Status of the European XFEL and plans for a SQS instrument

European XFEL User Workshop,
University Aarhus, Oct 29-31, 2008

Thomas Tschentscher
European XFEL Project Team, Hamburg, Germany

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This workshop

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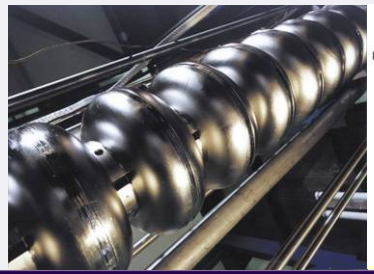
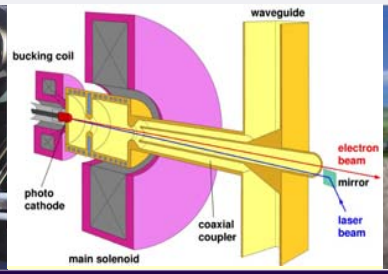
Project overview *European XFEL*

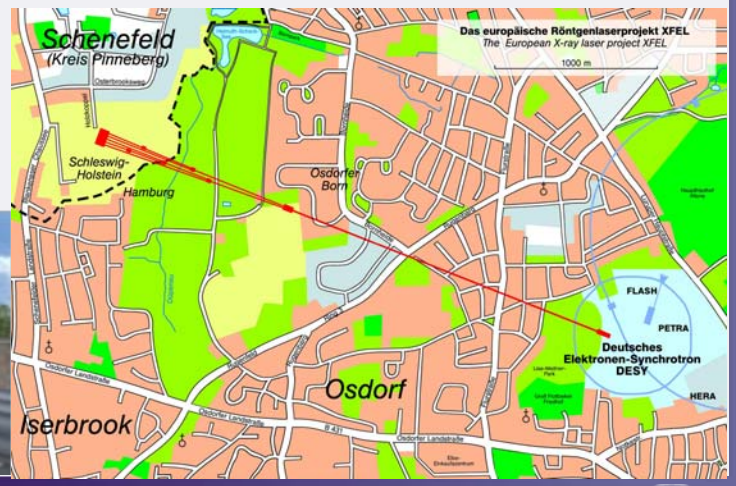
X-ray free-electron laser user facility with a 20 GeV super-conducting linear accelerator.

- Low emittance electron beams for SASE FEL process
- Several FEL undulators covering wide range of x-ray parameters
- Dedicated instruments for wide range of scientific applications

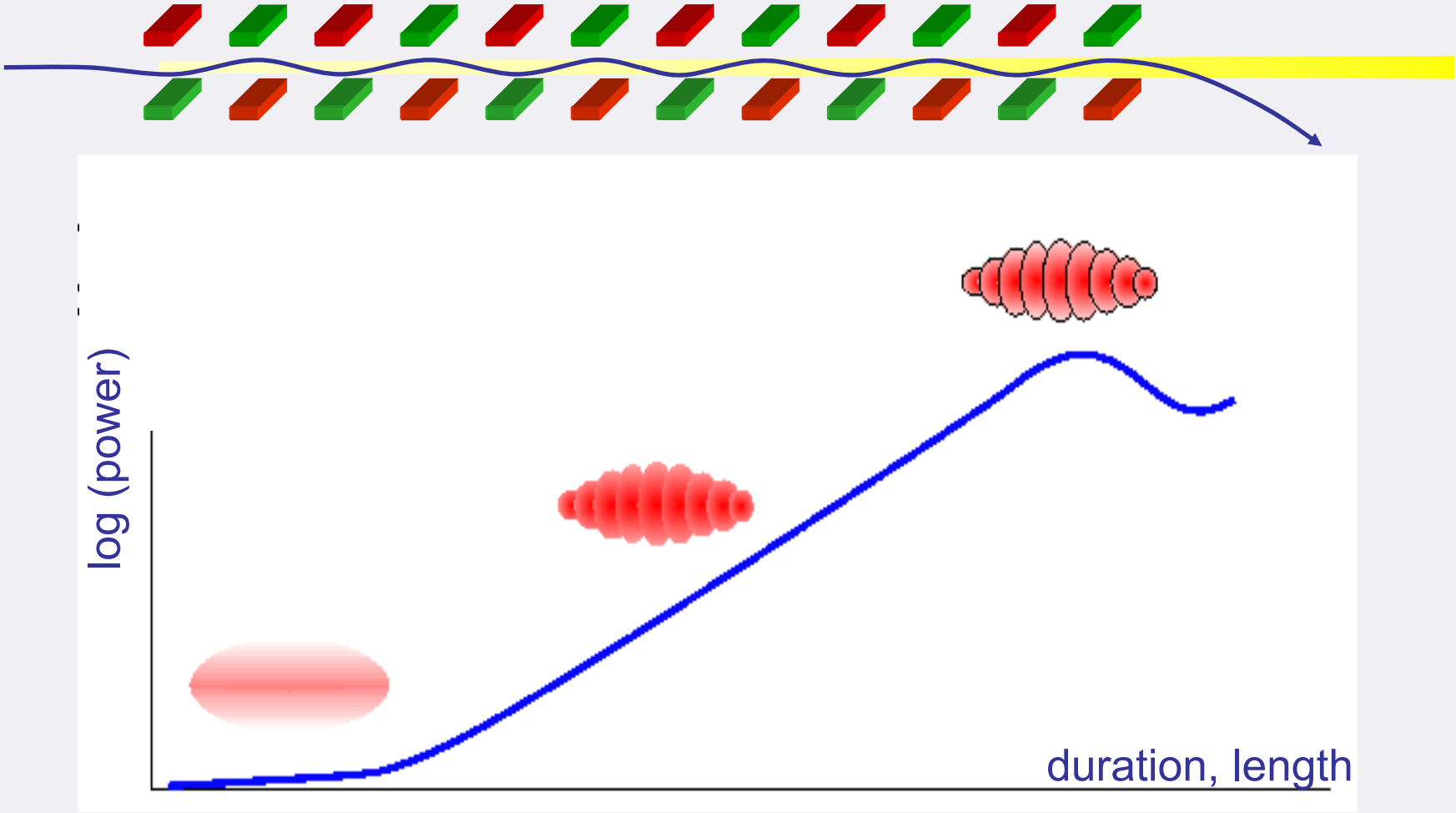
- Construction cost 986 M€
- First beam: 2013
- Full operation: 2015







Self-Amplified Spontaneous Emission (SASE)



Super-conducting accelerator

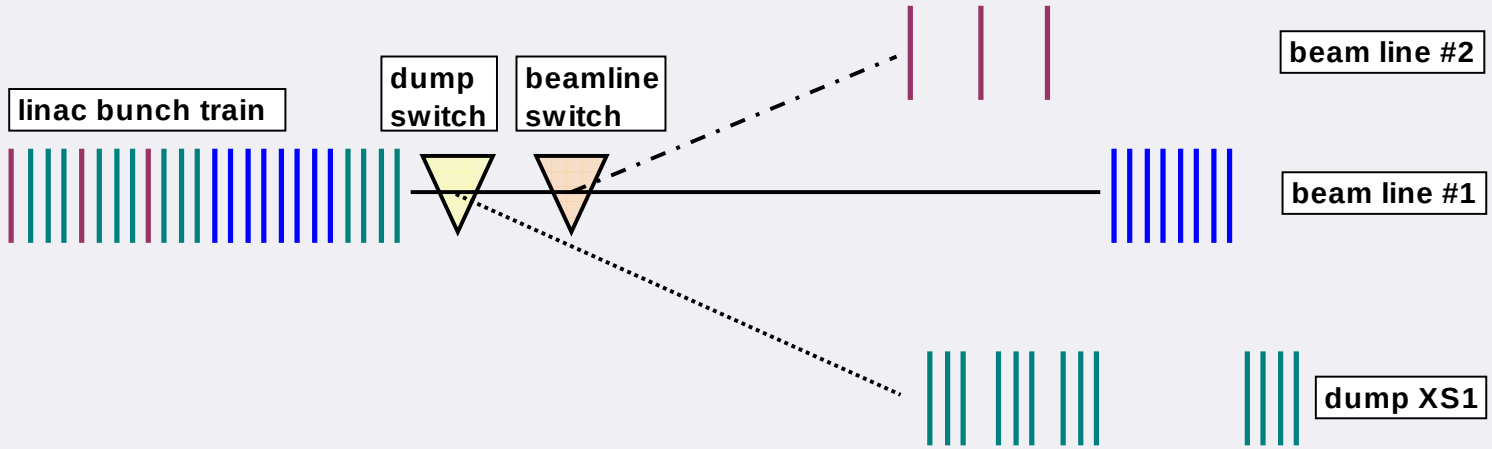
Superior qualities

- large cavity iris

  ⇒**reduced wakefields => smaller energy chirp**

- high stability due to intra-bunch feedback
- high flexibility of operation for simultaneous user experiments
- large number of delivered FEL pulses

  ⇒**Combination of peak & average brilliance**



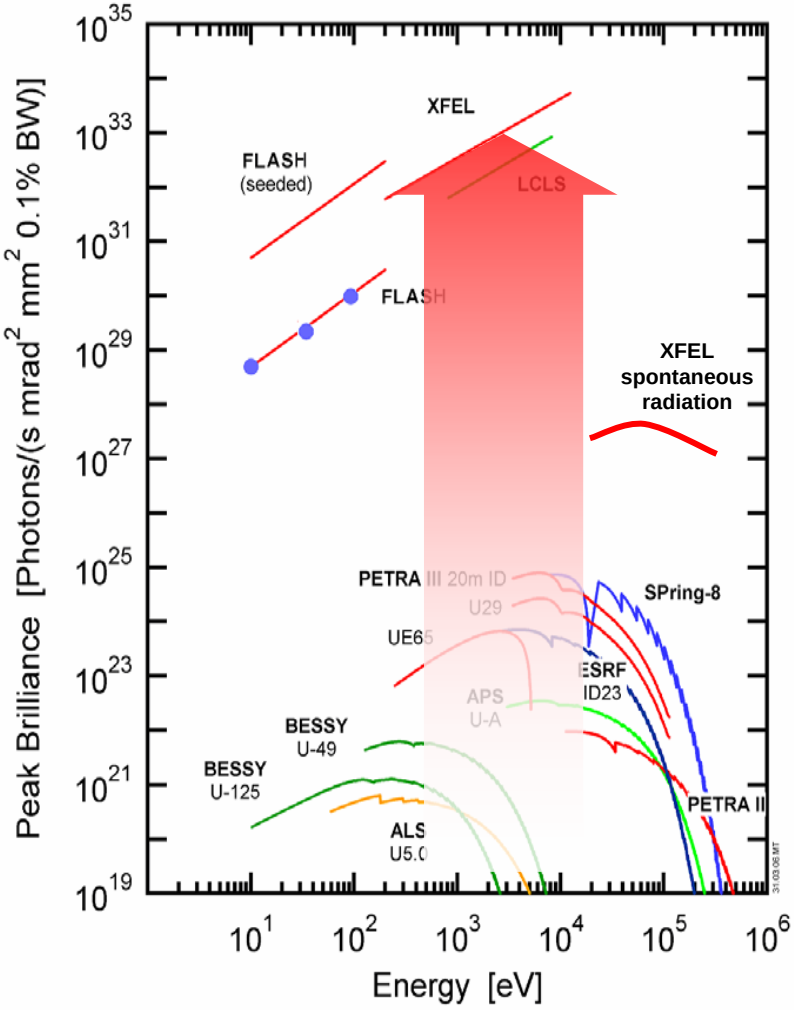
Properties of XFEL radiation

in the X-ray range (0.5-14 keV)

- pulse duration 100 fs
- pulse intensities 10^{12}-10^{14}
- diffraction limited
- degeneracy 10^{9}-10^{12}
- peak brilliance 10^{32}-10^{33}

Peak brilliance

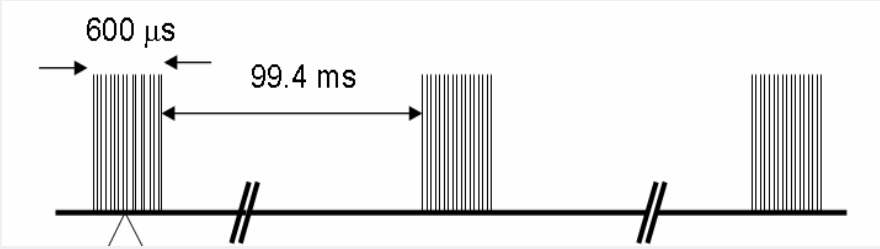
$$PB = \frac{Number\ of\ photons}{\Delta_x \Delta_{x'} \Delta_y \Delta_{y'} \times bandwidth \times \Delta_t}$$



High average brilliance

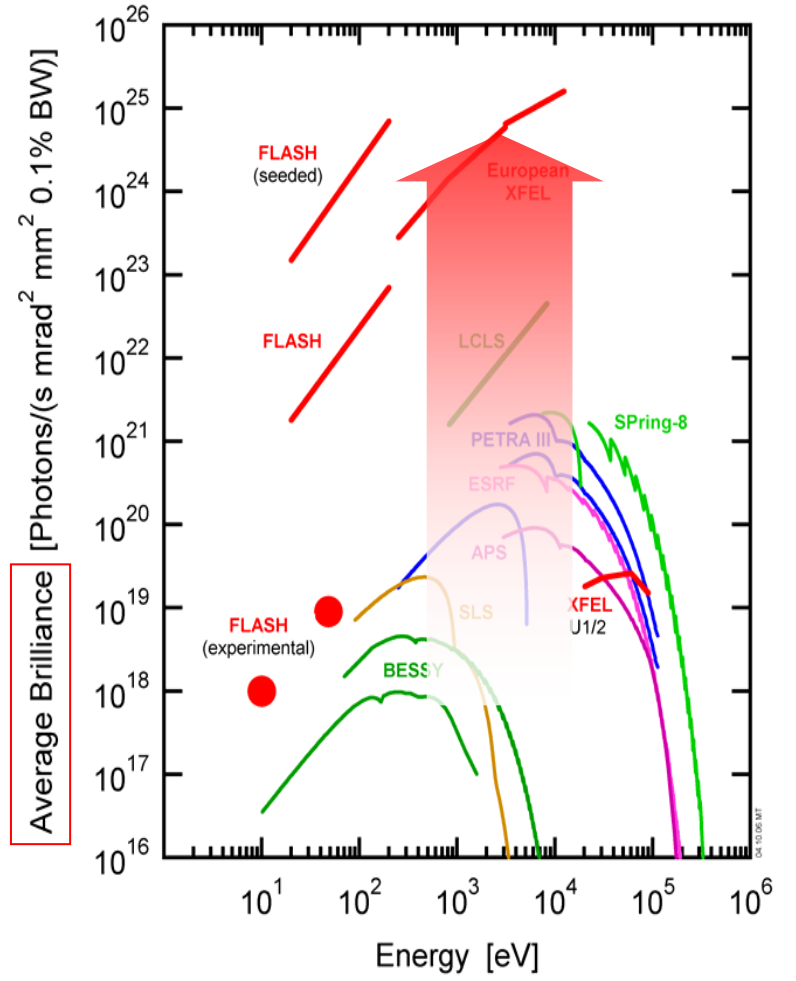
High repetition rates

- up to 30.000 pulses/s
- pulse train mode



Average brilliance

$$B = \frac{Number\ of\ \ photons}{\Delta_x \Delta_{x'} \Delta_y \Delta_{y'} \times bandwidth \times s}$$



Building the European XFEL as a User Facility

- intense interaction in preparation of TDRs in 2001 & 2006

European XFEL users' meetings

- last week of Jan in Hamburg – 2007, 2008, 2009, …

European XFEL instrumentation workshops

- SQS – Aarhus, Oct 29-31, 2008
- SPB – Uppsala, Nov 20-22, 2008
- …2009 …

Startup scenario

Limit design electron energy to 17.5 GeV

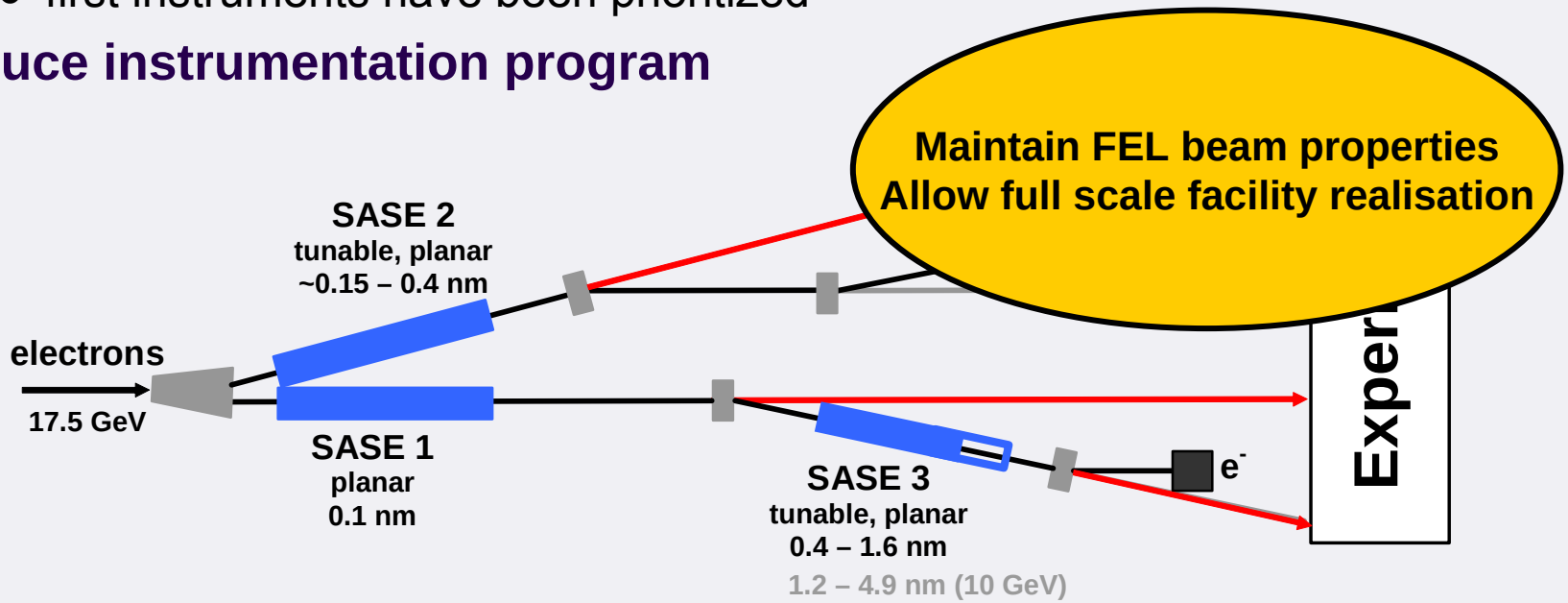
Provide SASE FEL radiation 0.1 – 1.6 nm

- maintain SASE radiators with slight modifications

Reduce number of scientific instruments to six

- first instruments have been prioritized

Reduce instrumentation program



Characteristics of initial sources

SASE 1 **as described in TDR (2006)**

- designed for reaching saturation at **12.4 keV** (closed gap)

SASE 2 **shortened by 5 undulator segments**

- designed for tunability range ~4 (**3.1 – 12.4 keV**)
- magnetic length now 185 m
- saturation length (12.4 keV, 19 mm gap) ~174 m

SASE 3 **planar device for linear polarization**

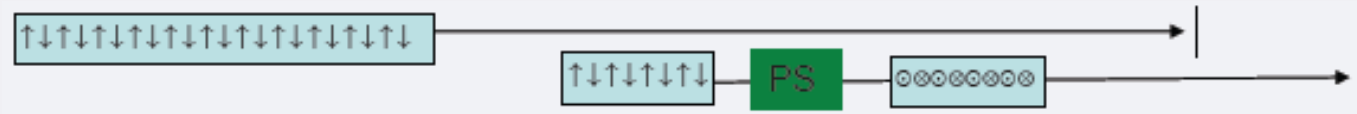
- designed for tunability range ~4
  - ⇒ 0.775 – 3.1 keV @ 17.5 GeV
  - ⇒ 0.250 – 1.0 keV @ 10 GeV
- 'conventional device'
  - ⇒ **higher reliability for commissioning & operation**
- magnetic length 105 m, saturation (3.1 keV, 19 mm) ~88 m
- R&D on possible upgrade scenarios has started

Possible paths towards variable polarization

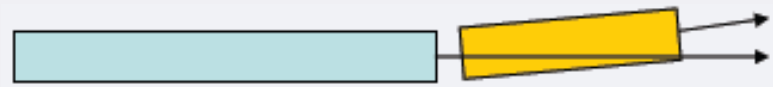
Several scenarios

(E.L. Saldin, E.A. Schneidmiller, M. Yurkhov, B. Faatz, …)

- **planar undulator followed by 2 crossed planar undulators**



- **planar undulator followed by helical (APPLE-type) undulator**



- **frequency doubler**

- **to be investigated: output intensity, polarization degree, electron trajectory and dynamics, separation & diagnostics of FEL beams**

Selection of first instruments

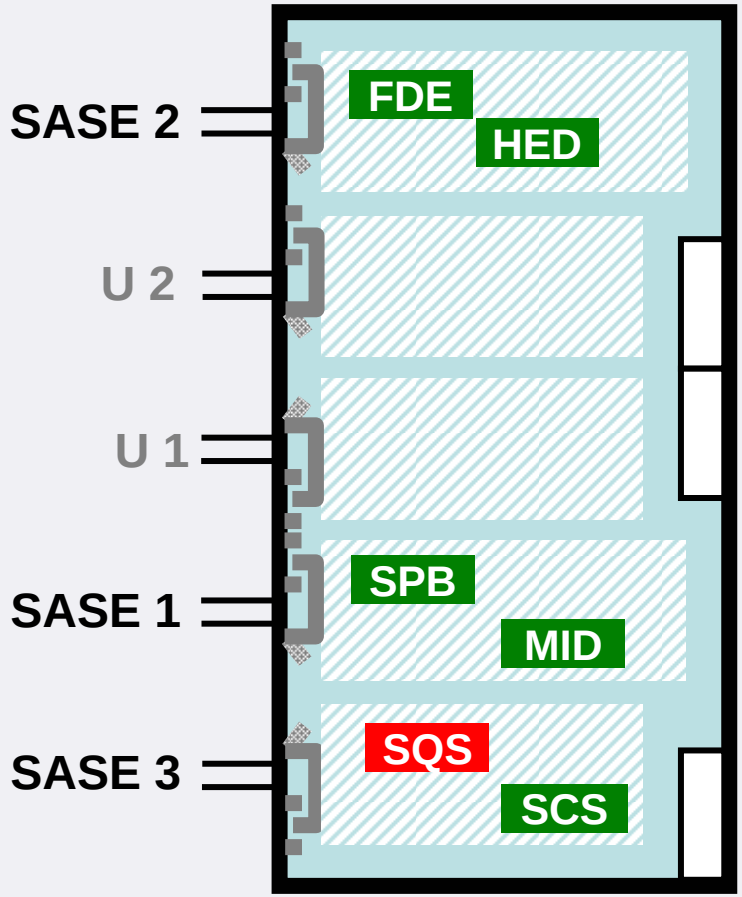
Hard X-rays

Soft X-rays

Instrument	Brief description of the instrument
SPB	**Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules** – Structure determination of single particles: atomic clusters, bio-molecules, virus particles, cells.
MID	**Materials Imaging & Dynamics** –Structure determination of nano-devices and dynamics at the nanoscale.
FDE	**Femtosecond Diffraction Experiments** – Time-resolved investigations of the dynamics of solids, liquids, gases
HED	**High Energy Density Matter** – Investigation of matter under extreme conditions using hard x-ray FEL radiation, e.g. probing dense plasmas.
SQS	**Small Quantum Systems** – Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena.
SCS	**Soft x-ray Coherent Scattering** –Structure and dynamics of nano-systems and of non-reproducible biological objects using soft X-rays.

Distribution of first instruments

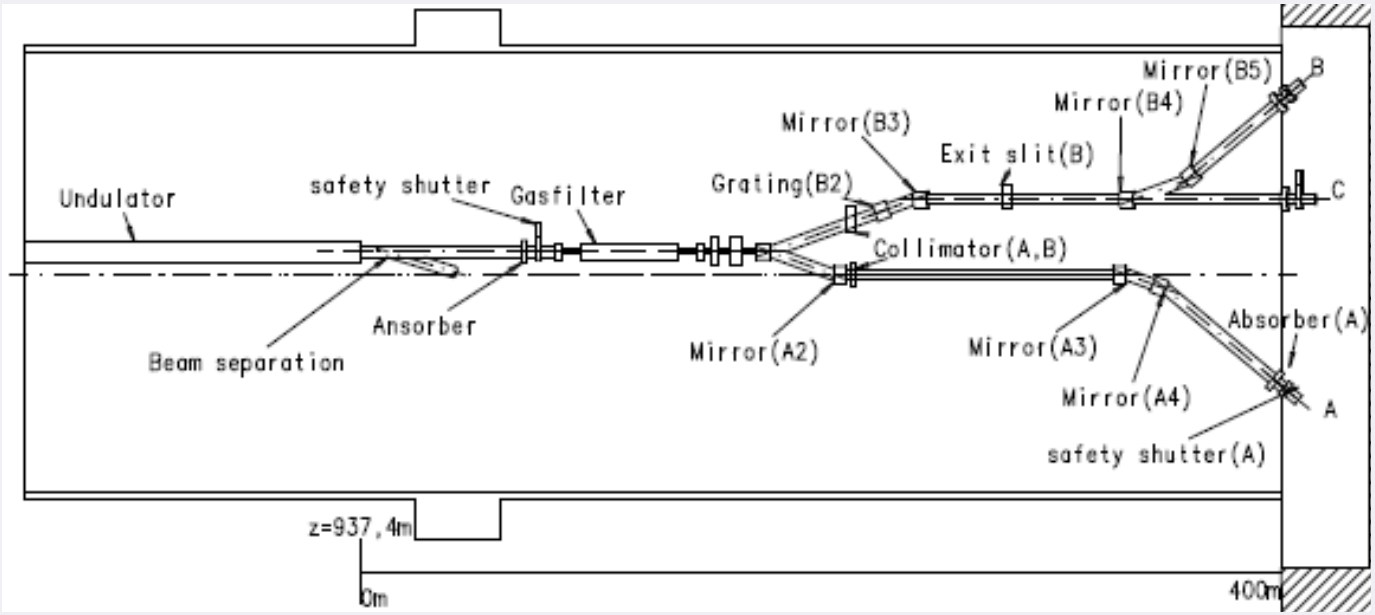
Source	Photon beam line characeristics
SASE 1	FEL radiation ~12 keV High coherence Spontaneous radiation (3rd, 5th harmonics)
SASE 2	FEL radiation 3-12 keV High time-resolution Spontaneous radiation (3rd, 5th harmonics)
SASE 3	FEL radiation 0.25 – 3 keV; High flux
	FEL radiation 0.25 – 3 keV; High resolution



TDR 2006 - SASE 3 photon beamline

Photon beamline

 # preservation of coherence (wavefront)
 # full bandwith & monochromatization
 # two separate beam transports



TDR 2006 - Small Quantum Systems

Scientific aims

- Investigation of atomic, ionic, molecular or cluster samples
- Linear processes
  - ⇒ **Inner-shell ionization in atomic ions**
    - **Astrophysical processes (x-ray absorption in interstellar clouds)**
    - **Probing atomic structure models at highest resolution using selective photon excitation of highly charged ions (Lamb-shift corrections, Zeeman spectroscopy)**
  - ⇒ **Scattering from ionic crystals captured in traps (dynamics after x-ray energy deposition; strongly-coupled plasma physics)**
  - ⇒ **Fragmentation processes of molecules of astrophysical interest**
  - ⇒ **Cluster studies**
    - **Atom-solid transition by spectroscopic studies with mass-selected clusters**
    - **Microscopic processed of x-ray energy deposition in matter**
- Non-linear processes
  - ⇒ **Multiphoton studies in the x-ray spectral region**
    - **Two-photon ionization processes and their applications**
    - **Two-colour experiments: *Dressed* atoms and *above-threshold ionization* measurements**
  - ⇒ **Dynamics of small molecules**
    - **Molecular wave packet dynamics**
    - **Investigation of laser-aligned molecules**
  - ⇒ **Time-resolved photo-fragmentation of small molecules**

TDR 2006 - Small Quantum Systems

Requirements

- ultra-dilute samples
- tunable soft x-ray FEL radiation
- spectroscopy: small bandwidth
- non-linear proc.: high intensity

X-ray beam requirements

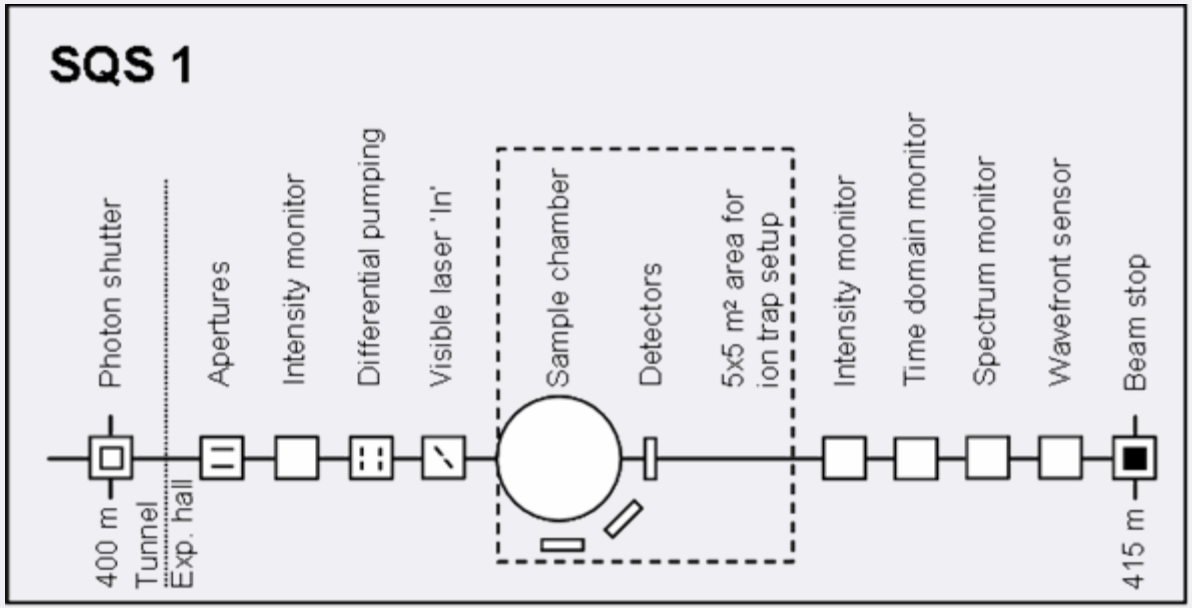
- photon energy
  - ⇒ **0.25 – 4.1 keV**
  - ⇒ **bw 10^{-3}-10^{-2} (high intensity)**
  - ⇒ **bw <10^{-5}-10^{-4} (spectroscopy)**
- beam size
  - ⇒ **1-100 µm**
- time domain
  - ⇒ **high rep. rate with Δt >10 µs**
  - ⇒ **< 30 fs pulse for non-linear exp.**
  - ⇒ **10 fs synchronisation**

Instrumentation

- photon diagnostics
  - ⇒**photon flux, spectral distribution, temporal dist., focus distribution, polarisation, synchronisation**
- sample manipulation & environment
  - ⇒**UHV conditions**
  - ⇒**gaseous and ion beams**
  - ⇒**confined volume (traps)**
  - ⇒**ion beam storage ring beyond scope of instrumentation ?**
- detector requirements
  - ⇒**particle detectors**
    - ⇒**space-, energy-, time-resolved**
  - ⇒**x-ray emission/fluorescence**
- optical laser
  - ⇒**tunable (0.2-12 µm)**
  - ⇒**few mJ pulse energy**

TDR 2006 - Small Quantum Systems

SQS using monochromatized FEL radiation



Monochromatic beam
- 10^{-4} bw

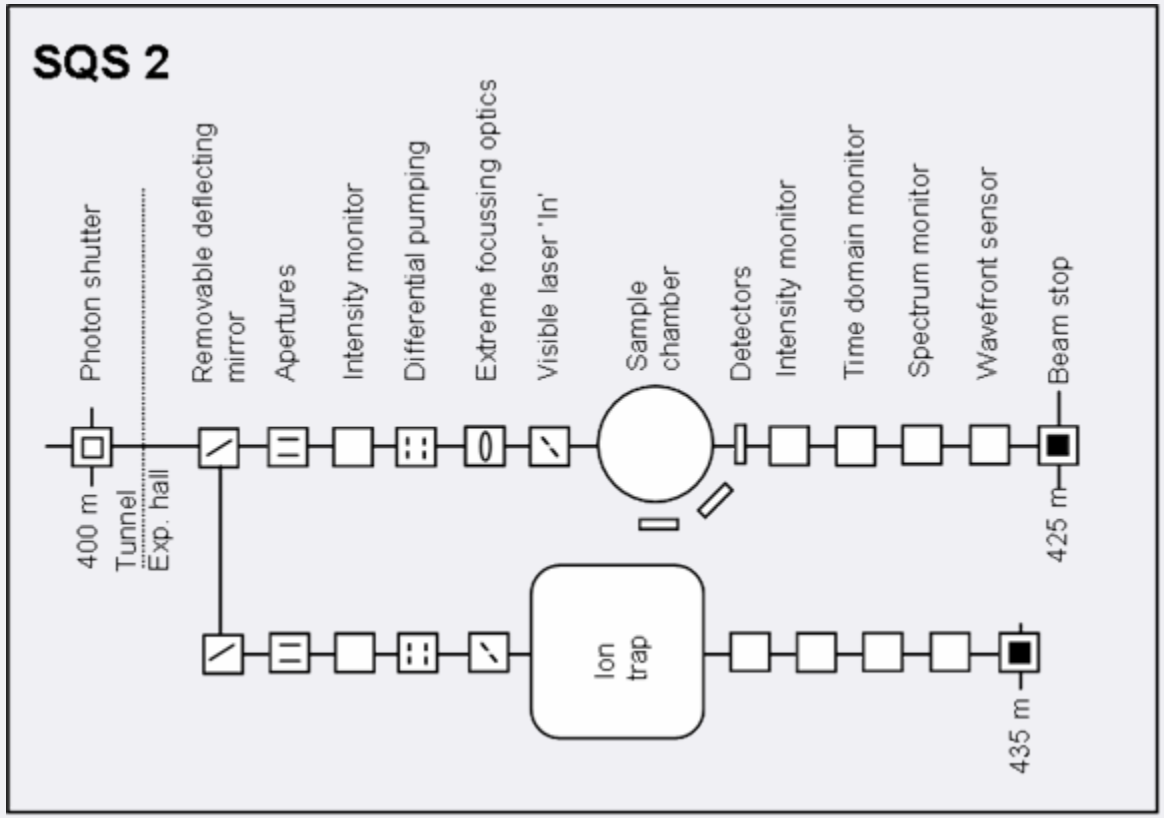
Refocusing mono. exit slit
- 5-100 µm spots

UHV vacuum chamber or ion trap setup
Optical laser
- frequency mult.
- OPA system

Photon diagnostics
- single-pulse
- on-line

TDR 2006 - Small Quantum Systems

SQS using natural monochromatization



Nat. monochromaticity
- **10^{-2}-10^{-3} bw**

2 branches for different focusing options
- **~1 µm spot**
- **100 µm spot**

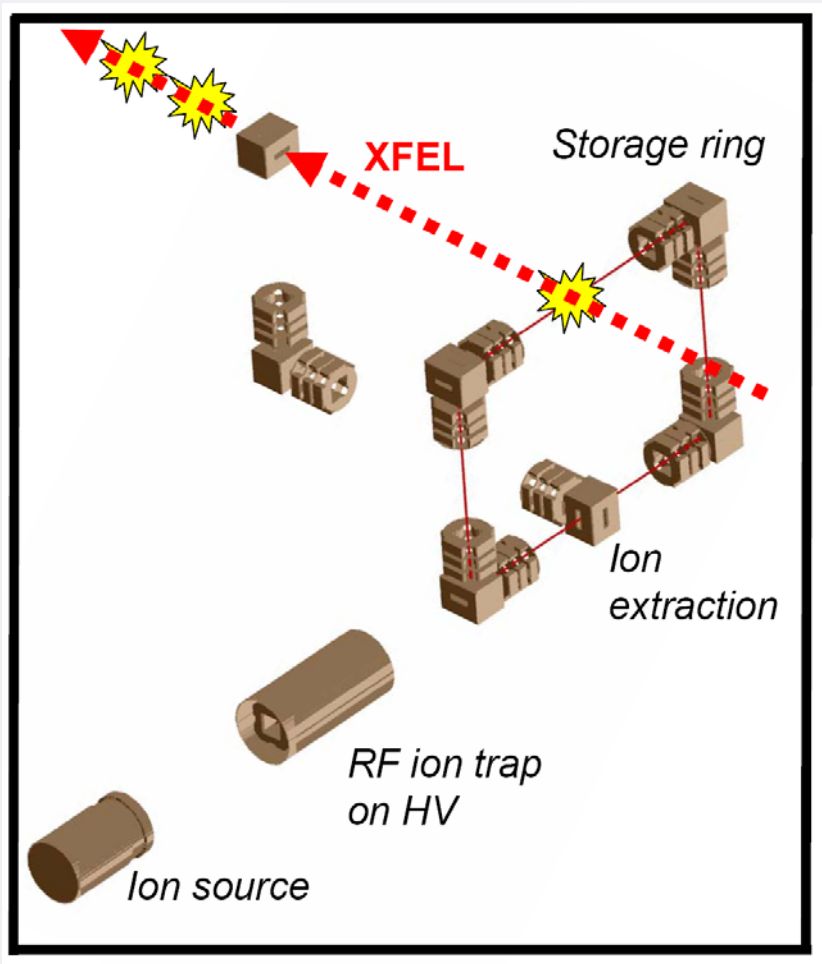
UHV vacuum chamber and ion trap setup
Optical laser
- **frequency mult.**
- **OPA system**

Photon diagnostics
- **single-pulse**
- **on-line**

TDR 2006 – Ion beam facility

Complex instrumentation

- permanent installation
- flexible setup enabling various options/techniques



Design:
H. Pedersen, L. Lammich et al.

Startup scenario

One SQS instrument prioritized

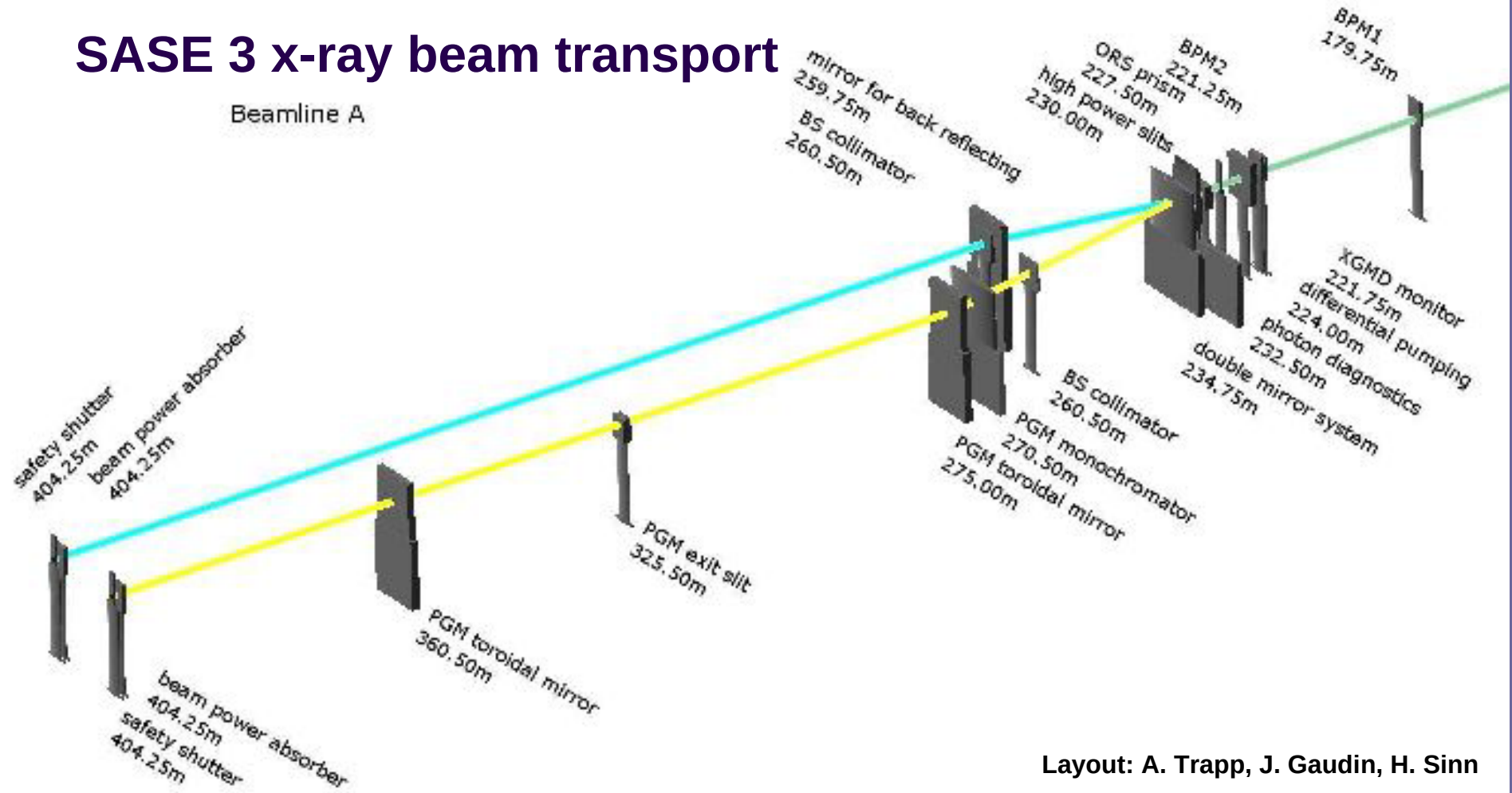
- emphasis on high intensity
  - ⇒**no monochromator**
  - ⇒**tight focusing optics**
- pump-probe experiments (vis. laser/x-ray)
  - ⇒**optical laser**
- interaction chamber provided by respective users
  - ⇒**no chamber & instrumentation foreseen (similar to FLASH)**
  - ⇒**no specific instrumentation (e.g. an ion beam facility)**

Selection requires review by user community

In order to rescope this instrumentation requires a clear & strong support by the user community

Current planning

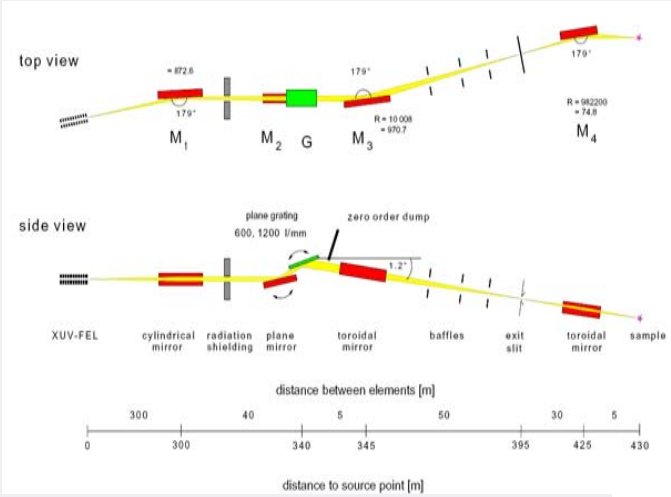
SASE 3 x-ray beam transport



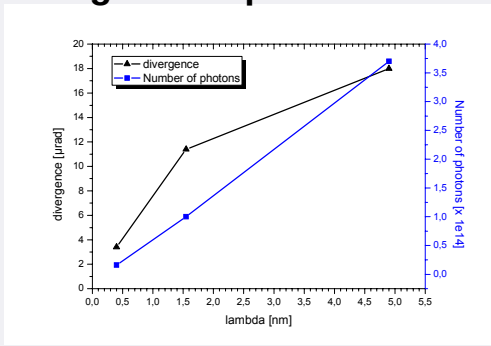
Layout: A. Trapp, J. Gaudin, H. Sinn

Monochromator design

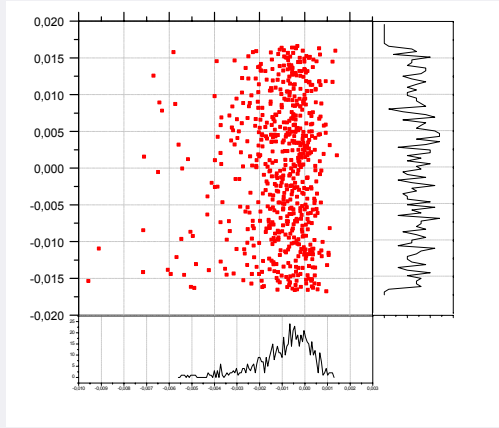
TDR 2001/6: PGM concept



Divergence & photon number



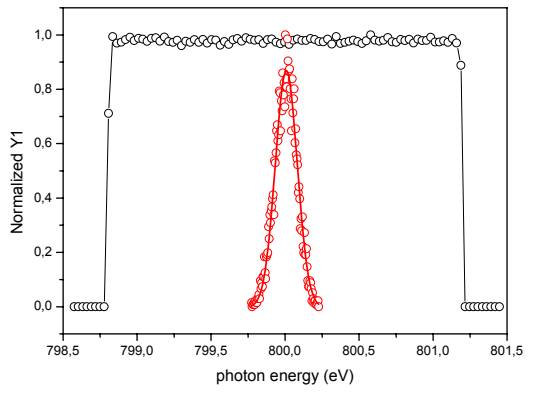
Focus spot @ 3100 eV with G2 (slit 200*200 µm)

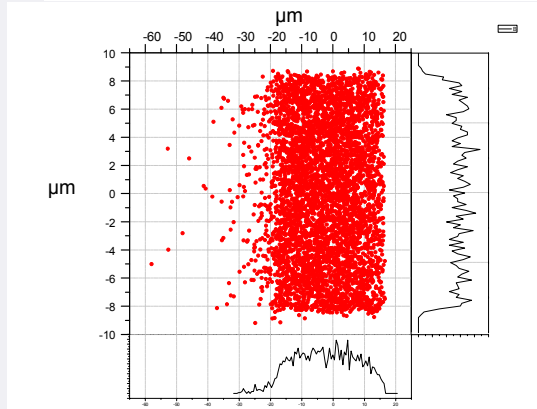


Source spectrum
800 eV with 0,3% bandwidth

Spectrum after at the sample
Bandwidth = 0,174 eV
Power resolution = 5e3

Simulations:
J. Gaudin

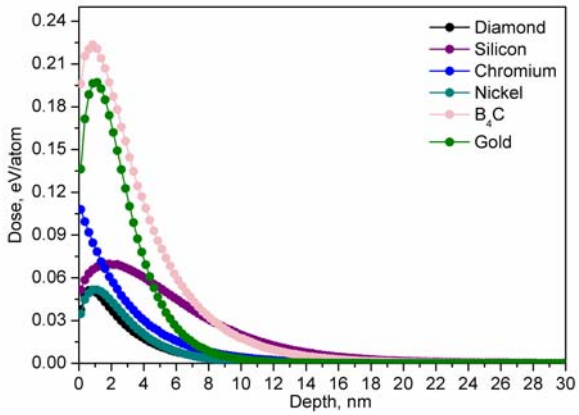




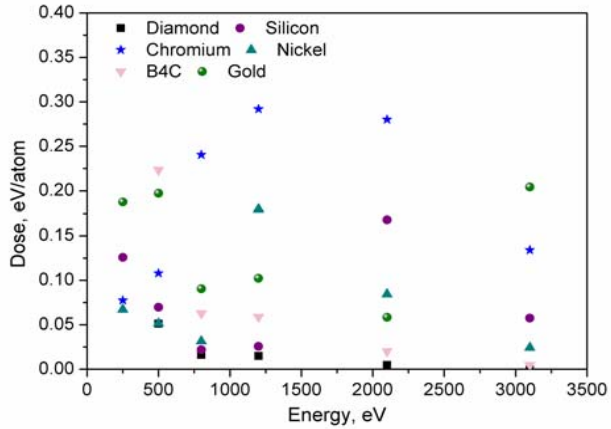
Focus spot @ 800 eV with G1
31 x 16 µm² (slit 200x100µm)

Interaction with highly intense FEL radiation

Damage



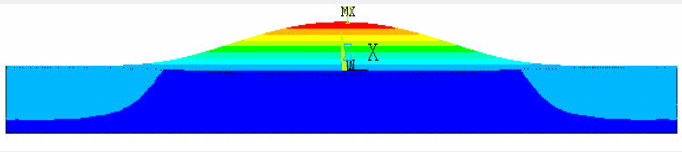
Absorption dose profile (hv=500eV)



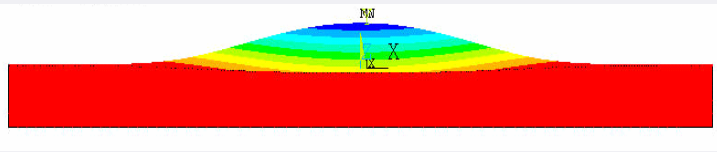
Maximum absorbed dose

Thermal effects

Simulations:
V. Altapova,
Fan Yang,
J. Gaudin



Deformation for 100 nm Au layer on Si substrate in mm

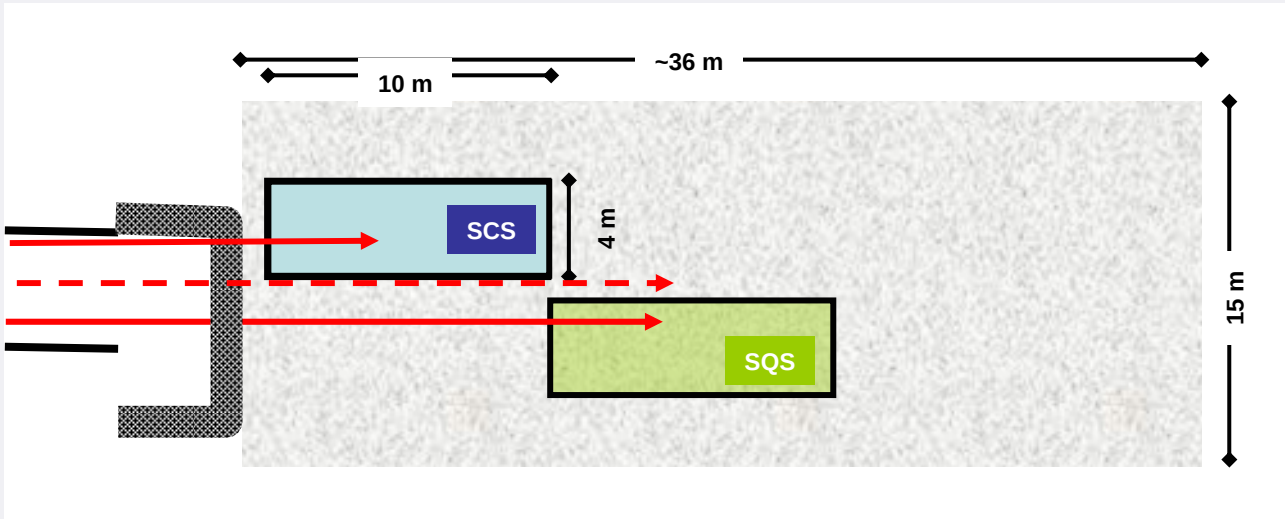


Stress for 100 nm Au layer on Si substrate in GPa

Experiments hall

X-ray/optical/control hutches

- two instruments: SQS & SCS
- optical laser
- beam separation 3–4 m



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European XFEL founding documents ready

Sep 22, 2008, Hamburg

Meeting of the International Steering Committee

- 14 International partners
  - ⇒**Funding secured**
- Finalize discussions on
  - ⇒**Convention**
  - ⇒**Articles of Association**

a rough time schedule …

2008+ Formation of user groups for first instruments

- Requirements for beam transport
- Scientific scope and layout instruments
- Infrastructure needs for instruments

2009+ Establish and review conceptual designs

- X-ray Optics & Beam Transport
- Scientific Instruments

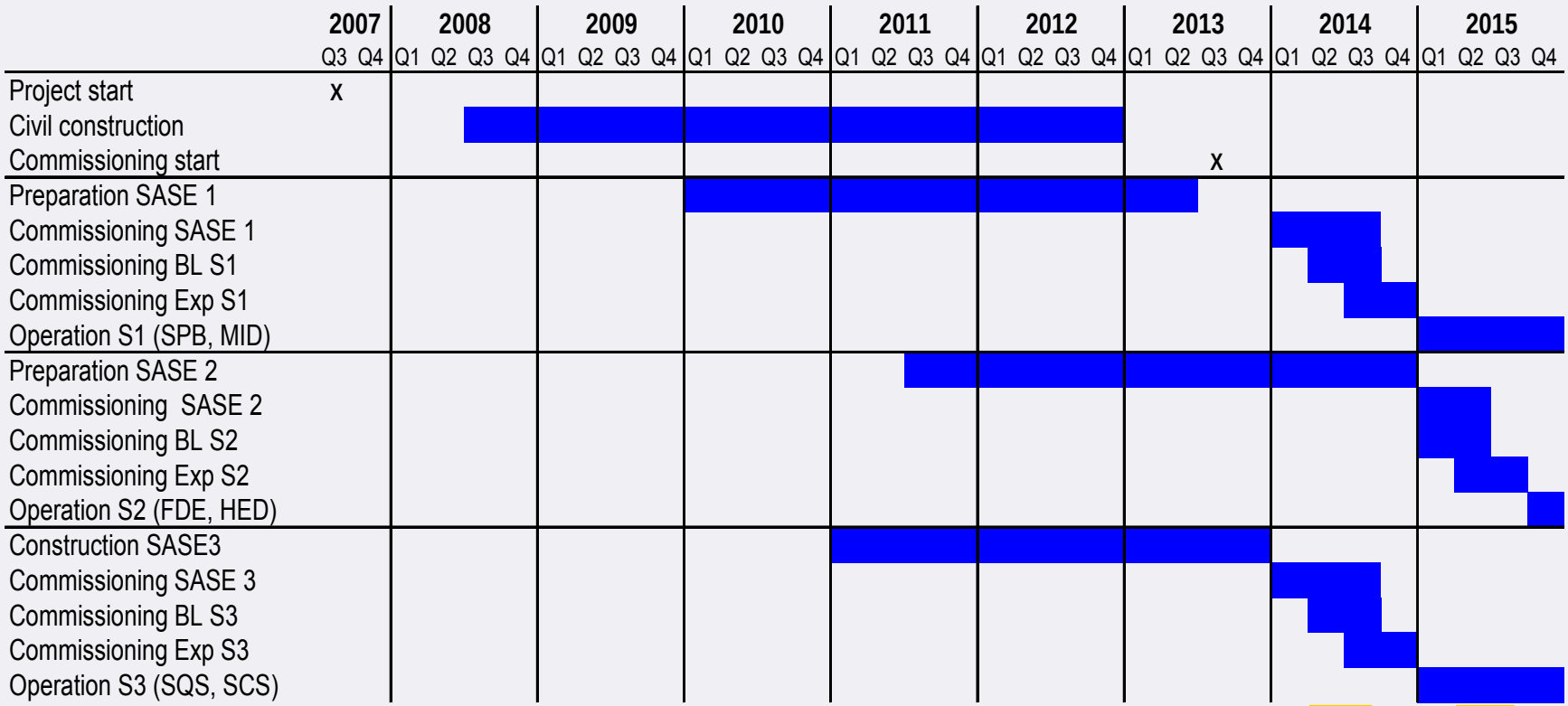
2010+ Establish and review technical designs

2011+ Construction and commissioning

2014 Involve Users in early experimental program

2015 Start full operation of most instruments

Time schedule



Commissioning SASE 1 & 3: SPB, MID, SQS, SCS

Commissioning SASE 2: FDE, HED

Operation SASE 1 & 3: SPB, MID, SQS, SCS

… in the case of SASE 3 beamline

Undulators

- SASE 1 ready for technical design

X-ray Optics & Beam Transport

- R&D (damage issues, wavefront preservation) & design
- Requirements for SPB & MID instruments
- Conceptual design beamline → Review ~2010
- Technical design beamline → Review ~2011

Scientific instruments SQS & SCS

- Definition of first experiments & instrumentation
- Conceptual design SQS & SCS → Review ~2011
- Technical design SQS & SCS → Review ~2012

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Plenary talks

	SESSION I: X-ray FELs and Small Quantum Systems
14.45-15.15	**Thomas Tschentscher** Status of the European XFEL and plans for a SQS instrument
15.15-15.45	**John Bozek** AMO Science at the LCLS - Instrumentation and First Experiments
15.45-16.15	Coffee/Tea
	SESSION II: Gas phase experiments
16.15-16.45	**Thomas Möller** Ultrafast processes of clusters in intense X-ray beams
16.45-17.15	**Robert Moshammer** Atomic and molecular fragmentation in intense XUV laser fields
17.15-17.45	**Michael Meyer** Pump-probe experiments in the XFEL regime
17.45-18.15	**Henrik Stapelfeldt** Laser aligned molecules as sample holders for FEL experiments
18.15-18.45	**Daniel Rolles** Multi-particle correlation measurements on atoms, mo nanoparticles
18.45-19.15	**Kyoshi Ueda** Atomic, molecular and cluster science using X-ray FEL
19.30-	Buffet dinner

	SESSION III: Experiments with ion beams
09.00-09.30	**Stefan Schippers** Photon-Ion experiment with hard X-rays: From PETRA III to the XFEL (Merged-beam technologies)
09.30-10.00	**Andreas Wolf** Photon induced fragmentation in molecular systems studied with fast beam imaging
10.00-10.30	**Mats Larsson** Experiments with stored ion beams
10.30-11.00	Coffee/Tea
	SESSION IV: Experiments with trapped particles
11.00-11.30	**José R. Crespo López-Urrutia** Soft x-ray laser spectroscopy
11.30-12.00	**Alexander Dorn** Tracing ultra-fast many-electron processes in the super-brilliant light of the XFEL via high-resolution MOTRIMS
12.00-12.30	**Todd Ditmire** Strongly coupled ion plasmas probed with the XFEL
12.30-13.30	Lunch

Working groups

THURSDAY, OCTOBER 30	
	SESSION I: Experimental techniques I
14.00-14.10	**Thomas Möller/Michael Meyer** Introduction
14.10-14.30	**Eckart Rühl** Experiments on Nano-Particles
14.30-14.50	**Tim Laarmann** X-ray Femtochemistry on small molecular systems
14.50-15.10	**Todd Ditmire** Studies on Clusters
15.10-15.30	**Daniel Rolles** X-Ray Fluorescence
15.30-16.00	Coffee/Tea (Physics Canteen)
	SESSION II: Experimental techniques II
16.00-16.20	**John Costello** Time-resolved Pump-Probe experiments
16.20-16.40	**Jonathan Marangos** Non-linear Processes in the X-Ray regime
16.40-17.00	**Marc Vrakking** Velocity-map Imaging
17.00-17.20	**Henrik Stapelfeldt** Molecular Alignment and Orientation
17.20-17.40	Conclusion
FRIDAY, OCTOBER 31	
	SESSION III:
09.00-09.30	Spontaneous contributions
09.30-10.30	Discussions and drafting of report
10.30-11.00	Coffee/Tea (Physics Canteen)

THURSDAY, OCTOBER 30	
	SESSION I: Ion Target preparation
14.00-14.10	**Henrik B. Pedersen/Stefan Schippers** Introduction
14.10-14.30	**Lutz Lammich** Fast Ion Beams
14.30-14.50	**Andreas Wolf** High energy ion beams and chrogenic storage rings
14.50-15.10	**Sascha Epp** Electron Beam Ion Traps (EBITs)
15.10-15.30	**Reinhold Schuch** Penning Ion Traps
15.30-16.00	Coffee/Tea (Physics canteen)
	SESSION II: Ion-XFEL interaction
16.00-16.20	**Michael Drewsen** Trapped ion-XFEL interactions
16.20-16.40	**Jean-Marc Bizau** Ion beam-XFEL interactions
16.40-17.00	**Ottmar Jagutzki** Detection of electrons and heavy fragments
17.00-17.20	**Andreas Schwarz** Dectection of Photons
17.20-17.30	**Discussion and conclusion**
FRIDAY, OCTOBER 31	
	SESSION III: **XFEL-beam and additional laser sources**
09.00-09.30	**Stefan Düsterer** Experience from FLASH
09.30-10.30	Discussions and drafting of report
10.30-11.00	Coffee/Tea (Physics canteen)

Working groups shall provide ample time for discussion !

Output of the working groups

Science

- identify scientific drivers for instrumentation

Technical issues

- FEL generation & x-ray beam delivery
  - ⇒ **photon energy, bandwidth, spot size, energy vs. power, …**
- SQS instrument implementation
  - ⇒ **techniques, instrumentation, detectors, lasers, …**
- needs for additional instrumentation
  - ⇒ **ion beam facility, …**

User community issues

- establish a SQS user group (list, email, future meetings, …)
- define process to resolve open issues

→ Brief report

- summarizing working group discussion
- suggested instrumentation
- proposed activities required to establish the instrumentation

Conclusion

- **European XFEL now enters a new phase of interaction with user community about details of science program.**
- **SQS instrument is undergoing review. Your input is crucial in this process.**
- **Scope limited in startup version compared to that of the TDR 2006.**

The European XFEL team is looking forward to working with you over the next years on defining and construc ting this instrument.

Acknowledgement

The European X-Ray Laser Project XFEL

International Workshop on the Science with and the Instrumentation for Small Quantum Systems at the European XFEL

October 29-31 2008, Department of Physics and Astronomy, University of Aarhus, Denmark

The study of Small Quantum Systems (SQS) of atomic, molecular, cluster, or crystalline character in gas phase experiments was one of the prioritized areas of science for the upcoming European XFEL facility as described in the Technical Design Report (available under www.xfel.eu) and includes studies of extremely dilute systems, of particles in traps, of non-linear processes using one- and two-color techniques and of ultrafast processes.

The workshop will bring together scientists interested in experiments using the SQS instrument at European XFEL facility both to review the science planned with this instrument, to discuss the requirements to the X-ray FEL beam delivery, and to initiate activities and collaborations on instrumentation and facilities needed at its photon endstations.

The workshop will include a series of invited lectures giving an overview of scientific and instrumental ideas for the SQS instrument followed by smaller working groups on specific instrumentation for the European XFEL facility.

Deadline Sep 1, 2008
YOUNG SCIENTISTS BURSARIES
for details see website

The workshop is co-funded by the European Commission through the Pre-XFEL project. This will allow free of charge access to the workshop, in particular cases support of travel cost might be possibleif requested by the speakers well in advance of the meeting. Hosting the workshop and support by the Department of Physics and Astronomy at the University of Aarhus is gratefully acknowledged.

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