

Adrian Mancuso





Reminder: SPB/SFX science

Reminder: The SPB/SFX instrument

Day one beam parameters

Sketch of first possible experiments

Requirements to instrumentation to perform these experiments











Imaging of "big" and "small" non-crystalline samples





Imaging of "big" and "small" non-crystalline samples





XFEL pulse

Imaging of "big" and "small" non-crystalline samples





XFEL pulse Imaging of "big" and "small" non-crystalline samples





The set of the set of





Crystallography of "small", "radiation sensitive" or "dynamic" samples

The set of the set of

























[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004









































Micron-scale KBs

Upstream interaction region

Nano-scale KBs

Refocusing CRLs

Downstream interaction region & 4Mpx AGIPD

Sample injector



XFEL Bird's eye view of instrumentation









XFEL Example: Serial crystallography



XFEL Example: Serial crystallography



XFEL Example: Serial crystallography


XFEL Example: Serial crystallography



Image courtesy A. Aquila, LCLS, SLAC

European

XFEL

Example: Serial crystallography



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Data: A. Barty, et al, J. Appl. Cryst. 2014

Image courtesy A. Aquila, LCLS, SLAC

24th April, 2015, 4th Collaboration Meeting of the European XFEL, DESY, Hamburg Adrian Mancuso, Leading Scientist, Single Particles, Clusters and Biomolecules (SPB) Instrument, European XFEL



XFEL Day one parameters for hard X-ray beamlines

Electron energy	17.5 GeV
Photon energy	8.4 keV
Repetition rate	100 kHz
Max. number pulses per train	60
Undulator K-value	3.9
Undulator Gap	10 mm
Pulse energy	2 mJ (slightly oversaturated)
Divergence	2.2 urad
Pulse duration	43 fs
Saturation length	58 m

H. Sinn, European XFEL



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Suitable for serial crystallography and more

H. Sinn, European XFEL

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9

Common requirements for day one experiments (non exhaustive list)

General requirements to do any of the planned Day-1 experiments

- um size beam
- cleanup apertures
- beam attenuator
- 2D detector
- gain calibration for detector
- detector debris shield (in practice)

- fixed target stage (all non jet)
- rotation stage (2D crystals only)
- efficient catcher (jet experiments)
- differential pumping (jet experiments)
- windowed gate valve? (jet experiments)
- post attenuator (SPI maybe)
- optical pump laser

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EuropeanXFELKB focussing optics



Preliminary granite support and vacuum tank designs

- Optics supported on granite plinths
- Vacuum tanks and controls / pumping infrastructure supported independently on stainless steel super-structure

XFEL KB focussing optics



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EuropeanXFELKB focussing optics



Optics have long lead times (polishing bottlenecks at JTEC)

Substrate / cooling design optimised by FEA and reviewed at FMB-Oxford PDR meeting to minimise thermal deformations





EuropeanXFELKB focussing optics



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Substrate / cooling design optimised by FEA and reviewed at FMB-Oxford PDR meeting to minimise thermal deformations



Possible delay hedged by alternative focusing system which supports crystallography FMB-Oxford competition sensitive, non-distributable

EuropeanSample delivery systems:XFELCompact and versatile liquid jet





Specifications

- Modular design
- Independent adjustment of nozzle and catcher
- Large opening angles for detectors
- Precise positioning



Ongoing development

Recovering catcher for sample recycling Integration of gas dynamic nozzles for sub-µm jets Detector protection Differential pumping and vacuum system

Slide courtesy J. Schulz, Sample environment group, European XFEL

Sample delivery systems: European **Compact and versatile liquid jet**





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Fing catcher for sample recycling gration of gas dynamic nozzles for sub-µm jets Detector protection Differential pumping and vacuum system

Slide courtesy J. Schulz, Sample environment group, European XFEL

Or

















EuropeanXFELInstrument beam stop









EuropeanXFELInstrument beam stop





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European XFEL



Adaptive Gain Integrating Pixel Detector

High repetition rate (4.5 MHz) 1MPix imaging detector



64x64 pixels/chip 2x8 chips/module modules/quadrant 4 quadrants/detector



Parameter	AGIPD
Energy Range	3-16 keV
Dynamic Range	10 ⁴ ph @12 keV
Single Photon Sens	Yes → Noise ~350e- rms
Storage cells/pixel	352 (analog)
Pixel size	200x200 μ m ² (squared)
Variable hole	Yes→ four independently movable quadrants
Veto capability	Yes

Status

- The full scale chip AGIPD1.0 exists
 - Fist test results show no major problems \rightarrow very encouraging
 - Measured parameters within the specification
- Mechanics design for 1MPix detector in advanced state
 - Initial tests of movement system successful
- Integration of the detector in the XFEL beamlines in progress



Slide: J. Sztuk-Dambietz, XFEL Image: AGIPD consortium



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Adaptive Gain Integrating Pixel Detector







Status

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> Slide: J. Sztuk-Dambietz, XFEL Image: AGIPD consortium

XFEL Controls, Analysis, Metadata



- Karabo controls must exist in time for commissioning without beam
- Some analysis code (e.g. CrystFEL for serial crystallography analysis) must be available to interpret measurements
 - inc. basic online analysis functions
 - inc. simple scripting analysis tools
- Metadata related to data (frames) such as pulse energy, I₀ and the diagnostic info must be accessible for analysis
 - Statistical analysis of serial crystallographic data increasingly valuable (correlation analysis, etc)





Installation & first experiments SPB/SFX

EuropeanXFELCartoon of installation plan

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XFEL Cartoon of installation plan



Aggressive installation requires ~6 months from "ready" hutches to seeing first beam

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EuropeanRidiculously optimistic route toXFELfast "1st measurements"

- Approximately focus optics
 - Using diagnostics screens, mirrors (or lenses)
 - Characterise beam size & coherence
 - 6 shifts
- Align sample delivery system
 - Using in-chamber diagnostic microscopes
 - Test with known sample
 - 2 shifts
- Confirm and refine detector geometry
 - Using "easy" nanocrystal sample
 - 2 shifts
- Taking data on a first sample
 - Requiring implemented serial crystallography analysis software
 - 5 shifts



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Installation & first experiments SPB/SFX

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fast "1st measurements"

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European

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Compare with LCLS \approx 6 weeks/instr.



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Installation & first experiments SPB/SFX

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European

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Total = 1+ weeks

These states ≠ commissioned

Compare with LCLS \approx 6 weeks/instr.

EuropeanXFELAcknowledgments

- SPB/SFX
 - Andrew Aquila (until Oct '14)
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 - Gannon Borchers
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 - Nadja Reimers (Central Instruments Engineering)
 - Stephan Stern
 - Tokushi Sato
 - Steffen Raabe
 - Chun Hong Yoon

A. P. Mancuso, A. Aquila, G. Borchers, K. Giewekemeyer & N. Reimers, Technical Design Report: Scientific Instrument SPB, 2013. <u>dx.doi.org/10.3204/XFEL.EU/</u> <u>TR-2013-004</u>



🚺 Universität Hamburg

ER FORSCHUNG | DER LEHRE | DER BILDU

für Bildung



wellcome^{trust}



DES

RESEARCH



XFE



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