Overview European XFEL

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Summary

- 1. Introduction - The Quest for Brilliance
- 2. From Storage Rings to Linear Accelerators
- 3. Scientific Case of the European XFEL
- 4. Status of the Project

Accelerator Based Light Sources

- **FIRST GENERATION:** Accelerators and storage rings built for other purposes, parasitically used as light sources

- **SECOND GENERATION:** Dedicated rings designed and optimised as light sources

- **THIRD GENERATION:** Dedicated rings built to maximise brilliance by reducing the beam emittance (electron phase space volume) and by the extensive use of undulators as light sources

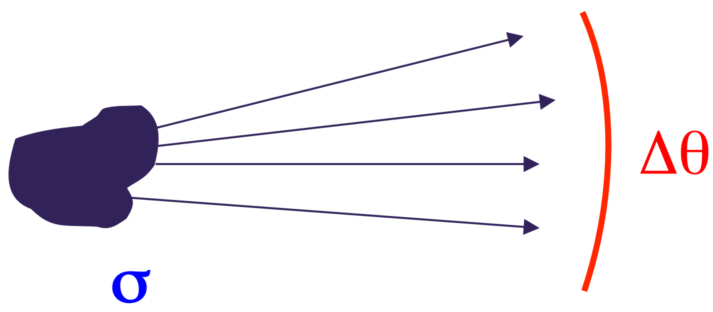
- **"FOURTH+" GENERATION:** Diffraction-limited VUV and X-ray sources, with full spatial coherence: "Ultimate" Storage Rings, Free-electron lasers based on Linacs, Energy-Recovery Linacs.

Brilliance/Spectral Brightness

FLUX OF PHOTONS IN UNIT SPECTRAL RANGE

(SOURCE AREA) X (BEAM DIVERGENCE)

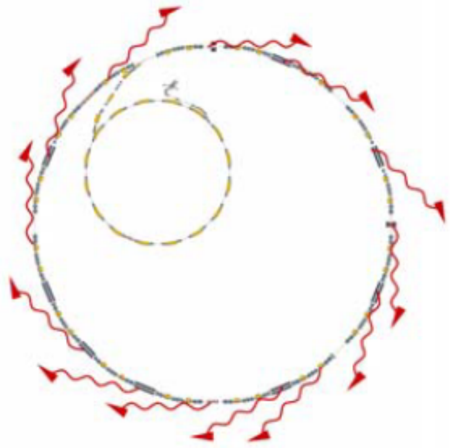
Units: photons/s/mm^2/mrad^2/0.1%BW



$$B=\frac{\Phi}{\sigma\,\Delta\theta_h\,\Delta\theta}$$

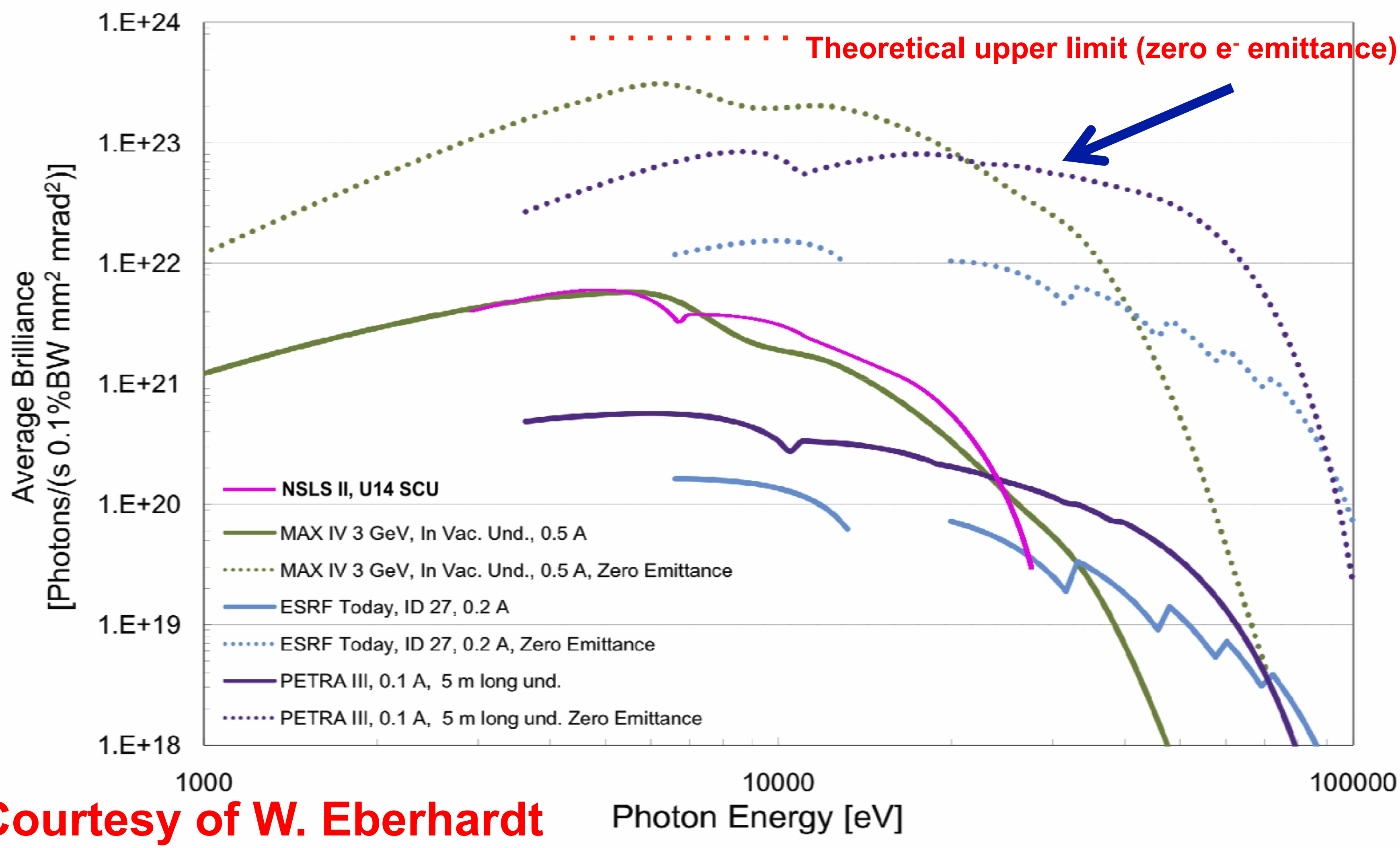
Important properties of storage ring sources

- High pulse-to-pulse reproducibility
- High stability of intensity, position, spectral properties
- High repetition rate
- Geometry allowing a large number of source points/beamlines and instruments operated in parallel



However,

Fundamental limits to storage rings brilliance



Courtesy of W. Eberhardt

Time Scales for Dynamics

Molecules

Phase relaxation
electronic transitions
vibrations

Intramolecular vibrational redistribution

Intermolecular energy transport

Electronic radiation lifetimes

10^{-9} s

10 fs | 100 fs | 1 ps | 10 ps | 100 ps | 1 ns | Time

Quantum kinetics
(carriers & phonons)

Energy transfer to lattice
Hot phonon effects

Phase relaxation
interband continuum/excitons

Phonon propagation

Intraband and intersubband
redistribution of carriers

Solids

Spatially coherent X-ray sources

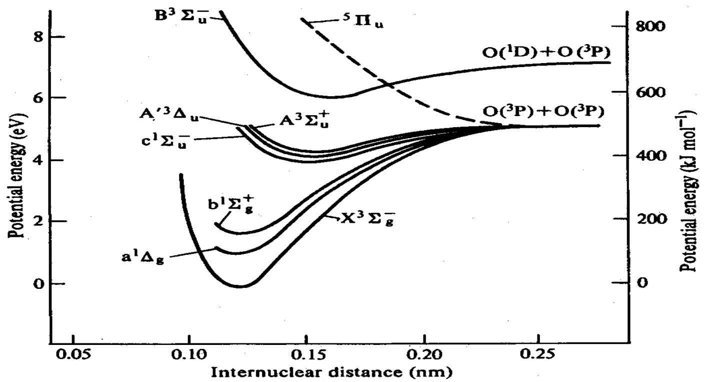
Compression of electron bunches to <100 fs preserving (or even increasing) the brilliance and number of photons per bunch is impossible in a storage ring configuration, where the same electrons run through the undulators ~ 10^6 times per second.

This can however be achieved in a single-pass machine such as a linear accelerator, with suitable bunch compressors.

In addition, in a linac, emittance ε is NOT conserved, but $\varepsilon_n = \gamma\varepsilon \sim$ const., with $\gamma = E/mc^2$. It is then possible to reach the condition in which $\varepsilon \sim \lambda$.

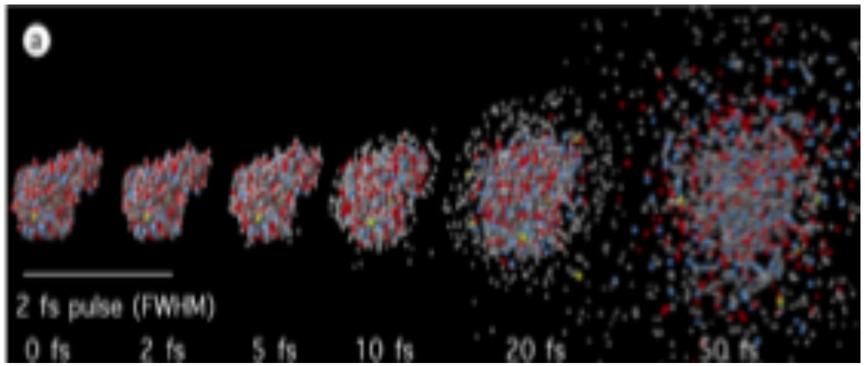
Wanted…A more brilliant X-ray source, with:

wavelength down to ~ 0.1 nm ==> *atomic-scale resolution*



ultrashort (<1 ps) pulses
==> "molecular movies"

ultra-high peak brightness
==>investigation of matter under extreme conditions…



transverse spatial coherence
==> imaging of single nanoscale objects, possibly down to individual macromolecules (no crystals)

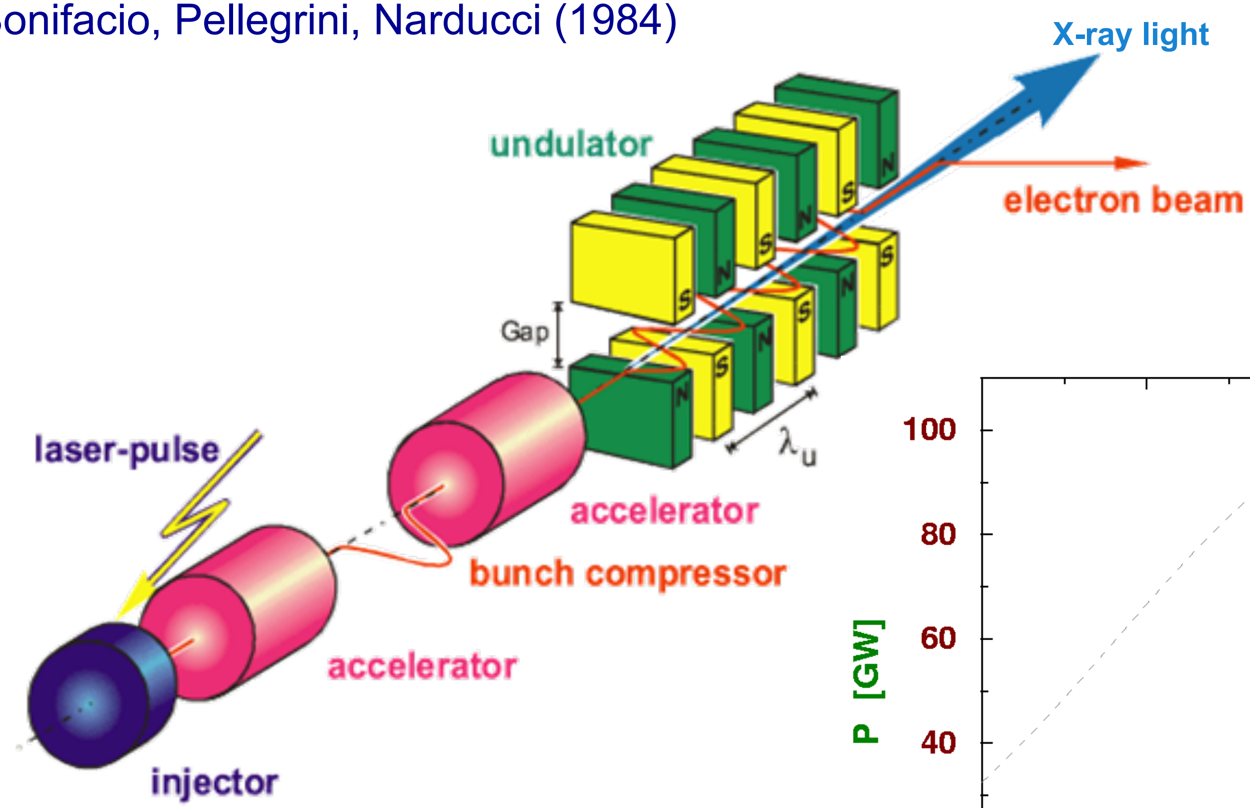
European XFEL

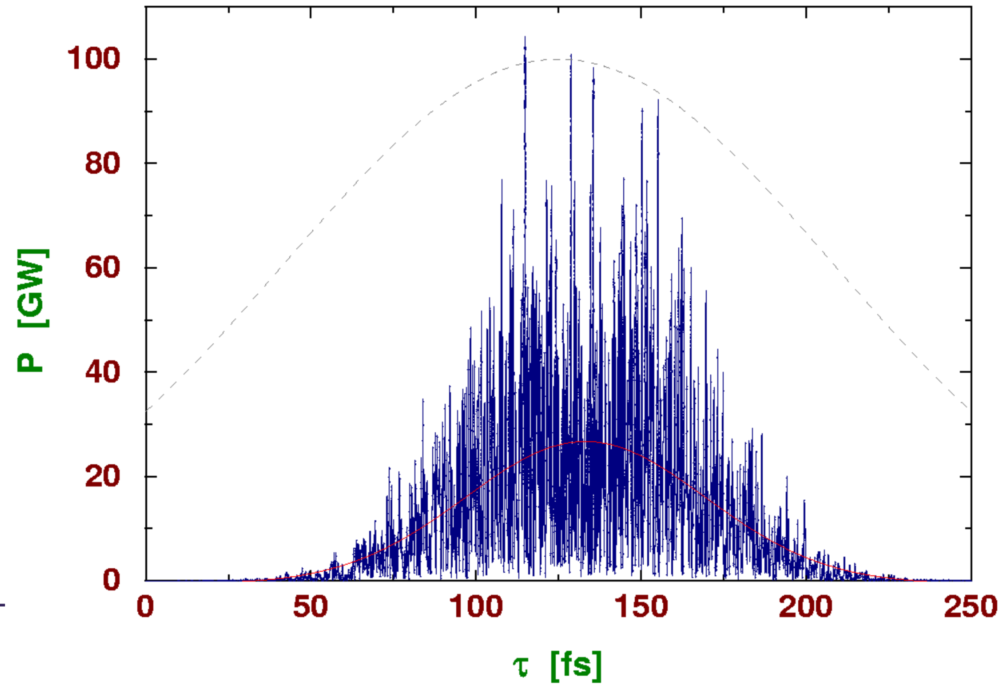
Free Electron Lasers

SASE – Self-Amplified Spontaneous Emission

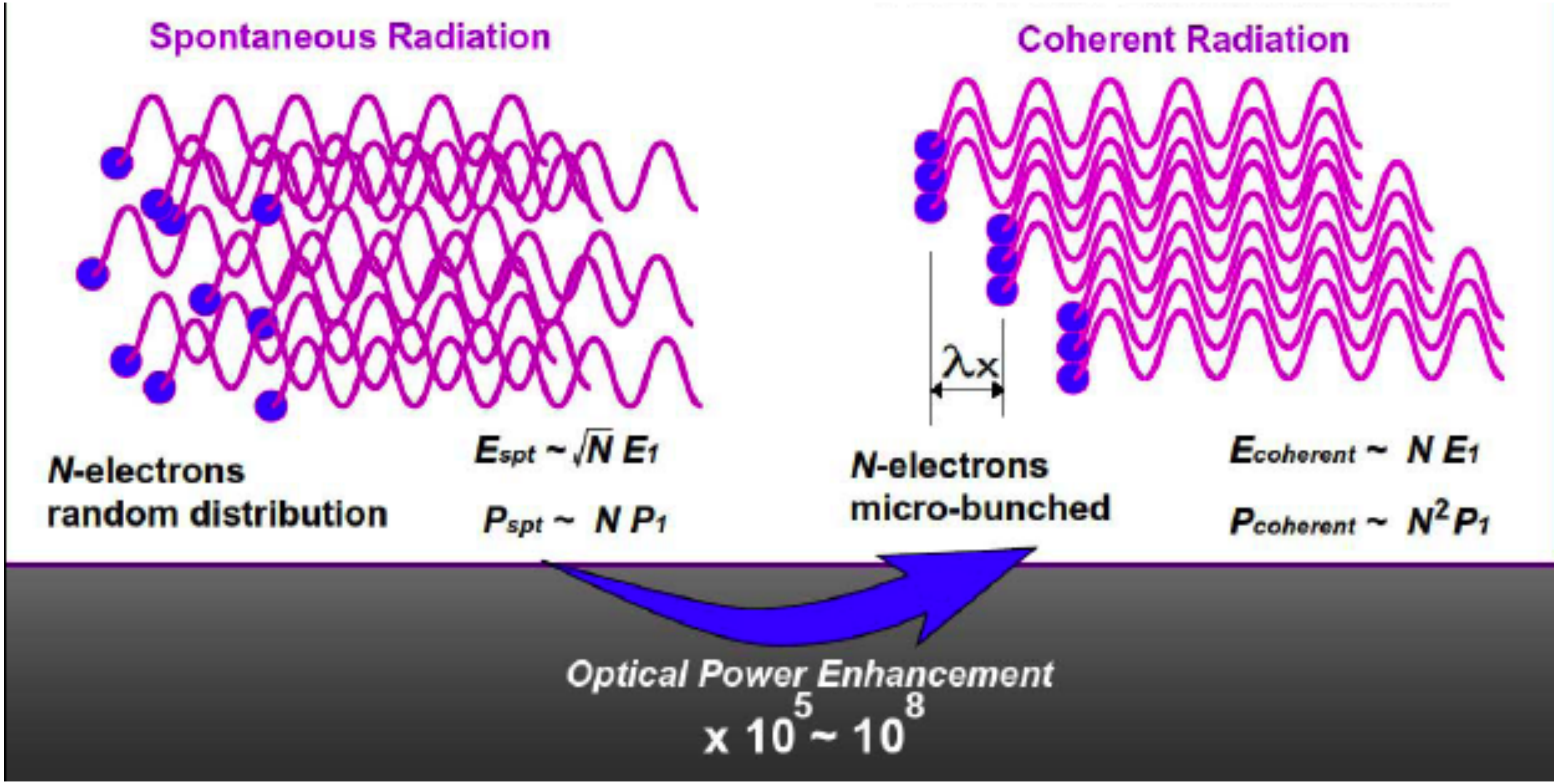
Kondratenko, Saldin (1979)

Bonifacio, Pellegrini, Narducci (1984)



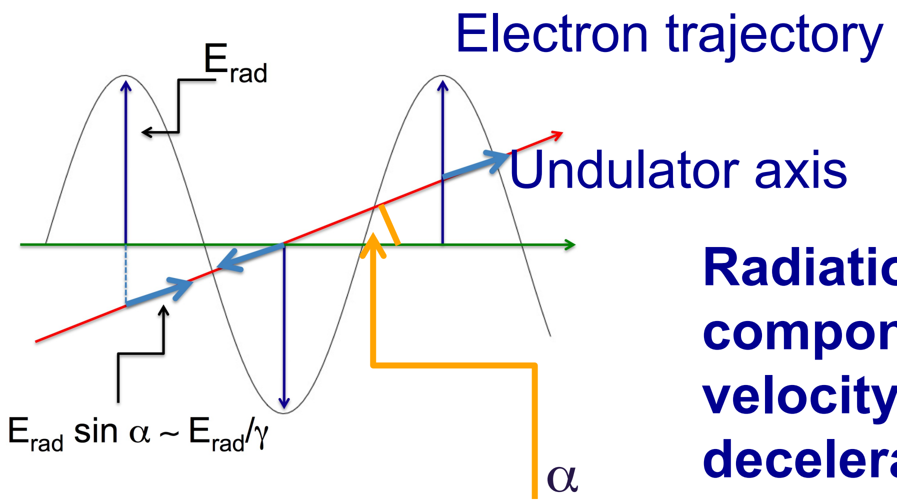


Spontaneous vs. coherent rad. in Undulators

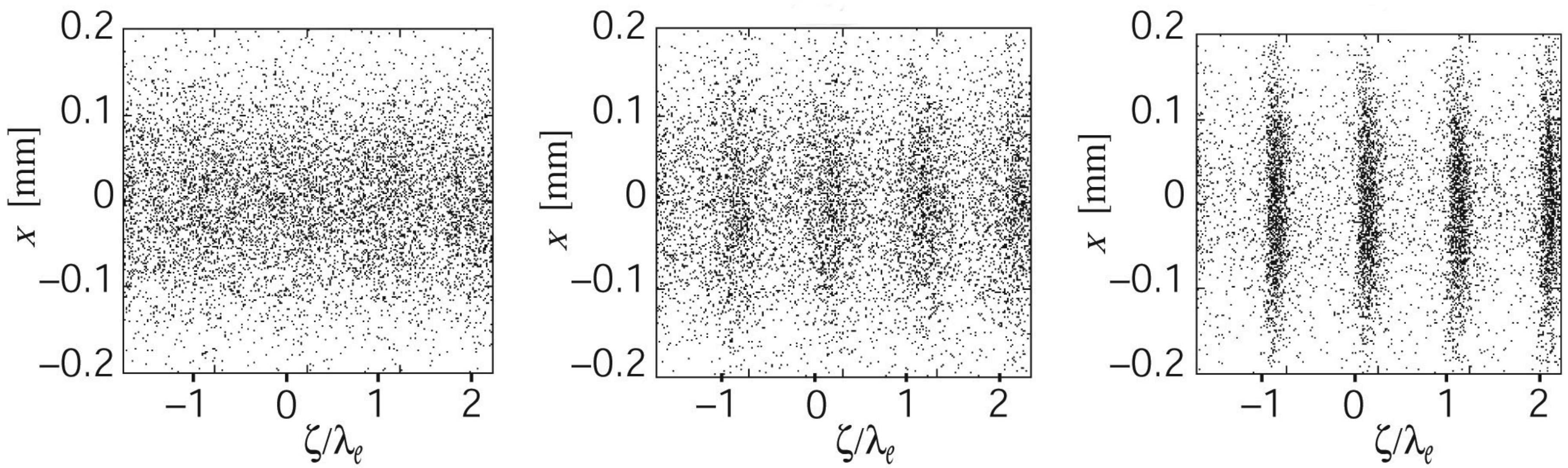


(after T. Shintake)

Origin of Microbunching

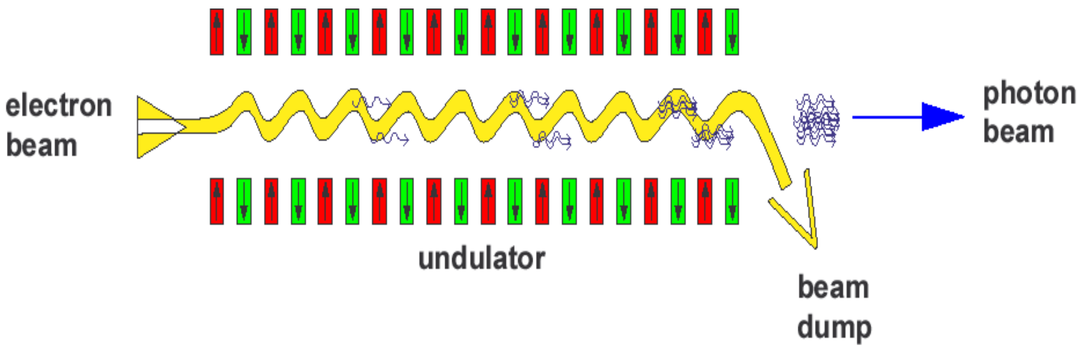


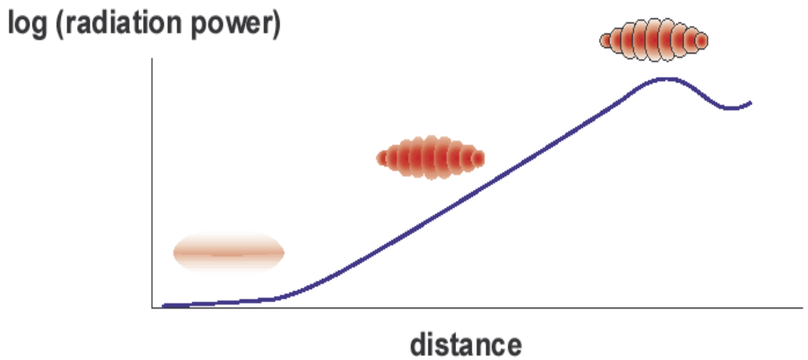
Radiation electric field has a small component parallel to electron velocity, which can accelerate or decelerate electrons



Self-Amplified Spontaneous Emission

Tightly collimated (low emittance) electron beam in a long undulator: coherent emission results from microbunching, produced by amplification of shot-noise density fluctuations at the resonant wavelength by the radiation, as it progresses through the bunch.

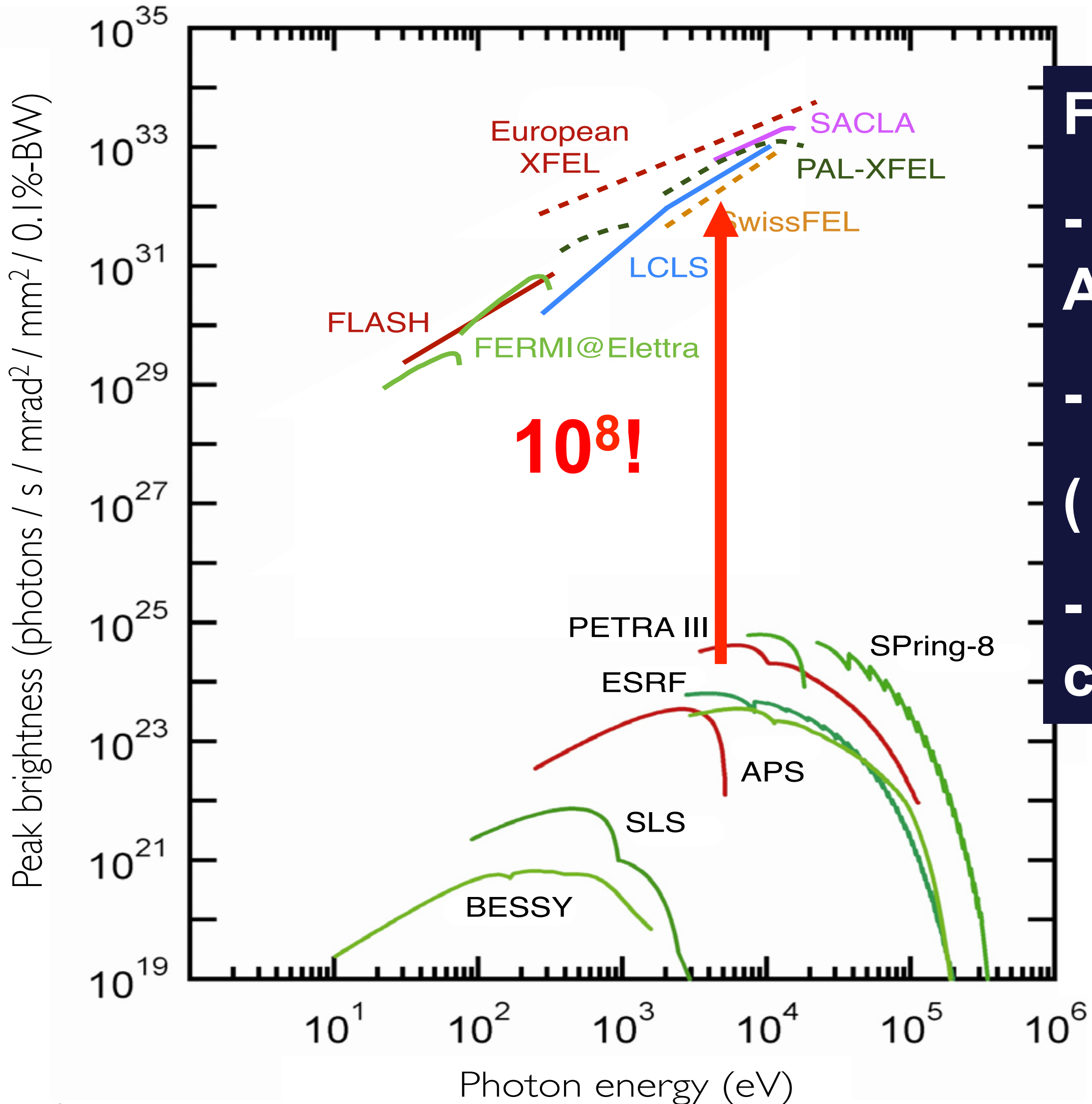




Peak Power:

~ 10 GW

Comparison of synchrotron and FEL sources



Free Electron Lasers:

- Based on Linear Accelerators

- Deliver ultrashort pulses

(< 100 fs = 0.1 ps= 10^{-13} s)

- (Transversely) Spatially coherent (laser-like) radiation

Today's state of the art

- **FLASH** – Ultraviolet and soft x-ray FEL user facility in Hamburg (down to λ ~ 4.5 nm), in operation since 2005
- **LCLS** (Linac Coherent Light Source) first hard X-ray FEL using 13.6 GeV electrons from SLAC Linac, first beam April 10, 2009
- **FERMI@ELETTRA** (Trieste, Italy) λ ~ 100 – 1 nm, "Seeded" FEL, First beam Dec. 2010
- **SACLA**, Spring-8, Japan, hard X-ray FEL, 8 GeV Linac, down to λ ~ 0.08 nm, First beam April 2011

European XFEL

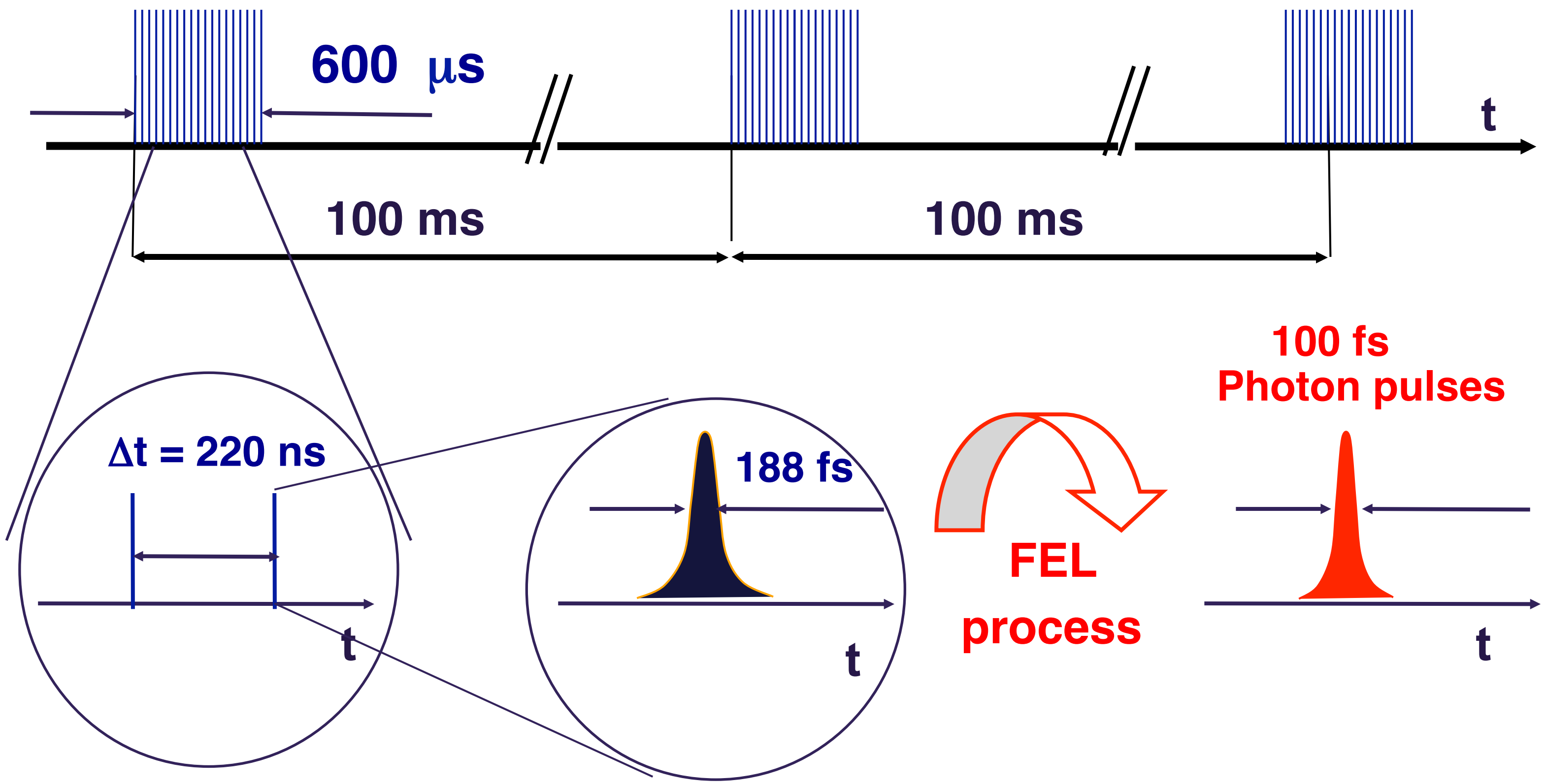
Comparison of the hard X-ray FEL Projects

Project	LCLS I, US	SACLA, JP	European XFEL	SwissFEL, CH	PAL-XFEL, KR	LCLS II, US
Max. electron energy (GeV)	14.3	8.5	17.5	5.8	10	4
Wavelength range (nm)	0.13−4.4	0.06−0.3	0.05−4.7	0.1−7	0.06−10	0.25 – 4.7
Photons/pulse	~ 10^{12}	2 x 10^{11}	~ 10^{12}	~ 3.6 x 10^{10}	10^{11}−10^{13}	2 10^{11} – 2 10^{10}
Peak brilliance	2 x 10^{33}	1 x 10^{33}	5 x 10^{33}	7 x 10^{32}	1.3 x 10^{33}	
Pulses/second	120	60	27 000	100	60	10^5 - 10^6
Date of first beam	2009	2011	2016	2016	2015	2019

European XFEL

European XFEL Project - Time Structure

Electron bunch trains
(with up to 2700 bunches à 1 nC)



Limits of Synchrotron for Bio-crystallography

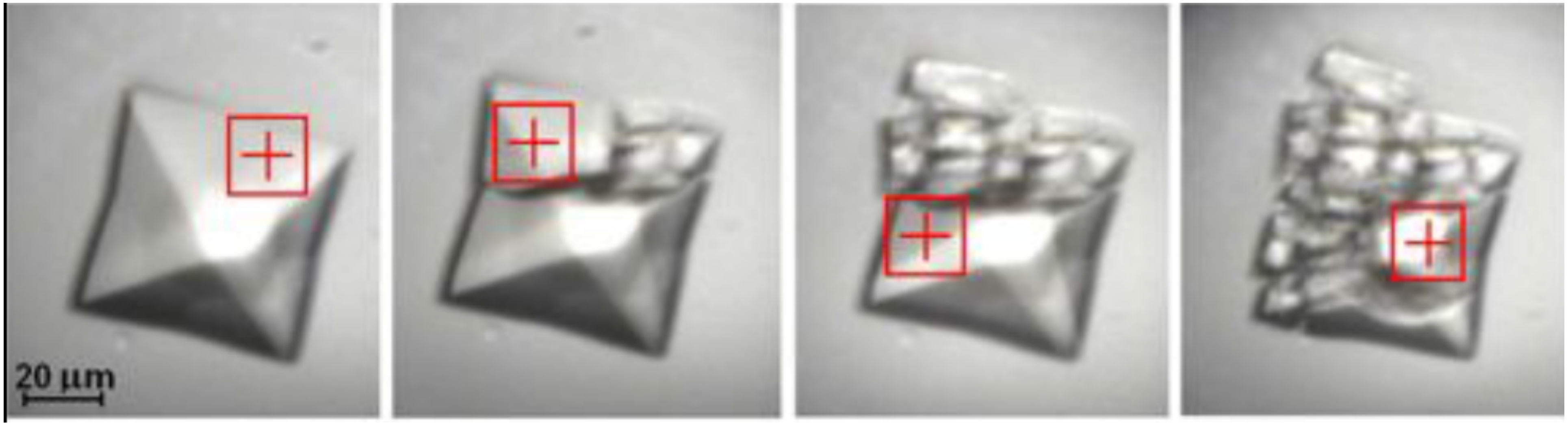
- In spite of its extraordinary success, synchrotron bio-crystallography meets some limitations:

  - Need for crystals > (10-100 μm)^3 (membrane proteins?)

  - Radiation damage limits resolution… freezing a partial remedy

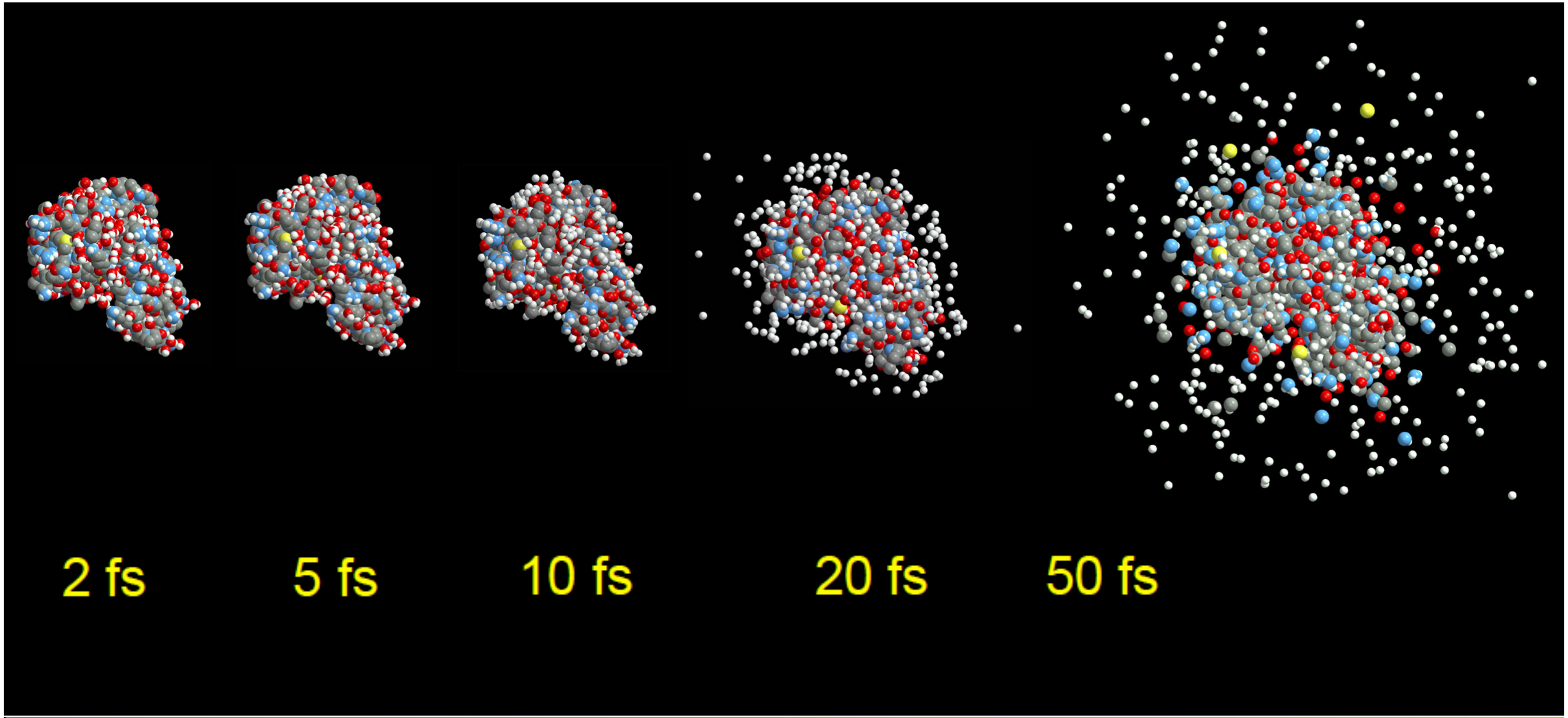
Crystal of Bovine Enterovirus 2 (BEV 2), 0.5 s, 10^8 ph/μm^2

D. Axford et al., Acta Cryst D68, 592 (2012)



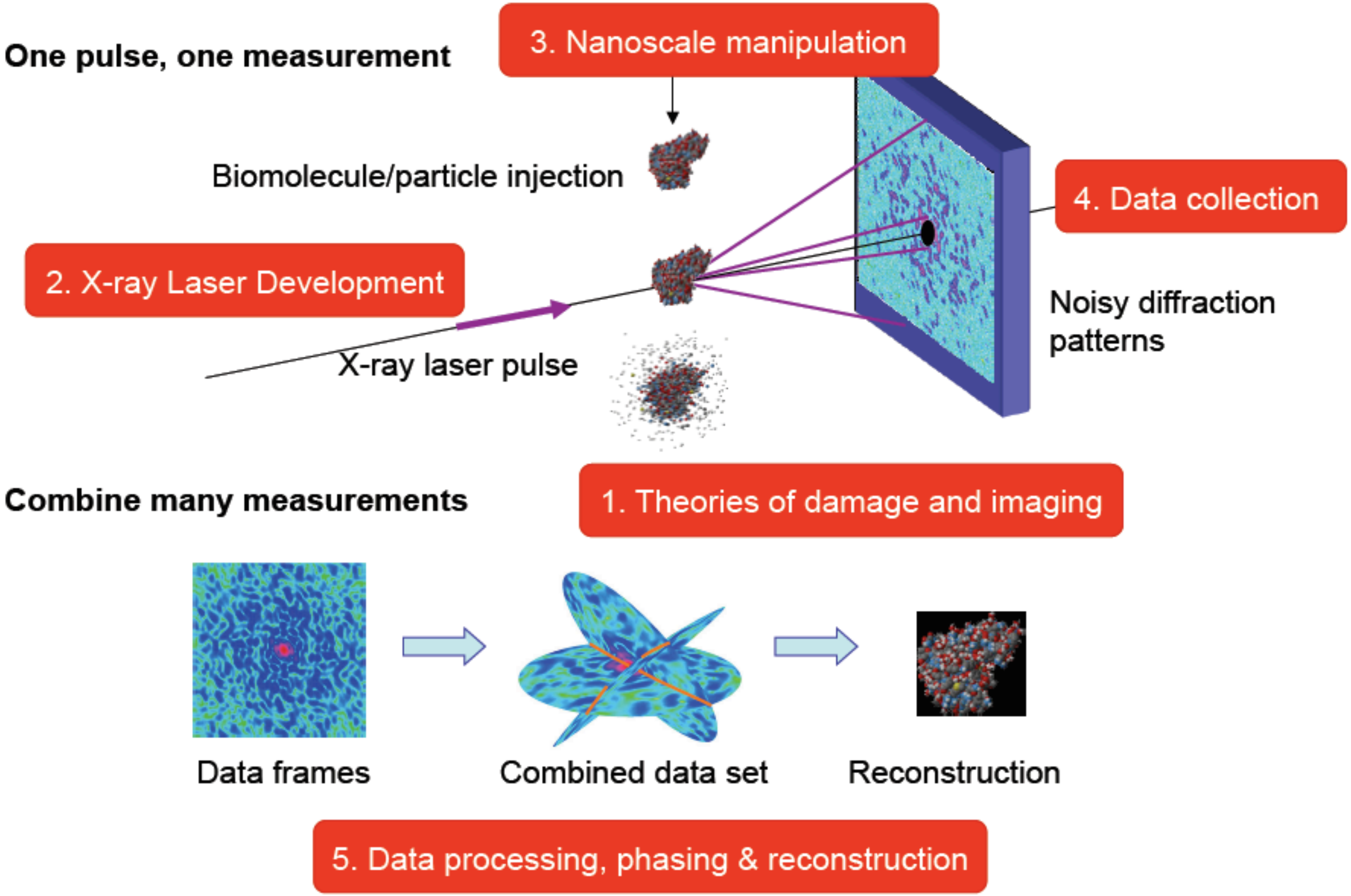
Speed may be the answer!

"Diffraction before destruction" ***1 fs = 10^{-15} s***



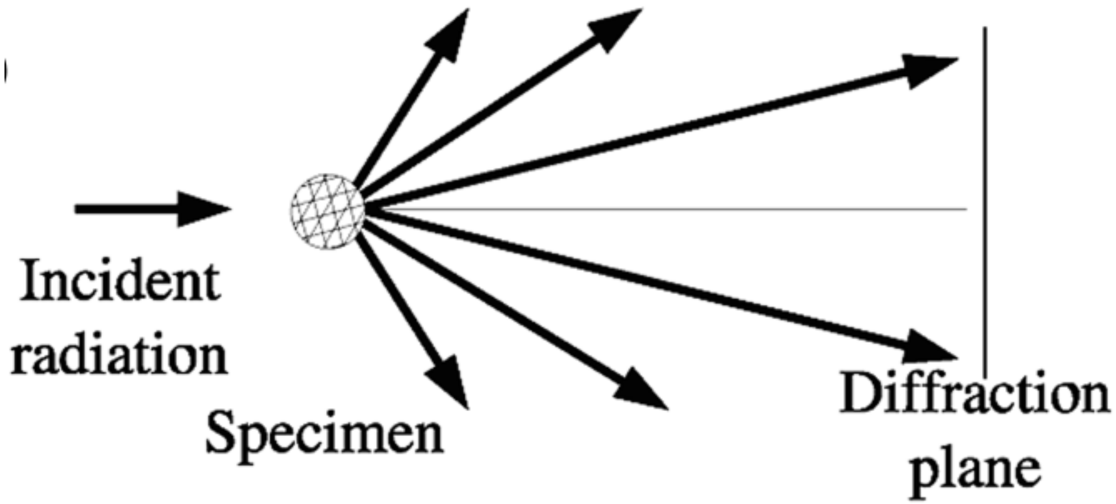
R. Neutze, R. Wouts, D. van der Spoel, E. Weckert, J. Hajdu, Nature **406** (2000)

Single-Molecule X-ray Imaging

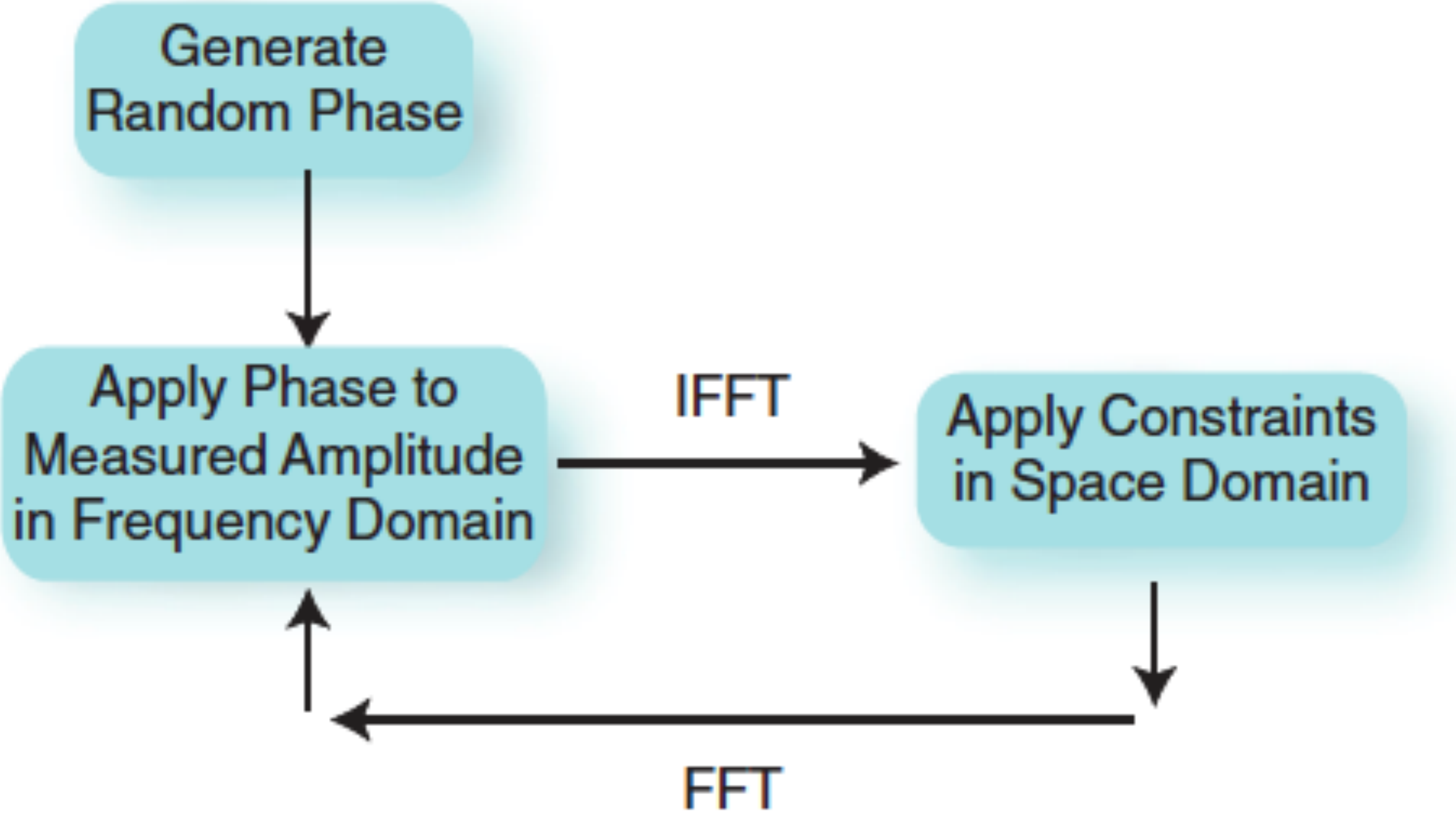


Phase retrieval, oversampling and all that

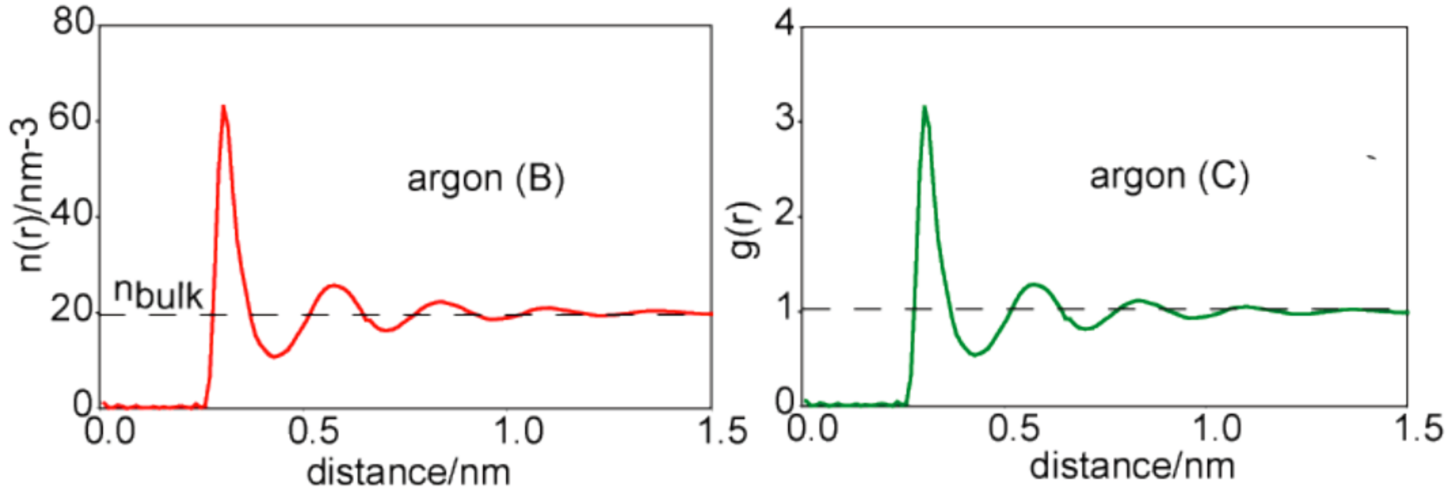
- D. Sayre, 1991:
- Phase can be retrieved and problem solved, for non-periodic objects, if sufficient information is collected, by "oversampling" diffraction pattern

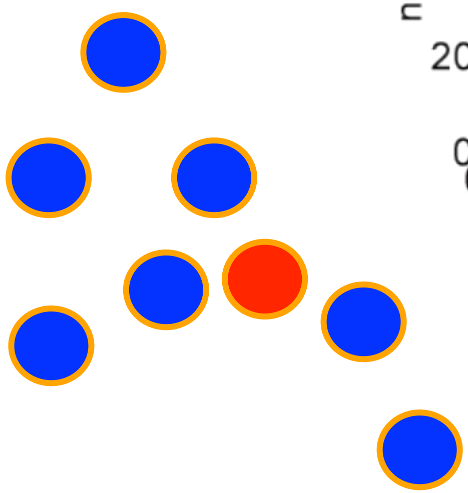


Reconstruction iterative algorithm in a nutshell



X-ray Diffraction: liquids!



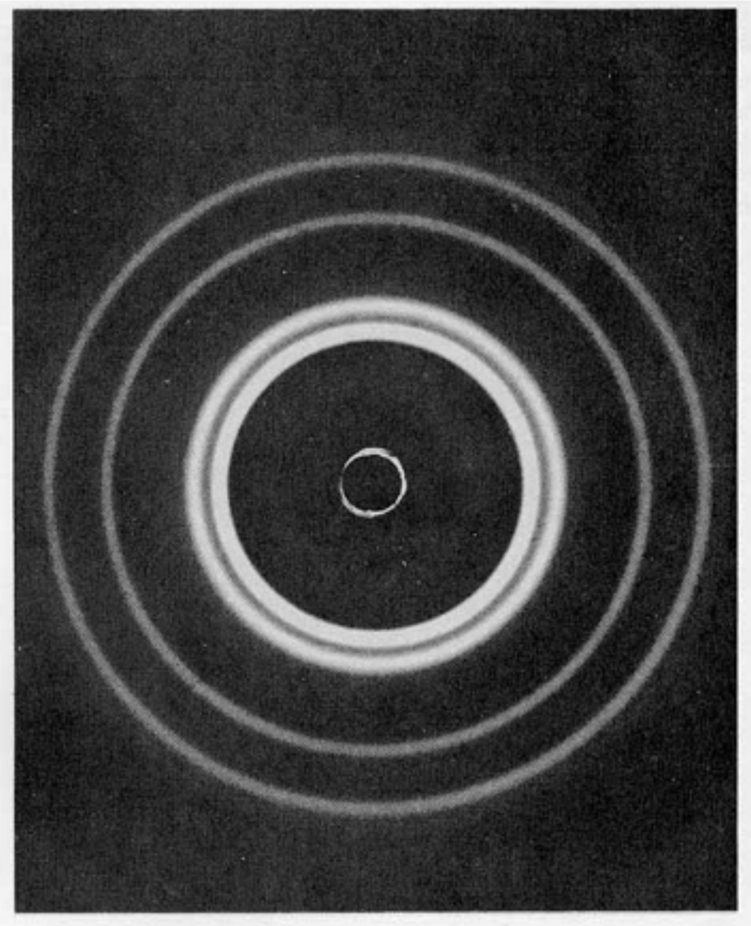


$$S(q) - 1 = \rho_o \int [g(\boldsymbol{r}) - 1]\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\, d\boldsymbol{r}$$

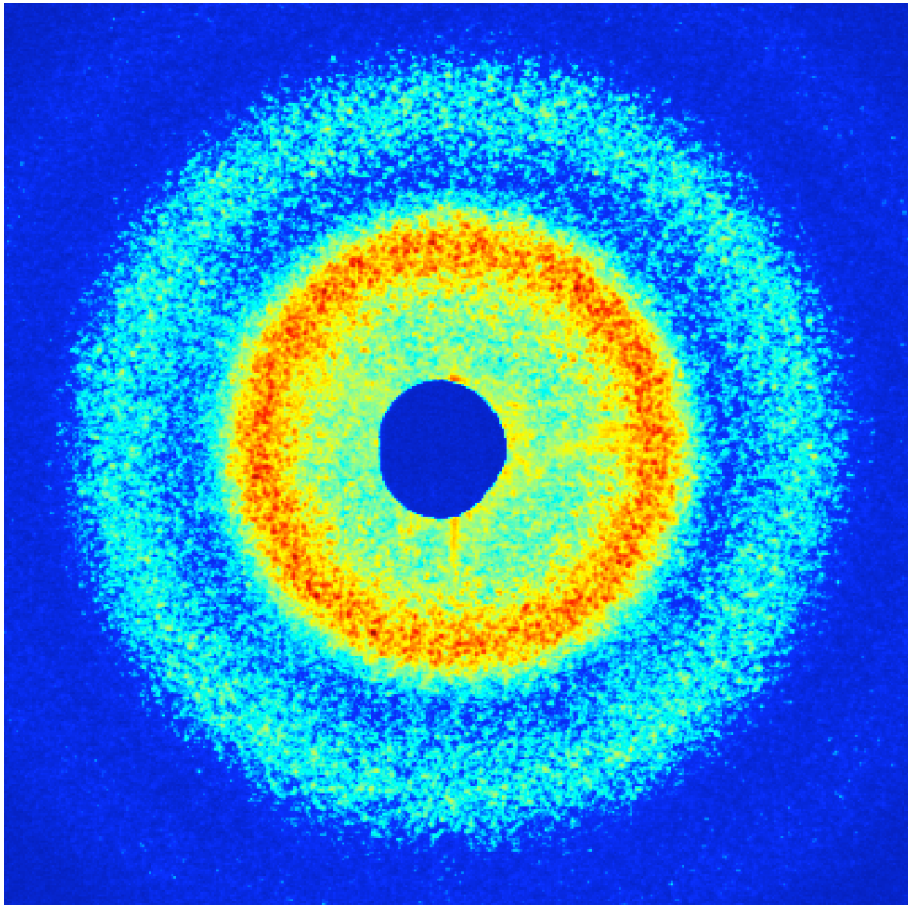
$$g(\boldsymbol{r}) - 1 = \frac{1}{\rho_o (2\pi)^3} \int [S(\boldsymbol{q}) - 1]\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\, d\boldsymbol{q}$$

Liquid

X-ray diffraction from liquids…



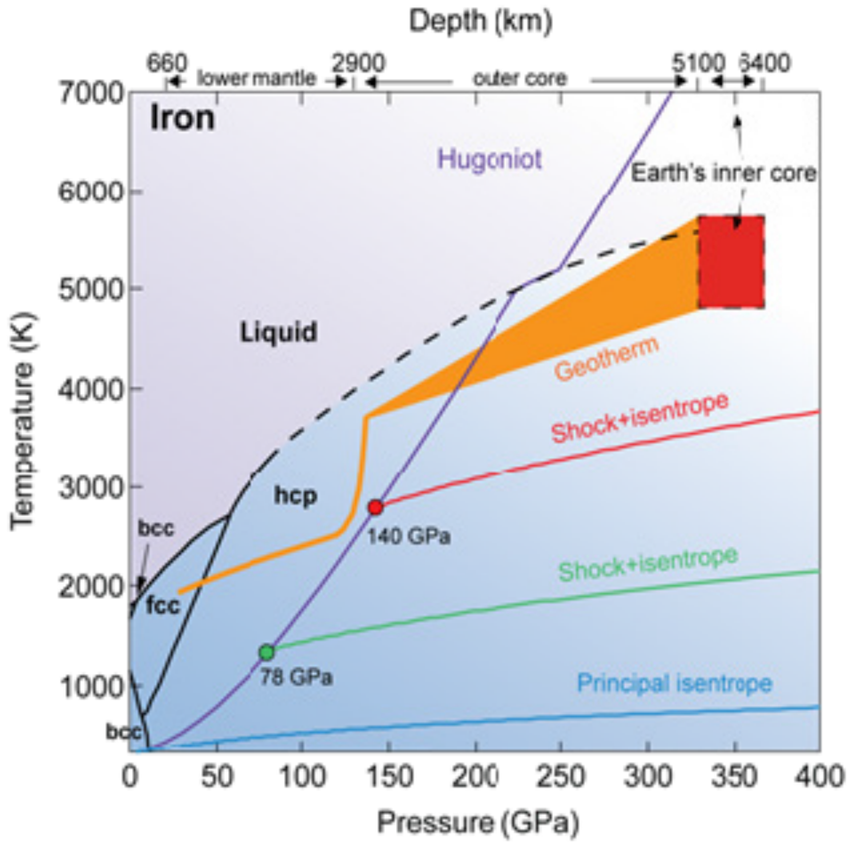
Slow, incoherent…

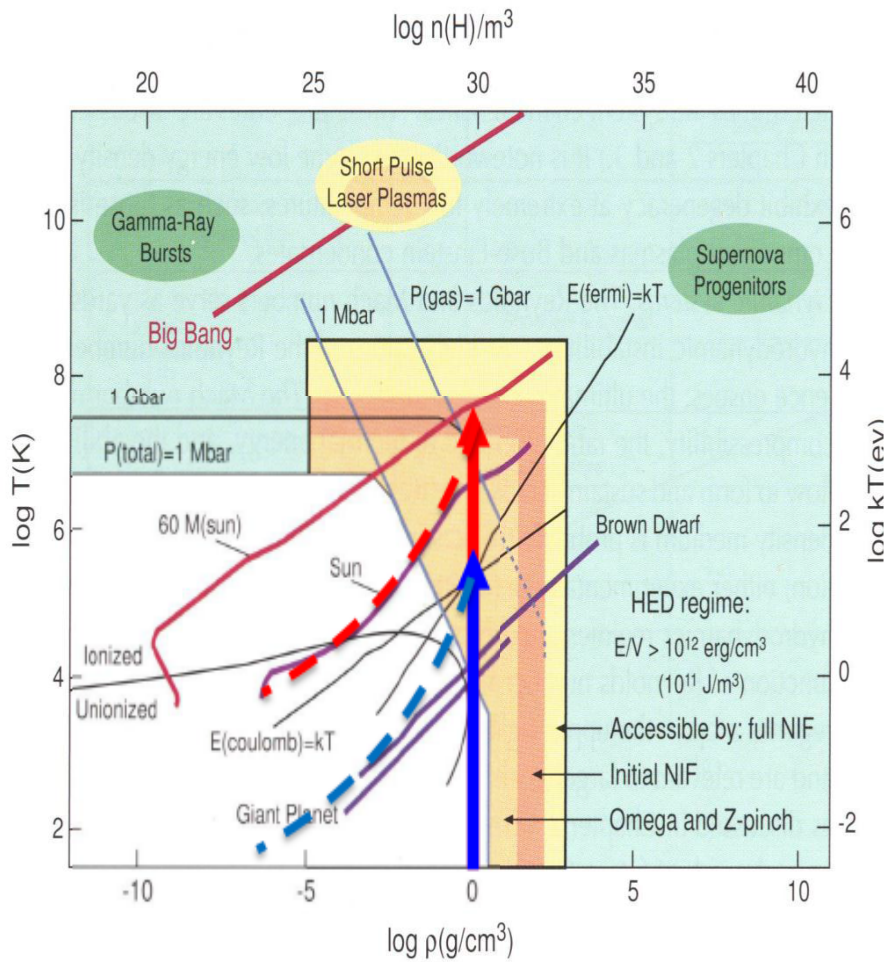


Fast, coherent => Speckles!
“Hologram”

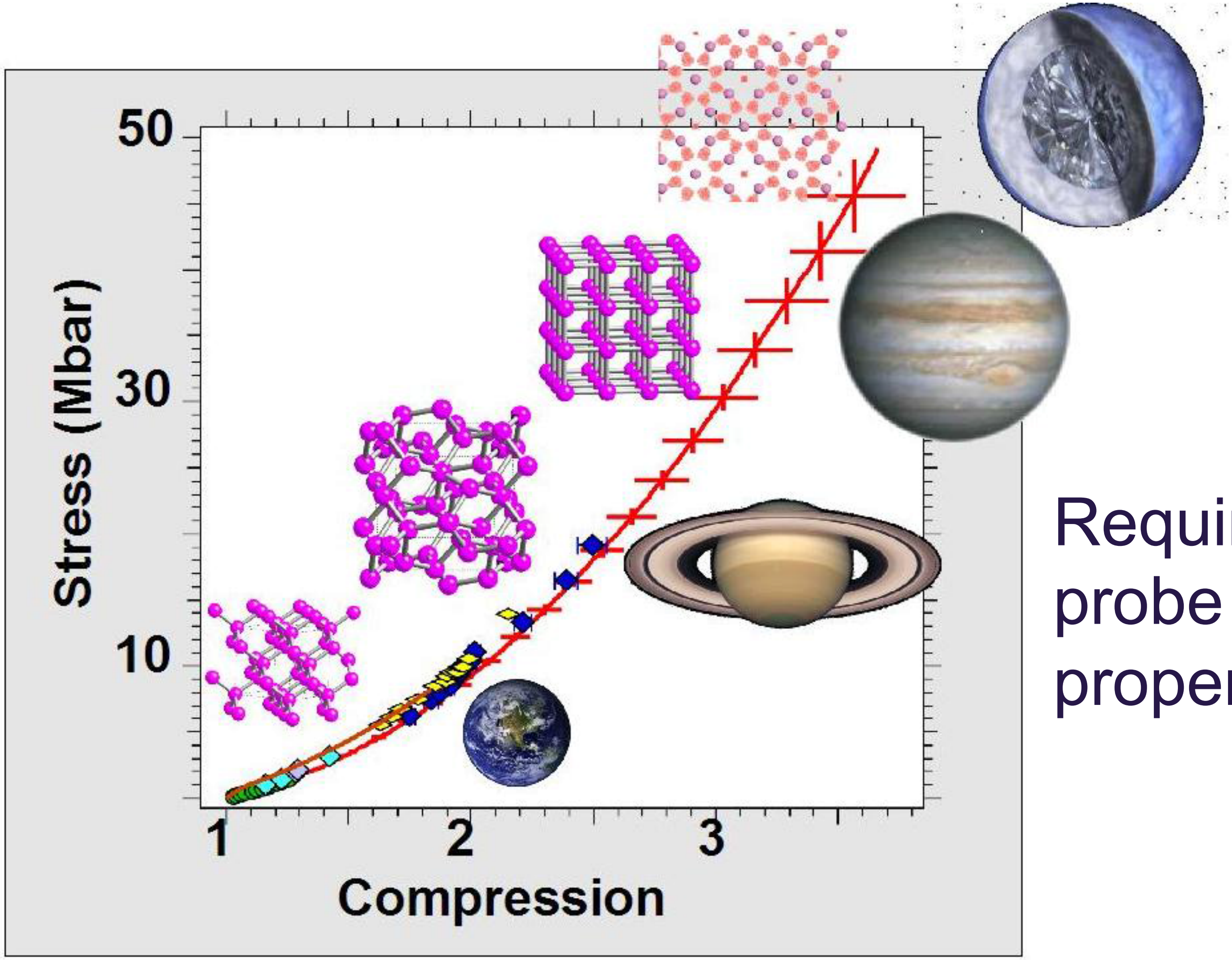
Laser excitation with ~ Terawatt (and up!) power

- Shock compression along Hugoniot (kJ, ~ ns pulse profile)
- Ramped (isoentropic) shock-free compression, with careful optimization of pulse profile
- Isochoric Heating (very short pulse, x-ray laser)





Structural transitions during laser pulse

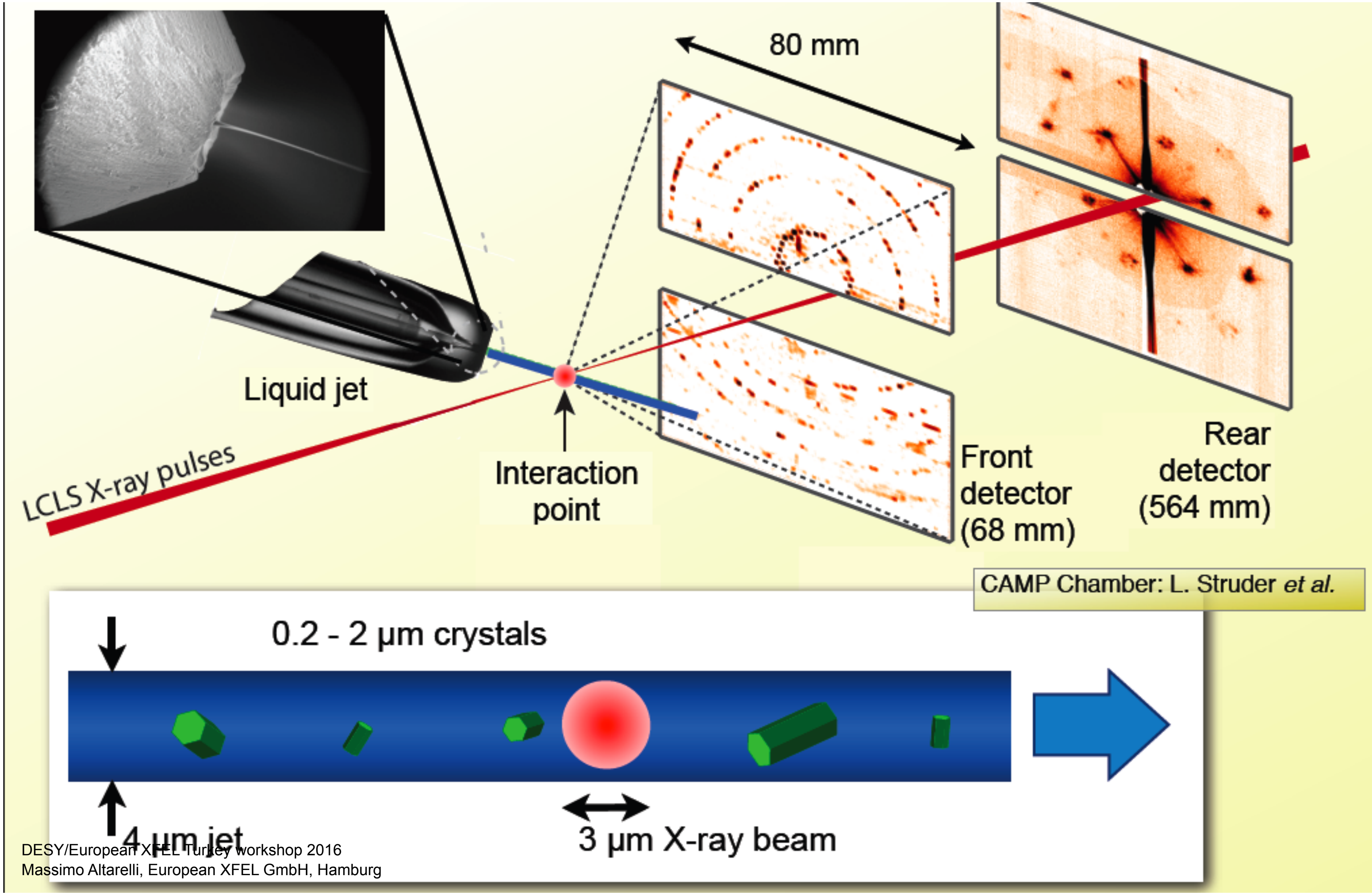


Requires fast probe of structural properties!

Examples of results from the LCLS, Stnaford

- Serial Femtosecond Crystallography of biomolecules: nanocrystals
- Liquid phases and nucleation: birth of a crystal
- Real time observation of vibrational modes of nanocrystals

Nanocrystallography at LCLS, H. Chapman et al.



“Serial Femtosecond Crystallography”, LCLS

Natively Inhibited *Trypanosoma brucei* Cathepsin B Structure Determined by Using an X-ray Laser

Lars Redecke *et al.*

Science **339**, 227 (2013);
DOI: 10.1126/science.1229663

Henry N. Chapman

2.1 Å resolution

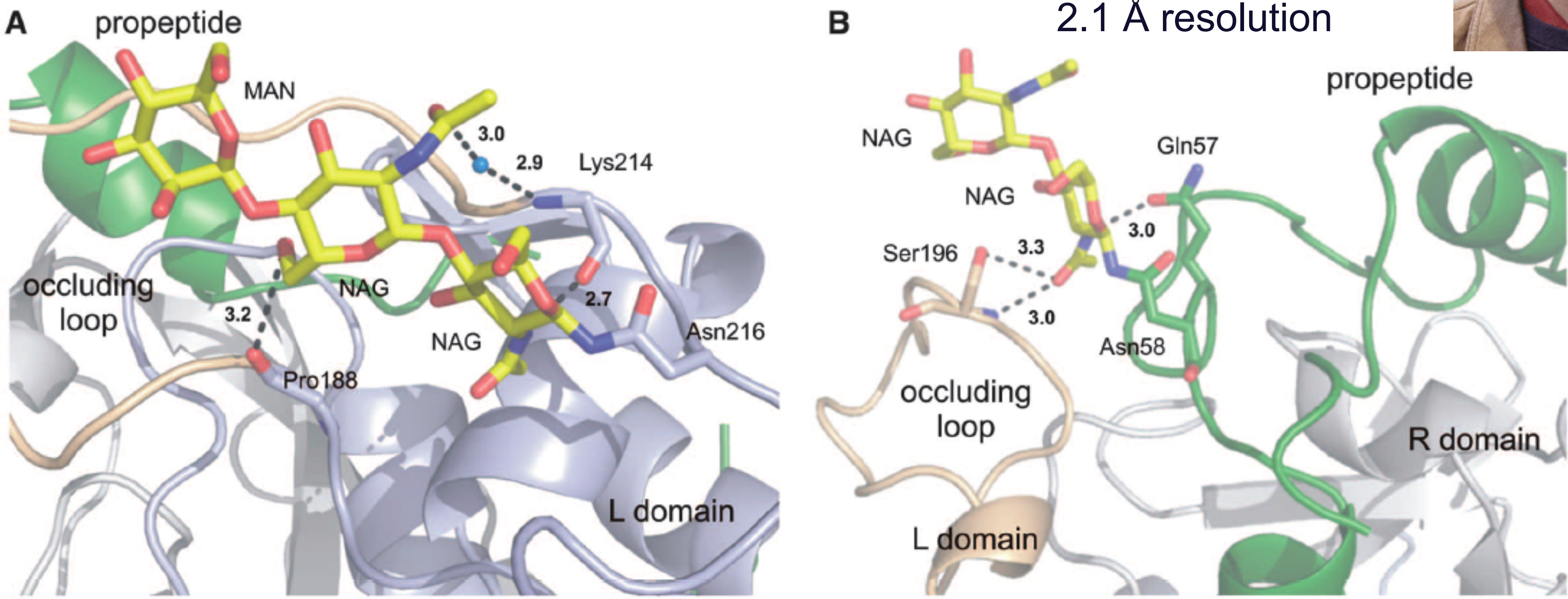


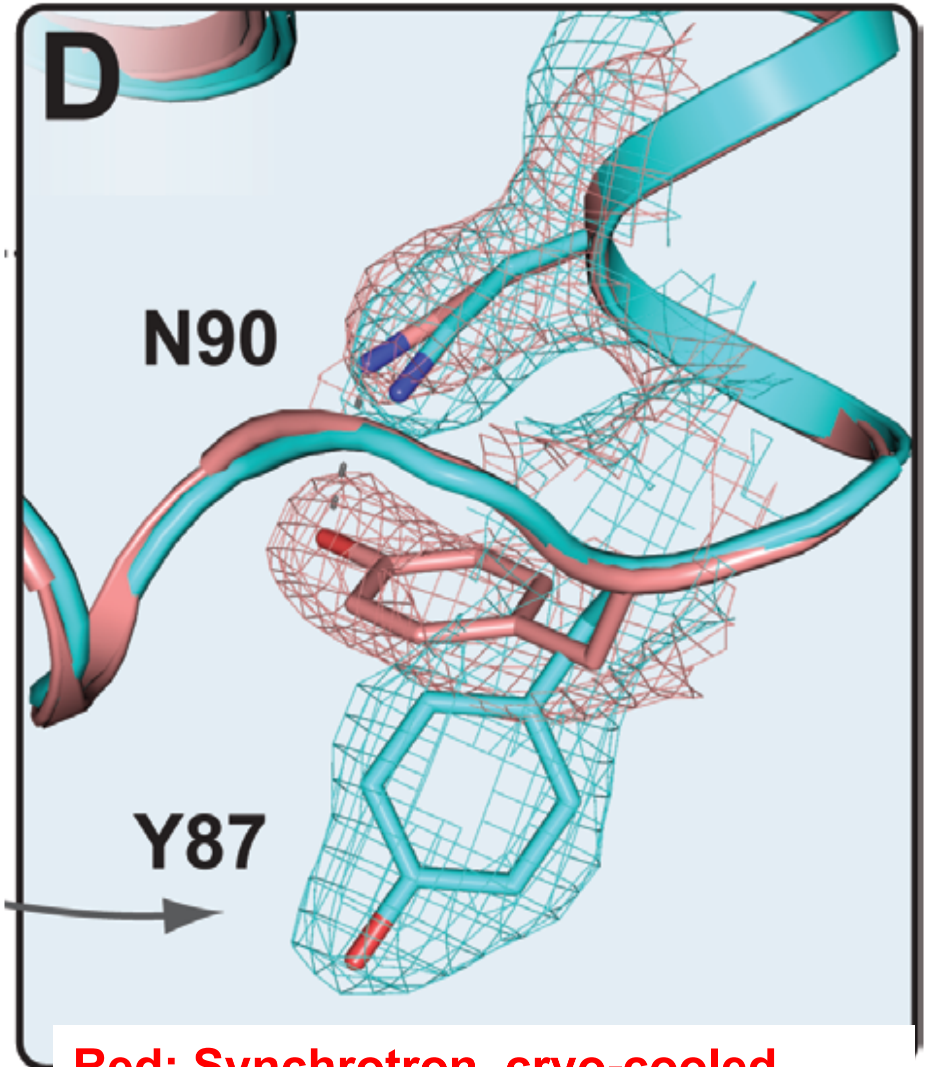
Fig. 4. Glycosylation of the TbCatB-propeptide complex. (**A**) Enzyme carbohydrate structure comprising two NAG and one MAN residue (yellow) N-linked to Asn^{216} C-terminal of the occluding loop (beige). The carbohydrate structure connects both occluding loop strands by two direct and one water-bridged H bond (black dashed lines). (**B**) Propeptide glycosylation site comprising two NAG units (yellow) at Asn^{58} within the kinked region of the propeptide (green). The propeptide carbohydrate structure forms an H bond to Gln^{57} of the propeptide and two H bonds to Ser^{196} at the tip of the occluding loop (beige), which stabilize its open conformation. Color codes correspond to Fig. 1C.

Science 342, 1521-1524 (2013)

Serial Femtosecond Crystallography of G Protein–Coupled Receptors

Wei Liu,[1] Daniel Wacker,[1] Cornelius Gati,[2] Gye Won Han,[1] Daniel James,[3] Dingjie Wang,[3] Garrett Nelson,[3] Uwe Weierstall,[3] Vsevolod Katritch,[1] Anton Barty,[2] Nadia A. Zatsepin,[3] Dianfan Li,[4] Marc Messerschmidt,[5] Sébastien Boutet,[5] Garth J. Williams,[5] Jason E. Koglin,[5] M. Marvin Seibert,[5,6] Chong Wang,[1] Syed T. A. Shah,[4] Shibom Basu,[7] Raimund Fromme,[7] Christopher Kupitz,[7] Kimberley N. Rendek,[7] Ingo Grotjohann,[7] Petra Fromme,[7] Richard A. Kirian,[2,3] Kenneth R. Beyerlein,[2] Thomas A. White,[2] Henry N. Chapman,[2,8,9] Martin Caffrey,[4] John C. H. Spence,[3] Raymond C. Stevens,[1] Vadim Cherezov[1]*

G-protein coupled receptor



Red: Synchrotron, cryo-cooled

Green: LCLS, nanocrystallography

Science 346, 1242 (2014): first time-dep. studies

STRUCTURAL BIOLOGY

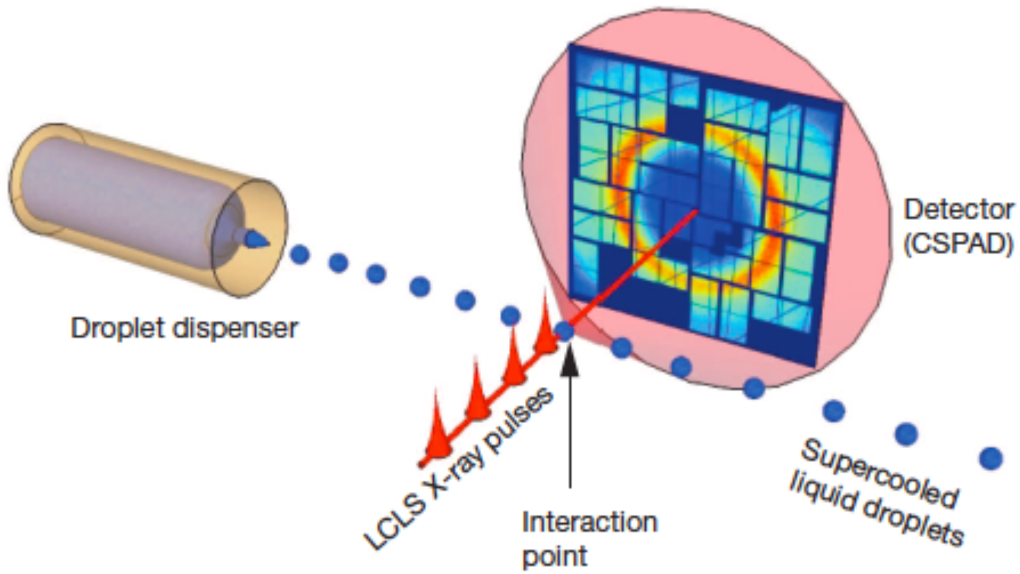
Time-resolved serial crystallography captures high-resolution intermediates of photoactive yellow protein

Jason Tenboer,[1] Shibom Basu,[2] Nadia Zatsepin,[3] Kanupriya Pande,[1] Despina Milathianaki,[4] Matthias Frank,[5] Mark Hunter,[5*] Sébastien Boutet,[4] Garth J. Williams,[4] Jason E. Koglin,[4] Dominik Oberthuer,[6] Michael Heymann,[7] Christopher Kupitz,[2†] Chelsie Conrad,[2] Jesse Coe,[2] Shatabdi Roy-Chowdhury,[2] Uwe Weierstall,[3] Daniel James,[3] Dingjie Wang,[3] Thomas Grant,[8] Anton Barty,[7] Oleksandr Yefanov,[7] Jennifer Scales,[1] Cornelius Gati,[6,7] Carolin Seuring,[6] Vukica Srajer,[9] Robert Henning,[9] Peter Schwander,[1] Raimund Fromme,[2] Abbas Ourmazd,[1] Keith Moffat,[9,10] Jasper J. Van Thor,[11] John C. H. Spence,[3] Petra Fromme,[2] Henry N. Chapman,[6,7] Marius Schmidt[1‡]

Serial femtosecond crystallography using ultrashort pulses from x-ray free electron lasers (XFELs) enables studies of the light-triggered dynamics of biomolecules. We used microcrystals of photoactive yellow protein (a bacterial blue light photoreceptor) as a model system and obtained high-resolution, time-resolved difference electron density maps of excellent quality with strong features; these allowed the determination of structures of reaction intermediates to a resolution of 1.6 angstroms. Our results open the way to the study of reversible and nonreversible biological reactions on time scales as short as femtoseconds under conditions that maximize the extent of reaction initiation throughout the crystal.

J. Sellberg et al., Nature 510, 381 (2014)

a

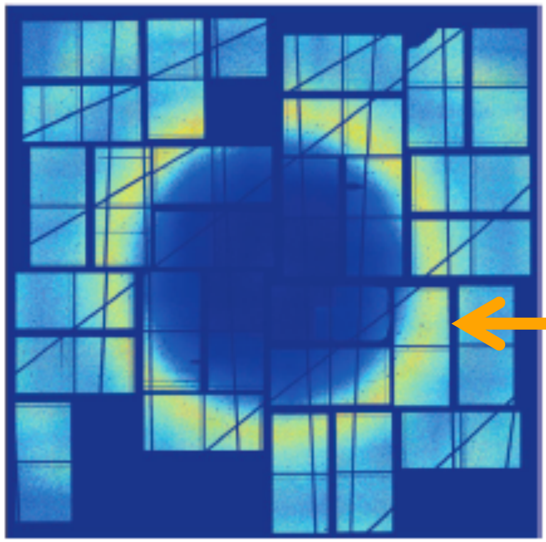


LCLS

Droplet size ~9 to 37 µm

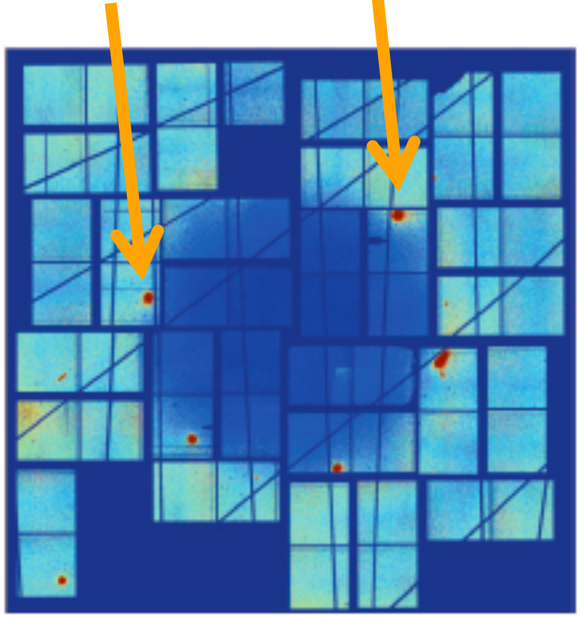
- Bragg peaks from ice

b

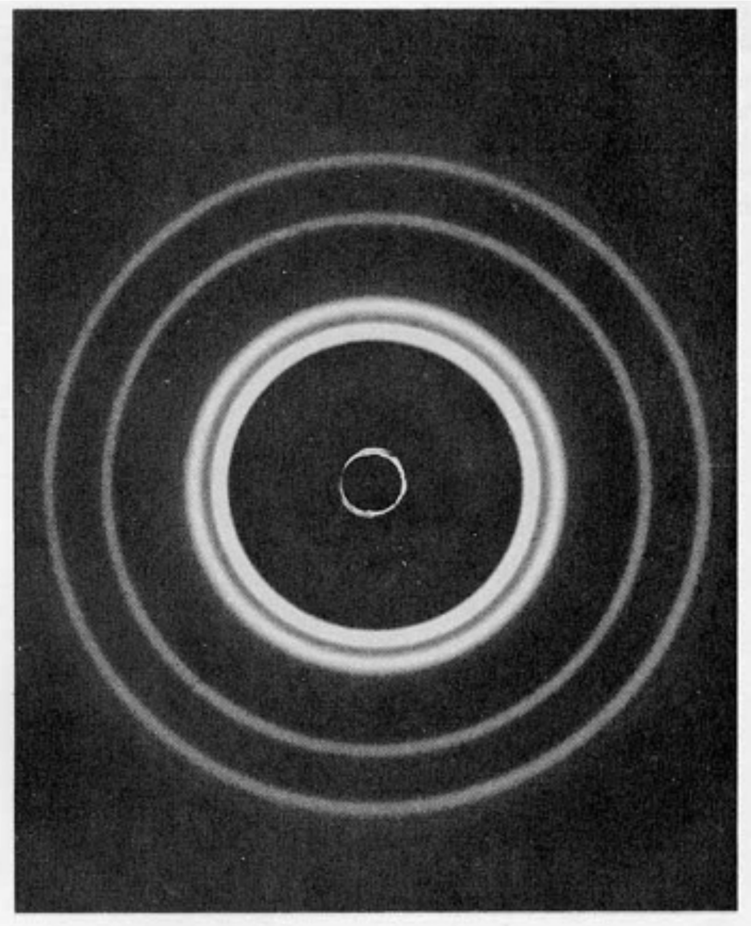


- Diffuse scattering from liquid

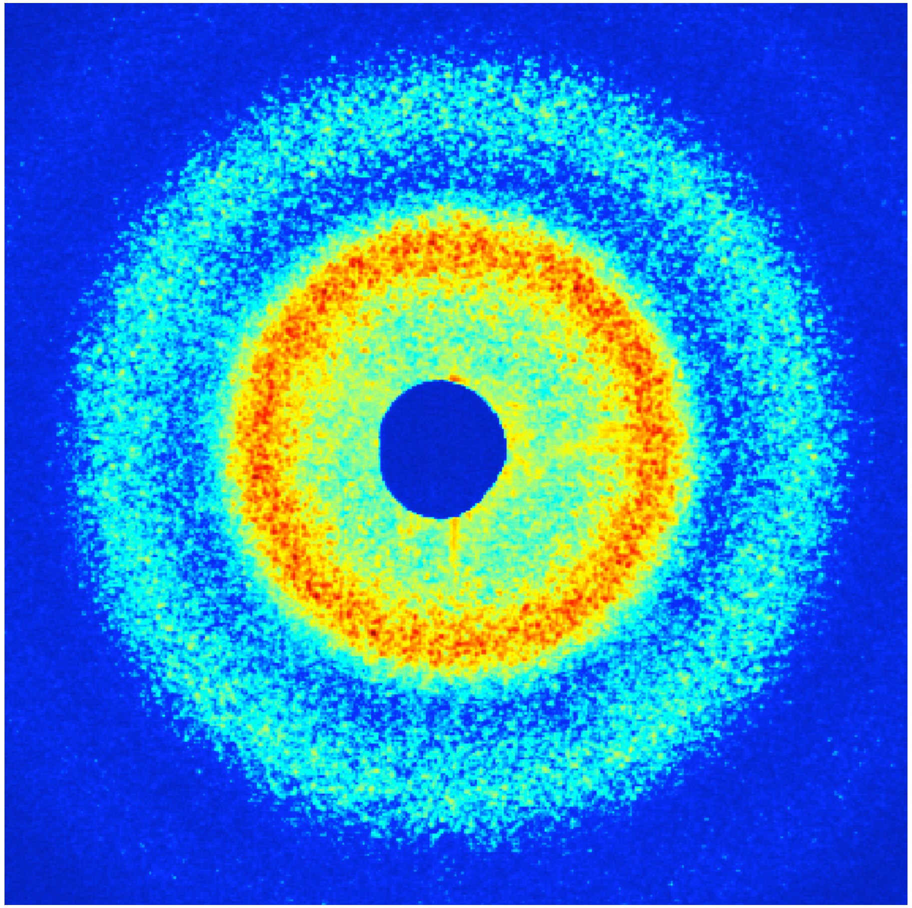
c



X-ray diffraction from liquids…

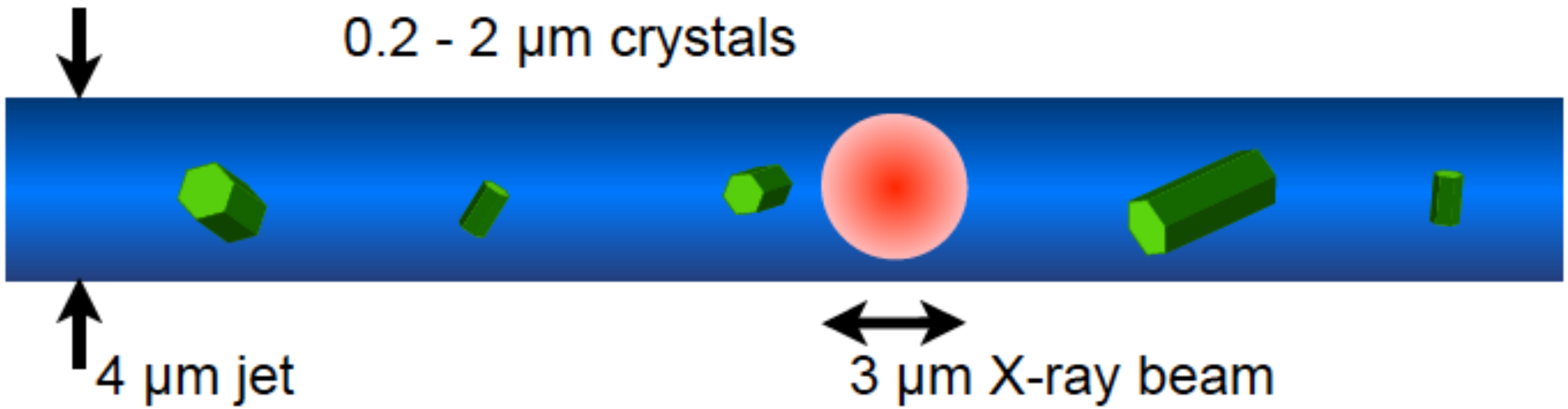


Slow, incoherent…



Fast, coherent => Speckles!
"Hologram"

Nucleation of solid phase from a freezing liquid

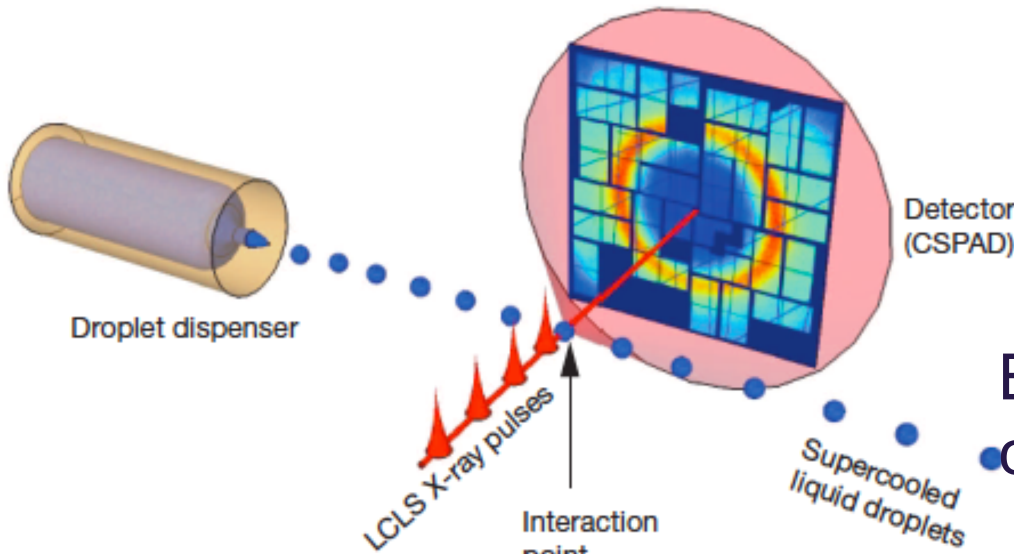


Instead of inserting micro or nanocrystals in a fluid, consider the emergence of nanocrystals in a freezing liquid – to address the open problems of *nucleation*

J. Sellberg et al., *Nature* **510**, 381 (2014)

J. Sellberg et al., Nature 510, 381 (2014)

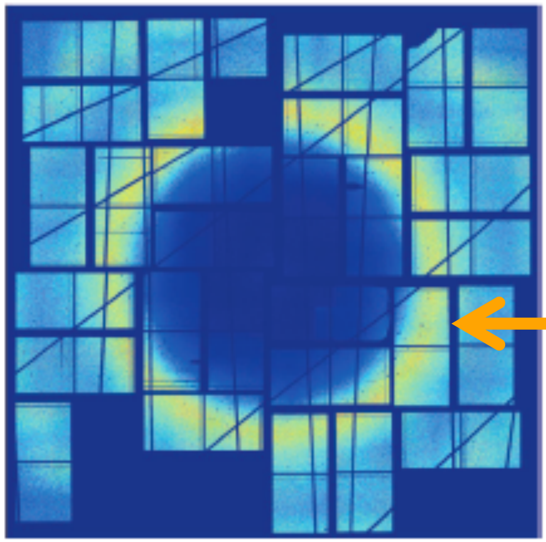
a



LCLS

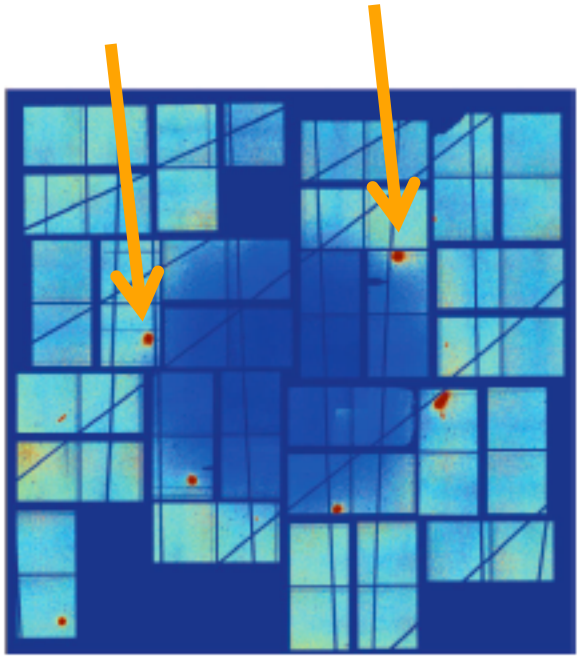
Droplet size ~9 to 37 μm
Bragg peaks from ice crystallites down to ~12 nm

b



Diffuse scattering from liquid

c



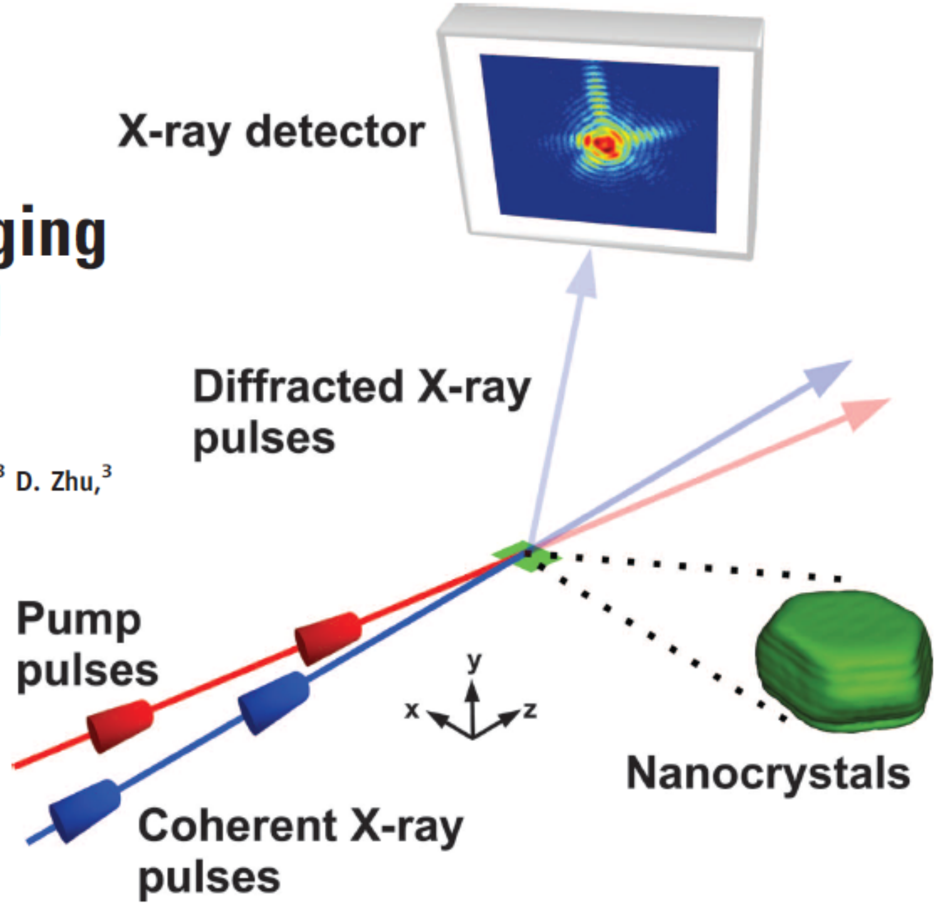
Gold nanocrystals

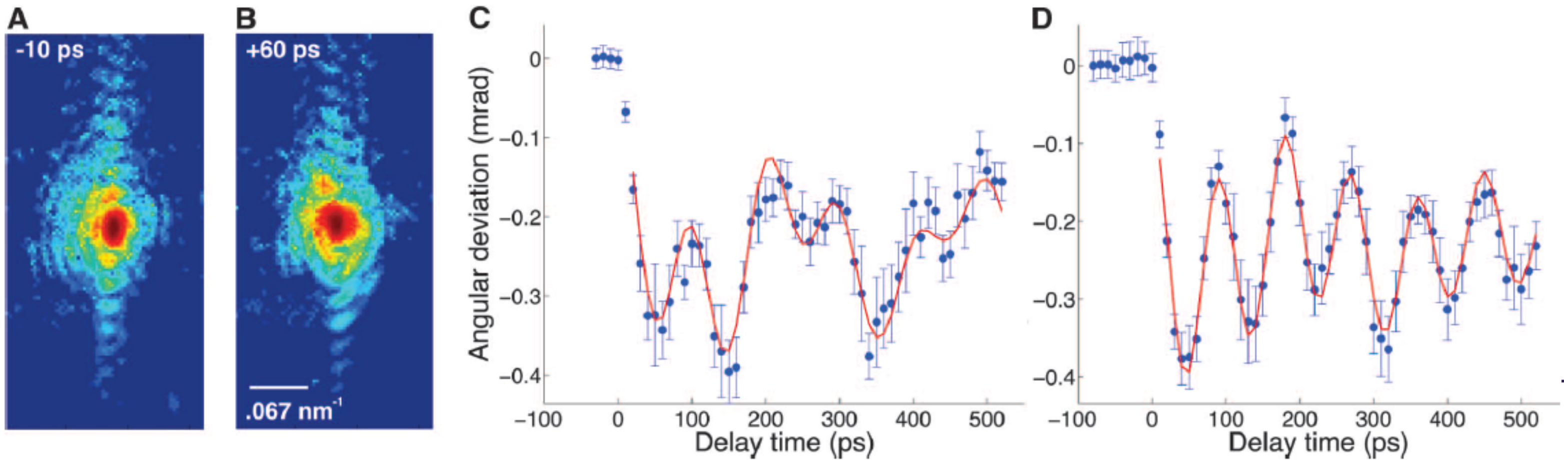
Ultrafast Three-Dimensional Imaging of Lattice Dynamics in Individual Gold Nanocrystals

J. N. Clark,[1*] L. Beitra,[1] G. Xiong,[1] A. Higginbotham,[2] D. M. Fritz,[3] H. T. Lemke,[3] D. Zhu,[3] M. Chollet,[3] G. J. Williams,[3] M. Messerschmidt,[3] B. Abbey,[4] R. J. Harder,[5] A. M. Korsunsky,[6,7] J. S. Wark,[2] I. K. Robinson[1,7]

Science **341**, 51-59 (2013)

- Pump-probe experiments

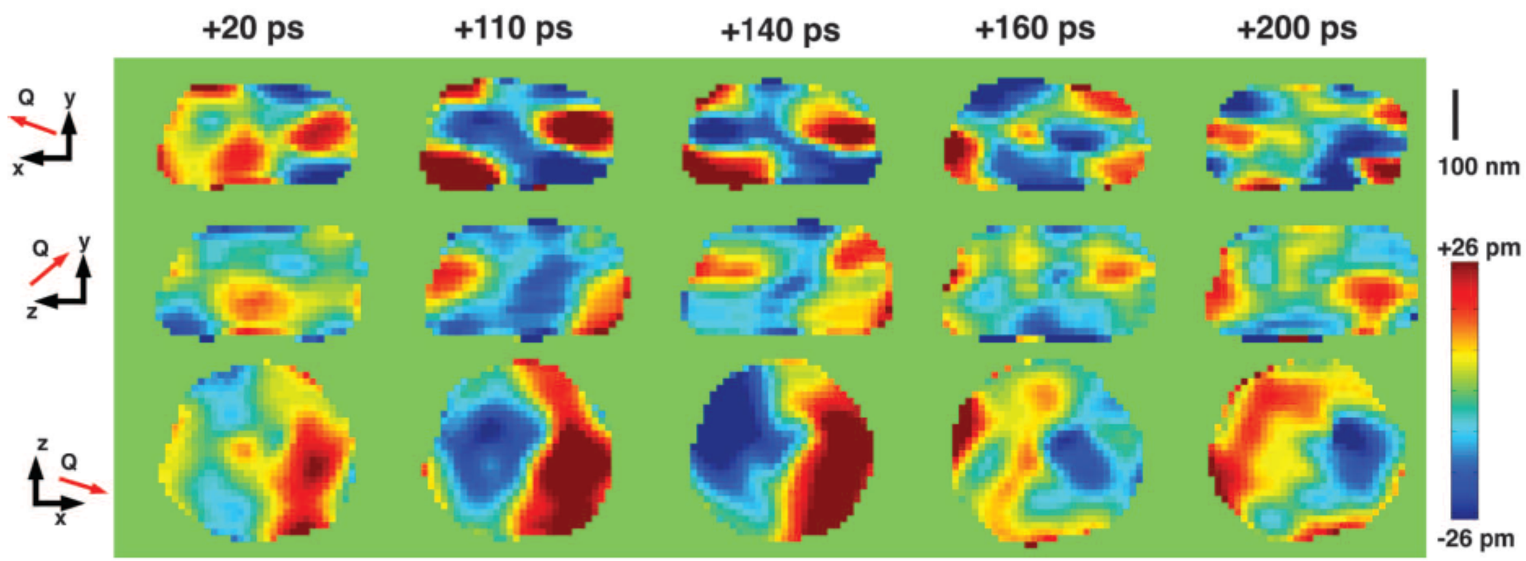




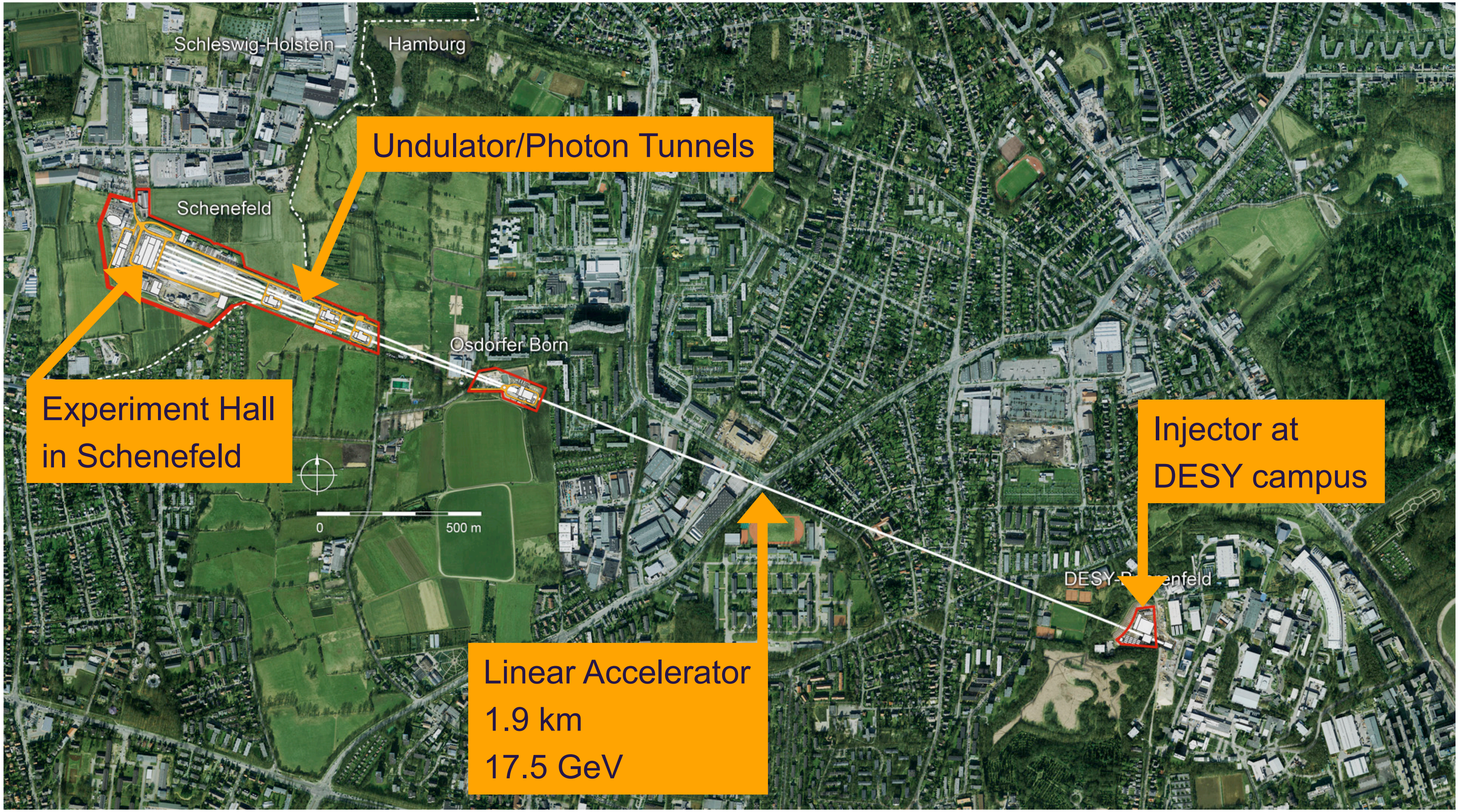
Imaging of vibrational modes

- Beyond the analysis of the Bragg spots position: imaging

Fig. 3. Imaging of acoustic phonons in a nanocrystal. Orthogonal cut planes through the center of nanocrystal I showing the projected displacement as a function of delay time. Three different viewing directions are shown. The direction of the displacement field is given by the ***Q*** vector in red. For clarity, the range of displacement has been truncated to ±26 pm instead of the full range of ±53 pm.



European XFEL: the most brilliant X-ray source

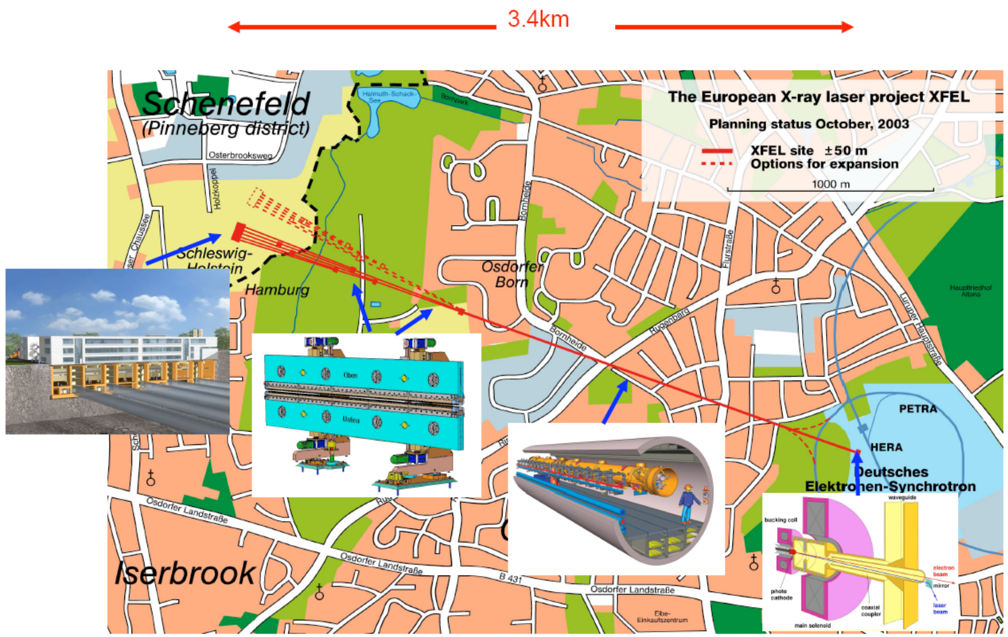


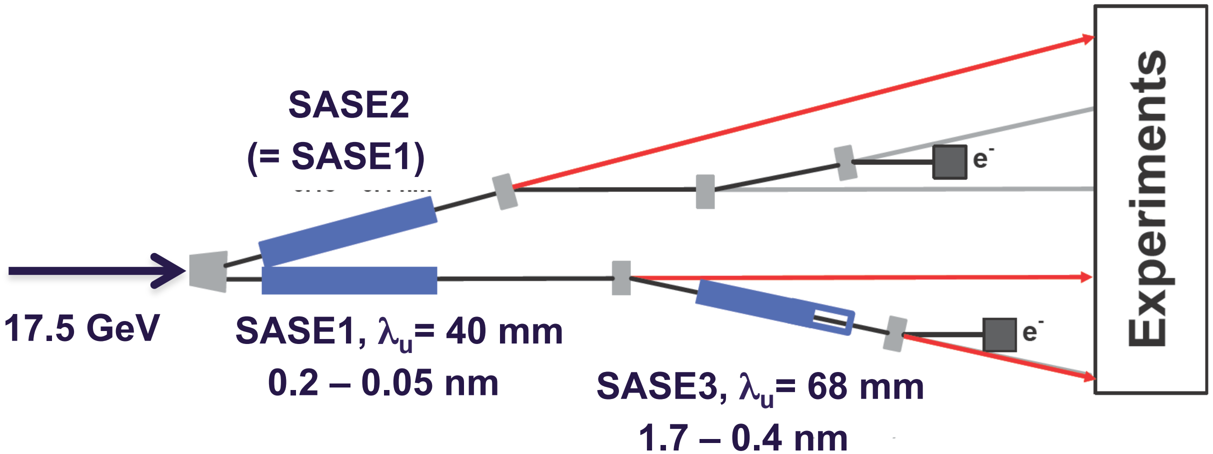
The European XFEL

Some specifications

- Photon energy 0.3-24 keV
- Pulse duration ~ 10-100 fs
- Pulse energy few mJ
- Superconducting linac. 17.5 GeV
- 10 Hz (27 000 b/s)
- 5 beamlines / 10 instruments
  - Start version with 3 beamlines and 6 instruments
- Several extensions possible:
  - More undulators
  - More instruments
  - Variable polarization
  - Self-Seeding
  - CW operation

First beam late 2016

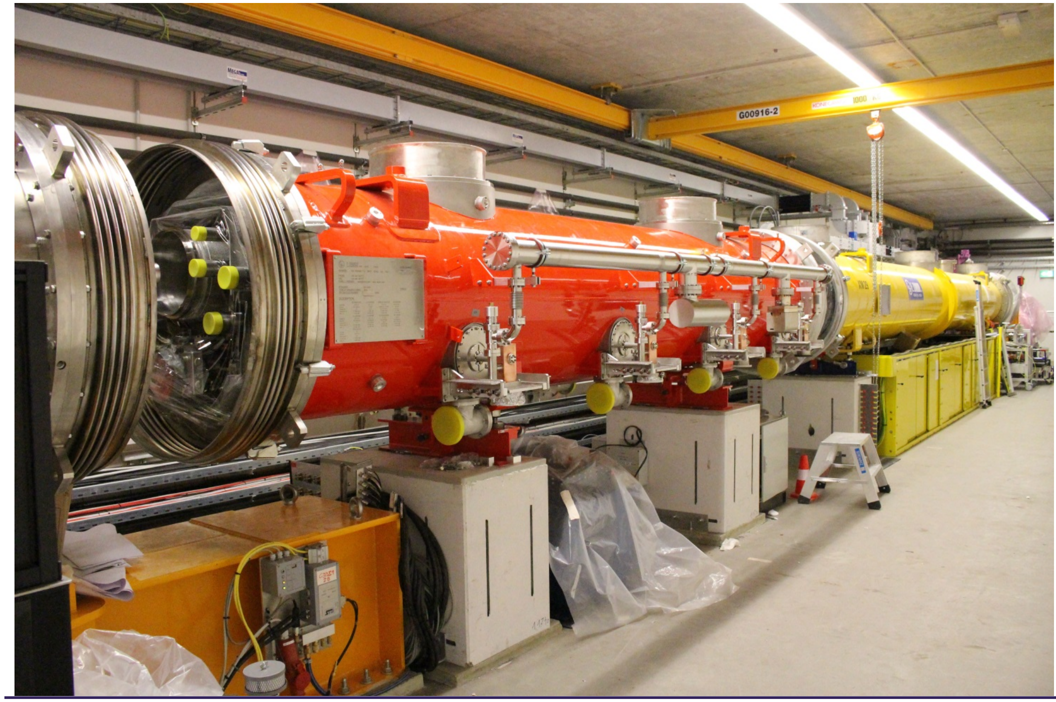


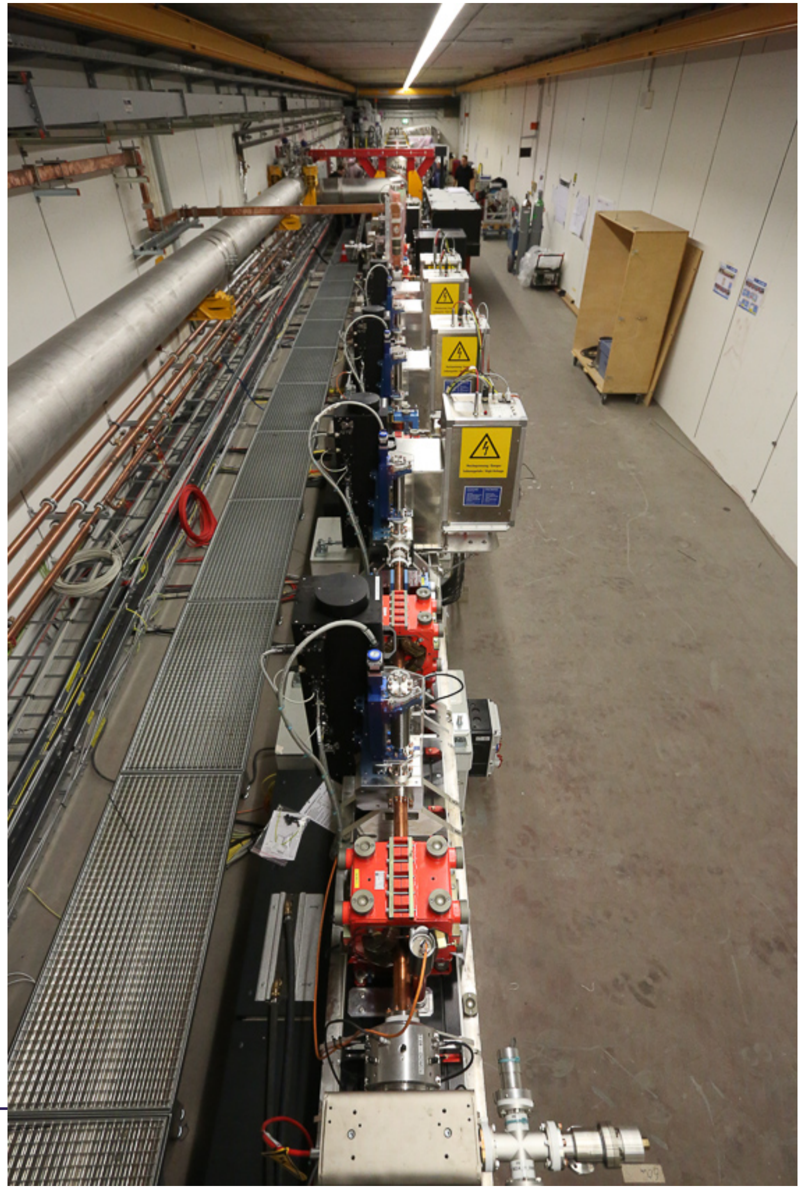


European XFEL

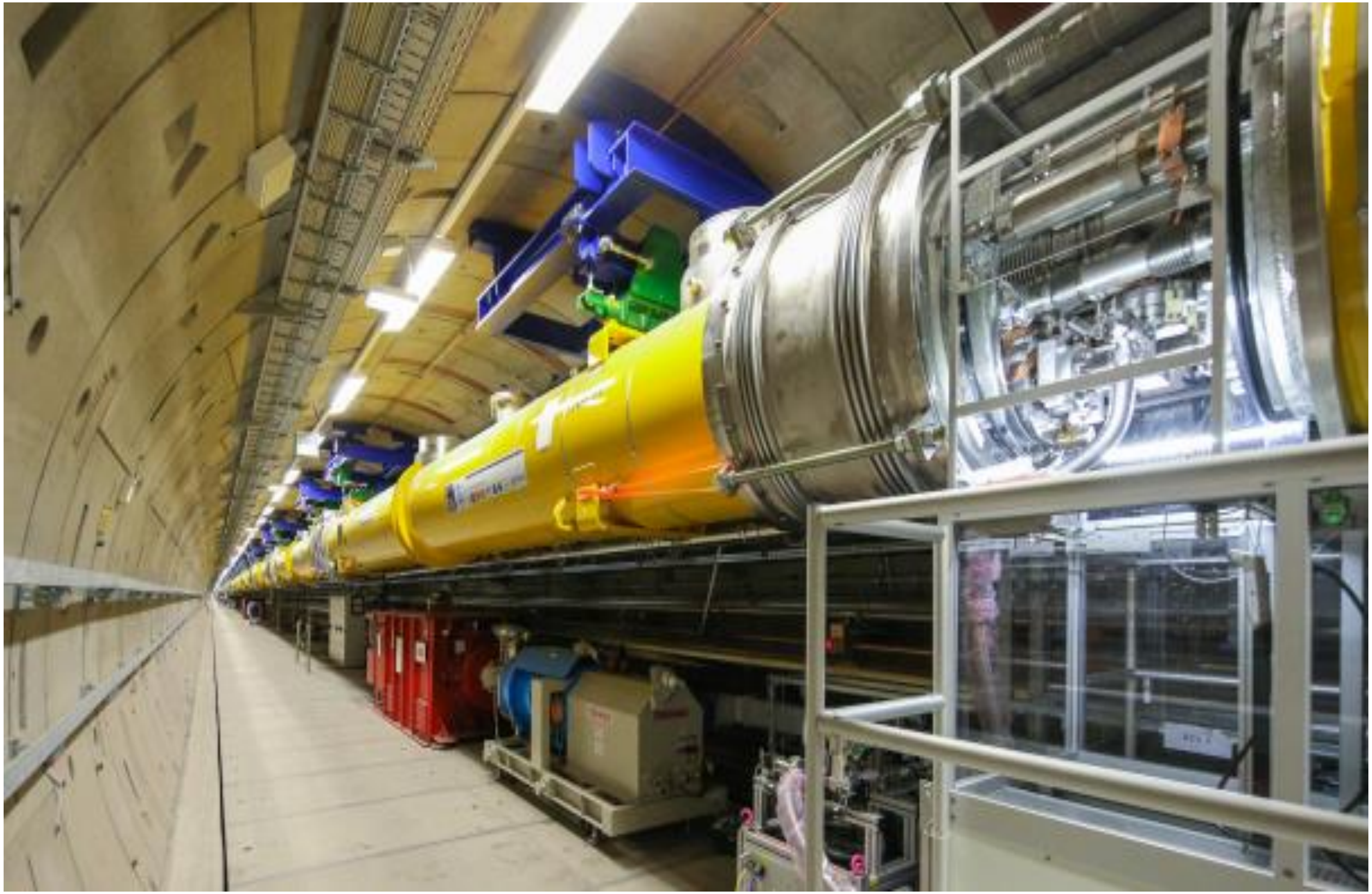
First accelerated e- beam in the injector

- **Injector commissioning started**, injector tunnel closed, cool down to 2 K successful.
- First 130 MeV Electron beam on 21.12.2015!





Linac Tunnel: 60 modules out of 100 installed



Undulator 5 m segment, made in Spain, Germany

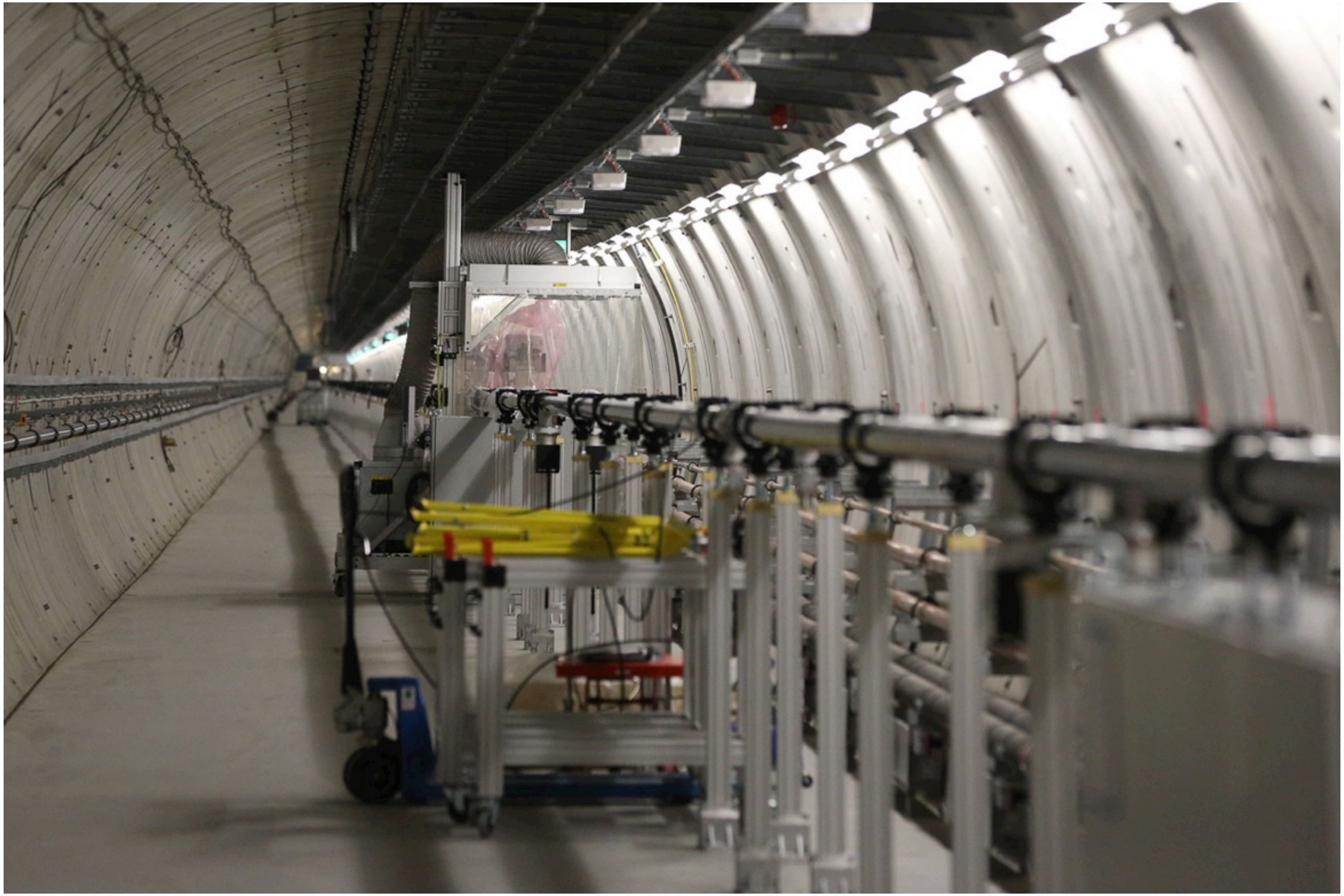
European XFEL

SASE1 undulator (35 segments) installed

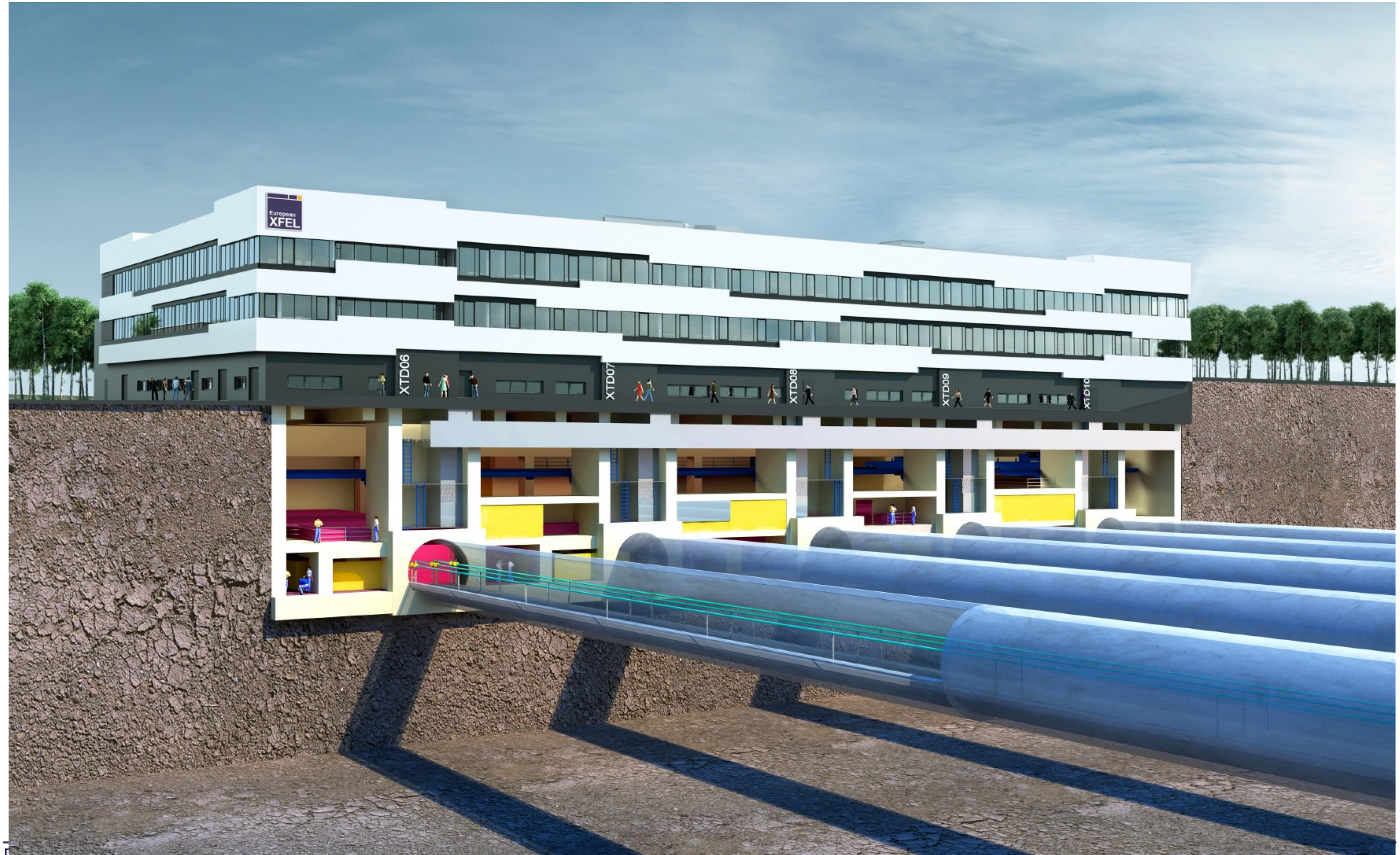
Optical elements of the SASE1 beamline

Photon diagnostics for the SASE1 beamline

Tunnel to Experiment Hall



Experiment Hall, Headquarters building



European XFEL

Scientific instruments

Hard X-rays

SPB/SFX: 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

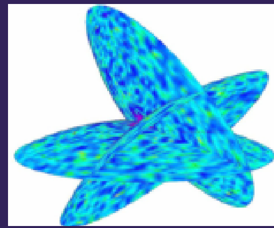
- Structure determination of nano-devices and dynamics at the nanoscale.

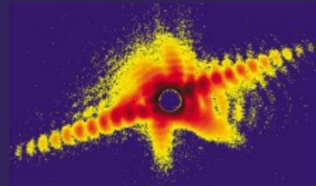
FXE: Femtosecond X-ray Experiments

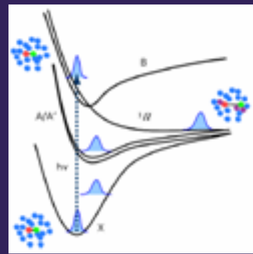
- Time-resolved investigations of the dynamics of solids, liquids, gases

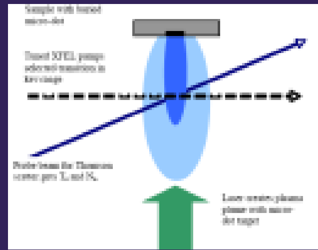
HED: High Energy Density Matter

- Investigation of matter under extreme conditions using hard X-ray FEL radiation, e.g. probing dense plasmas









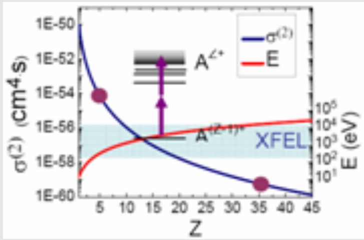
Soft x-rays

SQS: Small Quantum Systems

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

SCS: Soft x-ray Coherent Scattering/Spectroscopy

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



SASE1 stations FXE and SPB/SFX

SASE3 hutches construction in progress

Moving to Schenefeld Campus in June 2016

European XFEL

Timetable…

2016 Initial commissioning of linac, to bring electron beam in first undulator (SASE1). Enable first lasing.

FIRST CALL FOR PROPOSALS!

2017 Bring X-ray FEL beam to XHEXP.

Continue commissioning of accelerator.

Initial commissioning of X-ray beam transports and instruments.

Start “early user experiment” program (peer-reviewed).

2018 Reach full performance of accelerator.

Development of X-ray beam transports and instruments towards full performance.

Continue “early user experiment” program (peer-reviewed).

During 2nd half 2018 gear up towards full scope user program (peer-reviewed).

2019 Regular operation (4000 hrs for user programme).

- Thanks to all European XFEL and partner institutes members for the work presented here

- …and thank you for your attention