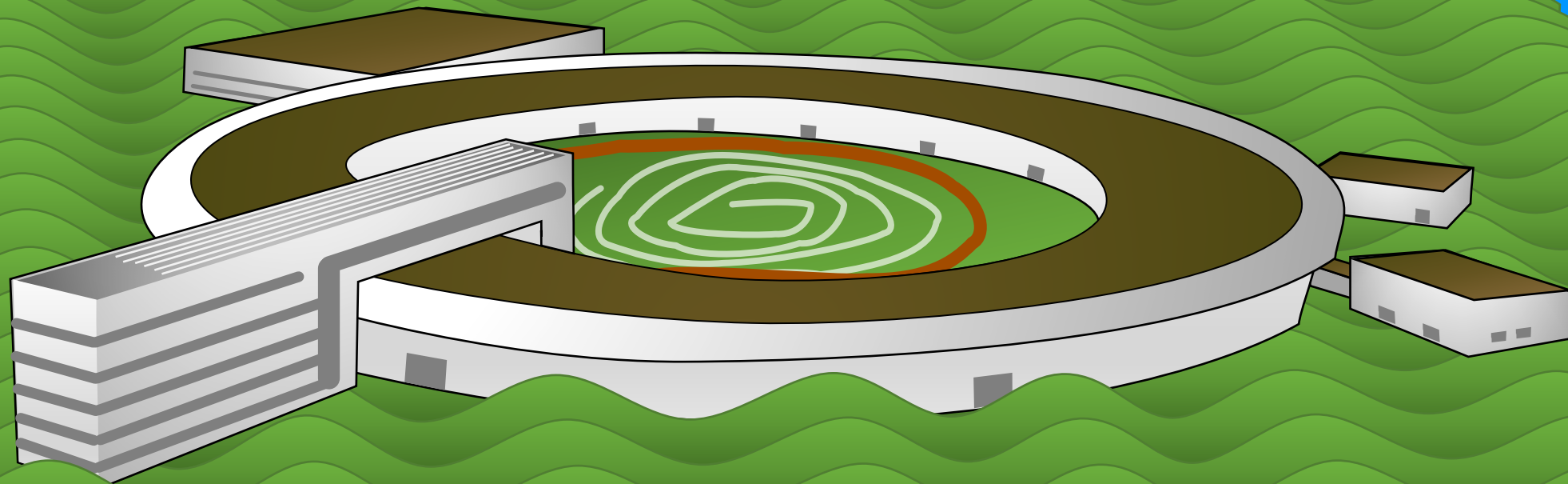


Opportunities for ML analysis and visualization at DanMAX

Mads Ry Jørgensen
mads@chem.au.dk
Innokenty Kantor
inkan@fysik.dtu.dk



Ministry of Higher Education
and Science



Region
Hovedstaden

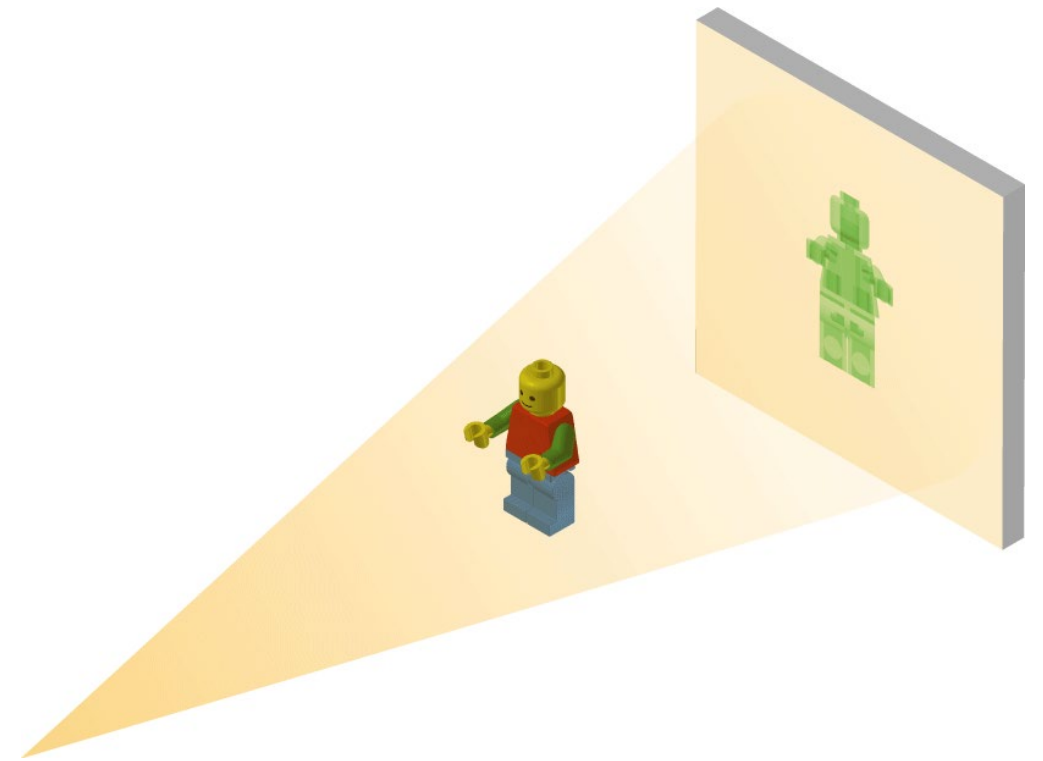
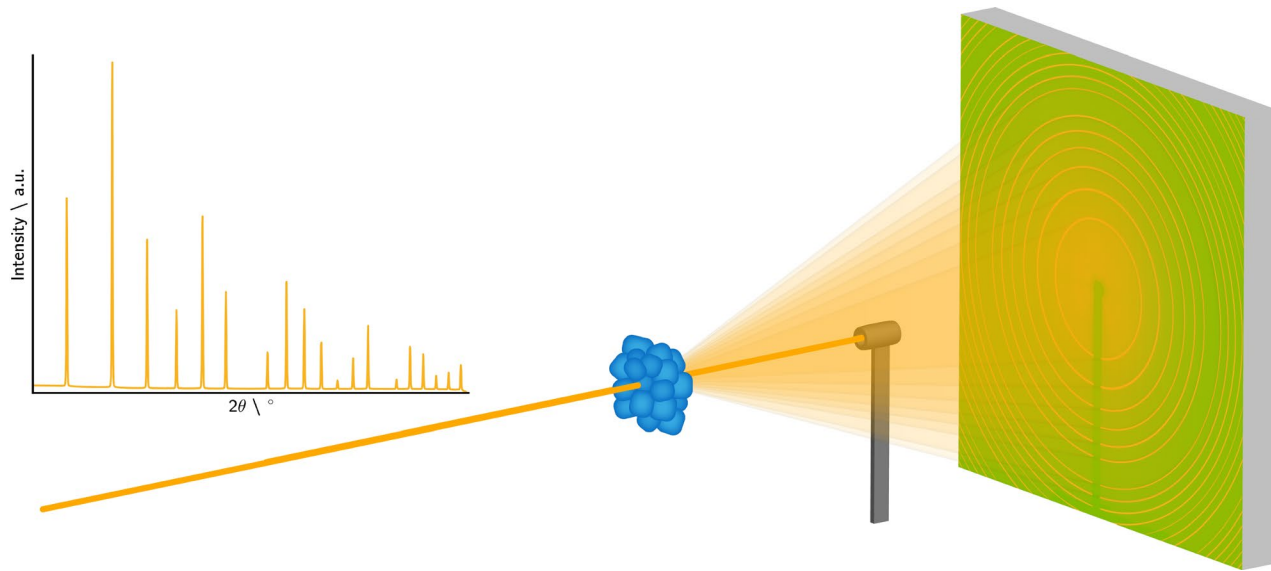


regionmidtjylland

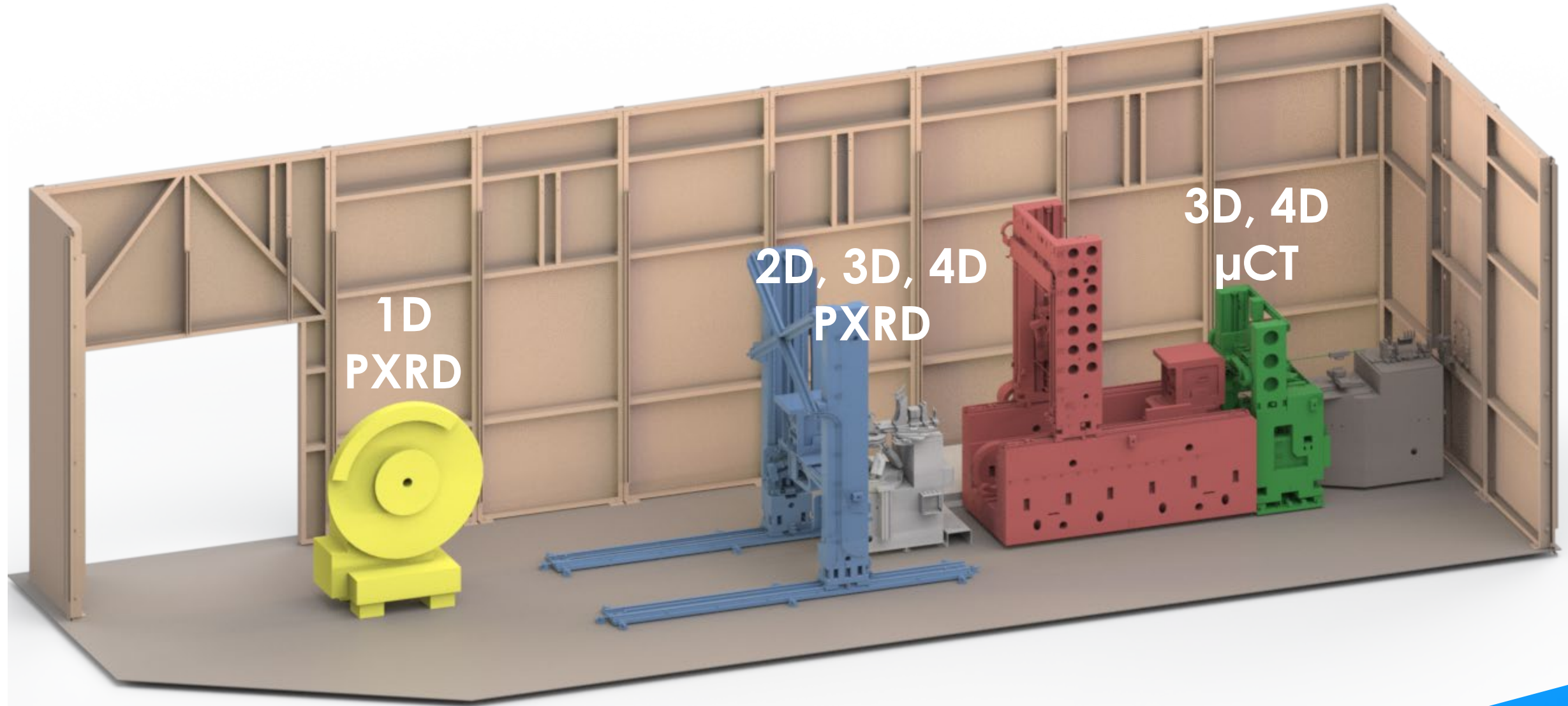


AARHUS
UNIVERSITY





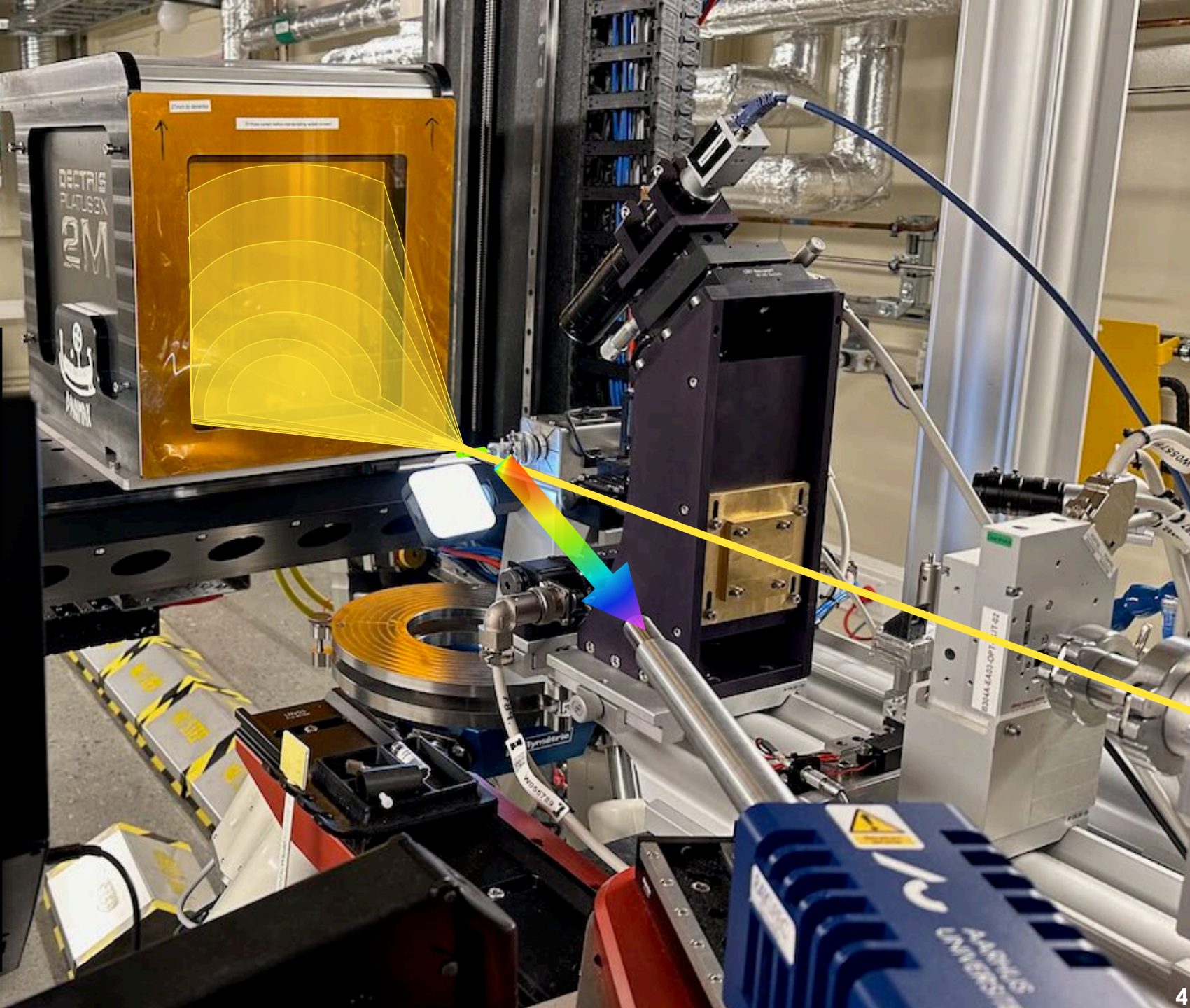
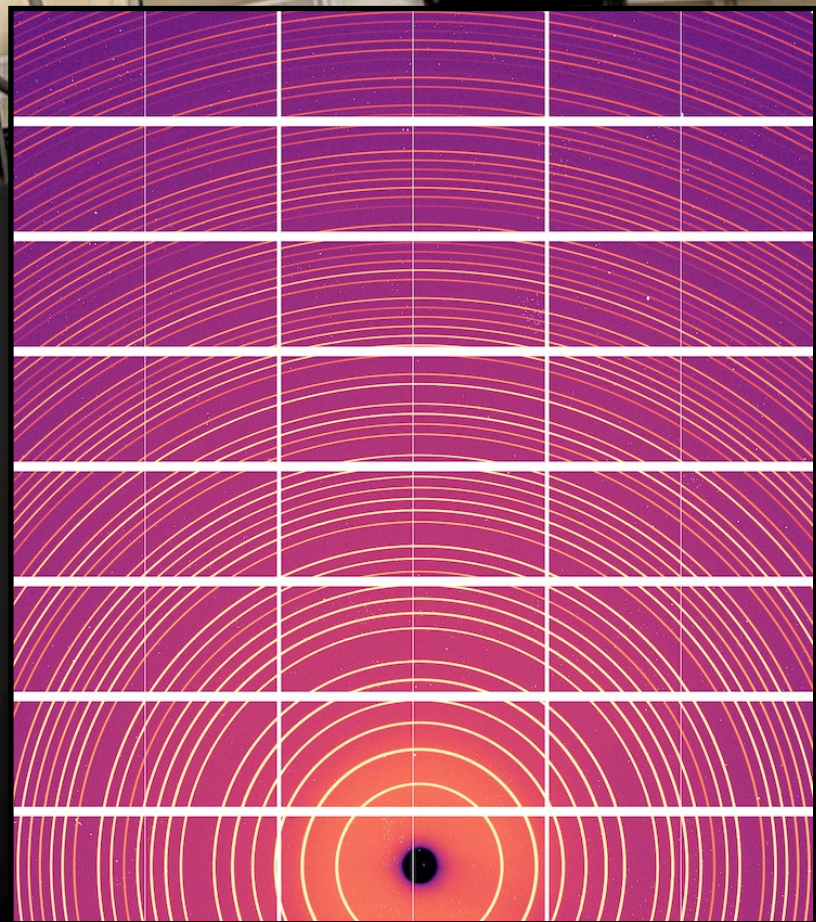
DanMAX: Real materials studied under realistic conditions at realistic time scales



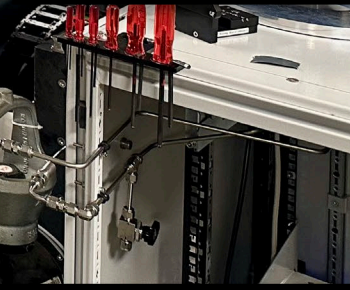
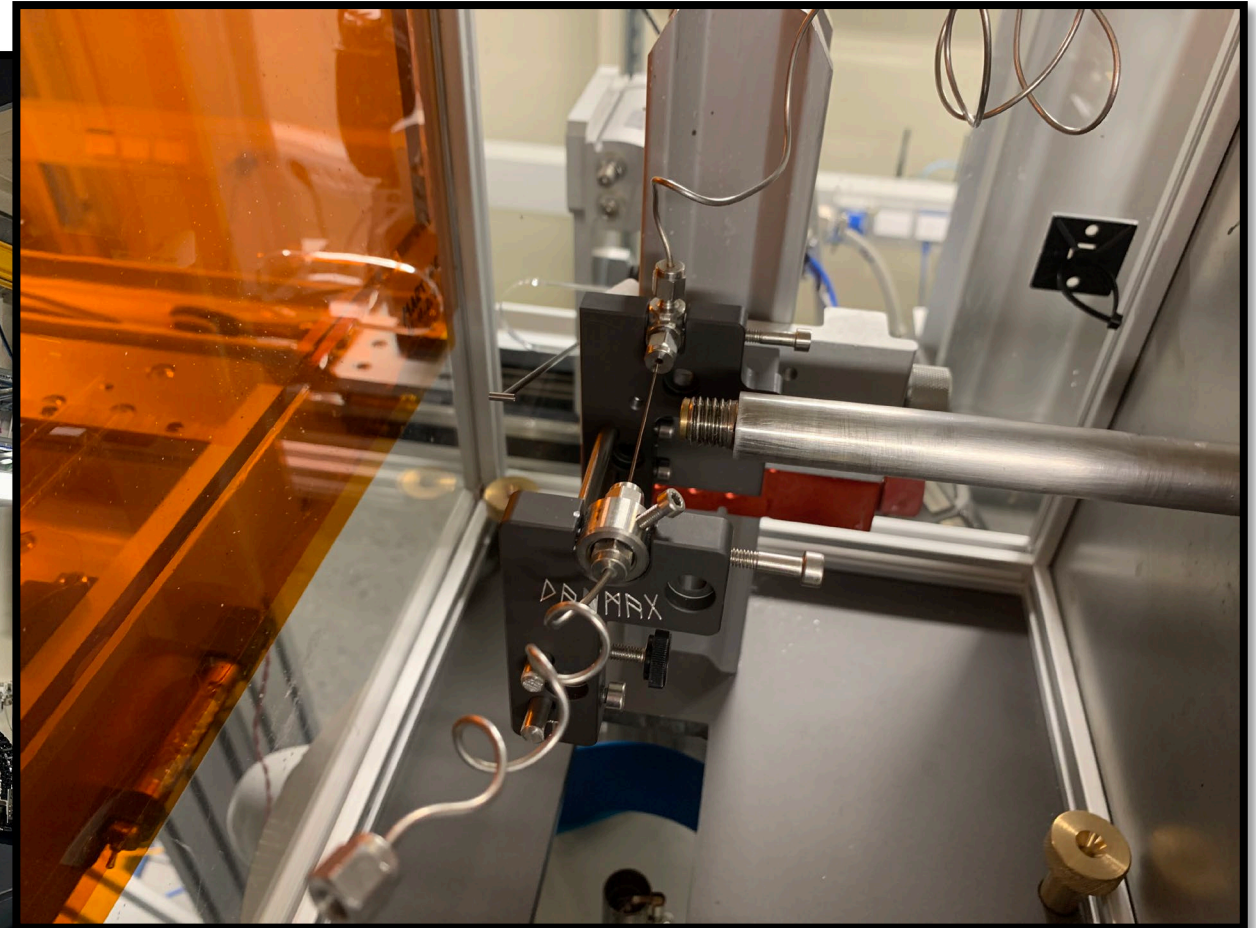
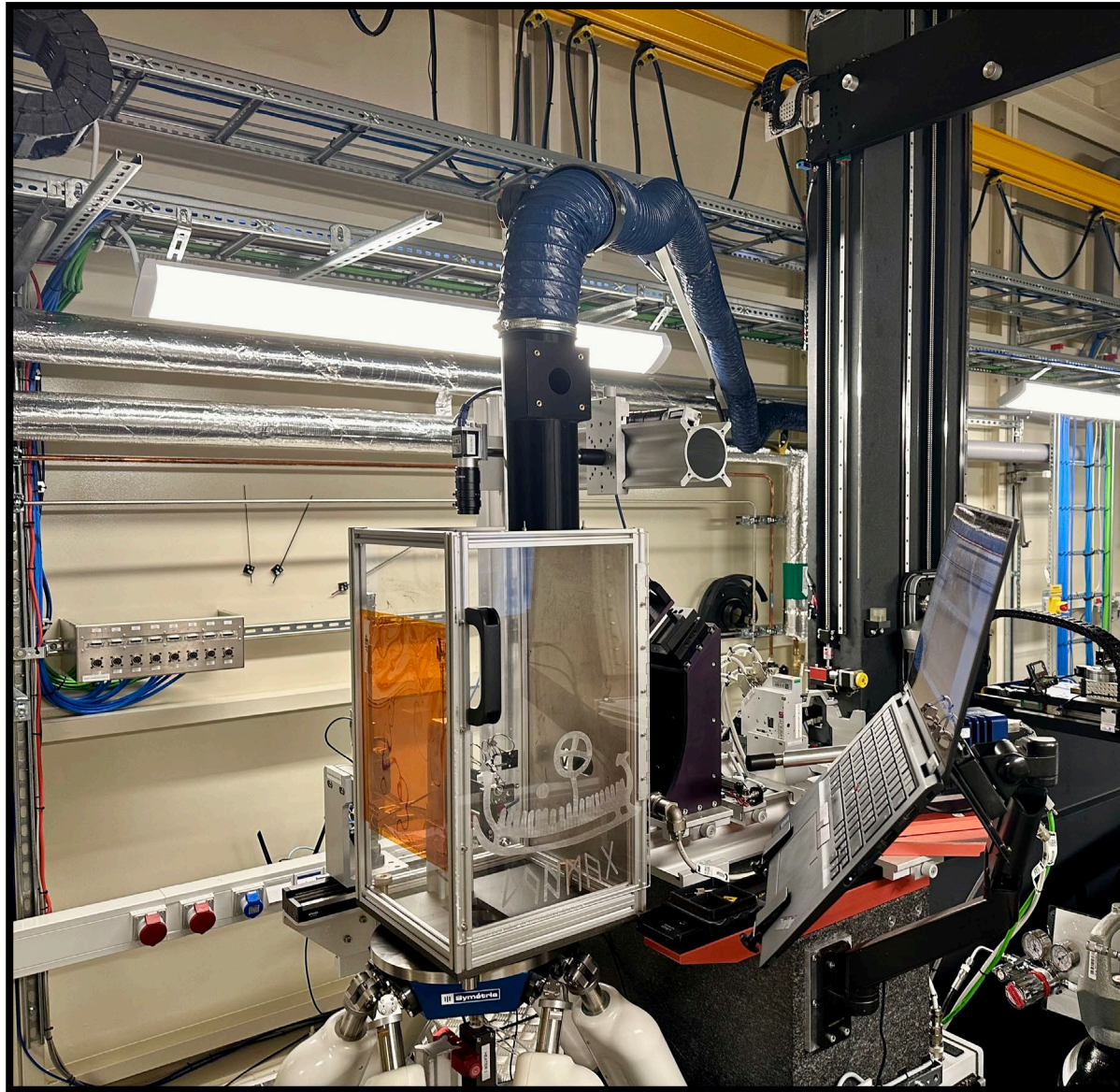
1D
PXR

2D, 3D, 4D
PXR

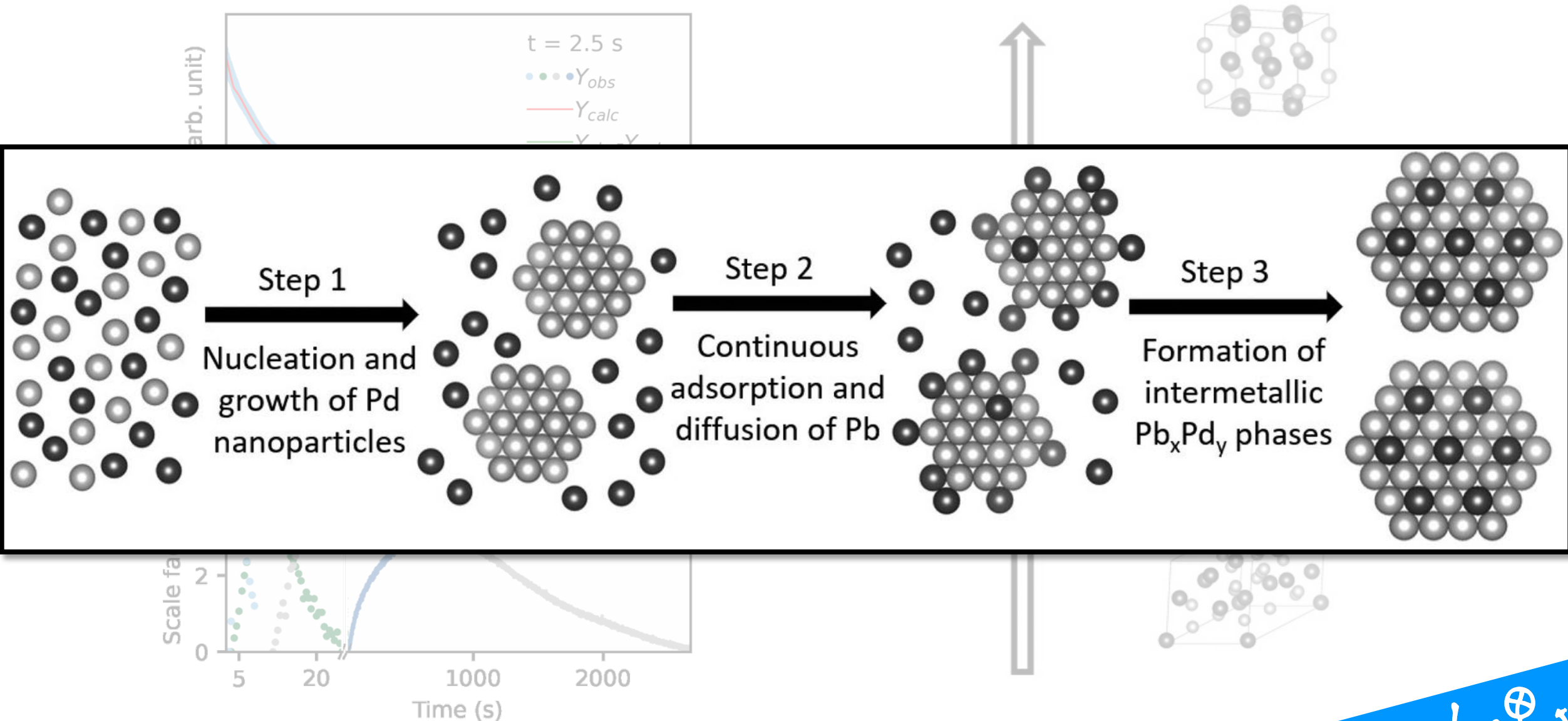
3D, 4D
μCT



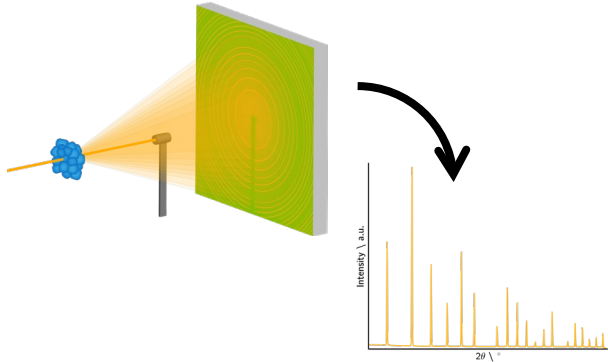
Solvothermal reactor



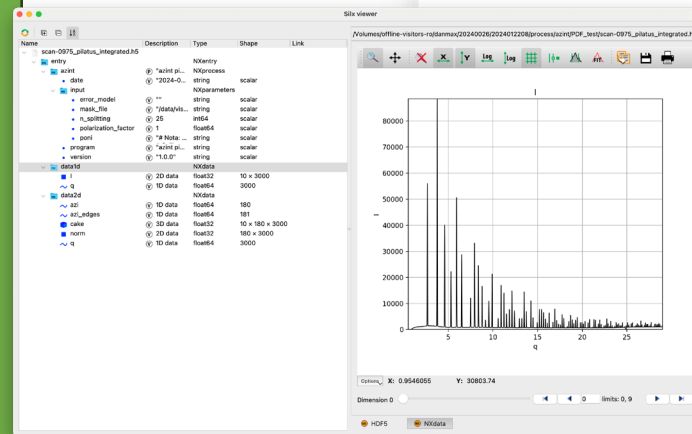
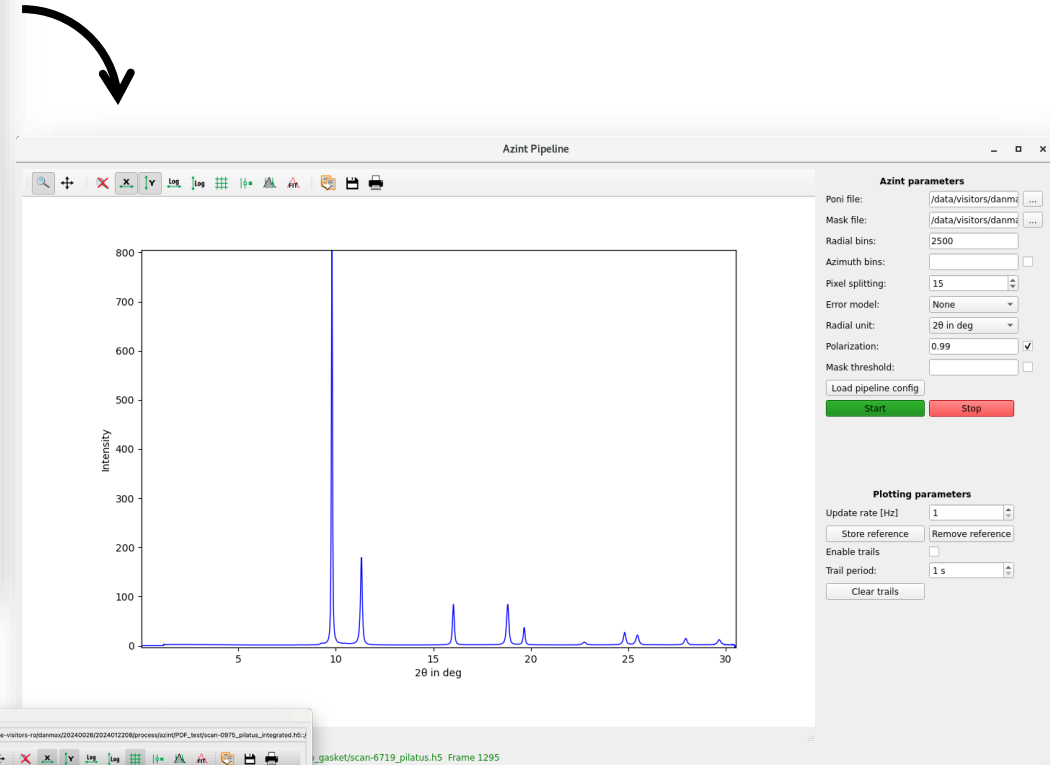
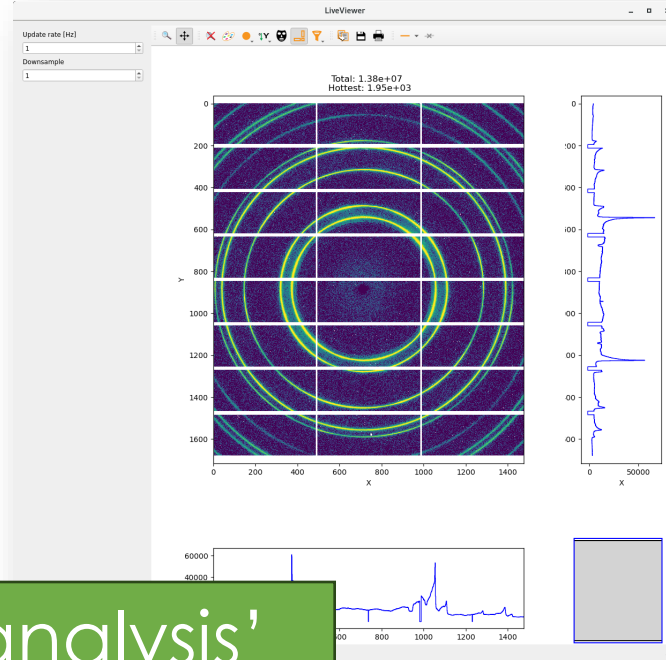
Investigating the formation of PbPd



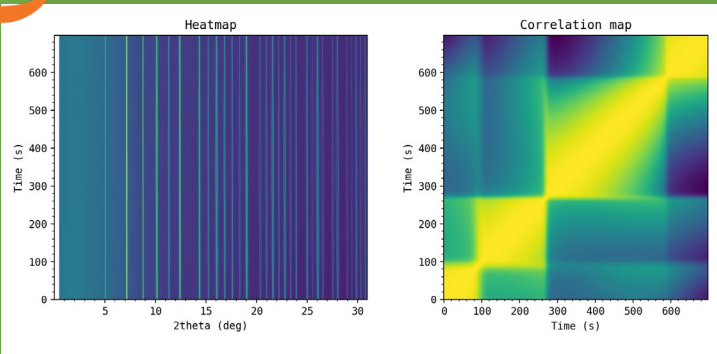
Live azimuthal integration - and quick analysis



Live integration (> kHz)
with live update using the
MATRFAIA* algorithm

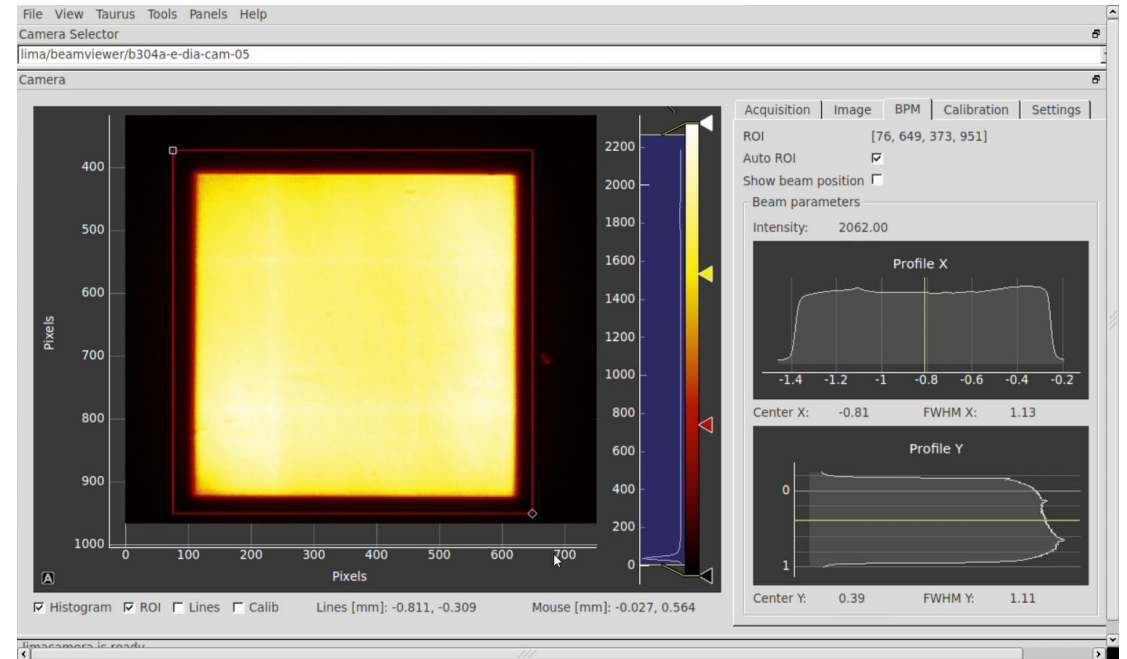
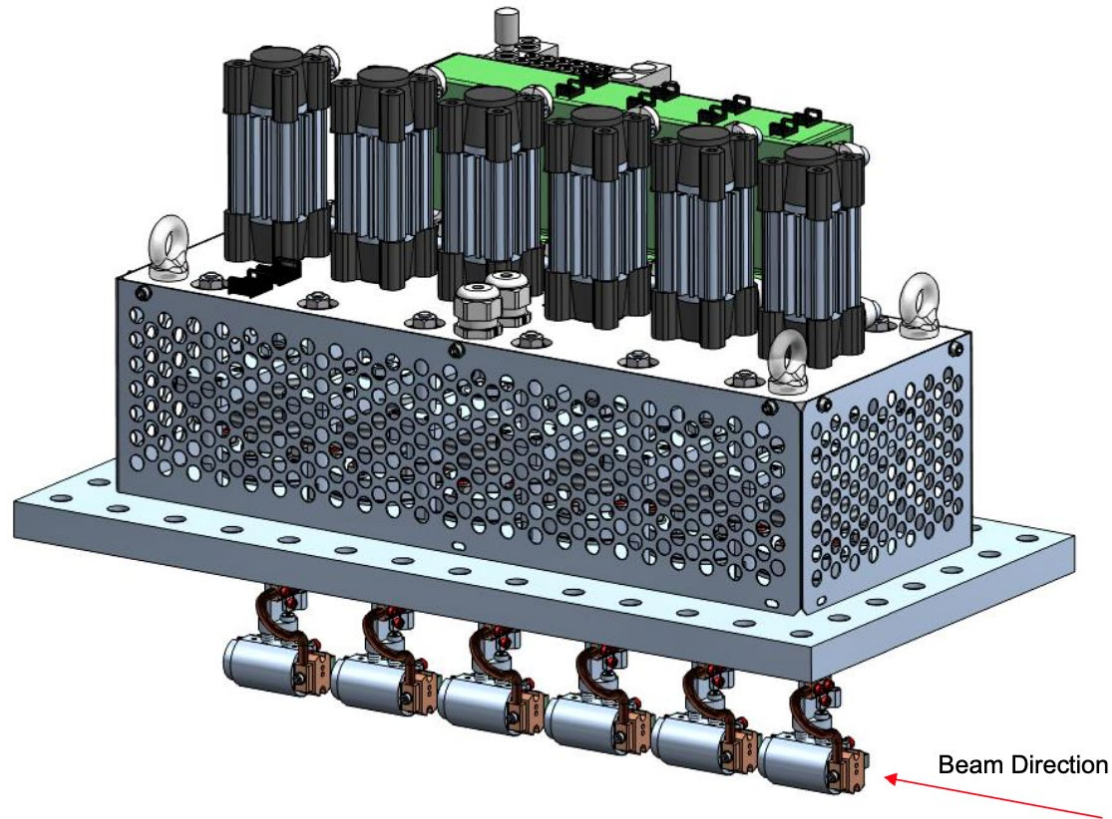


ML potential? 'Live analysis'

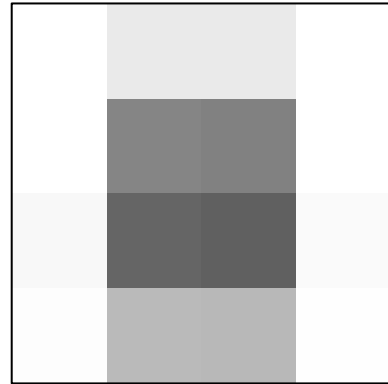


*A. Jensen *et al.*, J. Synchrotron Rad., 2022, **29**, 1420-1428

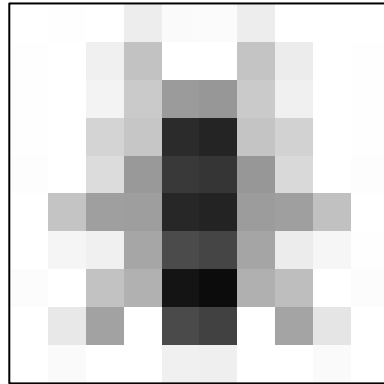
Beam focusing - imaging using μ XRD and μ XRF



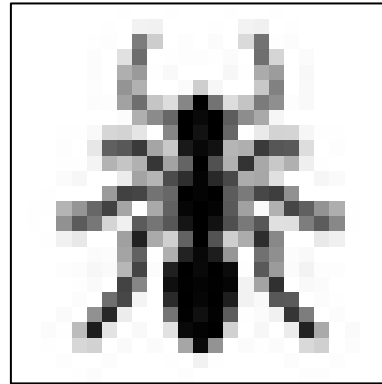
μ XRD (and μ XRF) mapping



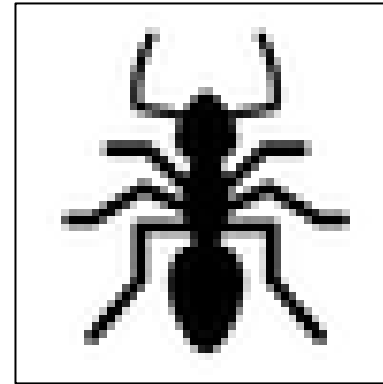
4 x 4 px



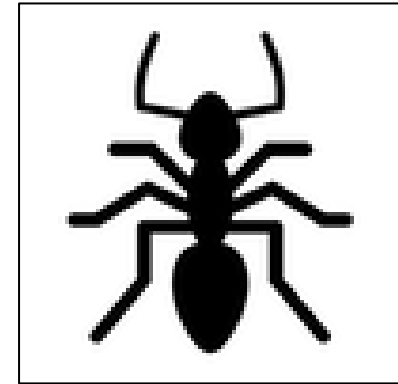
10 x 10 px



25 x 25 px

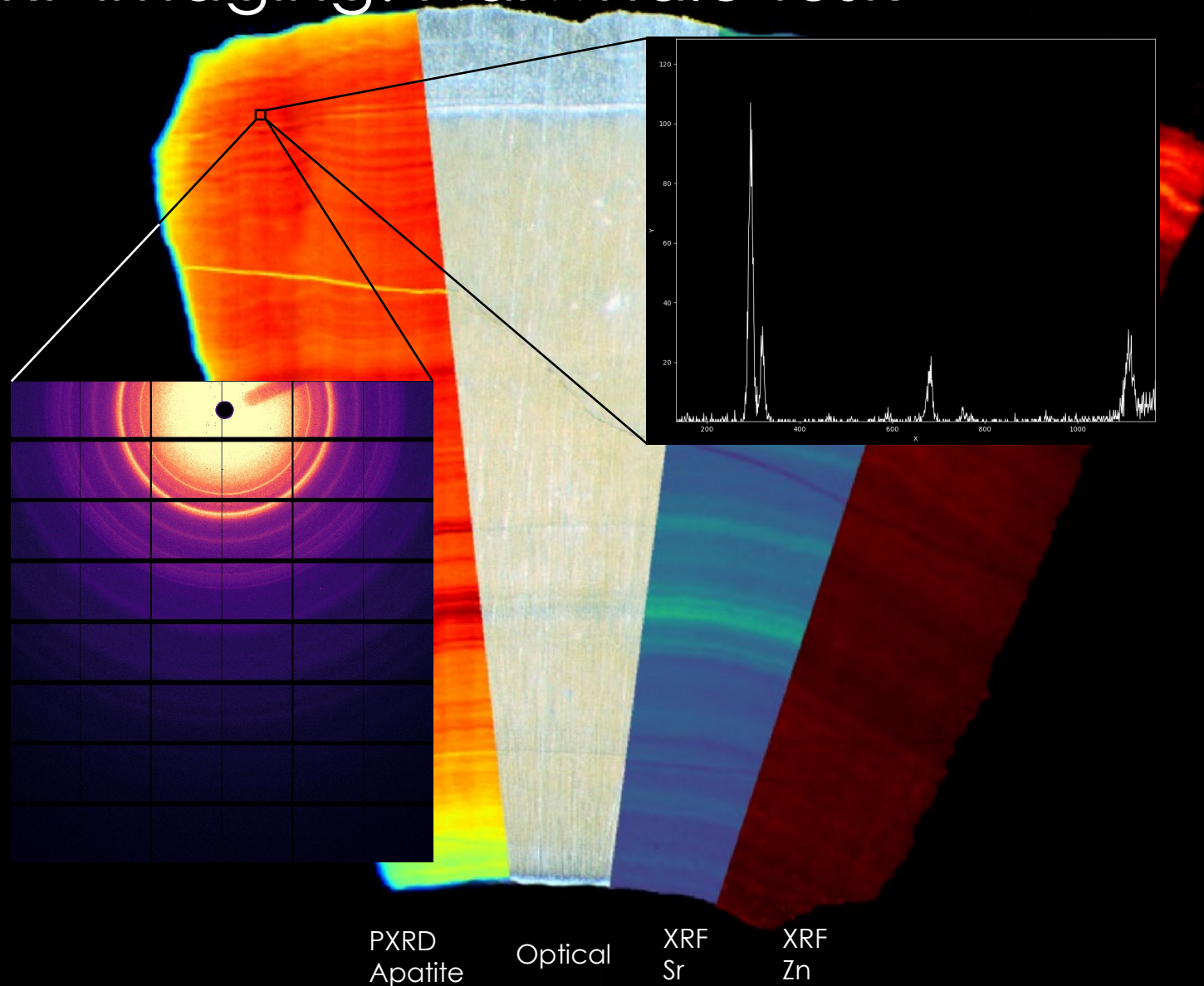


50 x 50 px



100 x 100 px

μ XRD + μ XRF imaging: Narwhale tusk



PXRd
Apatite

Optical

XRF
Sr

XRF
Zn

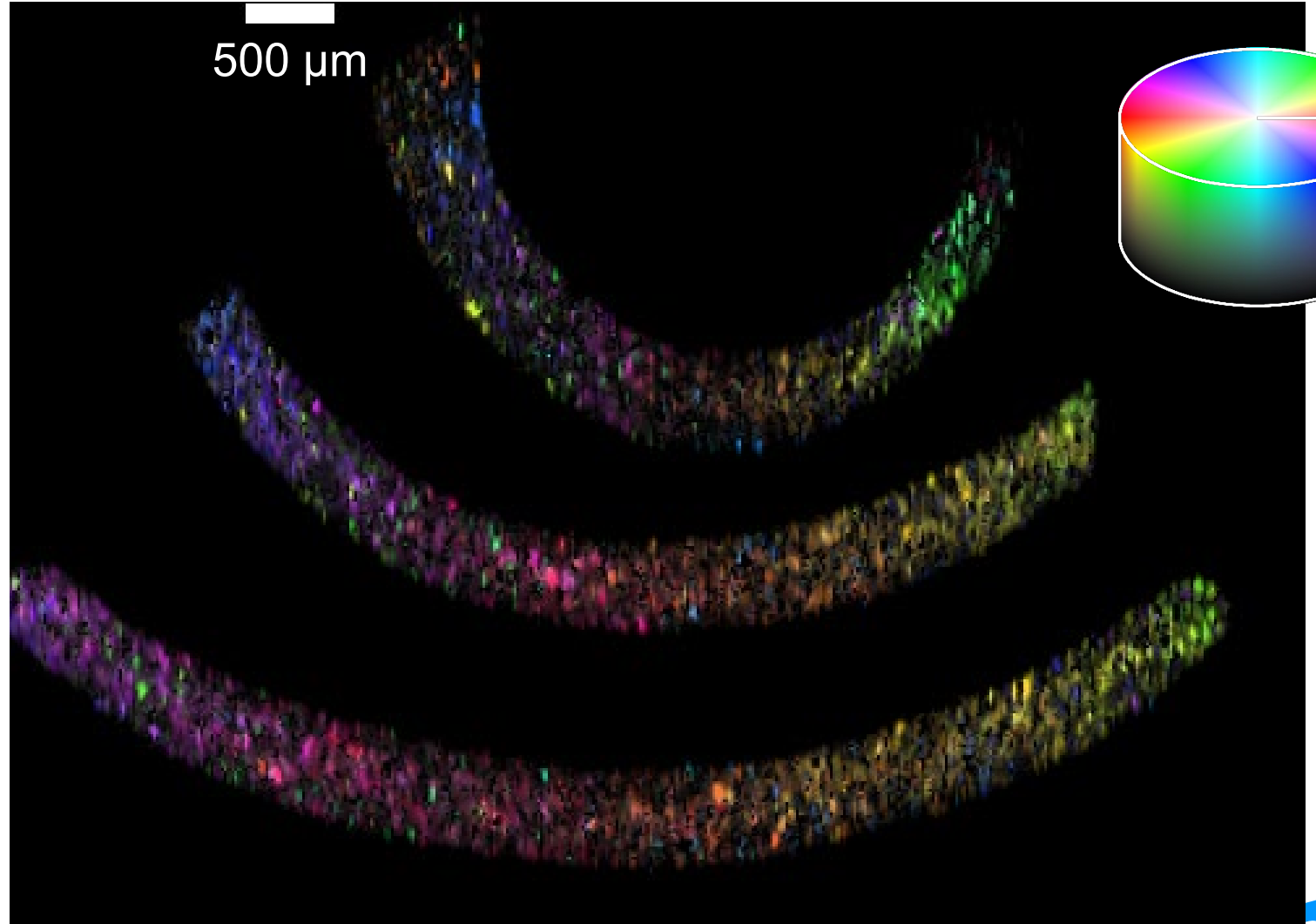
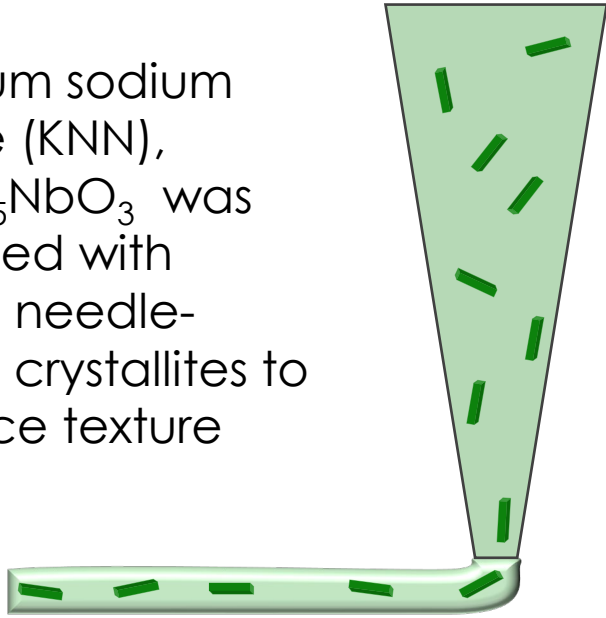


1 mm

~20 μ m beam
10 μ m step

3D-printing with template crystallites

Potassium sodium niobate (KNN), $K_{0.5}Na_{0.5}NbO_3$ was 3D printed with aligned needle-shaped crystallites to introduce texture

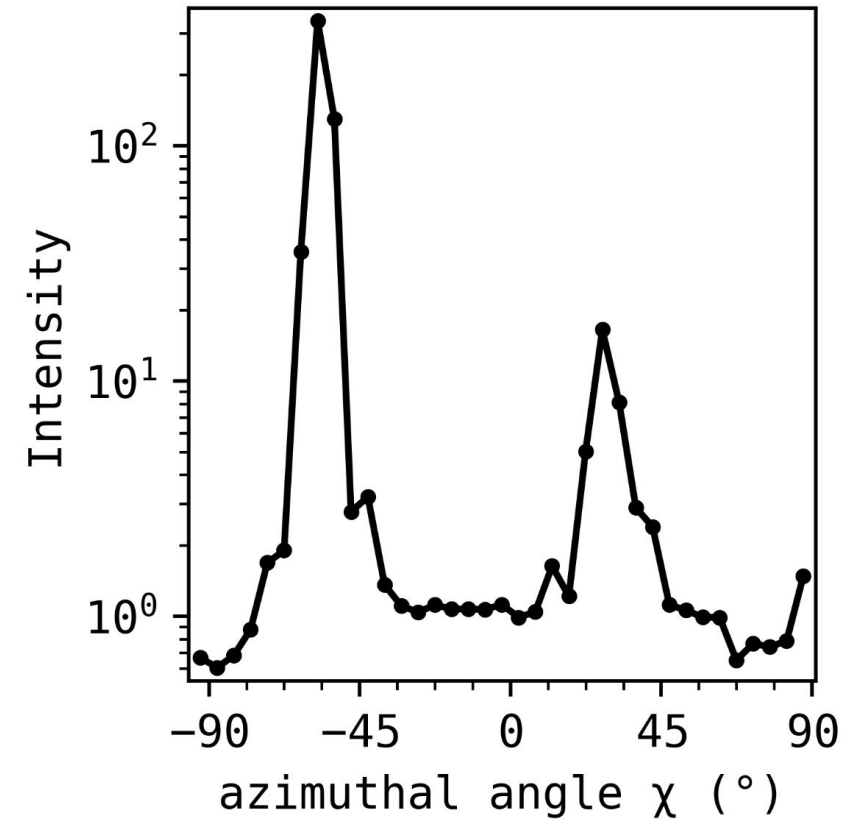
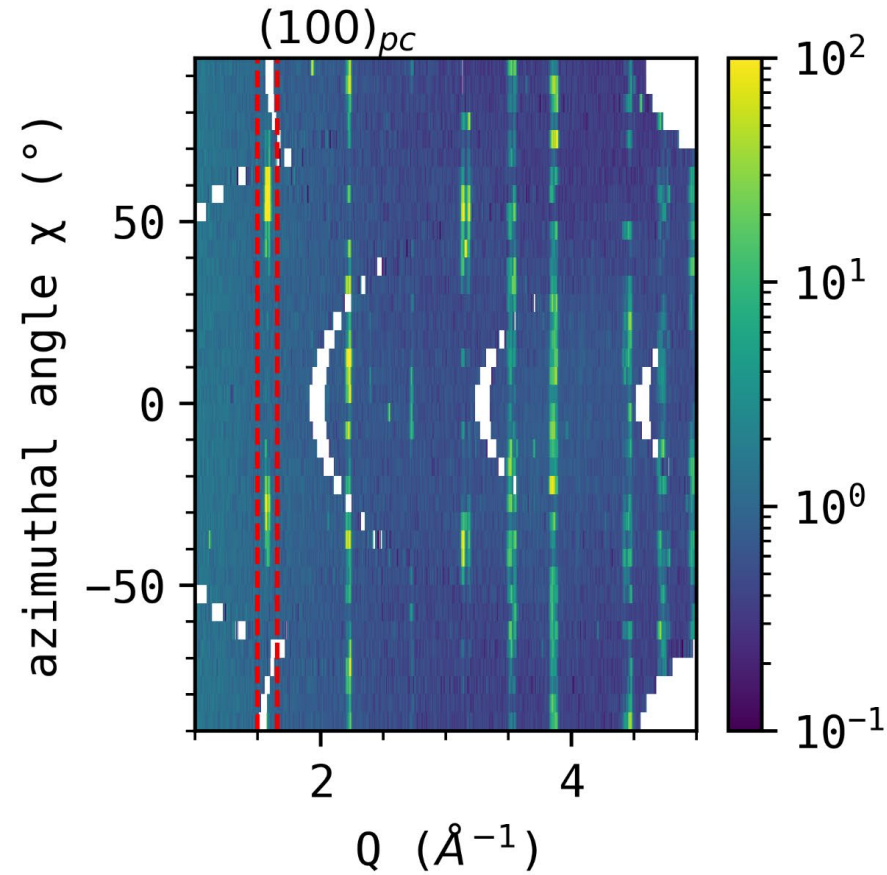
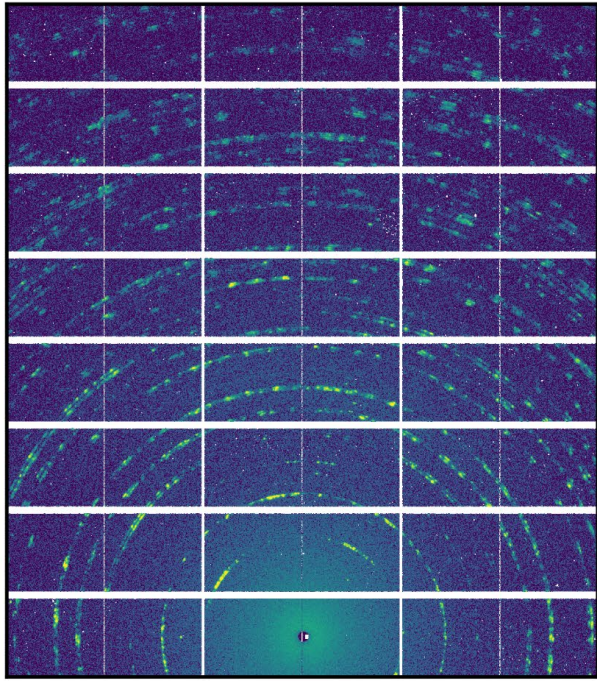


Collaboration
w. Astri Haugen

MAXIV



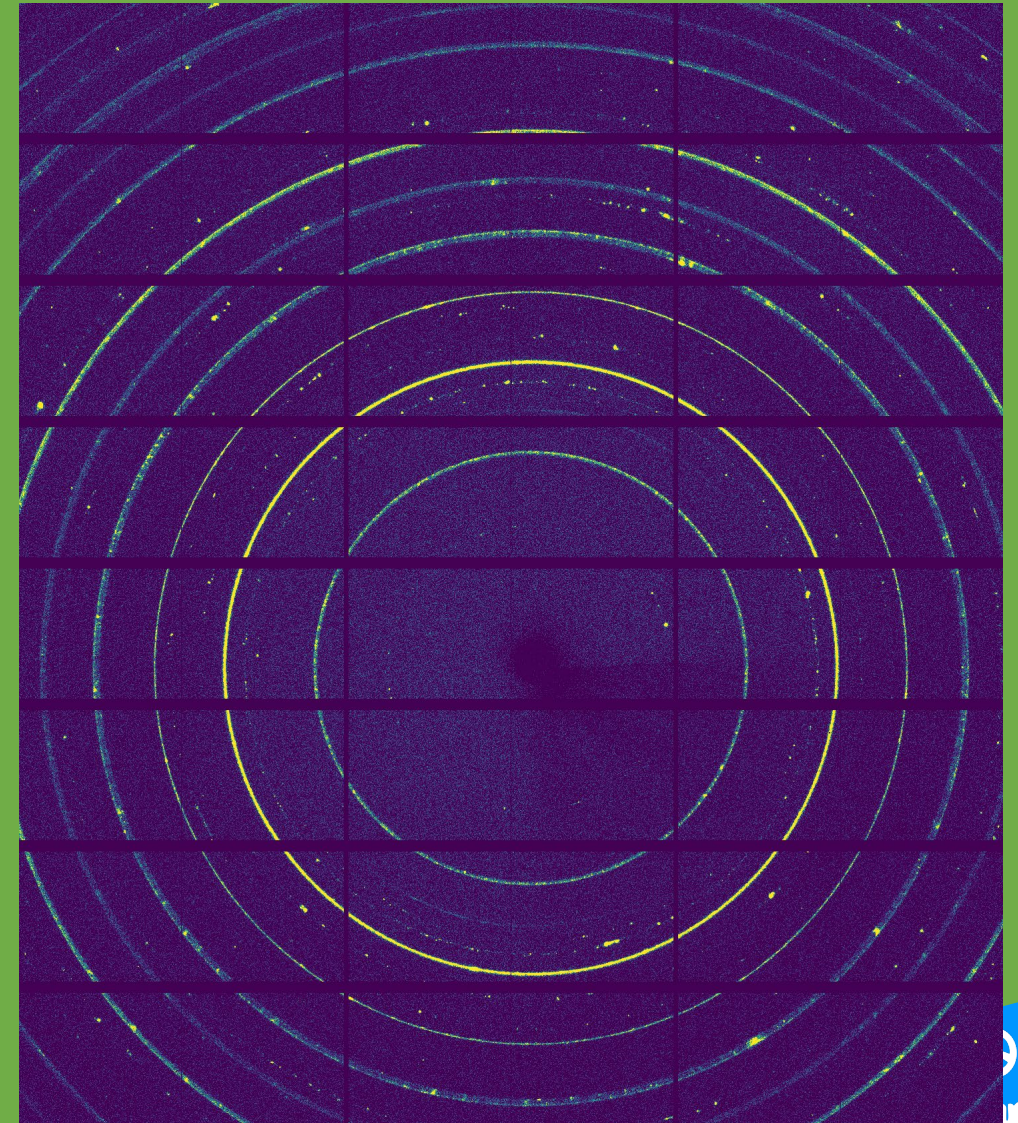
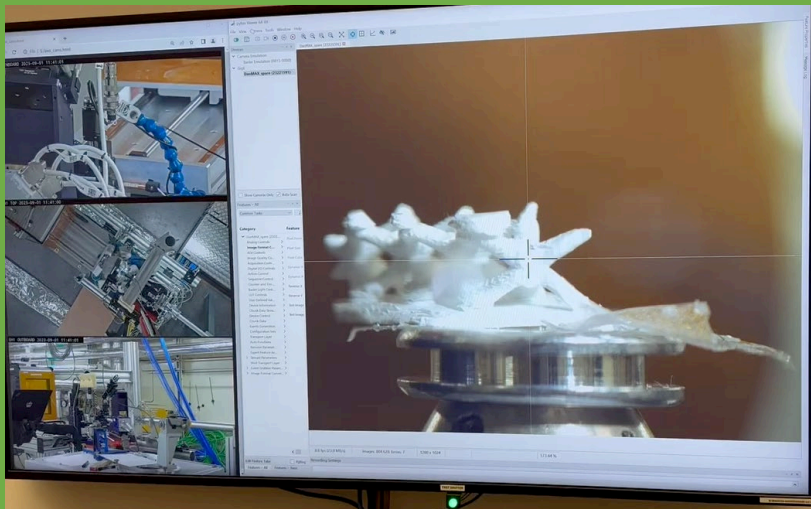
3D-printing with template crystallites



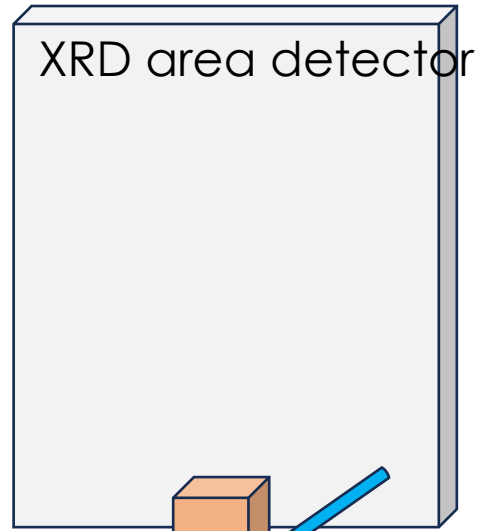
Large crystallites → Spotty diffraction data
Azimuthally binned data still show texture

ML potential?

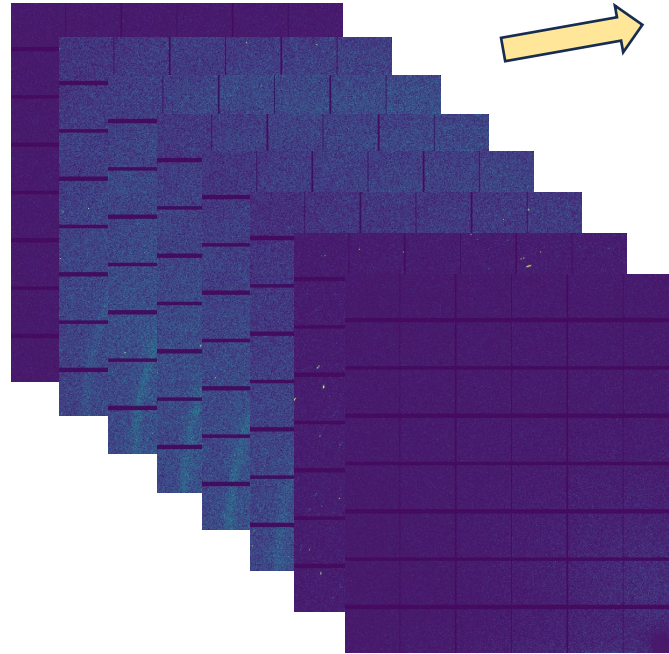
- Separation of diffraction signals based on appearance on 2D detector



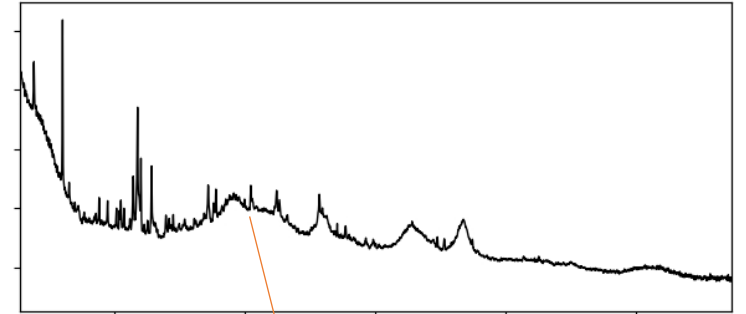
X-ray diffraction contrast tomography (XRD-CT)



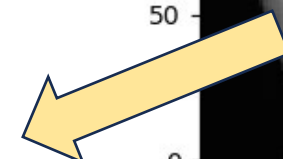
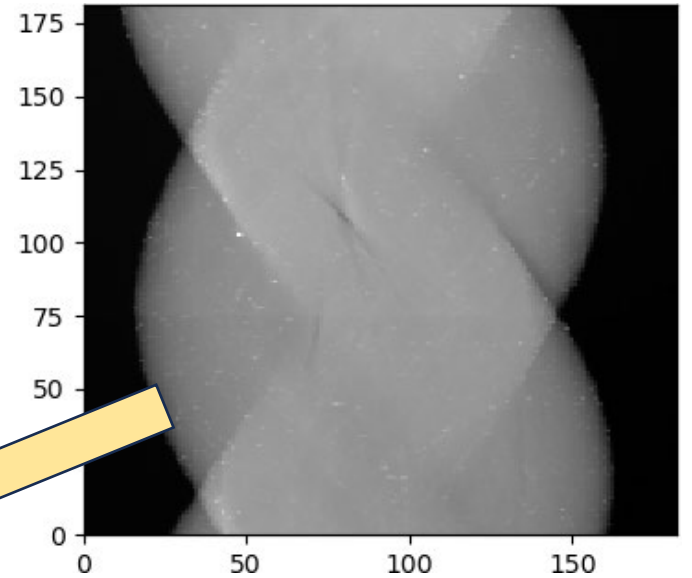
Diffraction patterns



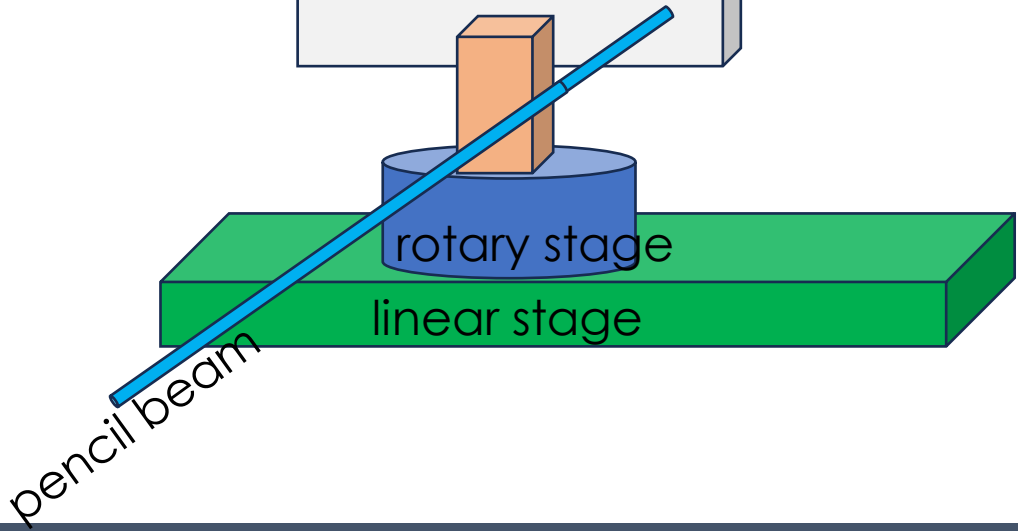
Azimuthal integration



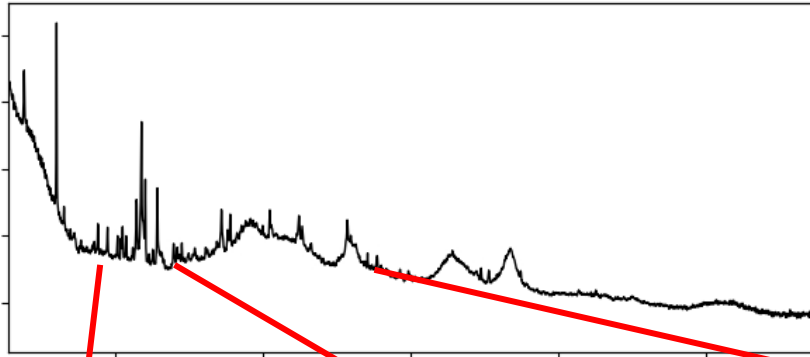
Sinogram at a given q (2θ)



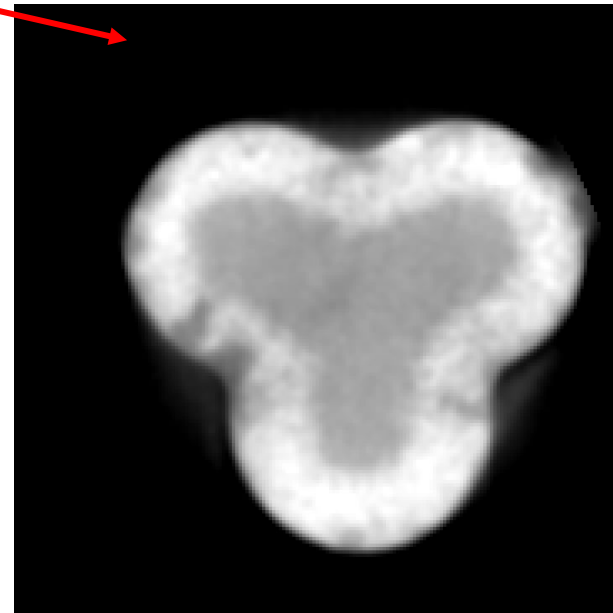
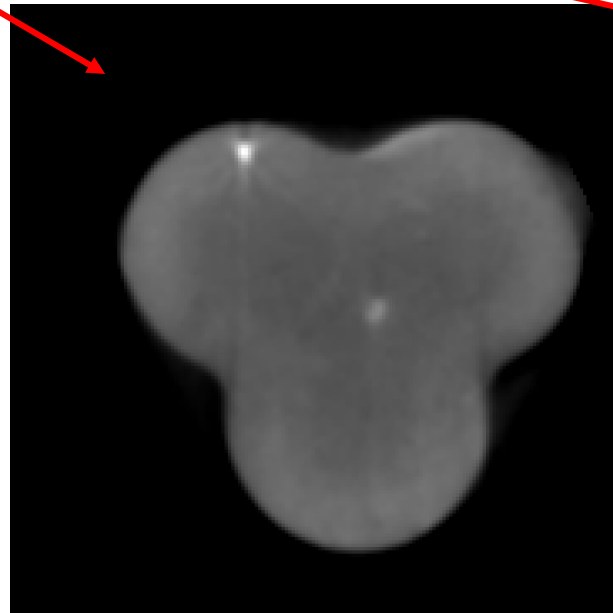
CT reconstruction



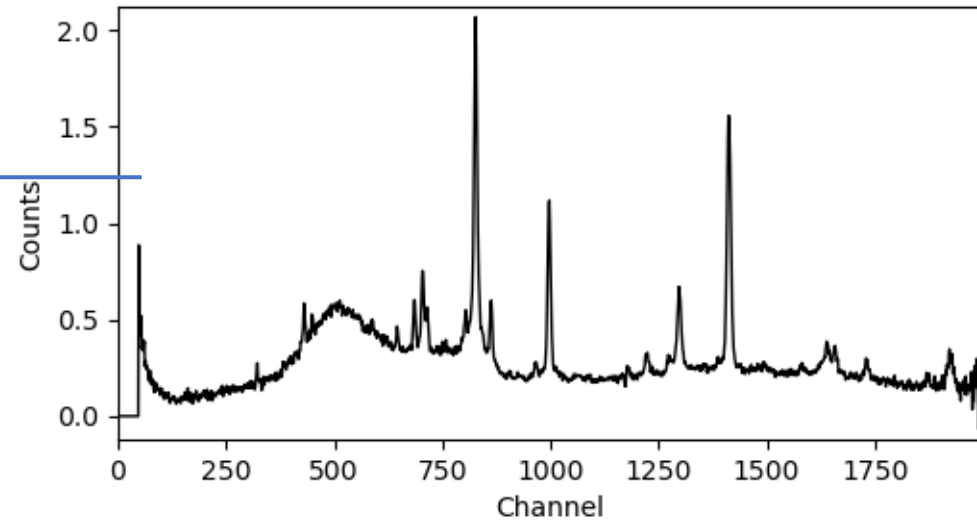
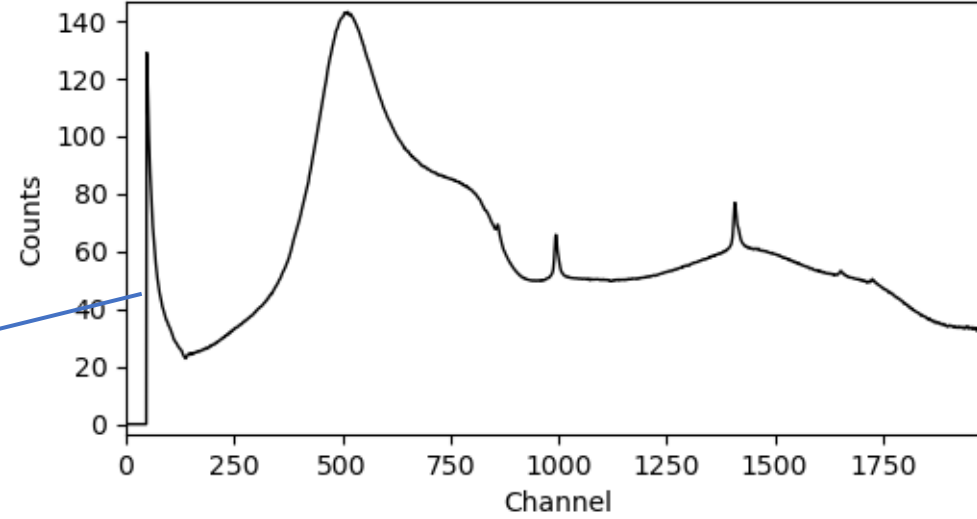
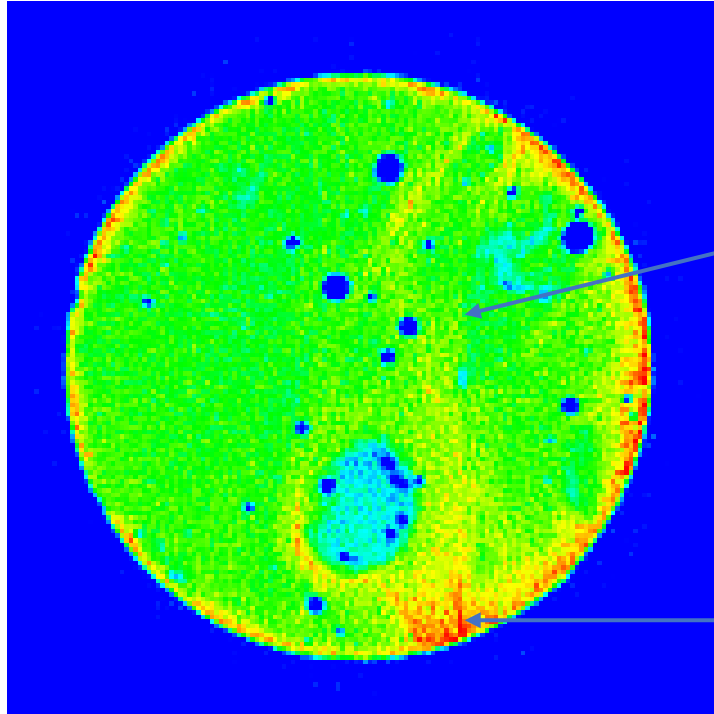
XRD-CT: contrast is generated by crystal structure



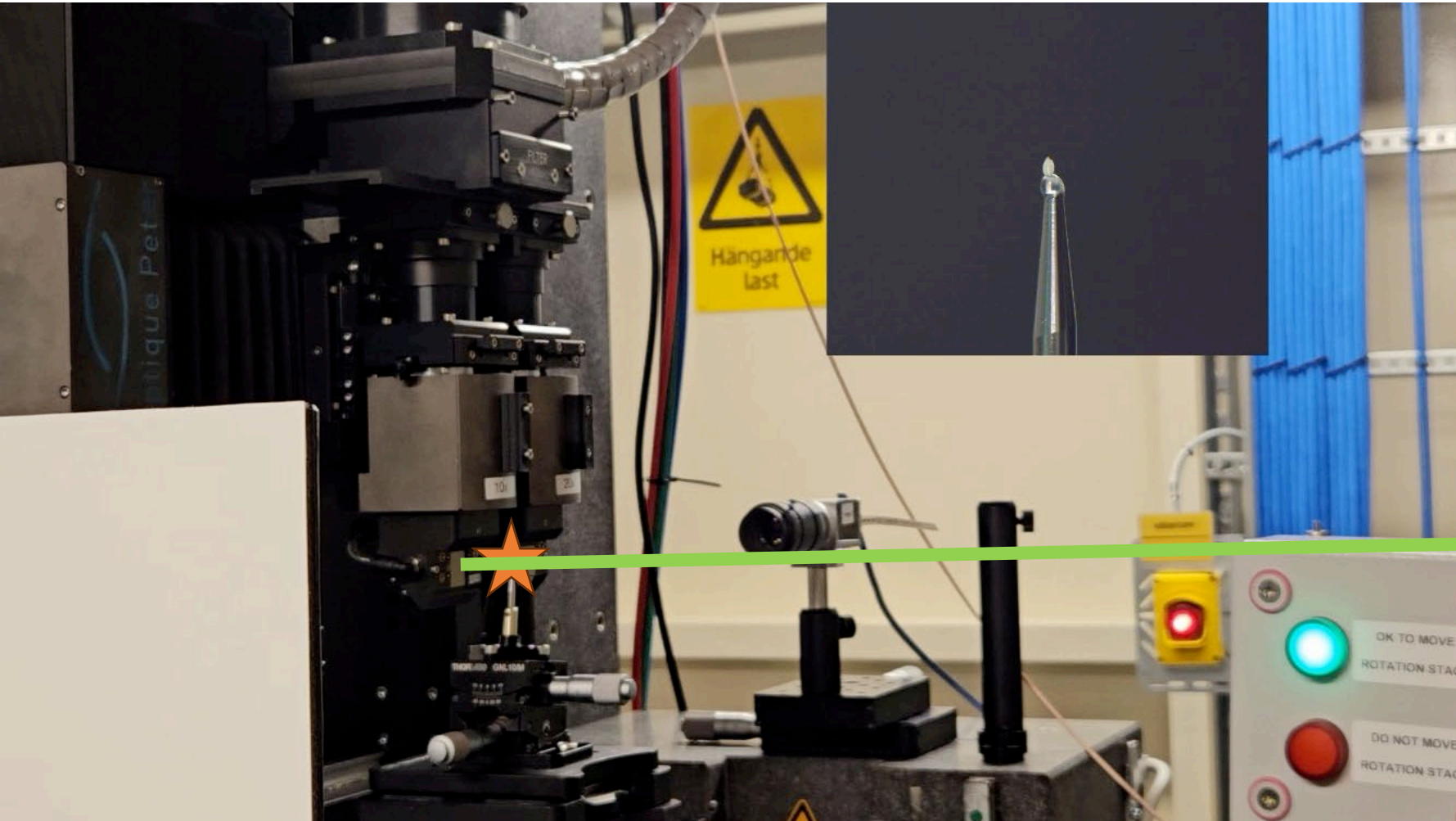
Typical parameters:
Resolution: $\sim 20 \mu\text{m}$
Sample diameter: 2-3 mm
Scan time: ~ 10 min per slice



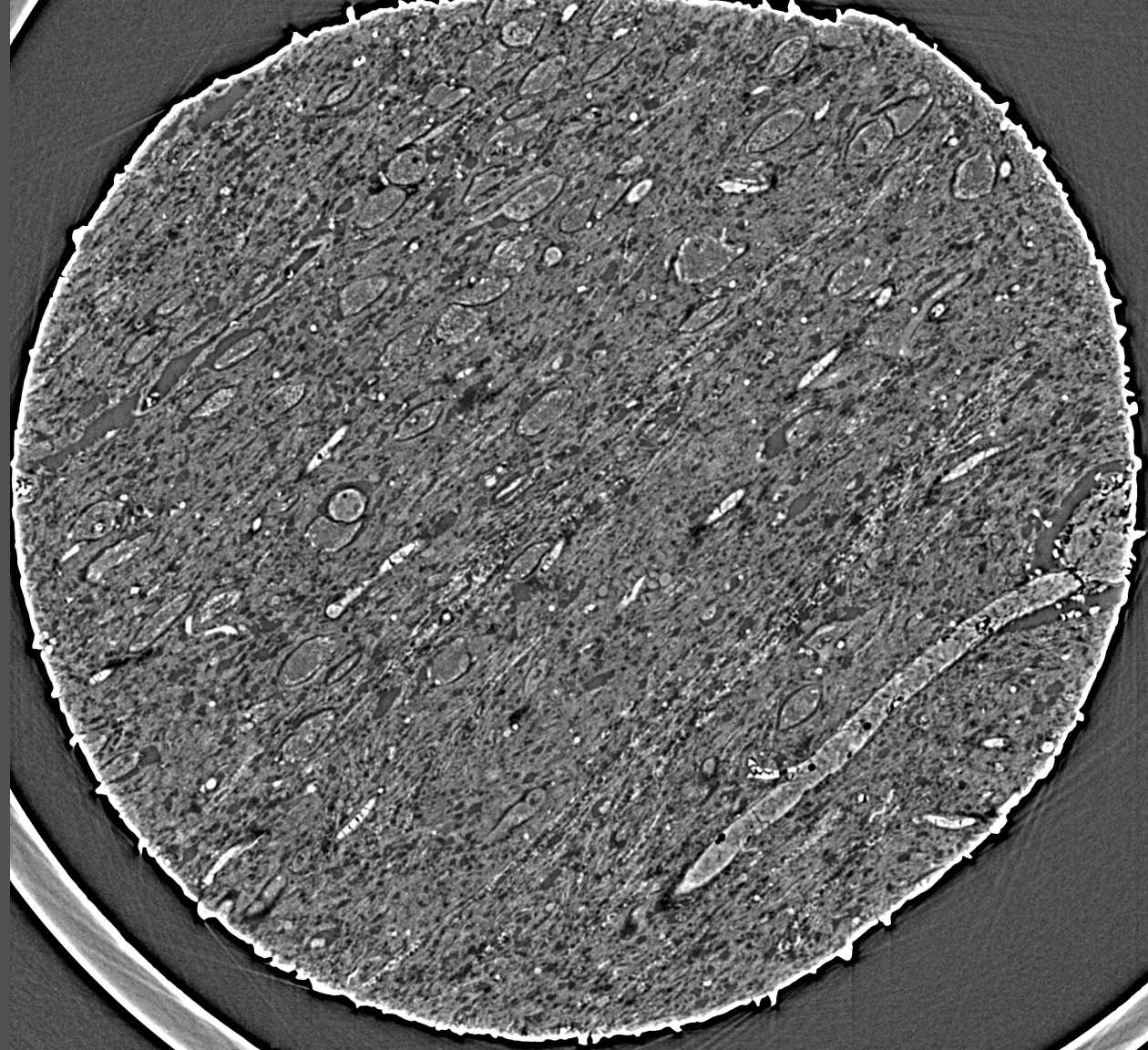
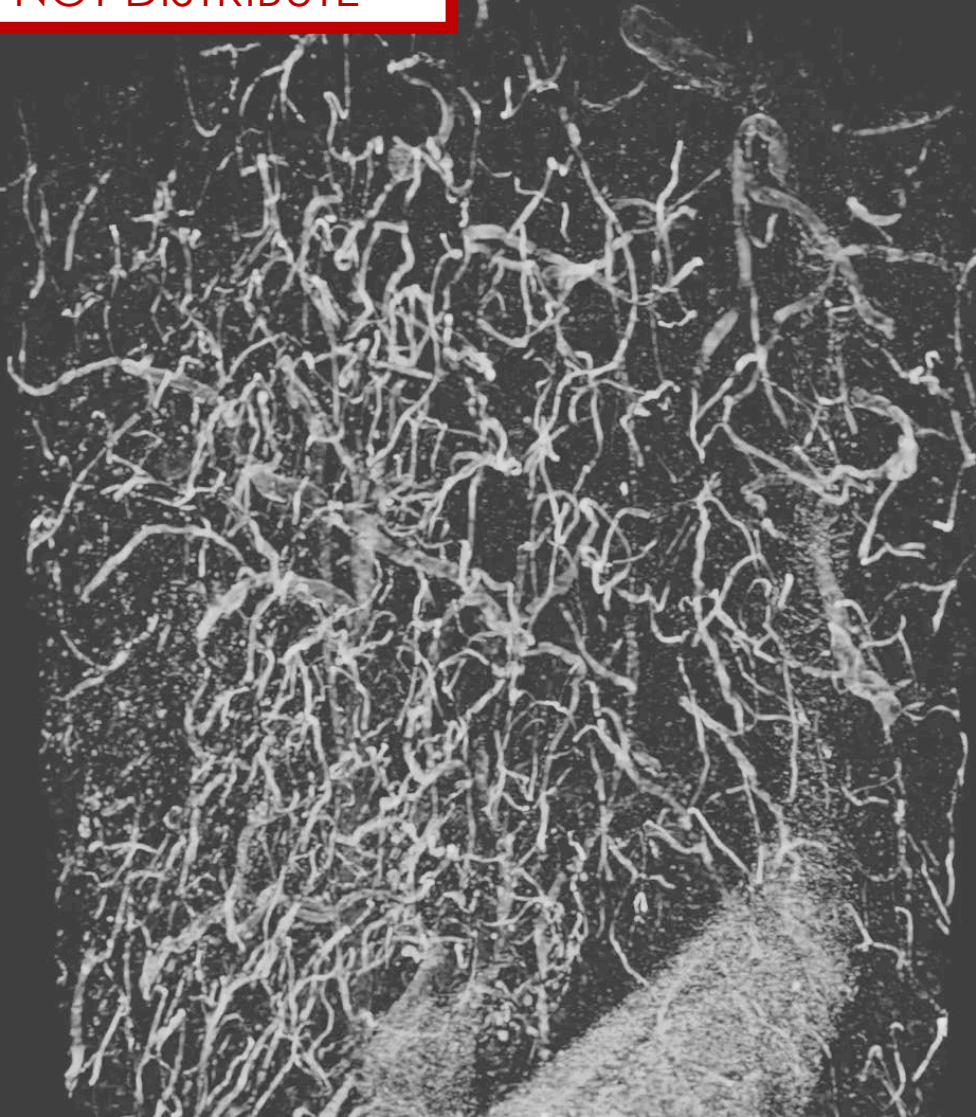
Problem: locating very weak peaks over intense broad background



Tomographic imaging



UNPUBLISHED DO
NOT DISTRIBUTE



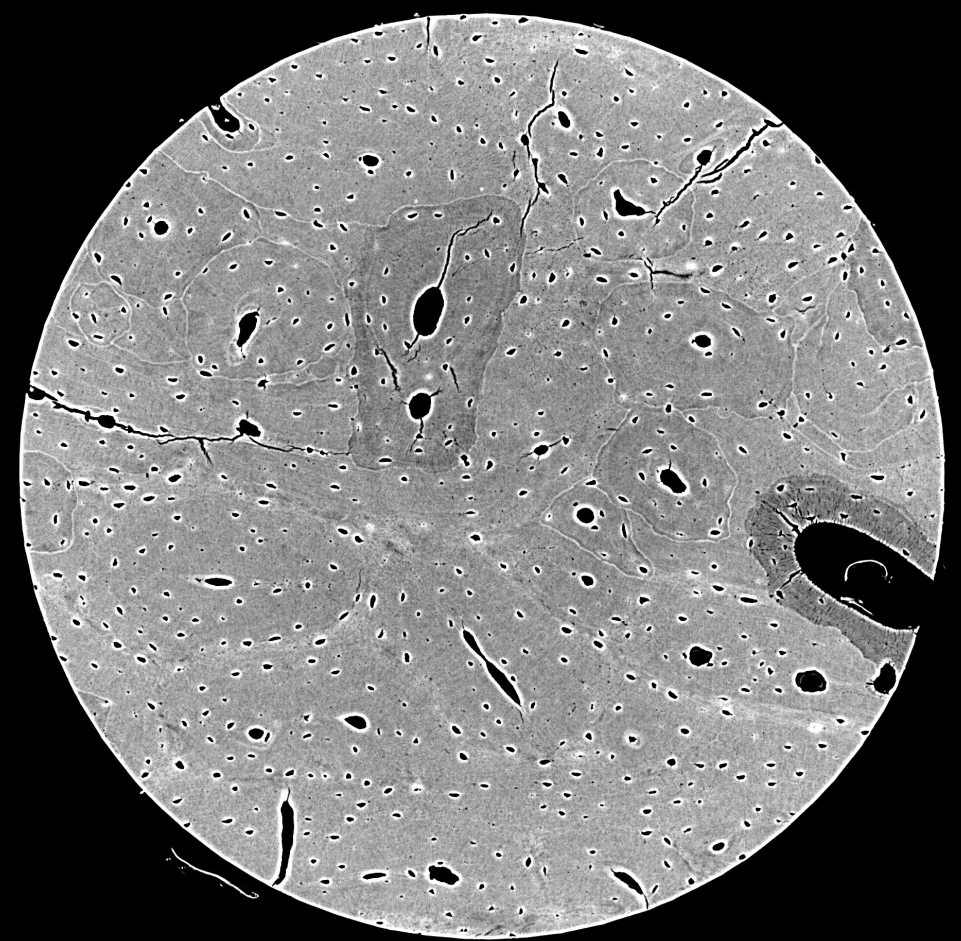
- Scan of **unstained** human brain
- Shows nerves, nerve bundles, and cells throughout the brain
- Measured in ~1 minute

Data:
Tim Dyrby and Emma Thomson
DTU

MAXIV



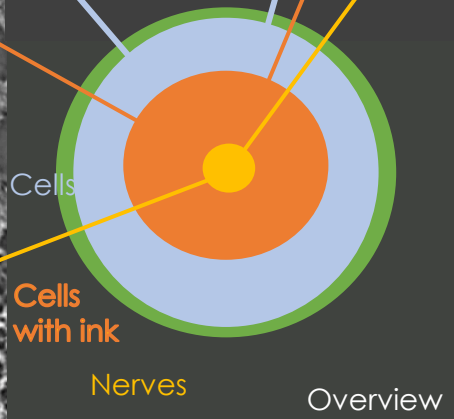
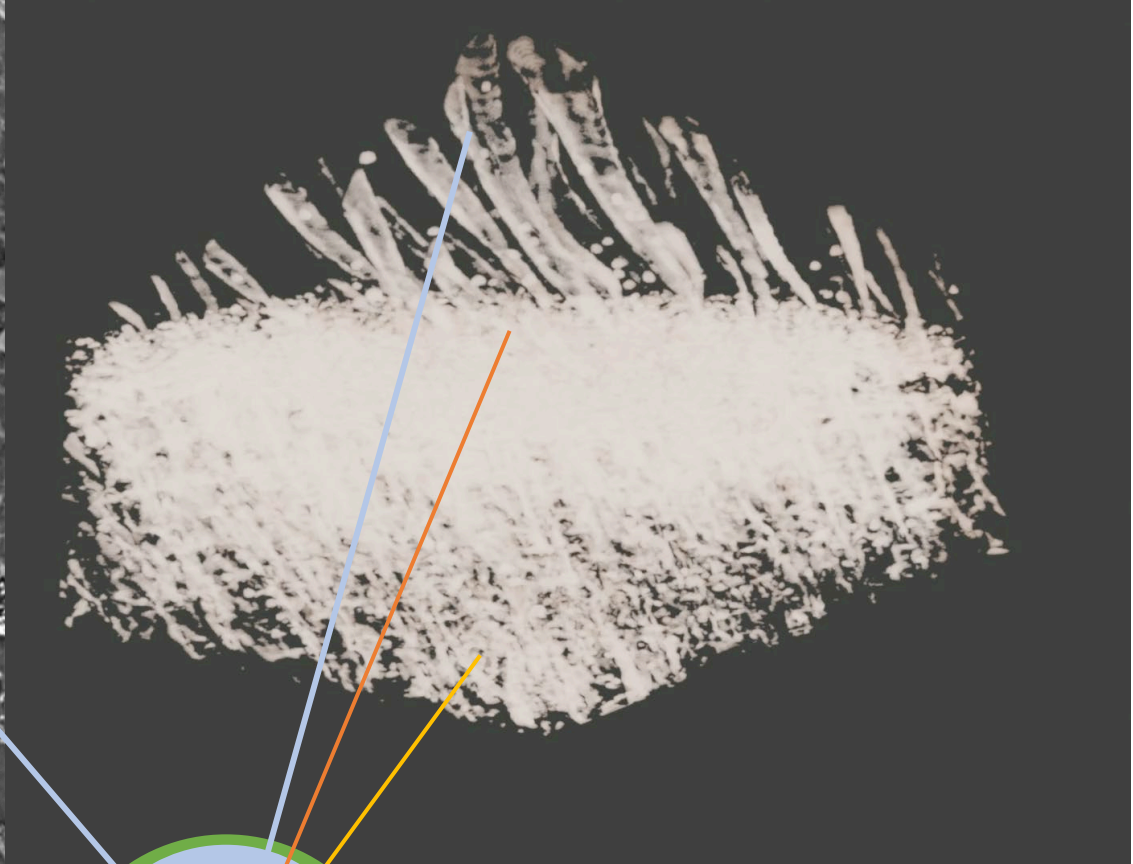
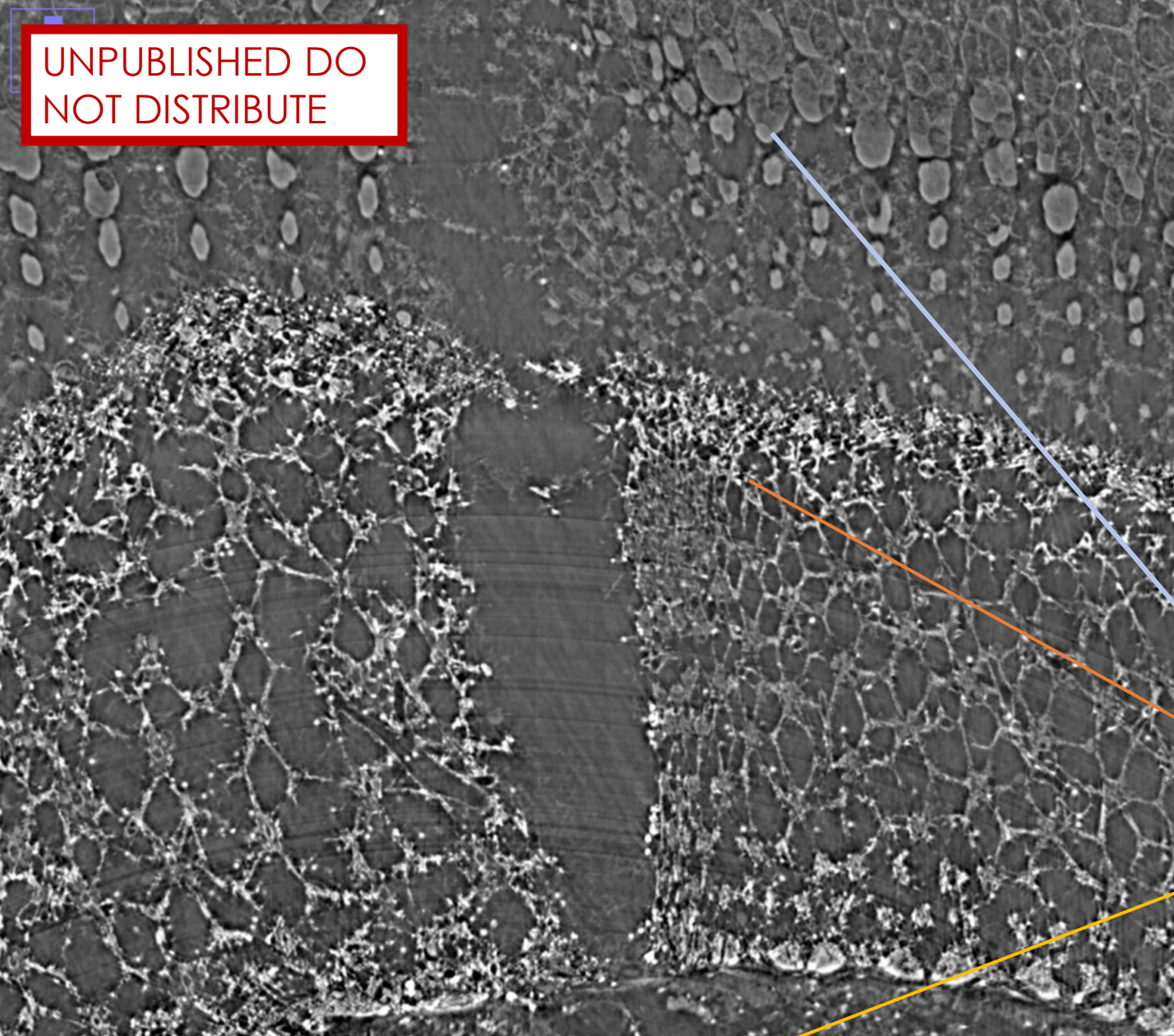
UNPUBLISHED DO
NOT DISTRIBUTE



- Ovine Bone.
- Clearly shows porosities
- See density variance in dense materials
- Measured in ~1 minute

Data:
Henrik Birkedal and Adrian Rodriguez Palomo
Aarhus University

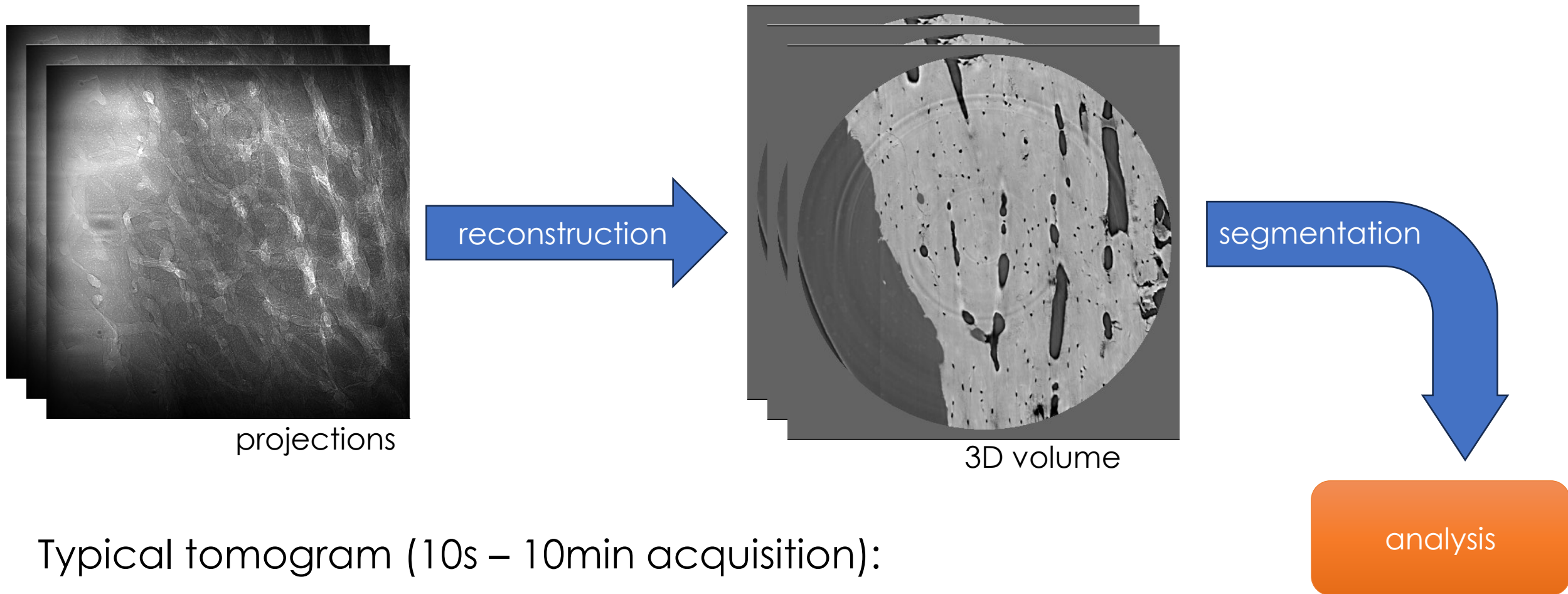
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- Scan of the mantis shrimp eye
- Pure phase scan, eye is **unstained**
- Full volume is 296 Gvox
- Measured in ~1 hour

Data:
Henrik Birkedal and Anne Marie Møller Faaborg
Aarhus University

AI/ML in tomography



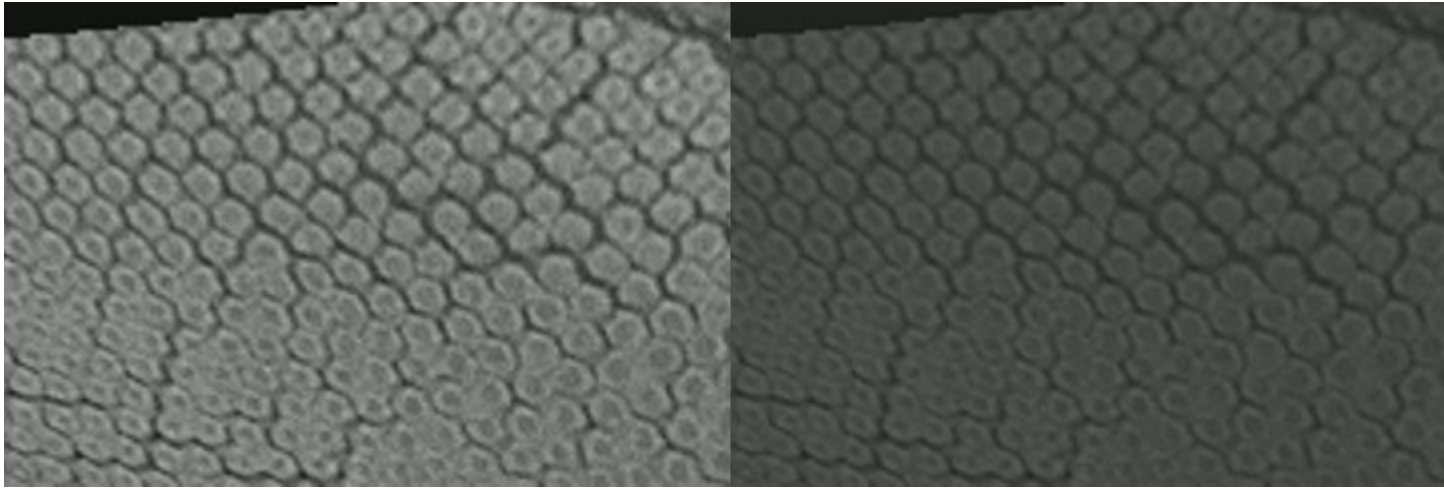
Typical tomogram (10s – 10min acquisition):

$2400 \times 2400 \times 2300$ (float32) = 53 GB

$4600 \times 4600 \times 2400$ (float32) = 203 GB

AI/ML in tomography

- Machine learning for segmentation and labeling
- Super-resolution enhancement

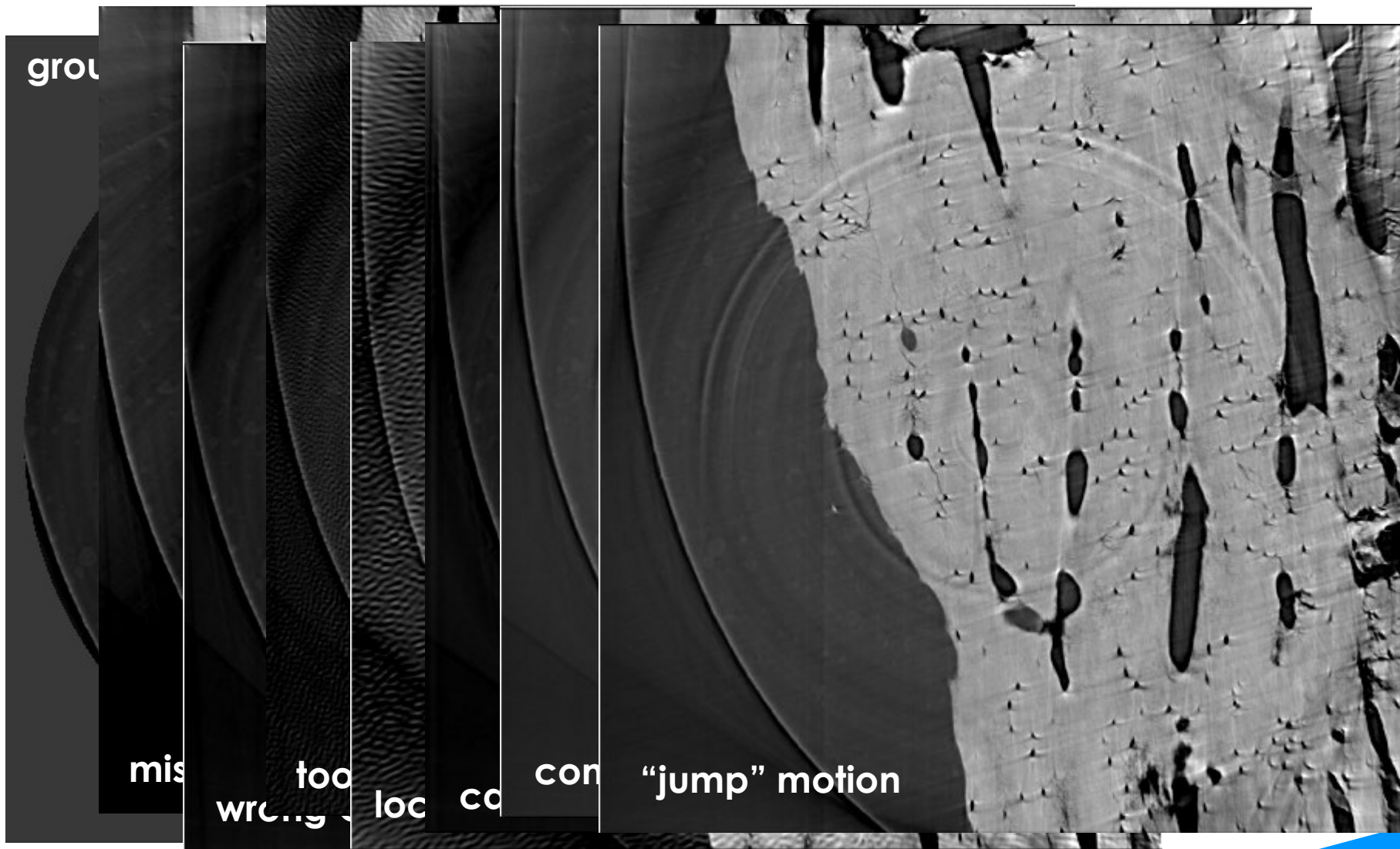


ML potential?

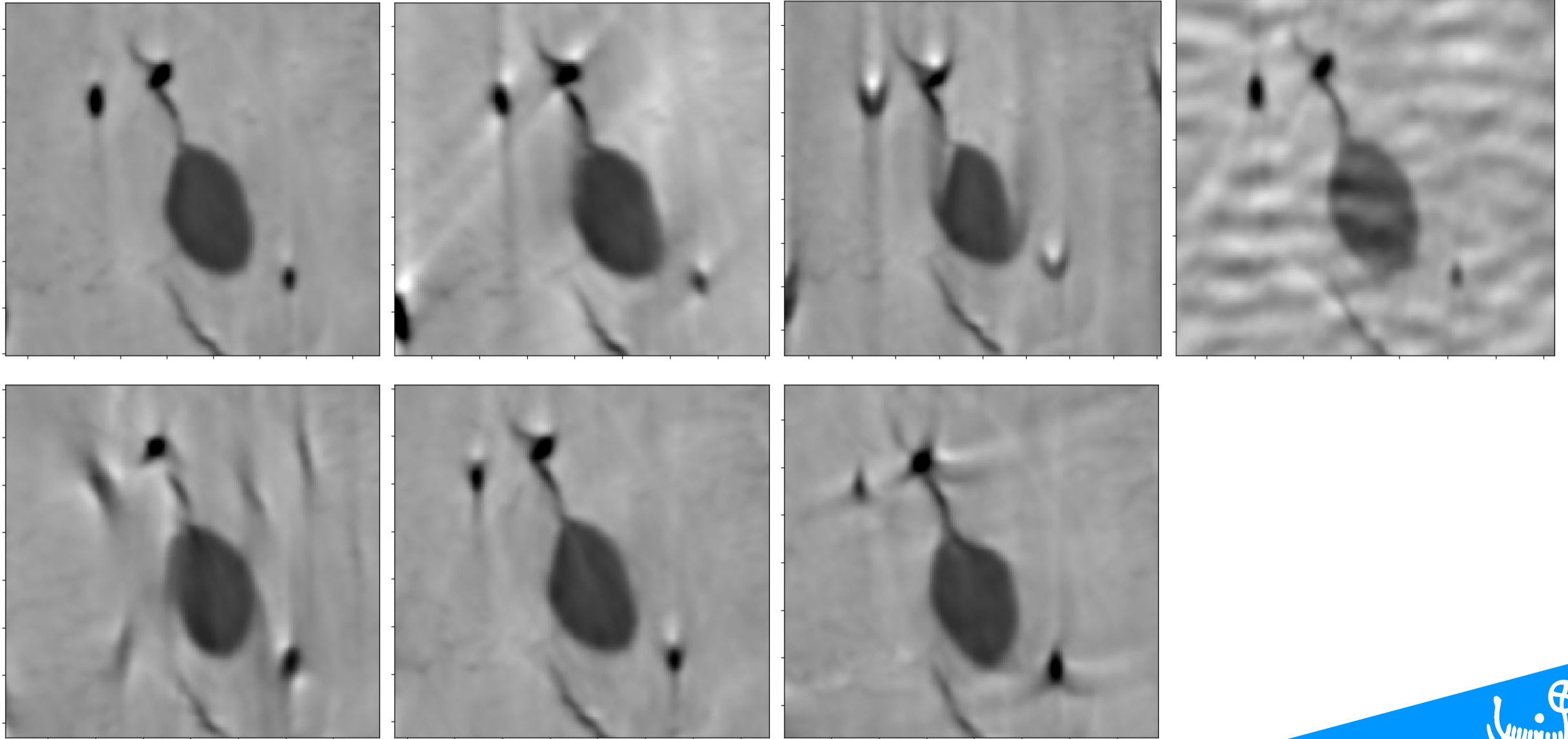
- Reconstruction artifacts identification

Reconstruction artifacts identification

- Can be done on single slice or fragments
- Requires a lot of experience to distinguish between them



Reconstruction artifacts identification





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