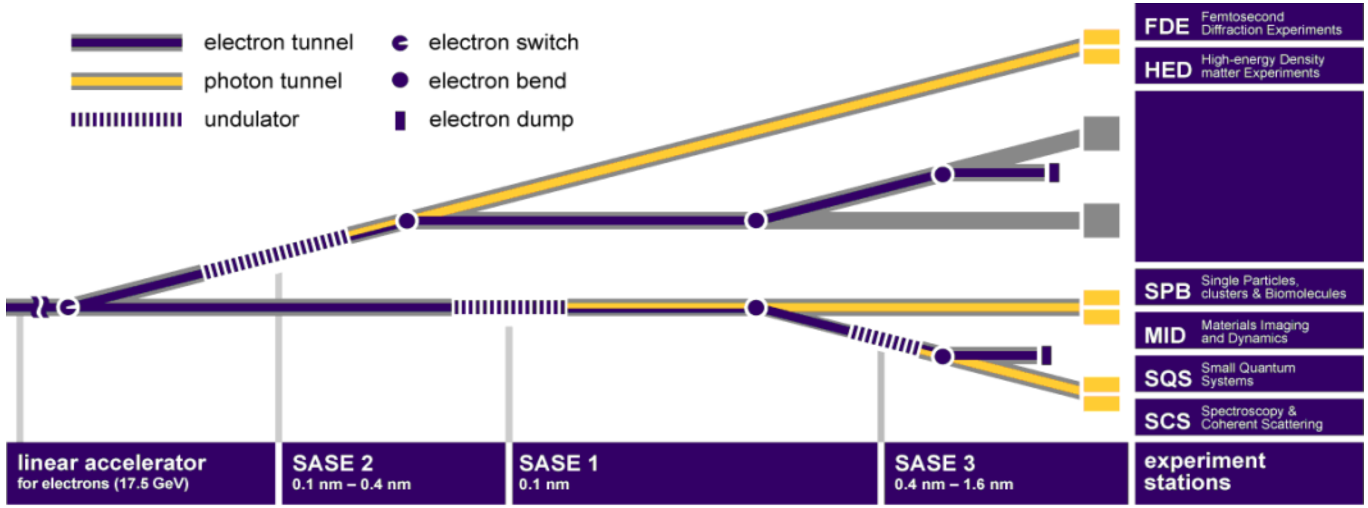
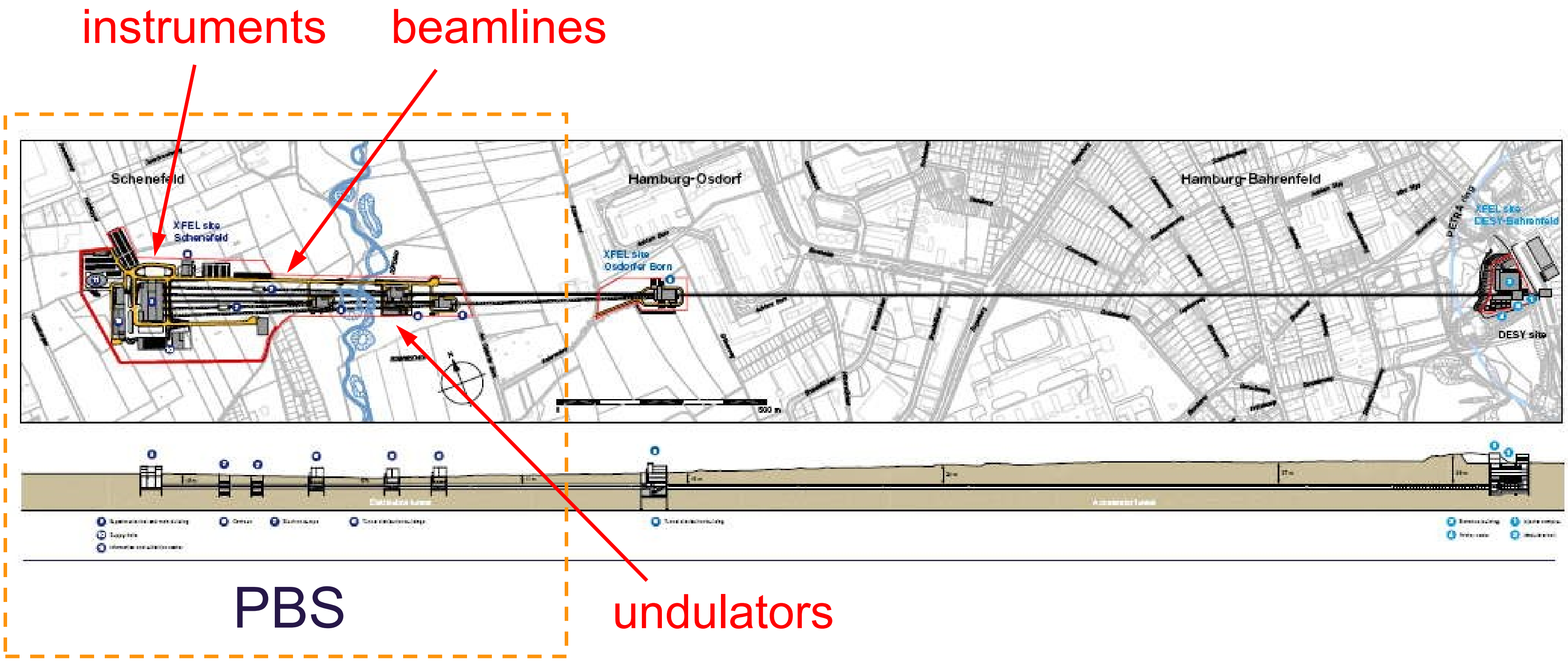
European XFEL Experiments

Serguei L. Molodtsov
European XFEL



What is Photon Beam System (PBS)?



- Photon Beam Systems comprise: undulators, beamlines, experimental stations (instruments), diagnostics, additional instrumentation
- Operation of the Photon Beam System is under direct responsibility of the European XFEL GmbH

Structure of PBS: Working Packages (WPs)

WP 71	Undulator Systems	J. Pflüger
WP 72	Simulation of Photon Fields	G. Geloni
WP 73	X-ray Optics &Transport	H.Sinn
WP 74	X-ray Photon Diagnostics	J. Grünert
WP 75	Detector Development	H. Graafsma
WP 76	DAQ & Control Systems	C. Youngman
WP 78	Optical Lasers	N.N.
WP 79	Sample Environment	N.N.
WP 81-86	Scientific Instruments	C. Bressler
		M. Meyer, N.N.

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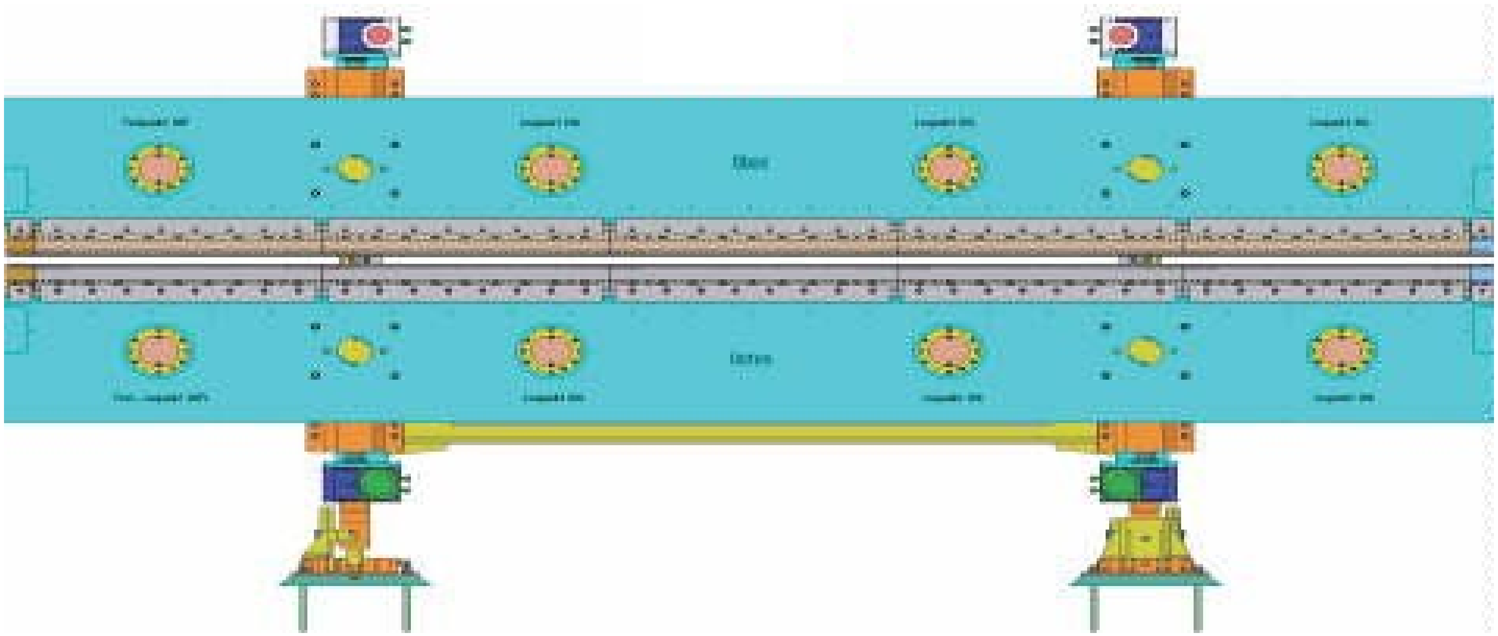
Undulators (WP71, J. Pflüger)

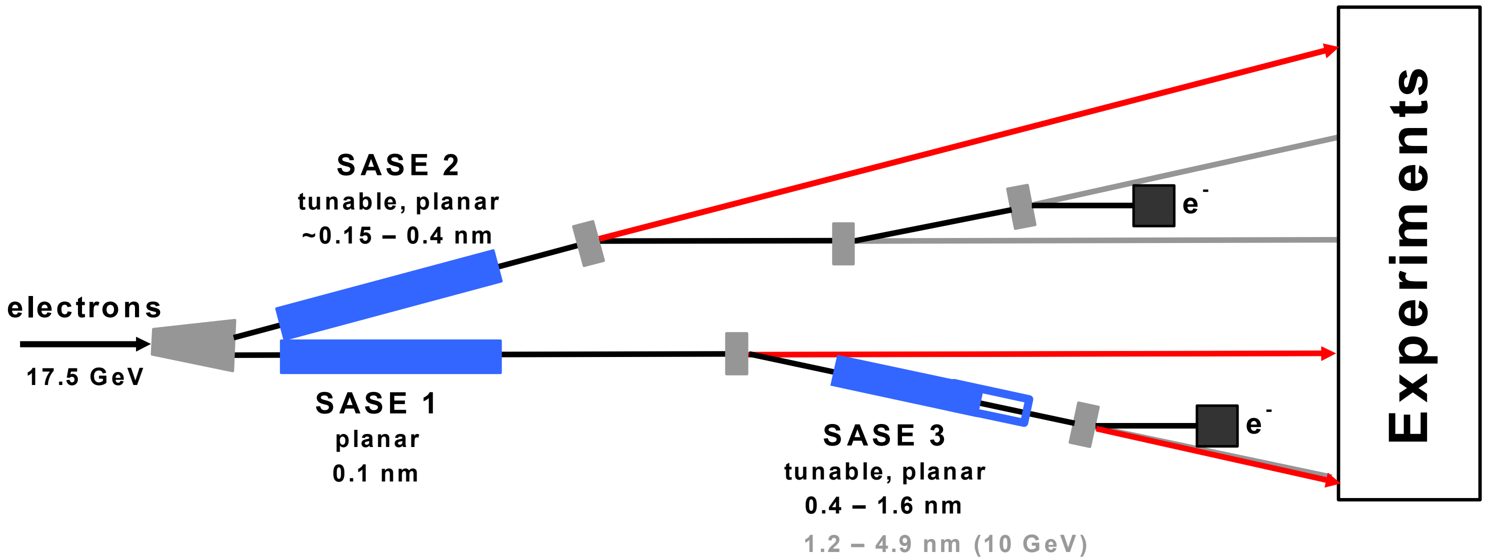


European XFEL

Start-up Scenario

Start-up design

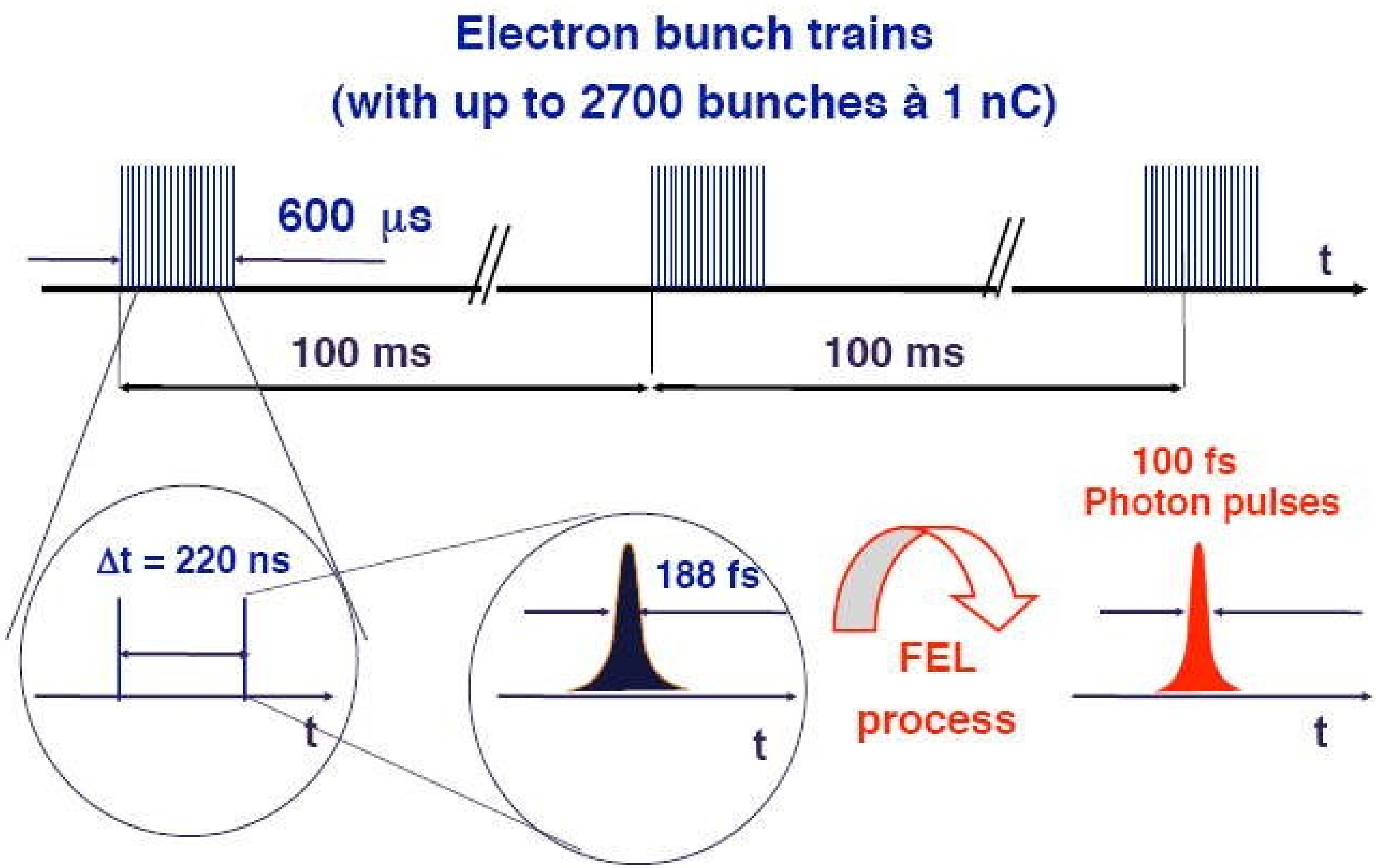
- Concentrate on SASE FEL radiation
- Provide as large as possible photon energy range
- For soft x-rays start with linear polarization (under reconsideration)
- Enable use of high harmonics and spontaneous emission in SASE beamlines



Undulators: FEL Parameters

Parameter	Unit	SASE 1	SASE 2		SASE 3		
Electron energy	GeV	17.5	17.5	17.5	17.5	17.5	10.0**
Wavelength	nm	0.1	0.1	0.4	0.4	1.6	6.4
Photon energy	keV	12.4	12.4	3.1	3.1	0.8	0.2
Peak power	GW	20	20	80	80	130	135
Average power*	W	65	65	260	260	420	580
Photon beam size (FWHM)	µm	70	85	55	60	70	95
Photon beam divergence (FWHM)	µrad	1	0.84	3.4	3.4	11.4	27
Coherence time	fs	0.2	0.22	0.38	0.34	0.88	1.9
Spectral bandwidth	%	0.08	0.08	0.18	0.2	0.3	0.73
Pulse duration	fs	100	100	100	100	100	100
Photons per pulse	#	10^{12}	10^{12}	1.6×10^{13}	1.6×10^{13}	1.0×10^{14}	4.3×10^{14}
Average flux	#/s	3.3×10^{16}	3.3×10^{16}	5.2×10^{17}	5.2×10^{17}	3.4×10^{18}	1.4×10^{19}
Peak brilliance	B	5.0×10^{33}	5.0×10^{33}	2.2×10^{33}	2.0×10^{33}	5.0×10^{32}	0.6×10^{32}
Average brilliance*	B	1.6×10^{25}	1.6×10^{25}	7.1×10^{24}	6.4×10^{24}	1.6×10^{24}	2.0×10^{23}

Undulators: FEL Pulses Structure



Superconducting LINAC technology provides 27.000 light pulses/s in burst-like structure. It makes XFEL.EU attractive for photon-hungry experiments.

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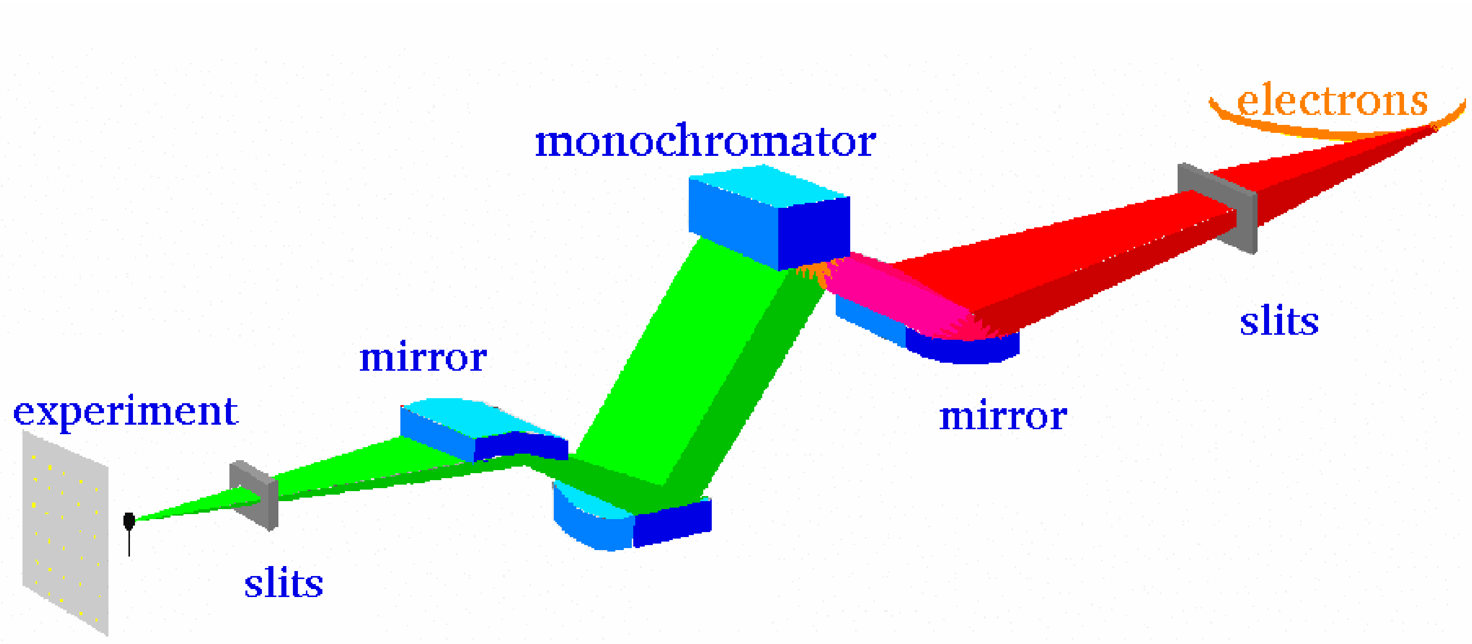
Beamlines (WP73, H. Sinn)



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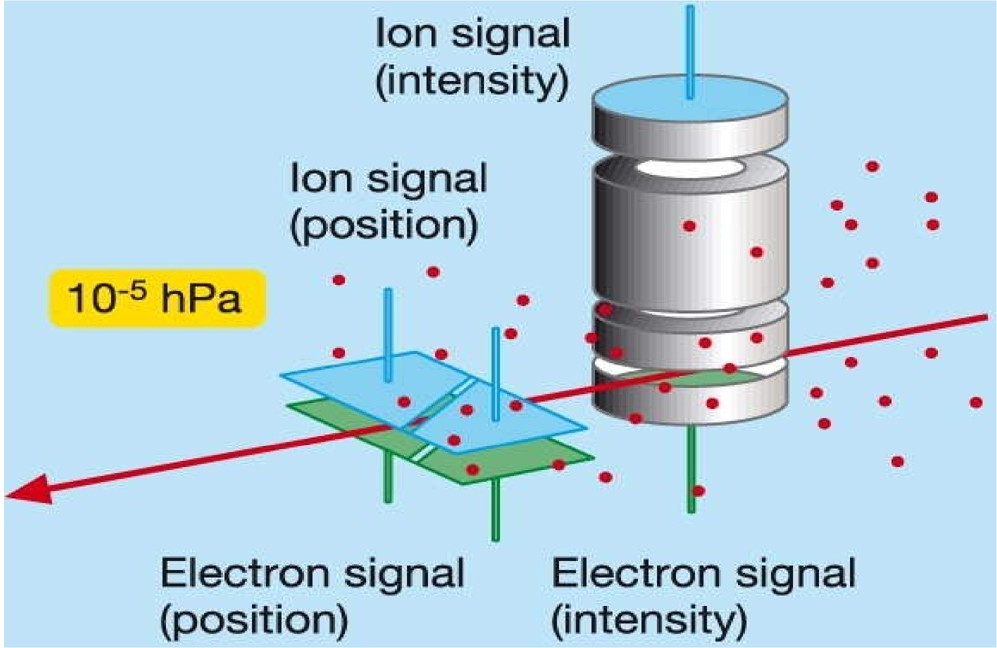
Diagnostics (WP74, J. Grünert)



The European XFEL

Scientific Instruments (WP81-86)

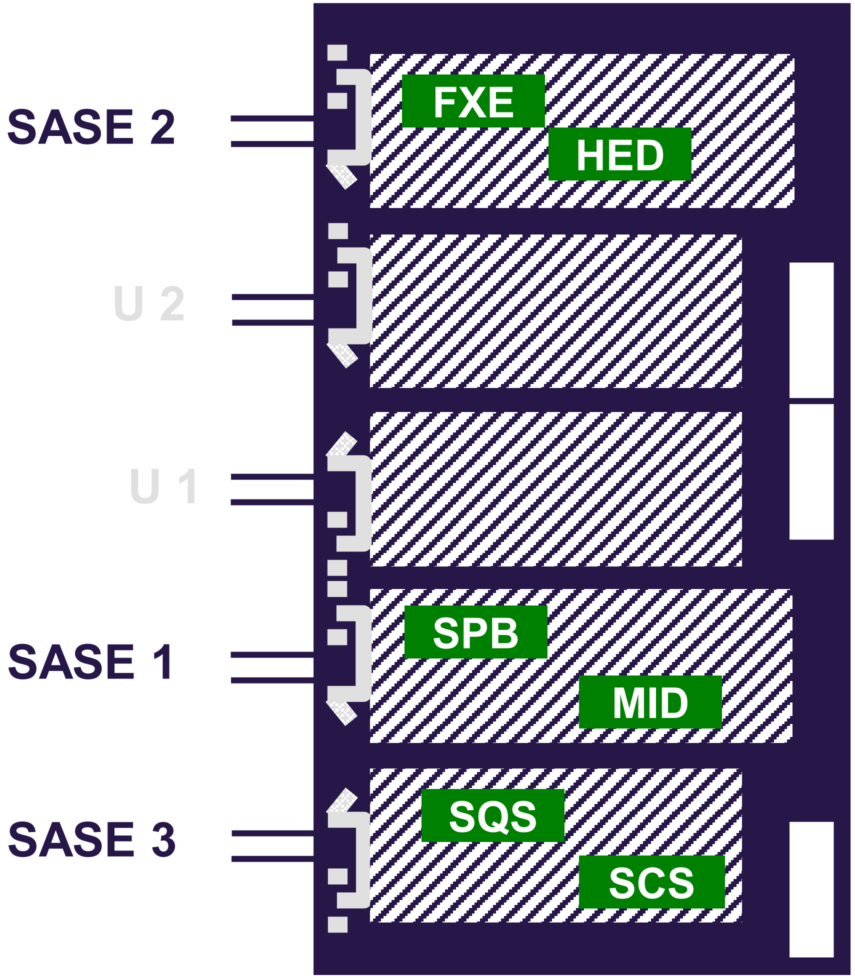
Selection of First Instruments

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.**
FXE	Femtosecond X-Ray 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 Spectroscopy and Coherent Scattering – **Electronic and atomic structure and dynamics of nano-systems and of non-reproducible biological objects using soft X-rays.**

Destribution of First Instruments

Source	Photon beam line characteristics
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 0.2 – 3.1 keV;** **High flux**
	FEL radiation 0.2 – 3.1 keV; **High resolution**



Instrument Workshops

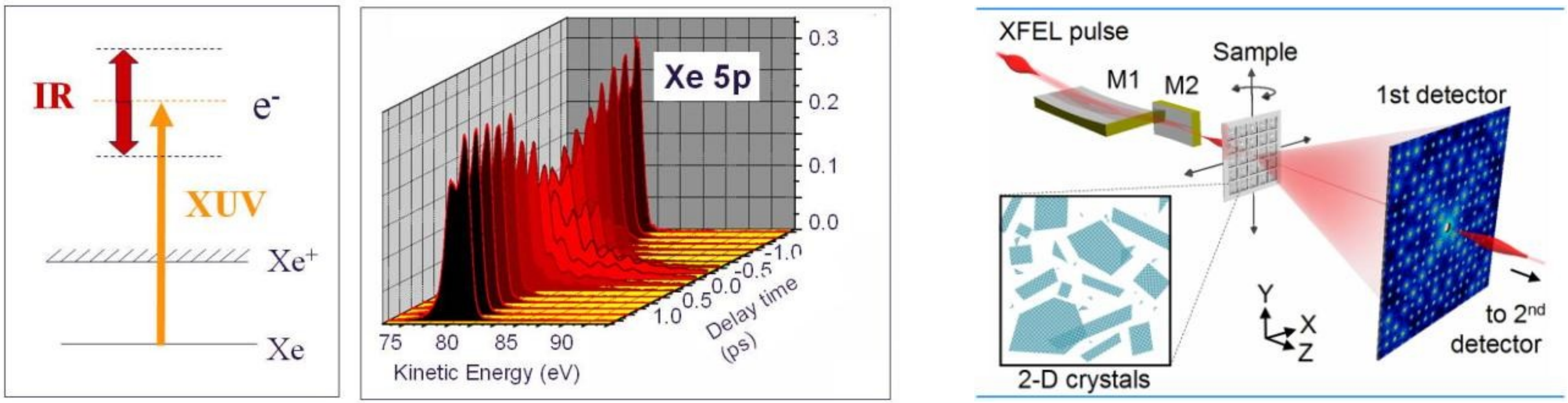
- Instrument Workshops:
  - SQS – Nov ’08, Aarhus, Dänemark
  - SPB – Nov ’08, Uppsala, Sweden
  - HED – Mar ’09, Oxford, UK
  - SCS – Jun ’09, Villigen, Switzerland
  - MID – Oct ’09, Grenoble, France
  - FDE – Dec ’09, Budapest, Hungary

- The Workshops brought together potential users of the instruments with purposes:
  - to review the areas of application of the instrument
  - to identify beam parameters and requirements to the experimental station(s) from the side of different experiments

Startup version instruments (Soft x-rays)

Small Quantum Systems (SQS)

- Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena

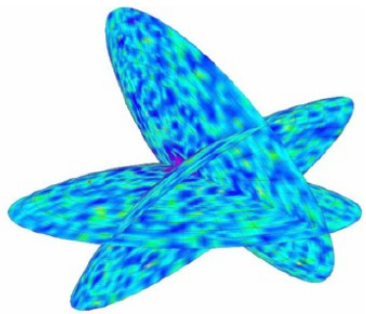


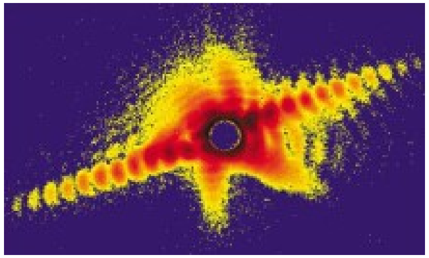
Spectroscopy & Coherent Scattering (SCS)

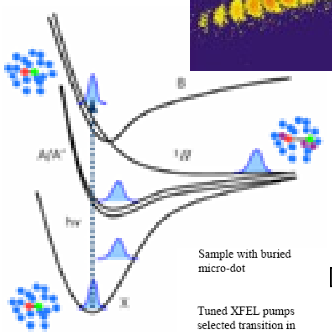
- Electronic and atomic structure and dynamics of nano-systems and of non-reproducible biological objects

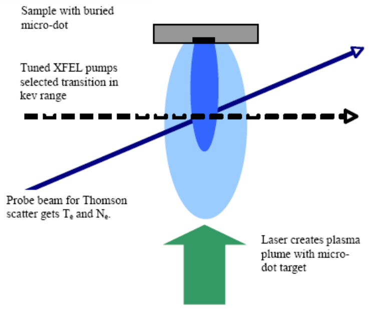
Startup version instruments (Hard x-rays)

- **Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB)**
  - Structure determination of single particles: atomic clusters, bio-molecules, virus particles, cells
- **Materials Imaging & Dynamics (MID)**
  - Structure determination of nano- devices and dynamics at the nanoscale
- **Femtosecond Diffraction Experiments (FDE)**
  - Time-resolved investigations of the dynamics of solids, liquids, gases
- **High Energy Density Matter (HED)**
  - Investigation of matter under extreme conditions using hard x-ray FEL radiation, e.g. probing dense plasmas









Small Quantum Systems (SQS)

University of Aarhus, 29-31 Oct 2008

- Organized by H. Pedersen, L. Lammich
- Program committee: G. Faigel, M. Larsson, J. Marangos, M. Meyer, Th. Möller, Th. Tschentscher, J. Ullrich, A. Wolf
- Participants: ~60 scientists from 11 countries

Two working groups (WG):

- Gas phase experiments (Th. Möller & M. Meyer)
- Experiments with ion beams and trapped particles (H. Pedersen & S. Schippers)

SQS Instrument

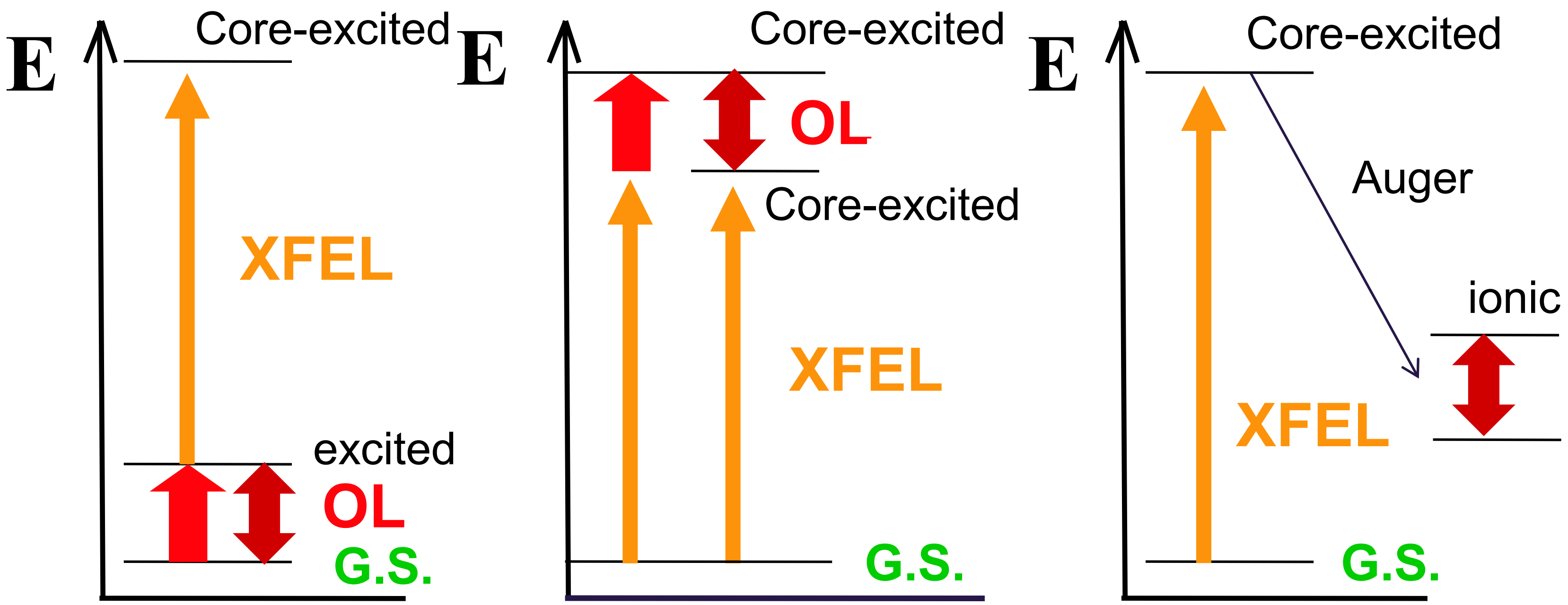
Major applications & instrumentation

- Ultrafast atom & molecular spectroscopy
- Strong field effects in SQS
- Highly excited ions
- Endstation for high field studies with opt. laser and particles energy analyser
- 2D detection & advanced diagnostics
- Additional location for user provided equipment (ion storage ring, etc.)

Requirements to x-ray delivery

	Photon energy [keV]	Tuna-bility	Polarization	Beam size [µm]	BW	Rep.rate	OL-PP/ X-PP
Initial	0.8 – 3.1	Yes	Linear	1, 100.	0.1%	5 MHz	Yes/Yes
Requested	~0.28 – 3	Yes	Variable	1, 100 unfocus.	0.1%	5 MHz	Yes/Yes
Status / Comments	t.b.e.	√	t.b.e.	√	√	√	√

SQS Details (M. Meyer)



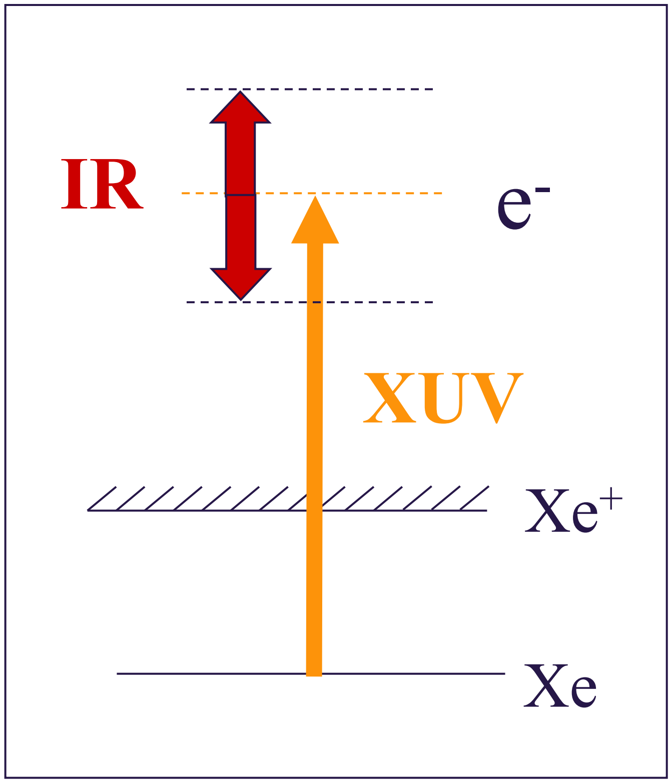
Laser-prepared state
Initial State Coupling

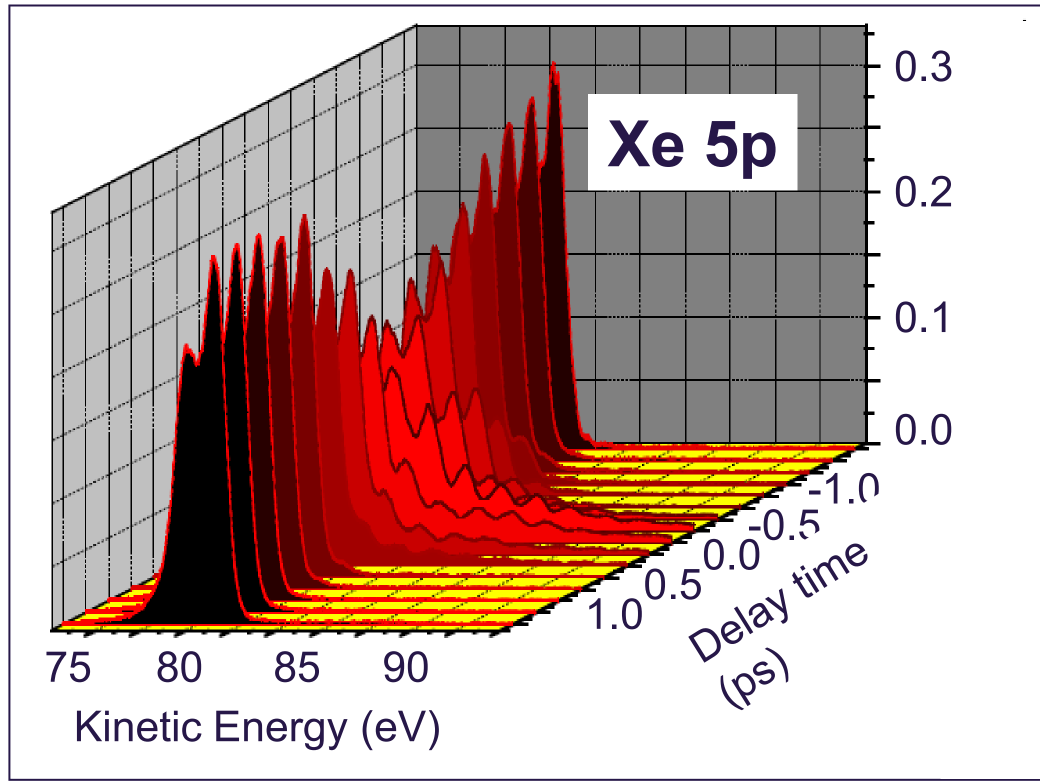
Two-color resonances
Coupling of AIS

Ionic state Coupling

SQS Details (M. Meyer)

FLASH: 13.7 nm, 20 μJ, 50 μm focus, 20 fs **Opt. Laser: 800 nm, 1mJ, 50 μm focus, 120 fs**





HHG : Toma et al. PRA 62, 0618015 (2000)

FLASH : 2007

Single Particle and Biomolecules (SPB)

University Uppsala, 20-22 Nov 2008

- Organized by D. van der Spoel, J. Hajdu
- Program committee: H. Chapman, G. Faigel, F. Pfeiffer, I. Schlichting, P. Szoke, Th. Tschentscher
- Participants: ~70 scientists from 10 countries

Three working groups:

- Instrumentation (H. Chapman)
- Simulation & rad. damage (G. Faigel)
- Data analysis & needs (D. van der Spoel)

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SPB Instrument

Major applications & instrumentation

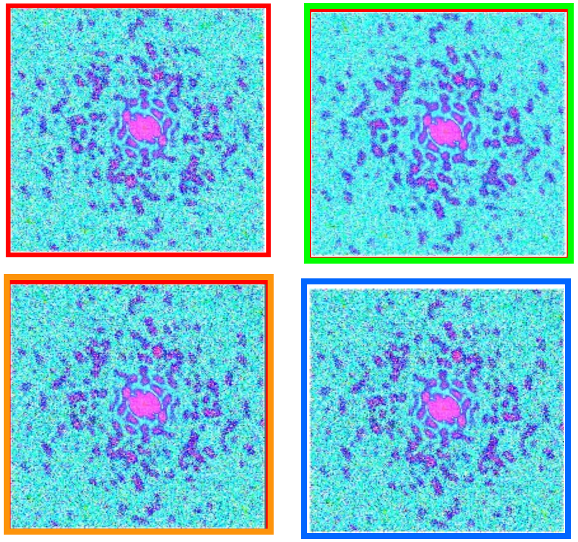
- Coherent diffraction imaging (CDI) from injected particles and bio-objects
- CDI from supported bio-objects (e.g. cells)
- Time-resolved diffraction from gas phase molecules New
- Laser techniques for aligning molecules New
- 2D detection & advanced diagnostics
- Various particle injection techniques

Requirements to x-ray delivery

	Photon energy [keV]	Tuna-bility	Polarization	Beam size [µm]	BW	Rep.rate	OL-PP/ X-PP
Initial	12.4	-	Linear	a.s.a.p.	0.1 %	5 Mhz	No*/No
Requested	~6 (?) – 12	-	-	0.1, 2, 5, unfocus.	-	~MHz	Yes (2x)/ No
Status / Comments	t.b.e.	√	√	√	√	t.b.e.	t.b.e.

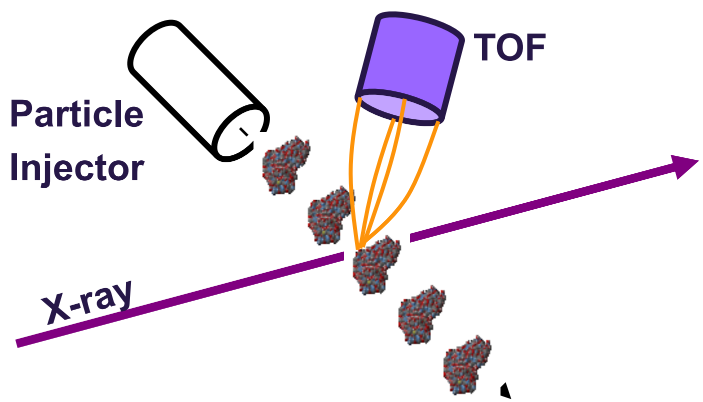
SPB Details

- **Use of high repetition rates**
  - Take benefit to collect needed amount of data
    - → Orientations
    - → Signal/orientation



10^5 – 10^7 patterns
req. for 3D reconstruction

- **Sample delivery**
  - Various methods with different benefits
    - → Jets
    - → Droplets
    - → Particles



Particle velocity ~200 m/s
→ traverse 1 µm : 5 ns

Issues

- Detector
- Jet→stability
- Particles→charge cloud
- Ion diagnostics→flight time

High Energy Density (HED) Experiments

University Oxford, 30 Mar – 1 Apr 2009

- Organized by J. Wark
- Program committee: P. Audebert, M. Fajardo, F. Faigel, G. Gregori, R. Lee, D. Riley, Th. Tschentscher
- Participants: ~60 scientists from 9 countries

Two working groups:

- X-ray instrumentation (D. Riley, Th. Tschentscher)
- Opt. laser instrumentation (P. Audebert, J. Wark)

Spokespeople nominated

P. Audebert, G. Gregori,
F. Rosmej, M . Tolley,
K. Sokolowski-Tinten, J. Wark

HED Instrument

Major applications & instrumentation

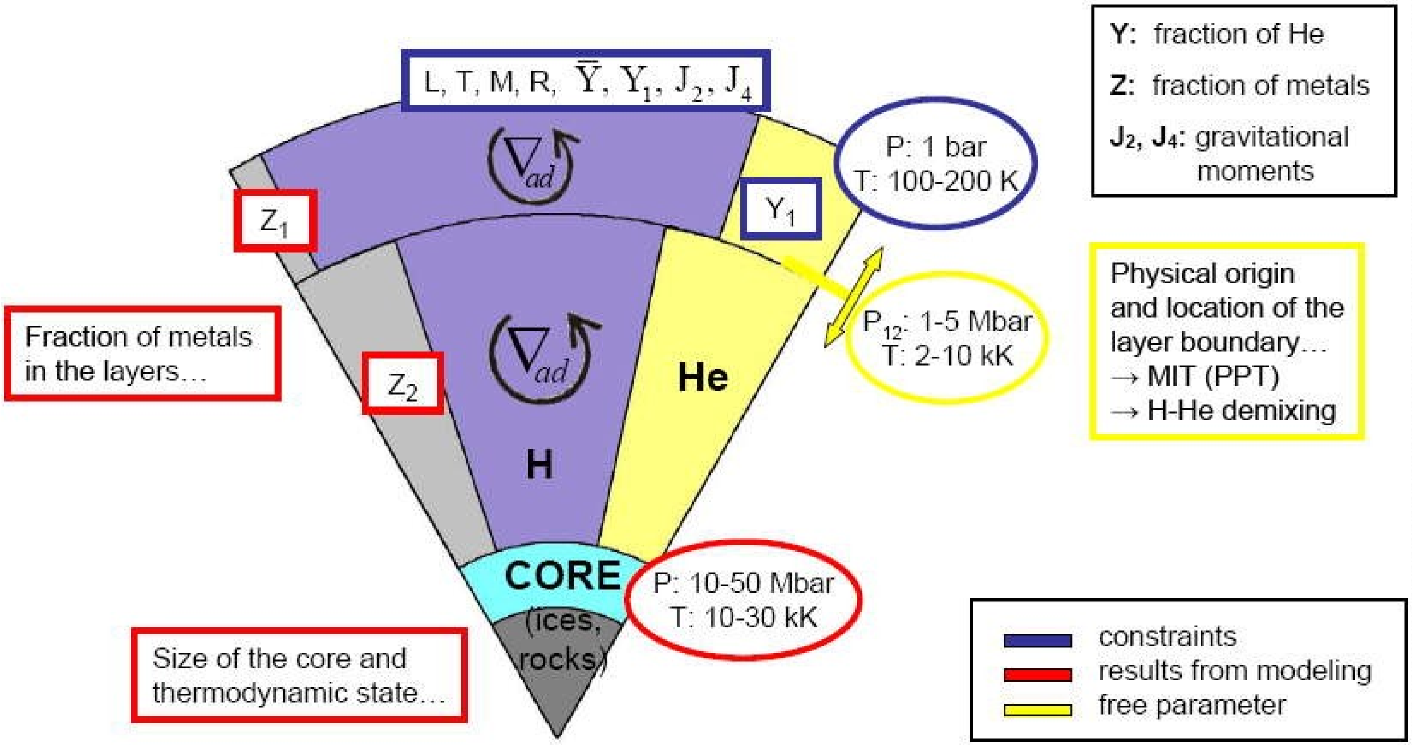
- Variety of hard x-ray techniques (scattering, diffraction, emission) to probe HED systems
- Isochoric & volumetric heating of matter
- Laser techniques for diagnosing are needed
- High energy laser for shock creation; extreme states of matter New
- 2D detection for imaging; fs-XSC for emission

Requirements to x-ray delivery

	Photon energy [keV]	Tuna-bility	Polariza-tion	Beam size [µm]	BW	Rep.rate	OL-PP/ X-PP
Initial	8 - 12	-	Linear	1 - 100	0.1 %	10 Hz	Yes/Yes
Requested	4 - 20	±3%	Linear	1,3,10,100 unfocus.	10^{-6}- 10^{-3}	10 Hz (+)	Yes/Yes
Status / Comments	t.b.e.	√	√	√(?)	t.b.e., 1-3%BW	t.b.e.	t.b.e.

HED Details (R. Redmer)

Standard three-layer structure model

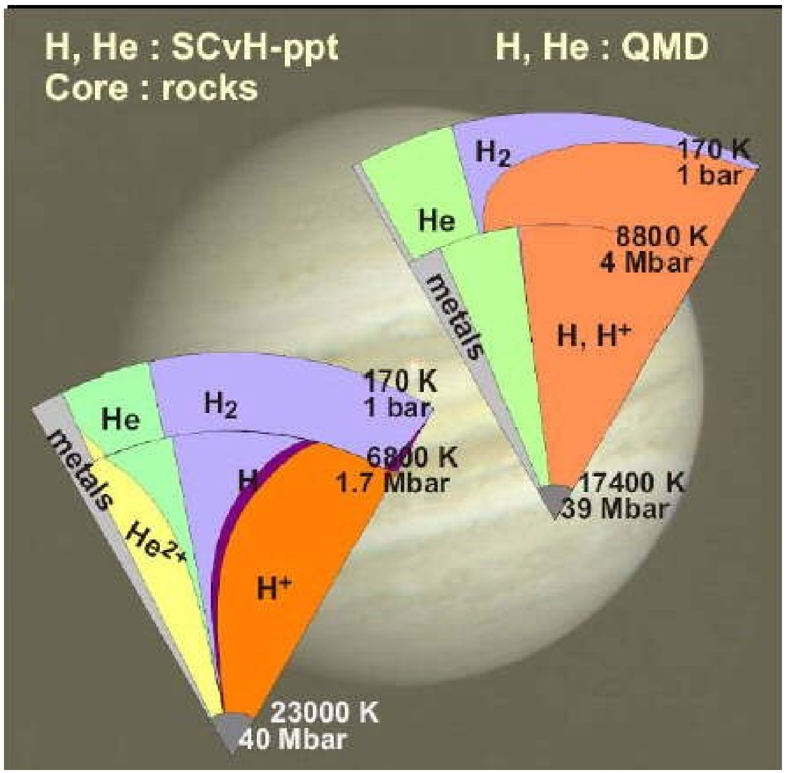


Apart from the transition pressure, interior models of this structure type are uniquely defined by the observables.

Most important input: Accurate EOS data for H and He as well as the representative of metals, e.g. H2O.

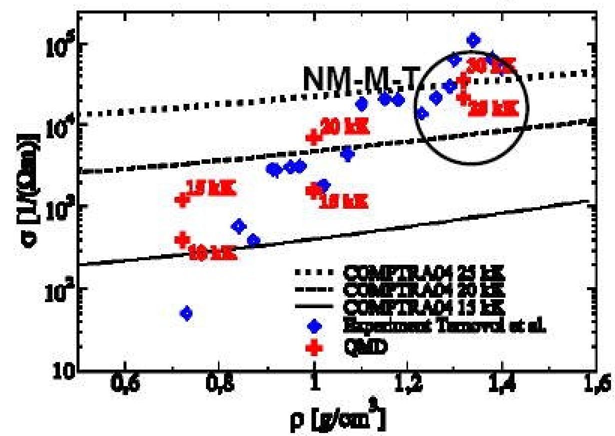
HED Details (R. Redmer)

Interior of Jupiter with LM-REOS



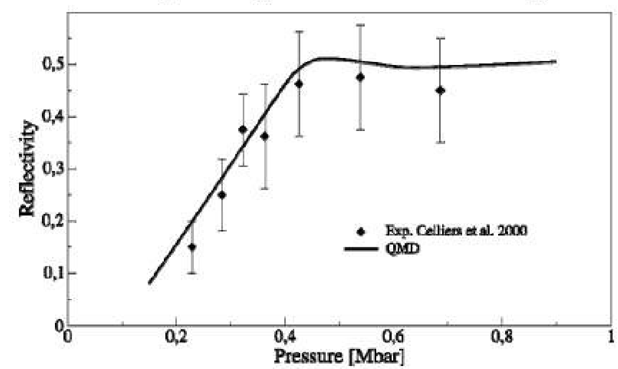
Distribution of chemical species for 2 models using different EOS

Helium: conductivity



A. Kietzmann et al, PRL **98**, 190602 (2007)

Hydrogen: reflectivity



B. Holst et al., PRB **77**, 184201 (2008)

Spectroscopy & Coherent Scattering (SCS)

PSI-SLS, Villigen, 2-4 Jun 2009

- Organized by R. Abela, B. Patterson
- Program committee: R. Abela, H. Chapman, G. Faigel, G. Grübel, Z. Hussain, M. Kiskinova, M. Kovalchuk, J. Luning, N. Mårtensson, S. Molodtsov, W. Wurth
- Participants: ~90 scientists, 14 countries

Three working groups (WG):

- Photon-in/photon-out & electron-out spectroscopic experiments (W. Wurth & Z. Hussain)
- Imaging, dynamics & photon correlation spectroscopy: Biological objects (I. Schlichting & I. Vartaniants)
- Imaging, dynamics & photon correlation spectroscopy: Magnetic Systems (G. Grübel & J. Luning)

SCS Instrument

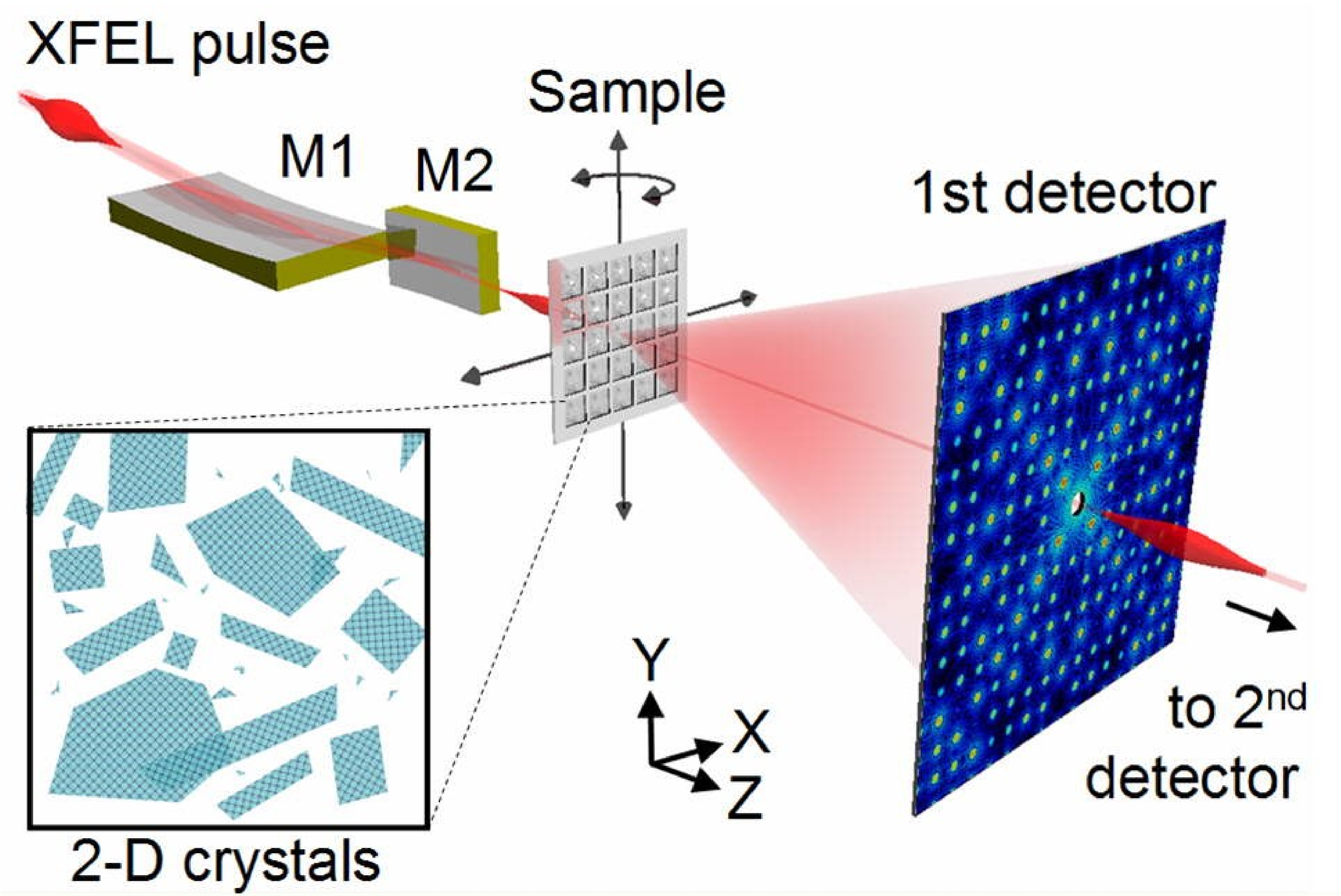
Major applications & instrumentation

- Electronic structure and excitations in solids & liquids
- Magnetism & magnetic structures including their dynamics
- Structure determination of nanosystems and bilogical units
- Endstation for x-ray spectroscopic studies
- 2D detection & advanced diagnostics
- Additional location for user provided equipment (e.g. CDI/XPCS chamber)

Requirements to x-ray delivery

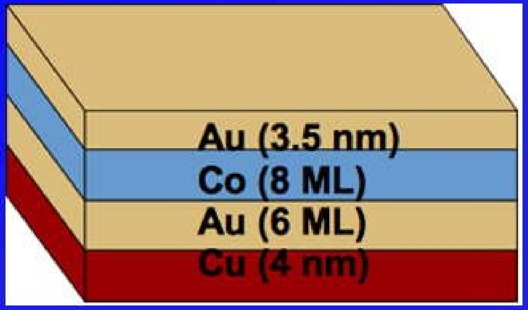
	Photon energy [keV]	Tuna-bility	Polarization	Beam size [µm]	BW	Rep.rate	OL-PP/ X-PP
Initial	0.8 – 3.1	Yes	Linear	1,10,100	0.01%	5 MHz	Yes/Yes
Requested	~0.28 – 2	Yes	Variable	1,10,100 unfocus.	0.003%	30 kHz	Yes/Yes
Status / Comments	t.b.e.	√	t.b.e.	√	t.b.e.	√	√

SCS Details (C. Kewish)



SCS Details (S. Kevan)

Spin Reorientation Transition in Au:Co:Au

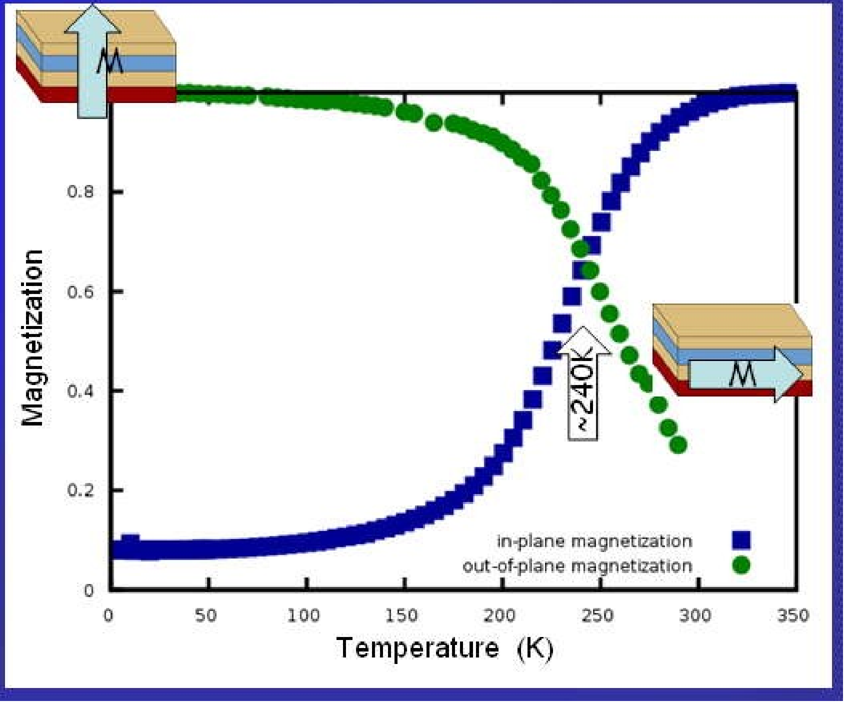


Ultrathin Co layers -> spin-reorientation transition. Preferred magnetization direction is determined by competition between shape and crystalline/surface anisotropy (Pescia *et al. PRL 65, 2599)*.

$$E = \{K_2(T) - 2\pi M_s(T)^2\}\sin^2(\theta) + K_4(T)\sin^4(\theta)$$

Magnetization rotates from out-of- to in-plane as a function of increasing temperature (Park *et al. APL 86 042504).*

Driving force in SRT is mostly temperature dependent interfacial magnetic anisotropy.



Materials Imaging and Dynamics (MID)

ESRF, Grenoble, 28/29 Oct 2009

- Organized by A. Madsen
- Program committee: J. Goedkoop, G. Grübel, O. Thomas, I. Vartaniants, Th. Tschentscher
- Participants: ~75 scientists from 10 countries

Two working groups:

- Coherent diffraction imaging (O. Thomas, I. Vartaniants)
- Photon correlation spectrosc. (C. Schüßler-Langeheine, G. Grübel)

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MID Instrument

Major applications & instrumentation

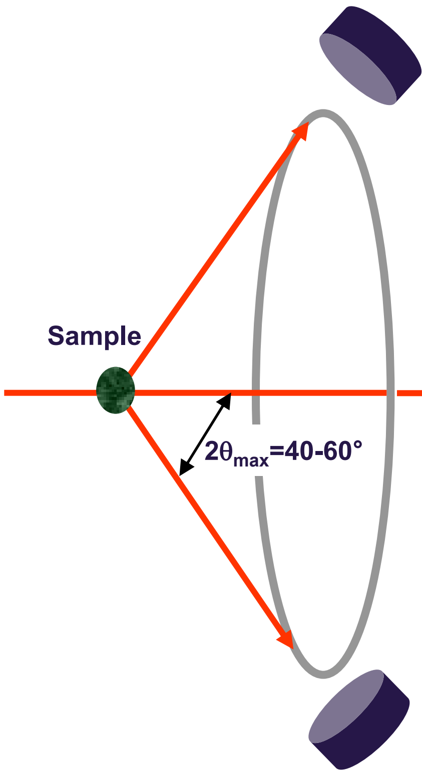
- Coherent diffraction imaging (CDI) from nano-structured objects & materials
- XPCS from amorphous and soft-matter systems (SAXS & large-q)
- 2D detects should match requirements; several detectors
- Large-q request puts constraint on detectors and exp. hall New

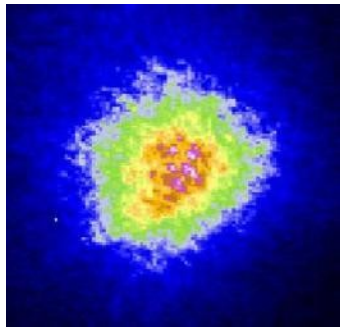
Requirements to x-ray delivery

	Photon energy [keV]	Tuna-bility	Polarization	Beam size [µm]	BW	Rep.rate	OL-PP/ X-PP
Initial	8-12, 36, 60-90	-	Linear	0.1 - 100	0.01	5 Mhz	Yes/Yes
Requested	~6 – 12(5), ~25	-	Vertical linear	1, 10, 25, unfocus.	nat., 10^{-4}, 10^{-5}	4.5 MHz	Yes/Yes
Status / Comments	t.b.e.	√	t.b.e.	√	√	√	t.b.e.

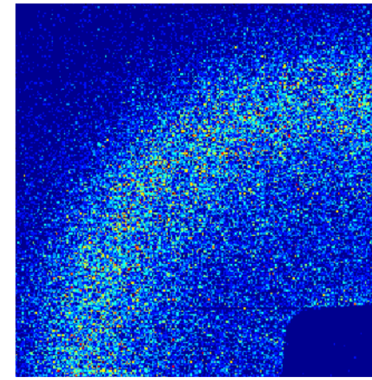
Combination of CDI and XPCS techniques

WAXS area

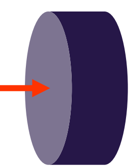




Large q-values
Multiple 2D detectors



SAXS area



Angular resolution requirements
→ Pixel size
XPCS – 4 µrad = 40µm@10m
CDI – 25-50 µrad = 100-200µm@4m

Requirements for CDI:
Ang. Resolution 100µrad; oversampling 2-4

Angular resolution requirements
→ Pixel size
XPCS – 4 µrad = 120 µm@30 m

Requirements for XPCS:
Pixel size < Speckle size: $S=(\lambda \times L)/D$

Femtosecond X-ray Experiments (FXE)

Hotel Benczur, Budapest, 9 – 11 Dec 2009

- Organized by G. Vanko
- Program committee: M. Bargheer, Ch. Bressler, F. Faigel, P. Glatzel, S. Johnson, J. Nielsen, A. Soldatov, S. Techert, Th. Tschentscher
- Participants: ~90 scientists from 16 countries

Two working groups:

- X-ray diffraction (M. Bargheer S. Johnson)
- X-ray spectroscopy (P. Glatzel, A. Soldatov)

FXE Instrument

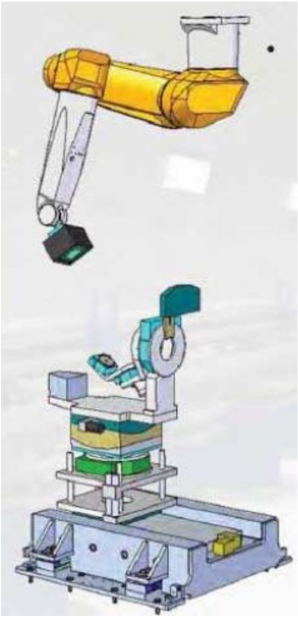
Major applications & instrumentation

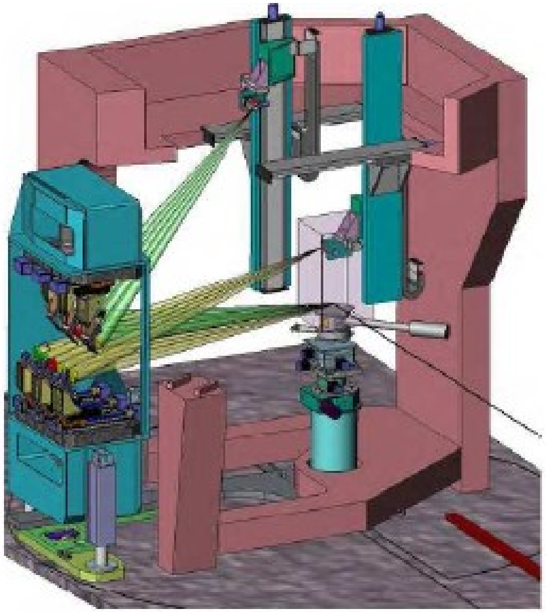
- Time-depend structural properties
- X-ray diffraction and spectroscopy techniques
- Solids and liquid samples (request for gas phase TR-XRD use SPB) New
- 2D detection for liquid and crystalline difraction New
- Integrate optical spectroscopy techniques New
- Reduced interest in X-ray pumping New

Requirements to x-ray delivery

	Photon energy [keV]	Tuna-bility	Polarization	Beam size [µm]	BW [%]	Rep.rate	OL-PP/ X-PP
Initial	3-12, 18-36	-	-	10 - 100	nat.,10^{-4}	5 MHz	Yes/Yes
Requested	~4 - 18	±3%	Linear	10, 100, line, unf.	nat.,10^{-4}	4.5 MHz	Yes/ No
Status / Comments	t.b.e.	√	√	√	t.b.e. , 1-3% BW	√	√

FXE Details

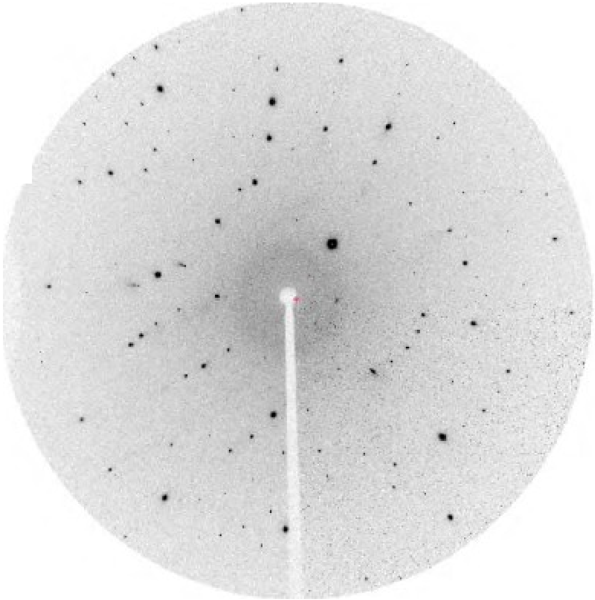




Complex instrument

- Diffraction
- Spectroscopy
- In-situ optical method

Single pulse Laue pattern



Large bandwidth request

- Chirp
- Single shot near-edge spectroscopy
- Laue-type diffraction

Roadmap to the Operational Facility

2007 Priority for undulators and instruments is determined

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

Thank you for your attention

and

you are very welcome to plan

experiments at the European XFEL