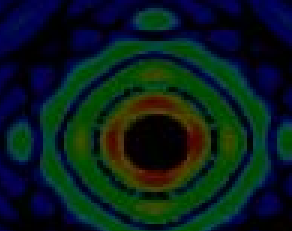


Summary & Final Discussion on Scientific Case



SPB-XFEL Workshop

Uppsala, November 2008

Franz Pfeiffer

What was presented ?

Instrumentation

- Thomas Tschentscher: Status of Euro-XFEL & SPB instrument
- Sebastien Boutet: Status of the CXI instrument at LCLS
- Christian David: Nano-Focusing XFEL beams
- Mike Bogan: Substrate-free sample injection
- Guenter Grossmann: Trapping particles
- Heinz Graafsma: Detectors (AGIPD)

What was presented ?

Concepts

- Janos Hajdu: Cell and Bio-particle experiments
- Uwe Weierstall: Serial crystallography
- Cameron Kewish: Coherent 2D membrane protein crystallography
- Colin Nave: Sub-micron crystals at XFEL and synchrotron sources
- Thomas Moeller: Structure determination of atomic clusters
- Jochen Kuepper: CDI of small but oriented biomolecules

What was presented ?

Coherent diffractive image formation & reconstruction

- Stefan Hau-Riege: Influence of radiation damage
- Pierre Thibault: Wave-front characterization
- Guyla Bortel: Classification & reconstruction of noisy diffraction patterns
- Filipe Maia: Image reconstruction of dynamic objects
- Veit Elser & Abbas Ourmazd: New reconstruction approaches

What did we learn ?

- Status of Machine & Instrument at LCLS is progressing
- Gained a more detailed picture of the design of the SPB instrument
- Great improvements in particle injection and alignment strategies
- Detector development is progressing and needs definitive input
- Wave-front characterization seems crucial for some experiments
- There might be alternatives to mirror optics (diamond FZPs, CRLs)
- Significant step forward in understanding & modeling radiation damage
- Great improvements in data analysis and reconstruction
- Observed several new approaches for 'Coherent Nano-Crystallography' (instead of: 'Crystallography without crystals')
- ...

Main scientific cases for the SPB instrument @ EU-XFEL

(as re-confirmed by the contributions presented at this workshop)

reproducible

- Structural information with atomic resolution of single particles
 - small (bio-)molecules, proteins, viruses, ...
 - other macro-molecular assemblies, etc.
- Structural information with atomic resolution of nano-crystalline assemblies
 - inorganic crystalline nano-clusters
 - protein nano-crystals (3D)
 - protein micro-crystals (2D)

non-reproducible

- 'Nano-radiography' (2D coherent imaging) of 'living' micro-organisms with nanometer resolution
 - pico-plancton
 - cells, ...

combination of these structural goals with pump-probe experiments to measure femto-second dynamics

Some Topics for Final Discussion

- Can we identify one or two specific bio-structures that we want to promote as 'scientific drivers' ?
- How important is the scientific case for 2D 'nano-radiography' at SPB,
 - if we consider competing techniques, *i.e.*, electron cryo-tomography
 - if we consider the non-ideal wave-length
- Desired future XFEL machine improvements
 - shorter pulses or more flux ?
 - how important is seeding for us ('longitudinal coherence') ?
- ...