A hard X-ray FEL multiscale microscope

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X-rays > 50 keV:

- Large Q-range
- Small correction terms

→ Amorphous materials
PDFs

- Flat Ewald sphere

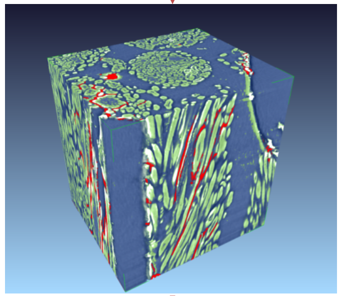
→ Diffuse scattering

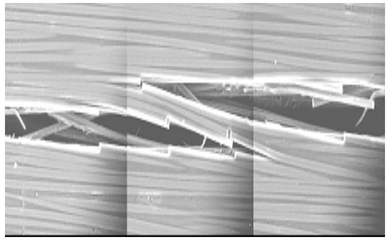
- Large penetration

→ Materials science
on hard materials

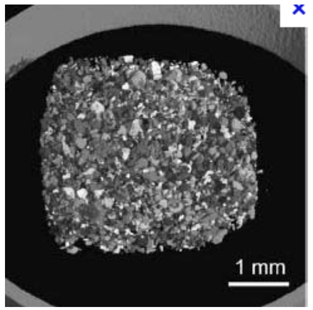
Devices are multiscale

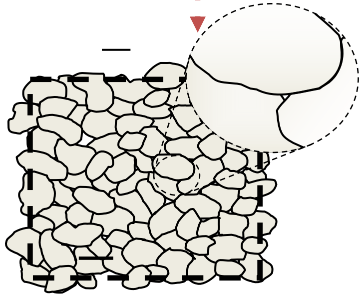
Composites for wind



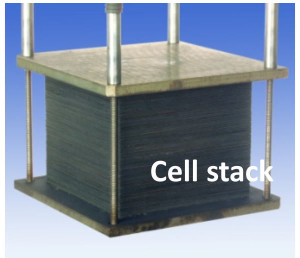


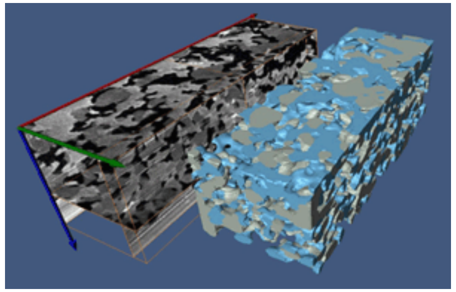
Batteries

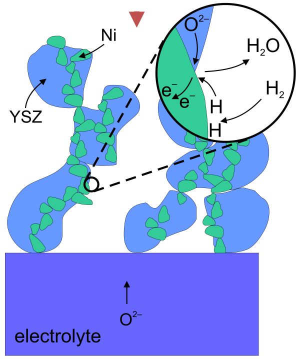




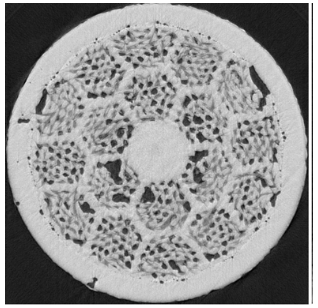
Fuel cells

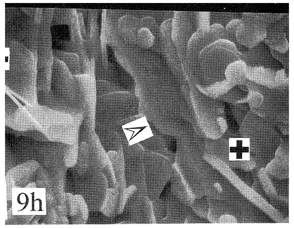






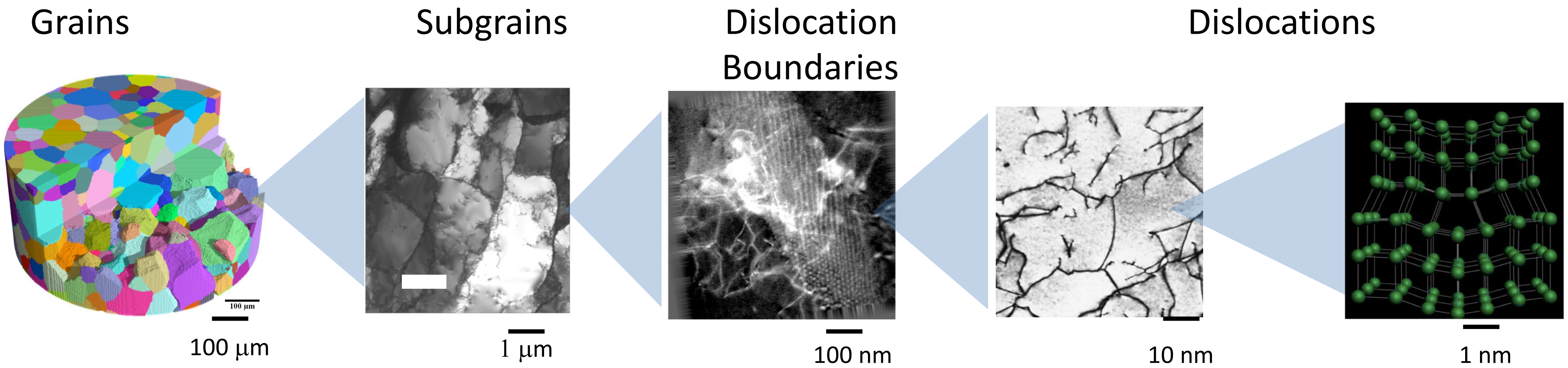
Superconducting cables





Structural materials are multiscale

Stength in metals determined by structure:



Scientific challenge: Predict dynamics and interaction between scales

Predict strength from first principles

Outlook: Materials design by computing

Specifications

Penetration: Tunable 30 keV -> 80 keV
Higher harmonics

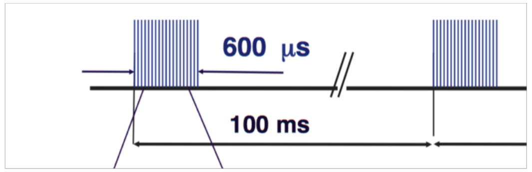
Materials science is a collection of rare events:

Repeated measurements

Realistic driving forces and sample environments
Electrical, mechanical, temperature

Local studies:
Zoom in and out

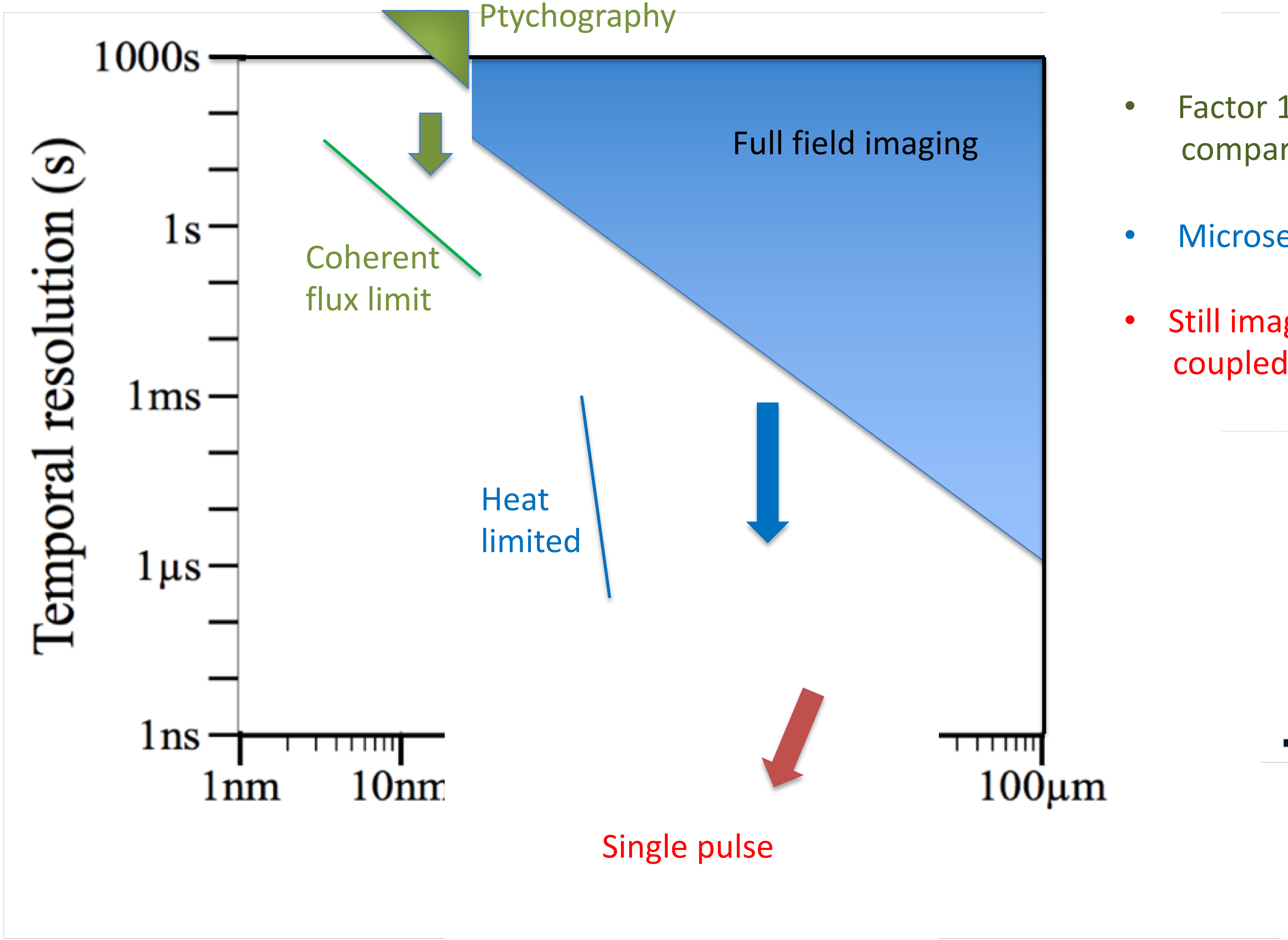
Limited by heating:
ΔT = 10 K in copper
No dissipation of heat during one bunch train
Full dissipation between trains



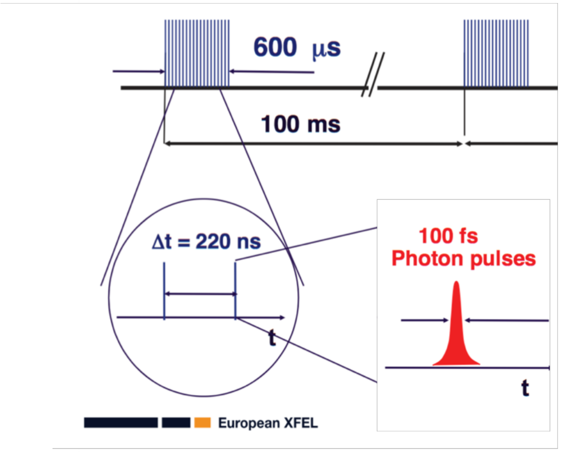
	Flux per pulse (ph/mm^2)	Flux per 500 pulses (ph/mm^2)
20 keV	1E11	2E8
40 keV	3E12	6E9
70 keV	3E12	6E9

Condense incoming beam to 30x30 microns

Full field Imaging at E-XFEL



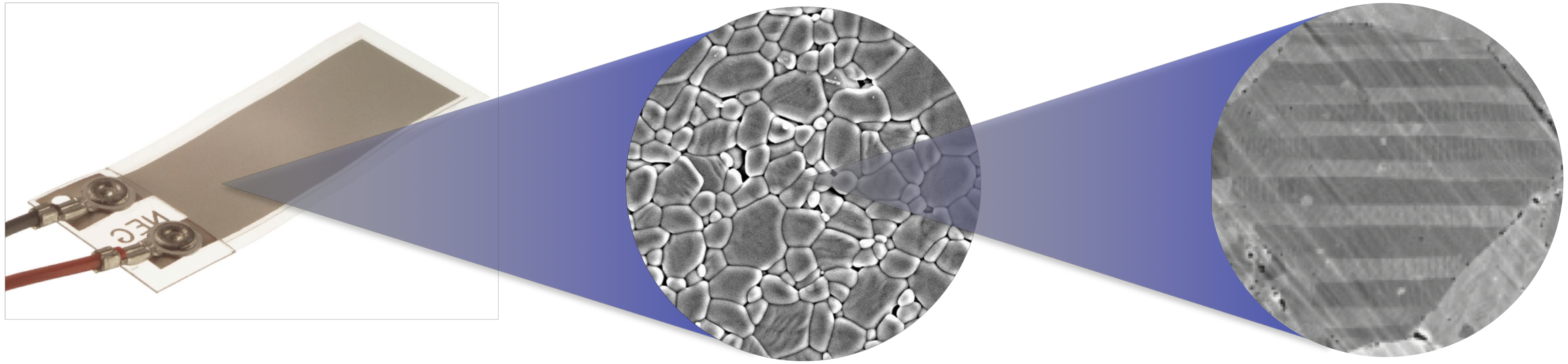
- Factor 100-1000 in coherent fraction compared to a synchrotron
- Microsecond movies
- Still images with 0.1 ps resolution coupled with classical imaging.



Domain evolution during phase transformations

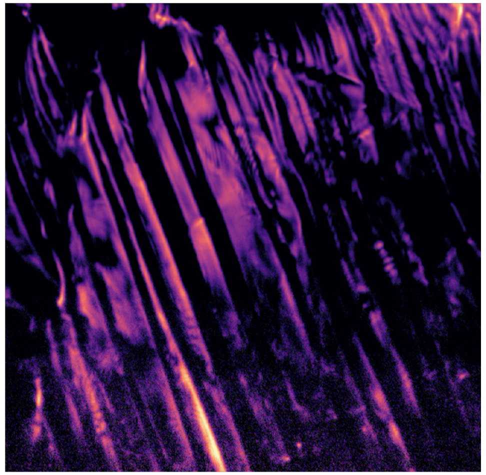
Synchrotron imaging on piezoelectrics:

Ceramic device ($10^{-2} – 10^{-3}$ m) | **Grain structure** ($10^{-4} – 10^{-6}$ m) | **Domain structure** ($10^{-5} – 10^{-8}$ m)



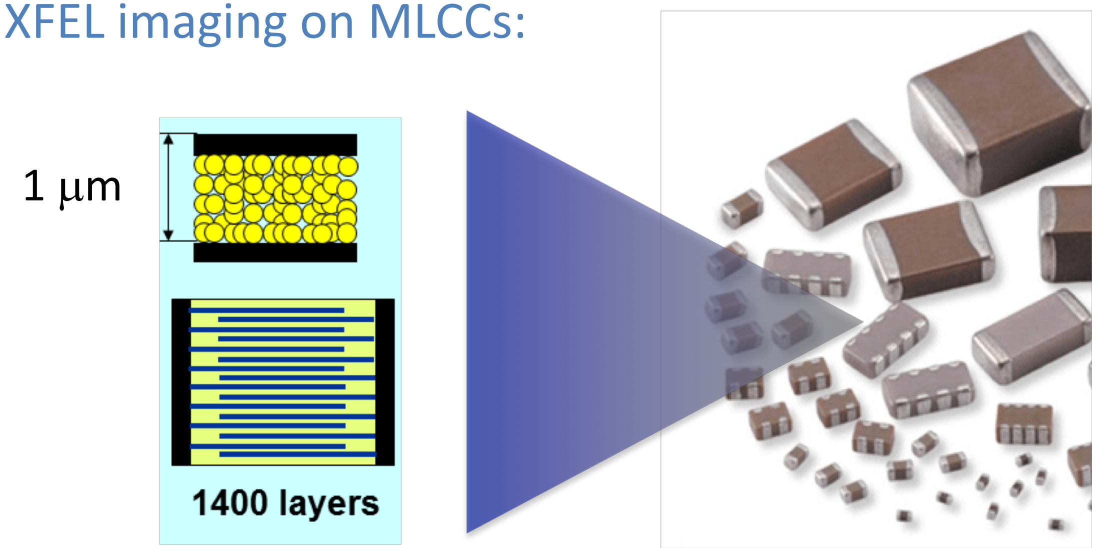
Diffraction tomography

Diffraction microscopy



$KNbO_3$ 10 Hz movie
17 keV, 200 nm resolution

Hard XFEL imaging on MLCCs:



Study of real device

Domain switching on ps-μs scale
Still images

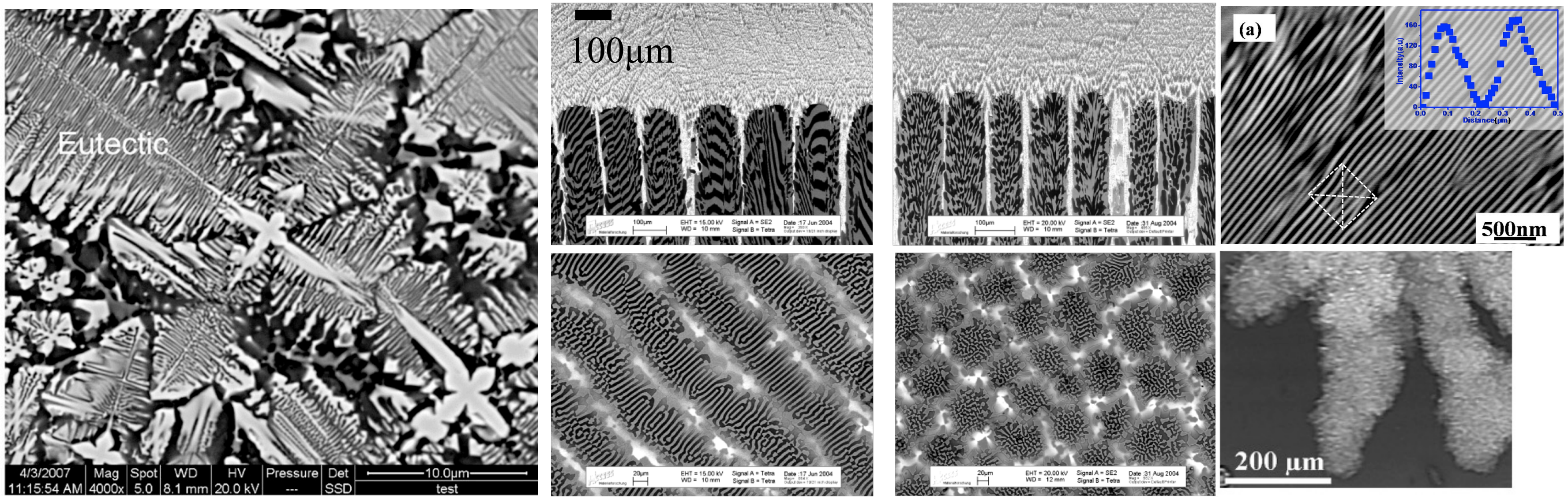
Eutectic and eutectoid transformations

NTNU

Group of Ragnvald Mathiesen

Applications: (most) casting alloys, solders & brazings, hydrogen storage, bulk metallic glasses, superplastic materials, metal-matrix composites, high-strength materials

Relevant systems: multicomponent, with non-isothermal fronts -> no model, limited insight

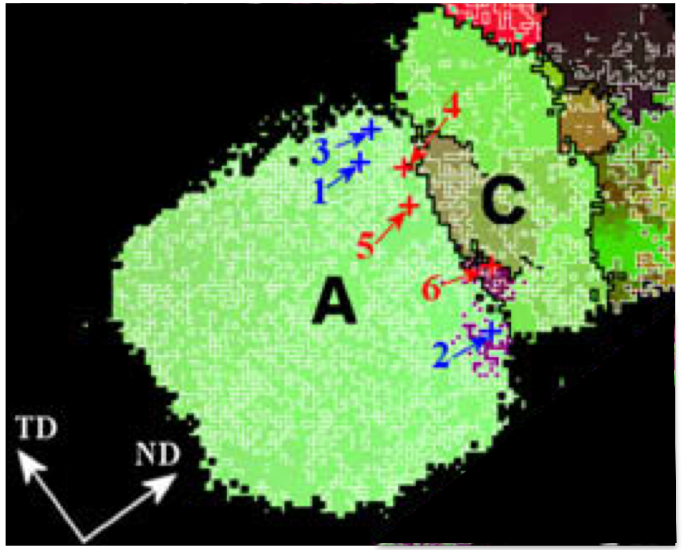


Mesoscale self-organised pattern formation @µs-ms time scales

Hard x-rays:
Solidification in real systems

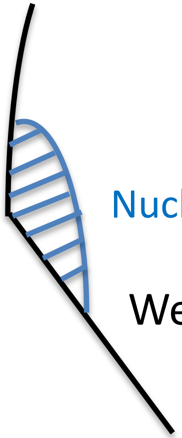
Nucleation

Synchrotron map of nuclei in Fe*



Resolution: 2 μm

Nucleation mechanims by Hard XFEL microscopy:



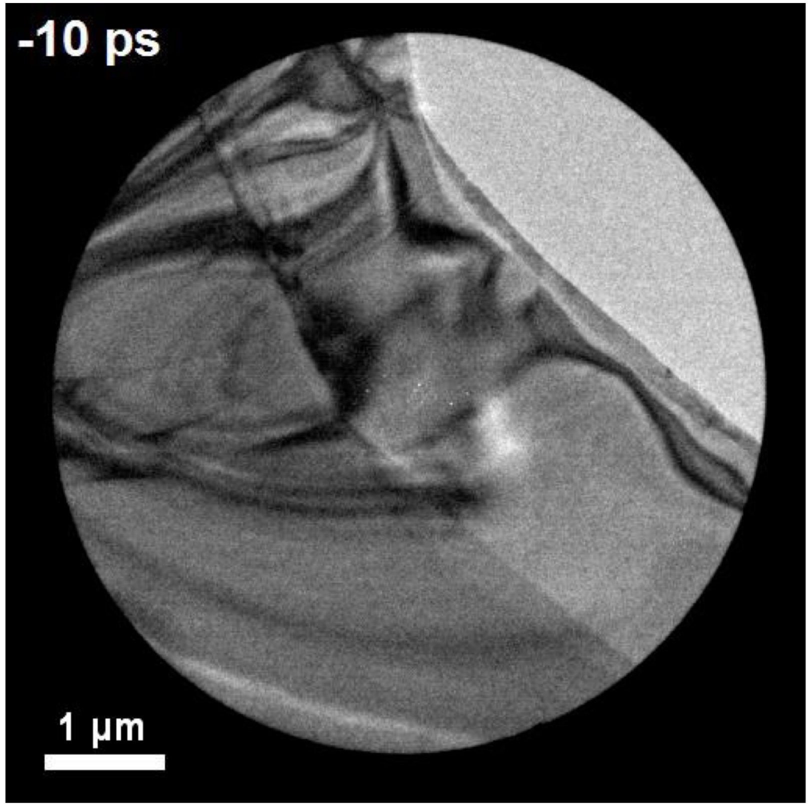
Rare events

Hierarchial structure ➧ hard x-rays
Snaphots with 100 nm spatial resolution

* S.S. West *et al.* *Scripta Mater*. **61** (2009) 875–878

Sound waves in thin foil

Electron microscopy*:

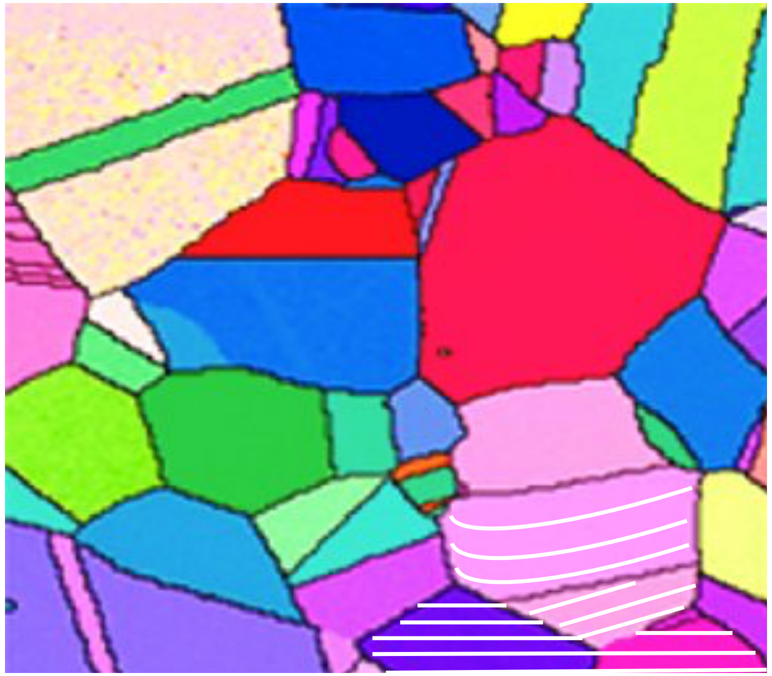


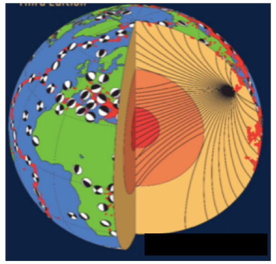
Rep. rate of 50 kHz.
Speed: 4-6 nm/ps

*D.R. Cremons *et al.* *Nature Communications* **7**, 11230 (2016)

Interaction of sound with obstacles

Hard XFEL diffraction imaging , stroboscopic:



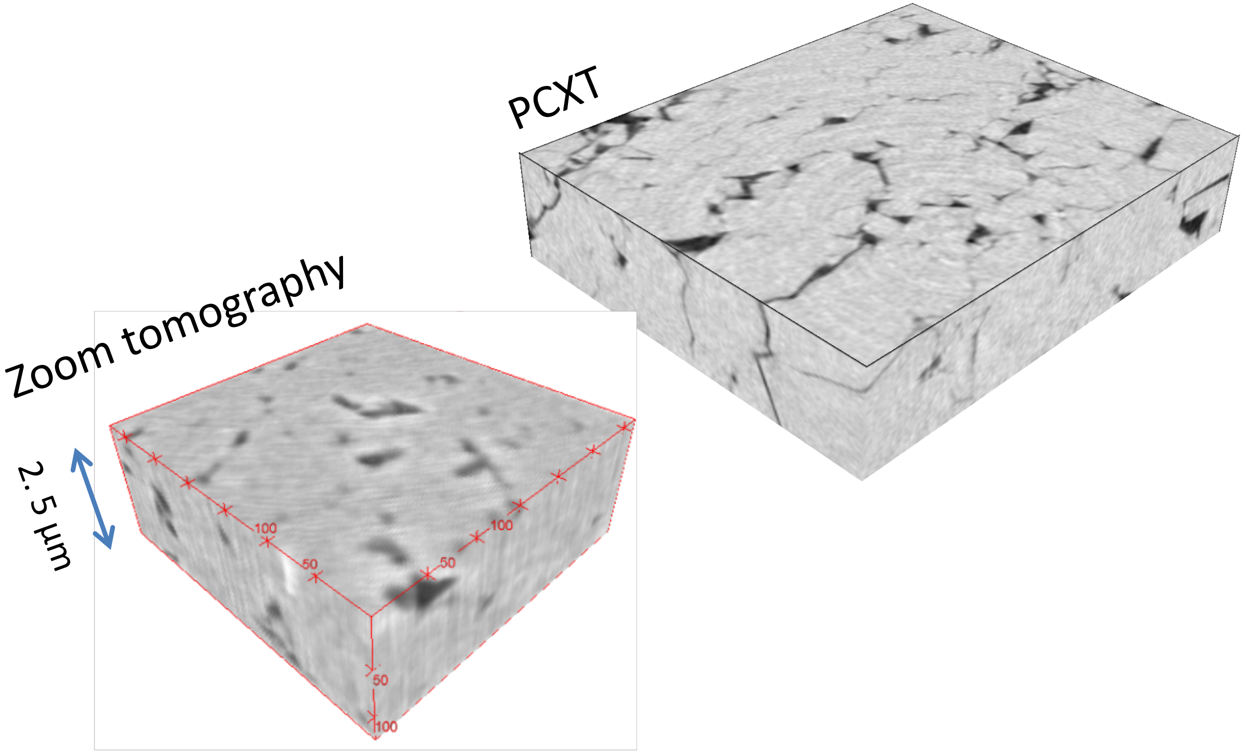


Fundamentals of heat/electrical conductivity
Seismology

Flow in porous materials (Chalck sample from oil drill)

Synchrotron imaging

- Zoom tomography (holotomography) - limited resolution
- Ptychographic X-ray nanotomography (PCXT)– limited to small samples



Hard XFEL bright field imaging

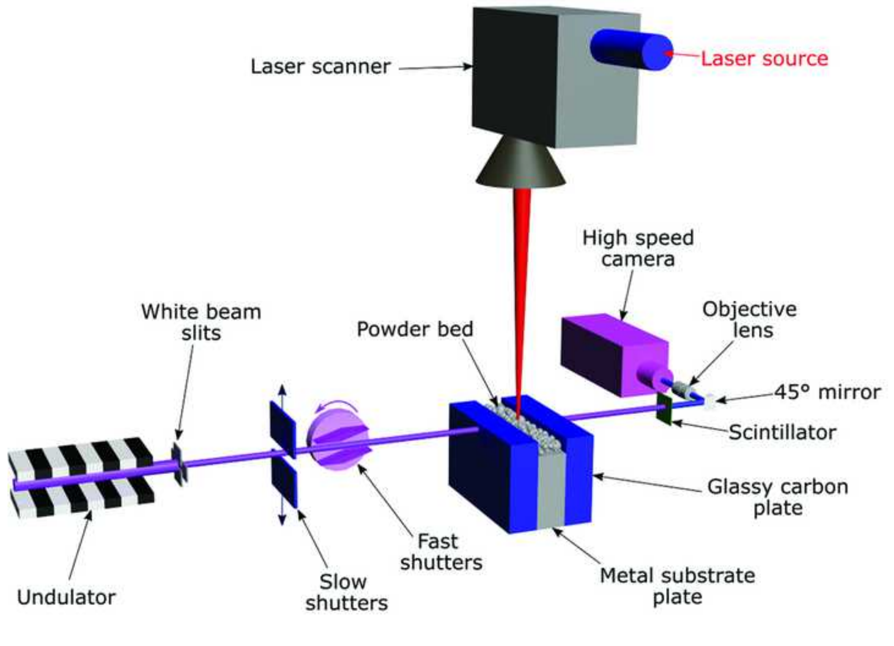
Coherence:

Develop local 3D ptychography.

µs resolution: See Haynes jumps

Welding and Additive Manufacturing

10 MHz synchrotron imaging of AM*:



(a)

Melt-pool dynamics and powder-spatter ejection

Hard XFEL imaging *:

Hard x-rays: Transmission studies
Time structure: match use of lasers

* *Parab et al. J. Synchr. Rad 25, 1467-1477 (2018)*

Electrical breakdown

Optical microsocopy

Lichtenberg figures /movies:

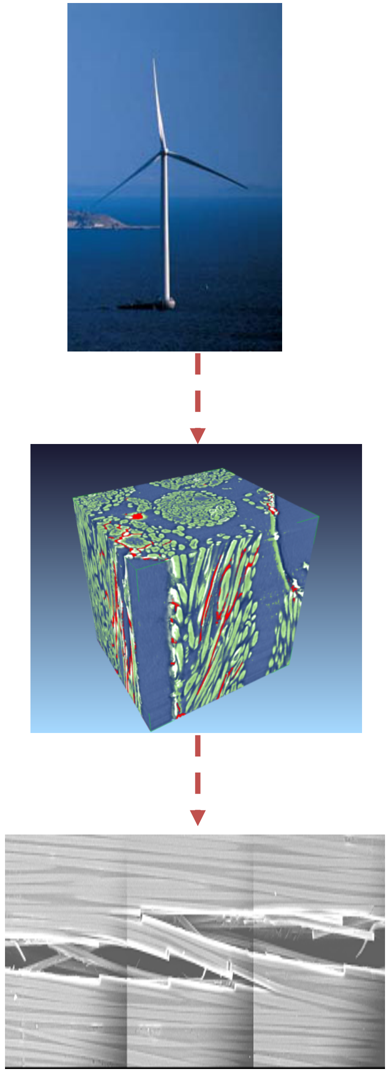
Entire process within ps or ns

Hard XFEL imaging: Partial breakdown in devices

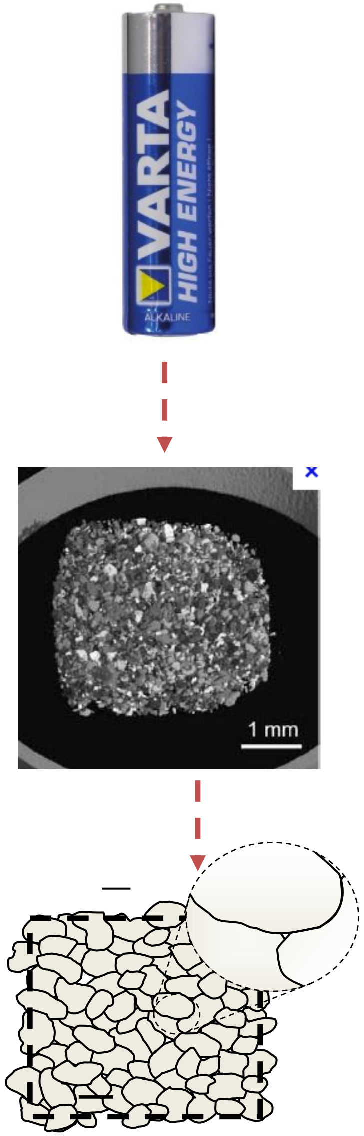
Multiscale reactions
Time resolution of ns to hours

Energy technologies are multiscale

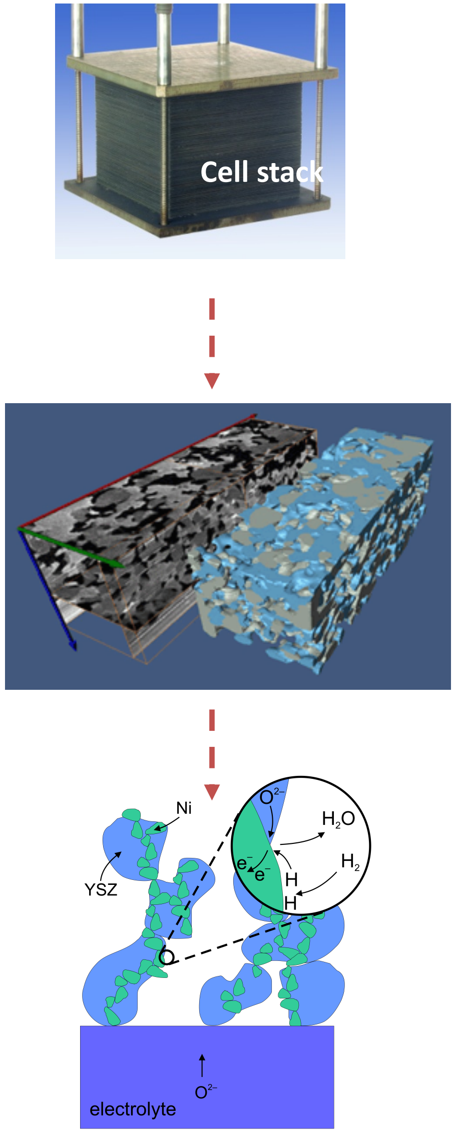
Composites for wind



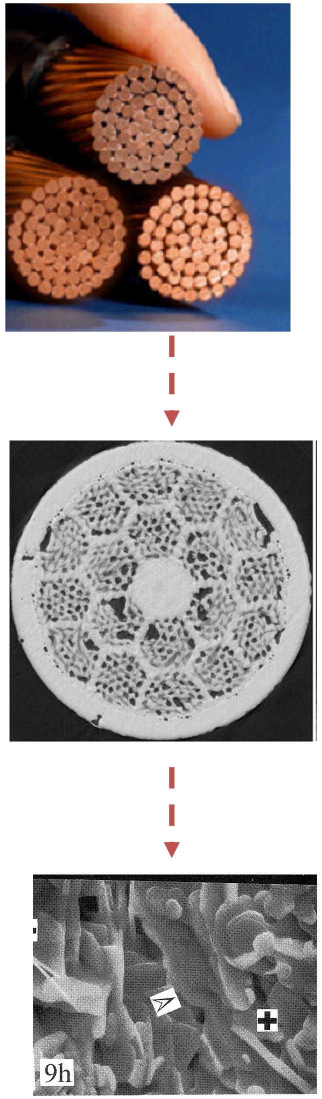
Batteries



Fuel cells



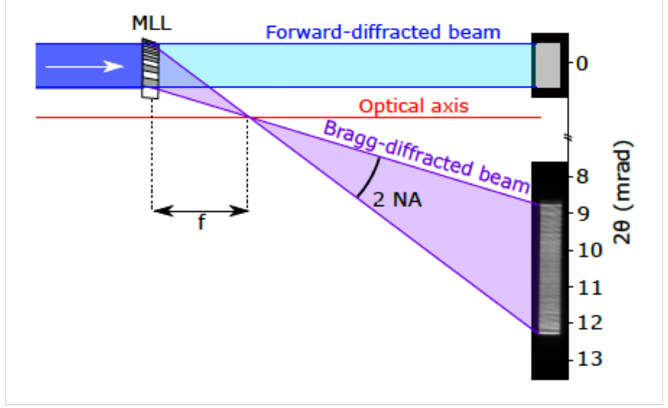
Superconducting cables



Challenges for XFEL work at 70 keV

Optics at 70 keV

Multilayer Laue Lenses:
high NA and efficiency



K.T. Murray *et al.* Multilayer Laue lenses at high X-ray energies: performance and applications. *Opt. Express*, *in print* (2019)

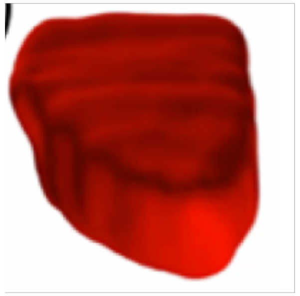
3D information from one image*:

- Diffraction based imaging + line beam => slice
- Compton camera -Confocal microscopy*

*: Ongoing work at DTU

Coherence in bulk specimens and at 70 keV ?

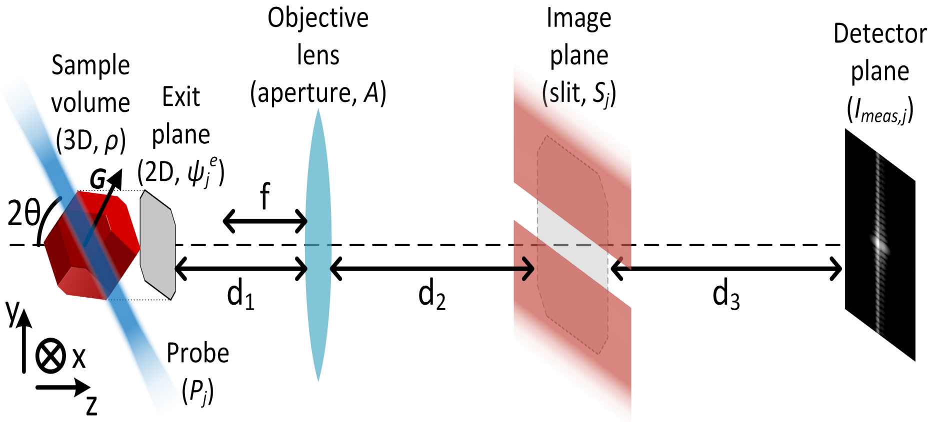
Bragg CDI in the bulk



13 nm resolution

A.F. Pedersen *et al. Opt. Express* **26**, 23411 (2018)
A.F. Pedersen *et al.*, submitted.

Bulk ptychography



A.F. Pedersen *et al.*, work in progress

So far only work at 8-17 keV

The case for 200 keV to 2 MeV

Harmonics + spontaneous emission background

Attenuation

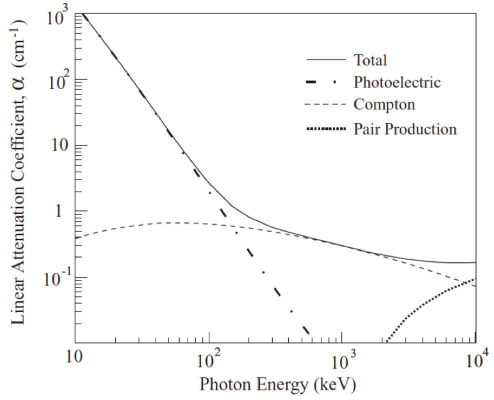
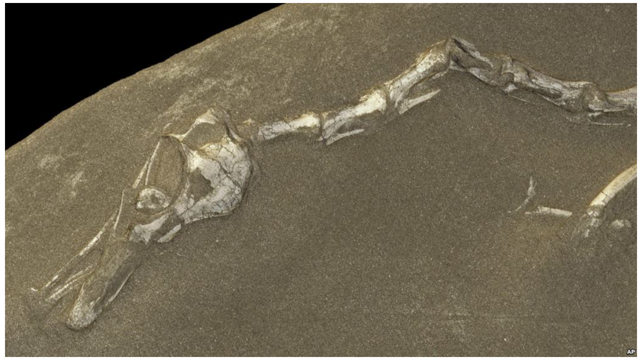


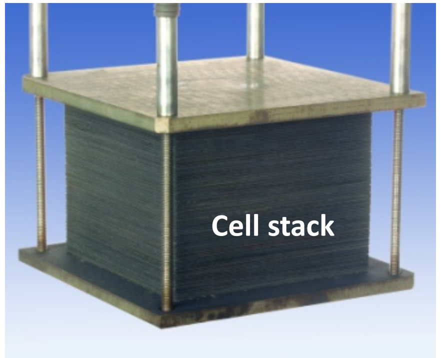
Figure 1. Linear γ-ray attenuation coefficients (proportional to the cross section) for photoelectric, Compton and pair-production interactions in Ge material as a function of γ-ray energy. The total absorption coefficient is also shown.

Compton camera

Applications



Fossils



Energy technology

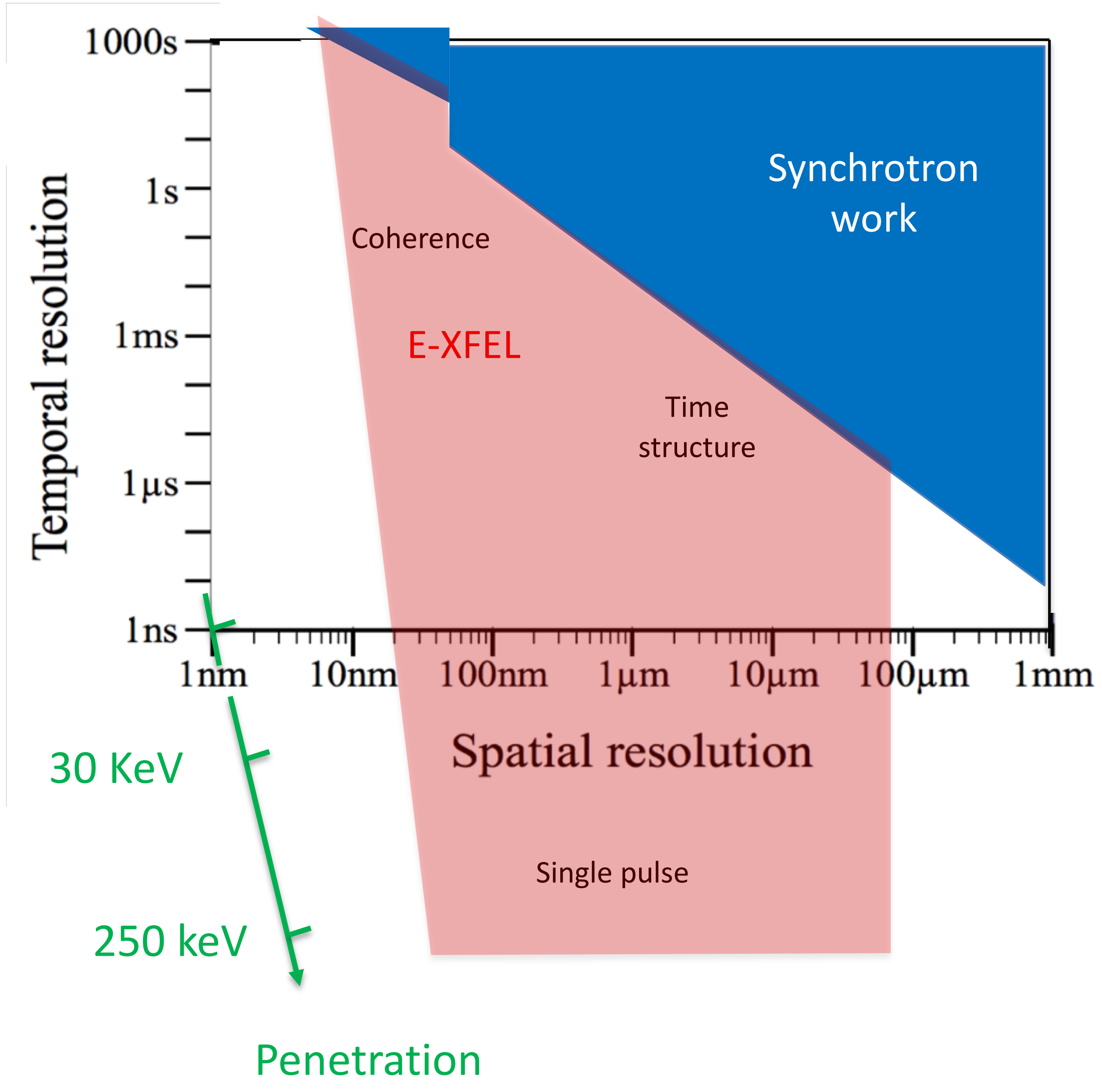
Also: Ewald sphere as in 100 keV TEM

for 3rd harmonic at 70 keV: λ= 0.05 Å.

Positron microscopy

Flux orders of magnitude higher than elsewhere on planet.

Case for a hard x-ray E-XFEL microscope



- Local studies on real life samples with high spatial and temporal resolution
- Repeated measurements with realistic sample environments
- Multimodal (imaging, diffraction, …) and multiscale