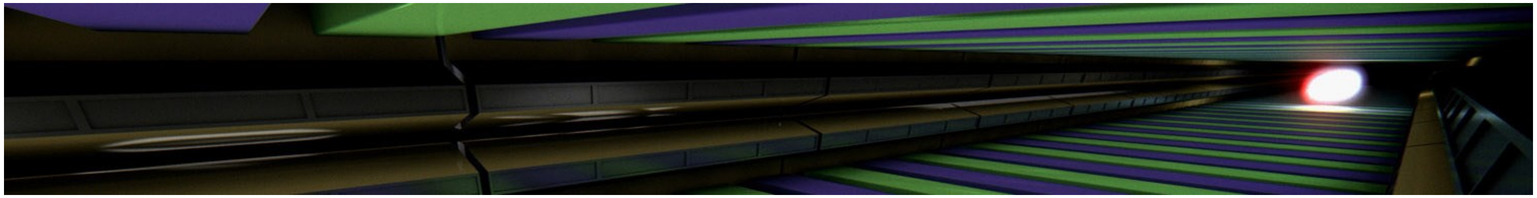

Materials Imaging and Dynamics Workshop: Early Science at MID

Jan 26-27, 2015

MID team:
A. Madsen, J. Hallmann, T. Roth, W. Lu (also TU Berlin),
G. Ansaldi, A. Schmidt, B. Kist (also TU Hamburg-Harburg)

European XFEL

Workshop Program

Monday, 26 January 2015

13:30	Welcome and status of MID instrument	A. Madsen	*European XFEL*
14:00	MID beam parameters and optics	T. Roth	*European XFEL*
14:30	MID sample environment and optical laser	J. Hallmann	*European XFEL*
15:00	Discussion		
15:30-16:00	**Coffee Break**		
16:00	XFEL science with nano-beams	C. Schroer	*DESY and Univ. Hamburg*
16:40	Correlations in space and time	C. Gutt	*Univ. Siegen*

Tuesday, 27 January 2015

9:00	Ultrafast XPCS	G. Grübel	*DESY*
9:40	Ultrafast pump-probe CXDI	I. Robinson	*University College London*
10:20-10:40	**Coffee Break**		
10:40	Ultrafast melting of colloidal crystals observed in pump-probe experiment at LCLS	I. Vartaniants	*DESY*
11:20	Ideas for microfluidics experiments at MID	S. Köster	*Univ. Göttingen*
12:00	AGIPD: A 2d pixel detector for XFEL.EU	H. Graafsma	*DESY*
12:40-14:00	**Lunch Break**		
14:00	New opportunities for 0.1-meV-resolution IXS at high-repetition-rate	Y. Shvyd'ko	*Argonne National Laboratory*
14:40	IXS for studies of collective dynamics: from glass forming systems to proteins	A. Sokolov	*Univ. Tennessee*
15:20	Dynamics studied by XFEL IXS	G. Monaco	*Trento University*
16:00-16:20	**Coffee Break**		
16:20	Ultrafast scattering exp. in materials science	P. Gaal	*HZ Berlin & Univ. Hamburg*
17:00	Femtosecond protein dynamics using split-delay line crystallography	J. J. van Thor	*Imperial College London*
17:40	**Discussion and Close Out**		

Past

- 2009: 1st MID workshop (Oct. 2009)
- 2011: Lead scientist hired, Advisory and Review Team (ART) established
- 2011: Publication of Conceptual Design Report (CDR)
- 2012: Engineering collaboration with ESRF
- 2012: 2nd MID workshop (Dec. 2012)
- 2013: Publication of Technical Design Report (TDR)
- 2014: First 3D instrument models ready, first Call-for-Tender published

Past, Present, and Future

- 2009: 1st MID workshop (Oct. 2009)
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- 2013: Publication of Technical Design Report (TDR)
- 2014: First 3D instrument models ready, first Call-for-Tender published
- 2015: 3rd MID workshop, all 3D models ready, all major CfTs out
- 2016: Reception of components, technical commissioning, installation
- 2017: Installation, first lasing, commissioning with beam, and early science
- 2018: User operation

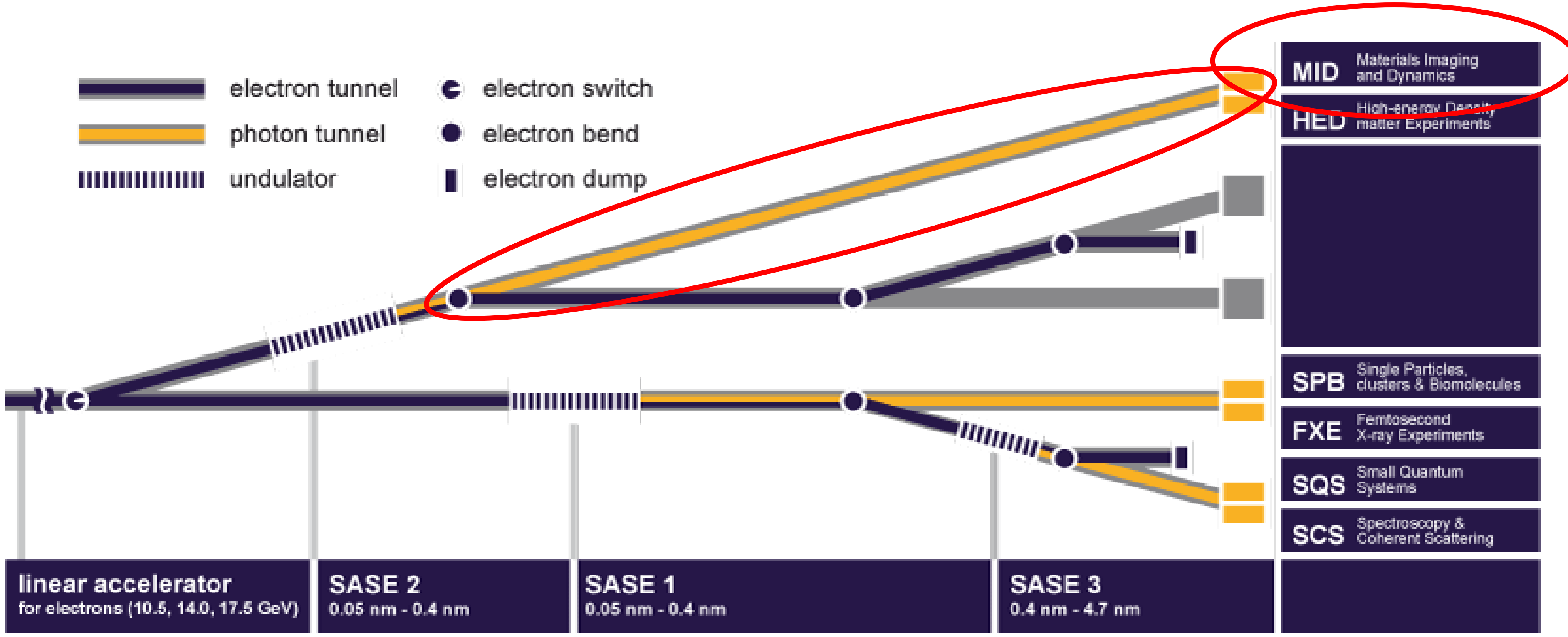
MID mission

The Materials Imaging and Dynamics (MID) instrument aims at the investigation of nanosized **structure** and nanoscale **dynamics** using **coherent radiation**. Applications to a **wide range of materials** from hard to soft condensed matter and biological structures are envisaged

(1st MID workshop, Oct 2009 @ ESRF, Grenoble)

Facility Outline

- MID @ SASE-2



MID Design Reports (CDR & TDR)

CONCEPTUAL DESIGN REPORT

Materials Imaging and Dynamics Instrument

A. Madsen

European XFEL GmbH, WP-83

September 2011

European X-Ray Free-Electron Laser GmbH
Albert-Einstein-Ring 19
22761 Hamburg
Germany

European XFEL

XFEL.EU TR-2013-005

TECHNICAL DESIGN REPORT

Scientific Instrument Materials Imaging and Dynamics (MID)

October 2013

A. Madsen, J. Hallmann, T. Roth, and G. Ansaldi for the Scientific Instrument MID (WP83) at European XFEL

European X-Ray Free-Electron Laser Facility GmbH
Albert-Einstein-Ring 19
22761 Hamburg
Germany

European XFEL

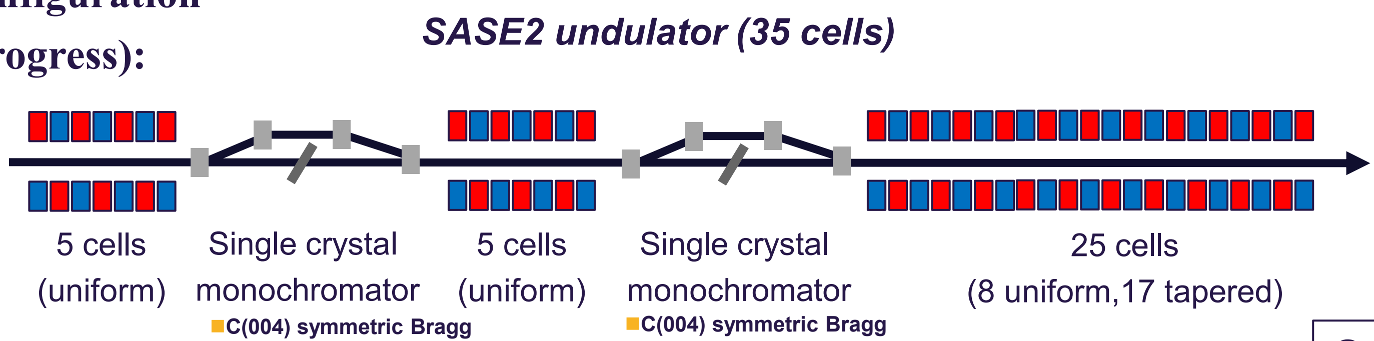
http://www.xfel.eu/documents/technical_documents/

Advisory and Review Team (ART):
G. Grübel, T. Salditt, G. Ruocco,
J. Hastings, H. F. Poulsen, I. Robinson

Seeding at SASE-2 from early on? YES!

- Self seeding concept (Geloni, Kocharyan, Saldin) using wake monochromators will be implemented at SASE-2
- Two seeding chicanes allow reducing the heat load on the diamond mono; high-rep rate operation within reach
- Commissioning of MID with SASE beam; seeding in a 2nd step but hopefully available from early on
- Chicanes also helpful for high harmonic lasing (>25 keV, future development…)

Possible configuration (work in progress):



G. Geloni et al.

Typical gain: factor 100 in spectral brightness due to seeding and tapering

I ~ 7×10^{12} ph/pulse in 10^{-4} BW @ 250 pC and 9 keV

Full specs (available from 2018)

- Full specification parameters

  8, 12.5, 14, or 17.5 GeV electron energy

  X-ray energy: **5 – 25 keV**, maybe higher (harmonic lasing)

  up to **10^{12} ph/pulse in pink SASE** beam (20-1000 pC)

  pulse duration: down to a few fs

  up to: **4.5 MHz** in a 600 µs train → 2700 pulses/train with 220 ns spacing

  10 trains/s → 27000 pulses/s (max)

  Self-seeding, pulse on demand, tapering, two-color

  Pink SASE beam (10^{-3} bw) or Si(220) or Si(111) monochromator

  Beamsize: **~1 – 100 µm, nanofocus** option

  Versatile **Optical laser** system, synchronized to X-rays, timing diagnostics

  X-ray **split delay line**, 0-800 ps delay ± 3 fs, 5-10 keV

  Possibility for **windowless** operation

  Standard sample environments, goniometer, scanner, SAXS/WAXS setup,

  Up to 8 m sample-detector distance at $2\theta = 55$ deg

Underground Experimental Hall

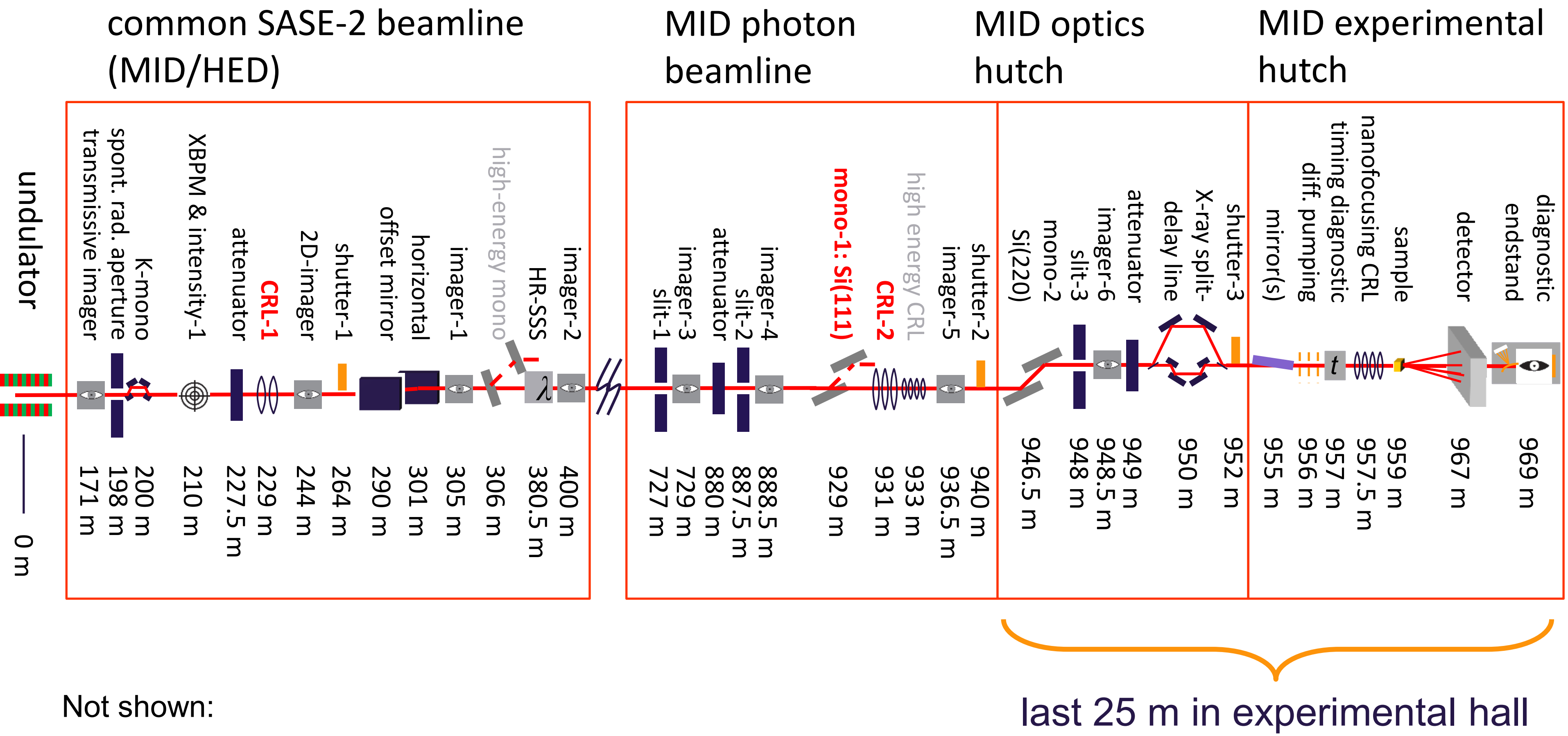
November 2011

MID Tunnel (SASE 2)


Aerial view of construction site,
Schenefeld, July 2014

Underground Experimental Hall

MID beamline overview



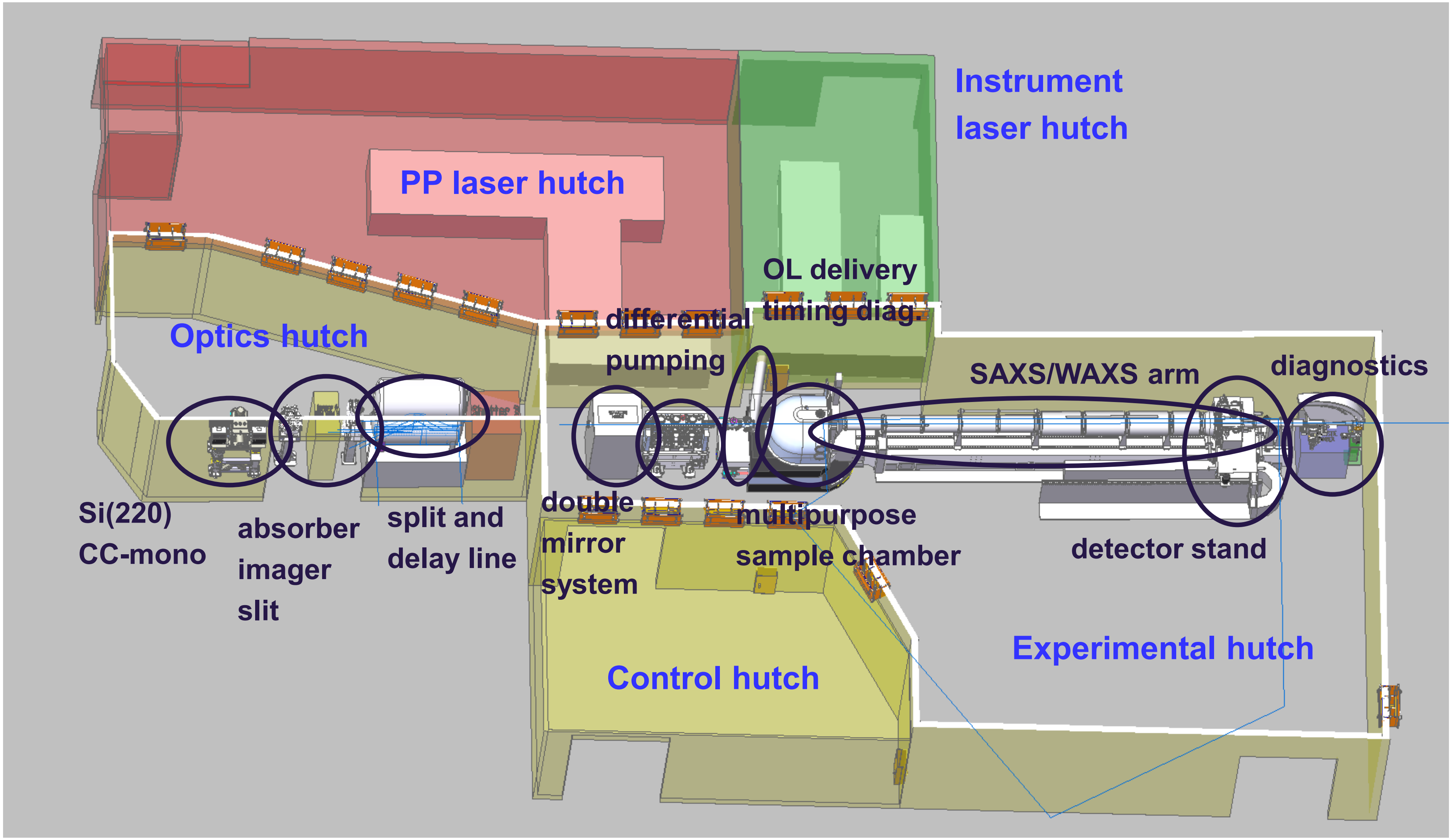
Not shown:

MCP at 303m (fine tuning of SASE)

Distribution mirror(s) at 390m and 395m (MID on central branch)

Beam loss monitors, PES

Schematic view of MID in exp. hall



European XFEL

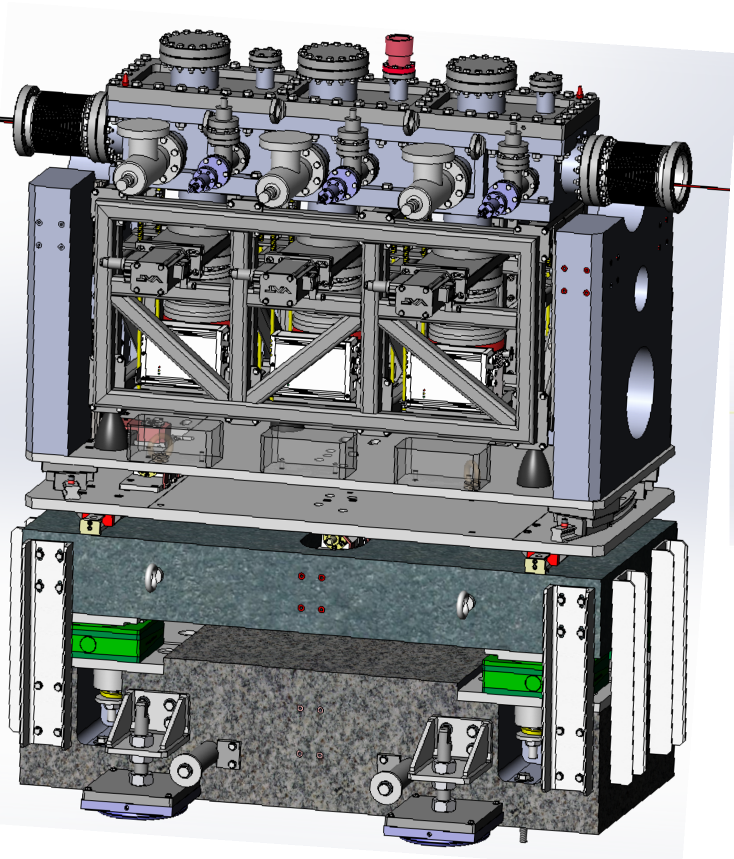
Design of MID components

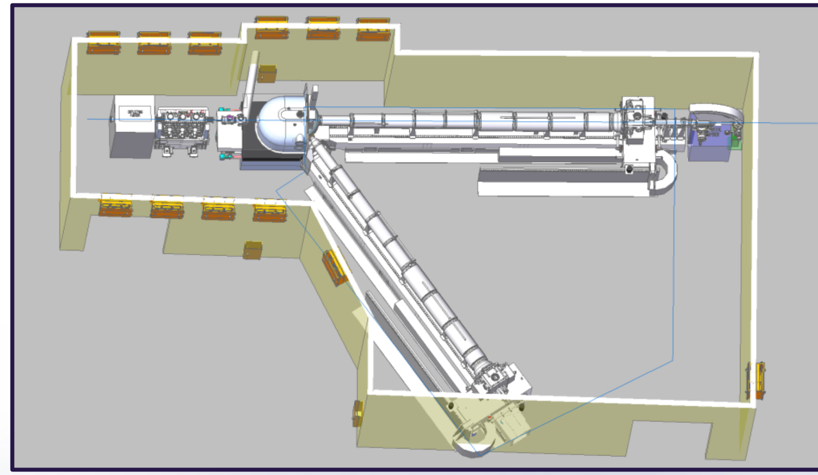
ESRF

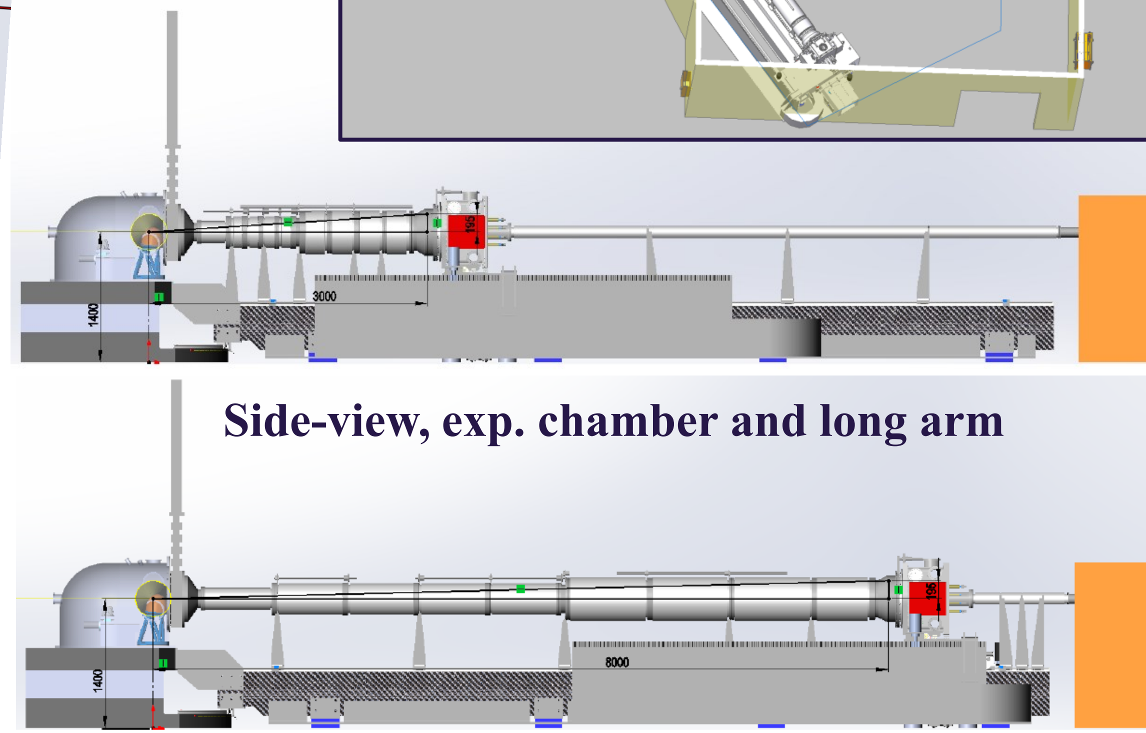
- Engineering collaboration with ESRF initiated in 2013
- Aim: co-designing together with MID team of
  - differential pumping
  - sample chamber
  - long, movable detector arm (SAXS, WAXS)
  - detector stand/detector integration

Design of MID components

Differential pumping section







Side-view, exp. chamber and long arm

Diff. pump section out for tender

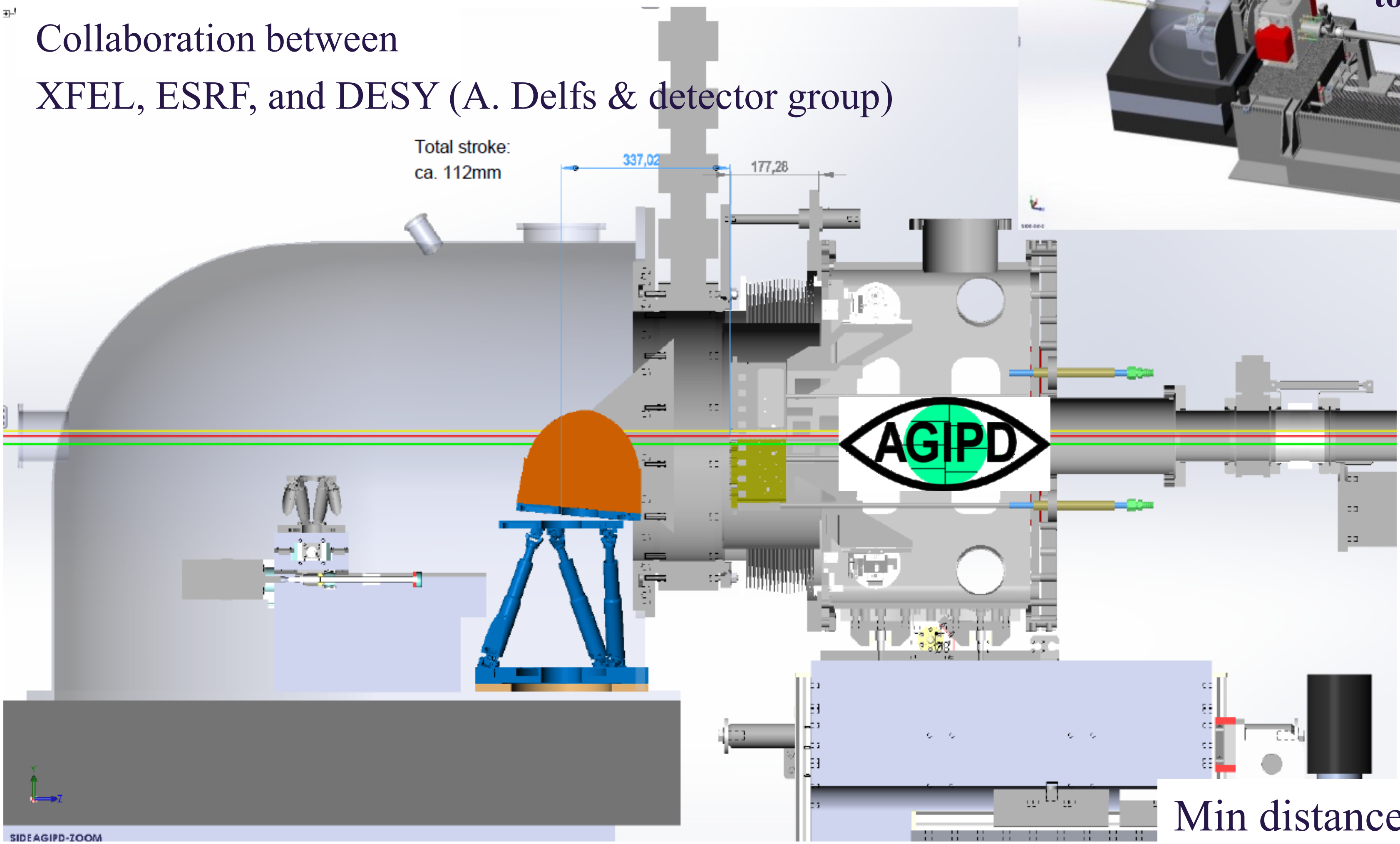
Finalize 3D models of chamber/arm/detector stand by summer 2015

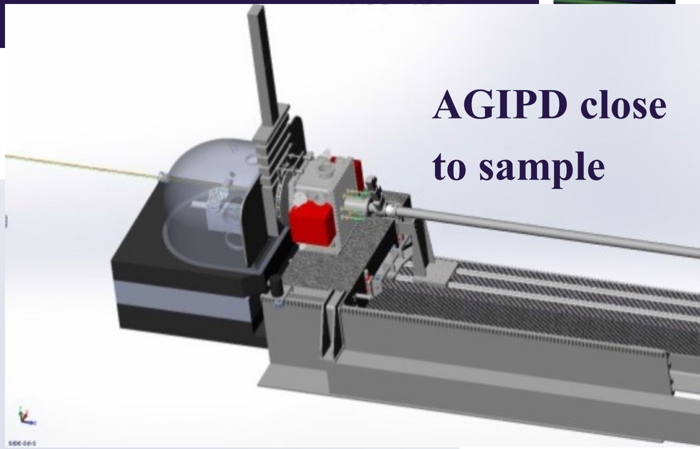
Design of MID components

Detector integration….

Collaboration between

XFEL, ESRF, and DESY (A. Delfs & detector group)





AGIPD close to sample

Min distance sample-detector: ~200 mm

Split-Delay Line (SDL)

Bundesministerium für Bildung und Forschung

FEL FSP-302

TU berlin

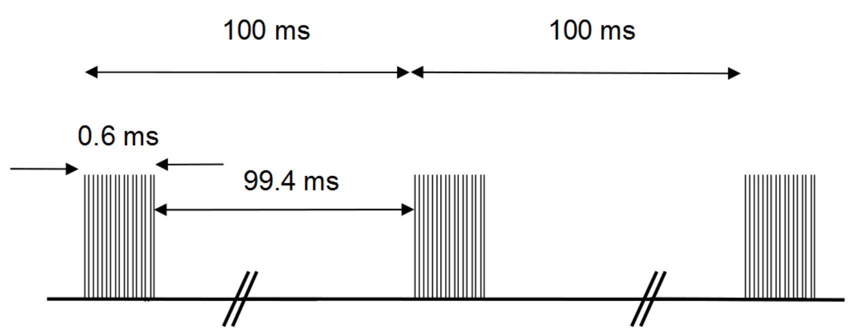
BMBF Verbundforschung Grant

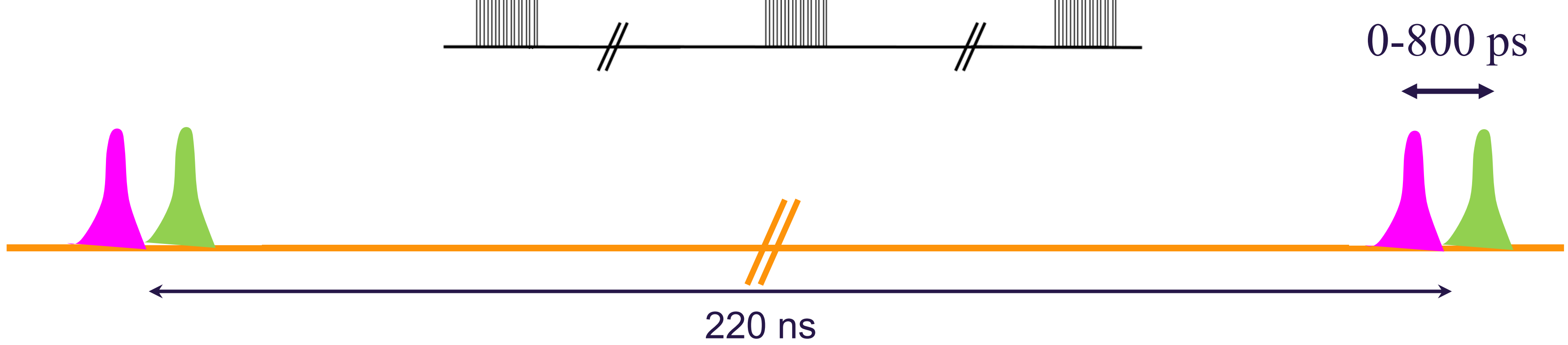
Collaboration TU-Berlin (Eisebitt) and XFEL (Madsen)

Construction cost + 2 year post doc position (W. Lu)

Aim of the SDL:

to enable modification of the photon pulse pattern (Δt < 220 ns)



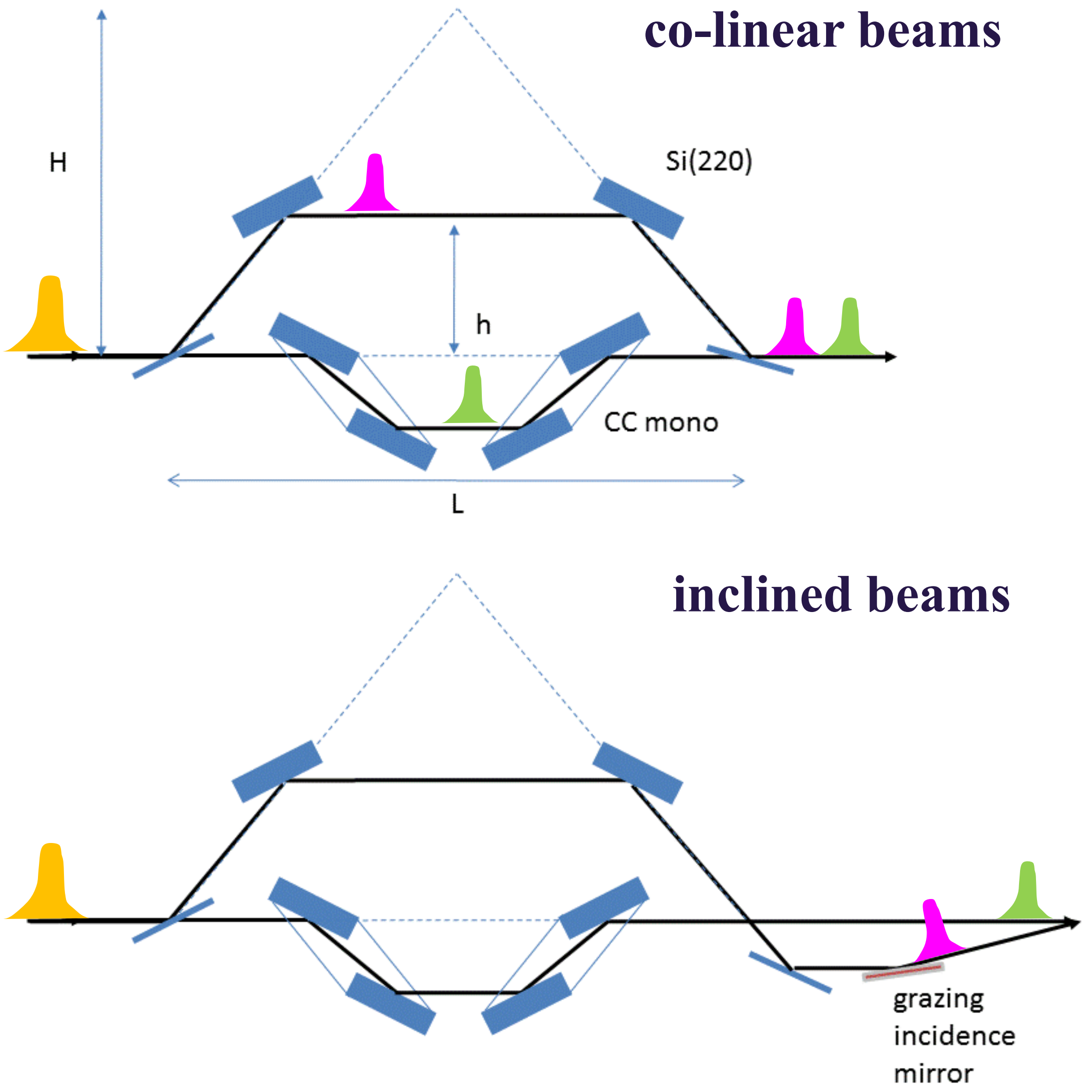


Hard X-Ray SDL Concept

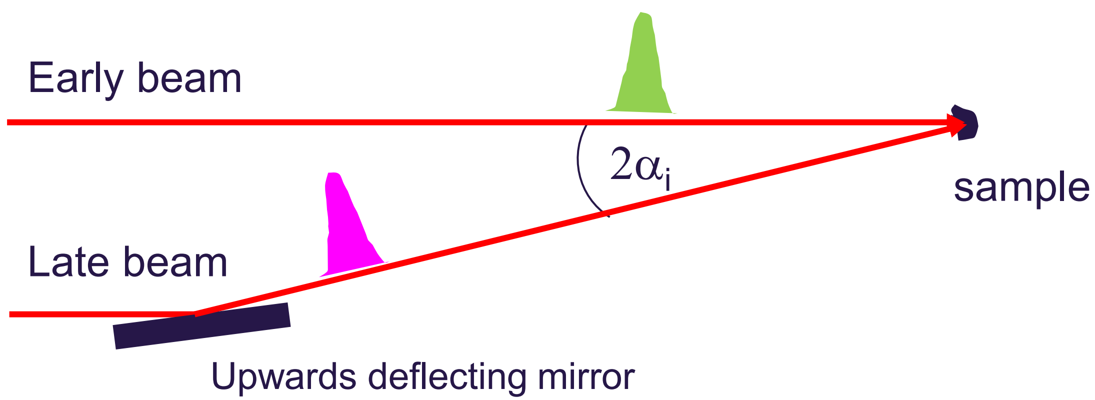
SDL at MID:

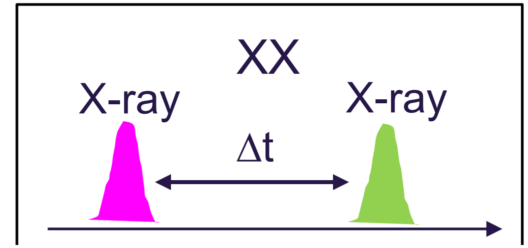
- 5 – 10 keV
- Few fs to 800 ps delay

Path length difference:
1µm → 3.3 fs



Inclined beams from split-delay line



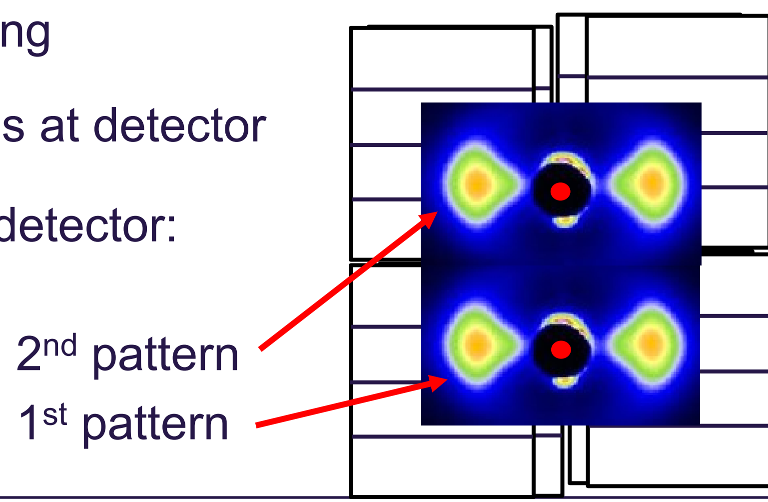


4 m mirror-sample distance, $2\alpha_i = 0.4$ deg

α_i even larger with coating

Separation of two beams at detector

Two images on AGIPD detector:



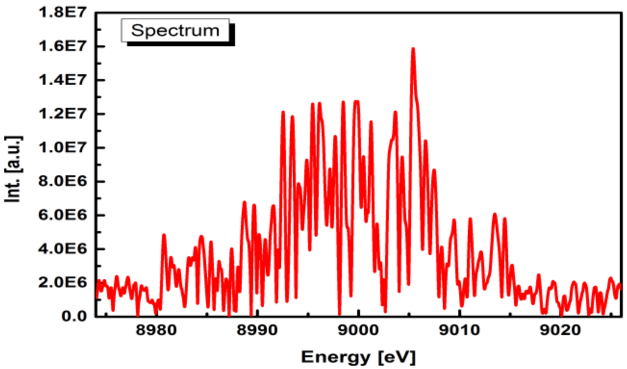
Split-Delay Line Simulations

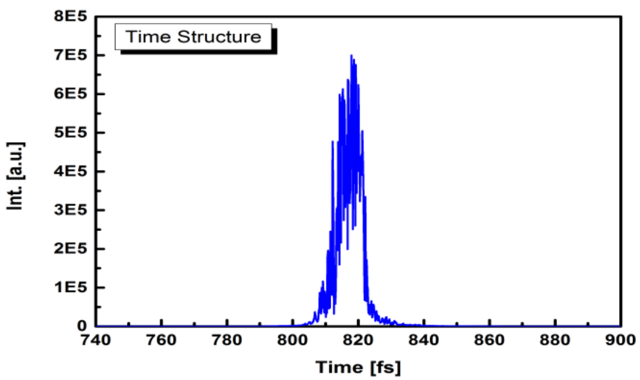
Bundesministerium für Bildung und Forschung

FEL FSP-302

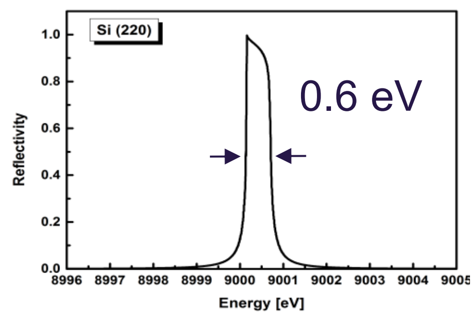
berlin

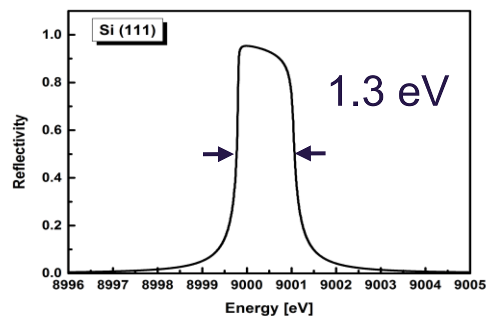
Input SASE pulse
9 keV, 20 fs



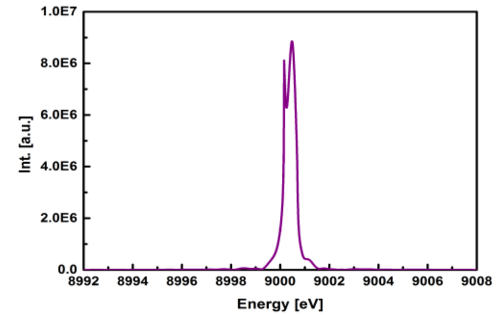


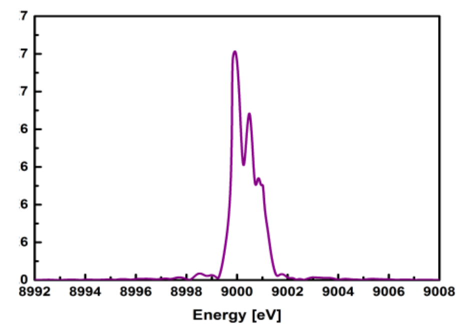
Pre-mono
Si(111) or (220)





Filtered input spectrum





Simulations: W. Lu, I. Agapov, G. Geloni

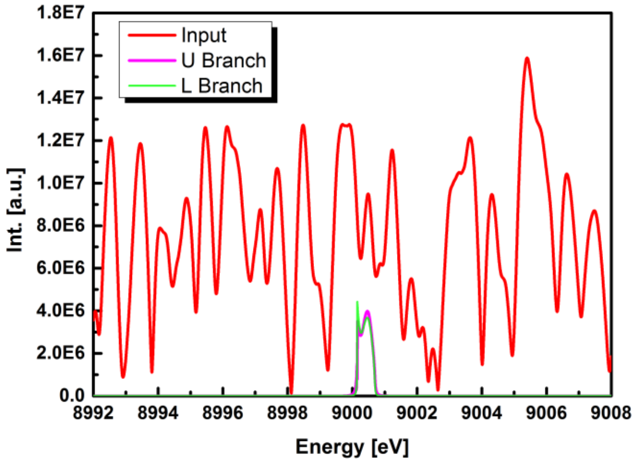
Split-Delay Line Simulations

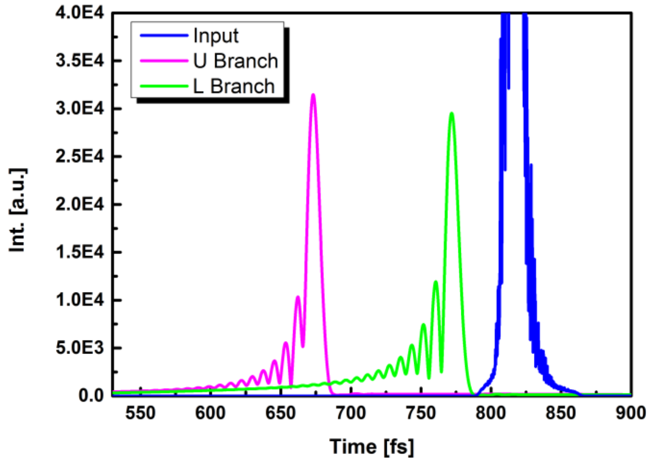
Bundesministerium für Bildung und Forschung

FSP-302

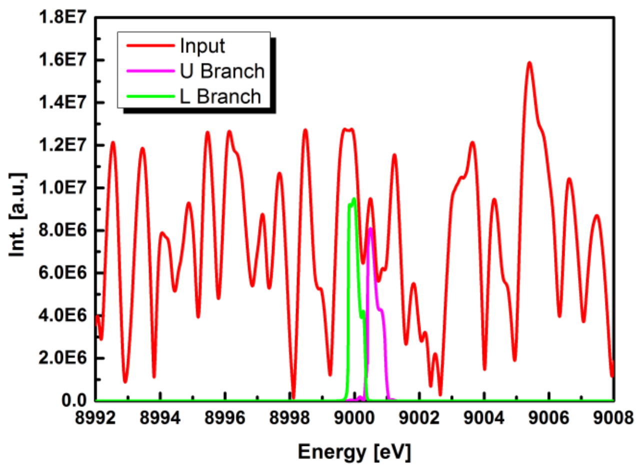
Spectrum output pulses

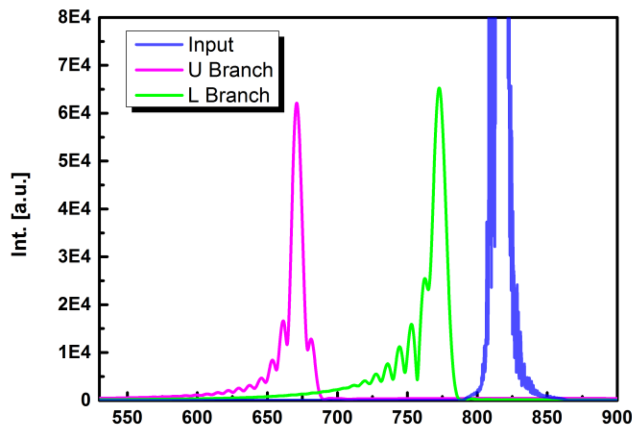
Time structure output pulses





Same energy:
Thin beam splitter
Low intensity (~1.1%)
Constant Int ratio



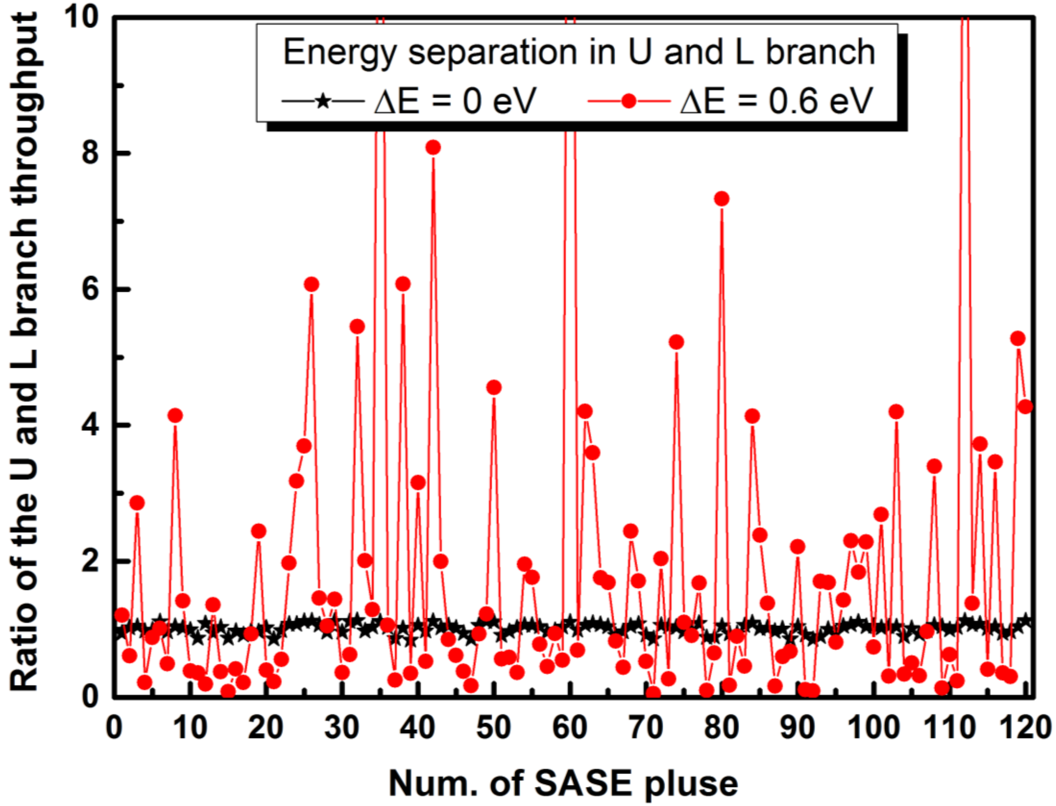


Small energy shift (0.6 eV):
3x thicker beam splitter
Higher intensity (~3.5%)
Fluctuating Int ratio

Simulations: W. Lu, I. Agapov, G. Geloni

Split-Delay Line Simulations

Bundesministerium für Bildung und Forschung

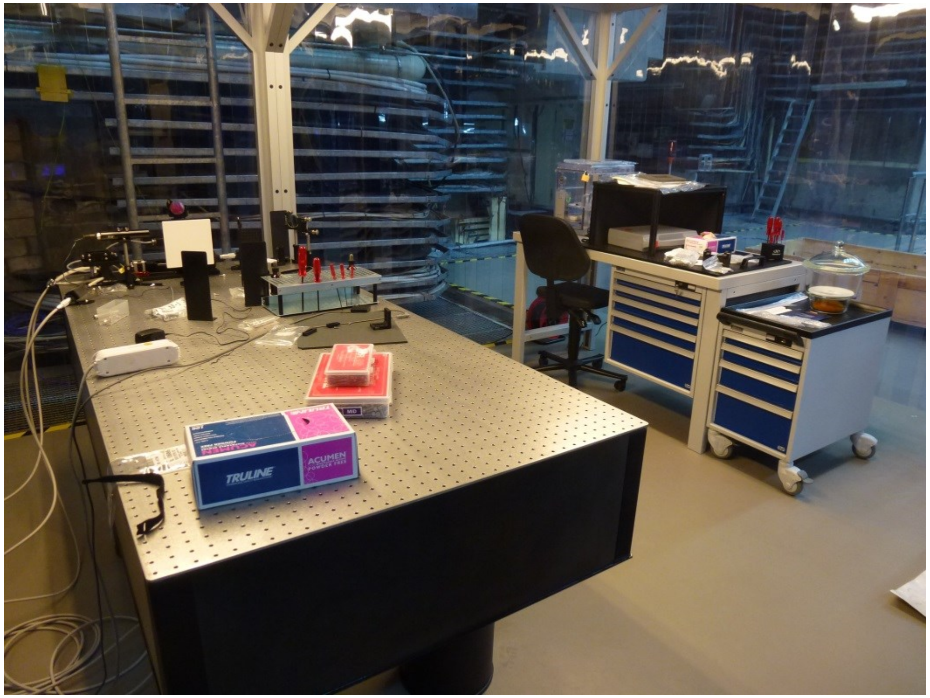


Simulation work will continue to address the throughput and intensity jitter in the self-seeded case

Simulations: W. Lu, I. Agapov, G. Geloni

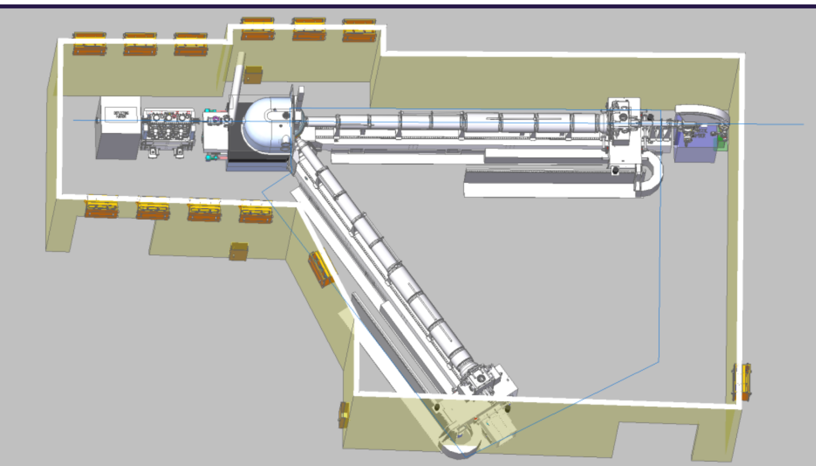
MID Laboratory for Technical Commissioning

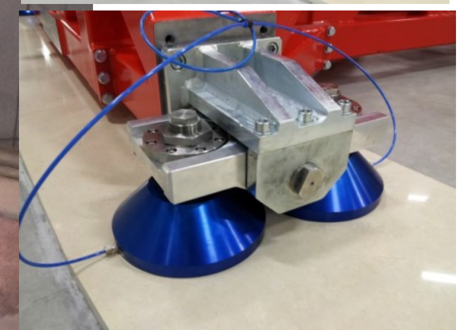
Hera South Lab



MID construction in Experimental hall

8 cm deep recess in concrete floor to prepare for high-quality polished granite floor





New RIXS instrument at ESRF

Work starts 1 March, by G. Pilloni (20 years experience from ESRF/ILL with such floors)

Suggested Beam Parameters for 1st Lasing and Commissioning

- Start-up beam parameters

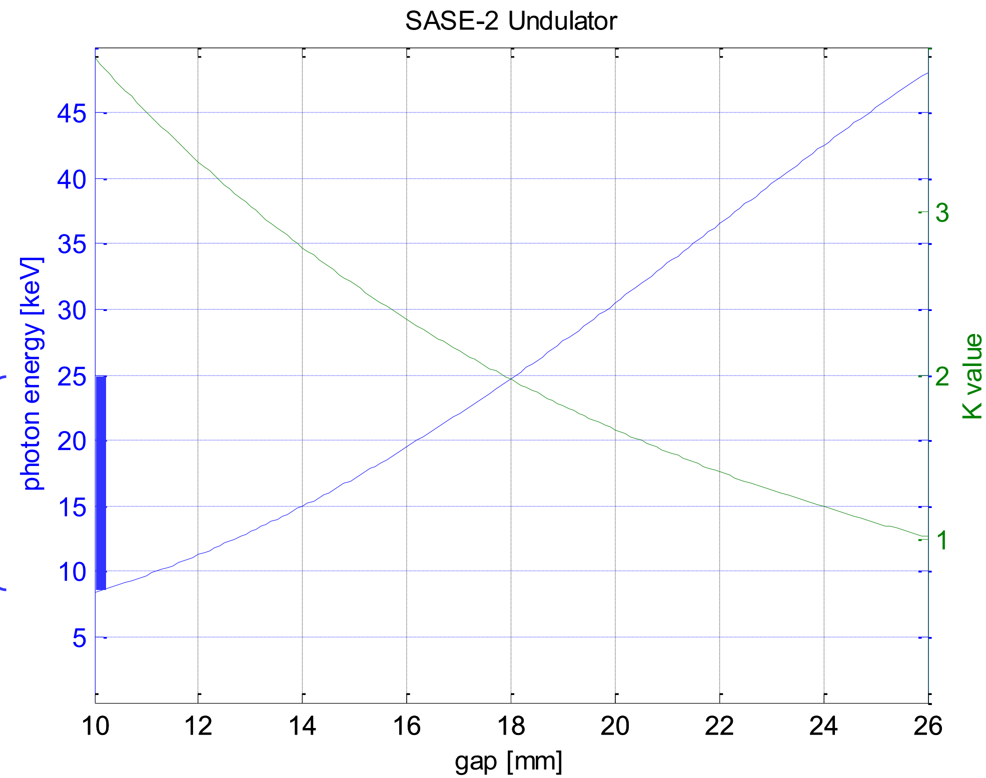
  17.5 GeV electron energy, 40 mm magnetic period

  X-ray energy: 8.3 keV (10 mm gap)

  maybe advantageous to start at 14 mm gap → ~15 keV

E_{max}: ~25 keV (defined by gain length)

E_{min}: ~8.3 keV



K value vs gap courtesy of J. Pflüger et al.

Suggested Beam Parameters for 1st Lasing and Commissioning

- Start-up beam parameters

    17.5 GeV electron energy, 40 mm magnetic period
    X-ray energy: 8.3 keV (10 mm gap)
    maybe advantageous to start at 14 mm gap → ~15 keV

    SASE, 500 pC bunch charge → $\sim 10^{12}$ ph/pulse
    pulse duration ~ 40 fs
    100 kHz in a 600 µs train → 60 pulses/train with 10 µs spacing

    Beamsize: ~1 – 100 µm, Pink SASE beam (10^{-3} bw)

    First lasing by SASE-2 undulator: April 2017
    First experiments at MID: Aug 2017
    Full TDR performance (machine and instrument): 2018

Commissioning phase. Rough outline

- 14 weeks counted from 1st lasing (15 Apr – 1 Aug, 2017)
- Expected 2 weeks of beamtime (max) during that period
- Preferably delivered in 12h shifts i.e. maximum 28 shifts for commissioning
- 1st goal: Commissioning of essential beam transport, diagnostics, instrument components, detectors, DAQ and control systems,…
- 2nd goal: Characterization of beam parameters: spectrum, intensity, coherence, stability,…
- 3rd goal: 1 or 2 demonstration-type experiments

From Commissioning to User Operation (Early Science, in progress…)

- Commissioning of MID ends in Aug 2017
- ~1000/3 h (max) user operation of SASE-2 in 2017
- MID and HED need to share the beam time available at SASE-2
- Establish **Early Science Program** for remainder of 2017
  - 1000/6 = 167 h = 14 shifts (2-3 experiments)
  - Addressed in a call for Early Science proposals
  - Interested groups competing for beamtime OR we organize in a few larger collaborations to conduct first experiments
  - Hopefully this WS will trigger some discussions...
- **Early Science** likely to continue into 2018

Early Science parameters, from Aug 2017

- Early science parameters (guesstimate):

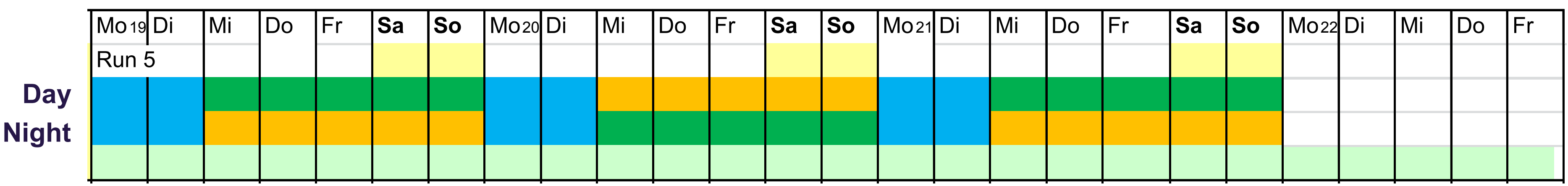
  X-ray energy ~**8.3 - 15 keV**,
  up to **10^{12} ph/pulse** in pink beam
  pulse duration: down to a few fs
  min. **100 kHz** in a 600 µs train → **60 pulses/train with 10 µs spacing**
  10 trains/s

  Beamsize: ~1 – 100 µm, maybe nanofocus option
  Pink SASE beam (10^{-3} bw) or Si(220)/Si(111) monochromator
  Possibility for windowless operation
  Standard sample environments, goniometer, scanner, SAXS/WAXS setup
  AGIPD detector
  Up to 8m sample-detector distance at 2θ=55deg
  Down to ~20 cm sample-detector distance, less maybe possible
  Optical laser system, 800 nm, not fully commissioned…

Steady State Operation Plans (full specs, from 2018)

Concept

- Beamtime proposals, peer-review, 2 allocation rounds/year (?)
- Typical 5 day slots; separated by machine maintenance day(s)
- Split day in two 12 hrs shifts, e.g. 10 am – 10 pm
- 12 h instr. operation and 12 h data analysis and/or minor exp. changes
- Change of setup on machine days only (e.g. Mon-Tue)
- Major modifications/installations during shutdown weeks



Example of 4 weeks at SASE-2:

Day shift (12 hrs; e.g. 10-22 hrs)
Night shift (12 hrs; e.g. 22-10 hrs)

- HED
- MID

Courtesy of W. Decking and T. Tschentscher

Steady State Operation Plans (full specs, from 2018)

- Annual operation of the facility

  4800 hrs accelerator operation for generation of x-rays
  - ➔ Peer-reviewed proposals [4000 hrs]
  - ➔ Internal activities [800 hrs]
    - Maintenance
    - R&D program & management contingency

- Total amount of user experiments
  - **12000 hrs** user time by operation of three instruments in parallel
  - ~200 user experiments / year (5 day slots)
  - **~33 user experiments**/year per instrument

Courtesy of W. Decking and T. Tschentscher