Ярче Миллиарда Солнц

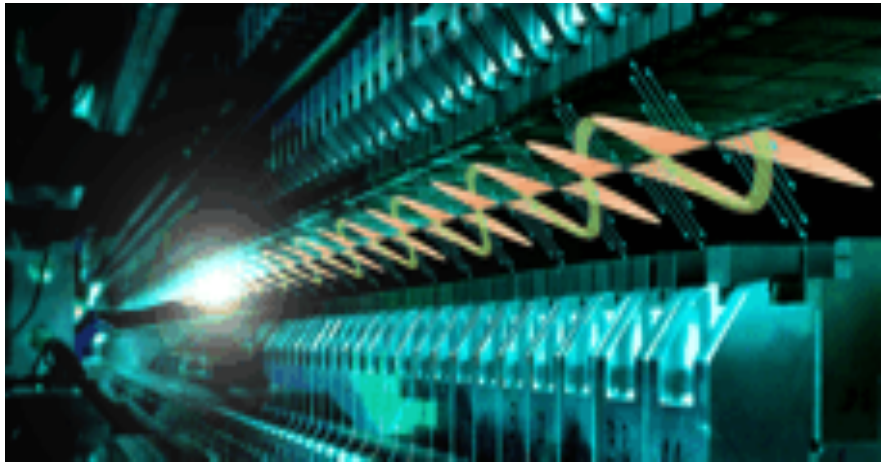
Сергей Молодцов

European X-ray Free Electron Laser, Hamburg

Technical University, Freiberg

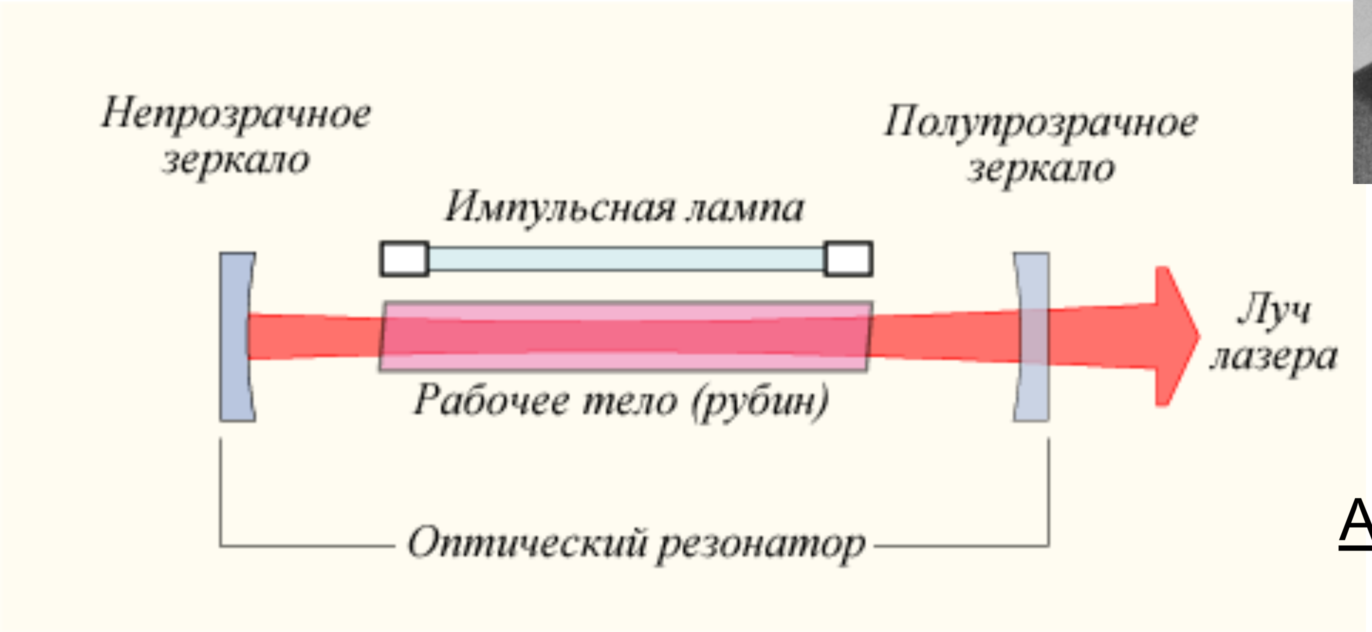
Technical University, Dresden

University ITMO, St. Petersburg



Super (PW) optical lasers

Nobel Prize 1964

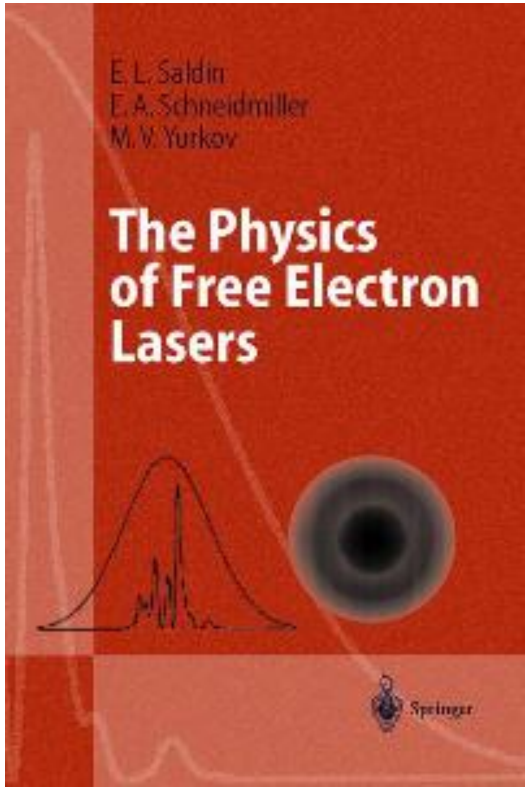


Николай Басов

Александр Прохоров

Charles H. Townes

Nobel Prize 2020 ???



E.L. Saldin
E.A. Schneidmiller
M.V. Yurkov

Innovation Prize, Helmholtz Zentrum Berlin

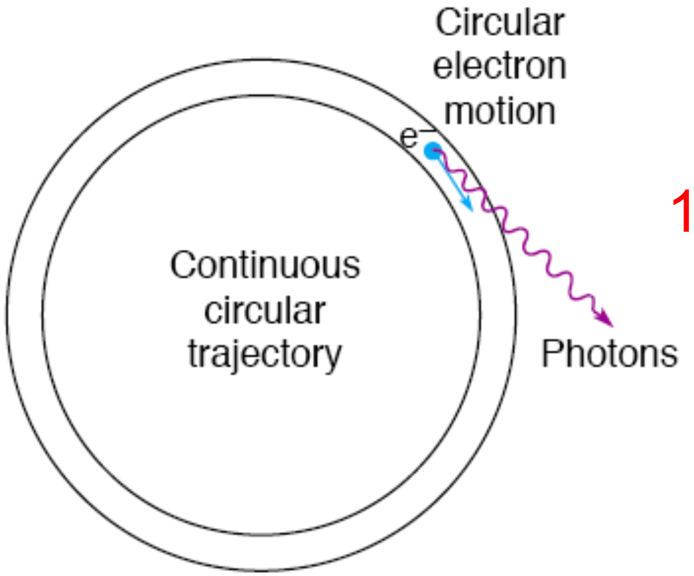
E. Saldin

Important dates in the history of science

Radiation from Electrons in a Synchrotron

F. R. Elder, A. M. Gurewitsch, R. V. Langmuir,
and H. C. Pollock
Research Laboratory, General Electric Company,
Schenectady, New York

May 7, 1947

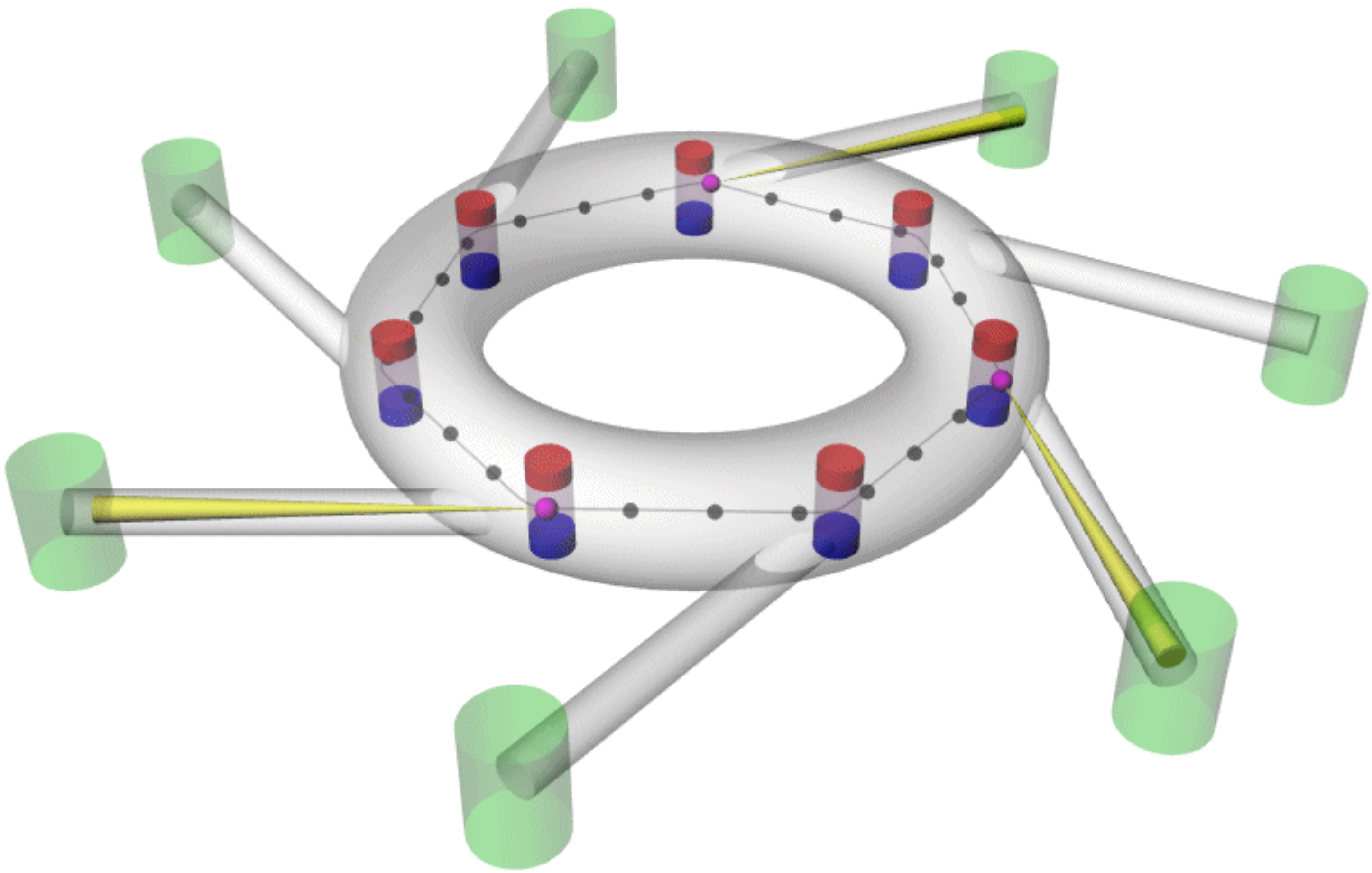


1947 First observation of synchrotron light

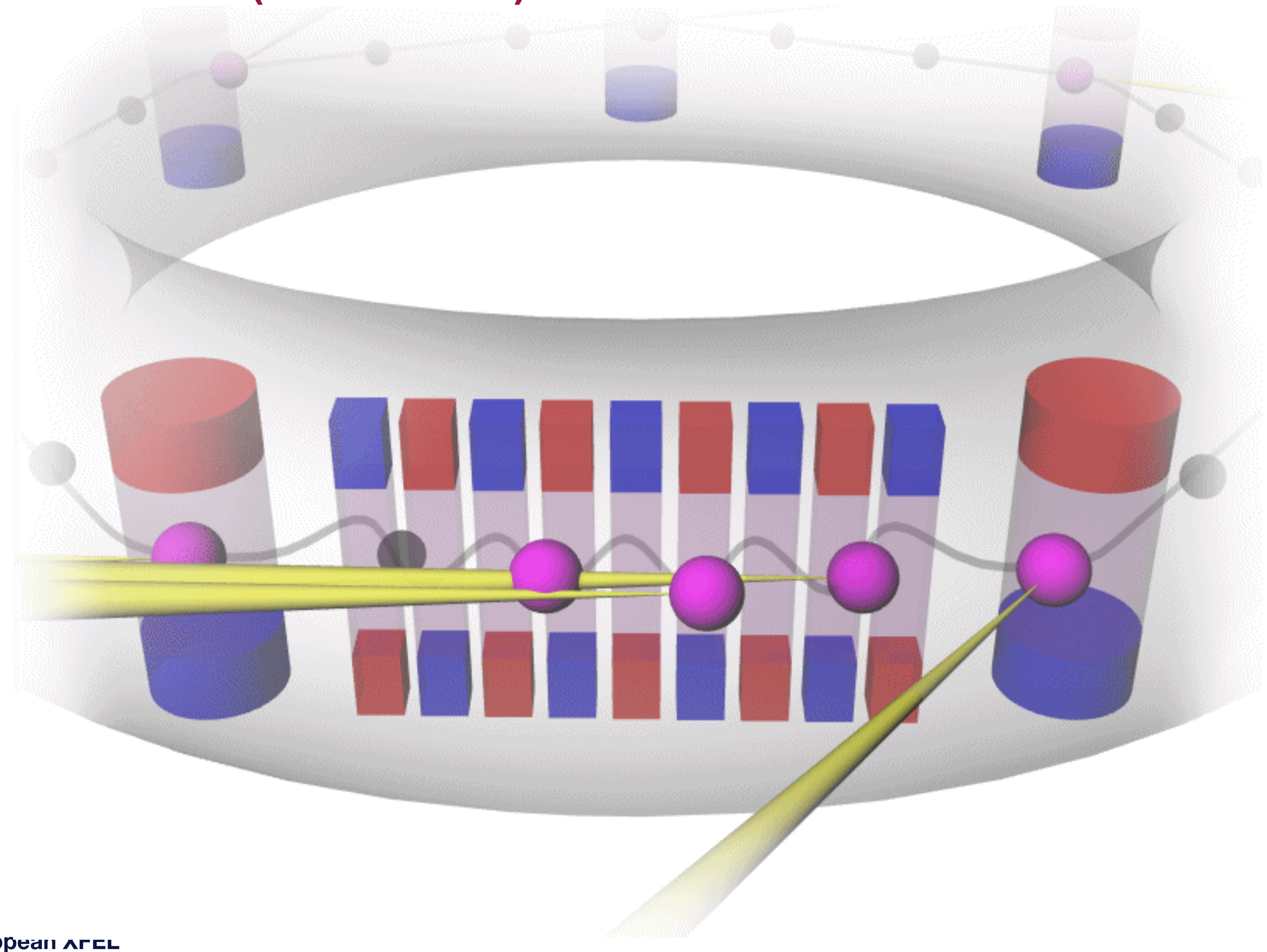
$$P = (3c^3)^{-1}\, 2q^2\, \nu^4\, a^2$$

P – radiated power; c – light velocity; q – particle charge; a – acceleration; ν - normalized energy

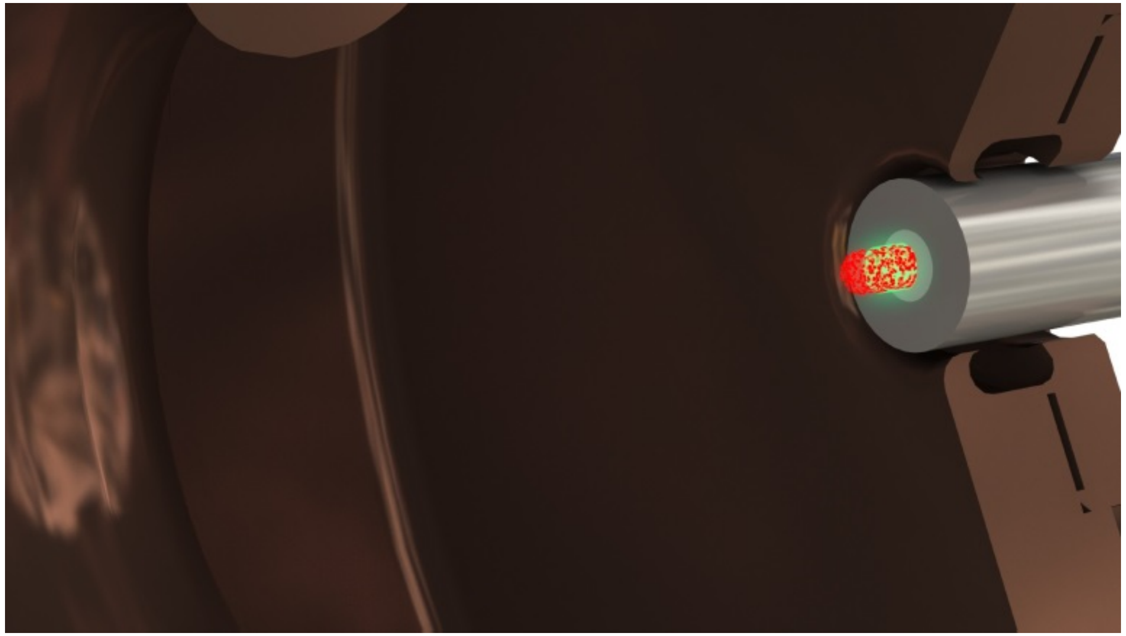
Synchrotron radiation (dipoles)



Synchrotron radiation (undulators)

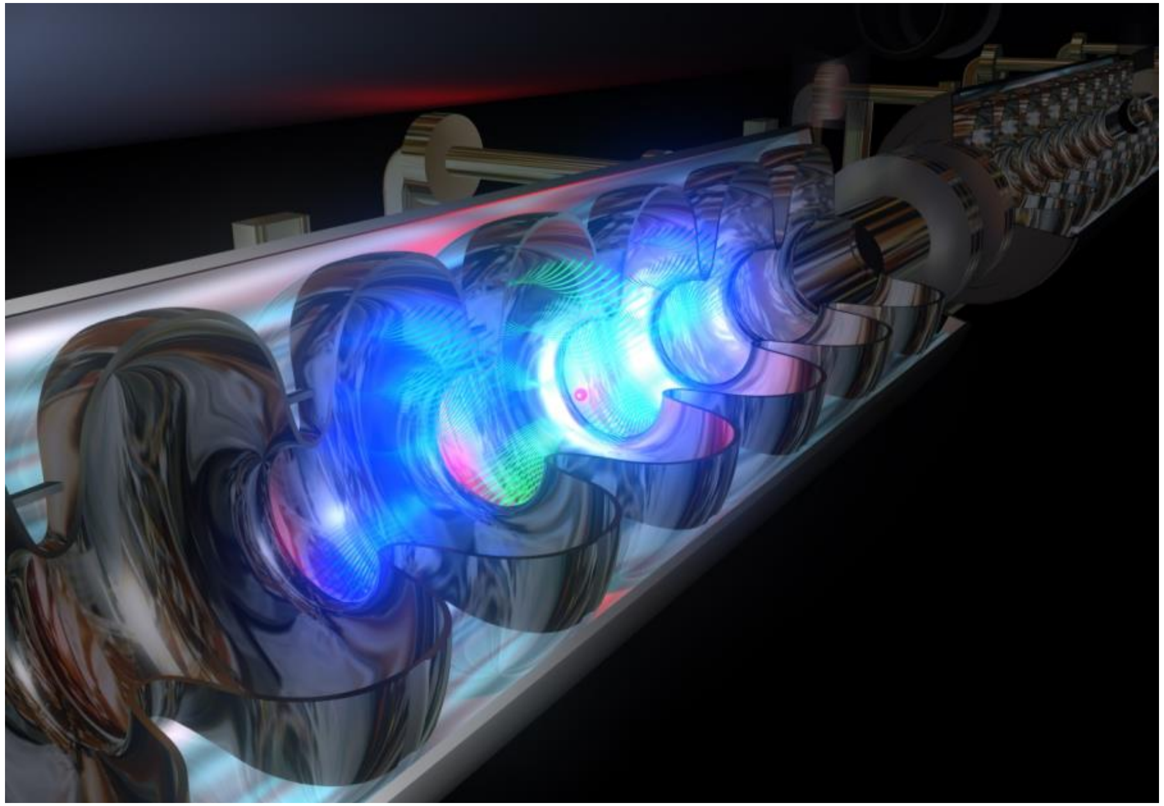


Injector: creating bunches of electrons



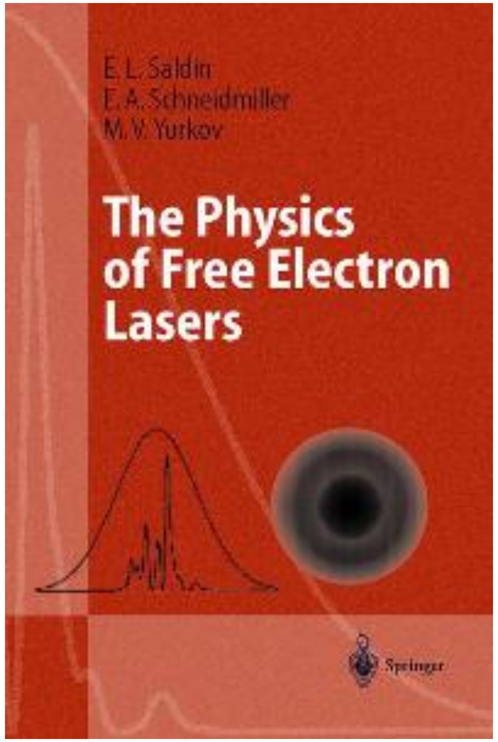
- Optical laser strikes Cs_2Te surface, releasing a cloud of electrons
- Electrons move into a magnetic field, shaping into a bunch
- Small accelerator module “fires” bunch into the main electron accelerator

Accelerator: electrons at close to light speed



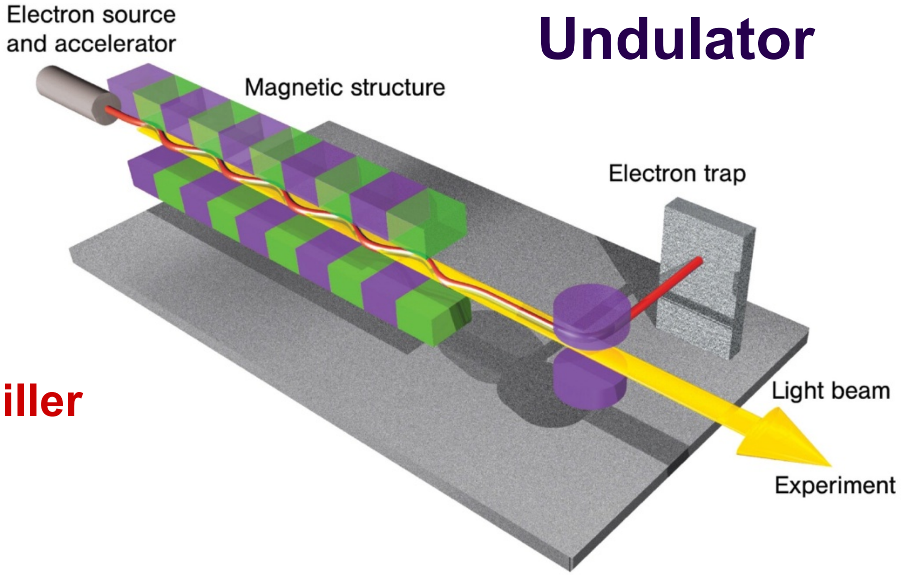
- 100 accelerator modules over 2 km bring the electron bunch to near light speed and high energies
- Superconducting niobium cavities powered by intense radio frequency accelerate electrons

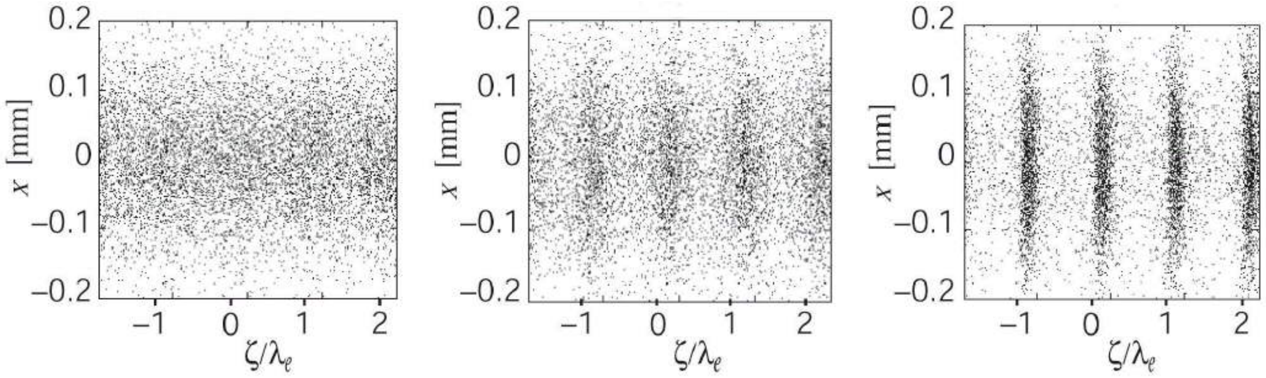
Basics of SASE FEL process



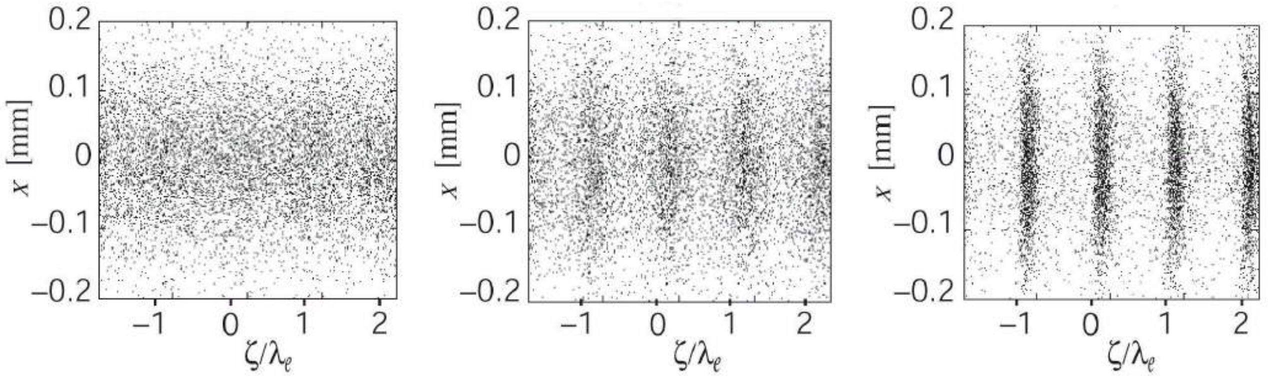
E.L. Saldin
E.A. Schneidmiller
M.V. Yurkov

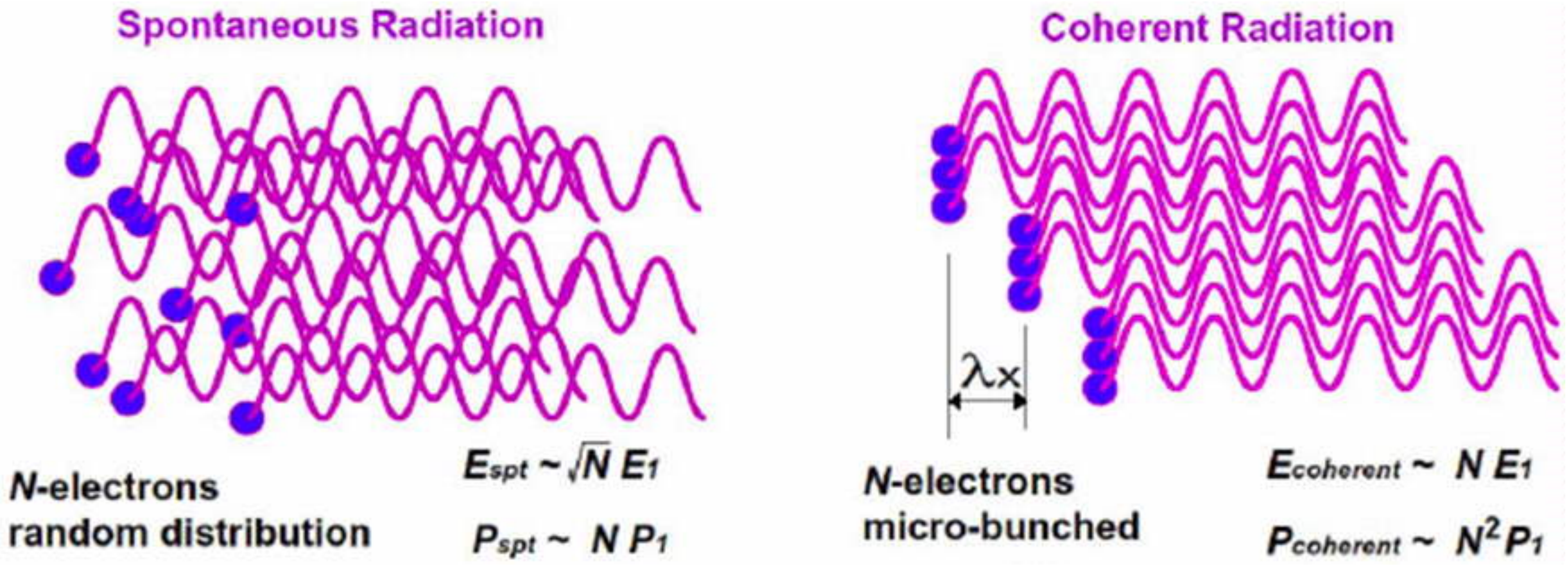
Undulator



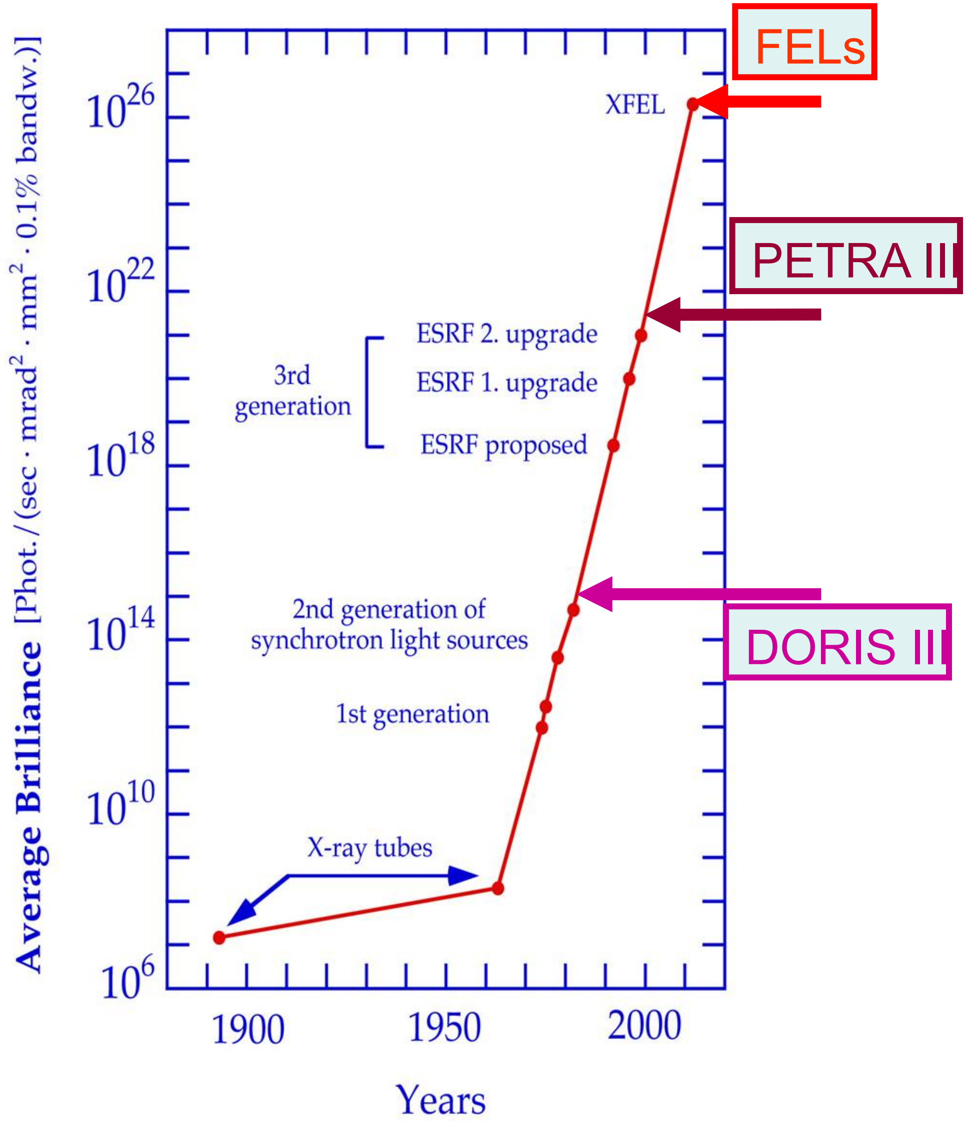


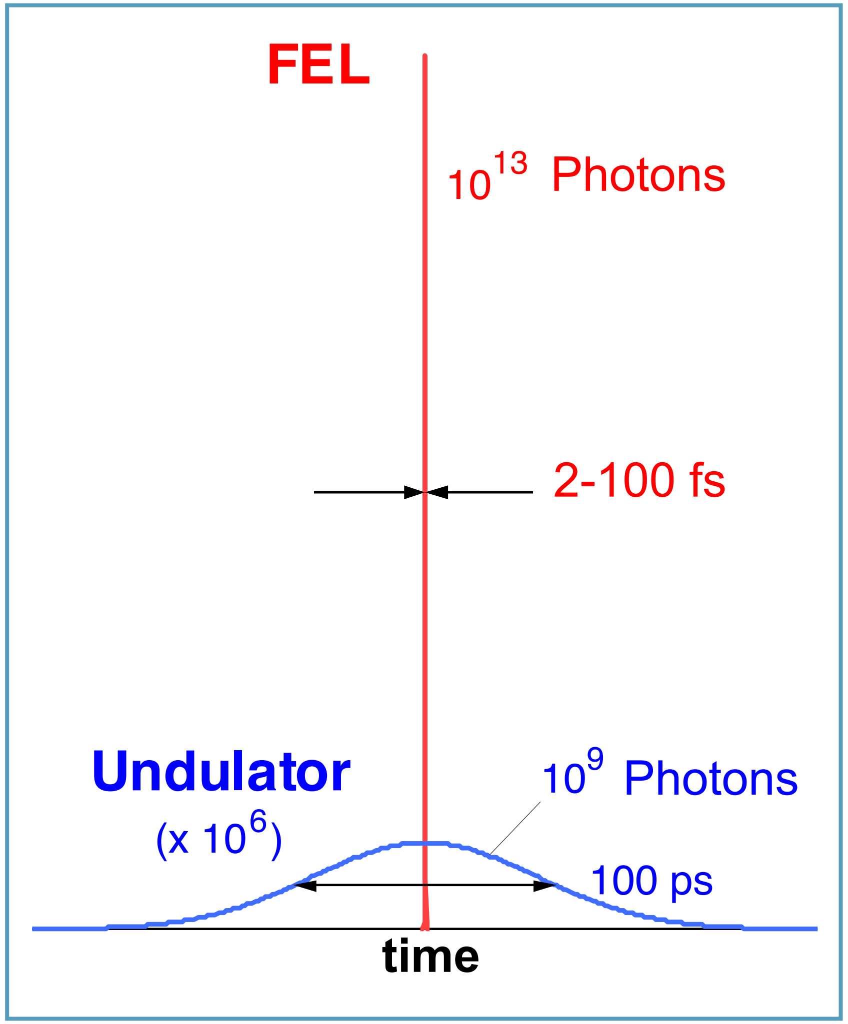
Spontaneous vs. coherent radiation in undulators





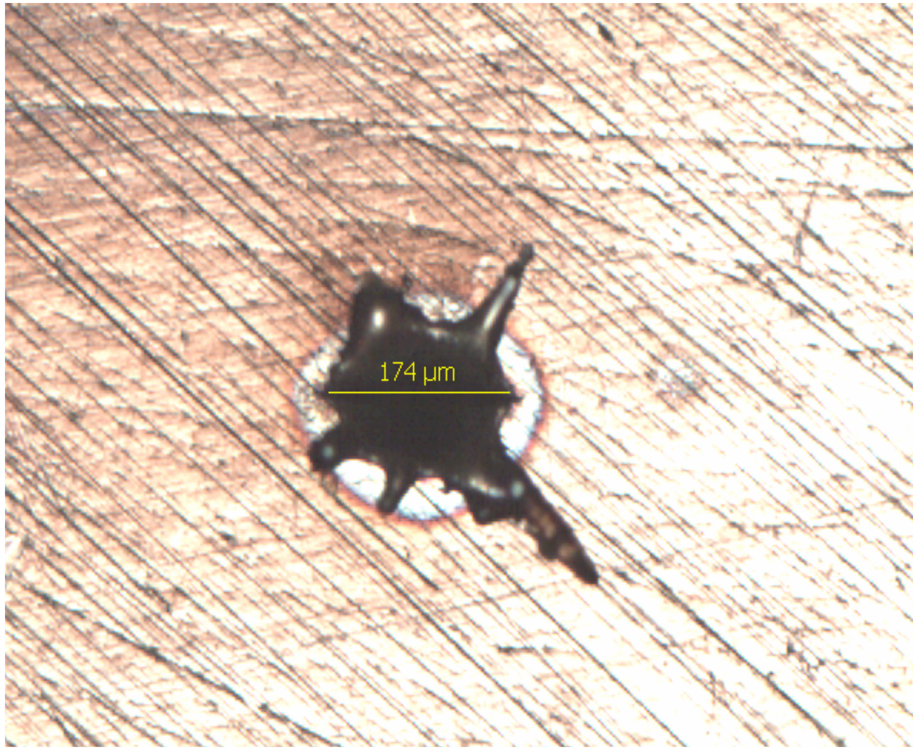
Main advantages of XFELs



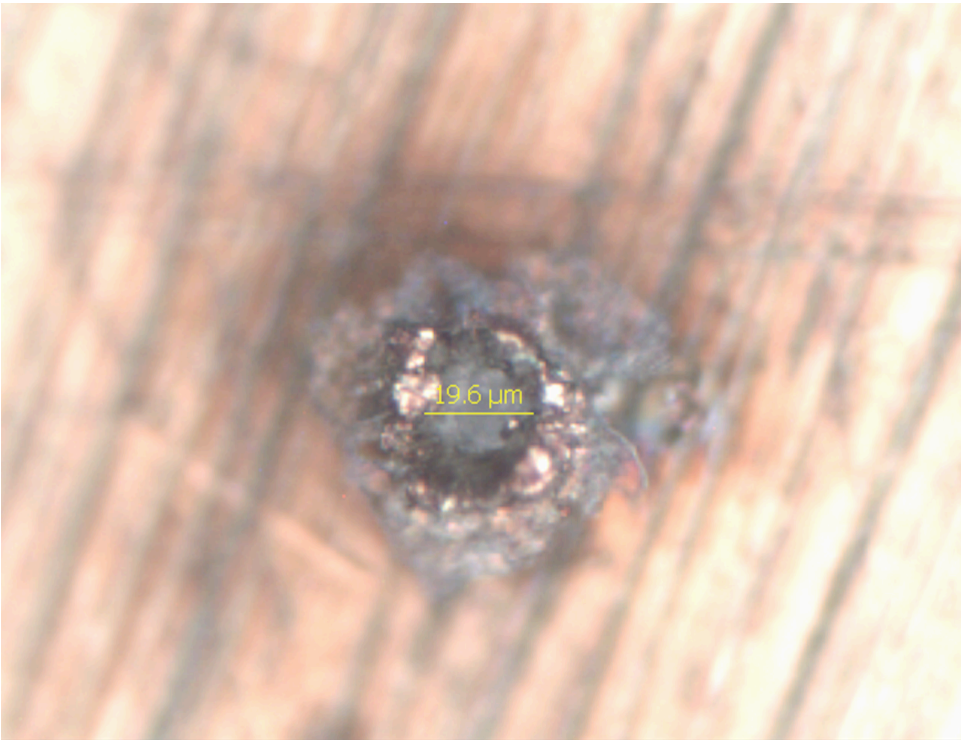


Drilling through 0.5 mm copper

Front side: 180 µm hole

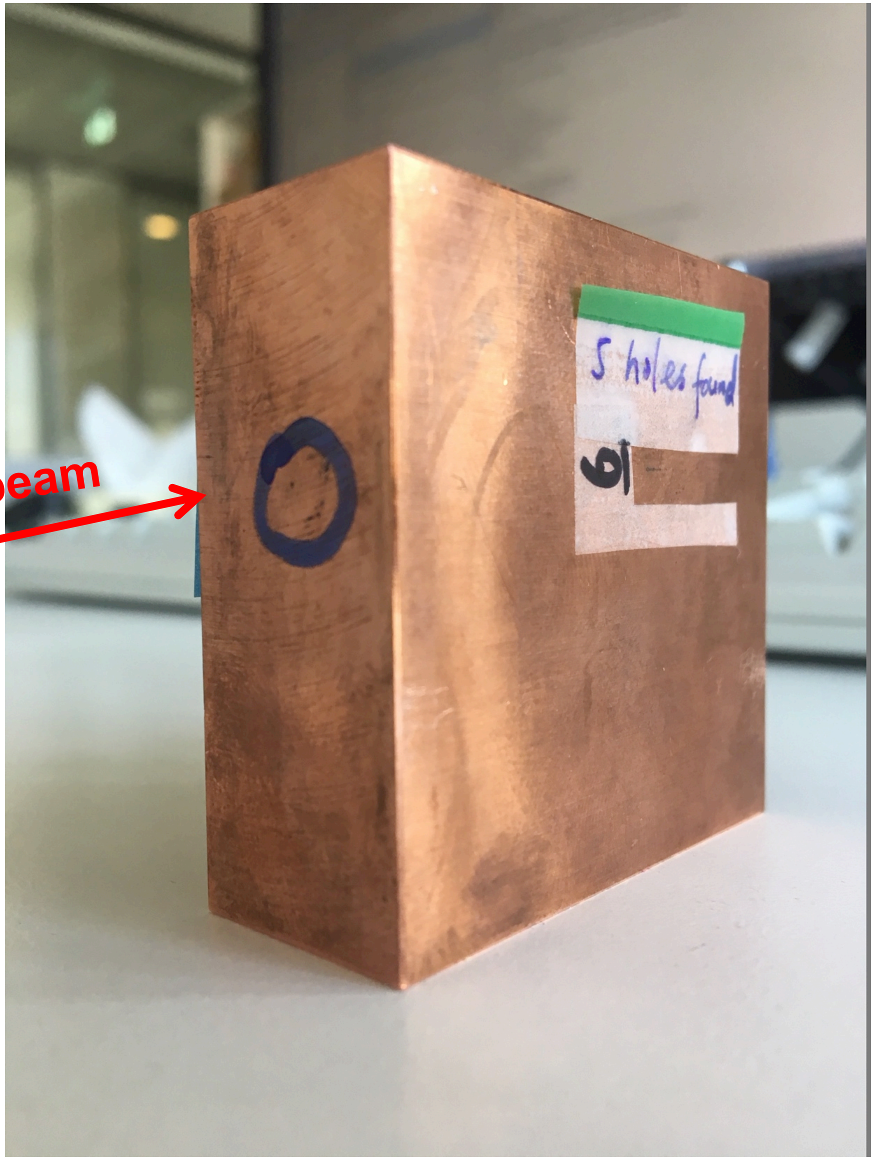


Back side: 20 µm hole



Drill through time: very short! (1 second or less)

Material test April 2018: Drill through 50 mm copper: 3 seconds!



Focus: 20 µm
9.3 keV, 1mJ/pulse

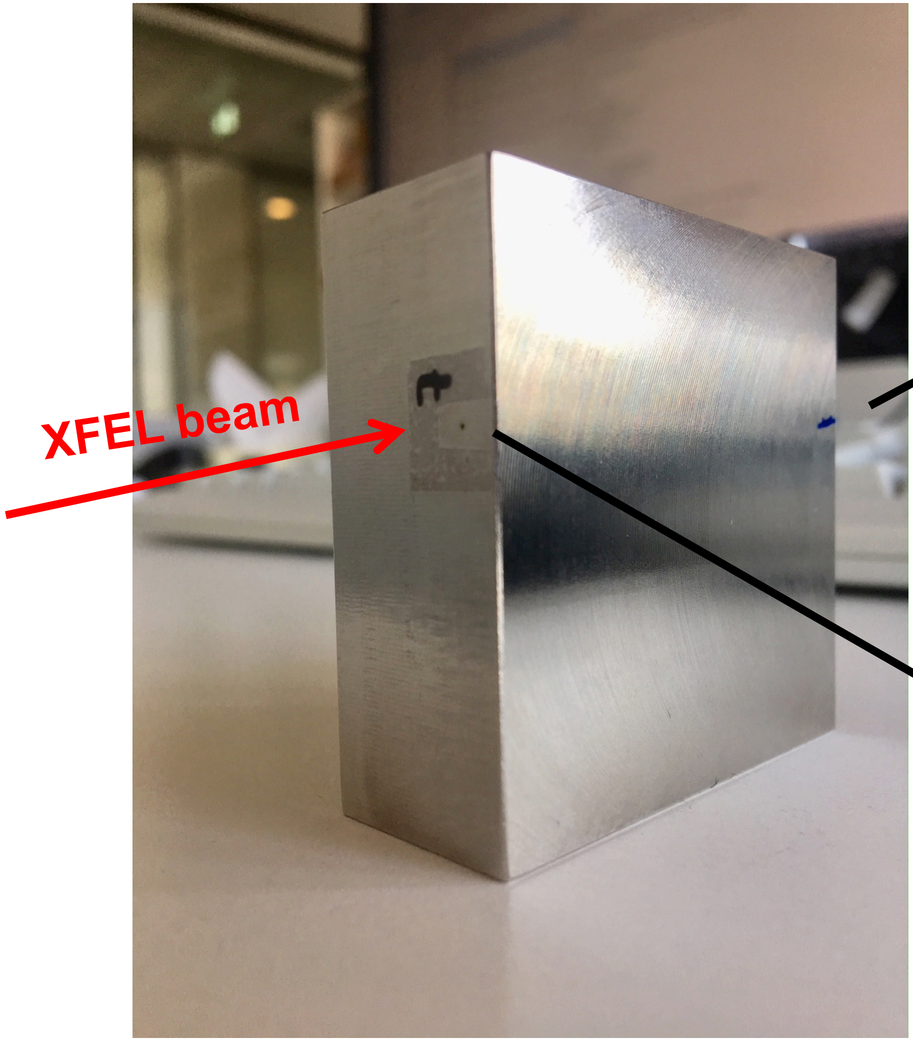
5cm/3sec = 16 mm/sec

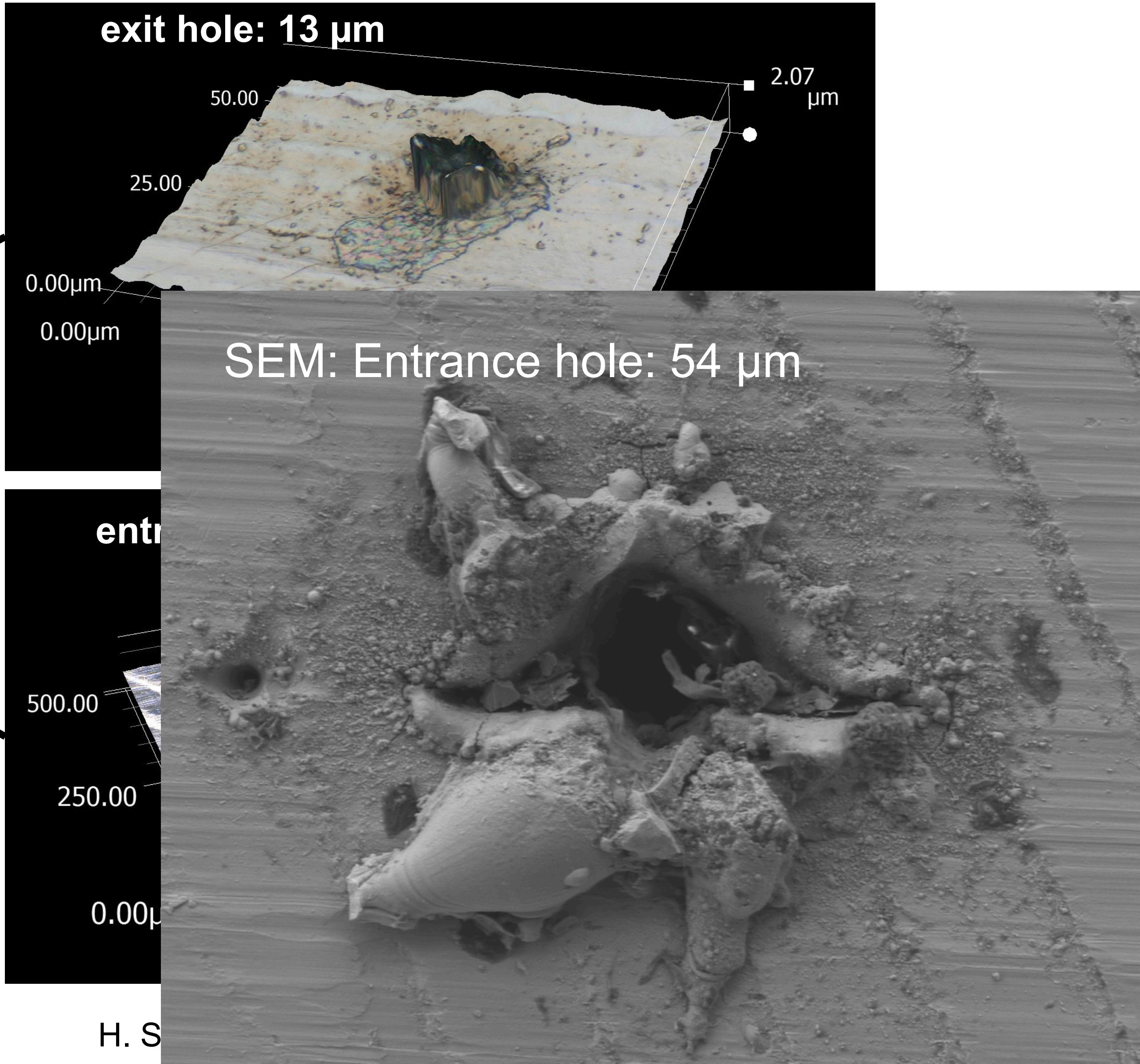
max. ablation rate: 10-15 µm/pulse

Propagation speed
during pulse train:
15 µm/1µs= 15 m/s = 54 km/h

Up to 150 mm drill-through copper slab was observed
200 mm thickness with reduced transmission

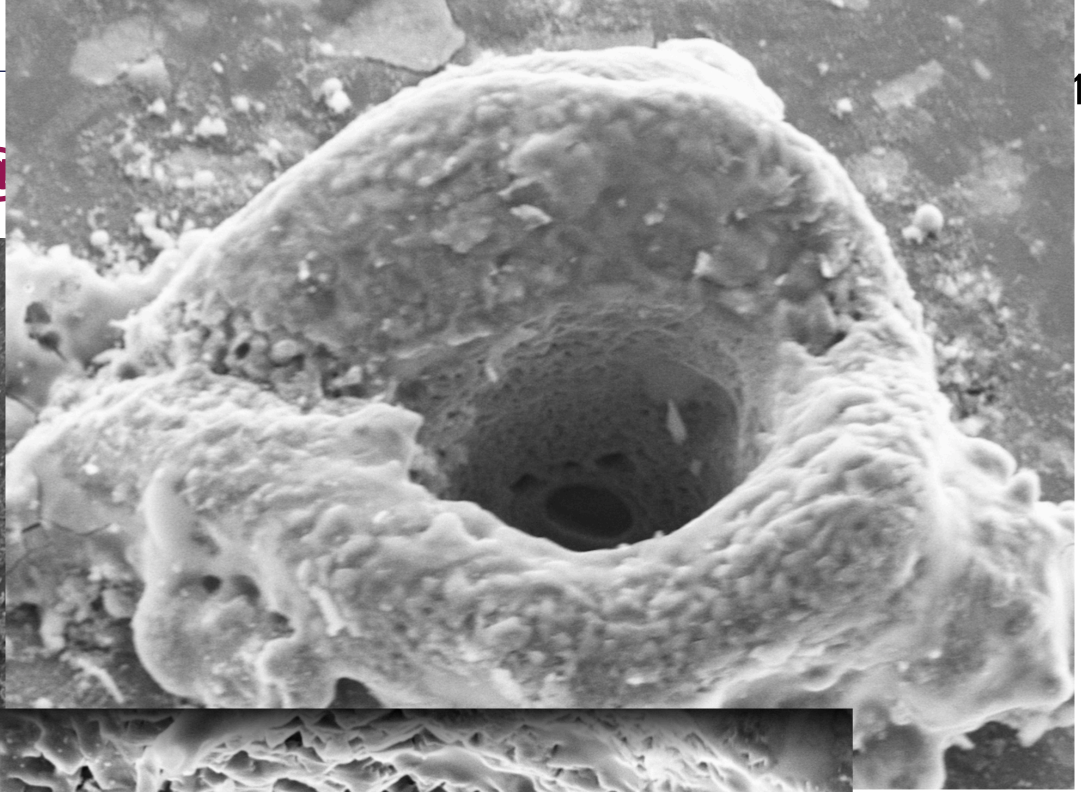
Drilling with XFEL beam through 50 mm of steel in 26 seconds

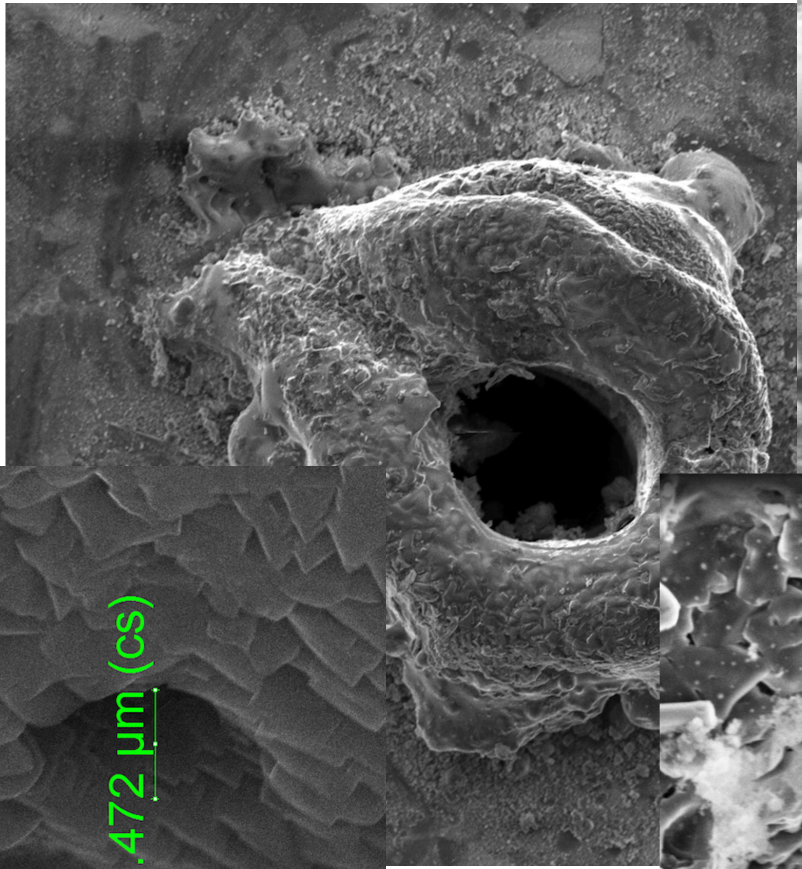


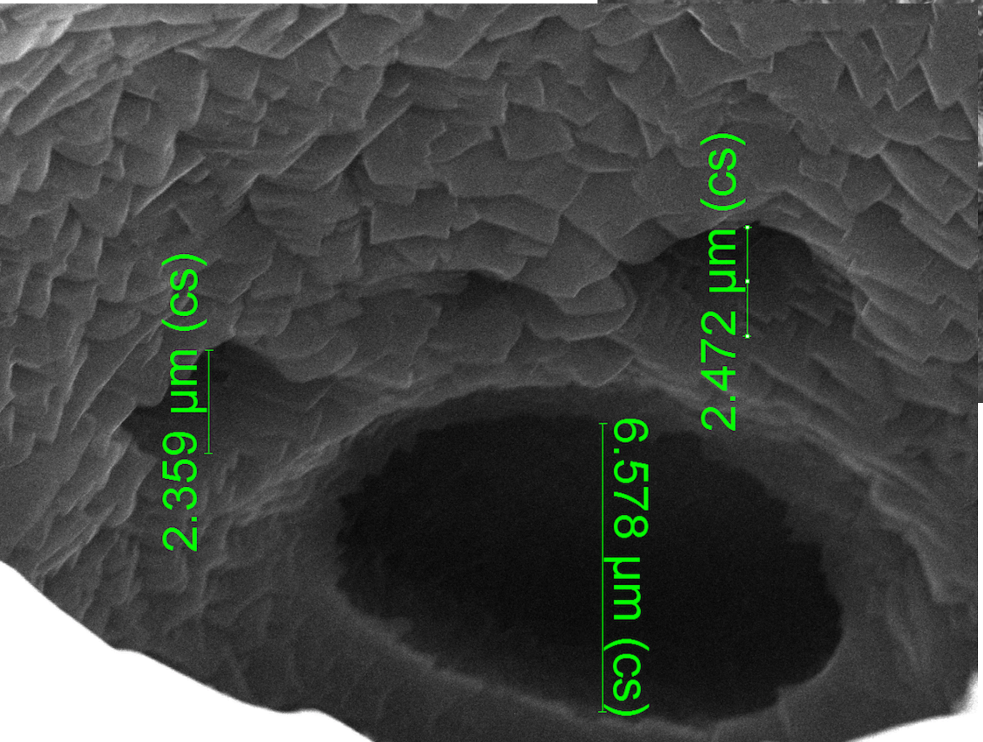


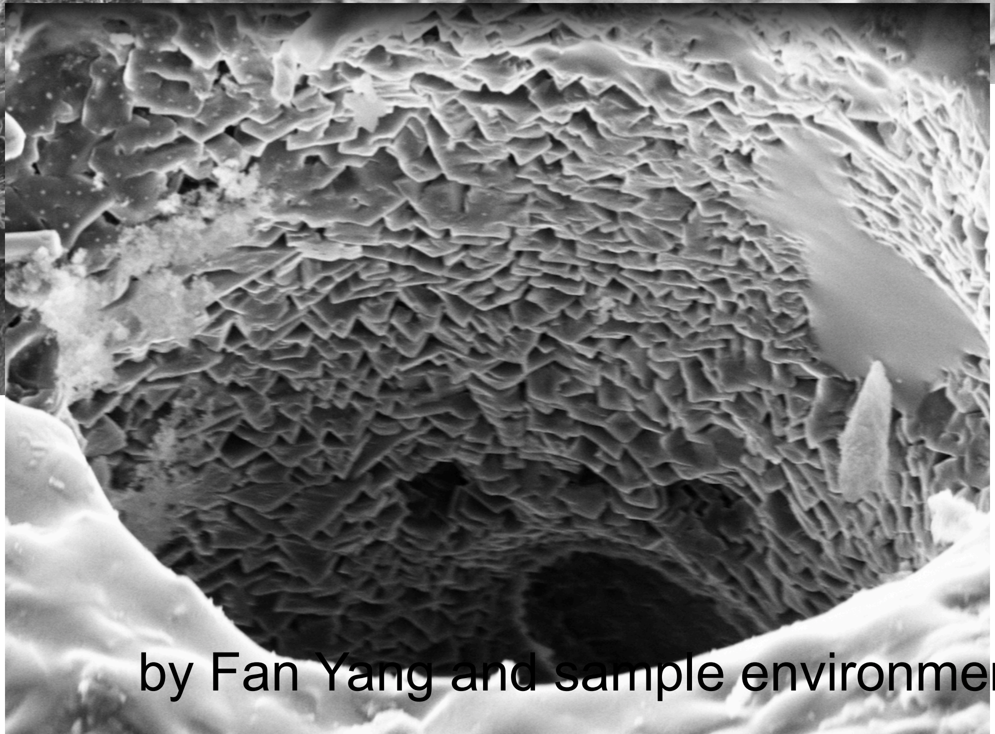
H. S

SEM pictures of B4C hole with 20 μm beam @



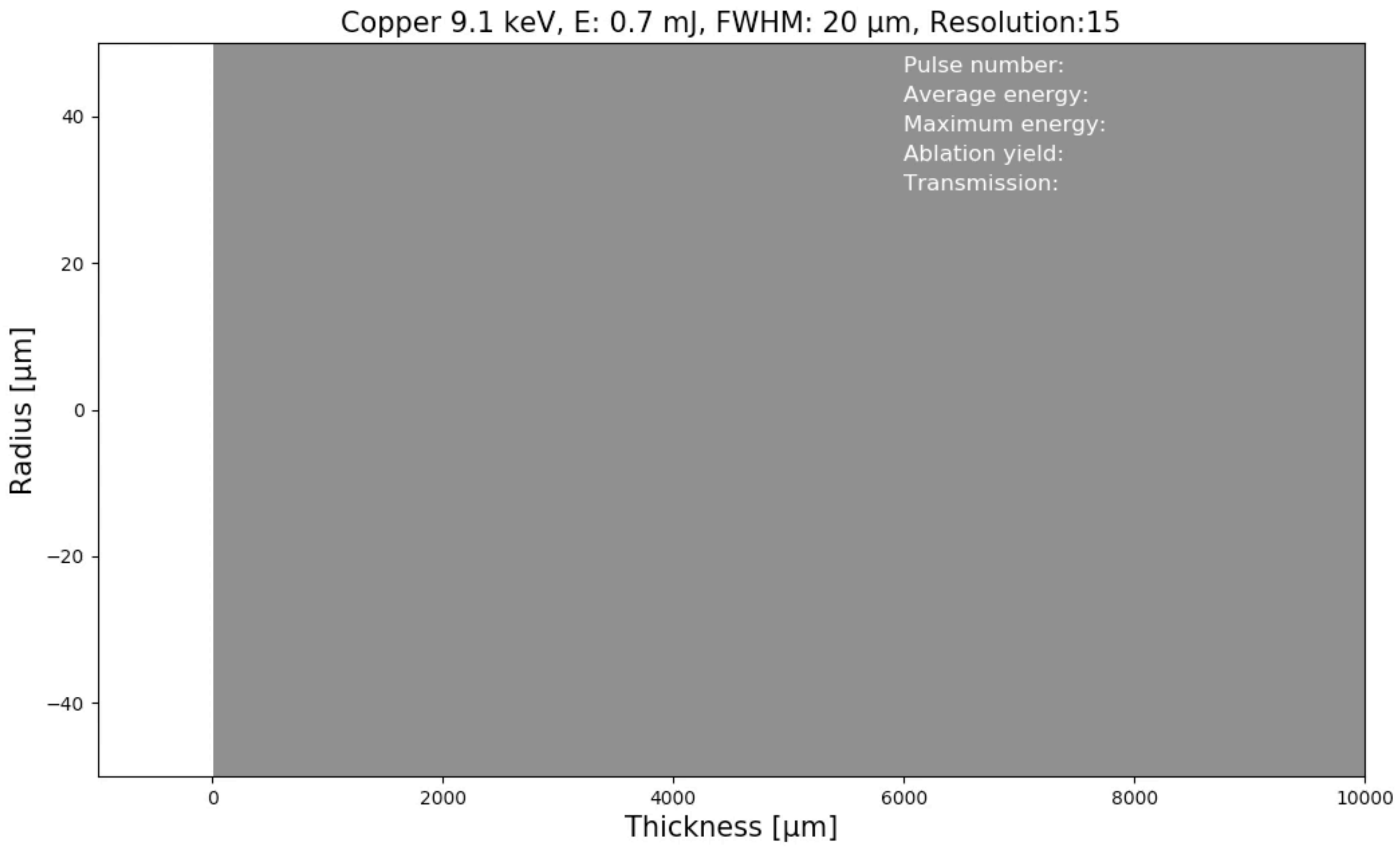






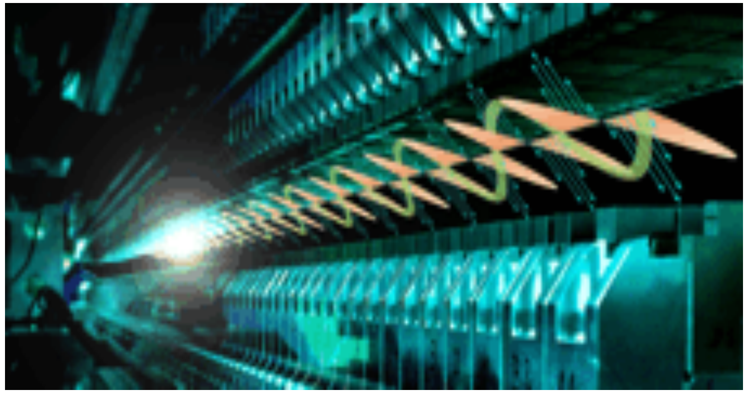
by Fan Yang and sample environment group

Movie of drilling process

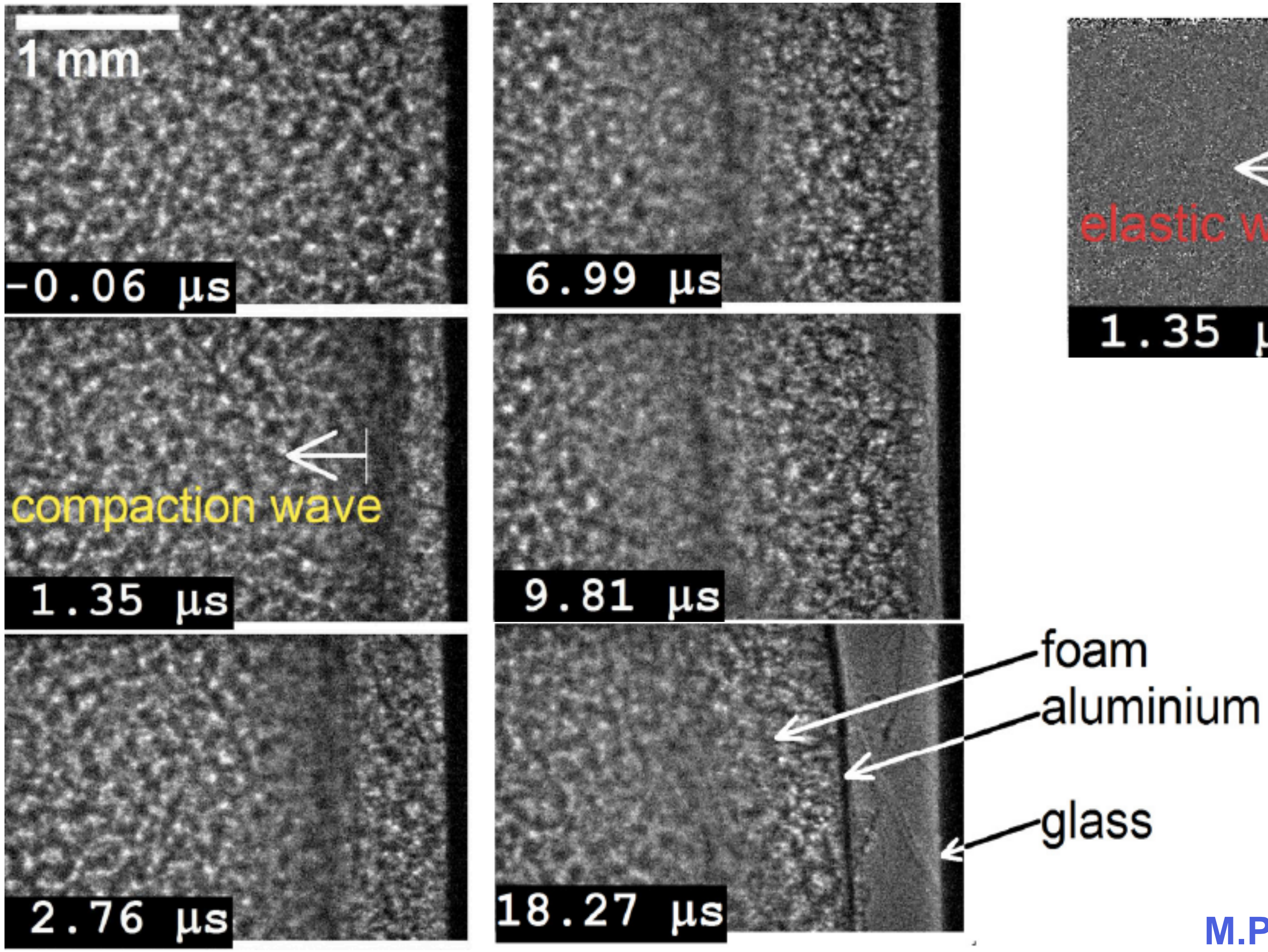


New Generation Sources
Free Electron Lasers (XFELs)

Main Applications



X-ray imaging of laser-driven shock compression



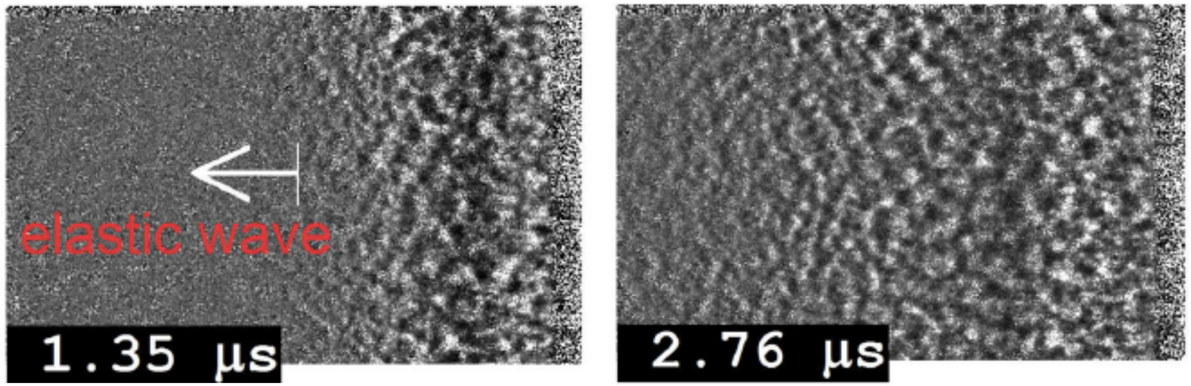


Fig. X-ray phase-contrast images of a polyurethane foam subjected to a laser shock applied on the right surface (the laser was directed through a glass plate onto an aluminium foil).

M.P. Olbinado, et al. *J. Phys. D* 51, 055601 (2018)

Compressional seismic wave

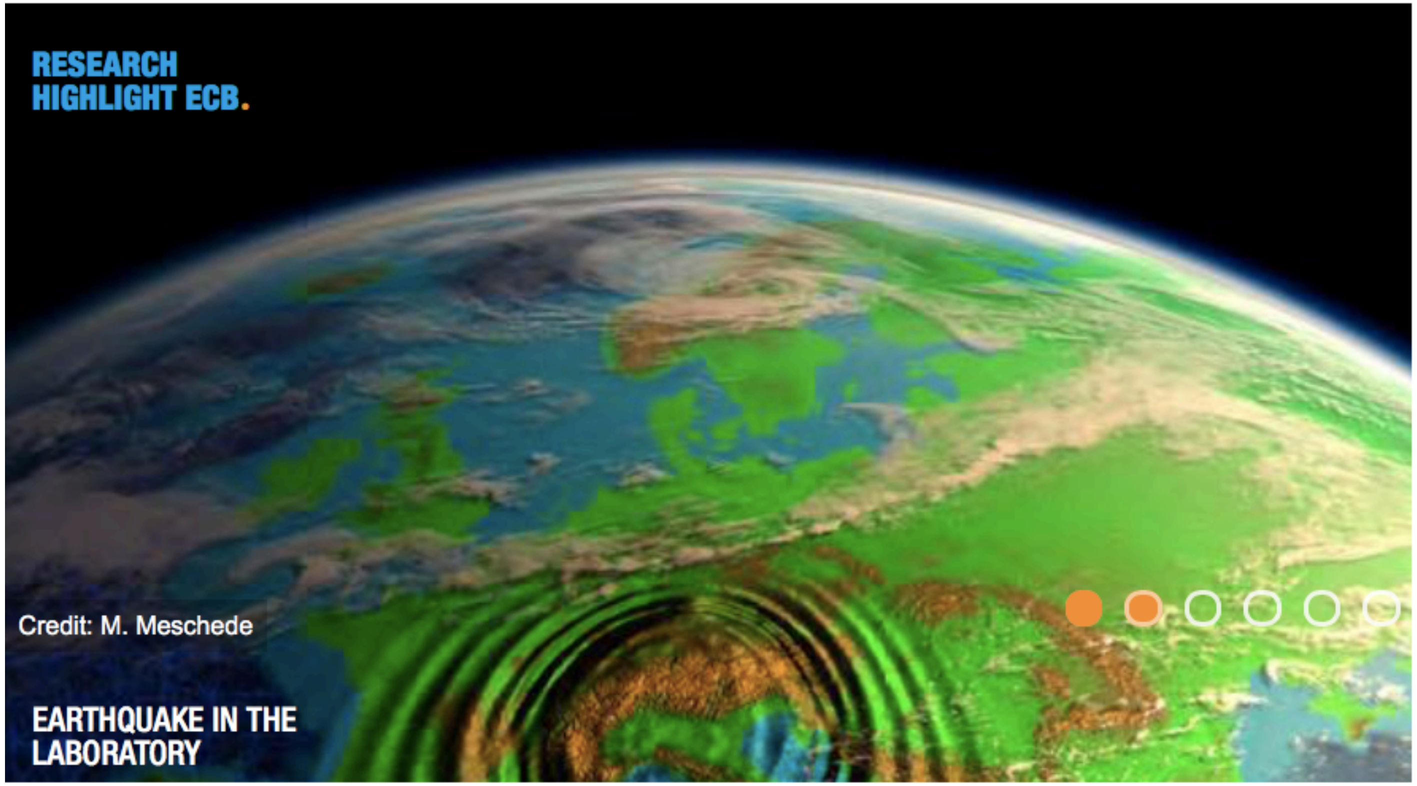


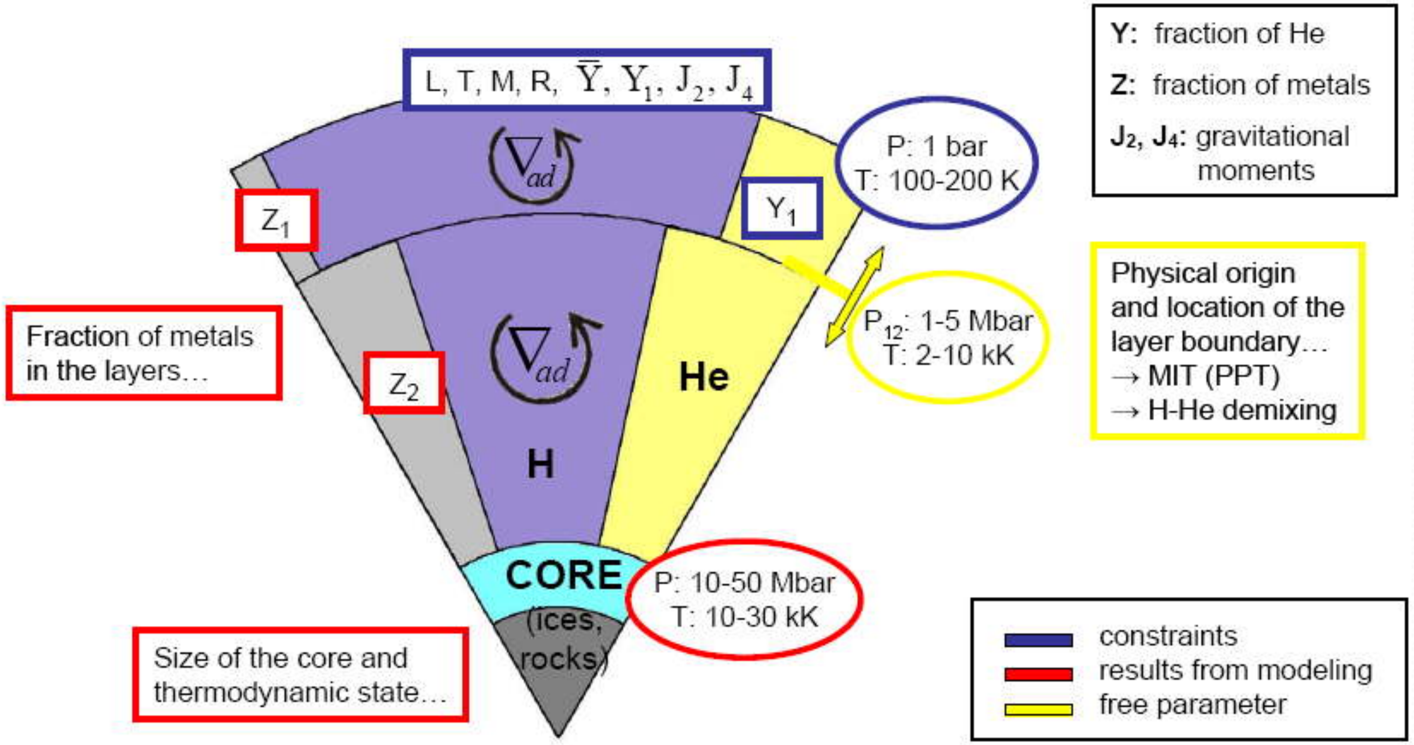
Fig. Propagation of a compressional seismic wave through $(Mg_{0.8}Fe_{0.2})O$ ferropericlase by employing a piezo-driven dynamic diamond anvil cell that allows to oscillate pressure at seismic frequencies was simulated.

H. Marquardt *et al.*
***Geophysical Research Letters* (2018)**

During pressure oscillations, X-ray diffraction images were continuously collected every 5–50 ms. The bulk modulus is directly calculated from these data at different pressures. Experiments show a pronounced softening of the bulk modulus throughout the spin crossover.

Planetarial models

Standard three-layer structure model



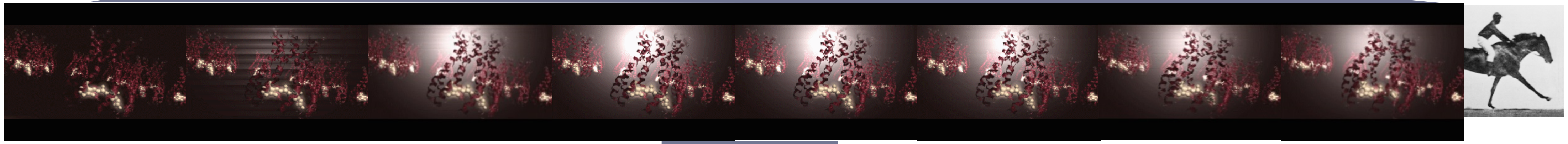
Apart from the transition pressure, interior models of this structure type are uniquely defined by the observables.

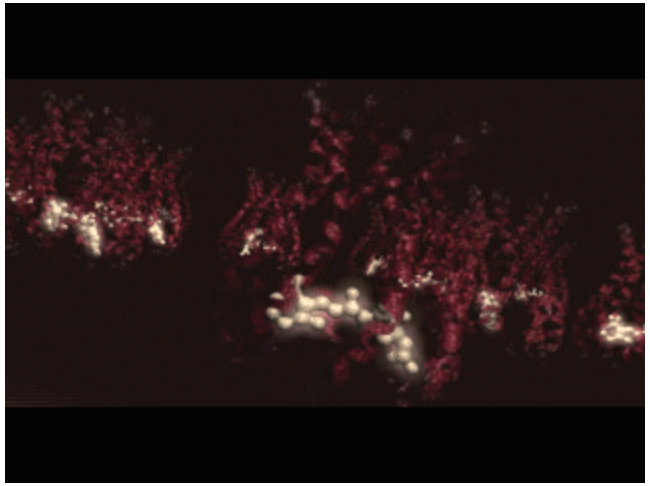
Most important input: Accurate EOS data for H and He as well as the representative of metals, e.g. H2O.

Making molecular movies

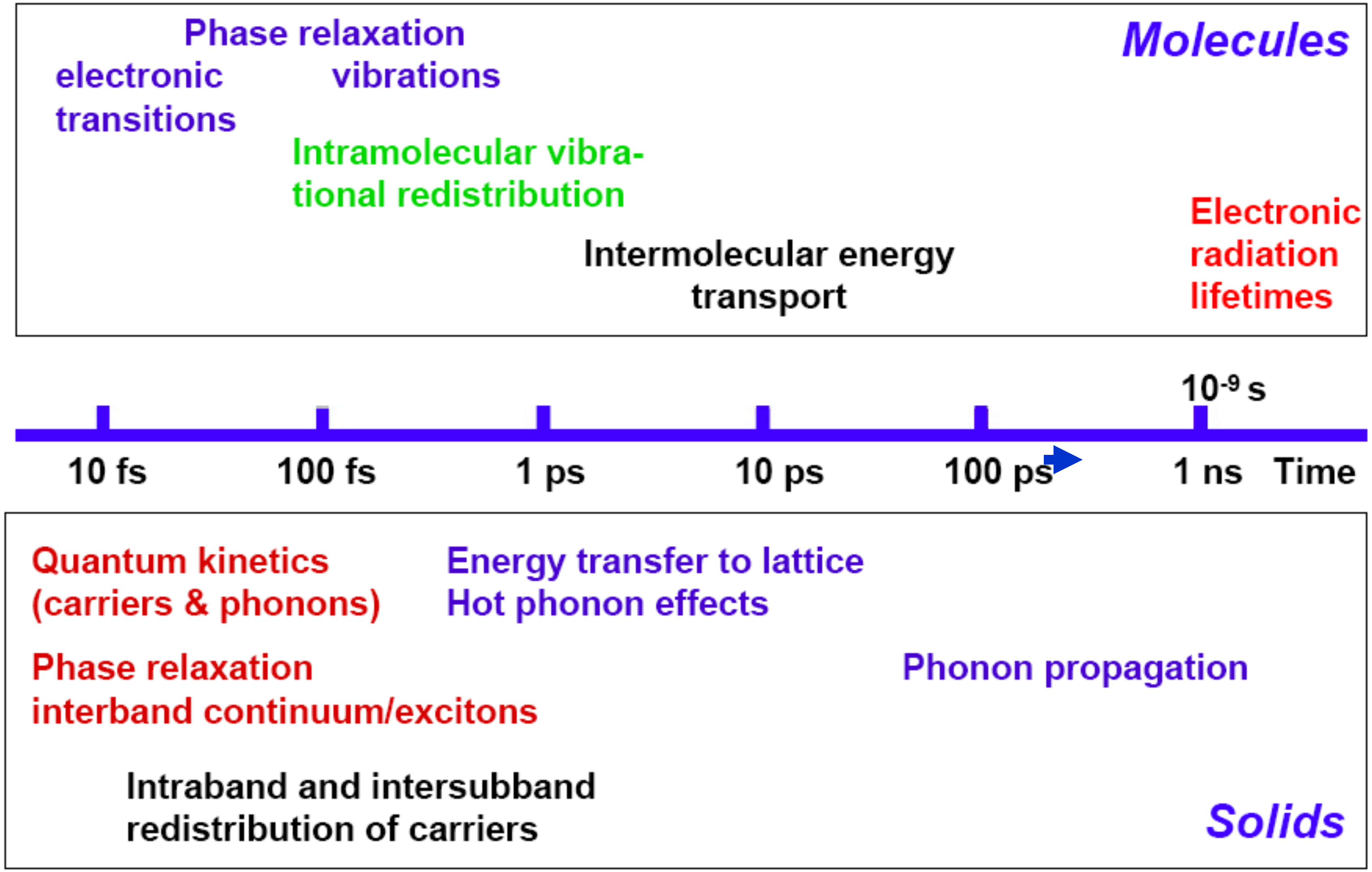
Eadward Muybridge
1892

European XFEL
2017



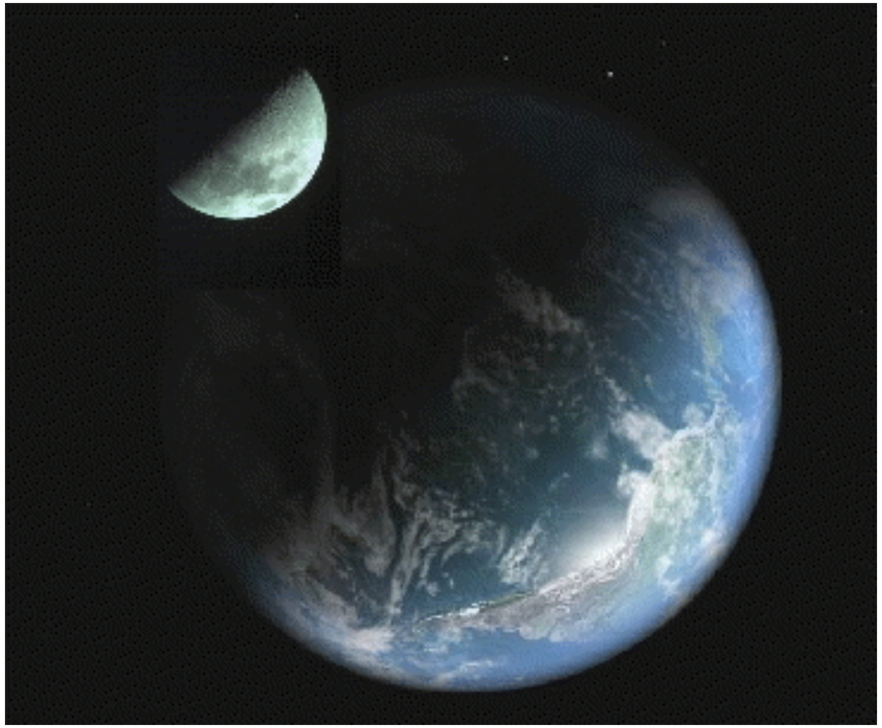


Time scales for dynamics



What is a picosecond?

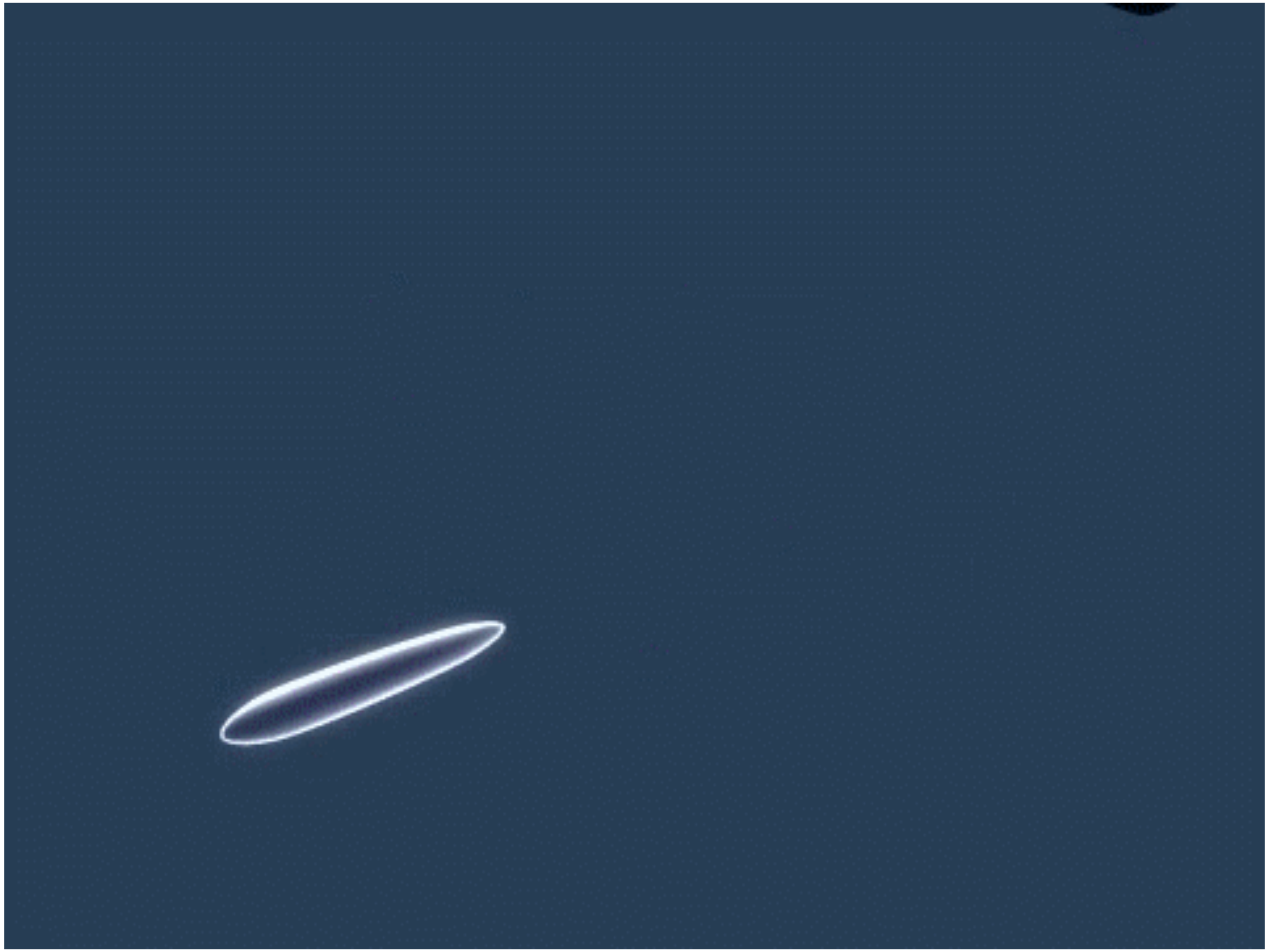
In 1 s light travels 300 000 km



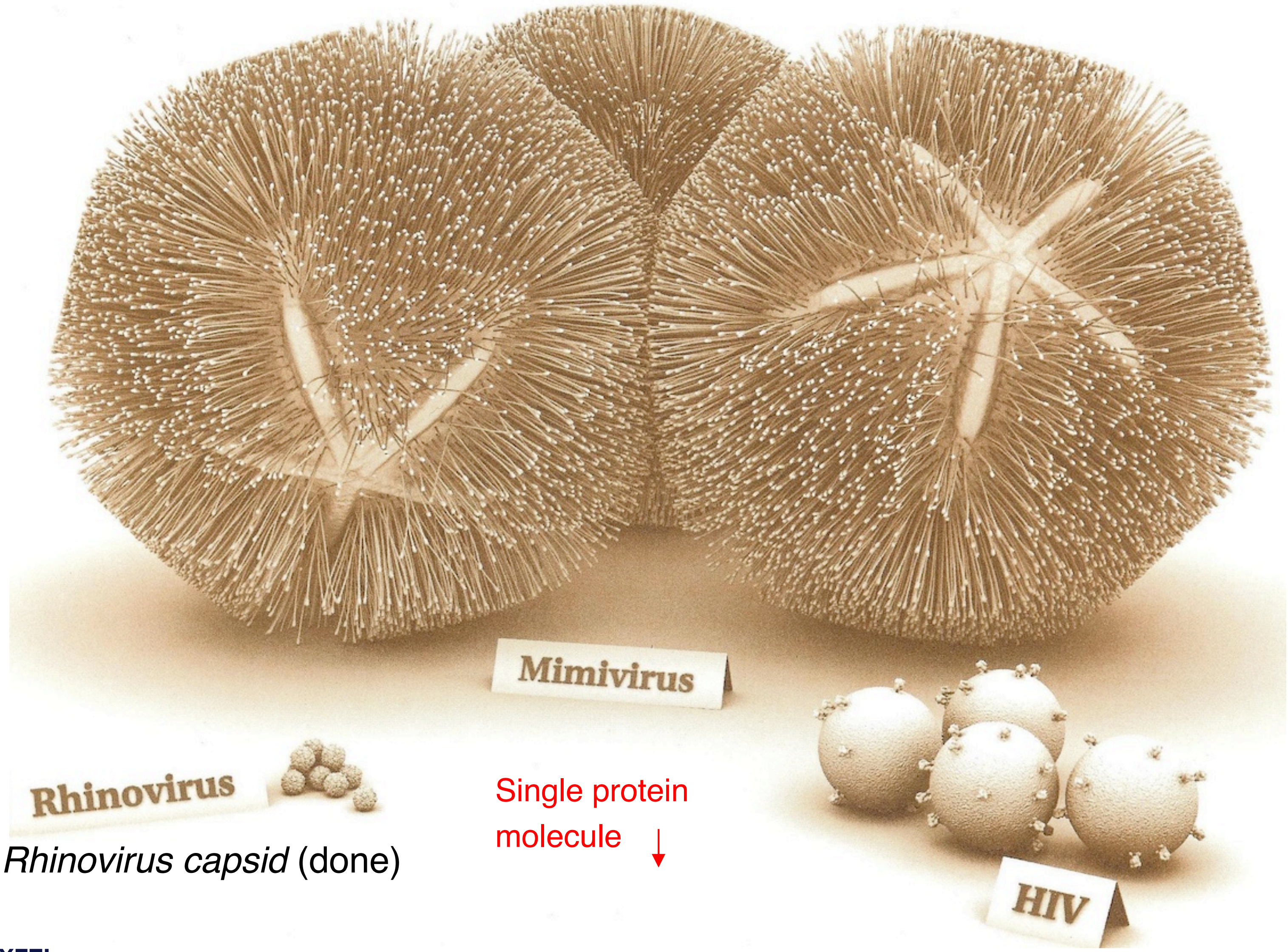
Distance between earth and moon is 384 000 km

In 1 fs light travels 0,3 µm

All these time-resolved in pump-probe experiments!



Tremendous variety of bio-objects to be studied



Rhinovirus capsid (done)

Single protein molecule ↓

http://www.americanscientist.org/issues/feature/2011/4/giant-viruses

Nobel prizes to synchrotron radiation work

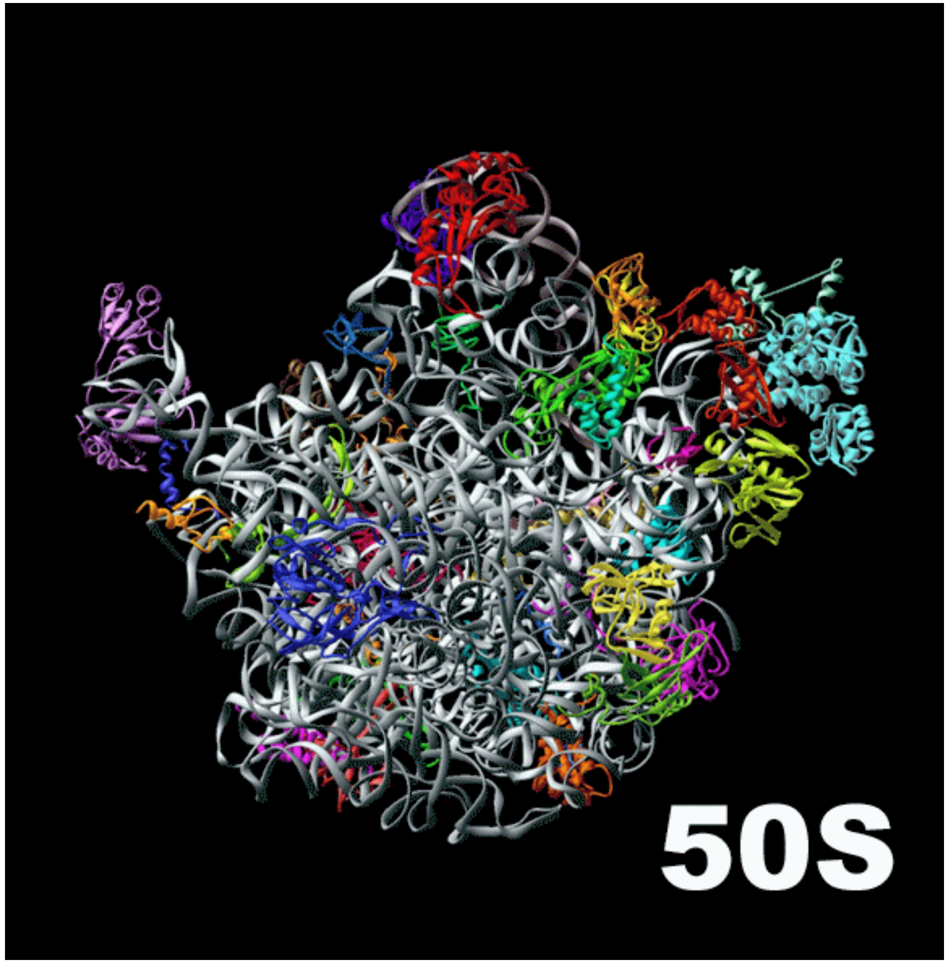
3 Win Nobel for Ribosome Research

From left, Venkatraman Ramakrishnan of the
Cambridge, England; Thomas A. Steitz of Yal
Institute of Science in Rehovot, Israel, will sha

2009 Venkatraman Ramakrishnan, Thomas Steitz & Ada Yonath

Working independently and using, among other things, the X-rays generated by powerful particle accelerators and prodigious computer calculations, the three winners and their colleagues succeeded in mapping the locations of the hundreds of thousands of atoms in the giant molecular complexes inside.

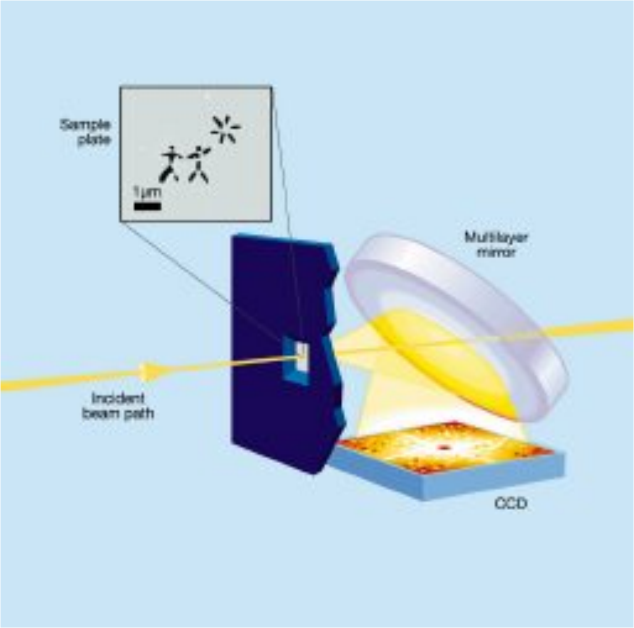
Ribosome: the Protein Factory of the cell



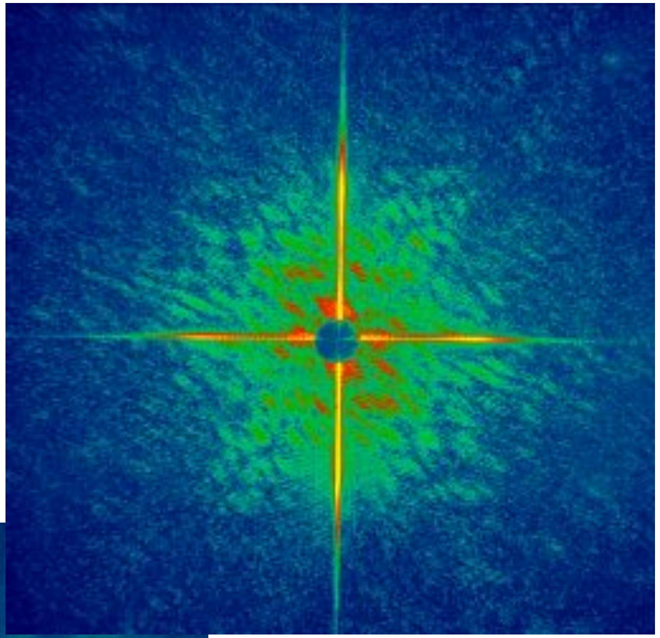
20 years of heroic efforts to crystallize Ribosomes!

Experiments at FLASH (H. Chapman, CFEL, Hamburg)

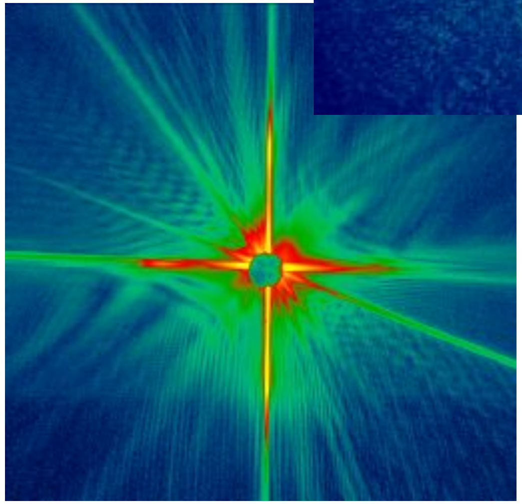
A single shot image



A nanoscale object can be imaged by a single femtosecond FEL pulse before the sample explodes

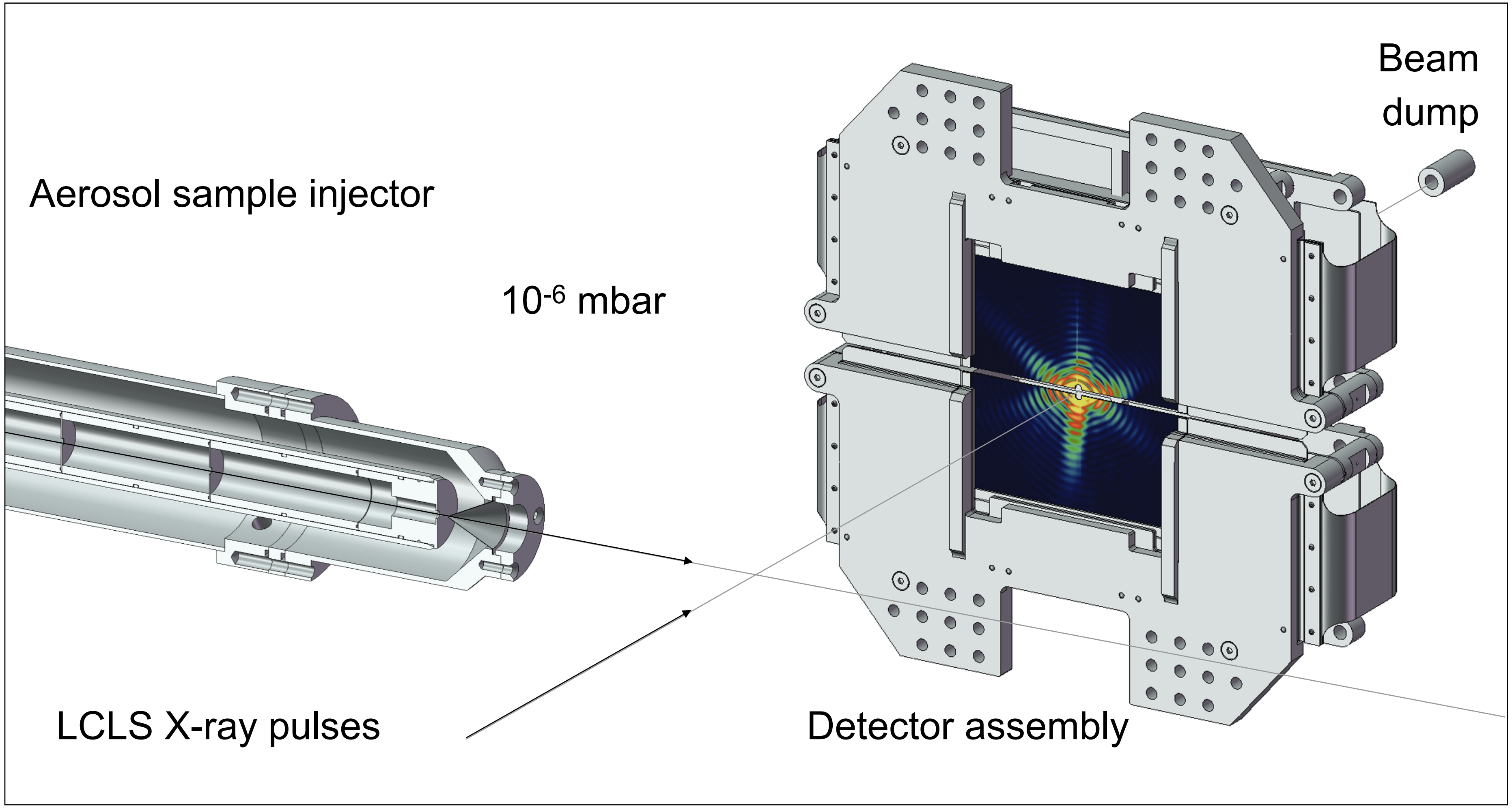


A coherent diffraction pattern recorded from a single 25 fs pulse



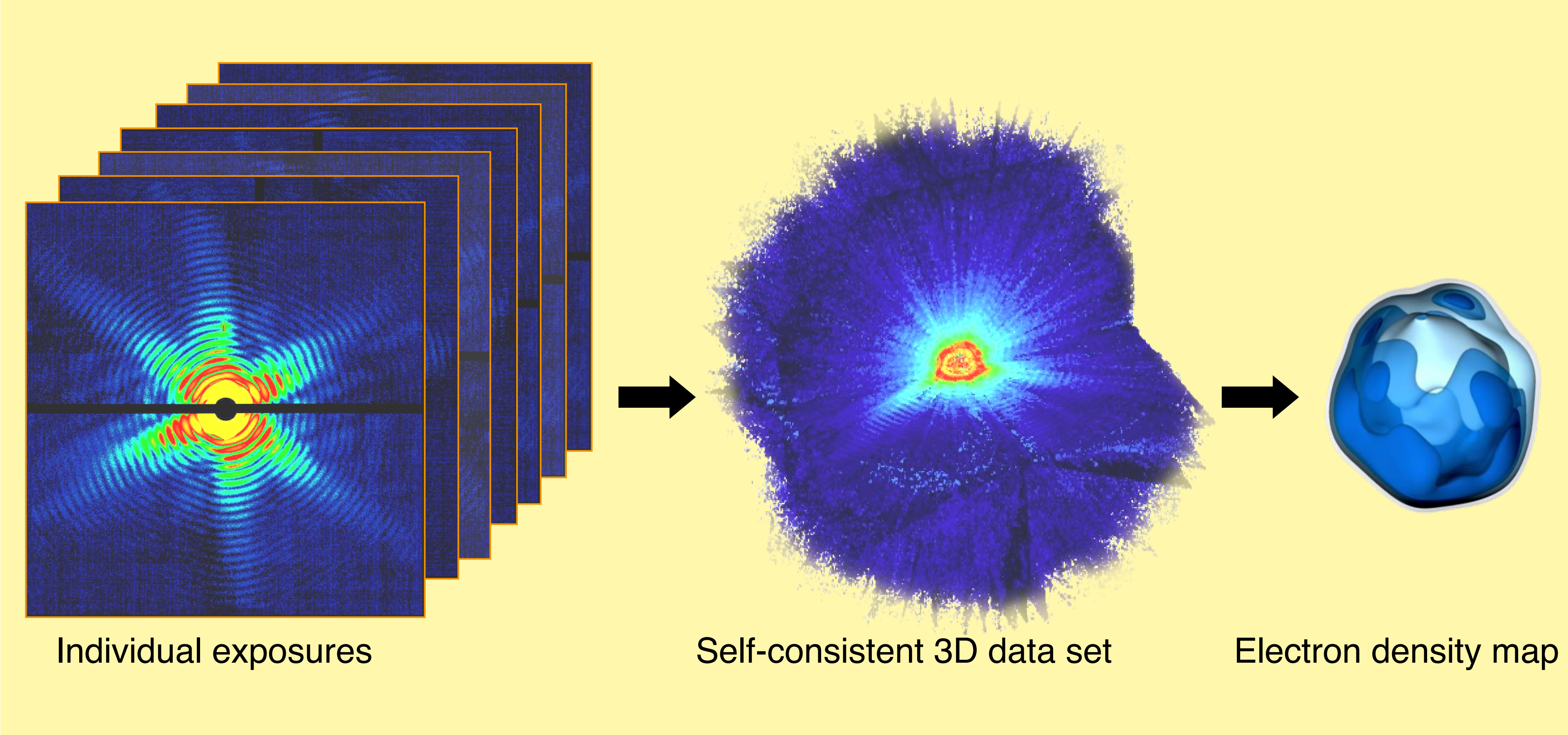
Diffraction pattern from a subsequent pulse showing that the sample was destroyed after recording the image

Single particle imaging (J. Hajdu, Uni Uppsala)



Measured hit rates match theoretical values

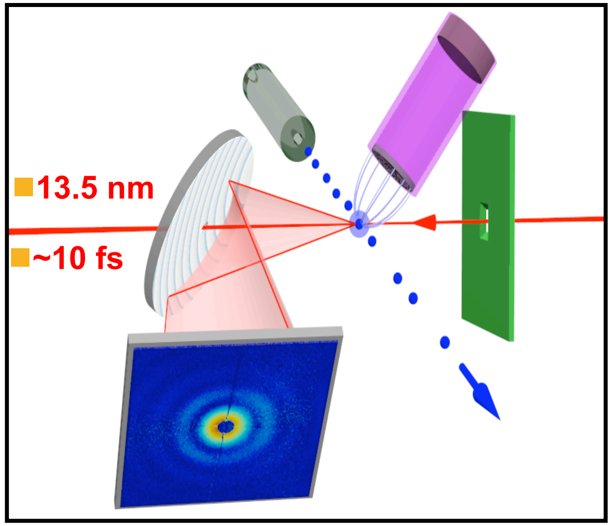
Single particle imaging (J. Hajdu, Uni Uppsala)

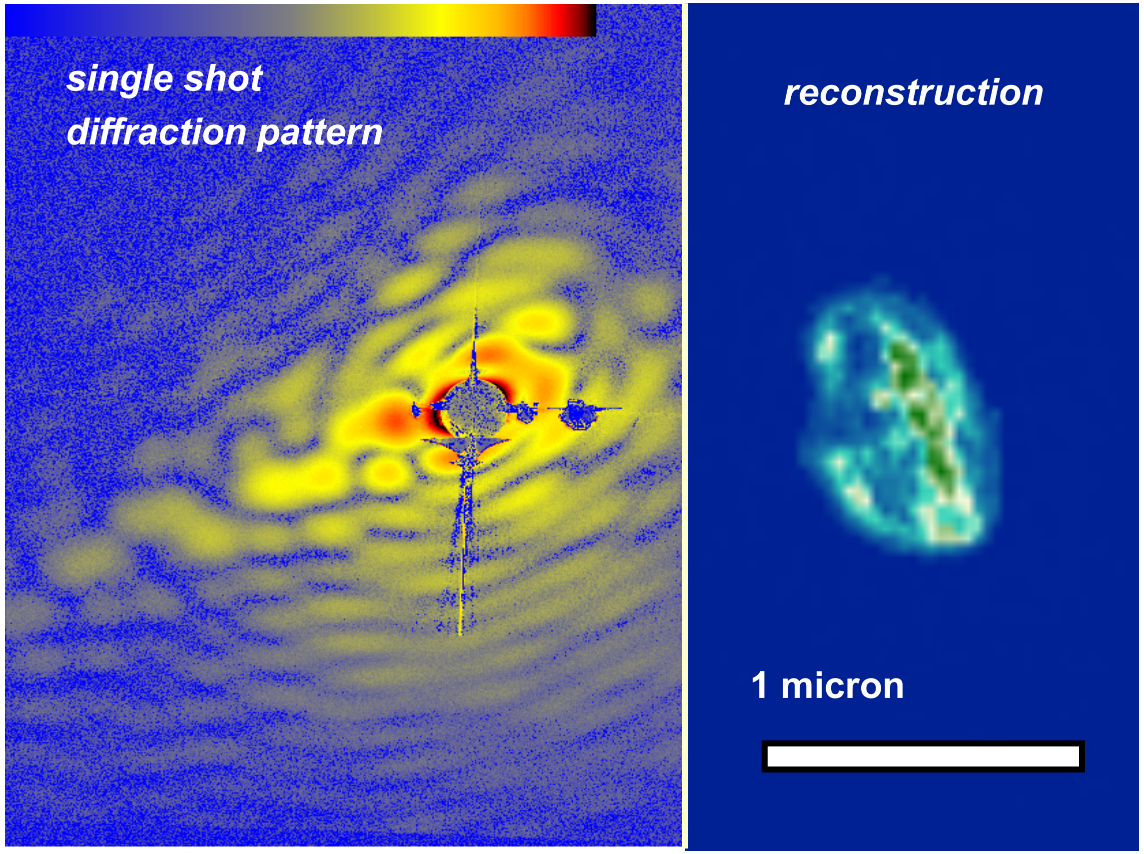


From 2D to 3D structure determination

Imaging picoplankton organism "on the fly"

- ***PICOPLANKTON** are the most abundant photosynthetic cells in the oceans (discovered in 1988)*



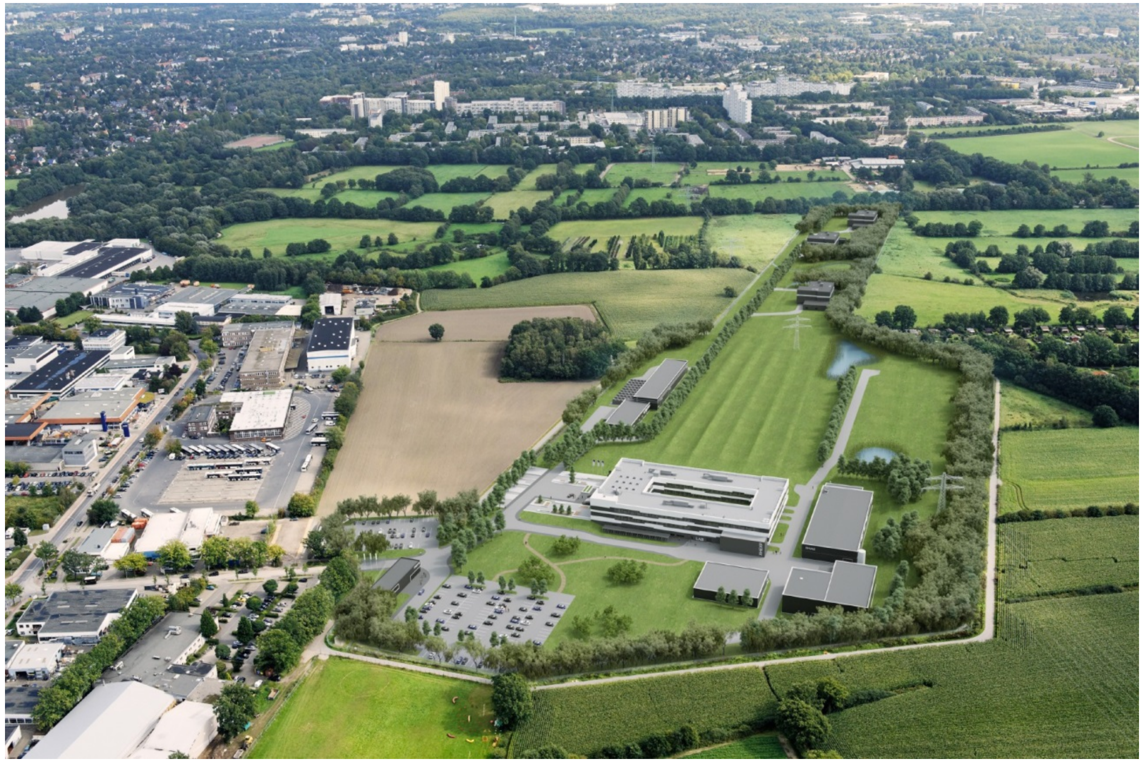


- ***This cell was injected into vacuum from solution, and shot through the beam at 200 m/s***

- J. Hajdu, I. Andersson, M. Svenda, M. Seibert (Uppsala)
- S. Boutet (SLAC)
- M. Bogan, H. Benner, U. Rohner, H. Chapman (LLNL)

European XFEL – a leading new research facility

The European XFEL is a research facility, which generates high-energy X-ray light to help scientists better understand the nature of matter.



Site at the start of user operation

Schenefeld & Hamburg, Germany

User facility with 360 staff (+ 230 from DESY)

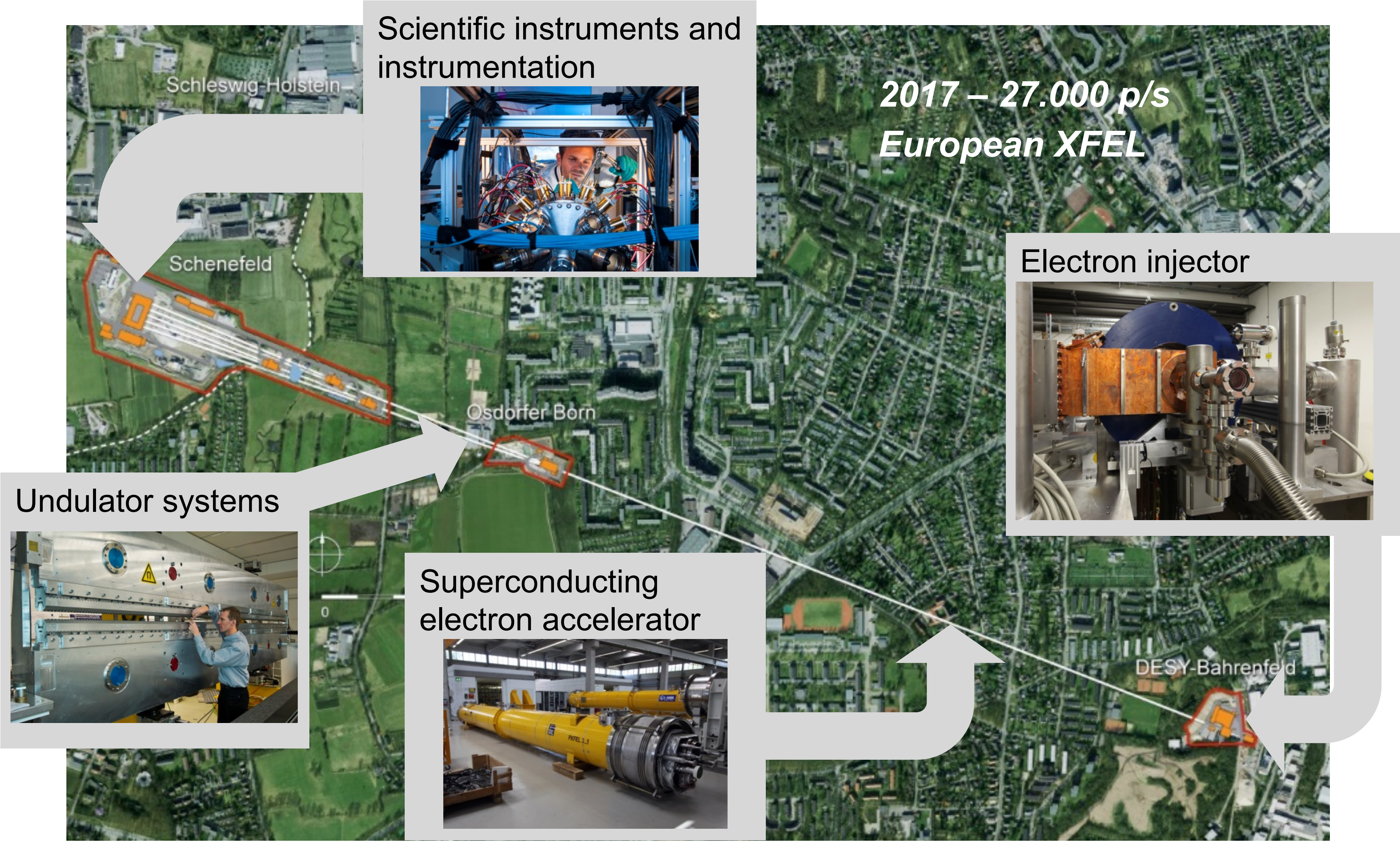
2017: Start of user operation

Hamburg, 30.11.2009: the European XFEL Convention Signing Ceremony

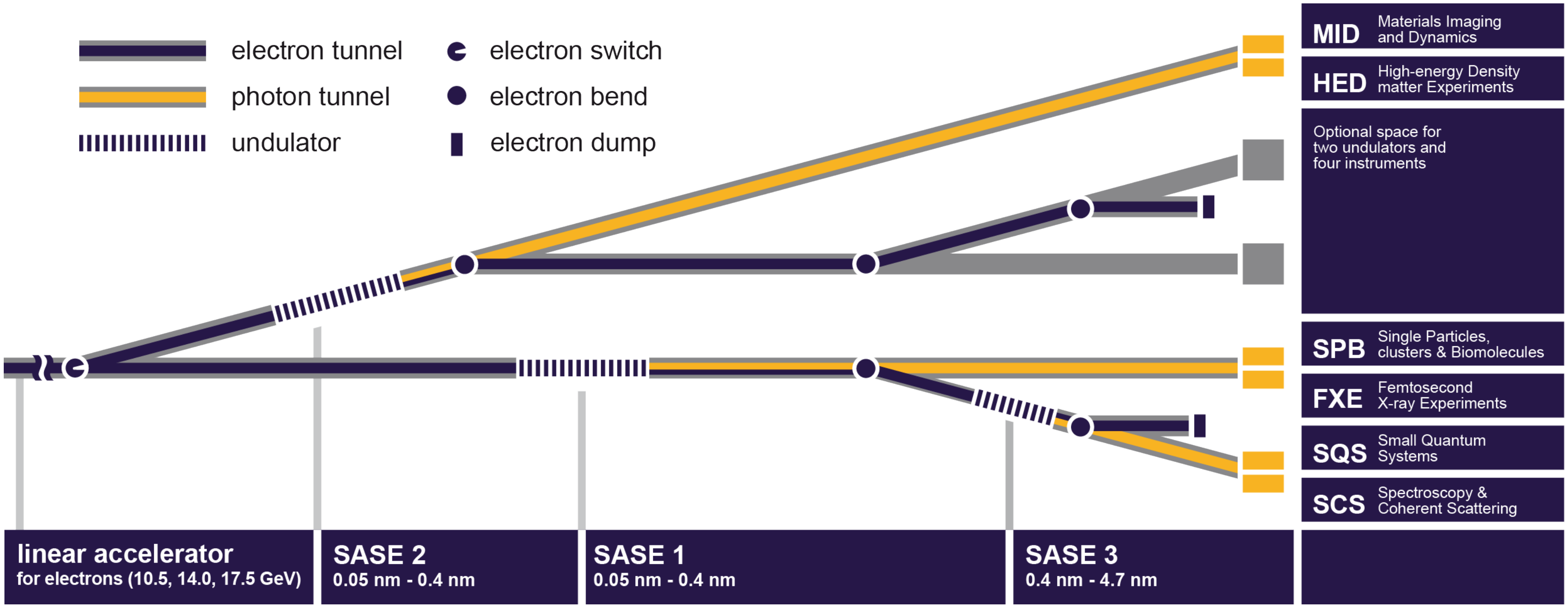
Total costs ≈1.500 MEUR, Shareholder & Scientific Coordinator – Kurchatov Institute

European XFEL - a leading new research facility

How it works – a closer look at the facility

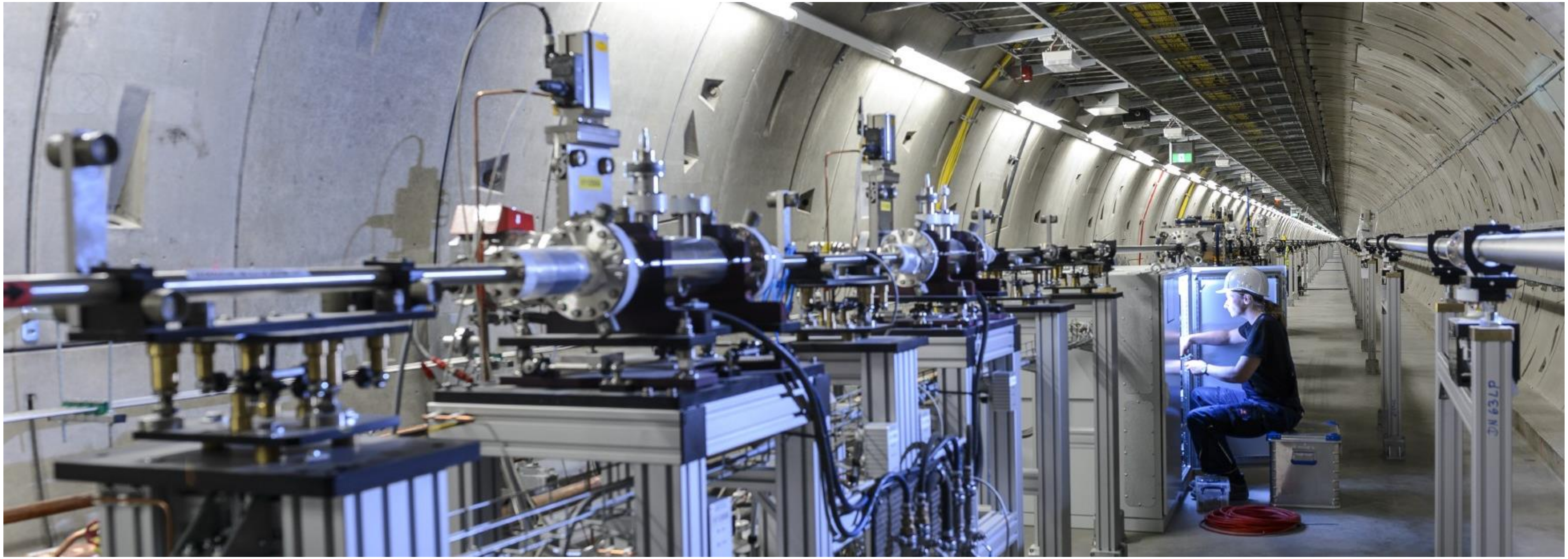


Beamline layout & experiment stations

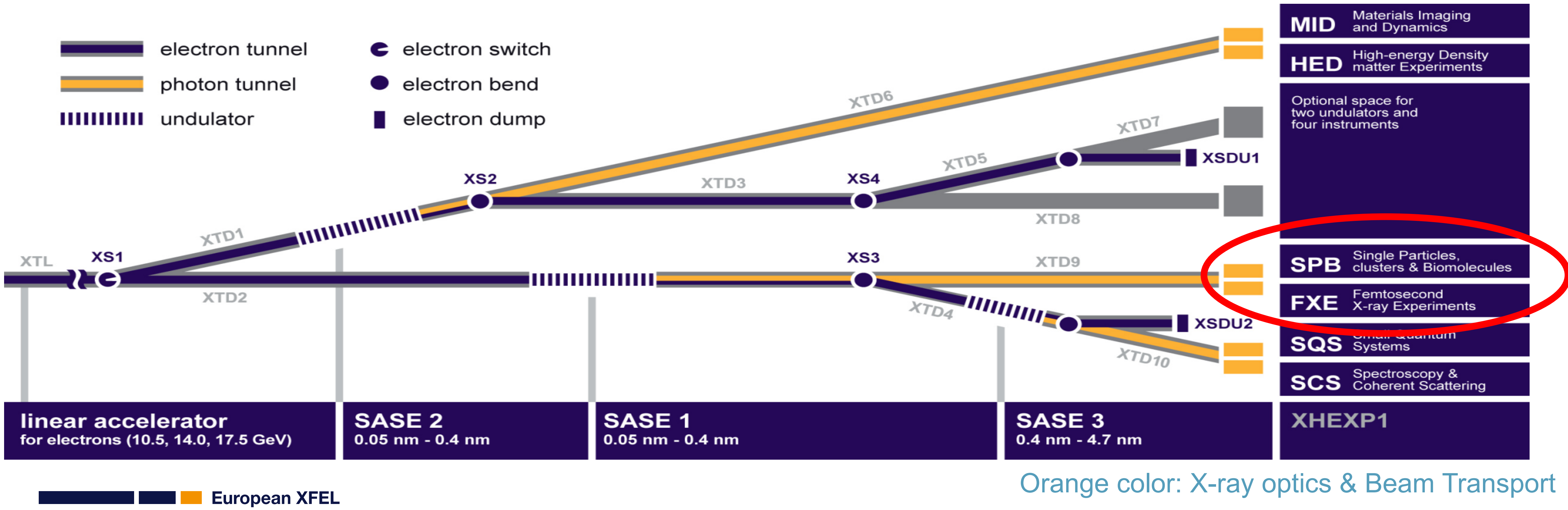


Undulators in tunnel

Photon beamlines

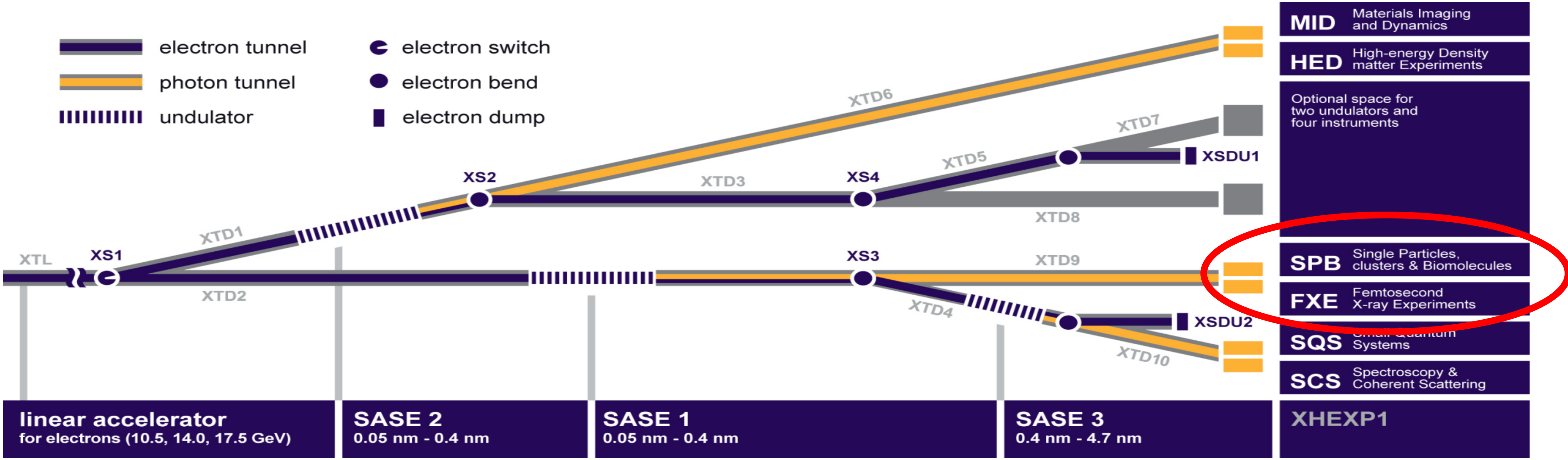


Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24 (Hard XR)	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 – 3 (Soft XR)	4.6 – 0.4



Orange color: X-ray optics & Beam Transport

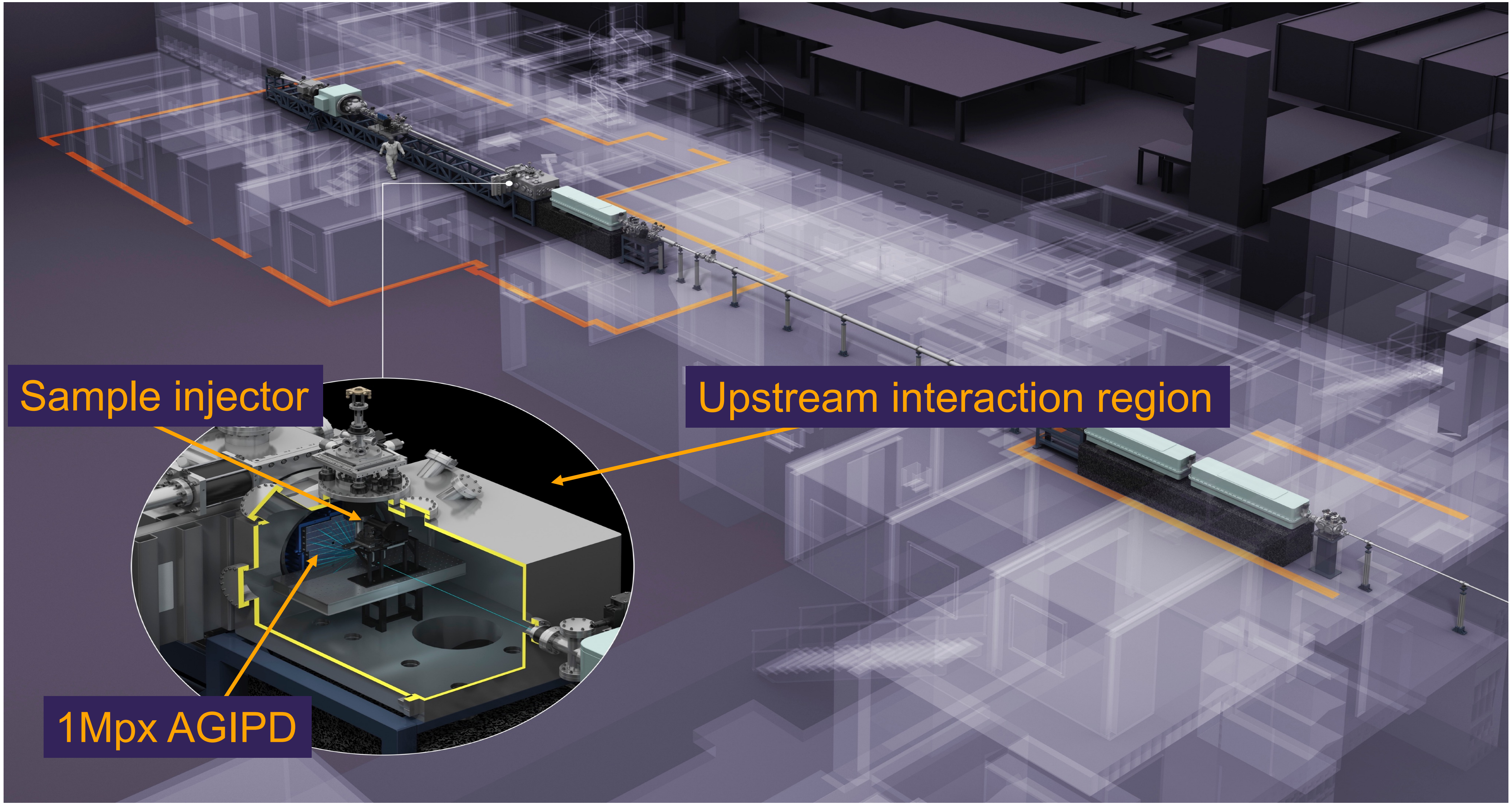
Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24 (Hard XR)	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 – 3 (Soft XR)	4.6 – 0.4



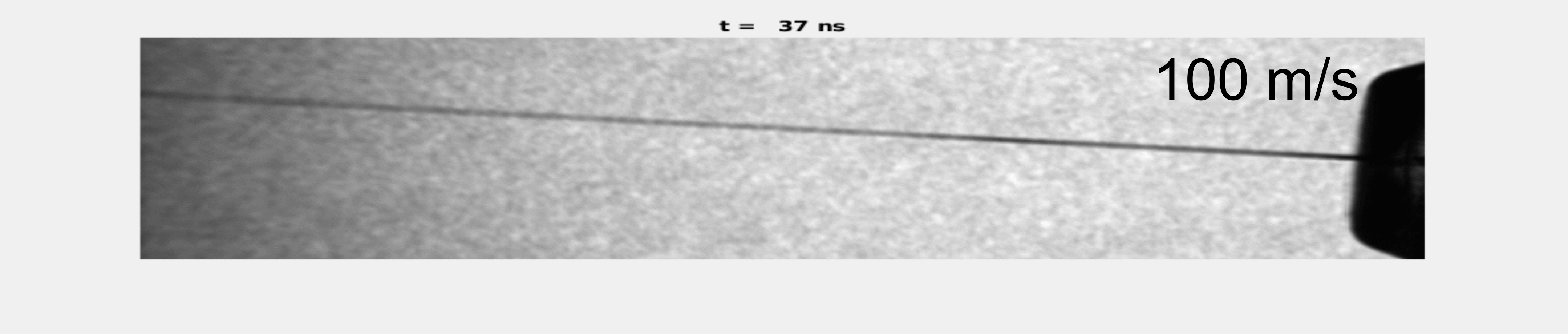
European XFEL

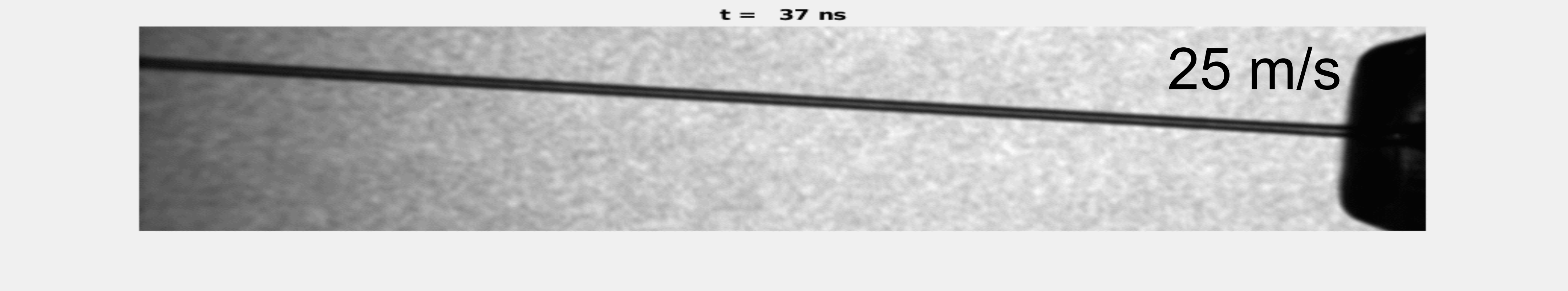
Orange color: X-ray optics & Beam Transport

Artist’s impression of the SPB/SFX Instrument



CFEL-designed jets recover in time for next pulse at 1.1 MHz repetition rate





Max Wierdorn, Claudio Stan

European XFEL

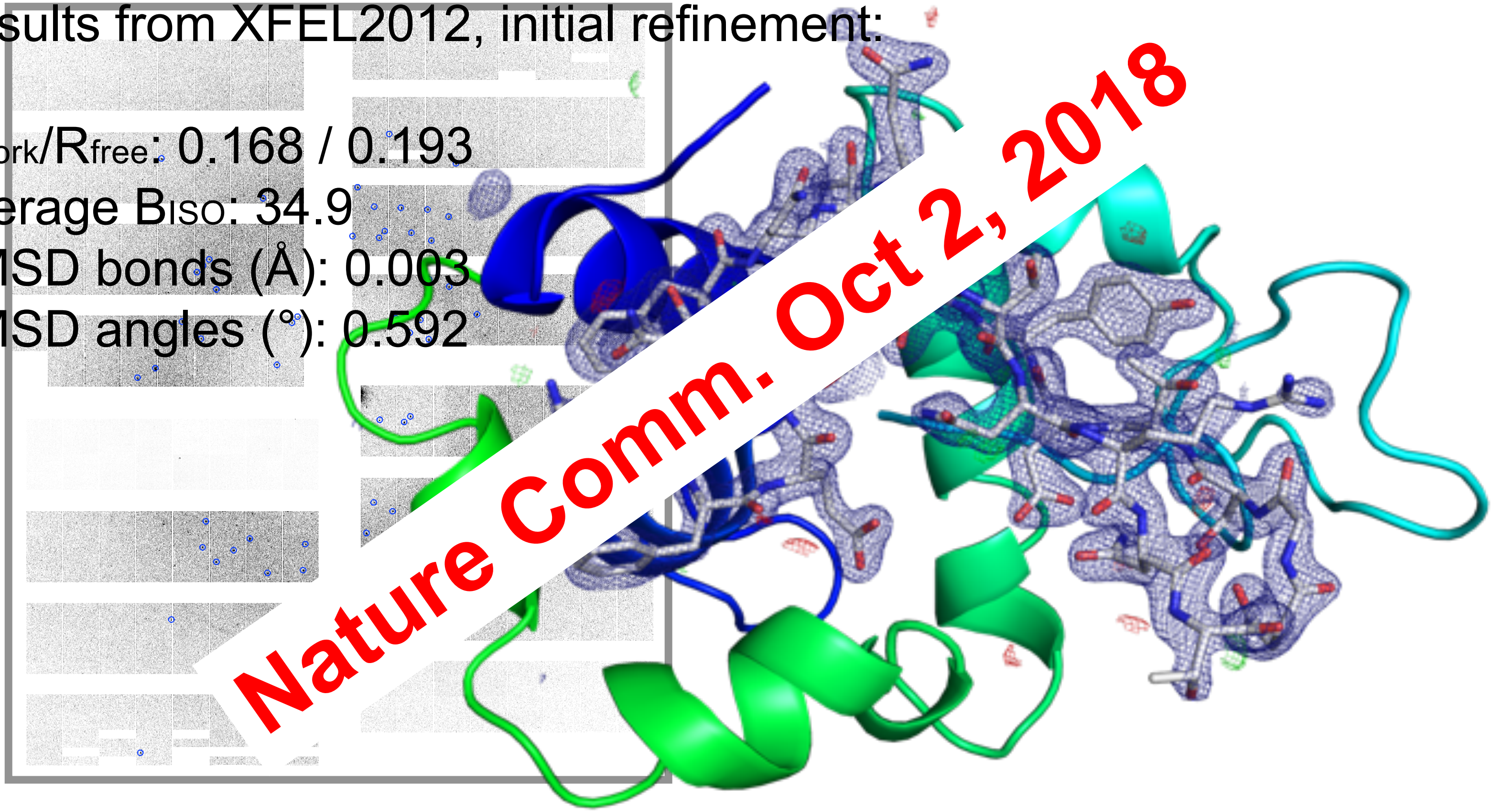
(courtesy A. Barty, H. Chapman)

CFEL SCIENCE

SPB/SFX experiment #2012 (A. Barty, CFEL): Many thousands of frames of diffraction data was collected and successfully analysed to give a structure!

Results from XFEL2012, initial refinement:

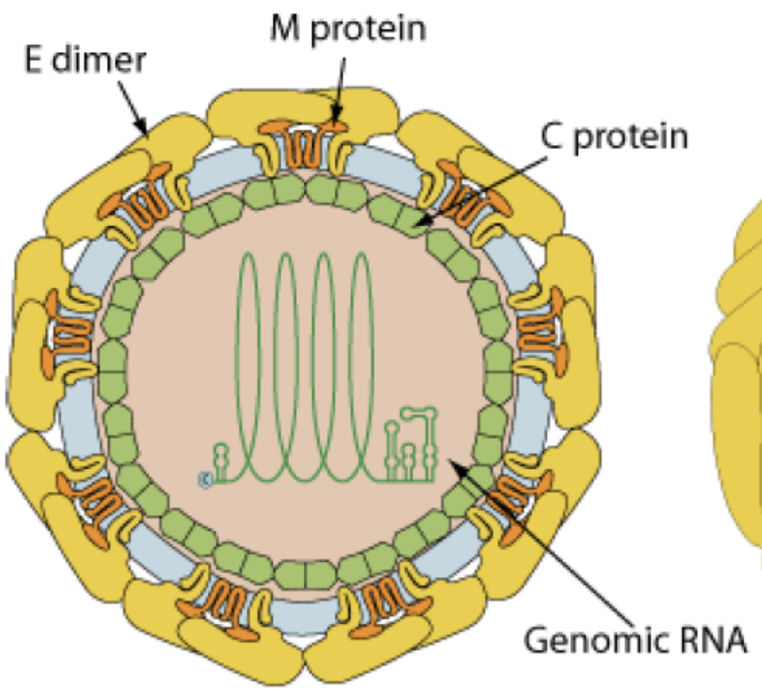
R_{work}/R_{free}: 0.168 / 0.193
Average B_{iso}: 34.9
RMSD bonds (Å): 0.003
RMSD angles (°): 0.592

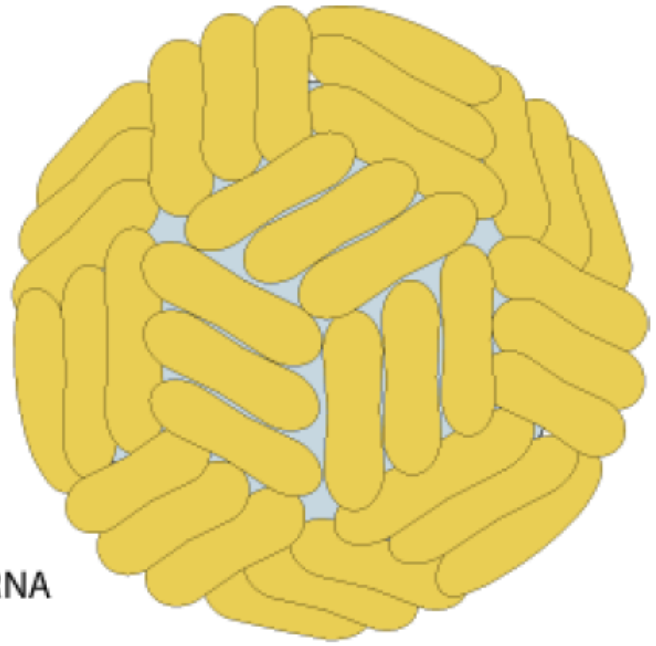


- This is the first realisation of the European XFEL's purpose—a complete experiment from start-to-end demonstrated in the very first user experiment at the facility at the SPB/SFX instrument (Data September 2017, Analysis November 2017). That is, structural biology works at XFEL!

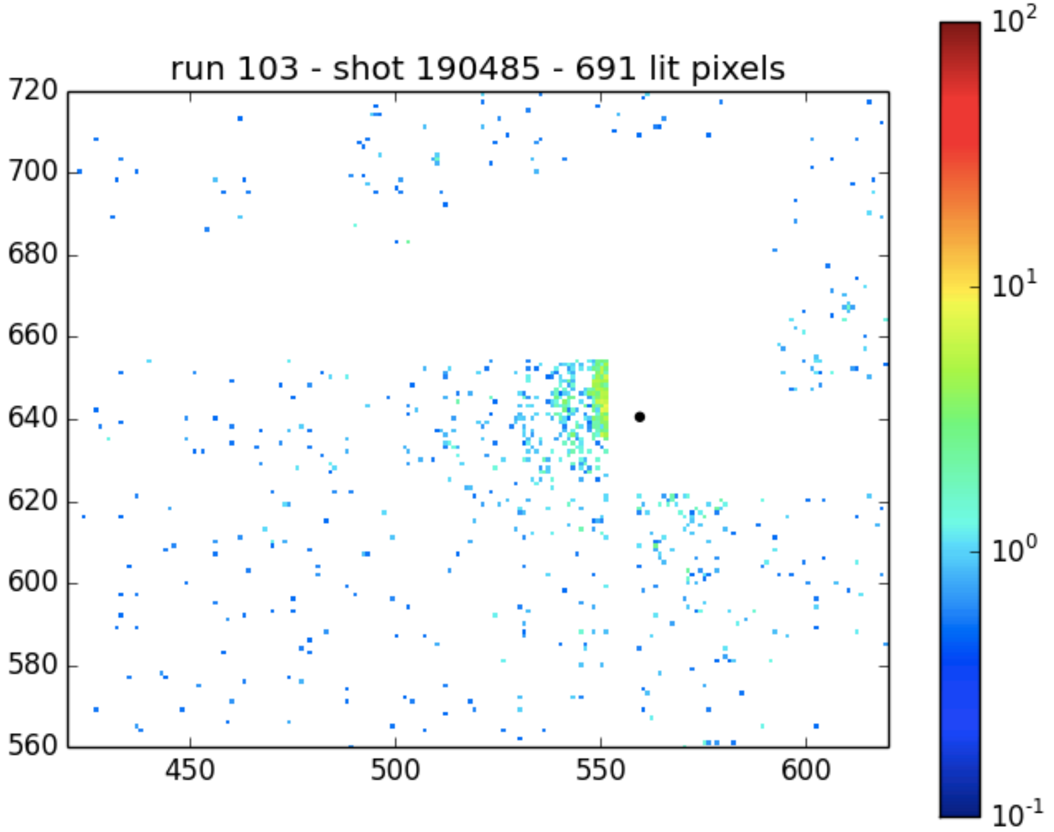
Courtesy Adrian Mancuso

SPB/SFX experiment #2145 (A. Egorov, Chumakov Center & Kurchatov Institute): Tick-borne encephalitis virus (TBEV) vaccine





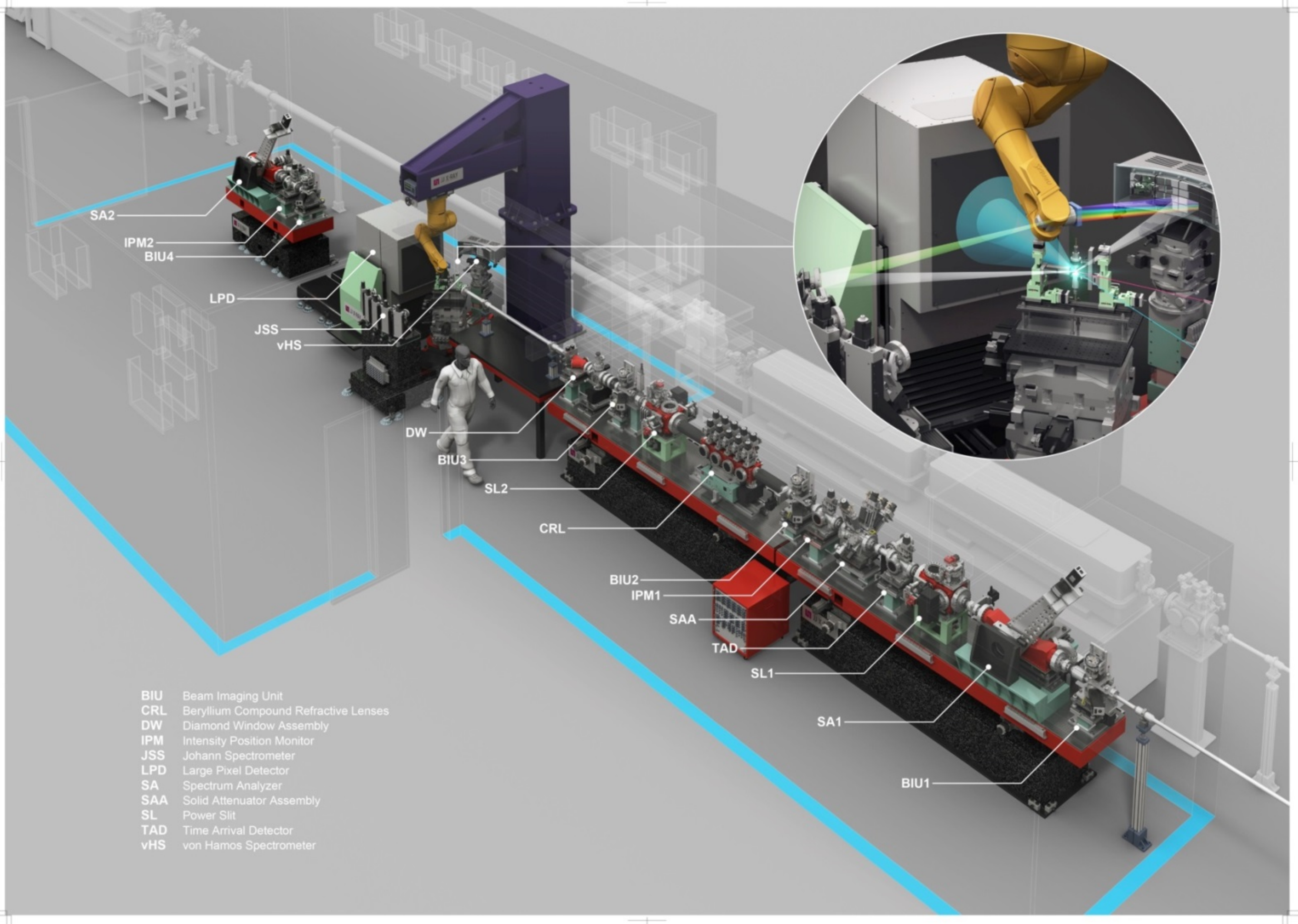
T=3-like organization of surface dimers



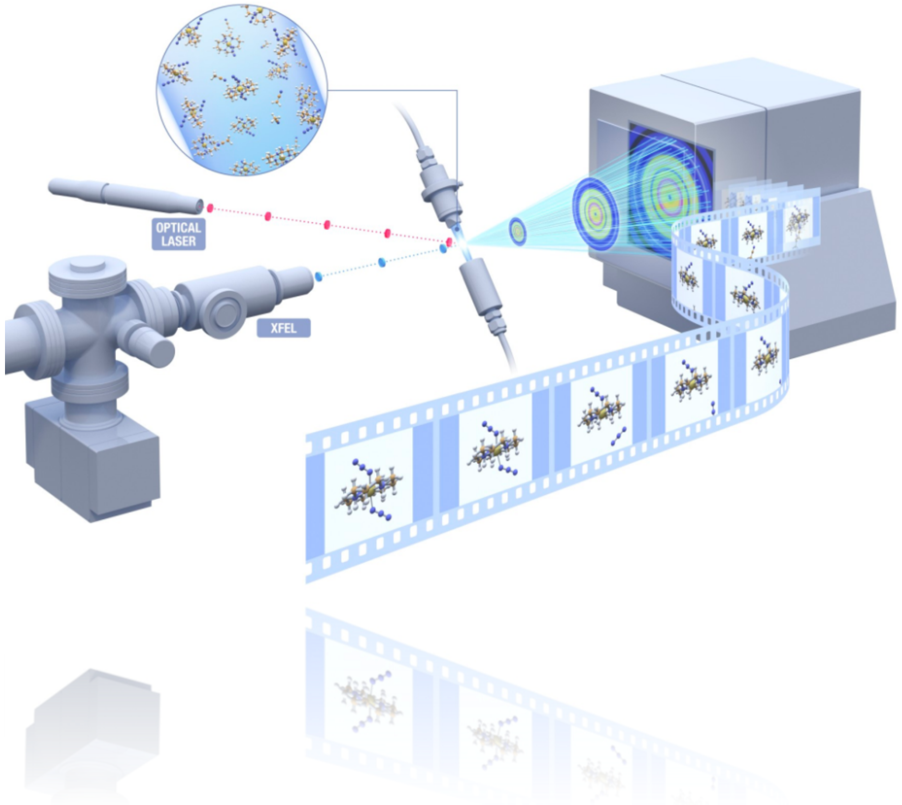
- During the beamtime for proposal 2145 (May 23-26, 2019) the sample of inactivated TBEV was successfully injected into XFEL SPB/SFX instrument chamber and more than 200 hits were observed!

Courtesy Adrian Mancuso

FXE – femtosecond X-ray experiments



Ultrafast photo-induced processes in liquids and solids

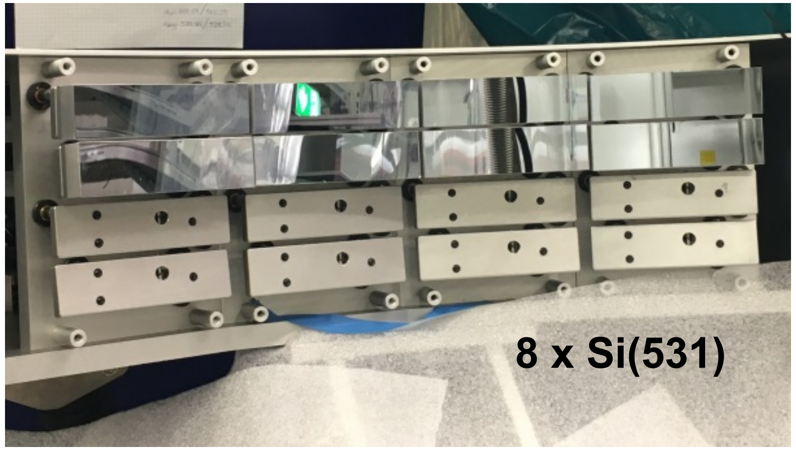


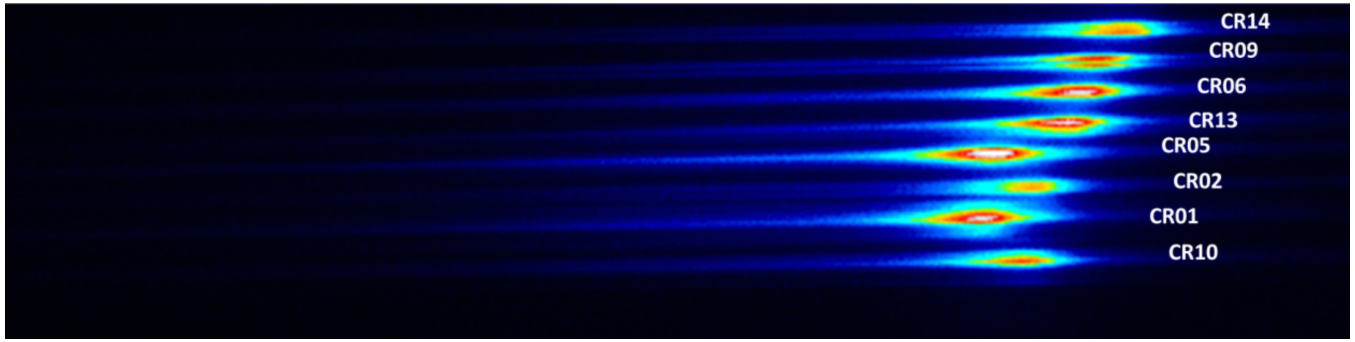
X-ray emission spectroscopy on $Fe(bpy)_3$ solution: #2016 (Gawelda et al.)

- 30 bunches, 9.3 keV, ~100uJ/pulse, focused to ~20 um

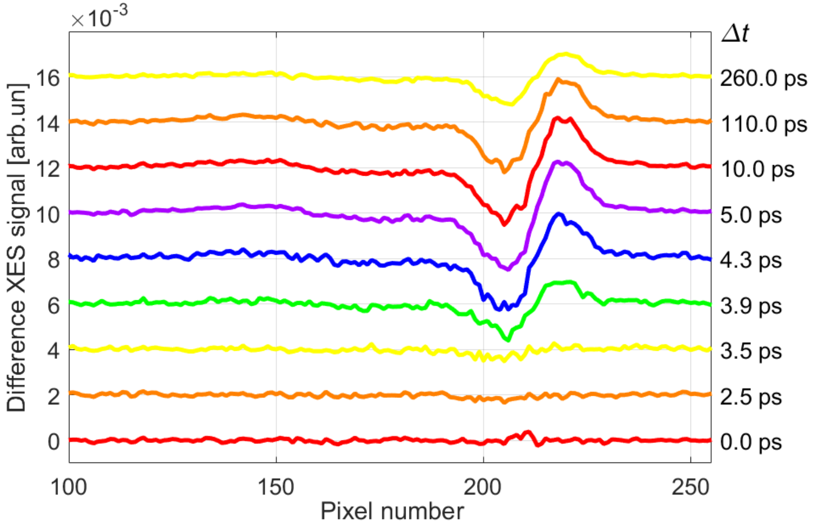
GreatEyes CCD detector

- von Hamos spectrometer

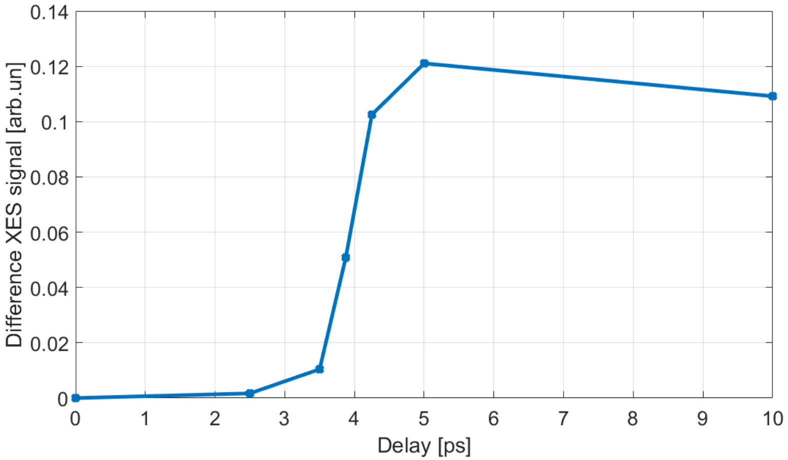




- Difference Iron K_β spectra



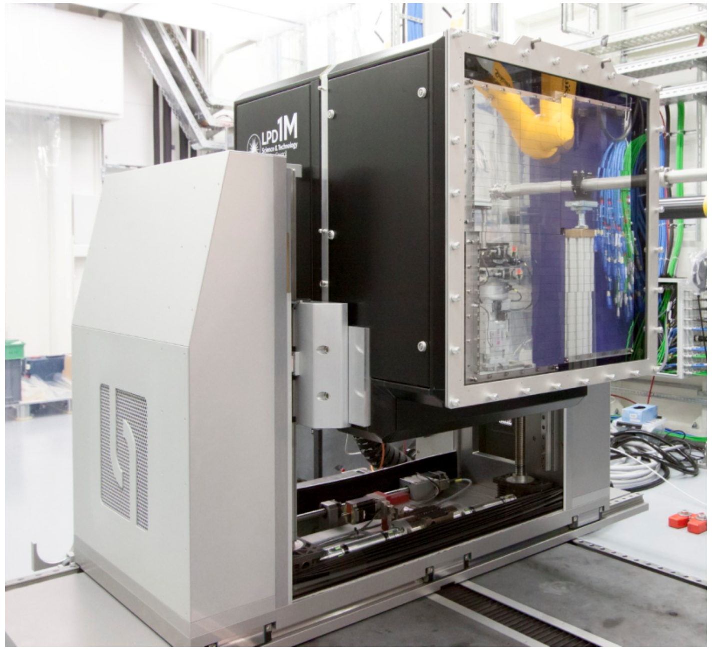
- Laser/X-ray delay scan



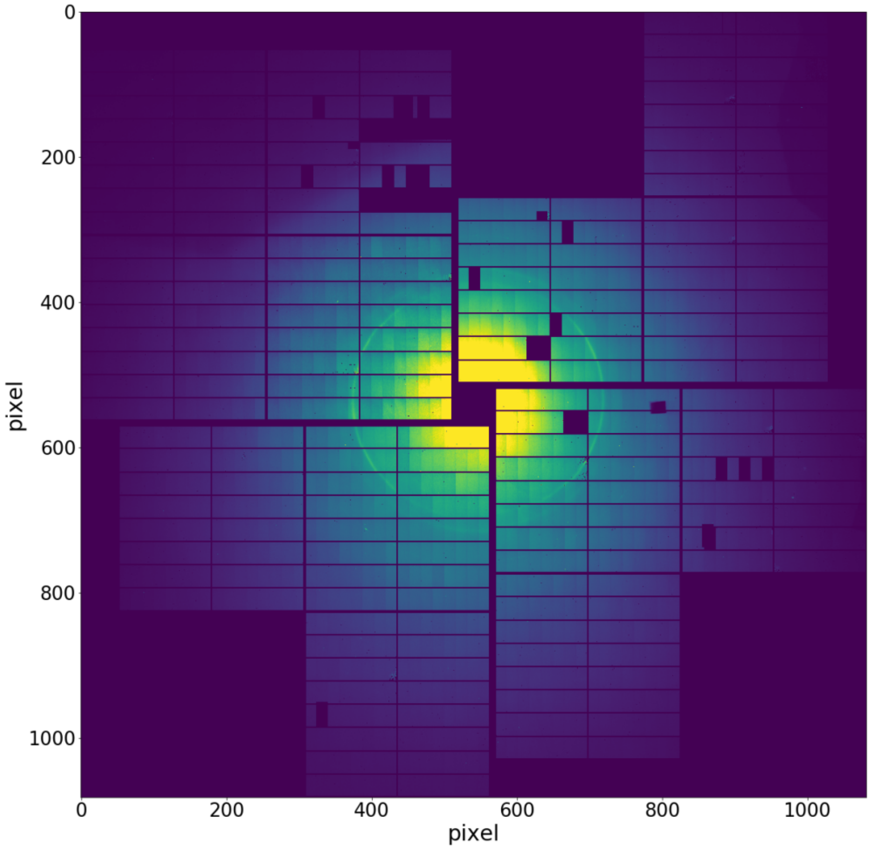
Scattering on aqueous $Fe(bpy)_3$ solution: #2016 (Gawelda et al.)

- 30 bunches/train, 9.3 keV, ~100uJ/pulse, focused to ~20 um

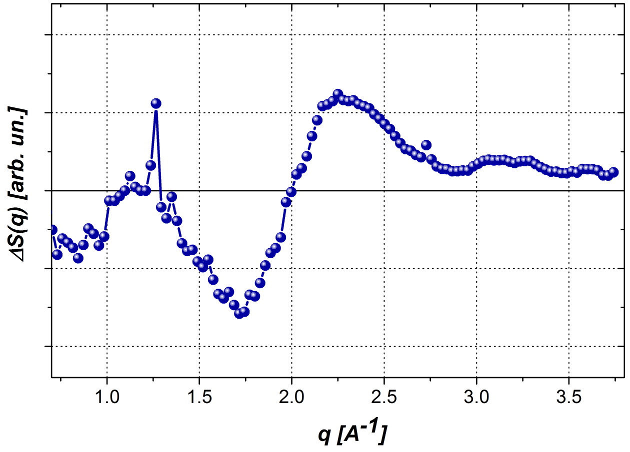
Large Pixel Detector, 4.5 MHz framerate



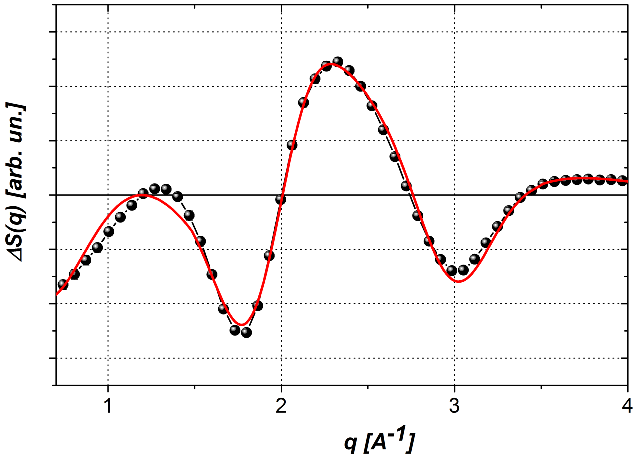
Scattering from 100 um jet, 5 trains summed



- FXE, 6 ps delay, ~ 2 min collection time

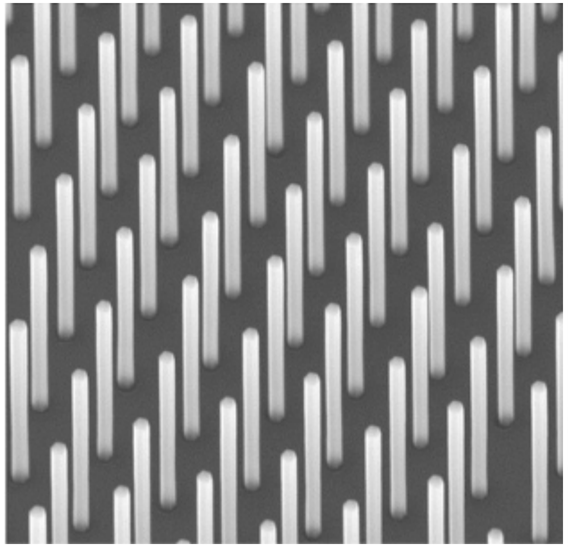


- Synchrotron, 100 ps delay, 8h collection time

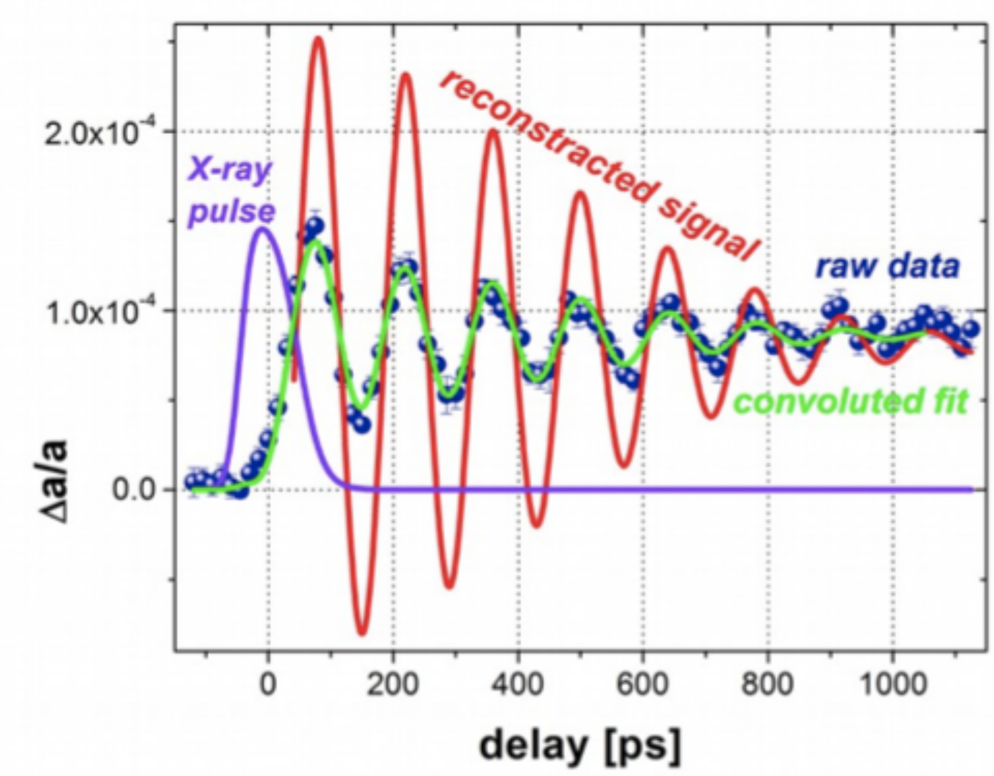


1st Russian Principle Investigator (PI): University ITMO (St. Petersburg)/A. Dubrovskii

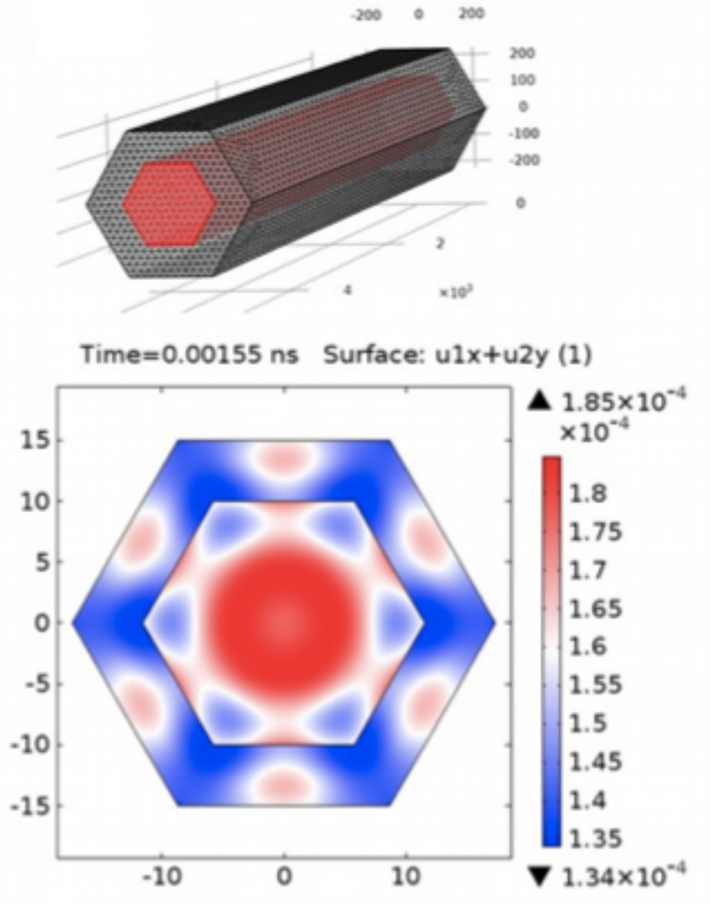
"Towards visualizing lattice dynamics and transient stain fields in semiconductor nanowires by means of ultrafast coherent X-ray diffraction and imaging"



Arrays of nanowires

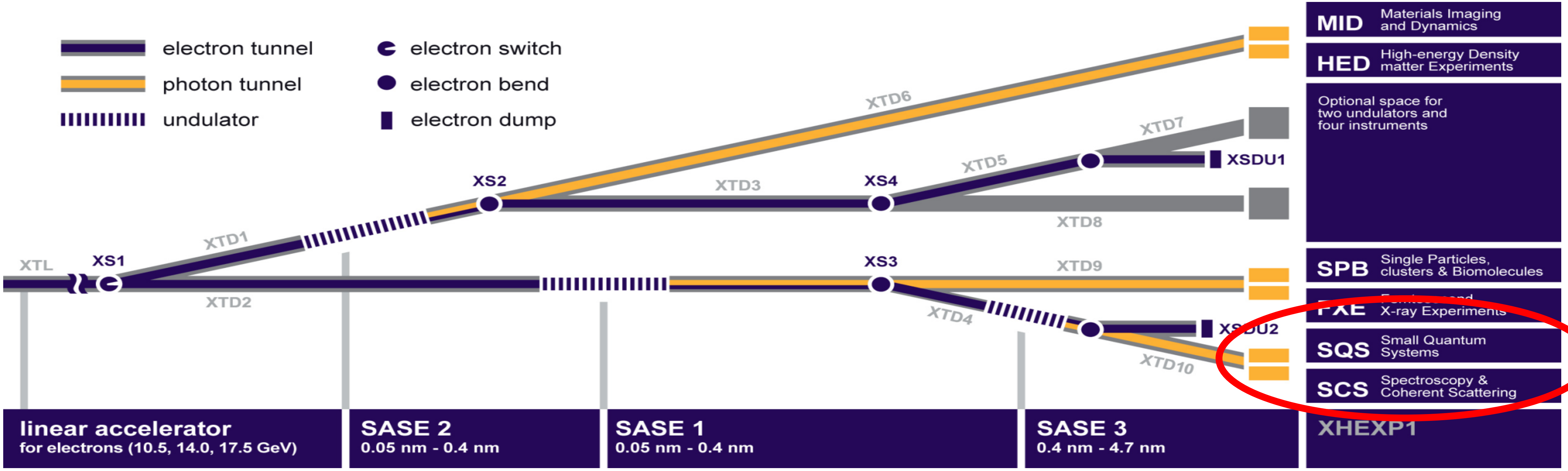


Diffraction peak response



FEM strain simulation

Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24 (Hard XR)	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 – 3 (Soft XR)	4.6 – 0.4



Orange color: X-ray optics & Beam Transport

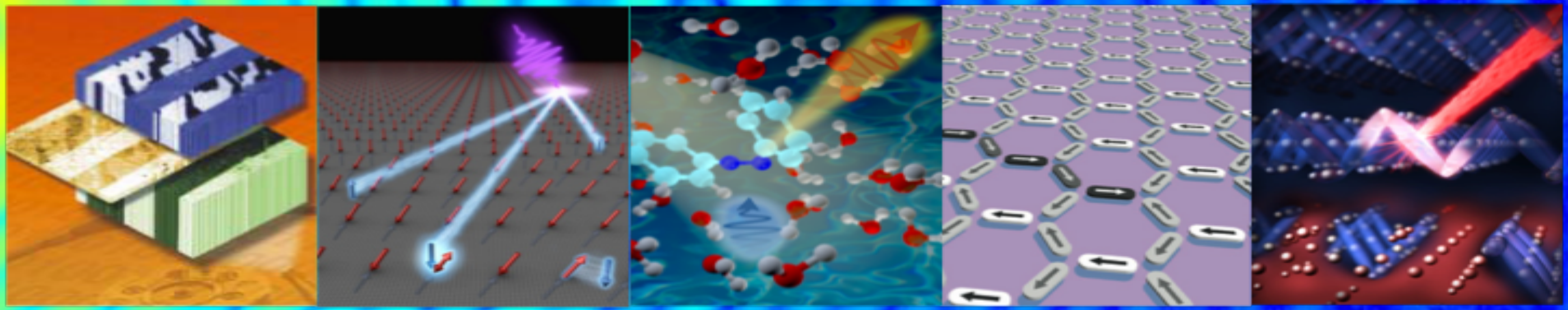
SCS (Spectroscopy & Coherent Scattering) science programme and techniques

Ultrafast Studies of electronic, spin and atomic structures on the nanoscale

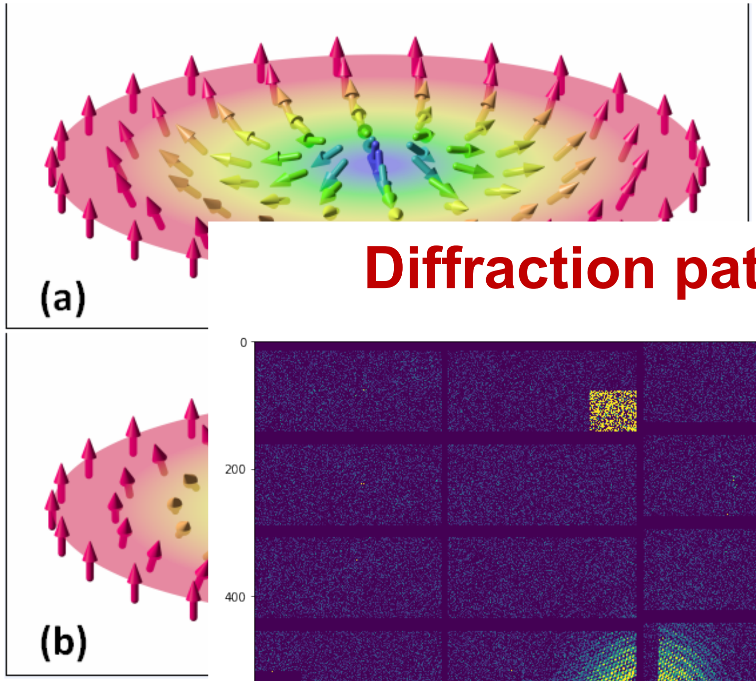
- Strongly correlated materials
- Femtomagnetism
- Applied material science
- Chemistry
- Catalysis
- Basic energy science

Pump-probe methods, single-shot experiments & nonlinear studies

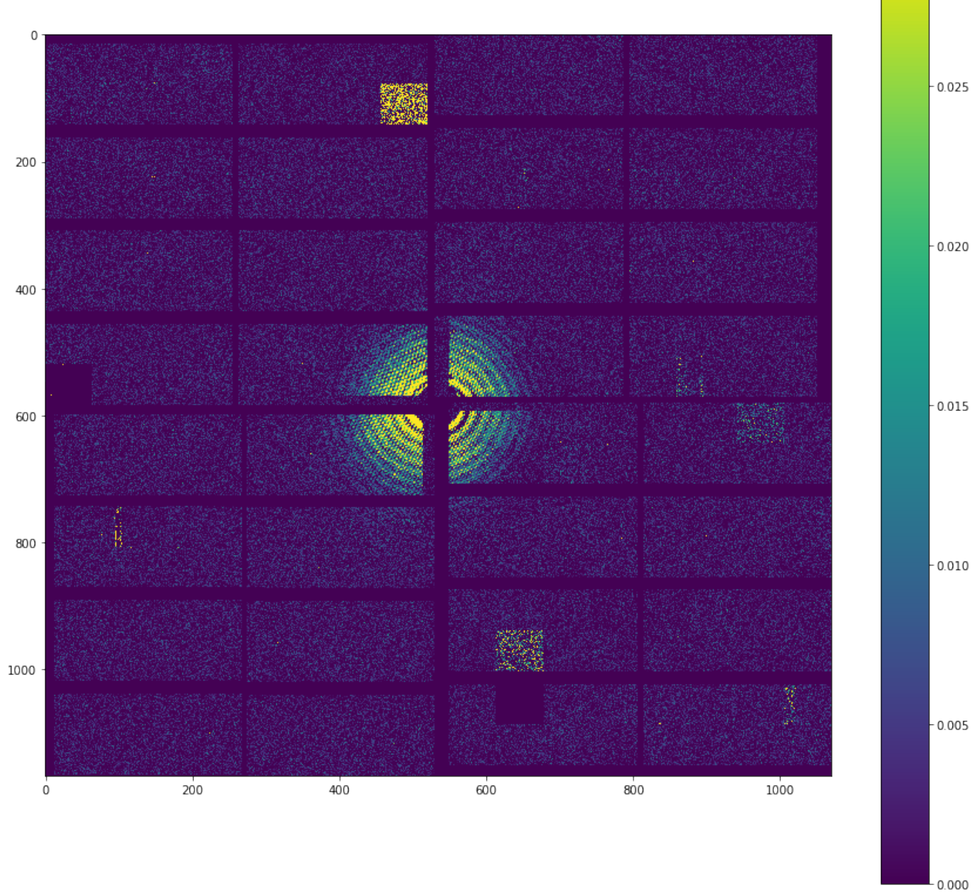
- X-ray absorption spectroscopy
- Resonant x-ray diffraction
- Coherent diffraction imaging
- Small-angle x-ray scattering
- Resonant inelastic x-ray scattering
- Reflectivity



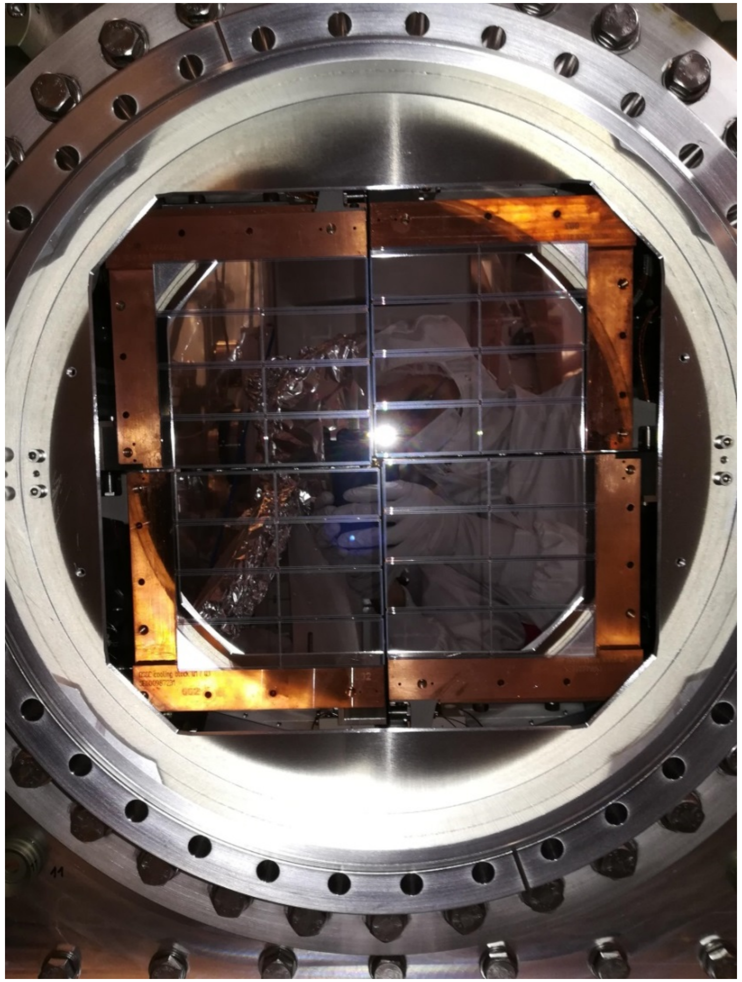
Dynamics of magnetic skyrmions



Diffraction pattern



DSSC detector in use for the first time



SQS (Small Quantum Systems)

Sorokin et al., PRL 99 (2007)
FLASH

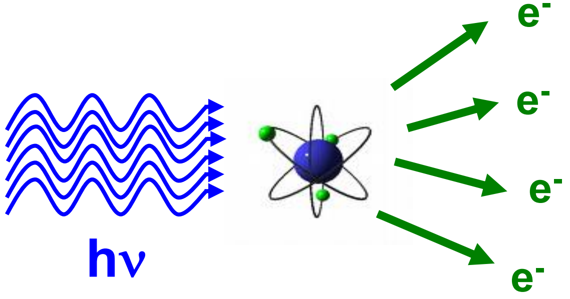
atoms, molecules, ions, clusters, nanoparticles

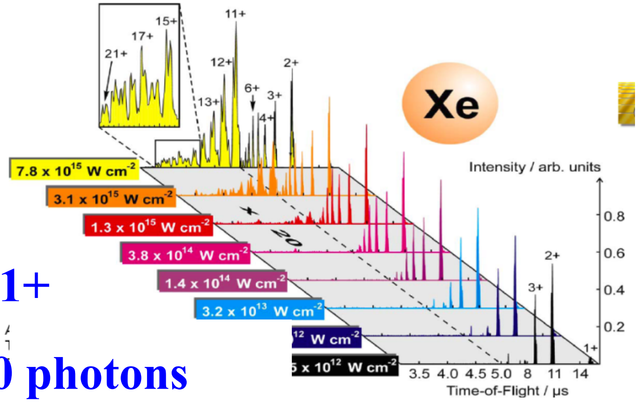
Non-linear phenomena

Intensity > 10^{18} W / cm^2

Multiple ionization

Multi-photon processes





Xe 21+
→ 50 photons

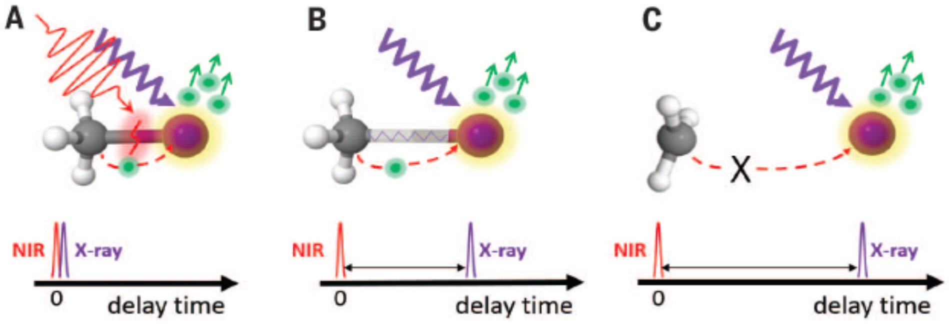
Time-resolved studies

Pulse durations: 2 - 100 fs

Pump-probe: NIR/XUV, XUV/XUV

Molecular dynamics

Element specific Soft X-rays



CH_3I → $CH_3^+ + I^{n+}$

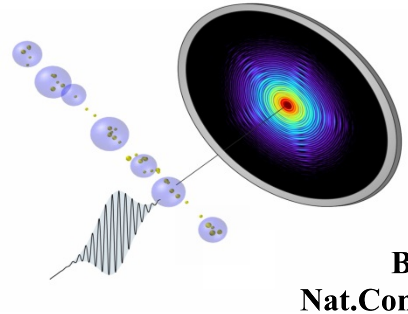
Erk et al., Science 345 (6194), 288 (2014)
LCLS

Imaging experiments

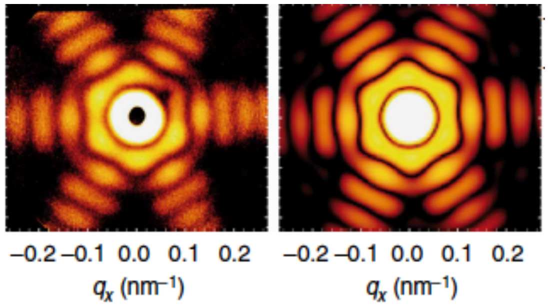
Spatial coherence

Size and shape selection

Cluster dynamics



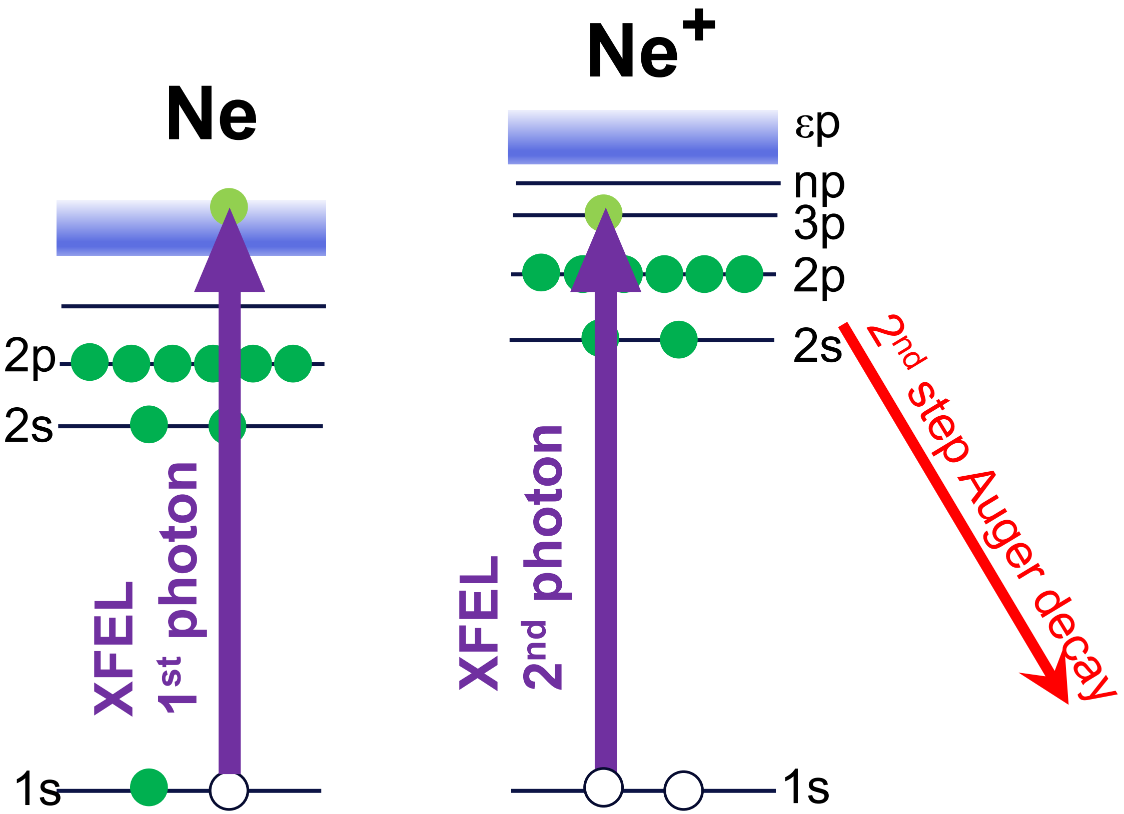
Barke et al., Nat.Comm.6, 6187 (2015)
FLASH



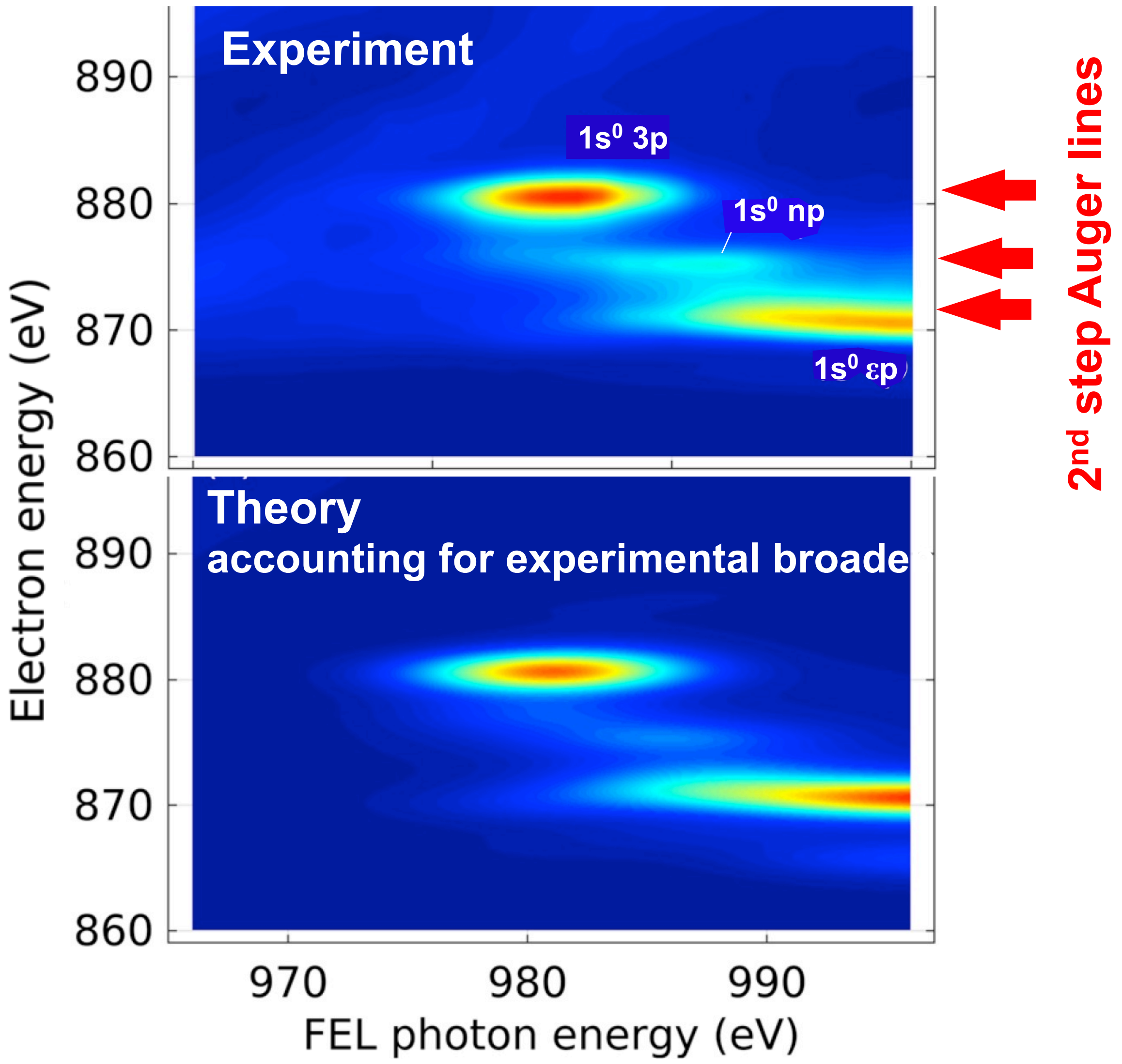
Ag nano-particles

Mapping resonance structures in transient core-ionized atoms

First user run at SQS, November 2018



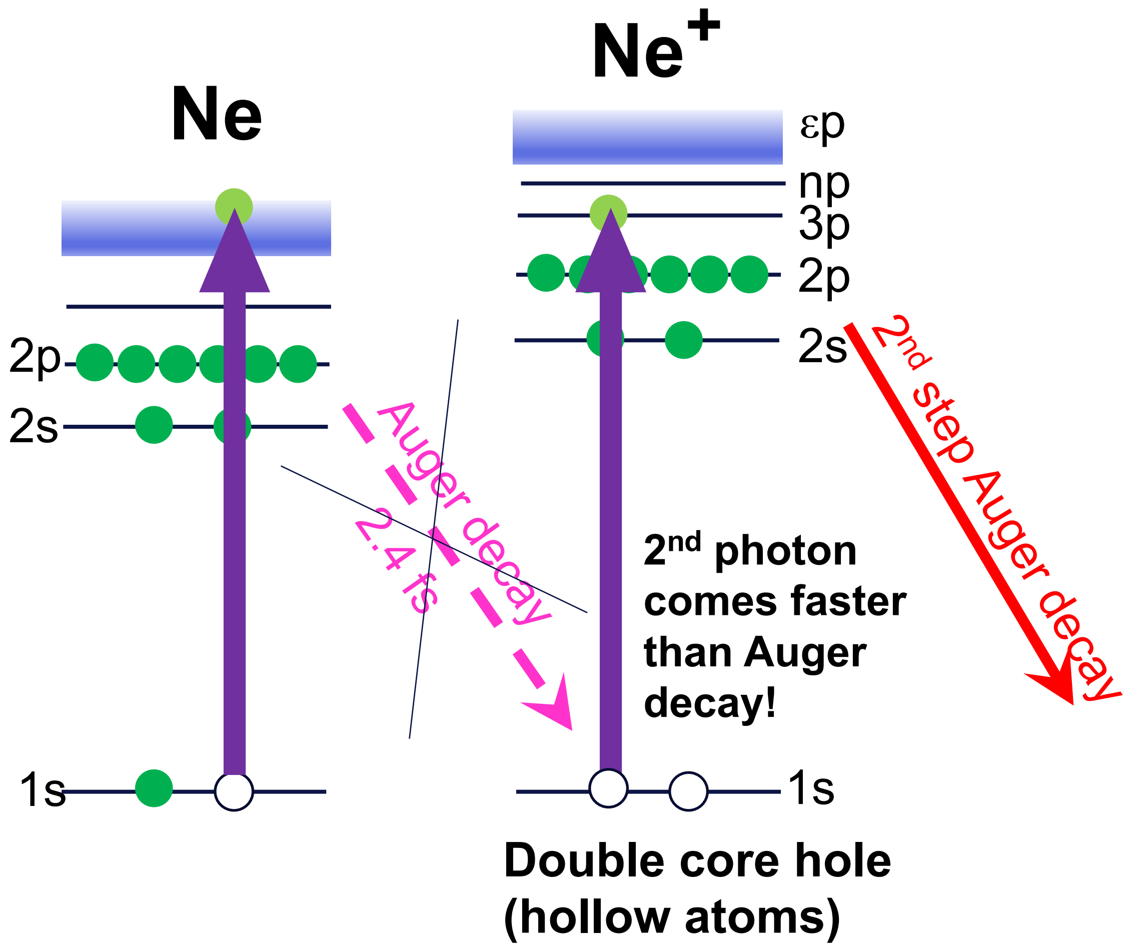
Double core hole (hollow atoms)

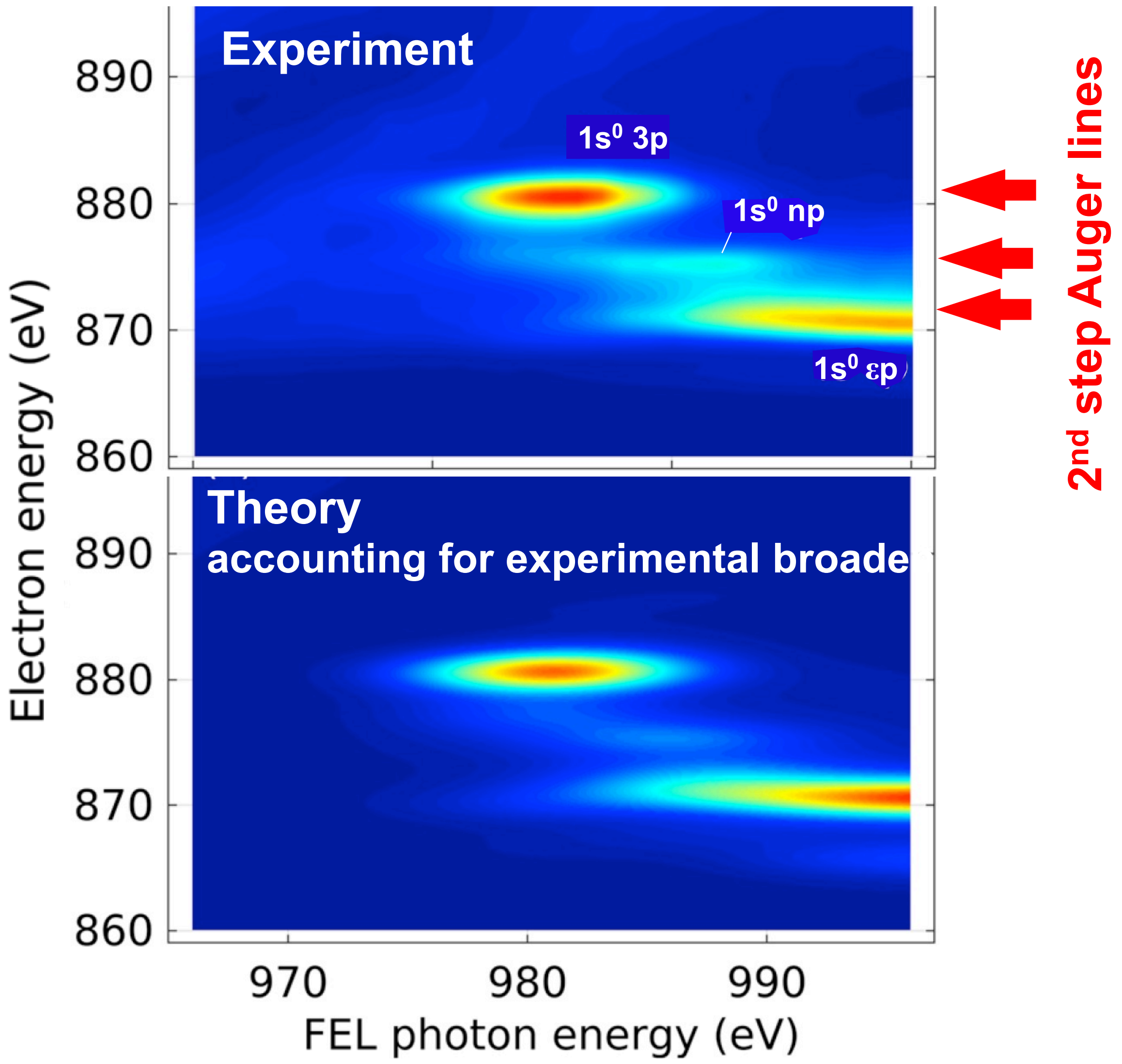


scanning 2nd step resonances

Mapping resonance structures in transient core-ionized atoms

First user run at SQS, November 2018

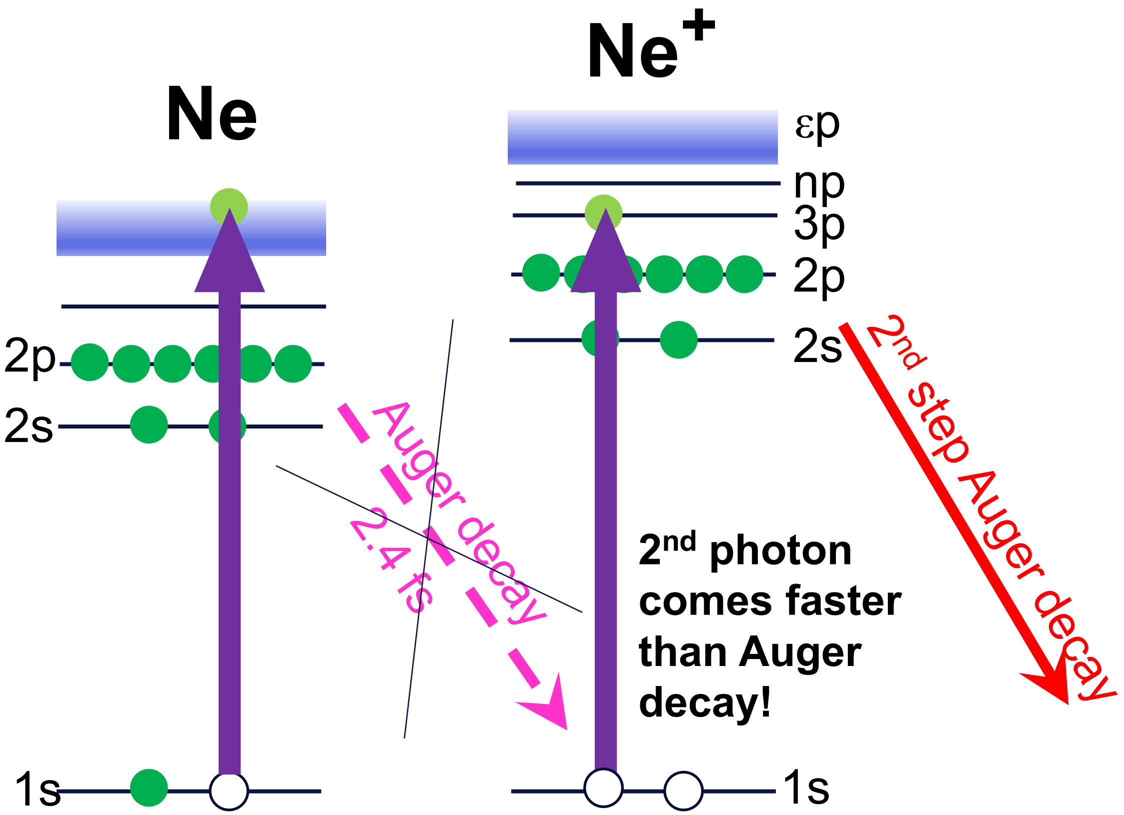


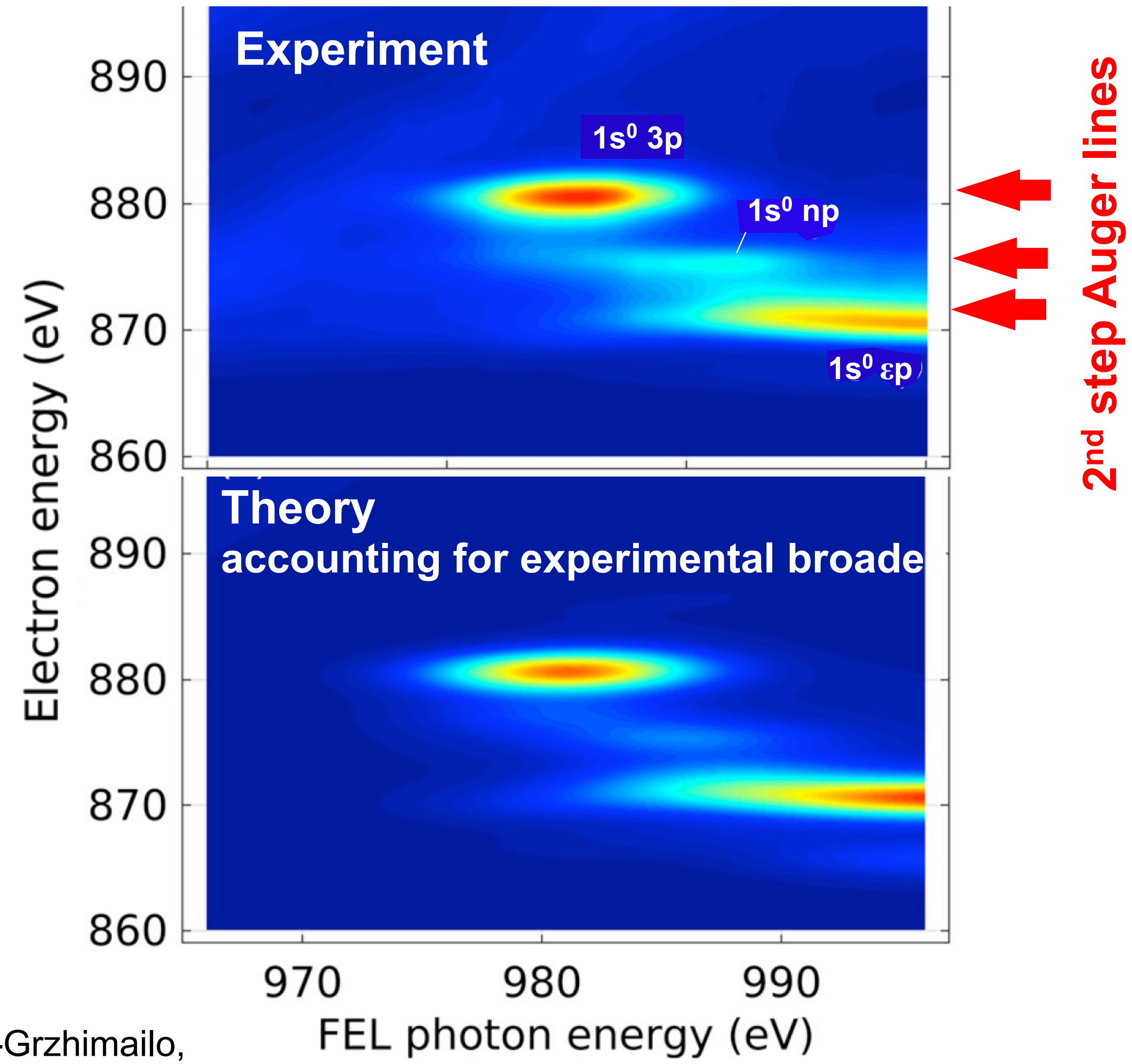


scanning 2nd step resonances

Mapping resonance structures in transient core-ionized atoms

First user run at SQS, November 2018



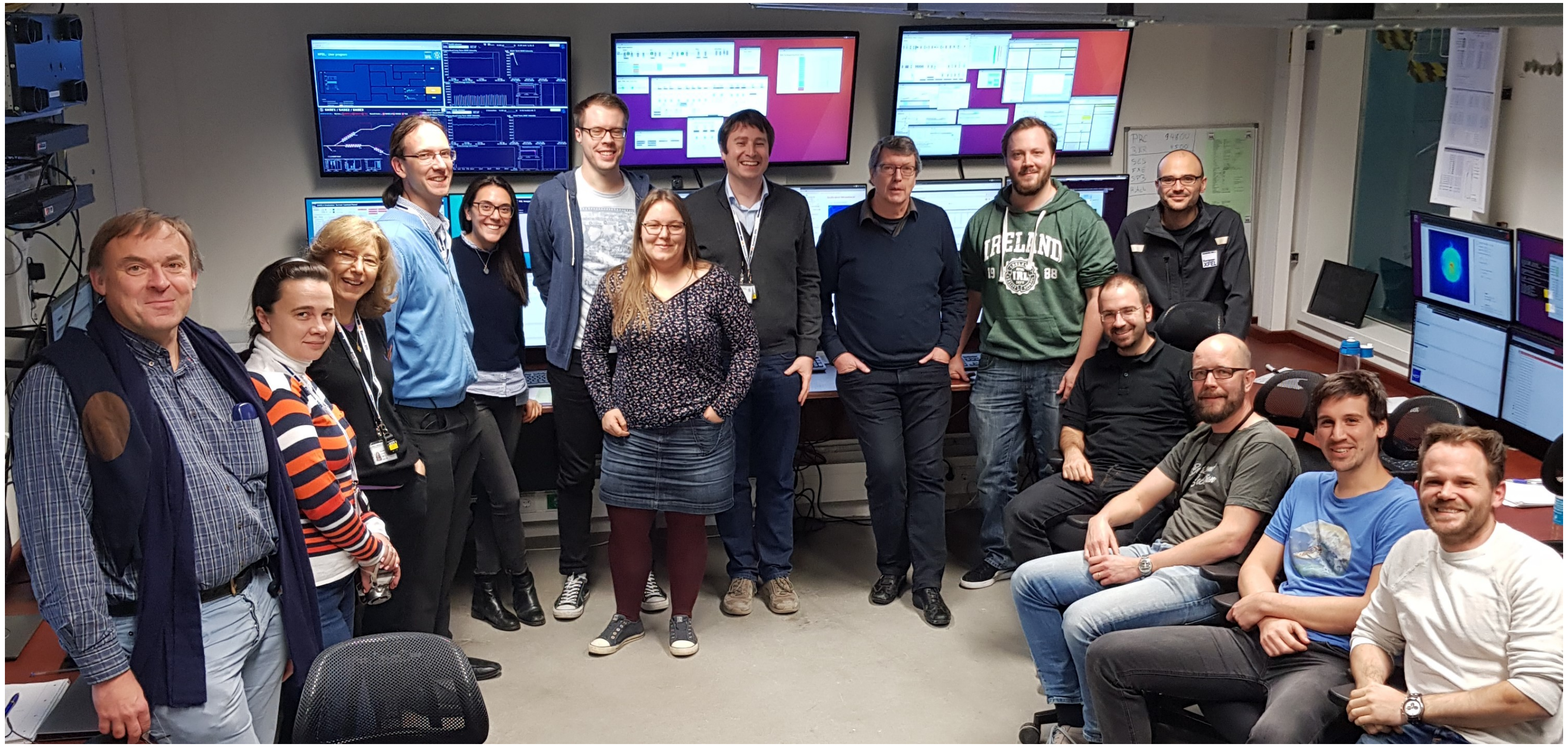


scanning 2nd step resonances

Theory:
A. Grum-Grzhimailo,
E. Gryzlova,
M. Kiselev

Phys. Rev. X **10**, 041056 (2020)

SQS First User Run Nov. 2018; a „Community proposal“



SQS: T. Mazza, T. Baumann, R. Boll, A. De Fanis, P. Grychtol, M. Ilchen, M. Meyer, J. Montano, Y. Ovcharenko,D. Rivas, V. Music, R. Wagner

Uni Kassel: Ph. Schmidt, C. Küstner-Wetekam, L. Marder

MPI Heidelberg: Ch. Ott, Th. Pfeifer

Uni Hamburg: M. Martins

DESY: B. Erk

Moscow State University: E. Gryzlova

Univ. Connecticut: N. Berrah

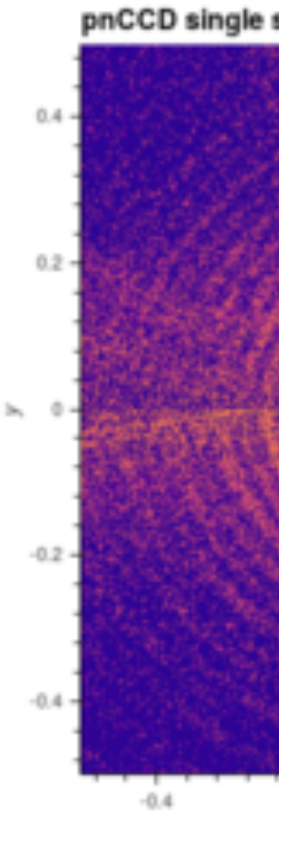
Kansas State University: D. Rolles, S. Pathak

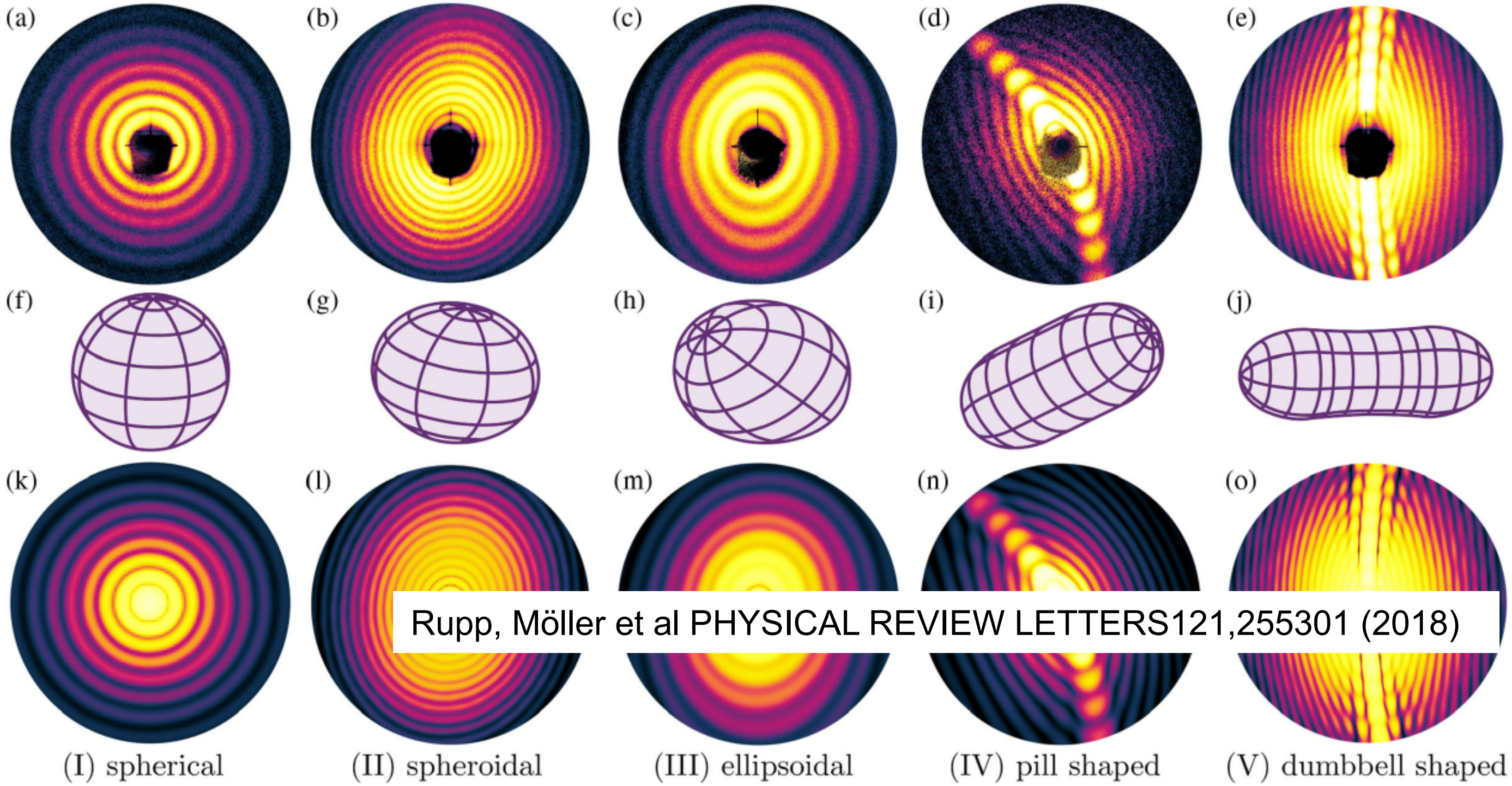
Lund Laser Center: P. Johnsson

Helium droplet doped with xenon and silver

pnCCD detector

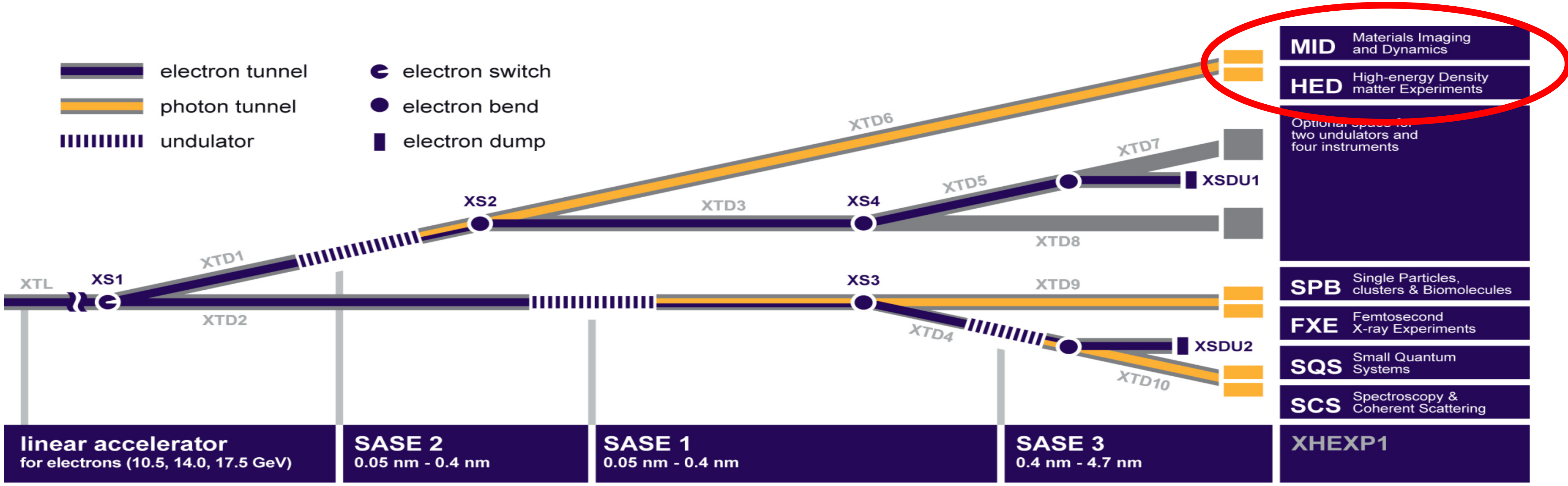
Diffraction pattern





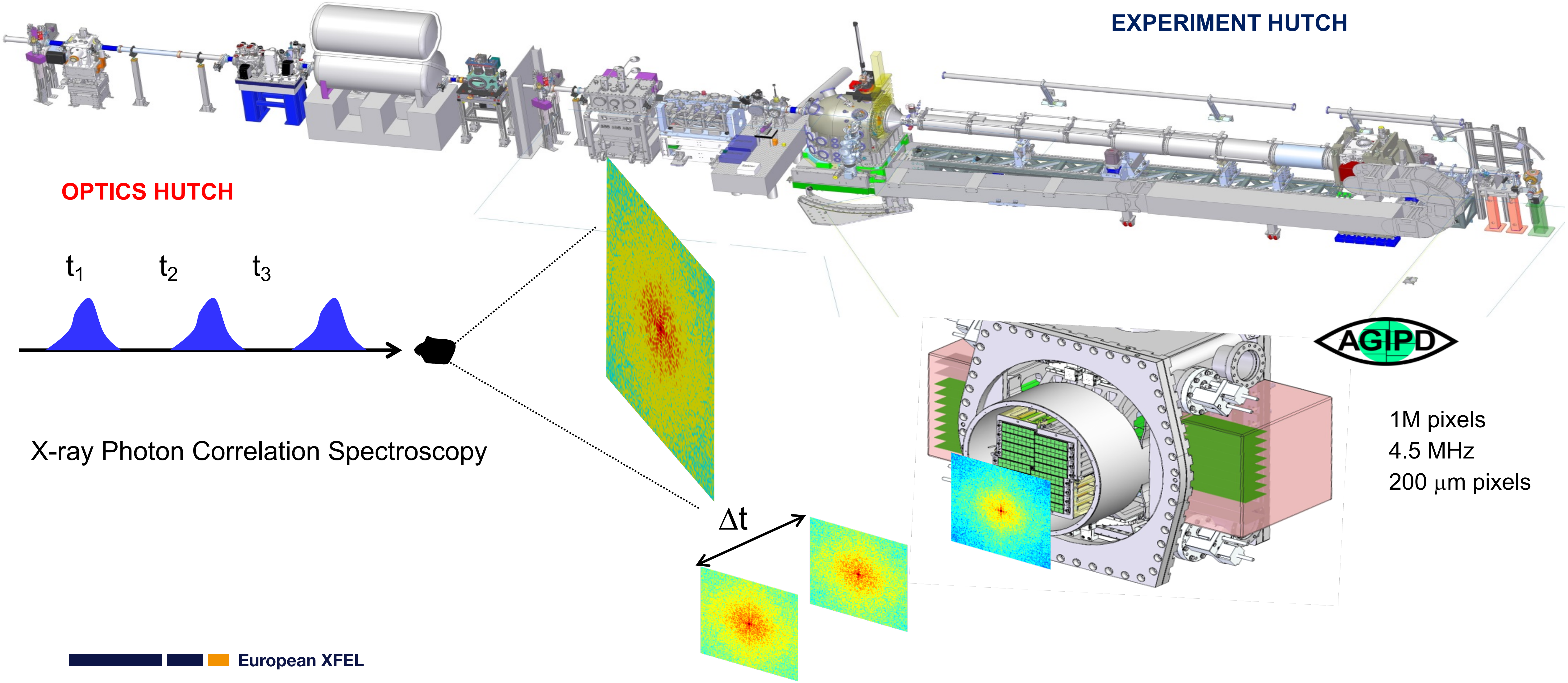
Rupp, Möller et al PHYSICAL REVIEW LETTERS121,255301 (2018)

Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24 (Hard XR)	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 – 3 (Soft XR)	4.6 – 0.4



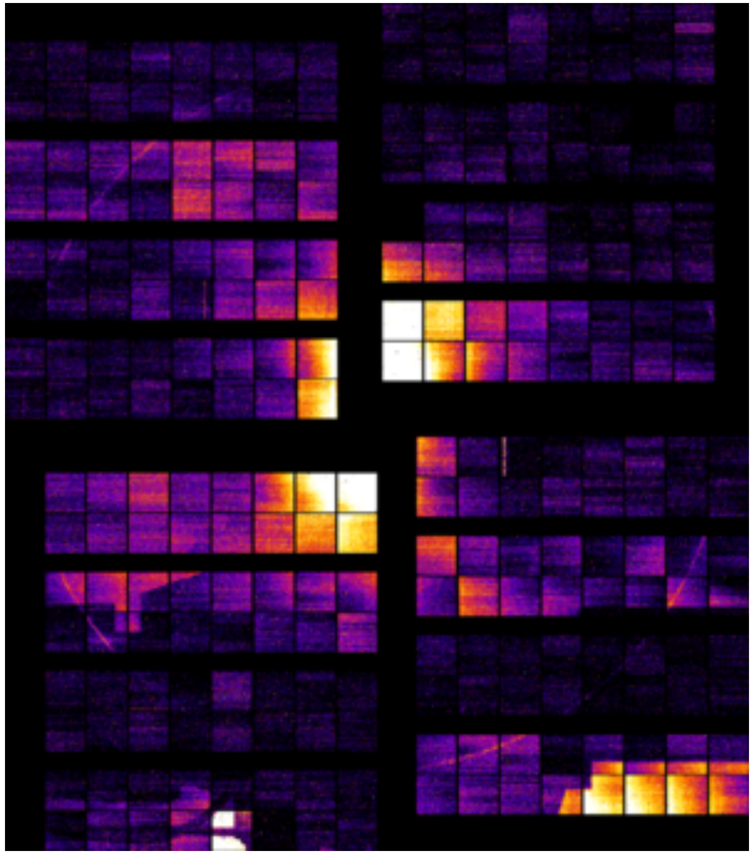
Orange color: X-ray optics & Beam Transport

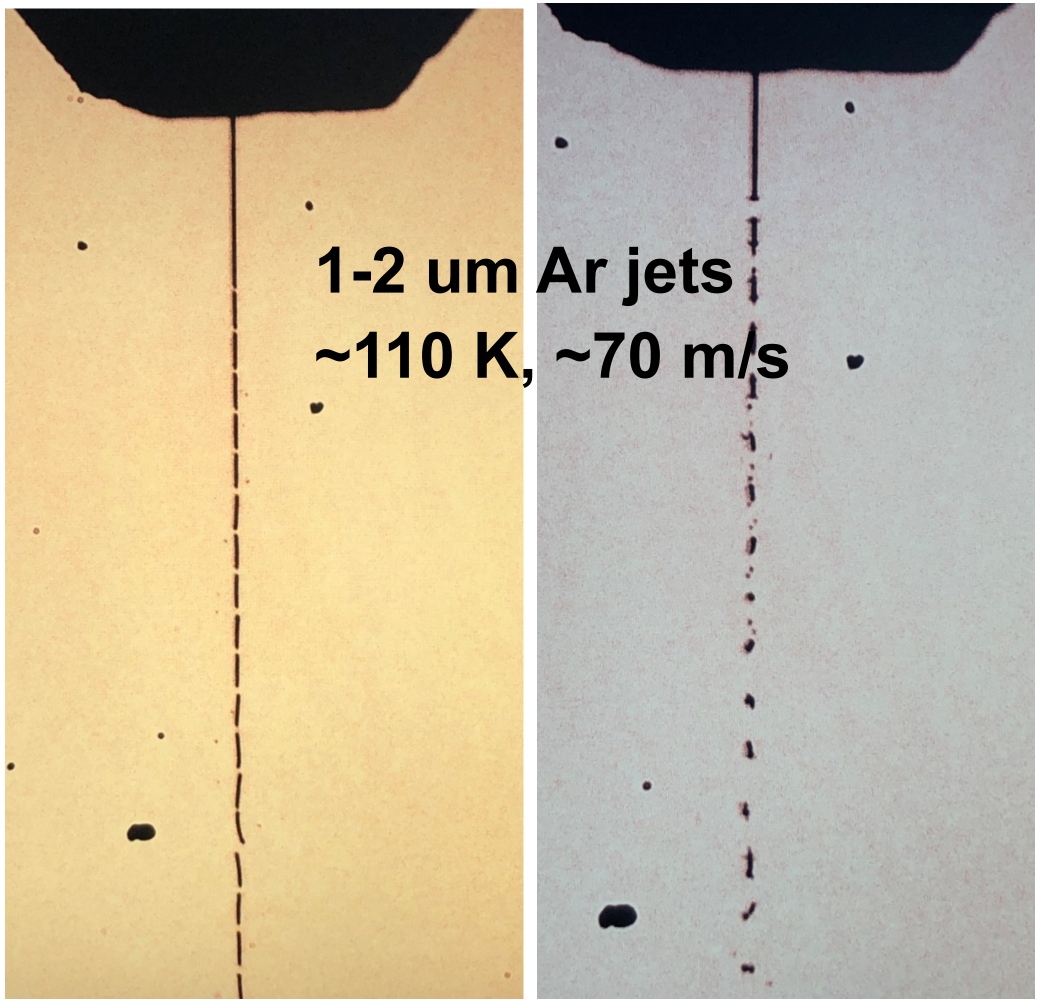
MID (Materials Imaging and Dynamics)



Local structural features in supercooled liquids during liquid-to-solid transition
R. Grisenti, proposal #2272, Uni Frankfurt, March 20

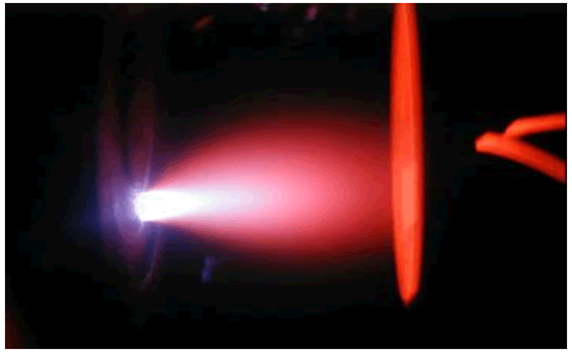
Diffraction pattern

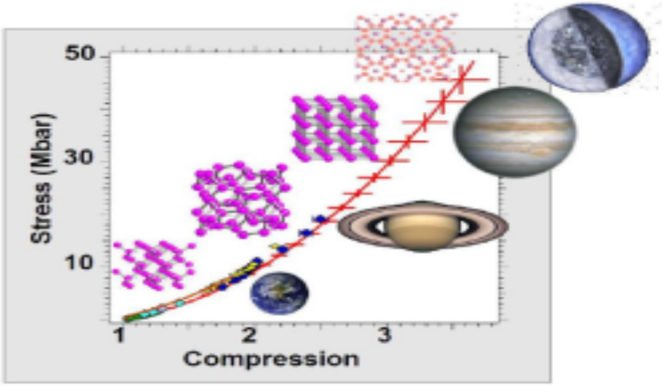


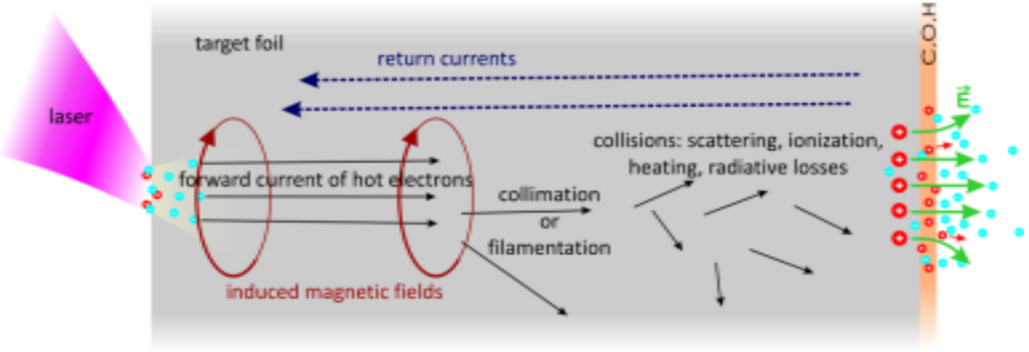


HED (High-Energy Density)

- Ultrafast dynamics and structural properties of matter at extreme states
  - **Highly excited solids**→ laser processing, dynamic compression, high B-field
  - **Near-solid density plasmas**→ WDM, HDM, rel. laser-matter interaction
  - **Quantum states of matter**→ high field QED (future upgrade)



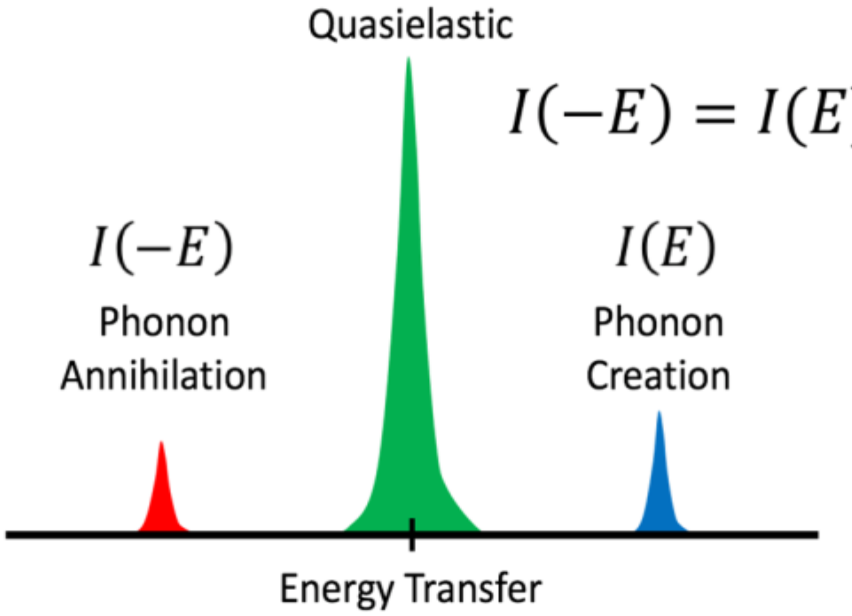


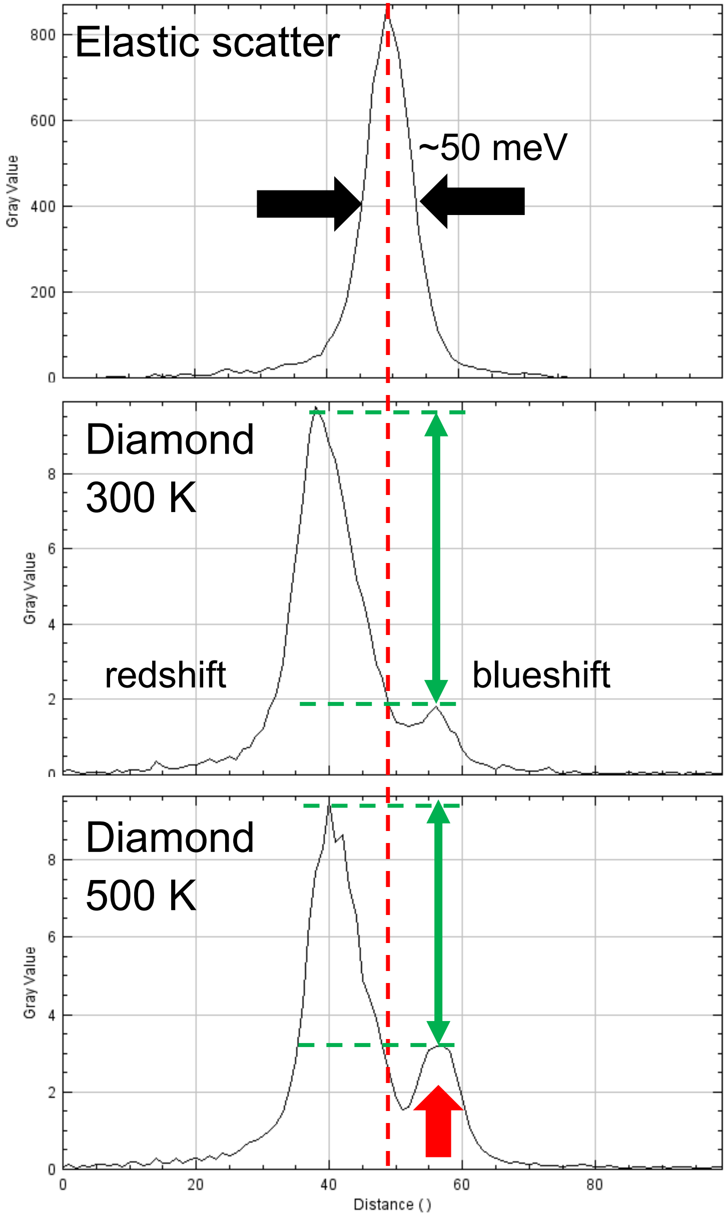


- Combination of high excitation with various X-ray techniques
  - Use of **various pump sources**: optical laser, XFEL, B-fields (60 T pulsed)
  - **Various X-ray probe techniques**: XRD, SAXS, XRTS, hrIXS, XI, XAS….

Phonons in single-crystal diamond

$$I(-E) = I(E)e^{E/k_B T}$$





You are welcome for cooperation at EuXFEL!