The SPB/SFX Instrument: An update

Adrian Mancuso
The Single Particles, Clusters and Biomolecules and Serial Femtosecond Crystallography Instrument

Adrian Mancuso
Aim of this (short) talk

- Reminder of the possible science at SPB/SFX
- Reminder of the basic instrumentation at SPB/SFX
- Describe the key elements of the “day one” instrumentation
- Describe the key elements of the “full” instrumentation
- Provide information about where you can find more detail about each part of the instrument
  - Documentation (papers & posters)
  - People
Reminder: SPB/SFX Science

Imaging of “big” and “small” non-crystalline samples
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Crystallography of “small”, “radiation sensitive” or “dynamic” samples

Imaging of “big” and “small” non-crystalline samples

The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

Overview SPB/SFX instrument

3-16 keV

Refocusing CRLs

Two mirror systems

AGIPD 2D detection


Overview SPB/SFX instrument

Two interaction regions
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

Overview SPB/SFX instrument

- SASE1 tunnel
- SPB/SFX optics hutch
  - 1 µm Focus KB Mirror System
  - 100 nm Focus KB Mirror System
- SPB/SFX Experimental hutches
  - AGIPD-1Mpix Detector
  - AGIPD-4Mpix Detector
- Beam Offset Mirror System
- Beam Dump
- Beam Diagnostics
- SFX UC Contribution

Coherent imaging

Pump-probe

Serial Crystallography
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

The SPB/SFX instrument at a glance

SPB/SFX Experimental hutch

The SPB/SFX instrument will setup a state-of-the-art experimental instrument to study the Femtosecond Crystallography (SFX) user consortium will setup a The combined contributions of the European XFEL and the Serial Serial Femtosecond Crystallography (SFX) user consortium will setup a...

...tion data can be obtained from samples Therefore, with such femtosecond snapshots high-resolution diffraction dose far above the conventional radiation damage limits can be x-ray-induced radiation damage effects take place. Therefore, a radiation methods at atomic resolution and to initiate and follow conformations with x-ray diffractive imaging. This approach can be applied to difficult-to-study, precious biological samples of the size down to single molecules accessible by other methods such as conventional x-ray crystallography, of dynamical conformational behaviour. for time-resolved studies, keeping biological samples close to their native conformation unperturbed by radiation.

Ultrashort x-ray pulses in the range of only a few up to several 100s of fs will be used to image the ultrafast structural dynamics of these samples with femtosecond time resolution. These pulses will be generated from the primary XFEL beam using the Kirkpatrick-Baez (KB) mirror system, which will be used to focus the beam to a small spot size of 3-16 keV operation range

- 3-8 keV B₄C coating
- 8-16 keV Ru Coating

100 nm scale and 1μm scale focal spots

2 nm height error specs

In production

Probably not day one

Beam conditioning (slits, etc.)

R. Bean, A. Aquila, L. Samoylova, A. P. Mancuso, “Design of the mirror optical systems for coherent diffractive imaging at the SPB/SFX instrument of the European XFEL”, submitted
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

Optics: Compound Refractive Lenses (CRLs)

Day one focusing system
To be installed in tunnel to produce ~1 μm focal spot at the upstream interaction region

Delivery dates:
Lenses — delivered
Mechanics — Q1 2016
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

SPB/SFX “Day one” overview

- Simplified subset of instrumentation for day one
- Initially single photon energy, 60 bunches per train
- One interaction region to start
- Well suited to supporting serial crystallography experiments
- Time schedule compatible with end 2016/start 2017
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

Upstream sample environment

Both delivery and diagnostic systems are included within the sample chamber

Test chambers: now
Chamber delivery date: Nov ’16
Sample delivery systems: earlier
AGIPD 1Mpix
- Currently:
  - Final design for integration into the beamline (by SPB/SFX)
  - Assembly of 1Mpix (FS-DS)

AGIPD 4Mpix
- Downstream, for crystallography and 2nd detection plane for upstream experiments
- In-vacuum motion (transversal (x) and longitudinal (z)), two movable halves, area 40x40 cm²
- Mechanical design with FS-DS, SPB/SFX, and external company

1Mpx Delivery date to XFEL: Aug ’16
Boring but important: Hutch and infrastructure
Boring but important:
Hutch and infrastructure

and a whole lot more...
Day one summary

- Limited, day one beam properties
  - 60 bunches / train, ~ 8-9 keV $E_{ph}$
- 1 μm scale focal spot from CRLs
- Sample delivery
  - Liquid jet sample delivery
  - Aerosol injection
  - Basic fixed target sample delivery
- 1 Mpx AGIPD for 2D detection
- Essential diagnostics (inc screens)
- First “early user” experiments to exploit these parameters
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument

Overall summary

- 3–16 keV instrument, 100 nm scale and 1 μm scale focal spots
- CRL refocussing for 2nd interaction region
- Two 2D detectors (AGIPD 1Mpx and 4Mpx)
- Additional “nice to have” diagnostics
- Transition from “day one” to “full” (two interaction regions) will occur over one (1) year from “early user experiments”
- Tight but feasible time schedule to “day one”
There’s much more to know:

- See on Friday:
  - Poster #2 – S. Stern, et al, SPB/SFX Instrument
  - Poster #19 – P. Thute, et al, SPB/SFX Sample environment
  - Poster #66 – V. Lyamayev, et al, Photon Beam-stop for the SPB/SFX Instrument
  - Poster #78 – P. Vagovic, et al, Monitoring the wave front by means of single 2D phase grating

- Or anytime this week:
  - Talk to any of the team—at the posters, dinner, lunch, etc

- Or talk to us anytime

- For more details contact: adrian.mancuso@xfel.eu
Even more relevant posters...

- Poster #27 – A. Allahgholli, et al, AGIPD - The Adaptive Gain Integrating Pixel Detector
- Poster #122 – J. Sztuk-Dambietz, et al, Laboratory Infrastructure for Detector Calibration and Characterization at XFEL.EU
- Poster #123 – S. Hauf, et al, Calibration Processing at the European XFEL
- Poster #12 – K. Giewekemeyer, et al, Towards 3D Single Particle Imaging using a model, non-crystalline system with weak 3D diffraction data

and much more…
Many thanks to **Steve Readman** for exceptional assistance with the project plan, and the **SFX Executive Board** for very constructive collaboration and support. Particular thanks to **all European XFEL groups supporting** (too many to mention).
Questions?
The Single Particles, Clusters and Biomolecules, and Serial Femtosecond Crystallography (SPB/SFX) Instrument