Imaging Techniques Scalable in Resolution, Volume, and Rate

Matter meets Information: Common Challenges and Perspectives

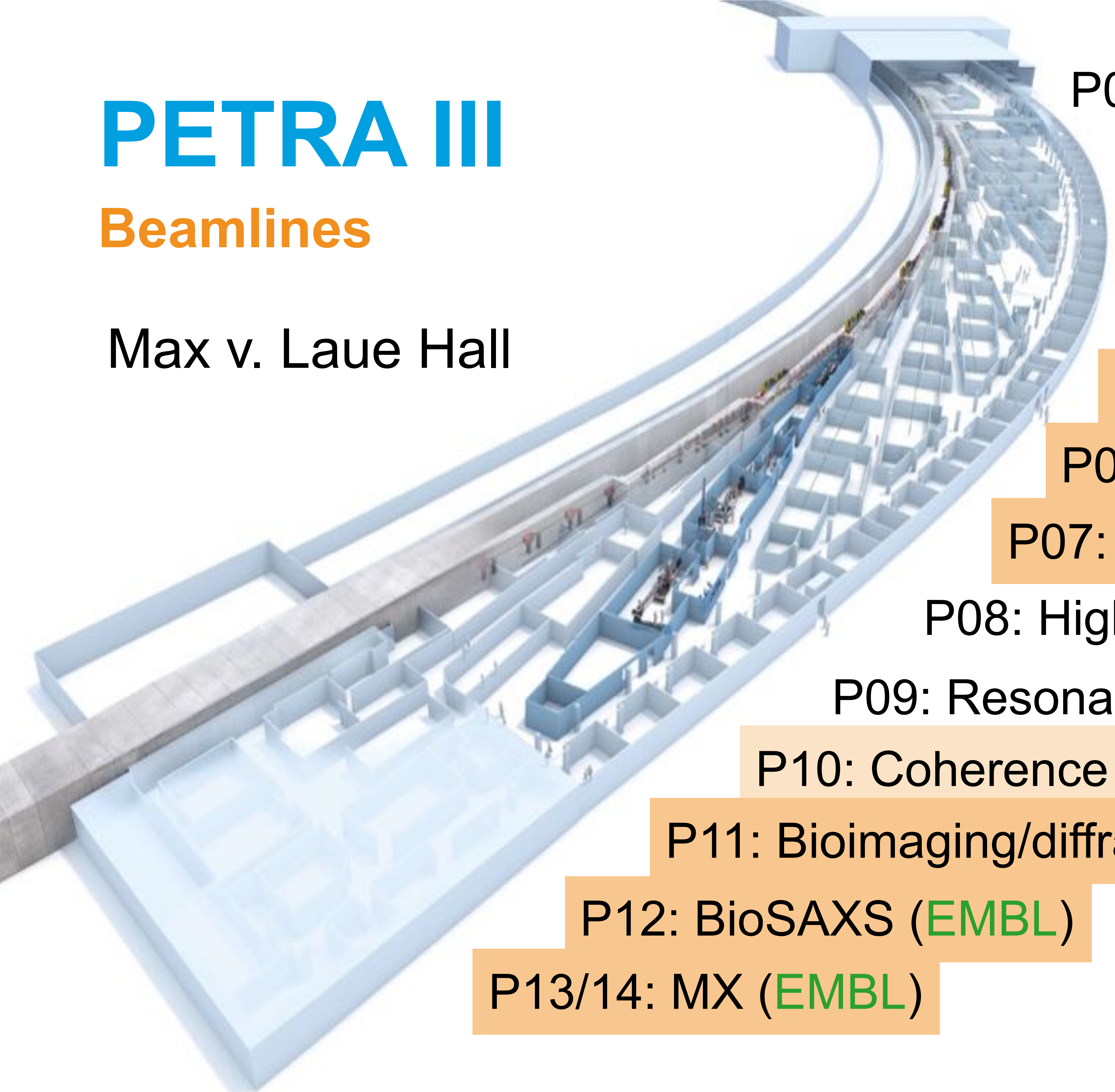
Christian. G. Schroer
DESY

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Photon Science as Data Source

PETRA III

Beamlines



Max v. Laue Hall

P01: Dynamics beamline, IXS, NRS

P02: Powder diffraction & extreme conditions

P03: Micro-, nano-SAXS, WAXS

P04: Variable polarisation XUV

P05: Micro-, nano-tomography (HZG)

P06: Hard X-ray micro-, nanoprobe

P07: High-energy materials sci. (HZG, DESY)

P08: High-resolution diffraction

P09: Resonant scattering/diffraction

P10: Coherence applications

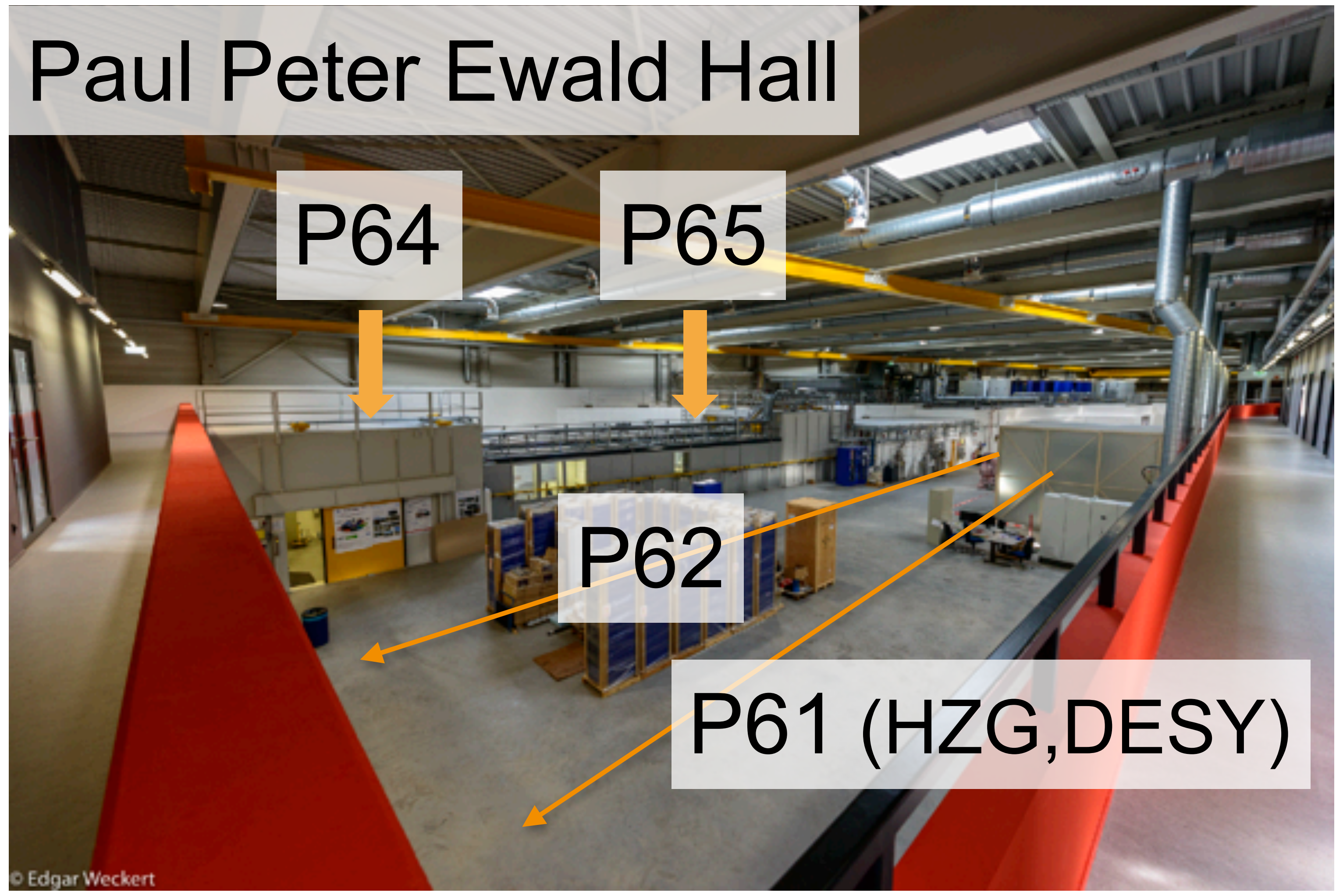
P11: Bioimaging/diffraction

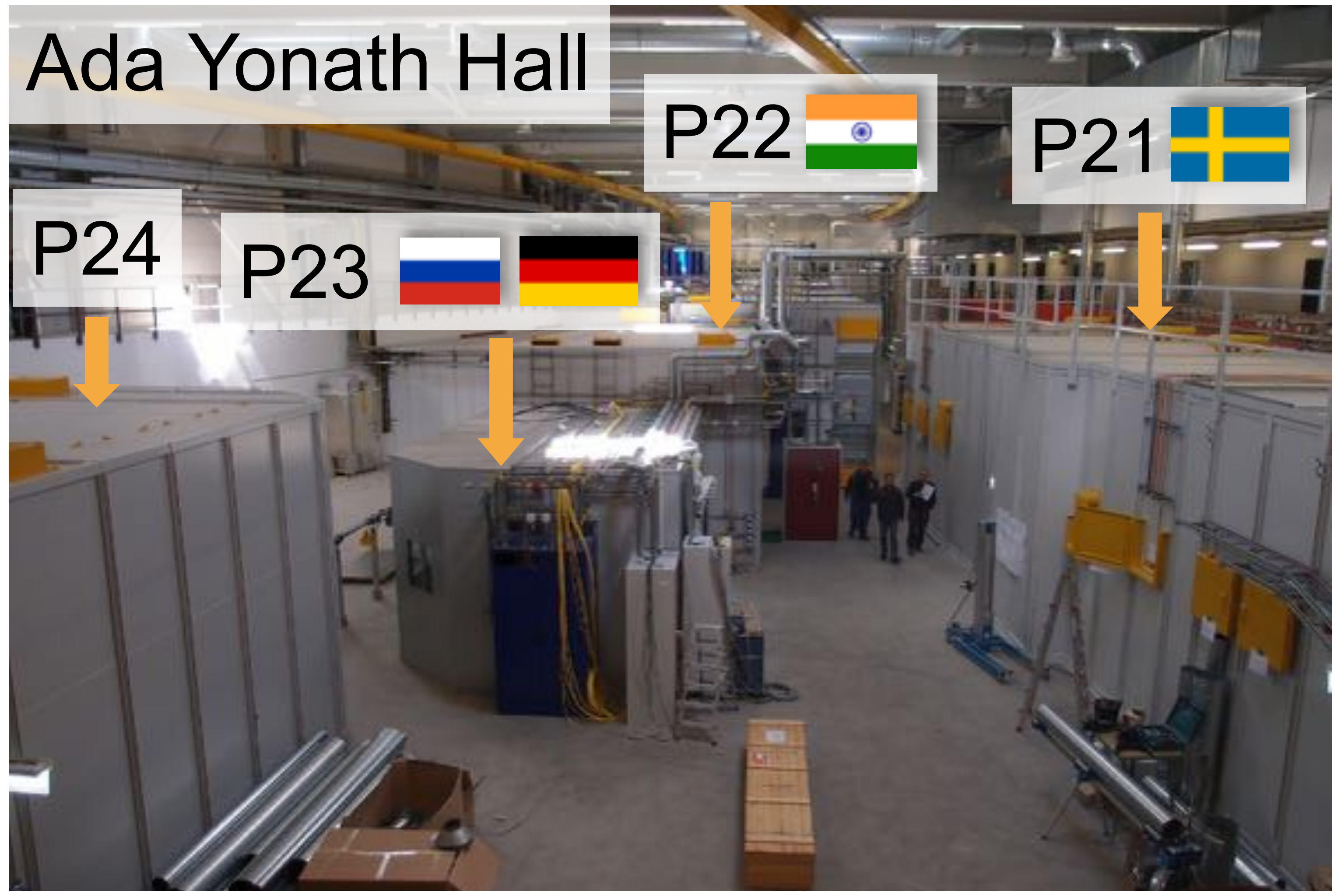
P12: BioSAXS (EMBL)

P13/14: MX (EMBL)

Verbundforschung

Federal Ministry of Education and Research





P21: Swedish materials science beamline (commissioning since Sept. 2018)

P22: Hard X-ray photoelectron spectroscopy

P23: In-situ and nano diffraction beamline

P24: Chemical crystallography

P25: TBD

P61: High-energy wiggler beamline (operational 2019)

P62: Small-angle X-ray scattering (planning phase)

P63: TBD

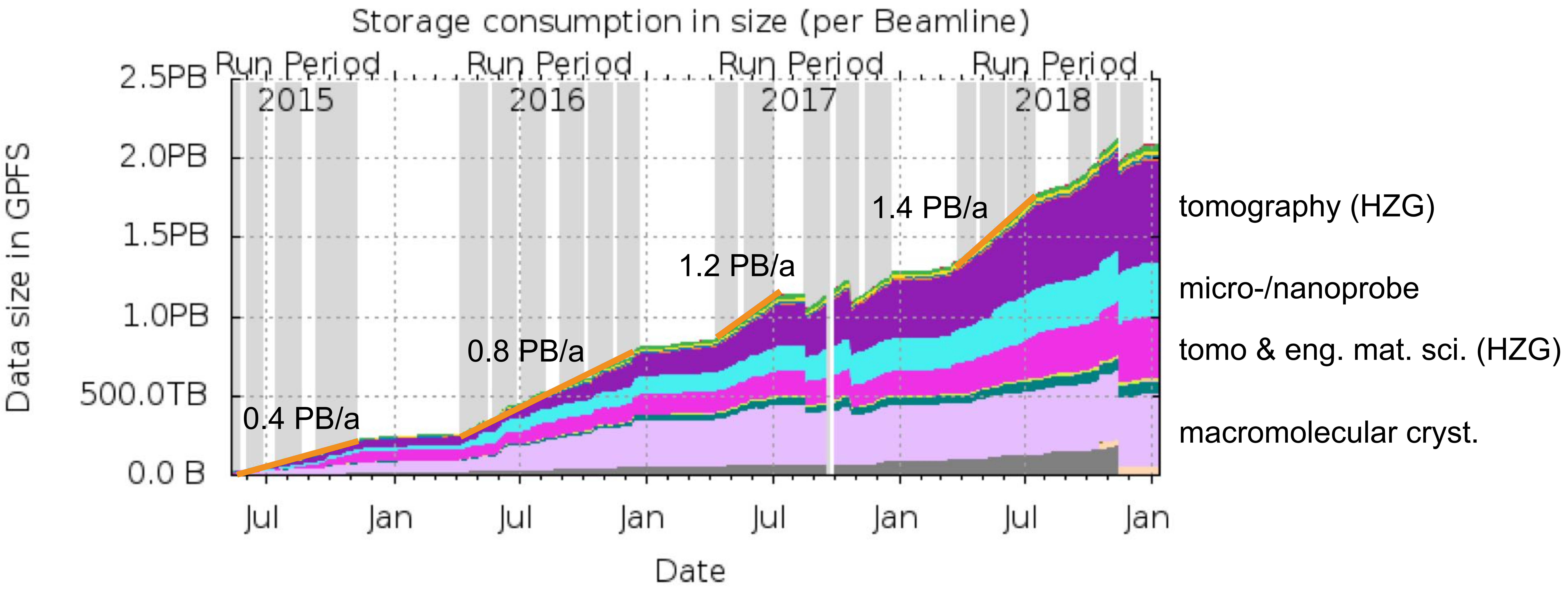
P64: Advanced XAFS

P65: Applied XAFS

P66: Time-resolved luminescence spectroscopy (operational 2019)

GPFS: Total Use per Beamline

Data rate increases with development of faster detectors

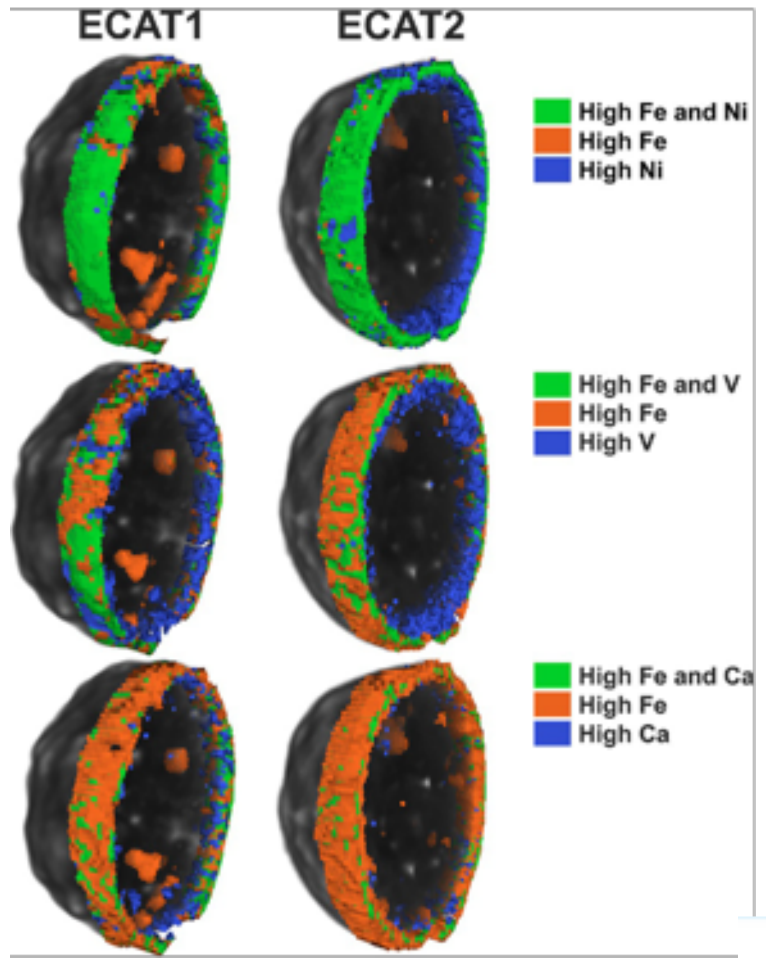


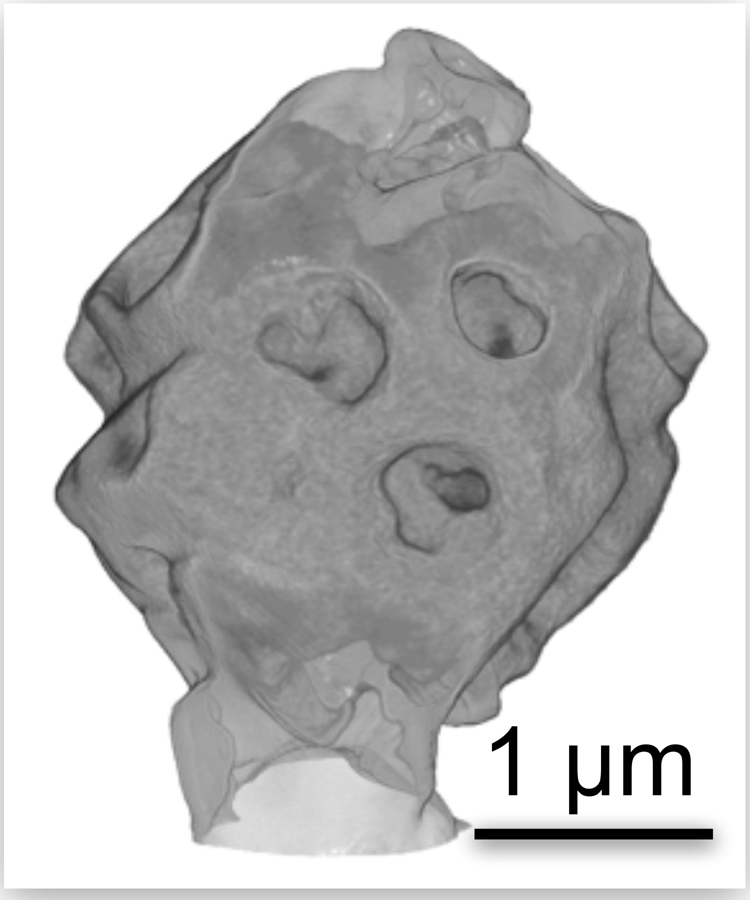
4 Beamlines generate 80 % of the data on GPFS

High Data Rate & Volume

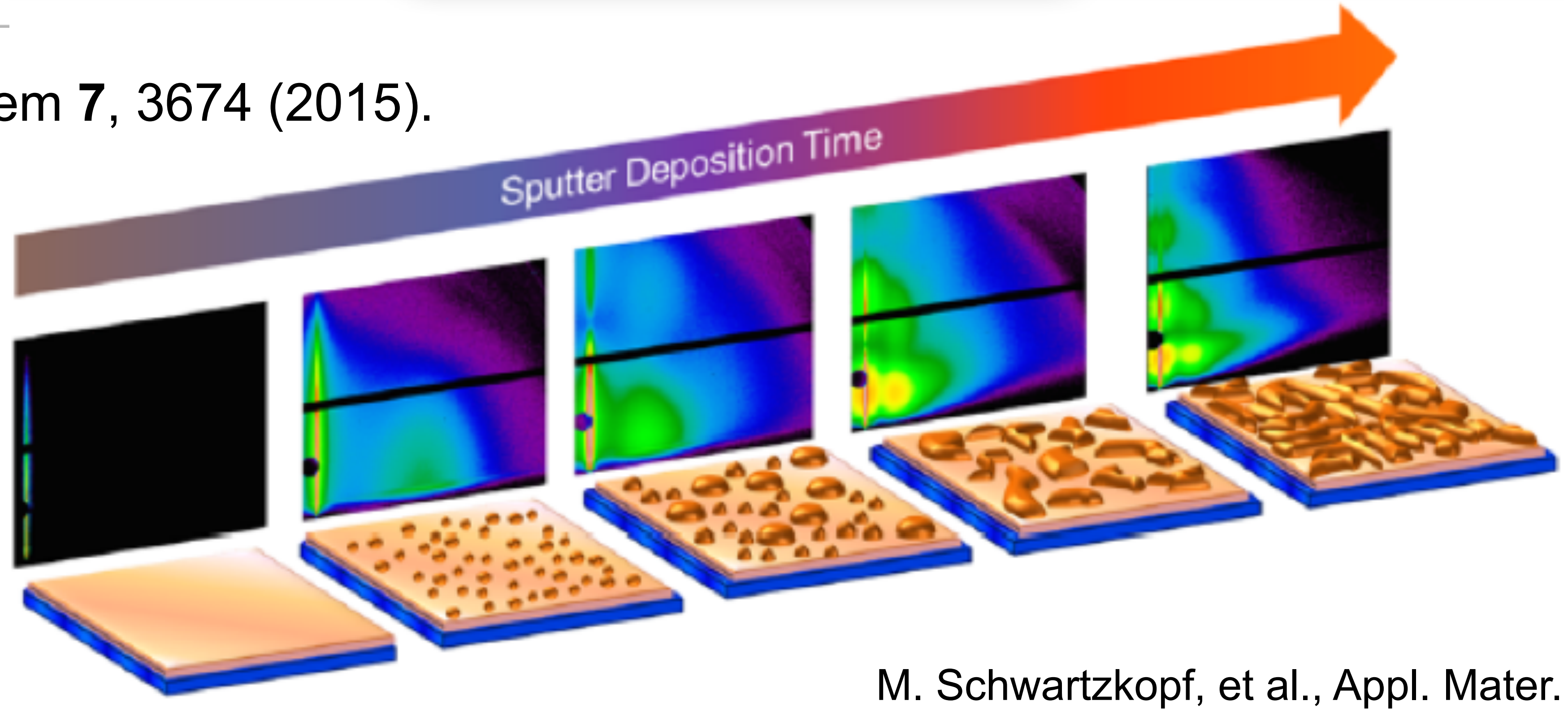
Space- and Time-resolved Experiments

- Measuring physical and chemical properties of complex materials in space (3D) and time
  - chemical composition
  - chemical state
  - structure (micro-, meso-, and macroscopic)
  - magnetic, electronic properties



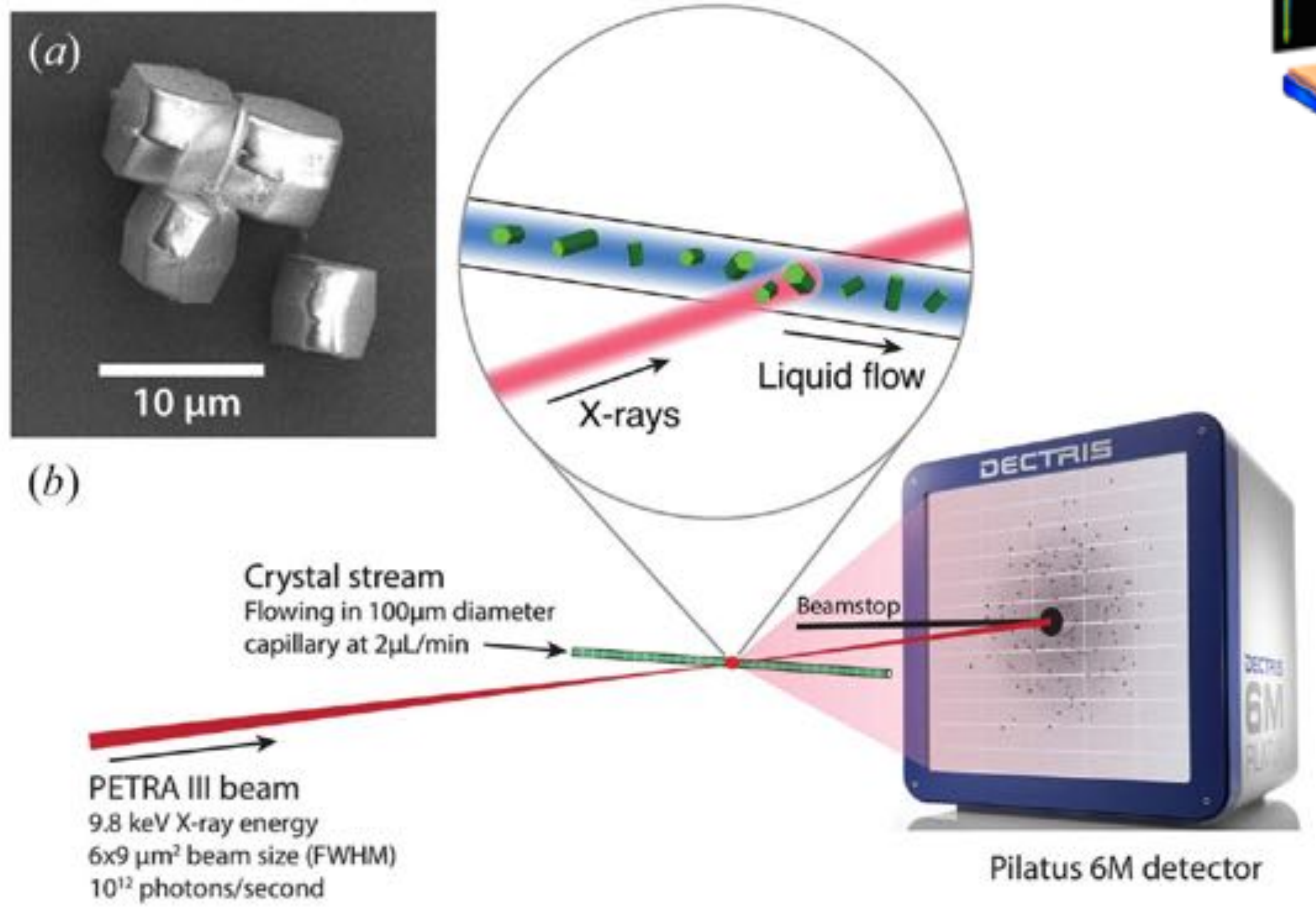


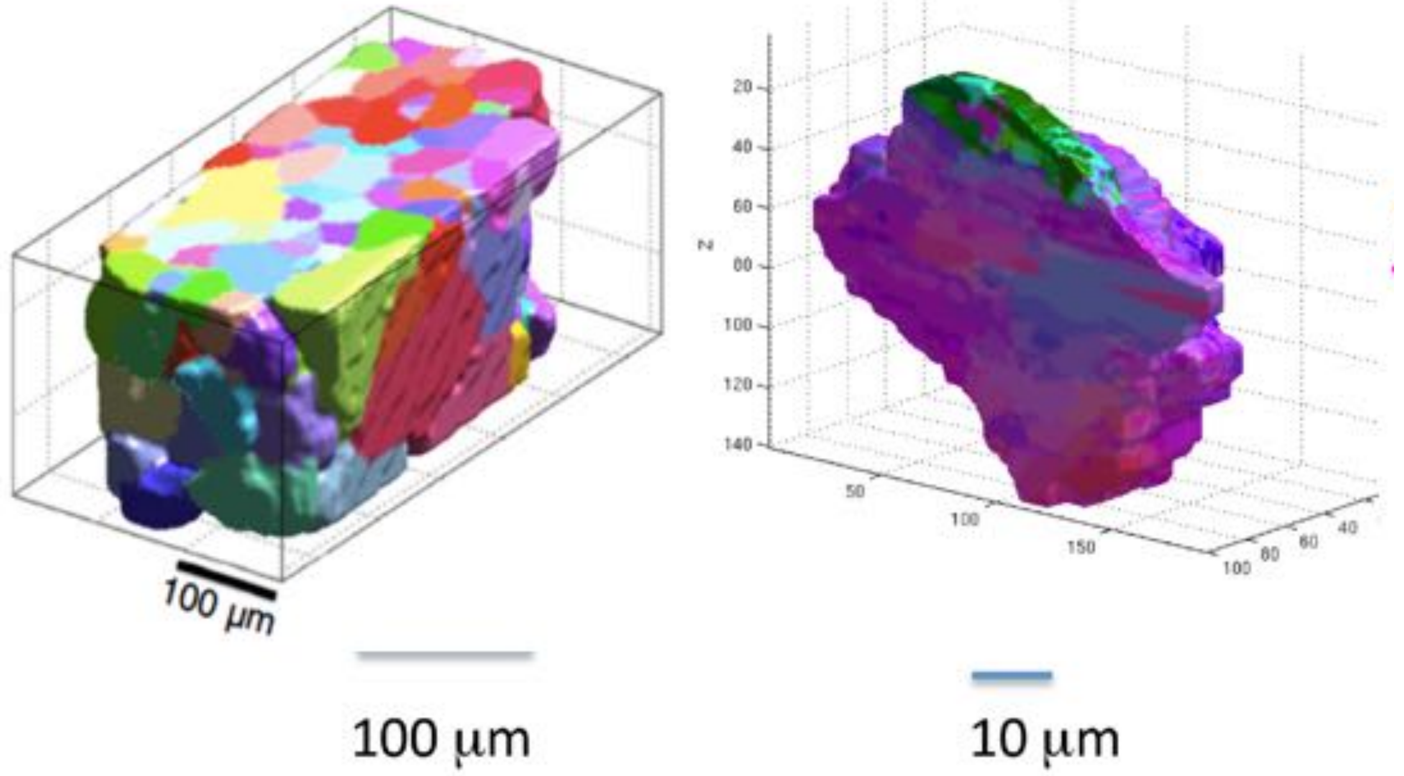
S. Kalirai, et al., ChemCatChem **7**, 3674 (2015).



M. Schwartzkopf, et al., Appl. Mater. Interfaces **7**, 13547 (2015).

- Serial crystallography: high-throughput single-pulse analysis of small crystals
  - solve structures of macromolecules that are difficult to crystallise,
  - time-resolved studies





F. Stellato, et al., IUCrJ **1**, 204 (2014).

High Data Rate & Volume

Large Inverse Problems

Most experiments involve inverse problems:

> Forward model: data taking processes are known and can be modelled

> Inverse model: given the measured data, what does the sample look like?

Data science:

> growth of data volume (next 10 years):

100 x - 1000 x increase in brightness (e. g., PETRA IV)
5 x more beamlines taking large data sets
10 x automation of data acquisition

➔ 10^4 - 10^5 x increased data rate

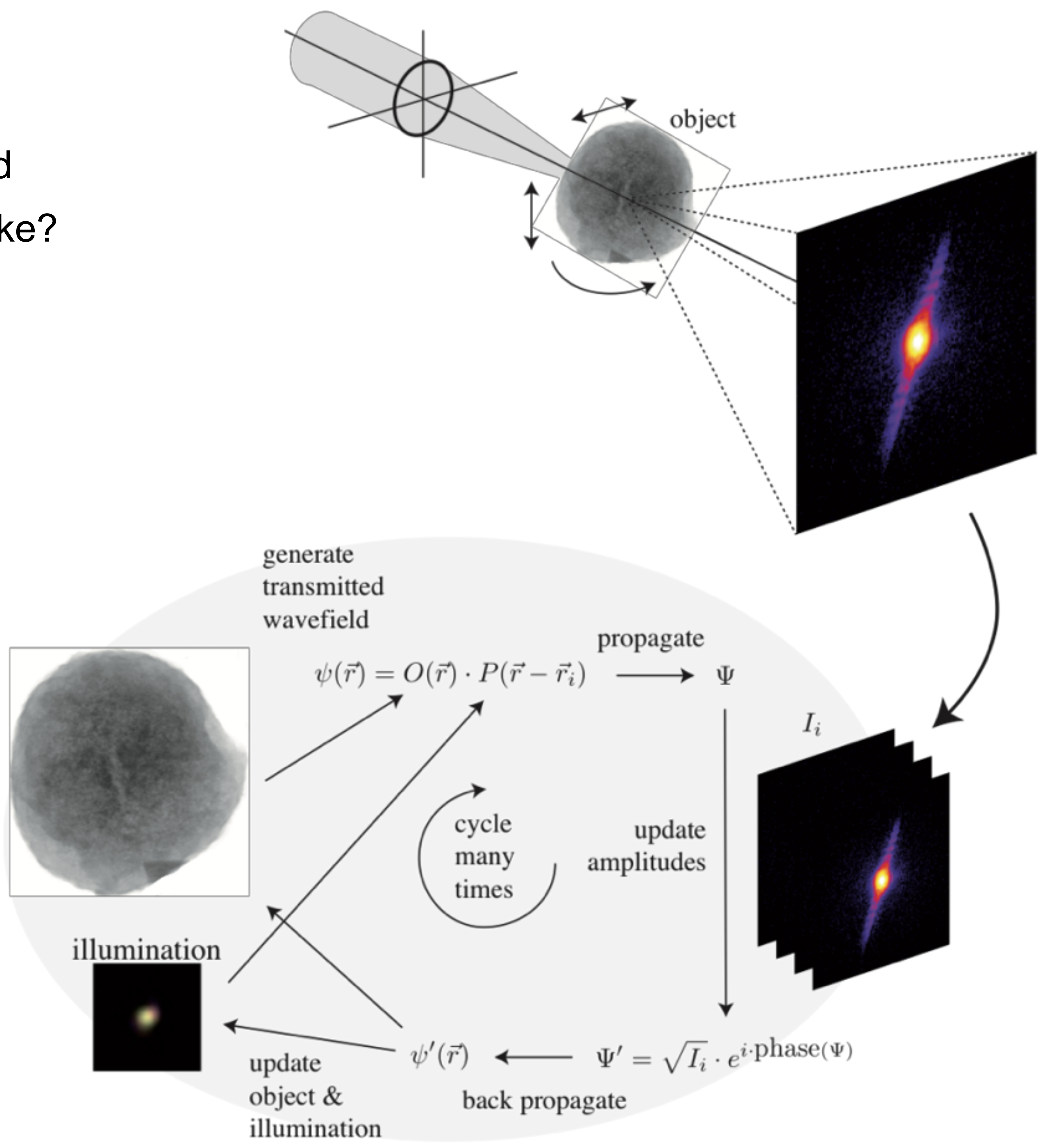
Scientific computing:

> today: data evaluation (pure number crunching time) is factor 10 - 100 too slow

> algorithms typically scale with (data size)$^{\alpha}$ ($\alpha \geq 1$), e. g. tomography: ~ size log(size)

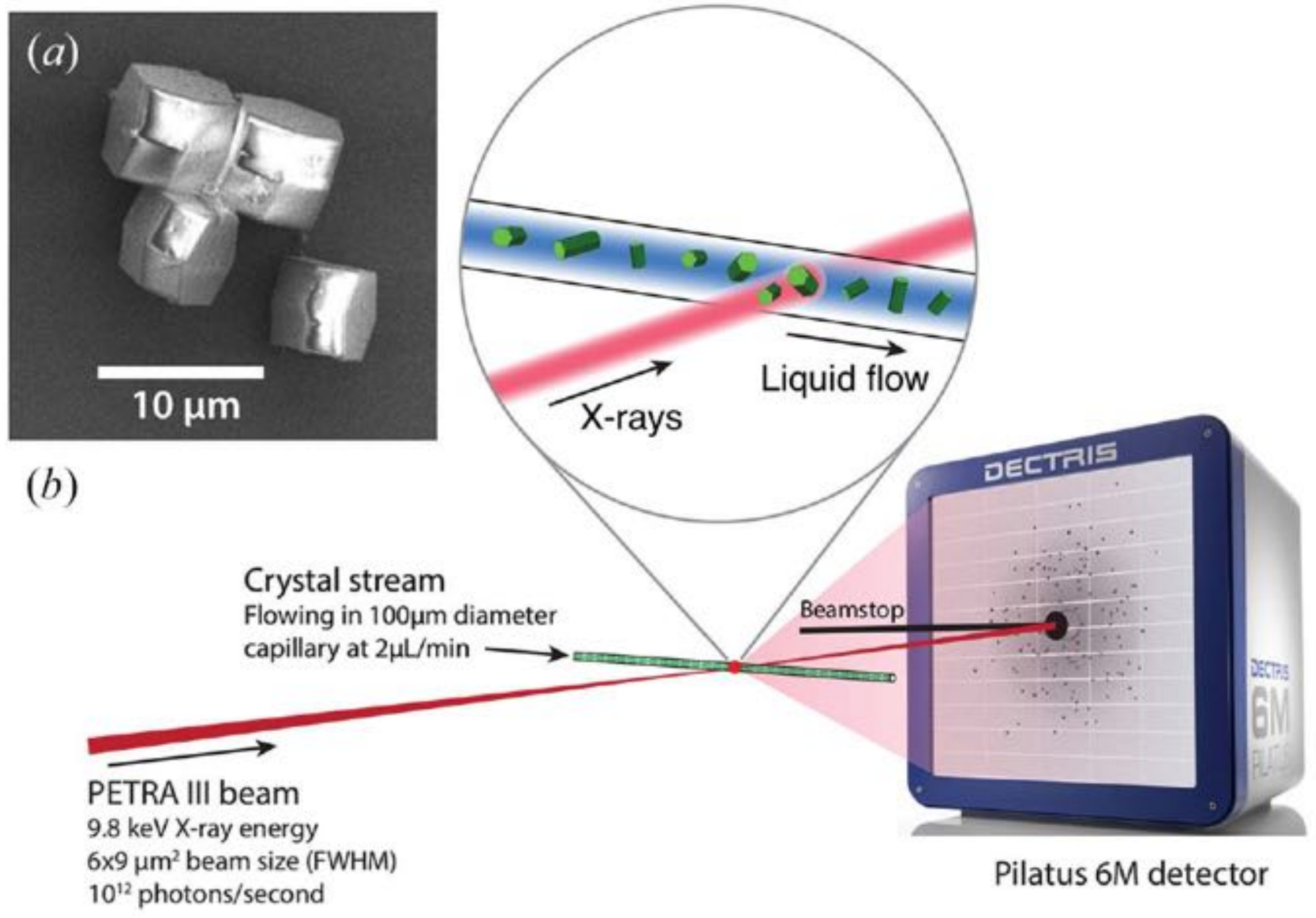
➔ new perspective on “raw data”
➔ clever algorithmic developments needed
➔ not solvable by brute force

Example Ptychography



High Data Rate (with Possibility to Trigger)

Serial Crystallography and Time-Resolved Crystallography



F. Stellato, et al., IUCrJ **1**, 204 (2014).

Demonstration experiment:

> lysozyme structure from series of microcrystals (6 µm diameter) at room temperature

> maximum single-crystal dose: < 0.3 MGy

> resolution: 2.1 Å

Record diffraction patterns of microcrystals flowing across the beam:

> record large number of frames (~ $1.5 \cdot 10^6$) (room temperature)

> select diffraction patterns (~ 40000) (triggering)

> index reflections in 3D reciprocal space and average

> solve structure from 3D reciprocal space data

High future potential:

> Scalable: increase flux and throughput: large number of crystals in short time

> Combine with pump-probe scheme for time-resolved studies with trigger upstream (resolution: transition time)

PETRA IV:

> detector frame-rate limited acquisition (up to ~10 MHz)

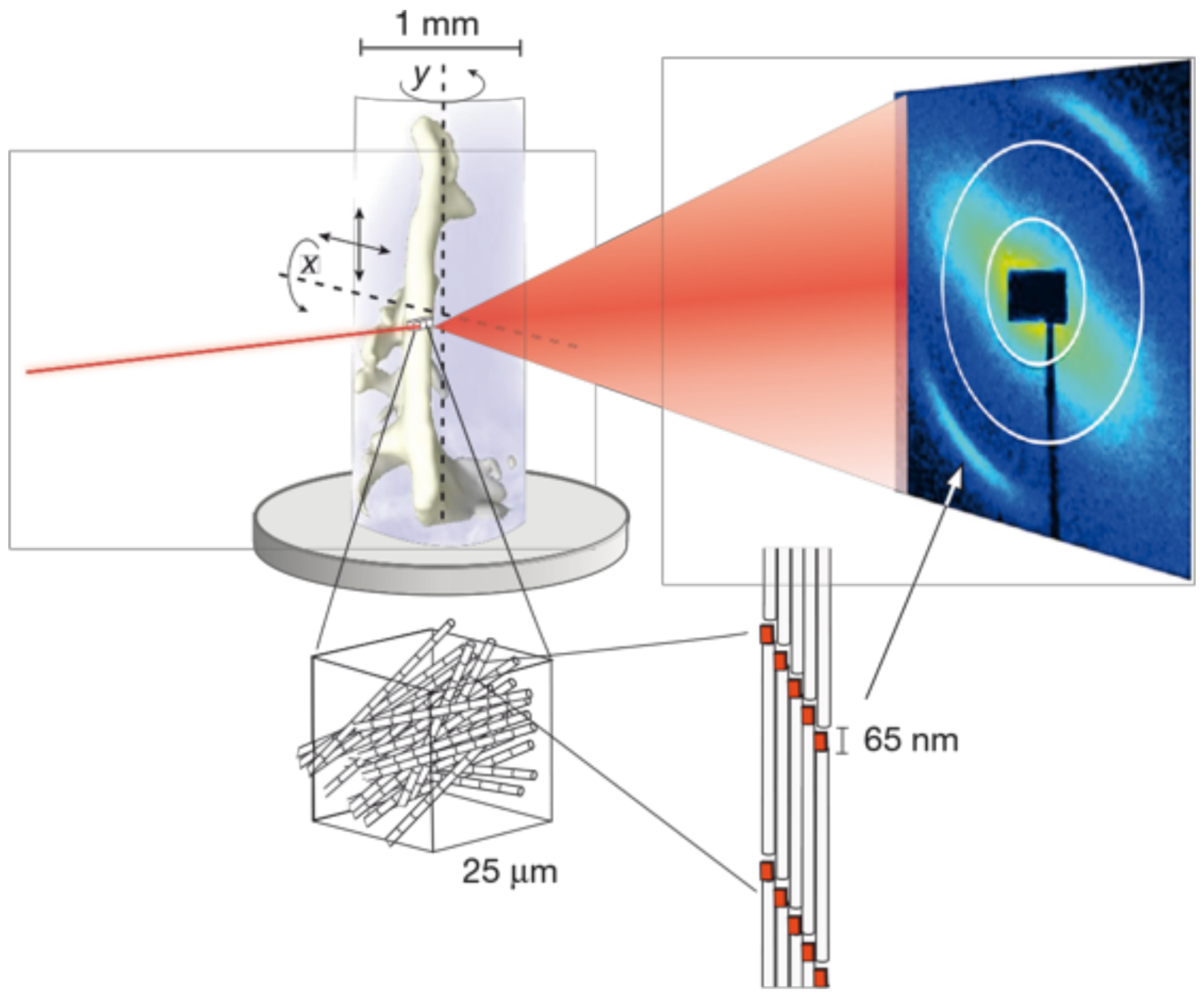
European XFEL:

> detector frame-rate limited acquisition (up to ~3500 Hz with current bunch structure)

> CW operation: > 100 kHz

SAXS-Tomography in 3D

High-Dimensional Data Sets



Liebi, M., et al., Nature, **527**(7578), 349–352. (2015).

Currently “heroic” experiment!

PETRA IV:

High resolution and
proper sampling possible!

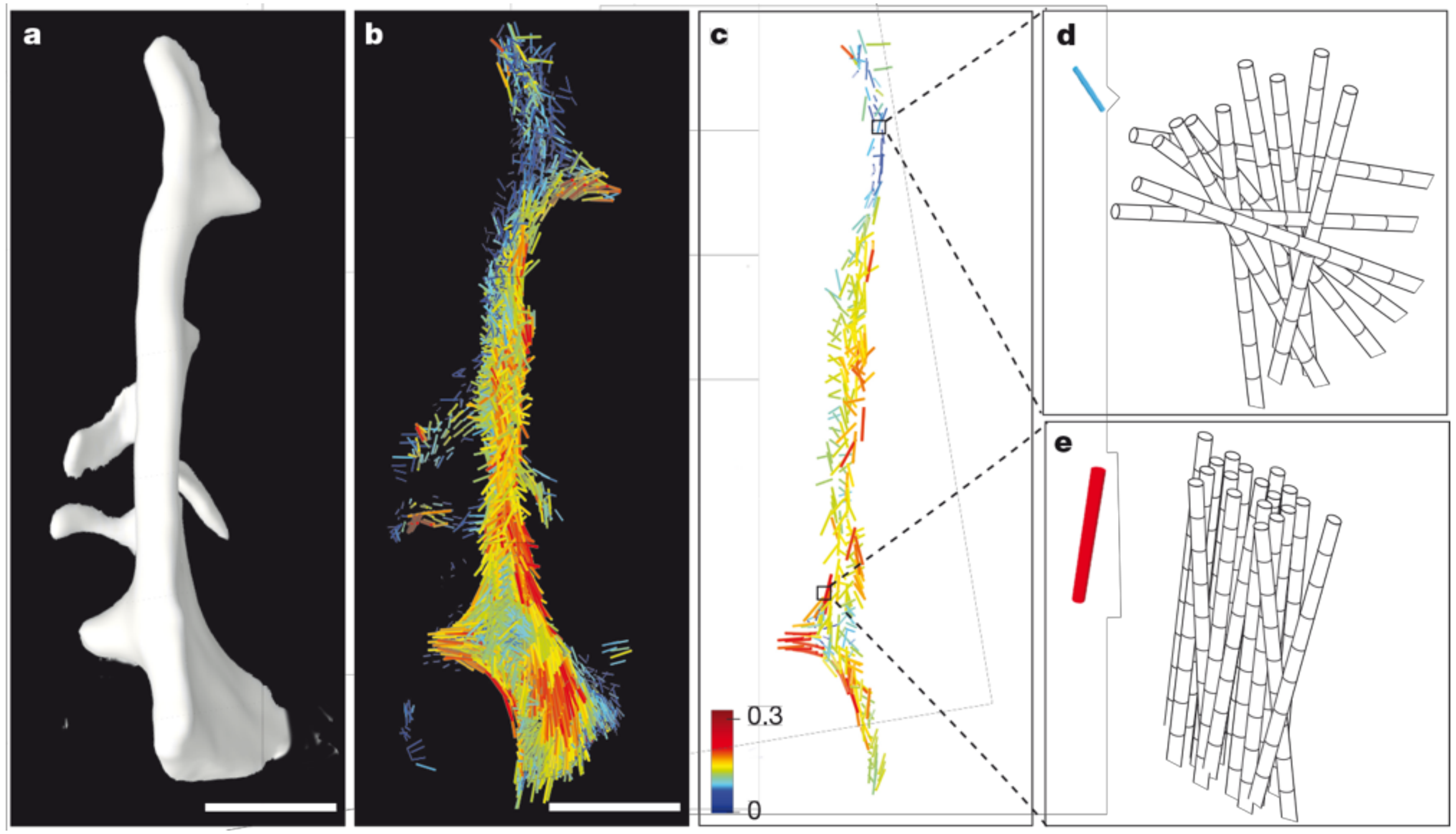
General SAXS-tomographic problem

6 dimensional map (3D reciprocal space as function of 3D real space)!

Scan in 4 dimensions

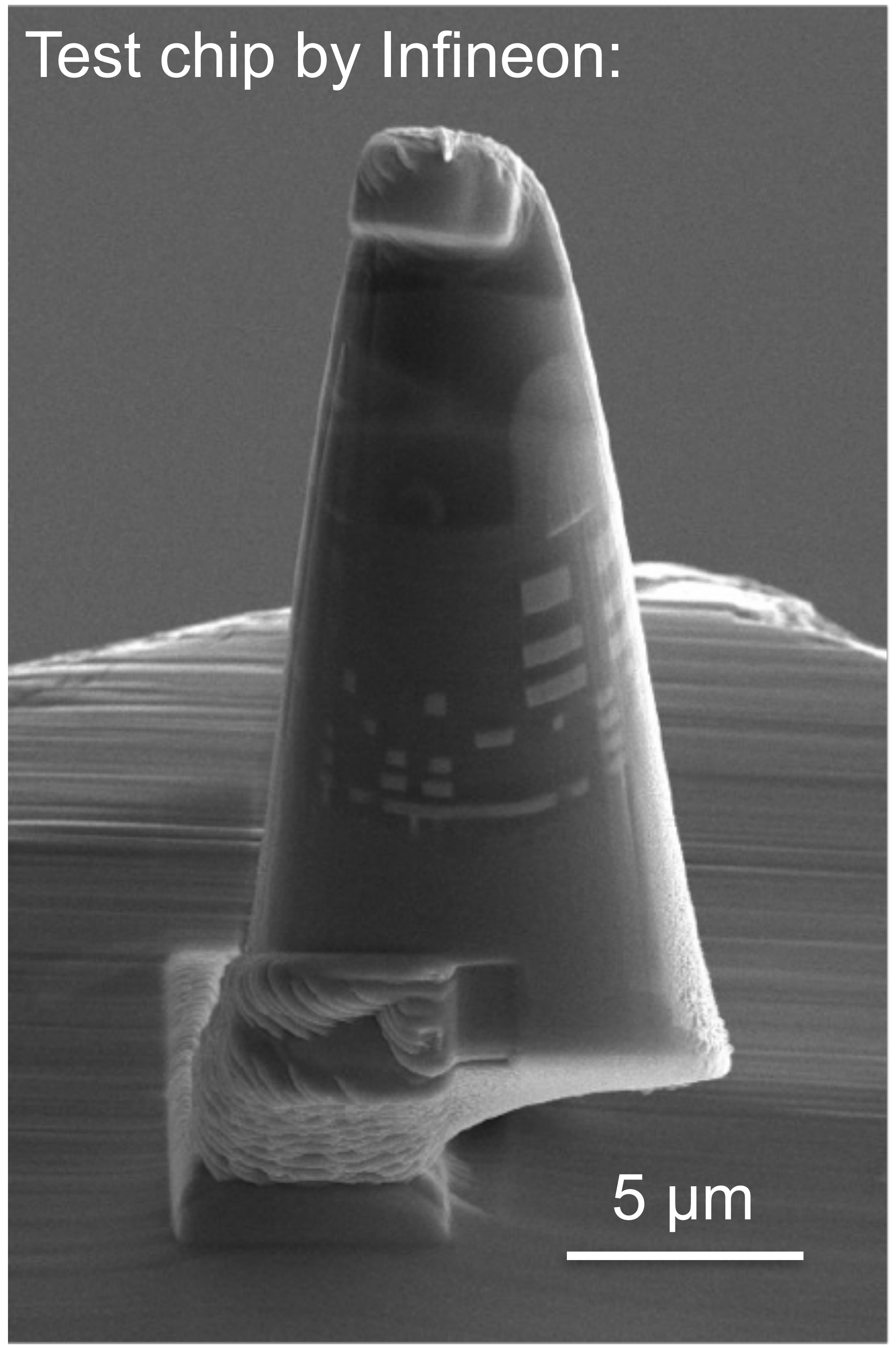
- 2x translation (horizontal and vertikal)
- 2x rotation (elevation and azimuth)

(currently very coarse sampling)



Multimodal Imaging

Various (X-Ray) Analytical Contrasts



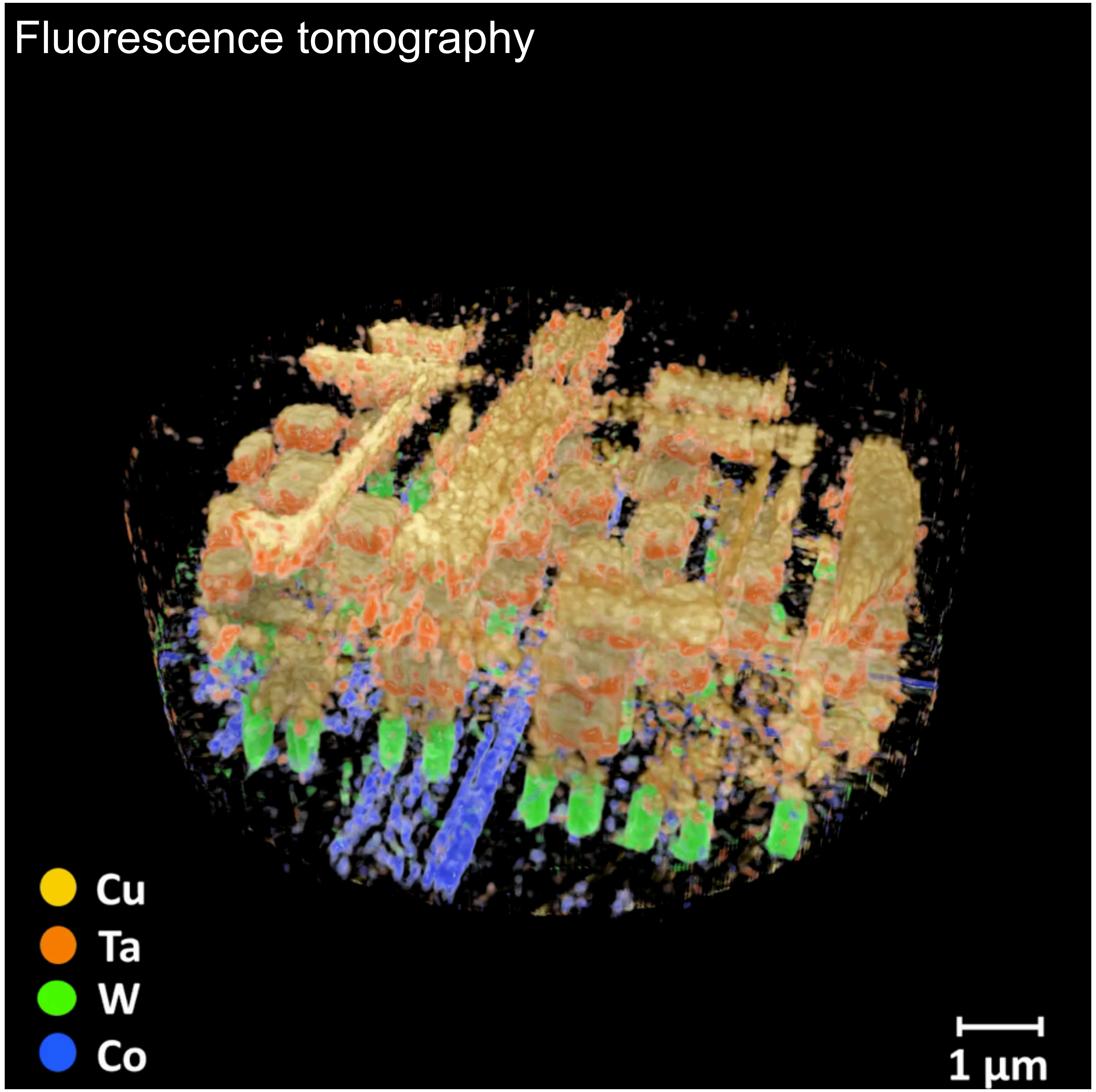
E = 18 keV

beam size: 61 x 80 nm^2

tomographischer scan:

> X-ray fluorescence
> diffraction & scattering

PhD research by
Maria Scholz



Master thesis of Lukas Grote

Multimodal Imaging

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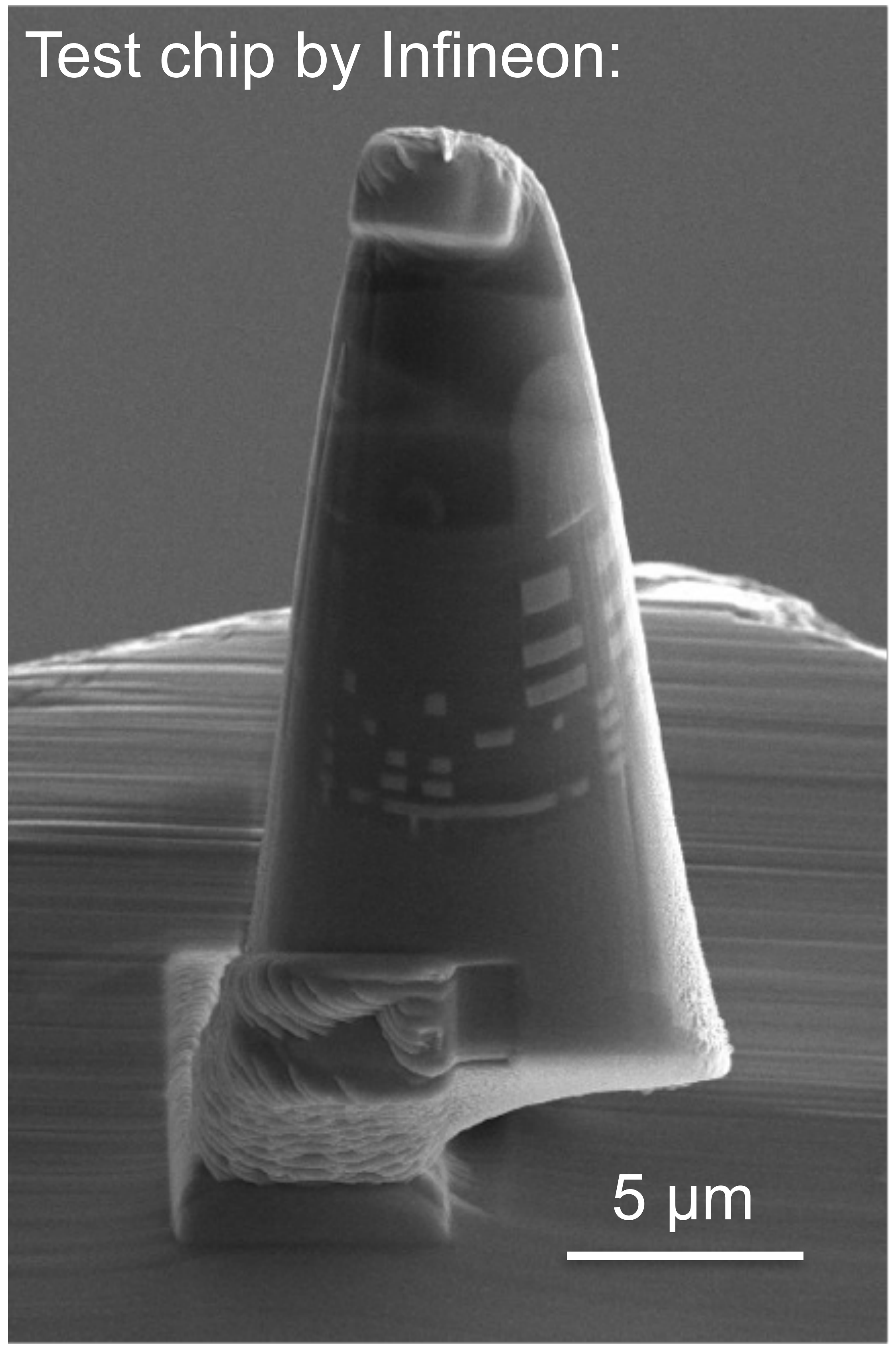

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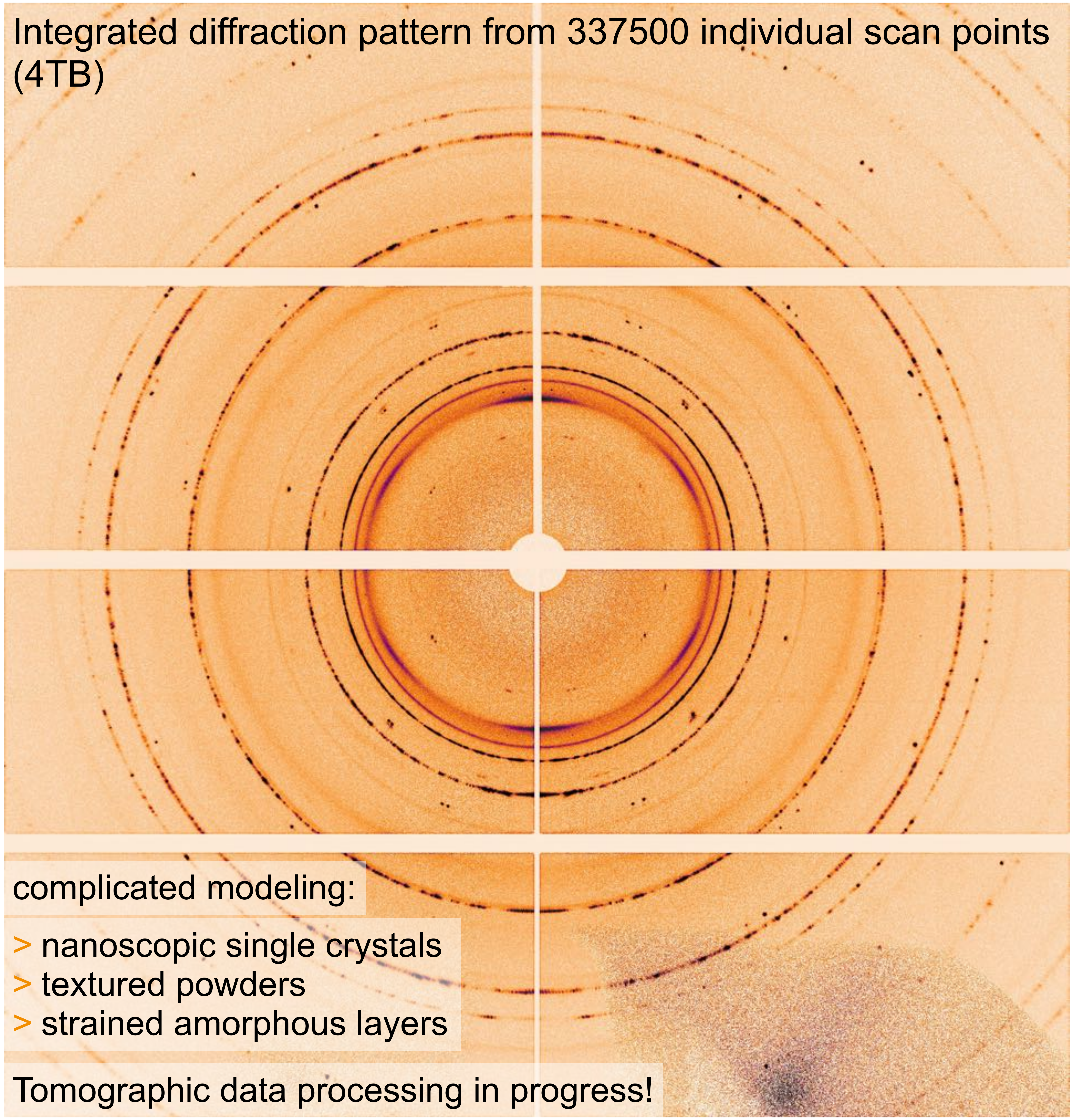


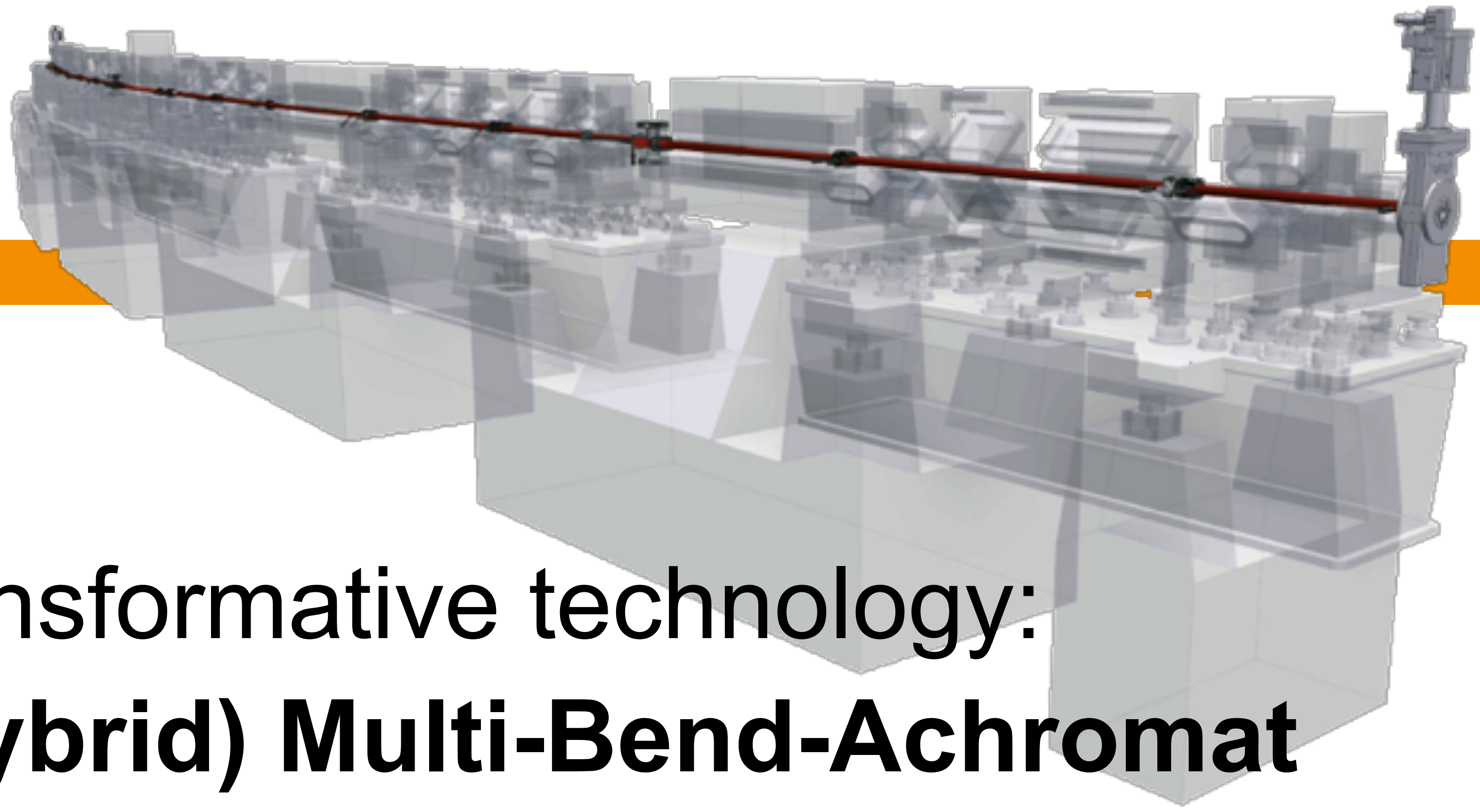

Refined tomographic models:
single crystal tracking
powder tomography
…
strained nano-crystalline Ti(II)O layer
W (110)
Cu (111)
Ta (111)
TiO2 (110)
horizontal compression
vertical expansion

PETRA IV

Ultra-Low Emittance Storage Ring

source size
& divergence:
155 µm x 6 µm
7.7 x 3.8 µrad^2

extended & divergent X-ray beam



source size
& divergence:
11 µm x 3.2 µm
1.7 x 1.5 µrad^2

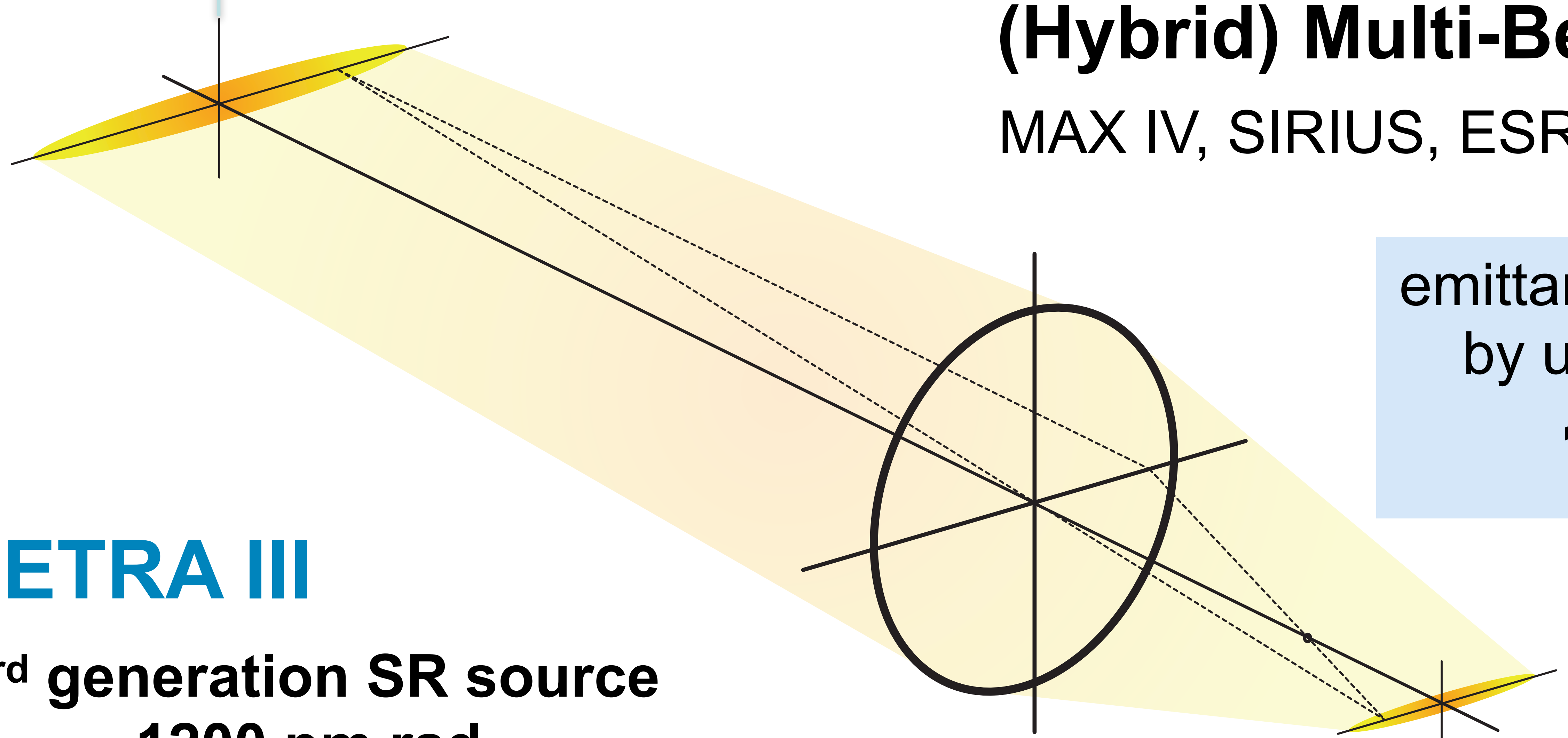
small & collimated X-ray beam

transformative technology:

(Hybrid) Multi-Bend-Achromat

MAX IV, SIRIUS, ESRF-EBS, APS-U, SPring-8-II

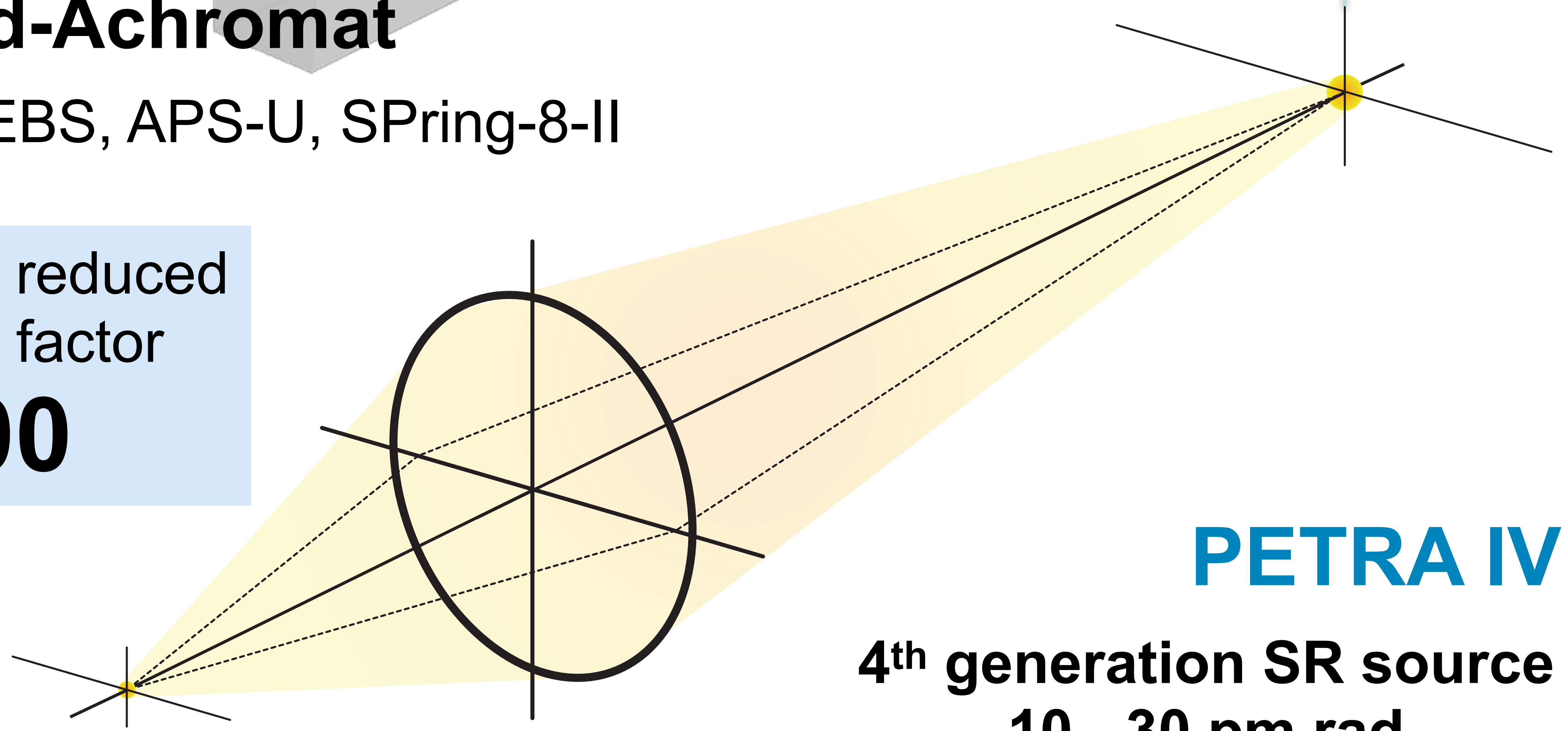
emittance reduced by upto factor
100



PETRA III

3rd generation SR source
1200 pm rad

Max. brightness: ~10^{21}
Coherence: ~0.1-1%



efficient nanometer focusing

PETRA IV

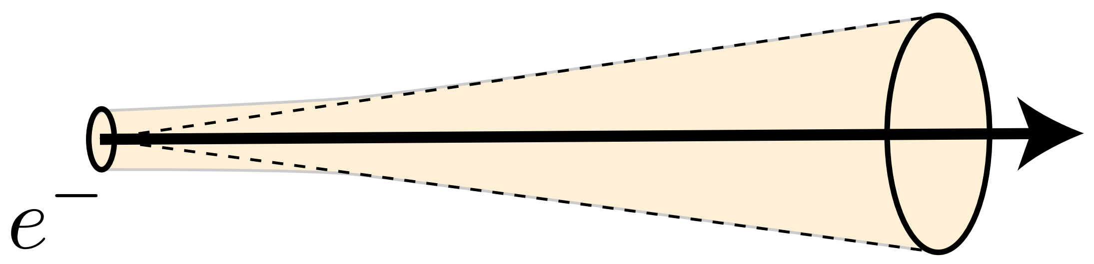
4th generation SR source
10 - 30 pm rad

Max. brightness: ~10^{23}
Coherence: > 25%

PETRA IV

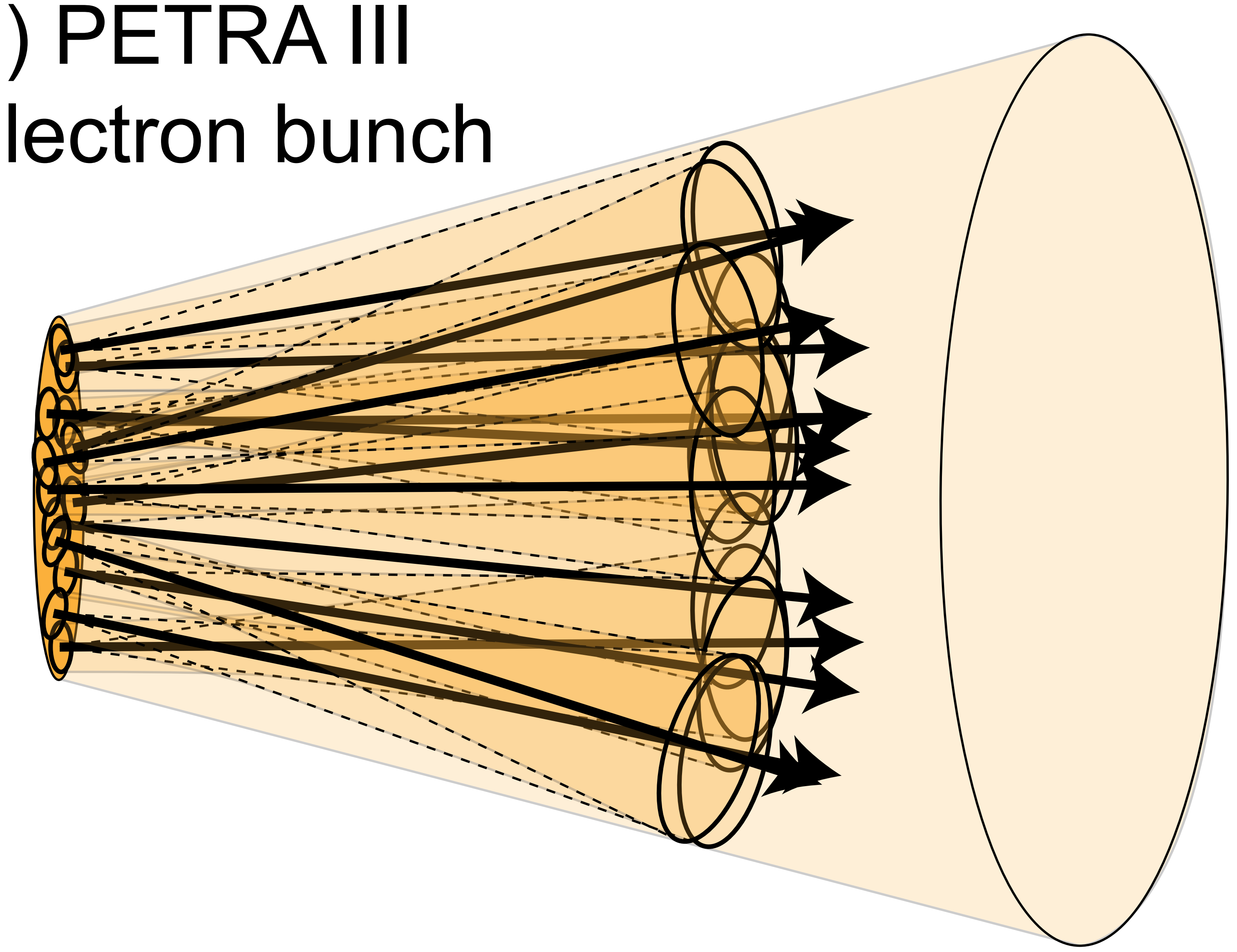
What makes the difference …

a) single electron

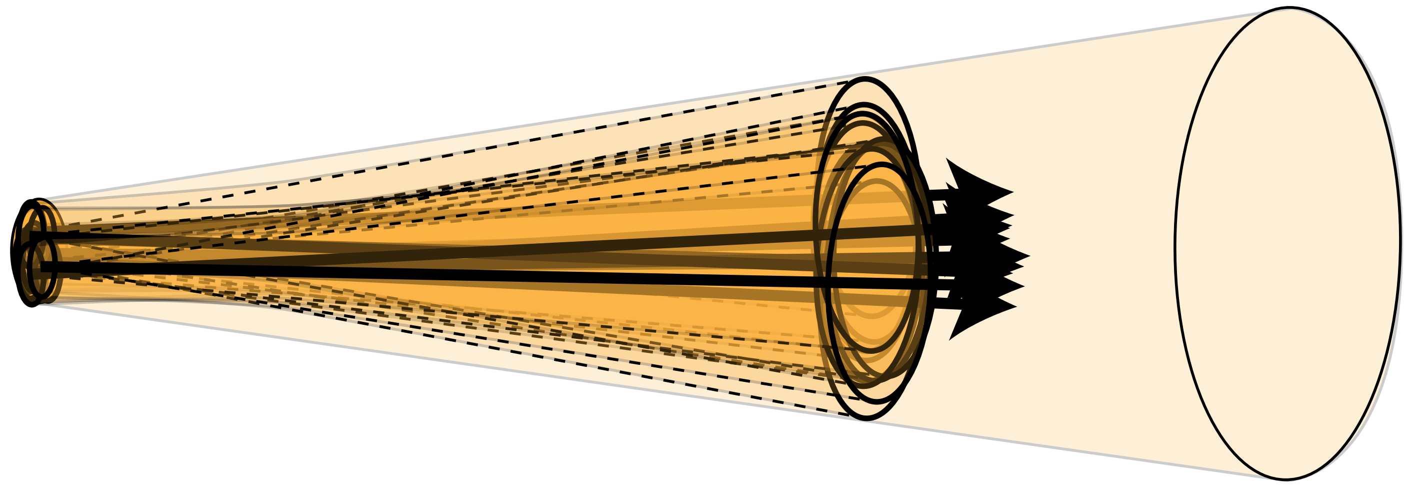


single-electron emission cone
(X-ray energy dependent)

b) PETRA III
electron bunch



c) PETRA IV
electron bunch



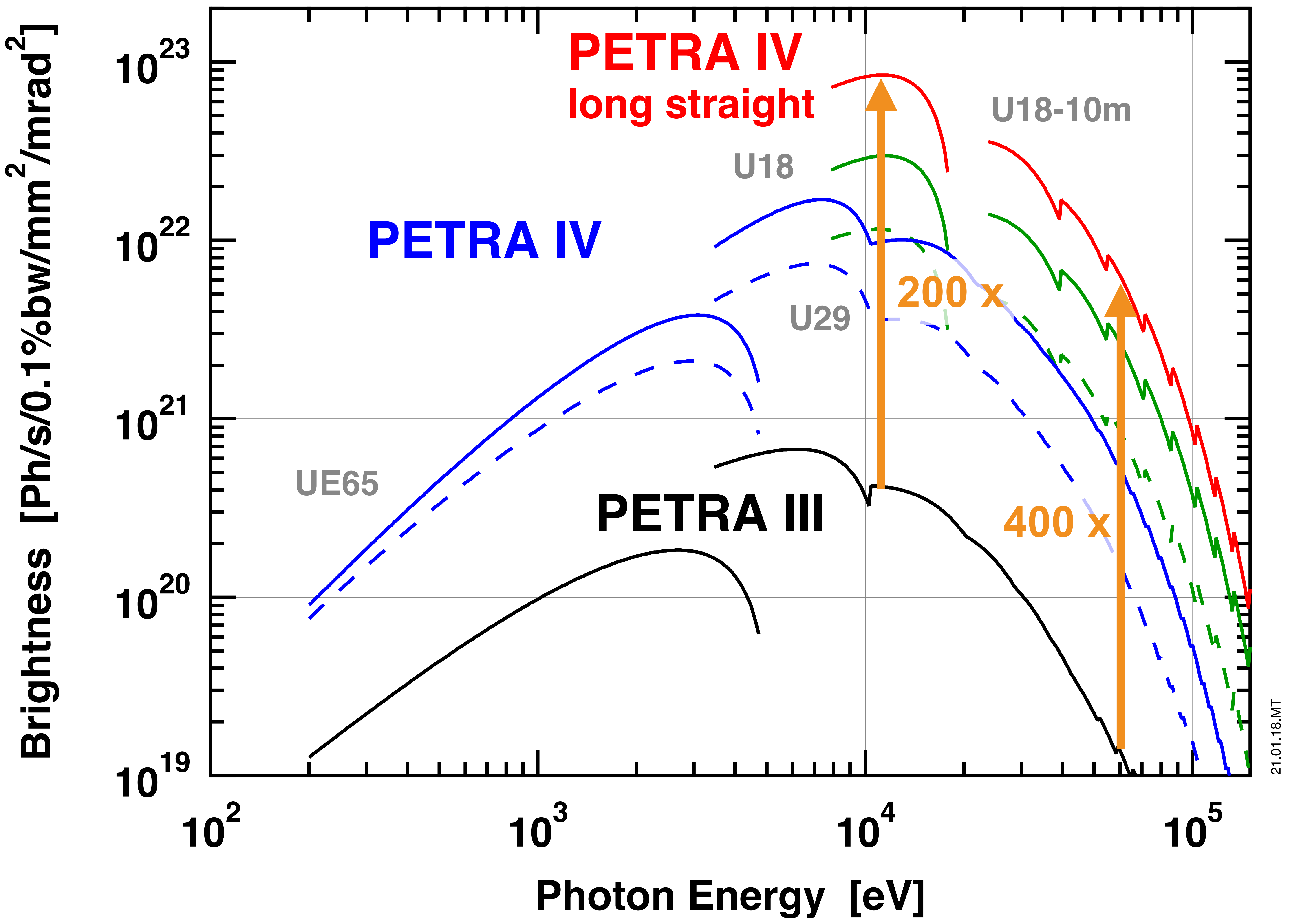
divergence and size of
electron bunches comparable to
single-electron emission cone

- ➔ (nearly) lossless focusing of the whole beam!
- ➔ **Diffraction limit**: optimal resolution in real and reciprocal space **AT THE SAME TIME**!
- ➔ PETRA IV can probe all length scales simultaneously, from atomic to macroscopic dimensions!

- ➔ ***In-situ*** 3D Microscope for **physical**, **chemical**, and **biological** processes

PETRA IV

Brightness



Based on current reference lattice:

- emittance:
  - → coherence mode: 20 x 2 pmrad²
  - → timing mode: 50 x 5 pmrad²
- undulators: 5 m, 10 m
- optimised beta (in 10 m section): 2 x 2 m²
- ring current: 100 mA

Brightness increase by

- → 200 x (hard X-rays)
- → 400 x (high-energy X-rays)

PETRA IV brightness at 100 keV
same as for 10 keV at PETRA III today!!

C. G. Schroer, et al., JSR **25**, 1277 (2018).

PETRA IV:

Ultimate 3D Microscope for Physical, Chemical and Biological Processes

Hard X-ray beam (nearly) diffraction limited:

➔ **Nanoprobes:** focus nearly full flux to nanobeam

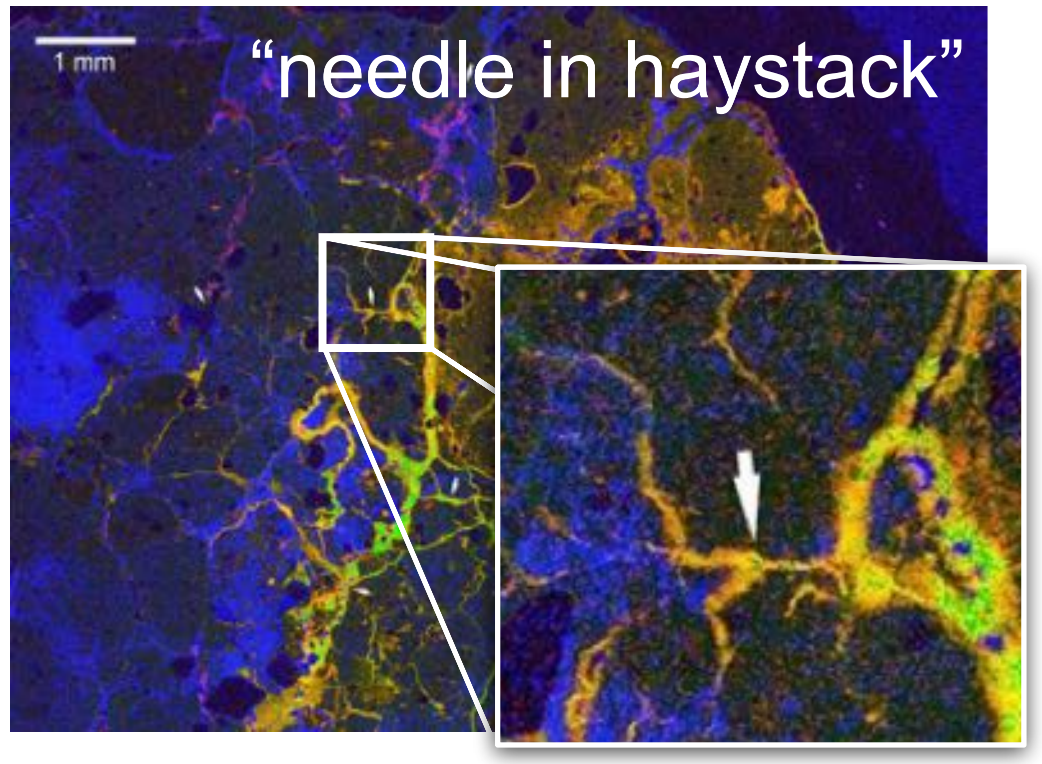
> up to **400 x faster** (movies rather than static images)

> up to **20 x better sensitivity** (signal-to-noise ratio)

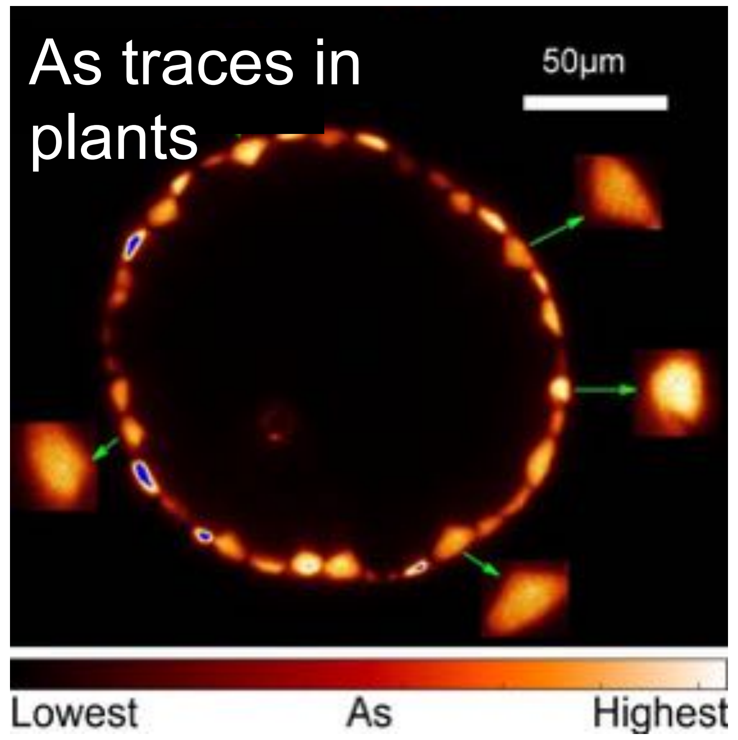
> up to **400 x larger field of view** or sample volumes ("needle in hay stack" problem)

➔ **Coherent imaging:**

> 4 to 5 orders of magnitude higher coherent flux density



CSIRO: gold deposit in clay



S. Mishra et al, J Exp Bot **67**, 4639 (2016).

New, unique properties:

➔ **Local quantitative measurements with all X-ray analytical techniques!**

➔ **Flux-hungry techniques go nano!**

> inelastic X-ray scattering,

> nuclear resonance scattering

> resonant magnetic hard X-ray scattering

➔ **High-energy X-ray techniques go nano!**

> Compton scattering

> Pair distribution function, …

➔ **Spatial resolution of coherent imaging: all spatial dimensions down to < 1 nm!**

> ptychographic imaging

3 GOOD HEALTH AND WELL-BEING

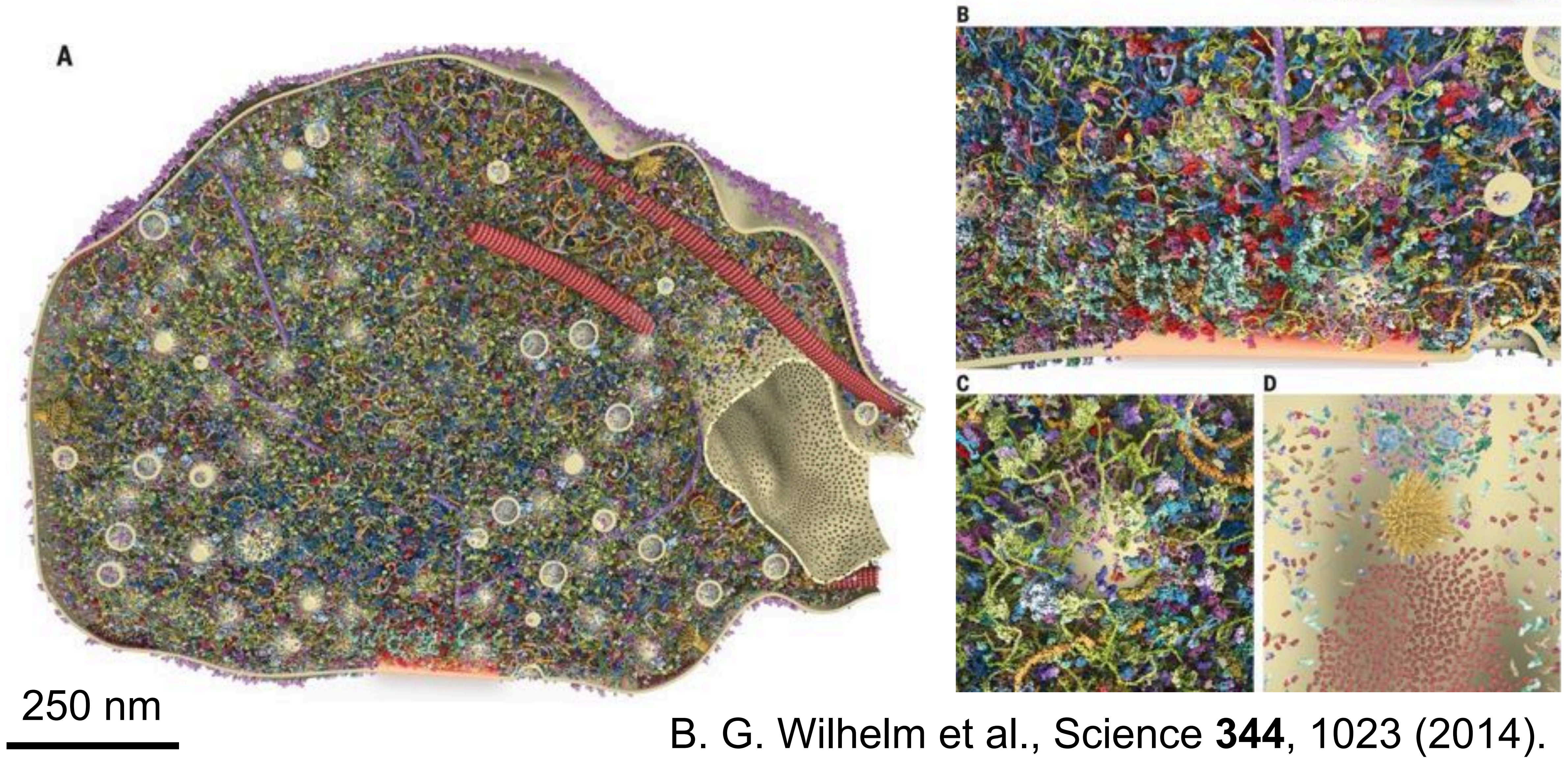
Example: Infection Research

Imaging infection pathways in tissues by high-resolution Compton tomography

Key question: how can a **virus binding at the surface** of a cell result seconds later in the **modification of a chemical reaction** occurring on the quantum level in an enzyme associated with gene transcription?

Major dream: **predictive multi-scale model** of the **structure** and **dynamics** of living organisms from molecules, macro-molecules, large assemblies to organelles, cells, and whole tissues.

Synaptic bouton: cellular complexity



B. G. Wilhelm et al., Science **344**, 1023 (2014).

PETRA IV: Compton nano-tomography

> **large-region-of-interest maps** of cellular and sub-cellular architectures

> low dose (Compton scattering at ~ 64 keV)

> ultra bright nanobeam at high X-ray energies
➔ high-resolution imaging of large volumes
(e. g., 100 μm^3 with 10 nm resolution, 10^{12} voxel)

requires
MHz acquisition rates!

Contribution to:

> Human Cell Atlas

> Human Brain Project

> …

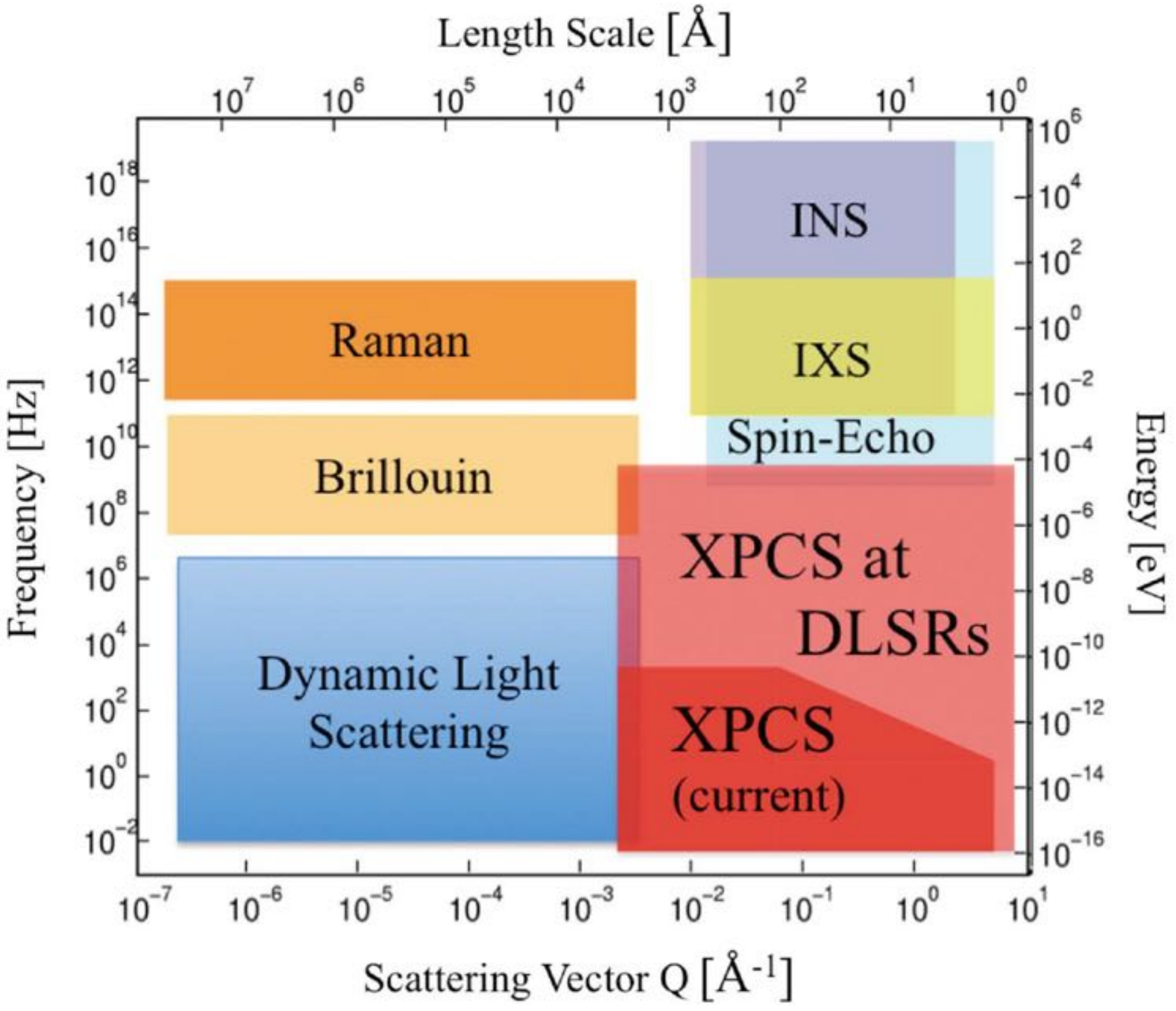
P. Villanueva-Perez, et al., Optica **5**, 450 (2018).

PETRA IV: Dynamics in Disordered Systems

Zooming in on dynamics of complex matter

X-ray photon correlation spectroscopy (coherence):

fast dynamics, non-equilibrium systems, image dynamic heterogeneity (locally), dynamics in nano objects



O. G. Shpyrko, J. Synchrotron Rad. **21**, 1057 (2014).

Signal-to-noise ratio in XPCS:

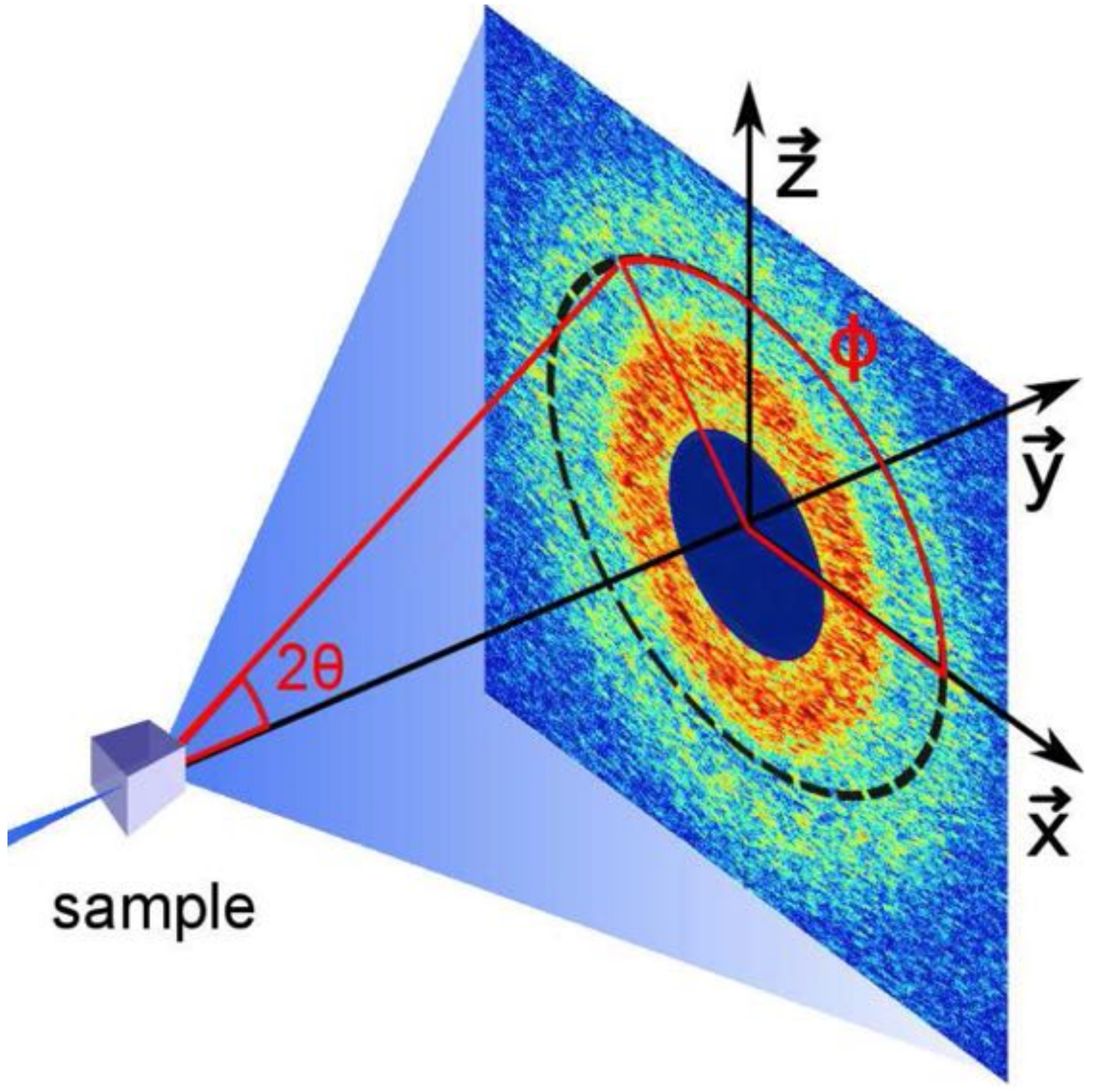
$$R_{\mathrm{sn}} = F_c \sqrt{T \tau n}$$

factor 100 in coherent flux F_c

factor 10000 in measurement time T or characteristic time τ

e. g., non-equilibrium dynamics, stimulated phase transitions, …

e. g., diffusion processes in aqueous solutions



S. Lee, et al., Opt. Expr. **21**, 24647 (2013).

requires multi-MHz acquisition rates!

data often very sparse (~10^{-2} photons per pixel)

Conclusion

Data and Computing Science Requirements in Photon Science

Data size:

> time-resolved studies ('movies' of processes)
> spatially resolved analytical data

} and combinations thereof (movies of images containing multi-dimensional data)

> large inverse problems, where all data points are "good"

Data rate:

> time-resolved studies
> serial crystallography (trigger)
> X-ray microscopy and tomography (with various analytical contrasts)

Data quality:

> fast time series at low count-rate (very sparse) images (e. g., XPCS)
> noisy data to avoid radiation damage (low dose)

Conclusion

Data and Computing Science Requirements in Photon Science

Users can no longer do data analysis by themselves

➔ support by facility needed

Online data analysis: does the experiment work?

fast (preliminary) data evaluation (on the fly) needed

➔ Machine learning?!

Experiments control:

fast feedback systems

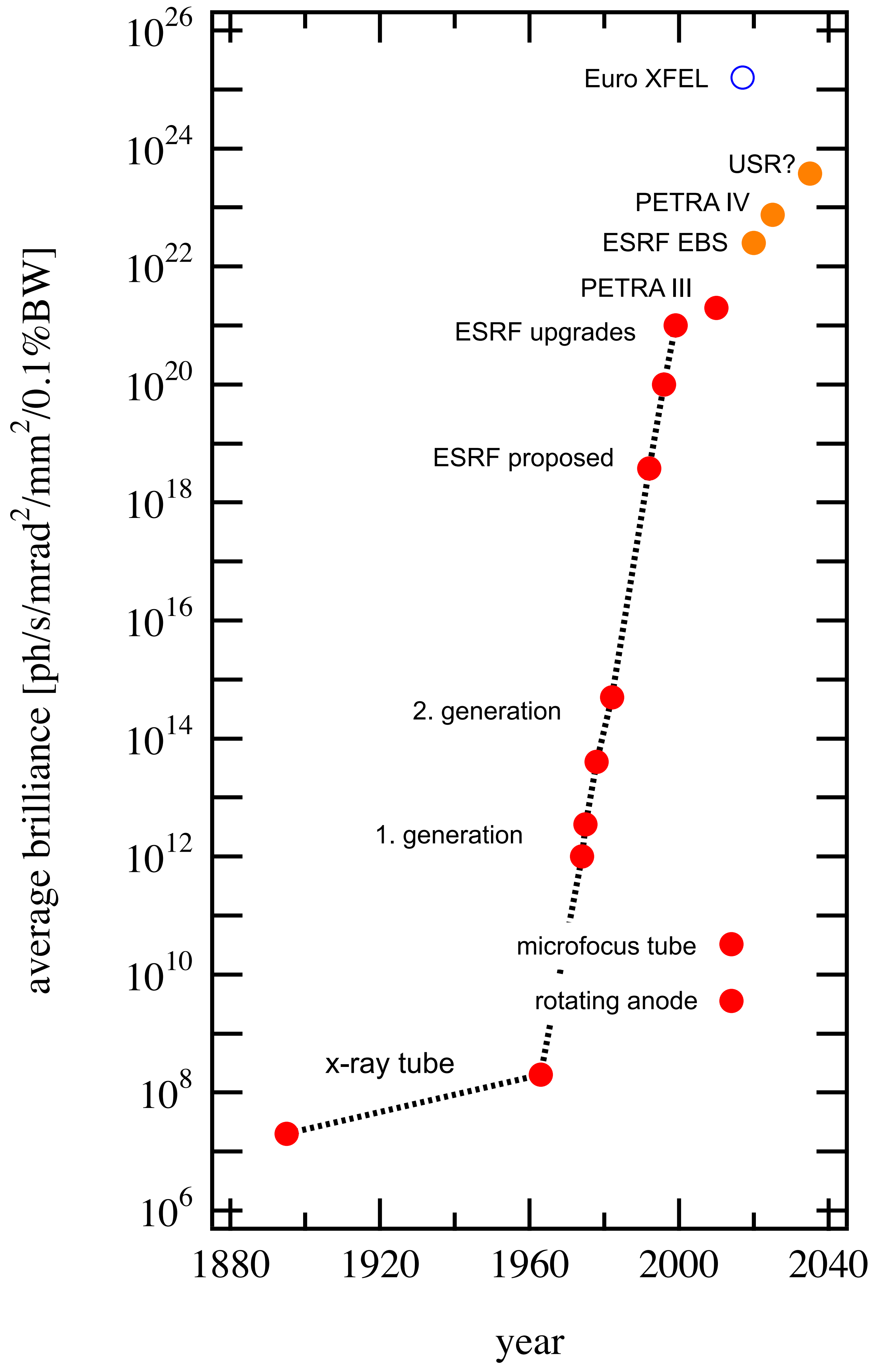
➔ Machine learning?!

Data evaluation:

significant improvement needed also on the algorithmic side (hardware growth does not keep up with needs)

➔ Moore's law: growth can not keep up with photons

Brightness of X-ray sources



10000 x more light per decade (since 1965)!!