MAX IV SAC

2.7.3

An Imaging Beamline Supporting Materials Science for Sustainability

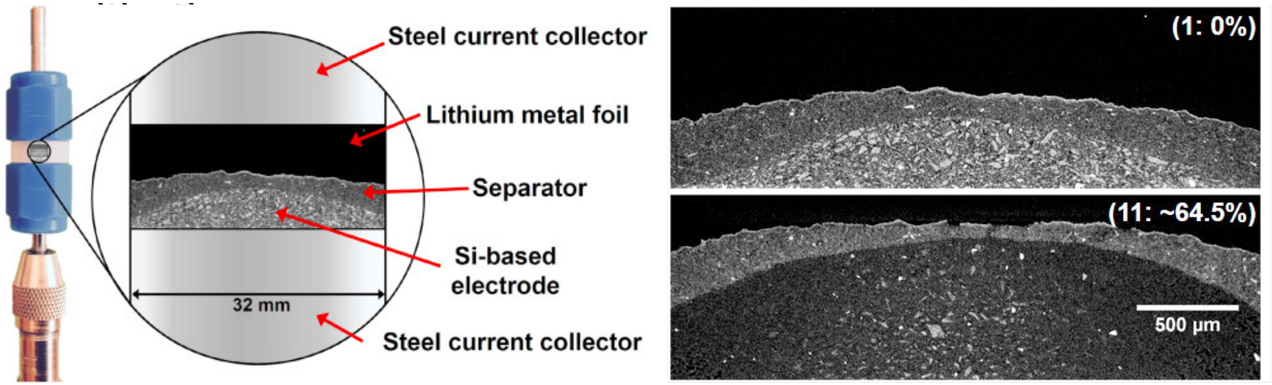
With input from the GTiMAX Expression of Interest

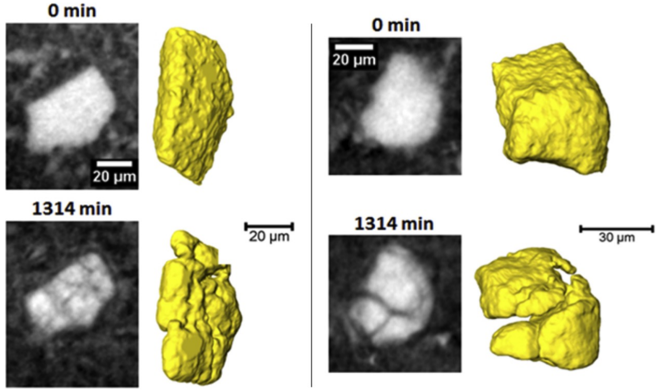
MAX IV

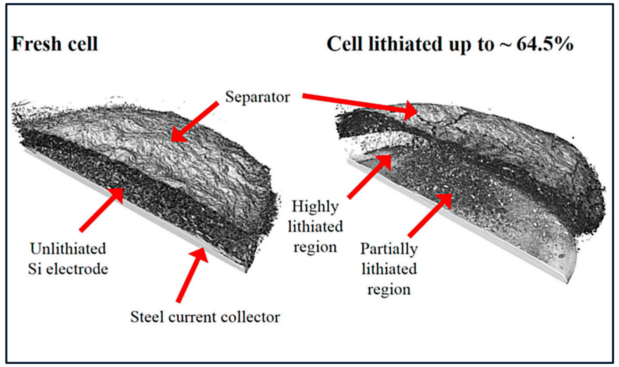
Scientific Background

Battery materials:

- Understanding processes that occur during charge/discharge cycles
- Follow microstructure evolution *in situ* to study, e.g., degradation/failure mechanisms, and to assess strategies for their



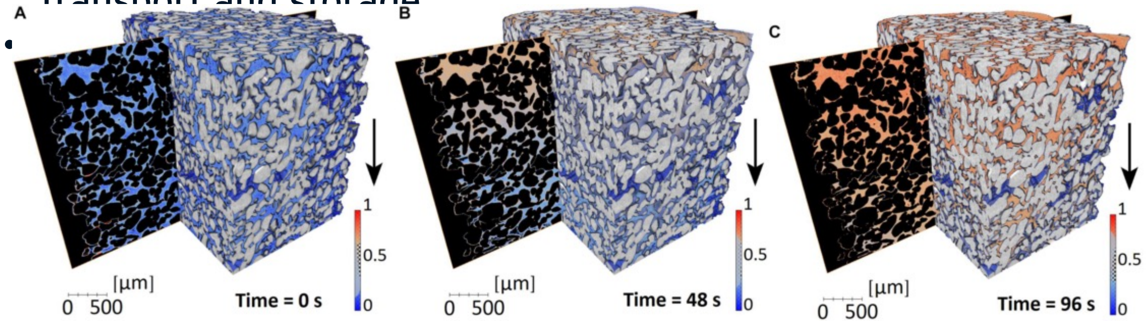




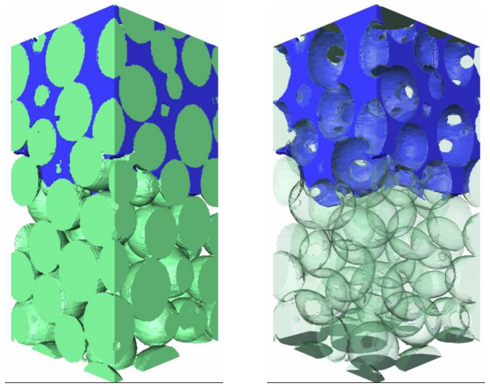
Tomography reconstructions showing microstructure evolution (right) and particle cracking (bottom left) in Si-based electrodes during lithiation (Paz-Garcia *et al.*, J. Power Sources, 2016)

Porous media:

- Understanding the structure–fluid transport–performance relationship, for more efficient, structured, porous materials for, e.g., catalysis
- Characterisation of hierarchical pore morphologies and 3D networks in, e.g., soil sediments and rocks for pollutant transport and storage



Above: 4D tomography time series showing solute transport at the pore scale, with lower (blue) to higher (red) concentrations
(F. Marone *et al.*, Front. Earth Sci., 2020)

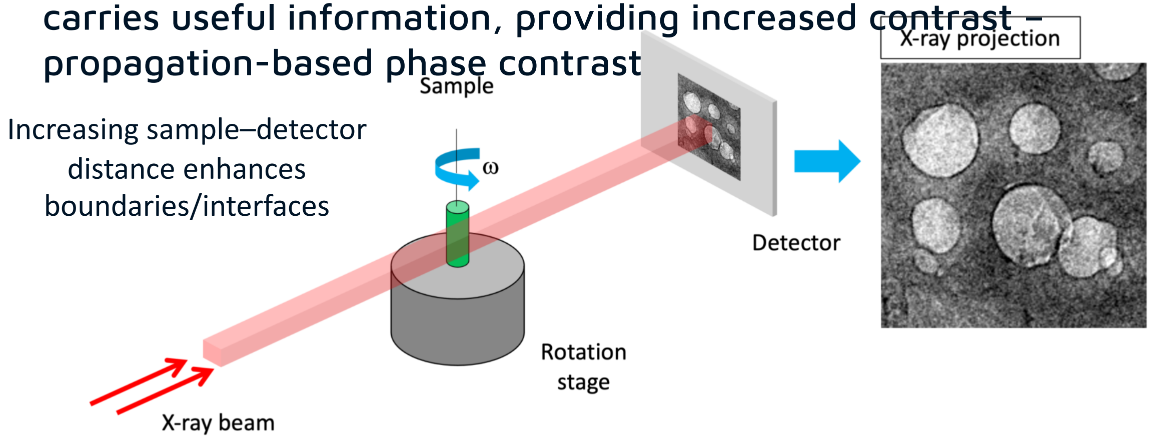


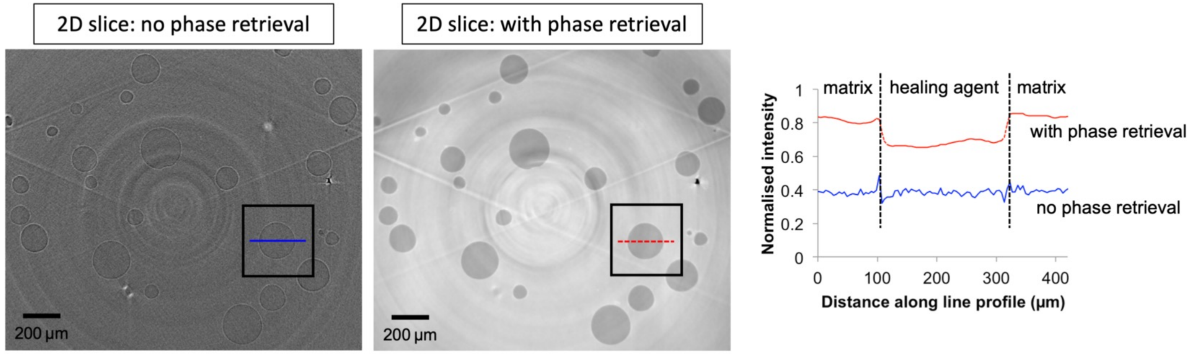
Left: Time series of tomography reconstructions tracking the movement of water through a porous bead pack.
Tomography acquisition rate: ~1 s^{-1}

Scientific Background

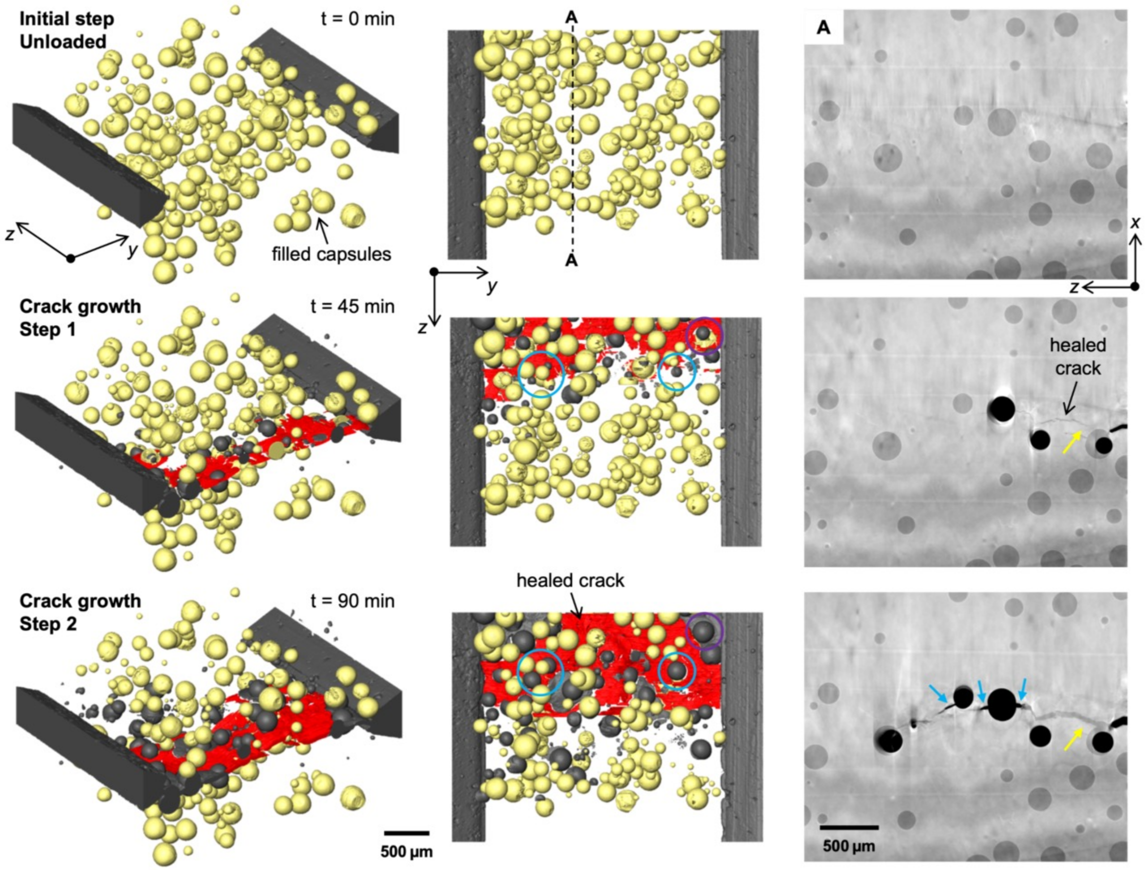
Phase contrast tomography:

- Many multi-material samples, e.g., composites, have weak absorption contrast between components due to similar X-ray attenuation
- Phase shift (scattered photons), e.g., at boundaries/interfaces, carries useful information, providing increased contrast – propagation-based phase contrast





Phase retrieval increases contrast between phases, enabling their segmentation (see right)

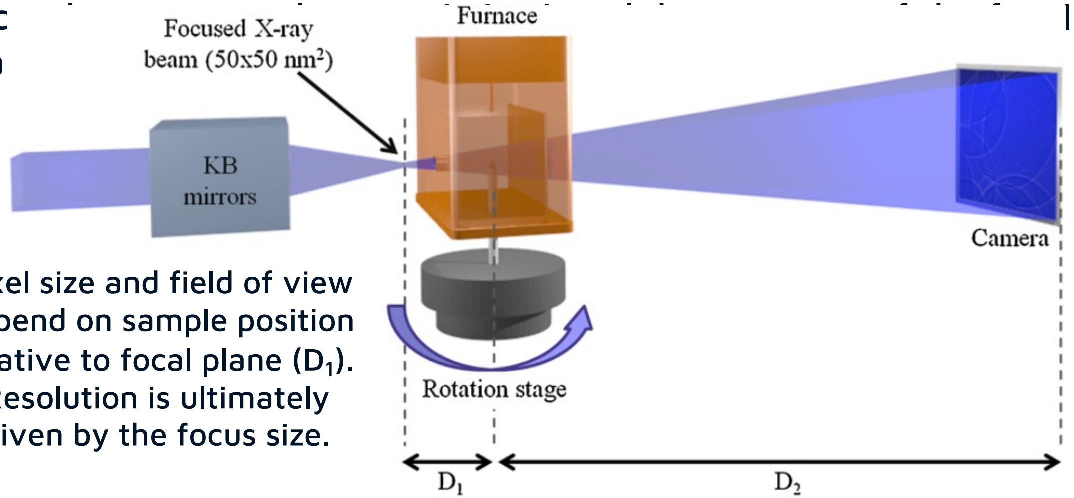


Showing crack healing in a polymer containing embedded microcapsules. When the microcapsules are ruptured by a growing crack, they release a polymerising agent into the crack plane, bonding (healing) the crack surfaces together.

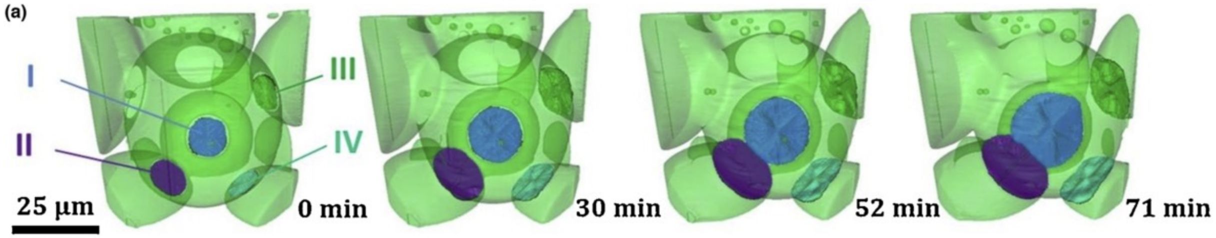
Scientific Background

Nanotomography (full-field):

- Understanding the physical mechanisms involved during, e.g., materials processing such as sintering, can require nanoscale 3D characterisation
- Can be achieved by focusing the X-ray beam and creating a sec
pla



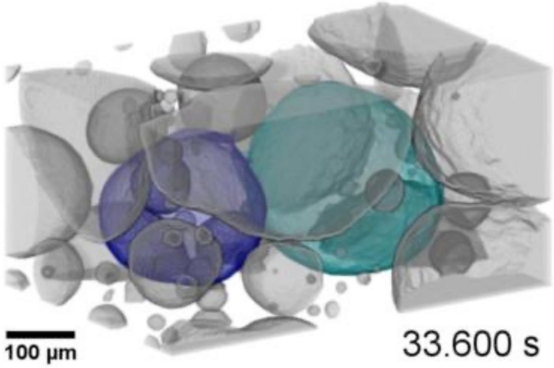
Pixel size and field of view depend on sample position relative to focal plane (D_1). Resolution is ultimately given by the focus size.



Schematic layout of an *in situ* 4D nano-imaging setup (ID16B, ESRF), used to study sintering of glass particles at 670°C and enabling neck growth (labelled I, II, III, IV) and curvature to be captured and followed with 100 nm pixel size (J. Villanova *et al.*, Materials Today 2017)

High-speed tomography:

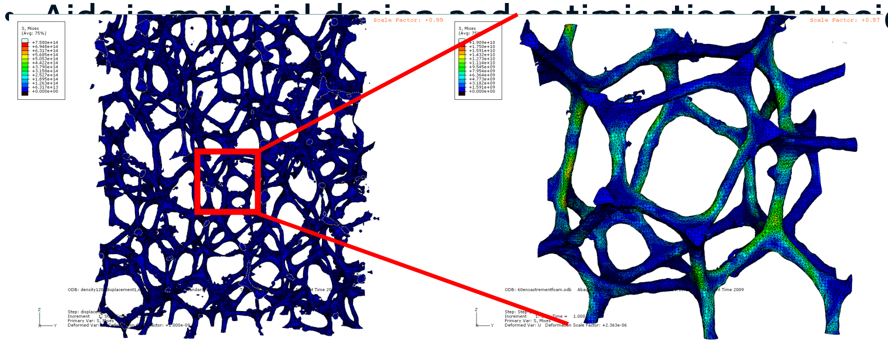
- Following *in-situ* processes with high temporal resolution, e.g., > 1 Hz
- Factors include, a high flux X-ray beam, high-speed cameras (kHz,



Time series of tomography reconstructions tracking bubble formation during aluminium foam development.
Tomography acquisition rate: ~1000 s^{-1}
(F. Garcia-Moreno *et al.*, Adv. Mater. 2021)

Multi-scale image-based modelling:

- Tomography provides structural information as input to material modelling
- Allows to simulate real, often complex 3D structures of interest
- Aids in material design and optimisation strategies



Finite element models generated from 3D images of a foam sample, to predict failure mechanisms under tensile load

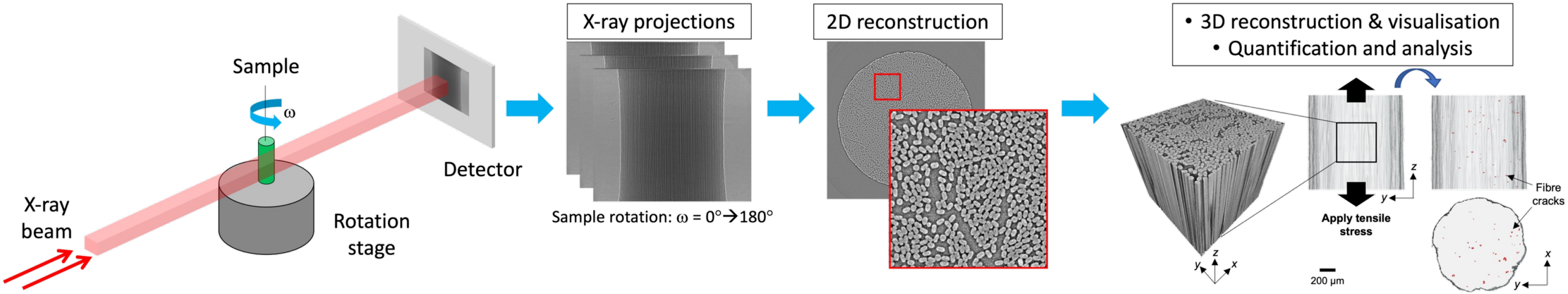
Beamline Overview

Beamline Parameters

- Energy range: 15–45+ keV
- Beam size at the sample position: ~1.5 mm
  - ~10 mm using beam expanding optics
- Spatial resolution: 100 nm–5 µm

Techniques

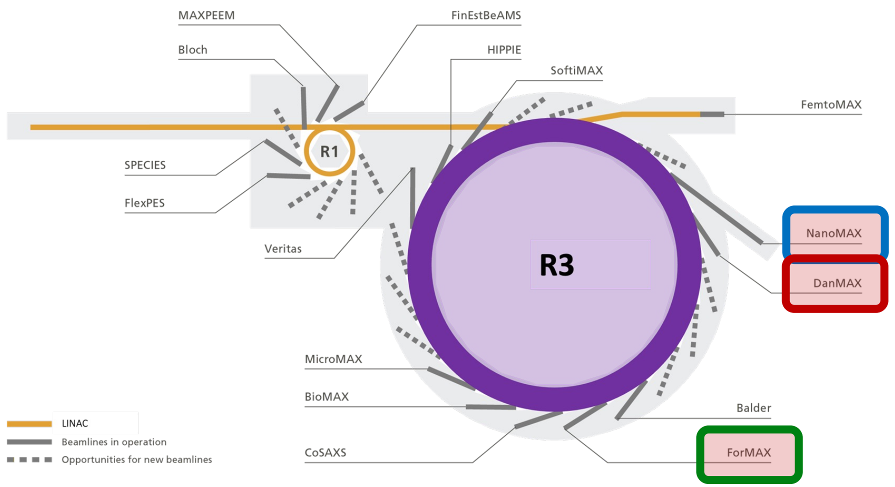
- X-ray microtomography (1–5 µm spatial resolution)
  - Absorption and phase contrast imaging
- Nanotomography (~100 nm spatial resolution)
- High-speed tomography for *in situ* imaging of dynamic processes
  - 20 Hz tomography acquisition rate



Illustrating the principal steps of the tomography pipeline.
The sample is a long fibre metal matrix composite, quantifying fibre cracks when subjected to a tensile stress.

Beamline in the MAX IV Portfolio

Beamlines at MAX IV providing full-field tomography



Proposed full-field tomography beamline

- Dedicated focus on tomography:
  - Absorption and phase contrast tomography
  - High-speed tomography (20 tomo/sec)
- Extended range of energies: 10–45+ keV (possibly up to 60 keV)
  - Increased penetration depth
  - Investigate higher Z materials
- Beam size: ~10 mm (using beam expanding optics)
  - Investigate larger, often more relevant, sample sizes
- 3D spatial resolution:
  - 1 μm–5 μm with standard microtomography
  - ~100 nm with nanotomography (using focussing optics)

ForMAX

- Energy range: 8–25 keV
- 3D spatial resolution: 1 μm–5 μm
- Other techniques: SWAXS, SWAXS imaging
- Focus on wood-based materials

DanMAX

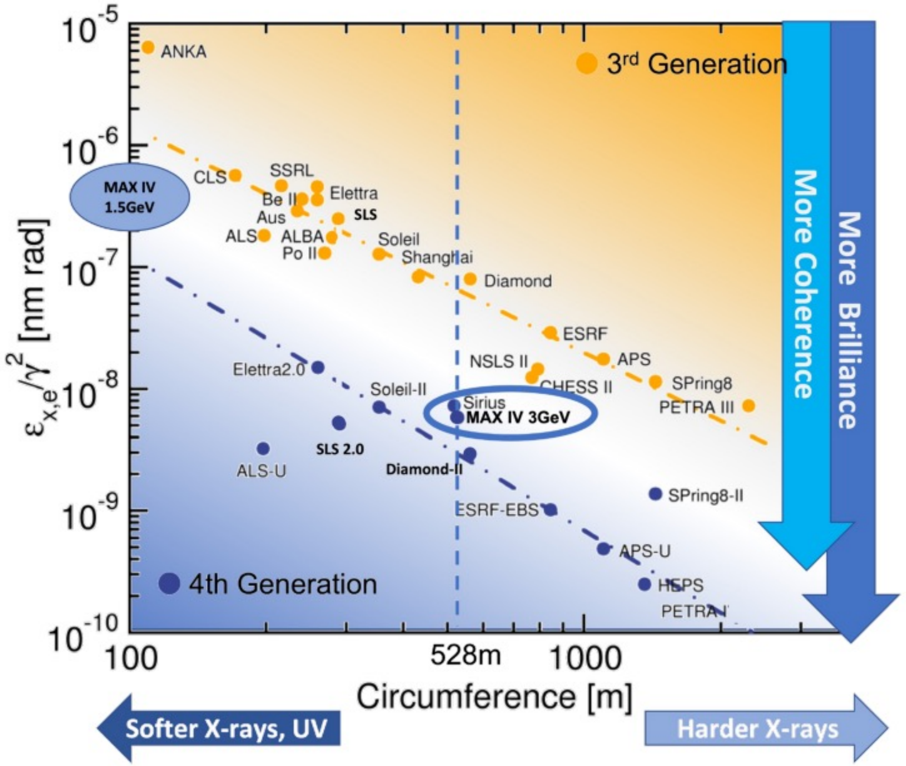
- Energy range: 15–35 keV
- 3D spatial resolution: 1 μm–5 μm (initially)
- Other techniques: Powder X-ray diffraction
- Materials Science

NanoMAX

- Energy range: 5–28 keV
- Spatial resolution (full-field): ~50 nm
- Other techniques: Ptychography, scanning X-ray diffraction imaging

Strategic Relevance

- Development and deployment of new materials requires dynamic imaging techniques to capture microstructure evolution during operational conditions
- 4^{th} generation synchrotrons offer unprecedented coherent flux, enabling high-resolution 4D imaging
- MAX IV lacks a dedicated full-field tomography beamline optimized for high-speed imaging
- Opportunity to take a leading role among medium-energy storage rings in developing tomographic imaging
- Development of energy materials:
  - e.g., microstructure evolution during battery charge/discharge
- Tackling environmental challenges:
  - e.g., fluid transport through pore networks, pollutant storage



"MAX IV has transformational opportunities to capitalize on the advances of modern spectro-micro-tomography techniques and further exploit the small emittance of our 3 GeV storage ring."
-MAX IV Strategic Plan 2023-2032

Comparison to Existing Beamlines (in Europe)

**Has a beamline that also provides full-field tomography in addition to powder diffraction techniques

I13
Diamond
8-30 keV
1 µm / 150 nm res.
****I12** (50-150 keV)

ANATOMIX
Soleil
5-25 keV
1 µm / 80 nm res.
****PSICHE** (15-50 keV)

???
MAX IV
10-45+ keV
1 µm / 100 nm res.

P05
PETRA III
5-50 keV
1 µm / 100 nm res.

ID19
ESRF
10-120 keV
1 µm res.

TOMCAT
Swiss Light Source
8-45 keV
1 µm / 100 nm res.

Also, at ESRF:
BM18
(hierarchical phase contrast tomography),
ID16
(nanotomography)