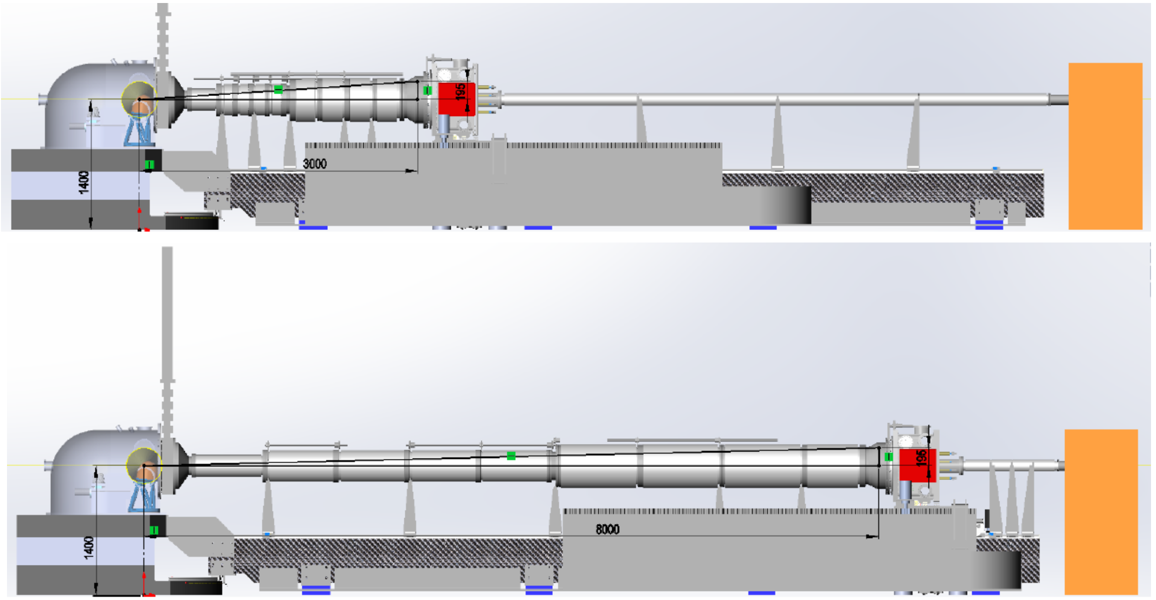


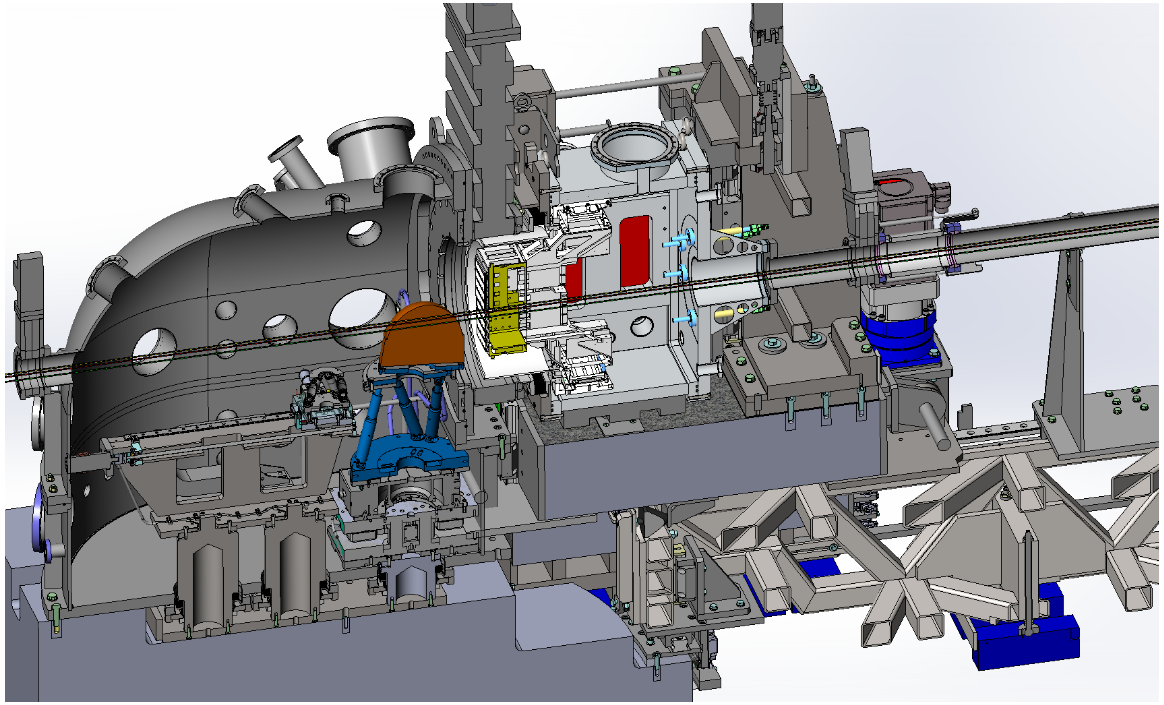
Large filed-of-view configuration (min sample-detector dist. ~ 22 cm)

Scattering Geometry



SAXS





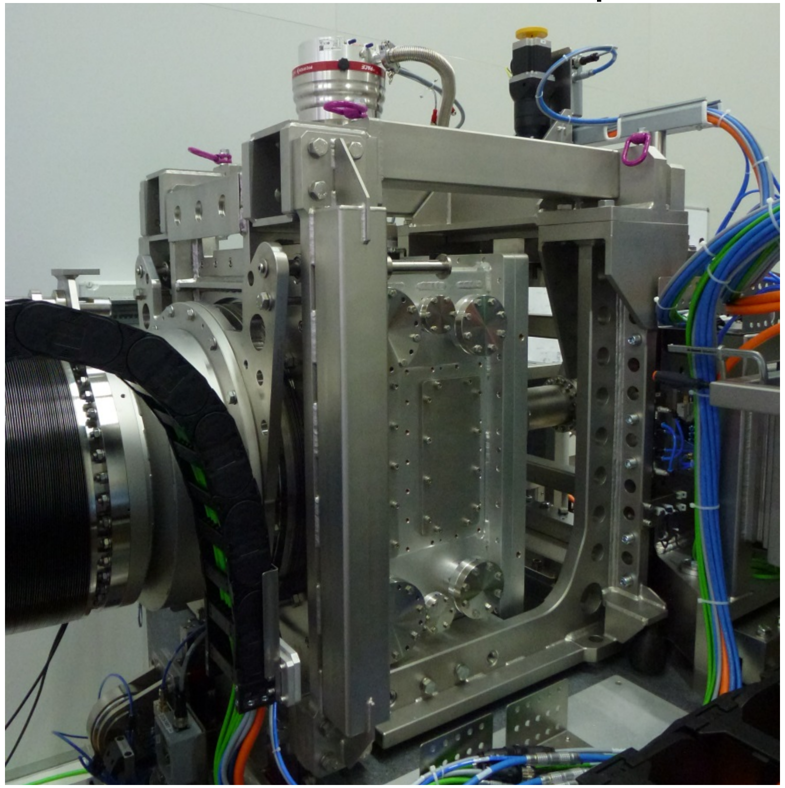
Detector ~20 cm from sample (large field of view config) or between 2 – 8 m (SAXS – WAXS)

2θ up to 50°

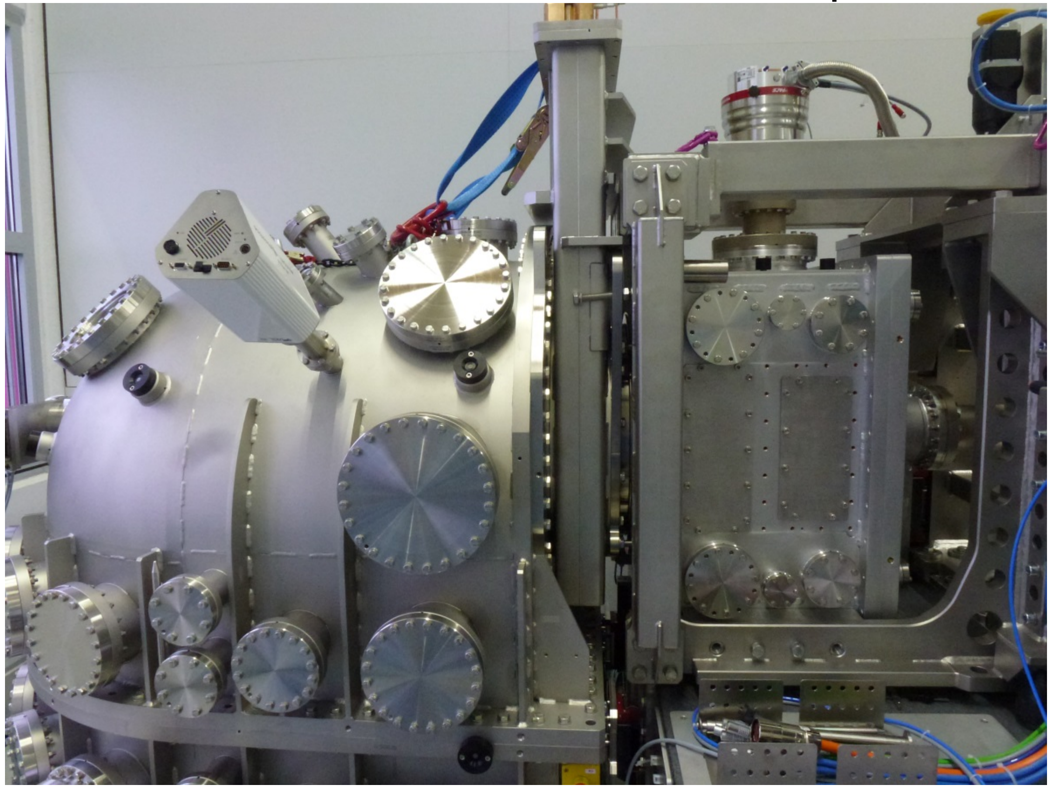
AGIPD detector size: ~ 20 x 20 cm, 200 μm pixels

Mechanical Integration of 2D Detector

AGIPD 8 m from sample

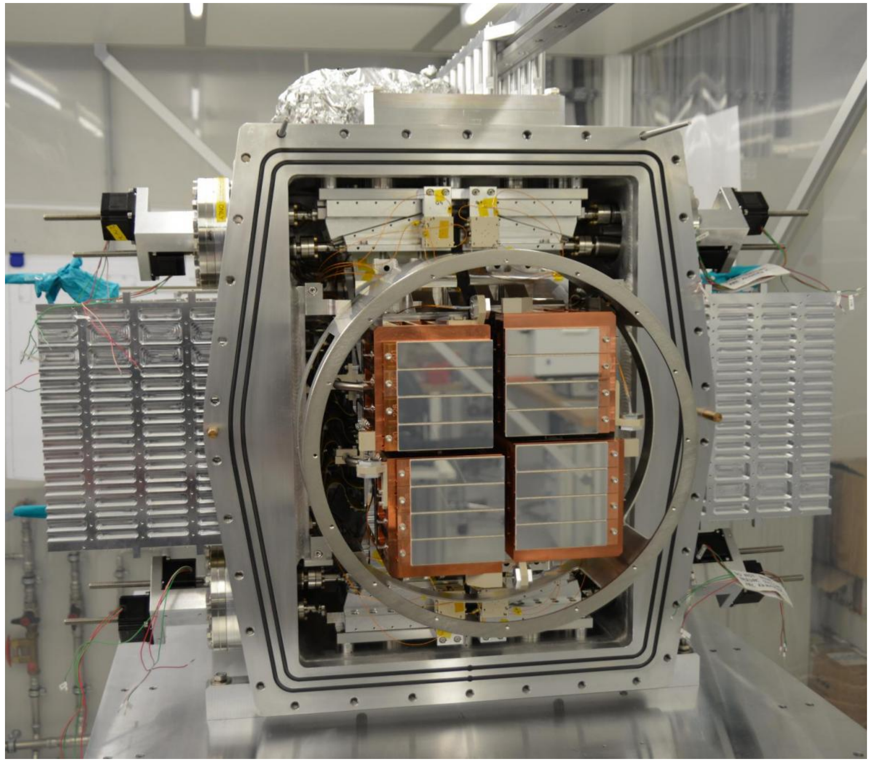


AGIPD ~20 cm from sample



- Use of AGIPD “dummy” to test mechanics and motion

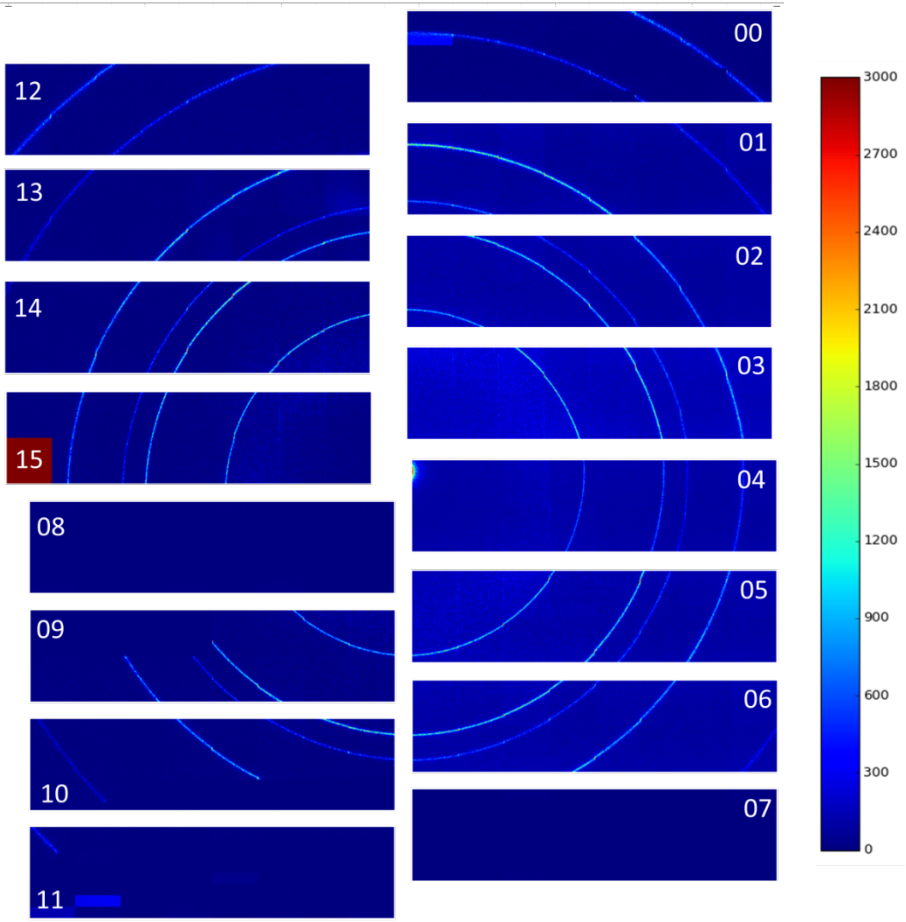
AGIPD Detector



AGIPD for MID (similar to SPB’s AGIPD)

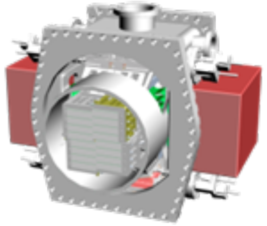
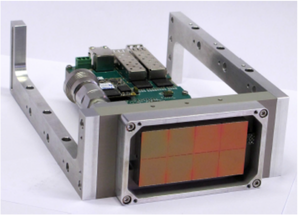
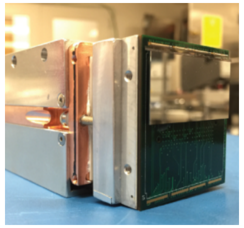
- ~1M pixels, 200 μm pixel size
- MHz rep rate
- Ready for 1st user experiments at MID

Al_2O_3 power rings (AGIPD calibration SPB)



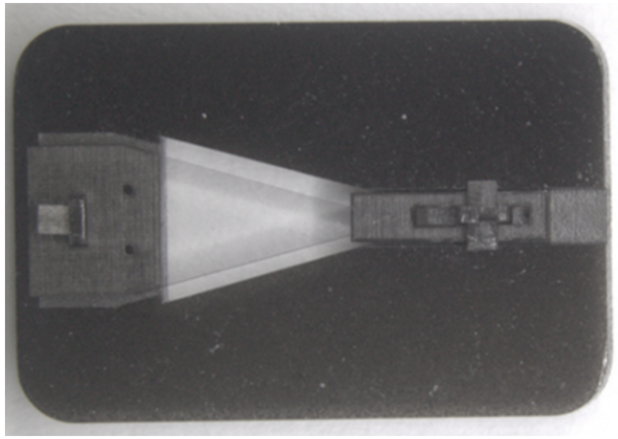
AGIPD coordinator H. Graafsma (DESY)
Slide adapted from Aschkan Allahgholi

Other Detectors for MID

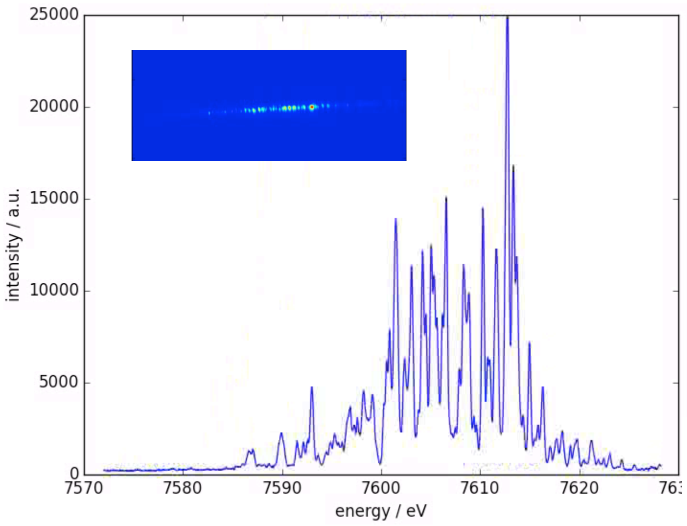
	AGIPD 1M	JUNGFRAU 1M	ePix 100 1M	GOTTHARD (-II)
				
Energy range (keV)	3-25	3-25	3-20	3-25
Dynamic range	10^4 ph/px/pulse @12 keV	10^4 ph/px/pulse @12 keV	100 ph/px @8 keV	10^4 ph/px/pulse @12 keV
Pixel size	200 × 200 μm^2	75 × 75 μm^2	50 × 50 μm^2	50 (25) μm
Noise	~1000eV	~200eV (HG)	<200eV	<750eV
Repetition rate	4.5 MHz	Currently 200kHz	120Hz	800kHz (4.5 MHz)
Number of storage cells	352	16	-	(Compact storage for full pulse train)
In-vacuum	Yes	Yes	Yes	No
(#mod) Array size	(4) 110×110mm^2 / mod	(2)40×80mm^2 /mod	(2)35×38mm^2 /mod.	(1) ~6×64mm^2 1280 (2560) pxl

Beam Diagnostics at Instrument

- Towards spectral analysis at MHz rate



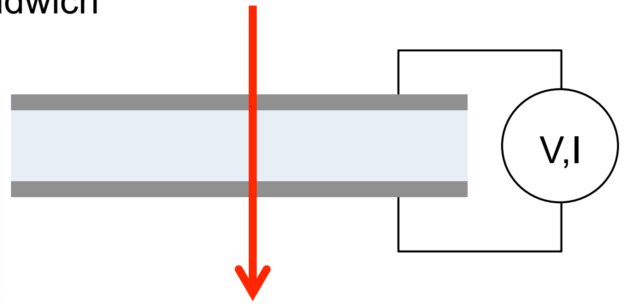
Diamond crystal bender
C*(220)

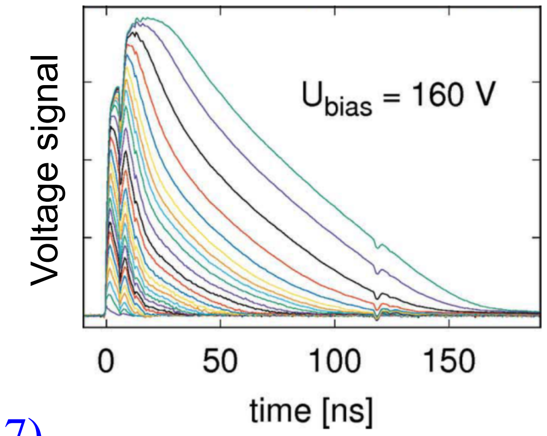


Pulse resolved spectra
recorded at LCLS (120 Hz)

- Non-invasive, MHz rate characterization of intensity and position

Diamond ionization chamber
Be-C-Be sandwich





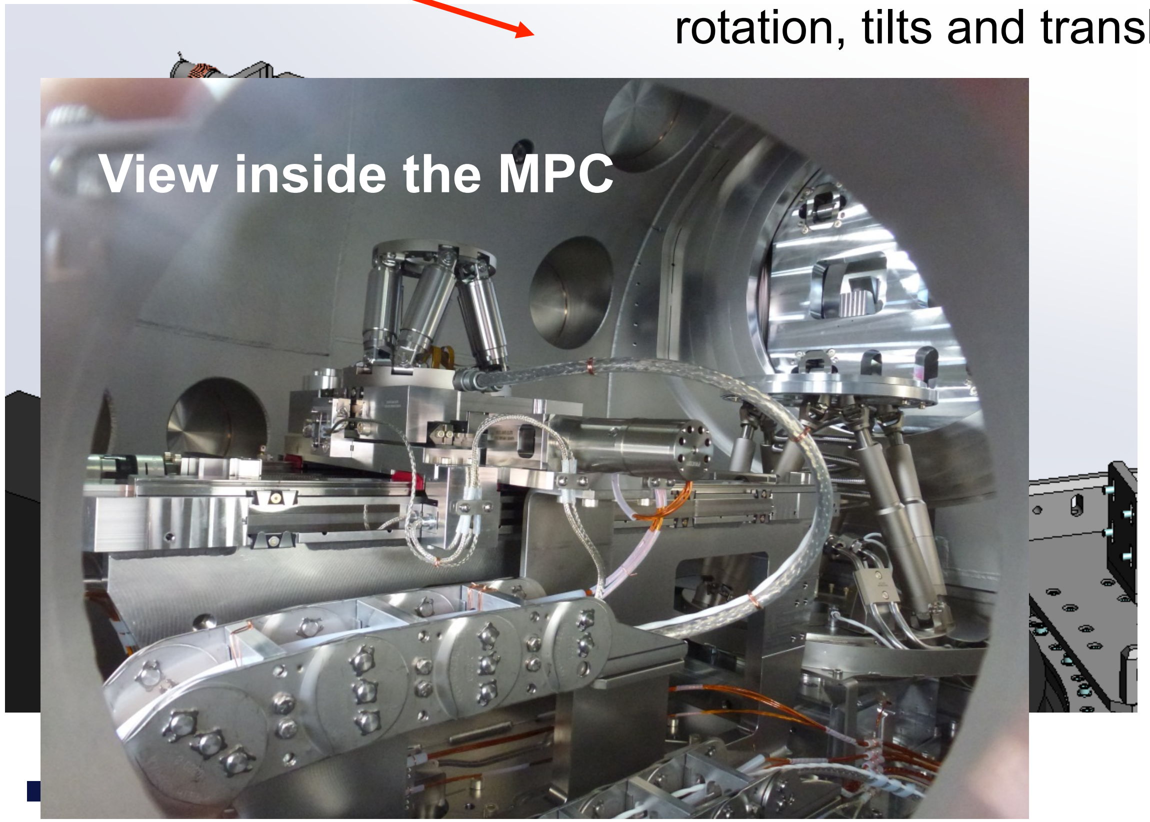
U. Boesenberg *et al.*, Optics Express **25**, 2852 (2017)
T. Roth *et al.*, J. Synchrotron Rad. **25**, 177 (2018)

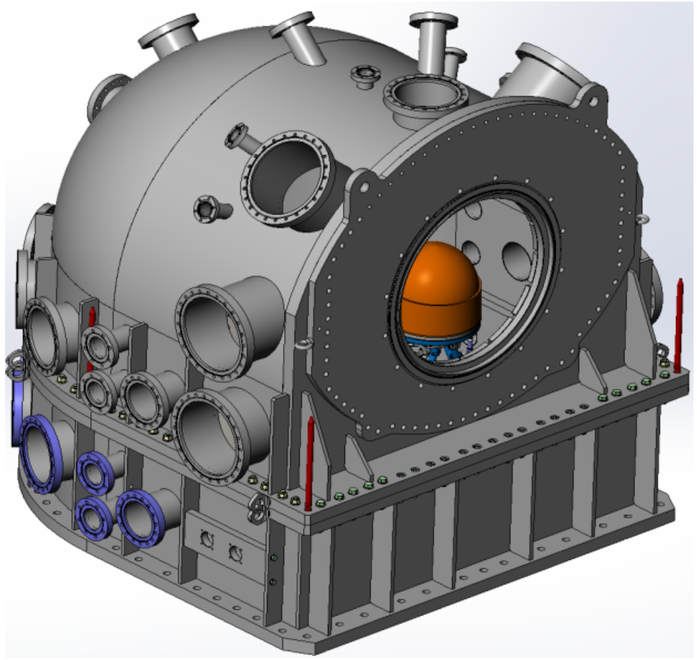
Experiment Chamber (MPC: Multi-Purpose Chamber)

1st stage (hexapod on linear stage)
(carries nanoCRL)

Beam

2nd stage (hexapod + Huber stack)
rotation, tilts and translations



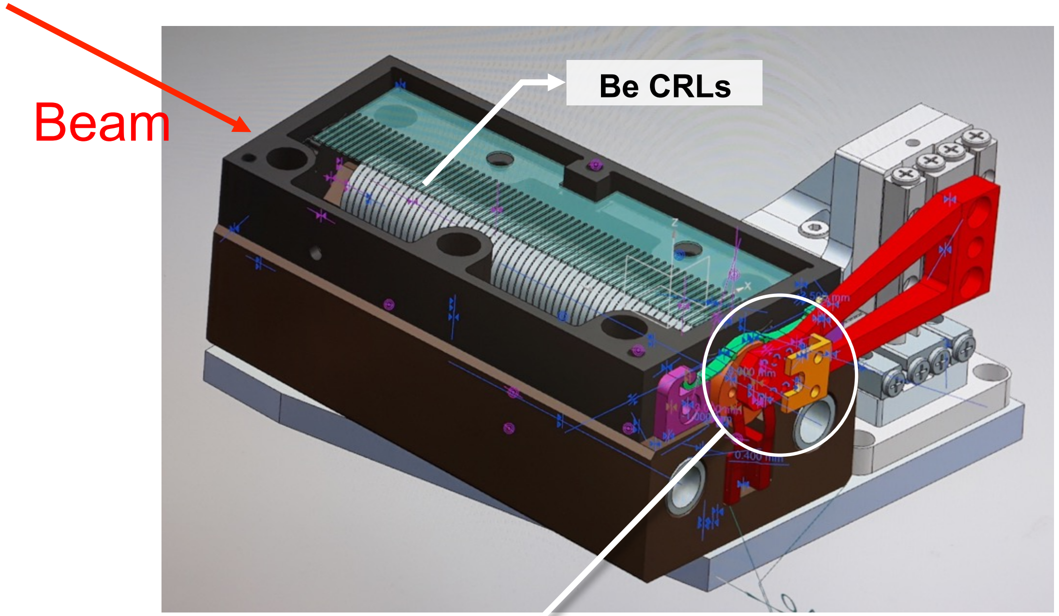


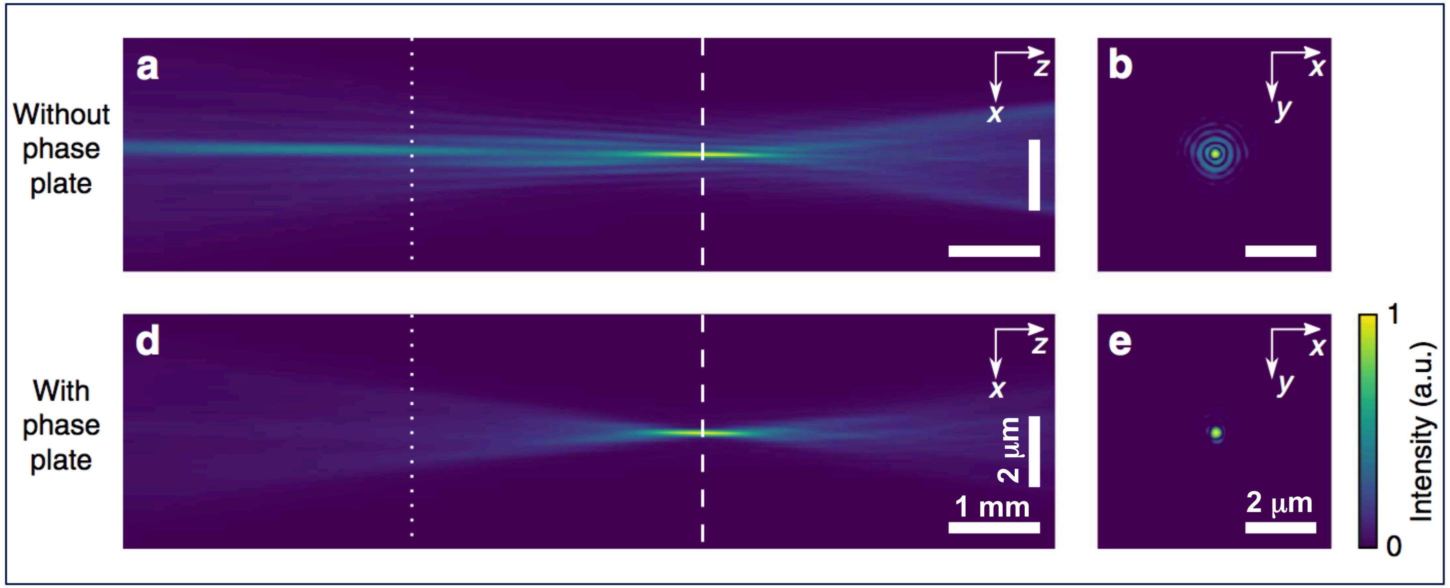
MPC operates under vacuum, windowless config.
Possibility to work without lid (in air or He bag)

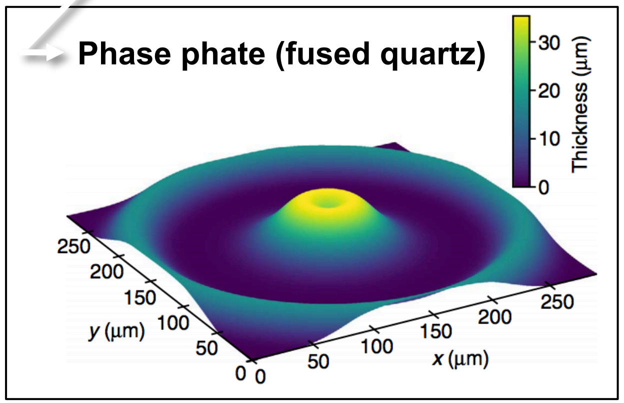
Sample environment:

- 10 Hz solid sample scanner
- Pulsed B field (Up to ~15T, 1 ms pulse)
- Cryostat (3,5K – 500K with <0,1K stability)
- Liquid jet
- ….

Nano-focusing CRL





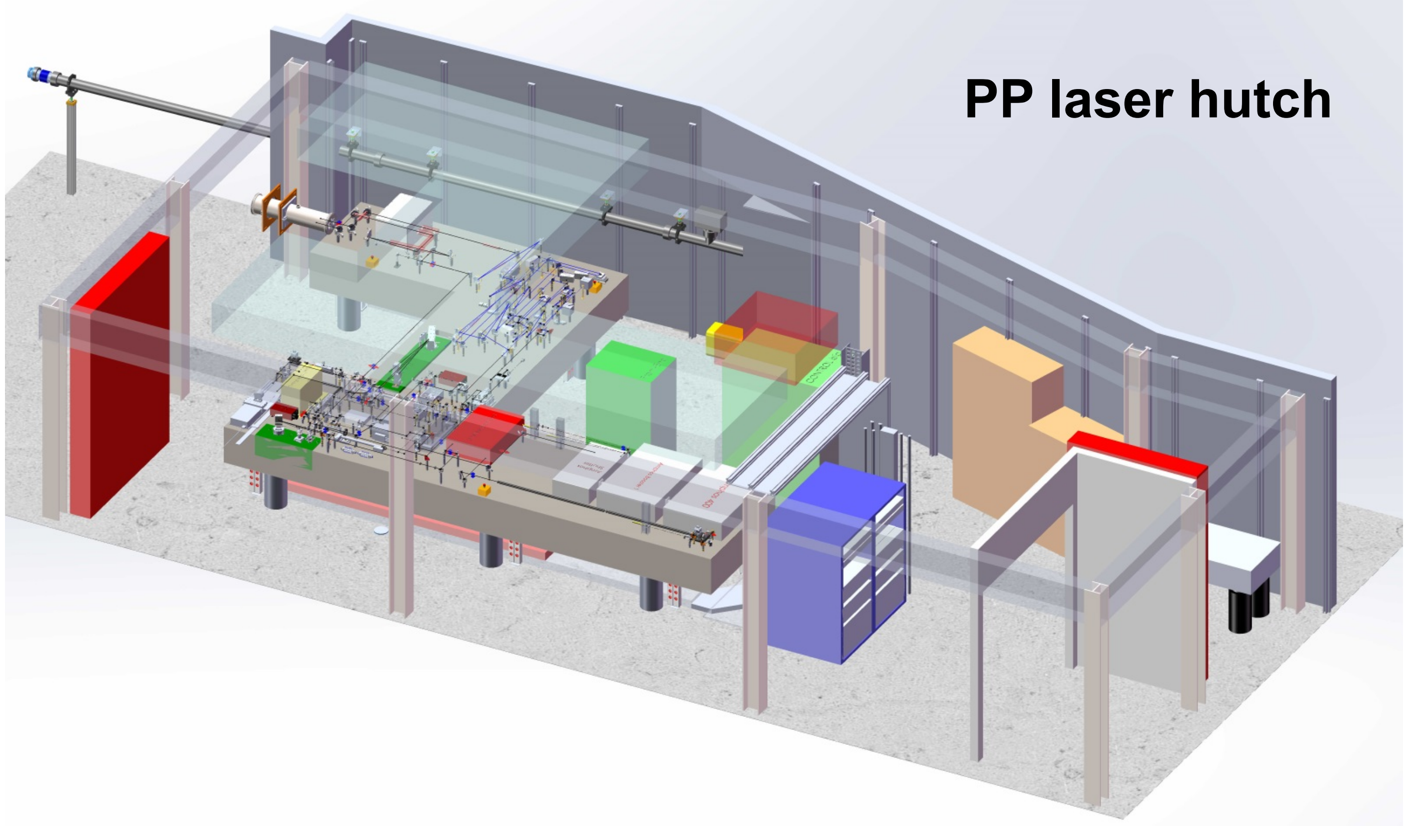


>> Aimed focus size is about 50 nm

BMBF project by Christian Schroer's Group
(X-ray nanoscience and x-ray optics in DESY)

NATURE COMMUNICATIONS | 8:14623 | DOI: 10.1038/ncomms14623

Pump-Probe fs Laser



Same pulse structure
("burst mode") as the X-rays

down to ~ 15 fs pulse duration
advanced cross-correlation scheme
(low jitter)

Set point	Rep-rate (MHz)	E_{Pump} (mJ) 1030 nm	NOPA	E_{NOPA} (mJ) 800 nm
1	4.5	1	I + II	0.05
2	1.13	4	I + II	0.3
3	0.188	21	I + II + III	1.5
4	0.1	40	I + II + III	2.5

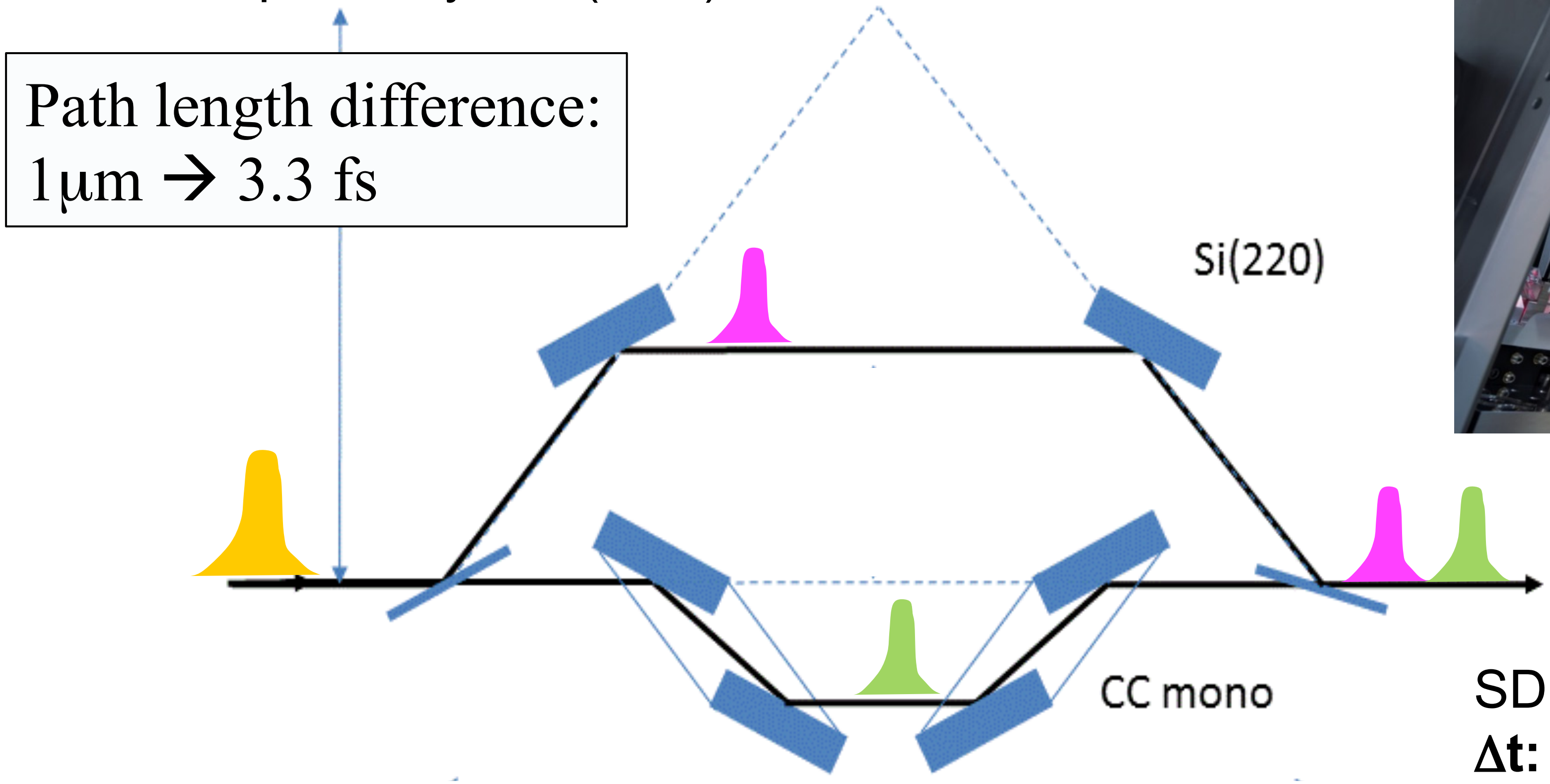
Slide from Max Lederer
XFEL Optical Laser Group

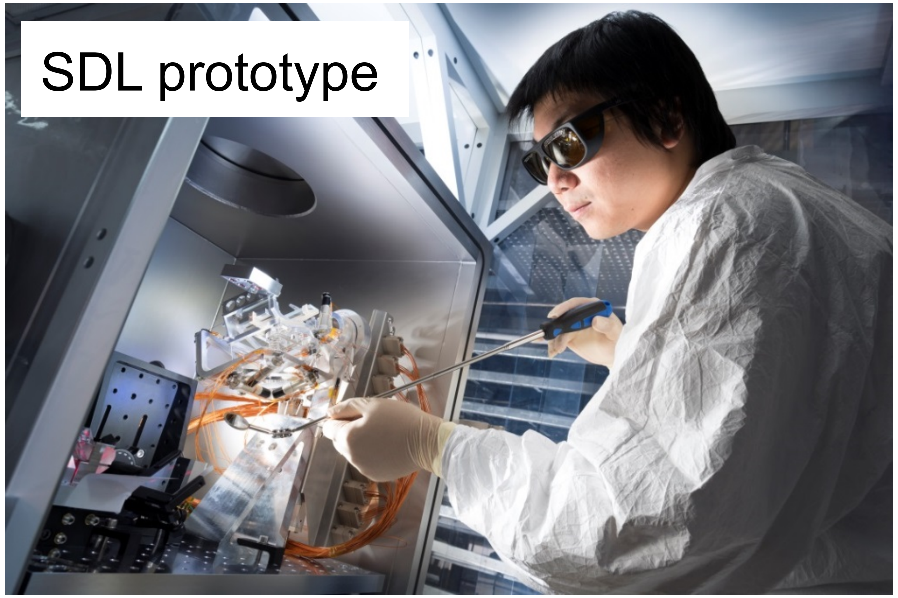
Pump-Probe ps/ns Laser

- Nanosecond to 20 ps dynamics study with Q-switched ns/ps laser
  - We plan to install a Q-switched ns/ps laser
  - It will be available second half of 2019
  - ns/ps might be too slow for phonons but still fine for certain phase transitions and dynamics

X-ray Split-Delay Line (SDL)

Need for split-delay line (SDL)





SDL under construction at XFEL.EU

Δt: -10 ps – 800 ps

E: 5 – 10 keV

Similar SDL projects at DESY, LCLS, SACLA,…

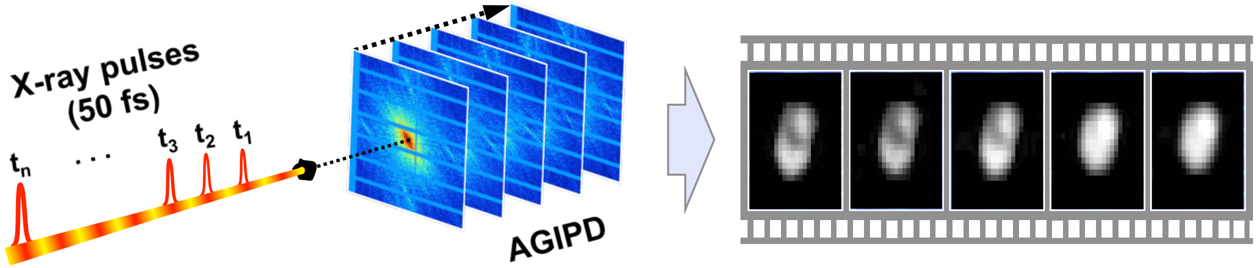
BMBF project by Stefan Eisebitt's Group (TU Berlin, Max-Born-Institut)

MID specifications

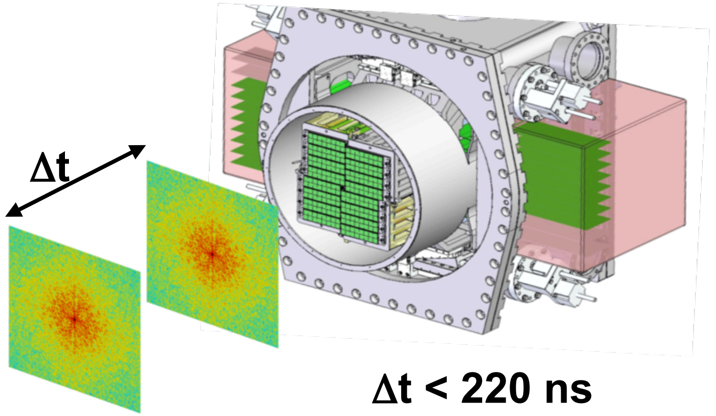
- 5-25 (9-14) keV X-rays, focusing with CRLs: down to few µm, nano-focusing option
- synchronized optical fs laser (available in end 2019)
- pink SASE (bw ~10^{-3}), Si(111) or Si(220) mono
- SASE-2 is the undulator where self-seeding will be implemented first (2019-2020?)
- Up to 4.5 MHz i.e. Δt = 220 ns spacing. Integers n·Δt possible (n=30 tested).
  1, 30, 120, 300, … pulses/train tested so far. 10 trains/s
- 0 - 800 ps spacing using split-delay line (SDL) (abailable in late 2019 or early 2020)
- pulse energy ~1 mJ = 6 x 10^{11} photons/pulse at 10 keV. Pulse duration <100 fs
- window-less setup (differential pump) or sample in air/He (diamond window)
- 2D detectors (AGIPD, ePix, Jungfrau), attenuators, slits, diagnostics,…
- pulse resolved energy dispersive spectrometer
- liquid jet, cryostat, B-field, fast sample scanner, hexapods, goniometer,…

Possible Dynamics Measurement Scheme

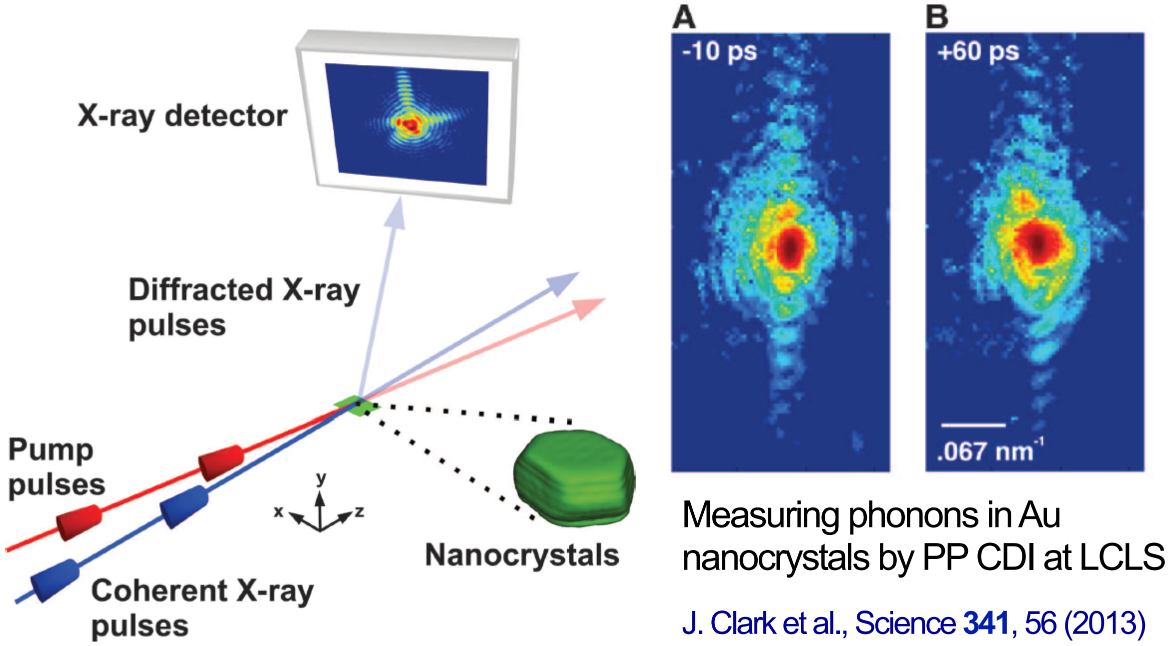
- Movie mode with XFEL pulses
  (Max 4.5MHz (220 ns) frame rate: XPCS, CXDI, etc.)



- X-ray speckle visibility spectroscopy type Exp.
  with different pulse width of XFEL pulses



- Pump-prove mode with ns/ps laser systems

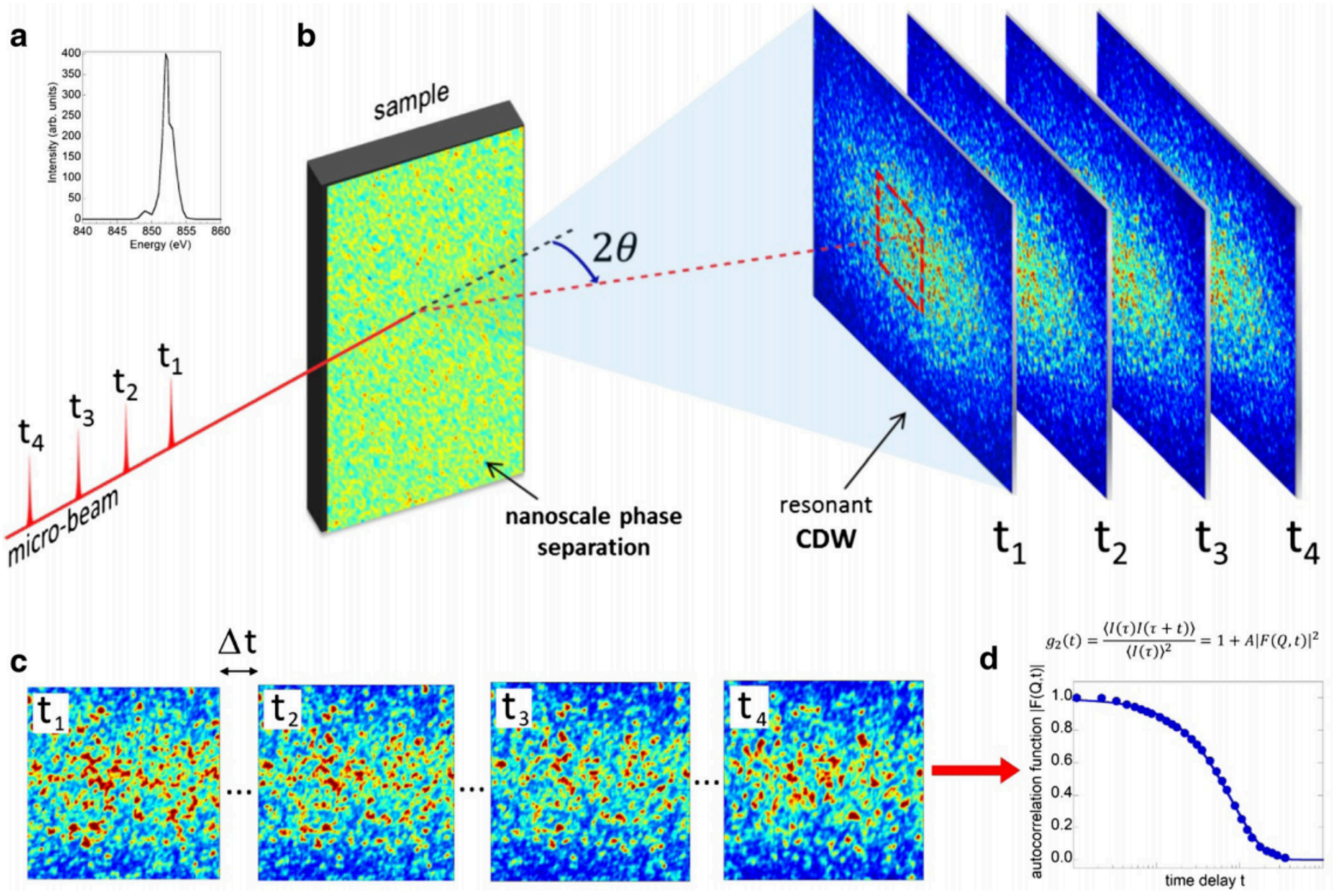


Measuring phonons in Au nanocrystals by PP CDI at LCLS

J. Clark et al., Science **341**, 56 (2013)

ns/ps too slow for phonons but
fine for certain phase transitions,
critical dynamics, surface dynamics,…

First Main Measurement Scheme at MID
Example of X-ray Photon Correlation Spectroscopy (XPCS)



Nanoscale Dynamics in Complex Materials by Resonant X-Ray Photon Correlation Spectroscopy (rXPCS)

Alessandro Ricci

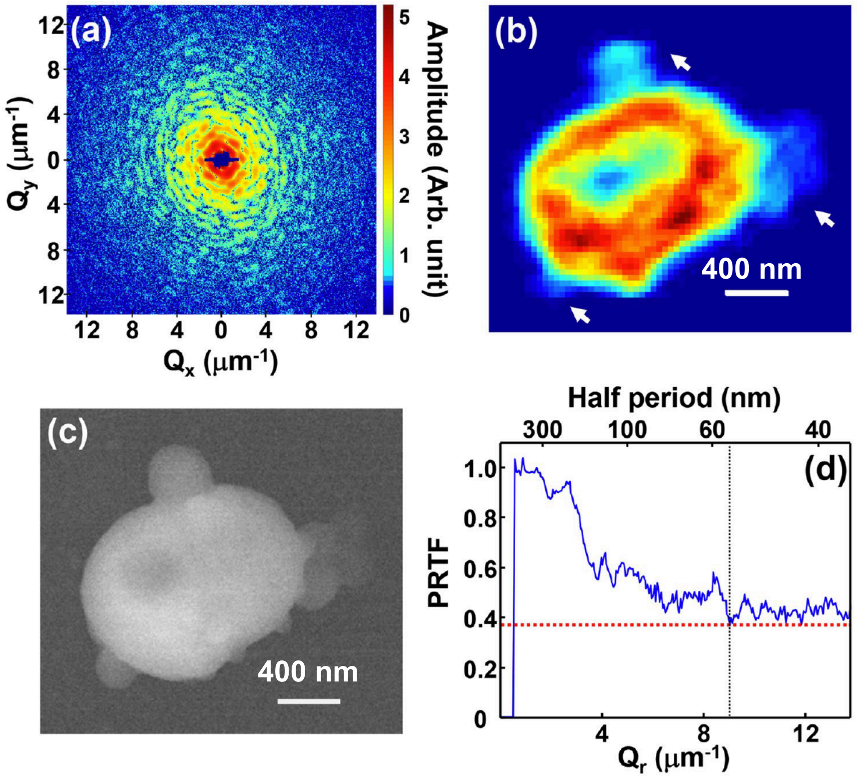
J Supercond Nov Magn
DOI 10.1007/s10948-014-2907-3

Fig. 1 Resonant X-ray photon correlation spectroscopy experiment. **a** The integrated intensity of resonant CDW peak in $La_{1.72}Sr_{0.28}NiO_4$ as a function of energy. The scattering intensity is strongly enhanced setting the energy to the Ni L_3-edge. **b** A sample showing nanoscale phase separation is illuminated by a coherent X-ray micro-beam. A time series of diffraction patterns is collected keeping external condition as stable as possible. **c** The time-dependent coherent diffraction patterns are characterized by the presence of speckles that represent the granular local structure of the material showing an inhomogeneous landscape of charge-ordered domains in the illuminated spot. **d** In order to determine the correlation time τ that characterizes the CDW domains dynamic, the intensity autocorrelation function can be calculated. This would allow to probe dynamics on timescales as short as the time spacing Δt of the collected time series

Second Main Measurement Scheme at MID
Example of Coherent X-ray Diffractive Imaging (CXDI)

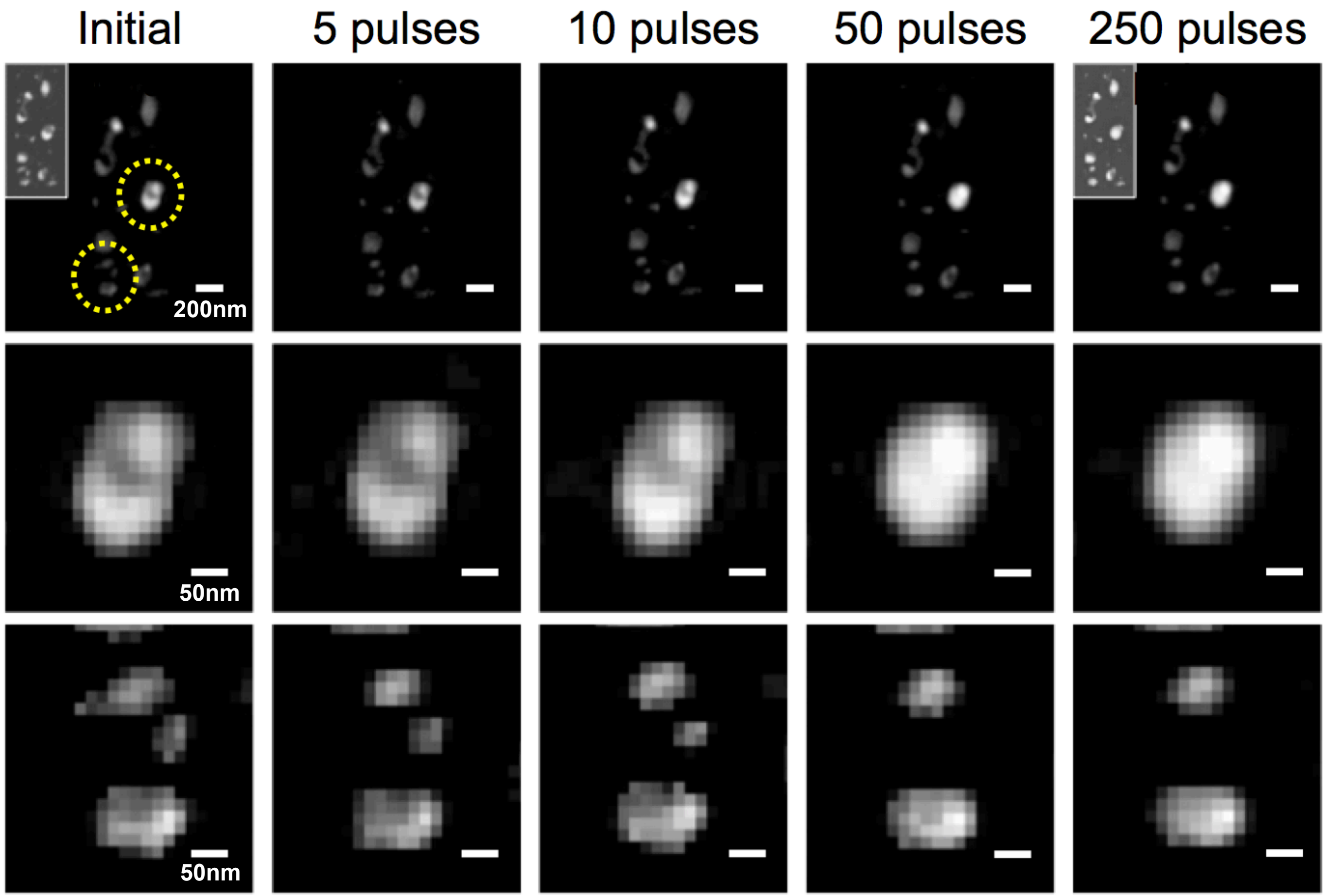
Visualization of a Mammalian Mitochondrion by Coherent X-ray Diffractive Imaging

Yoonhee Kim[1], Chan Kim[1,2], Ou Young Kwon[1], Daewoong Nam[3], Sang Soo Kim[4], Jae Hyun Park[4], Sunam Kim[4], Marcus Gallagher-Jones[5,6], Yoshiki Kohmura[5], Tetsuya Ishikawa[5], Changyong Song[3,5], Giyoong Tae[1] & Do Young Noh[1]



SCIENTIFIC REPORTS | 7: *1850* | DOI:10.1038/s41598-017-01833-x

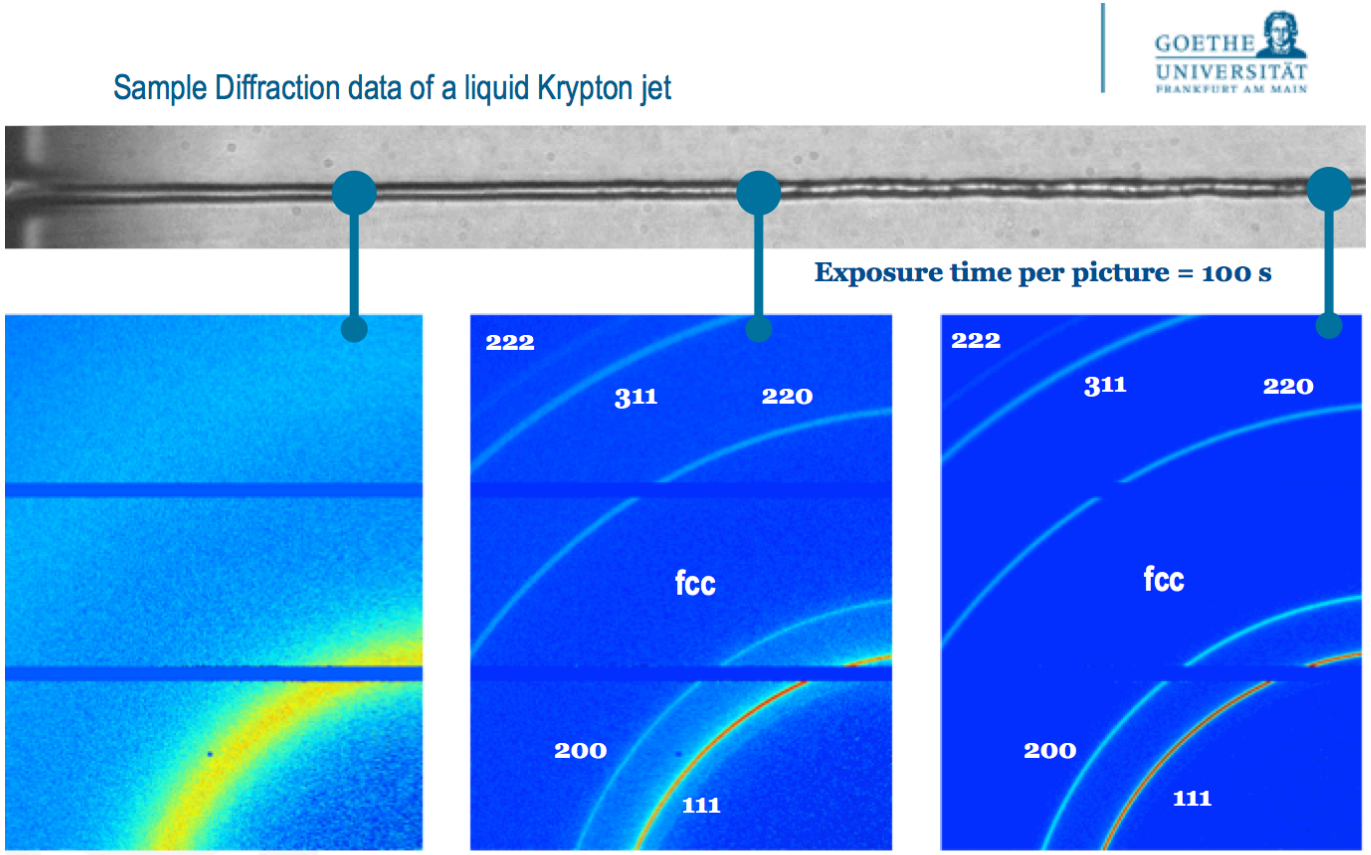
Laser Induced Diffusion Process of AuNi alloy



(532 nm, 0.2 mJ/cm^2/pulse)

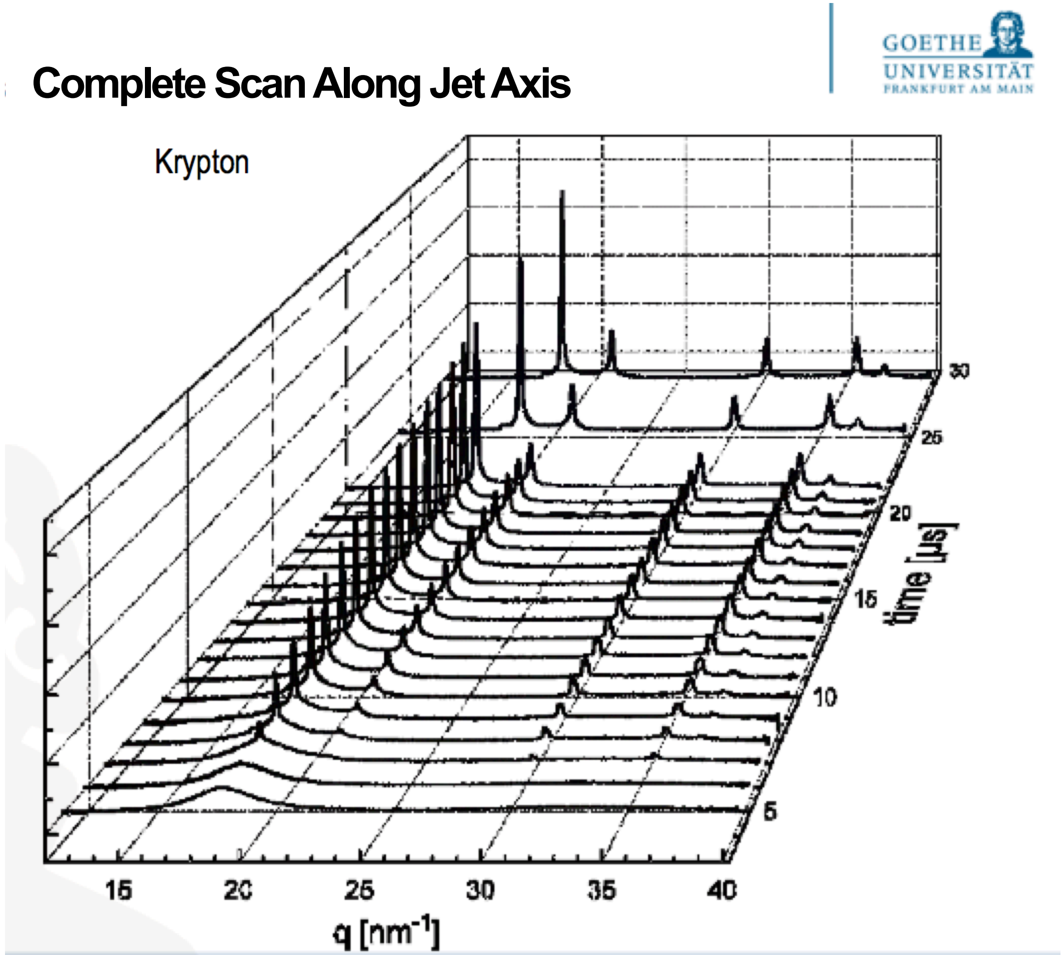
Scheduled User Experiment #1 at MID
Liquid to Solid Phase Transition in Supercooled Atomic Liquids

Sample Diffraction data of a liquid Krypton jet



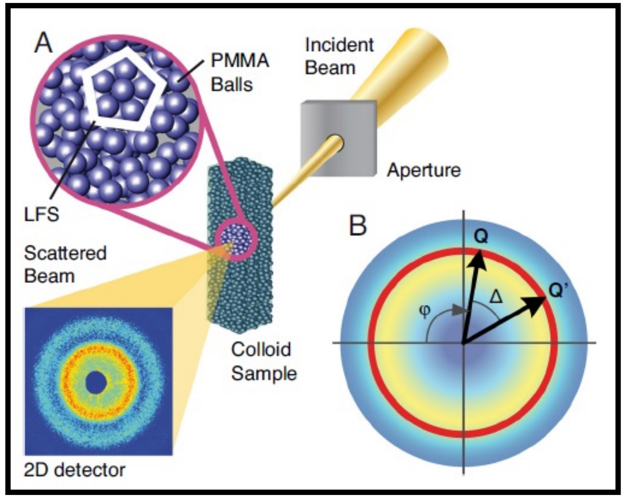
Data taken from a Ø 5 µm Krypton jet at P03 (DESY) with 13 keV Photons
Nozzle temperature T = 117 K

Complete Scan Along Jet Axis

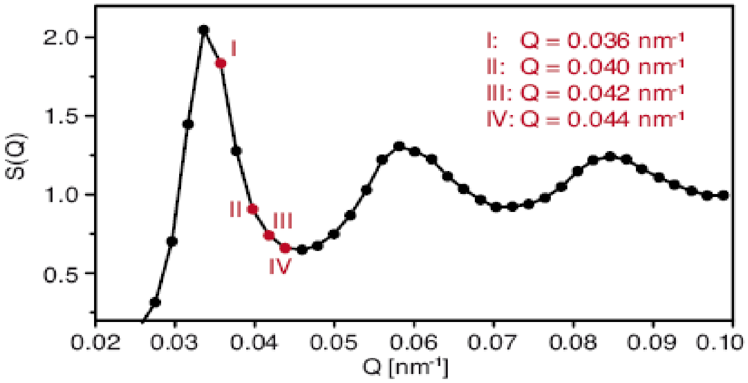


Robert Grisenti's Group (Göthe Univ.)
& Anders Madsen's Group (MID, E-XFEL)

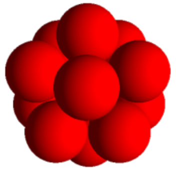
Liquid to Solid Phase Transition in Supercooled Atomic Liquids

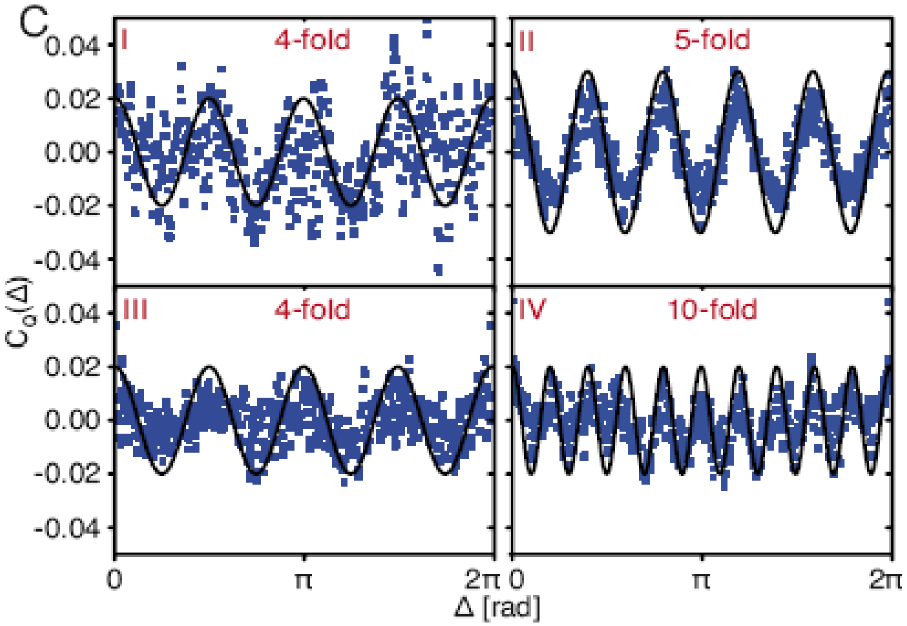


$$g(\boldsymbol{r}) - 1 = \frac{1}{\rho_o (2\pi)^3} \int [S(\boldsymbol{q}) - 1]\, \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\, \mathrm{d}\boldsymbol{q}$$



$$C_Q(\Delta) = \frac{\langle I(Q,\varphi) I(Q,\varphi+\Delta)\rangle_\varphi - \langle I(Q,\varphi)\rangle_\varphi^2}{\langle I(Q,\varphi)\rangle_\varphi^2}$$





P. Wochner et al., PNAS, 106, 11511 (2009); F. Lehmkühler et al., J. Appl. Cryst. 47, 1315 (2014);
M. A. Schroer et al., J. Chem. Phys. 144, 084903 (2016)

Scheduled User Experiment #2 at MID
Laser-Induced Cavitation Dynamics Studies by Time-resolved X-ray Holography

(a) Schematic of the experiment.
(b) Oscillation trajectory R(t) of a bubble. The period T is set by the laser repletion rate.
(c) Simulated hologram of a 600 nm large bubble at FN = 10^{-3} for 50 nm pixel size (blue density profile shown in (e)).
(d) Azimuthally integrated intensity profiles I(r) as function of the radius.
(e) Phase shift extracted from simulated density profiles (red and blue) of the water distribution inside the bubble for varied interaction strength of bubble wall and volume.

Christian Schroer's Group (DESY)
& Tim Salditt's Group (Univ. Göttingen)

First Result from SASE1 instruments at European XFEL

nature COMMUNICATIONS

ARTICLE

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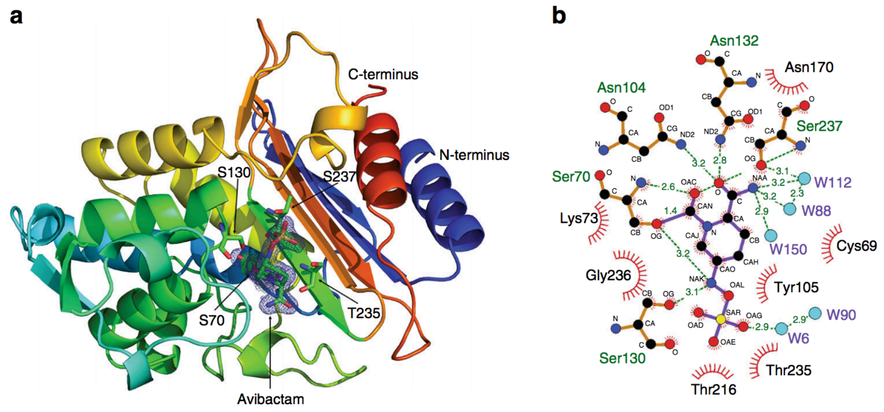
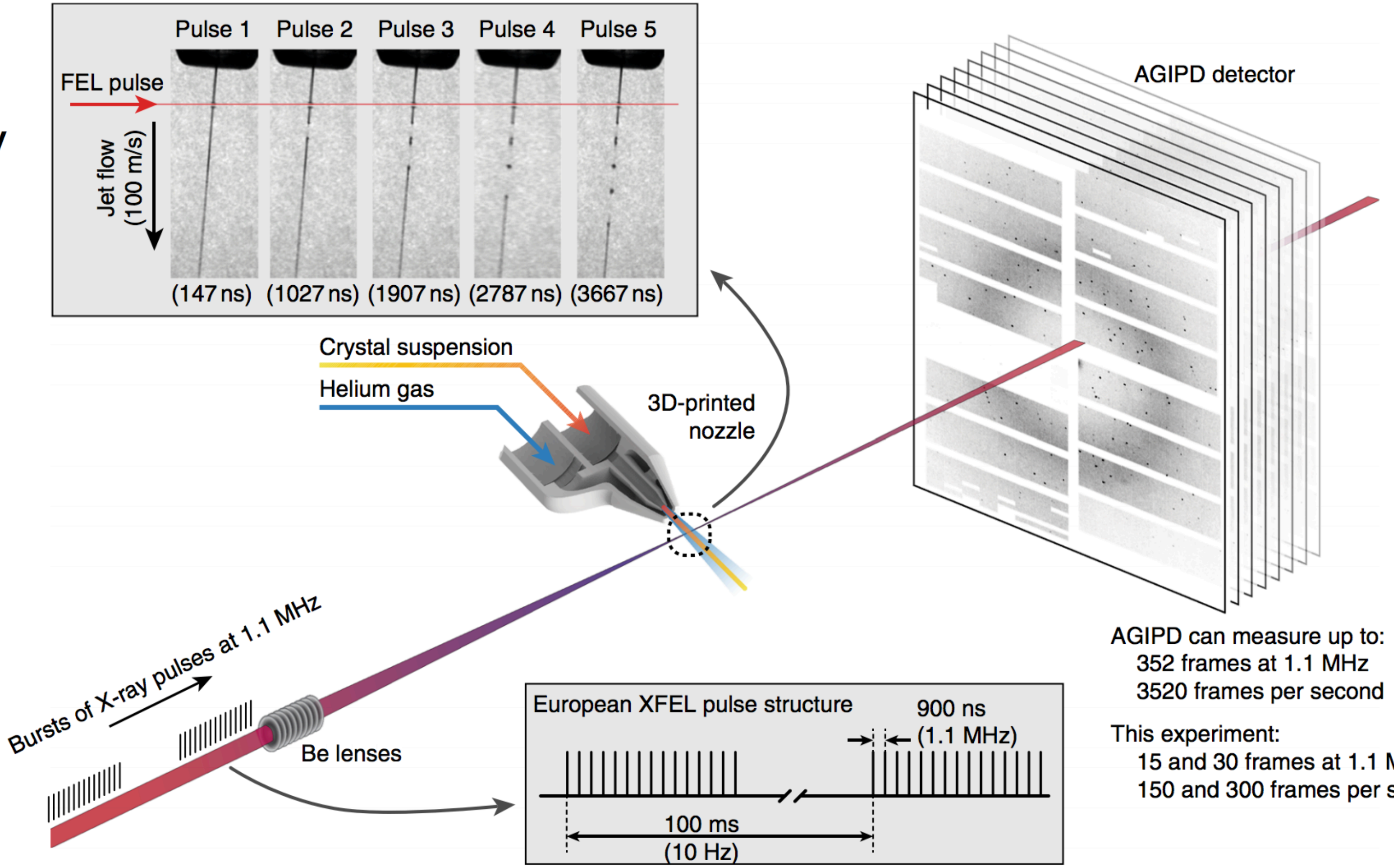
Megahertz serial crystallography

Max O. Wiedorn et al.#



Structure of CTX-M-14 β-lactamase determined by MHz SFX

Sketch of MHz Serial Crystallography



AGIPD can measure up to:
352 frames at 1.1 MHz
3520 frames per second

This experiment:
15 and 30 frames at 1.1 MHz
150 and 300 frames per second

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First Data Processing Results from XFEL2012 – 17 November 2017

Open Collaboration with over 100 participants

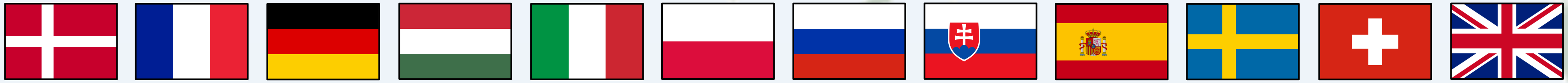
1. SPB/SFX instrument scientists
2. XFEL detector, AGIPD
3. Sample preparation
4. Jets & diagnostics (sample delivery)
5. Analysis
6. XFEL sample environment
7. Data storage & controls & software

Conclusion and Future Works

- European XFEL is ready for a various static and time-resolved experiments.
- A successful x-ray delivery to MID end-station was done in December 2018 and MID crew are preparing a first user experiment.
- Future works
  - Successful user operations and inhouse research.
  - Femtosecond pulsed laser systems will be installed and their timing with x-ray pulses will be confirmed.
  - SDL unit will be intalled and tested.
- For further information: chan.kim@xfel.eu, mid-info@xfel.eu


Hopefully see you at XFEL in near furture !!!
And thanks for your kind attention !!!

Questions ?



Potential for biomolecular imaging with femtosecond X-ray pulses

Richard Neutze*, Remco Wouts*, David van der Spoel*, Edgar Weckert†‡ & Janos Hajdu*

** Department of Biochemistry, Biomedical Centre, Box 576, Uppsa*
S-75123 Uppsala, Sweden
† Institut für Kristallographie, Universität Karlsruhe, Kaiserstrasse
Germany