High-resolution X-ray tomography

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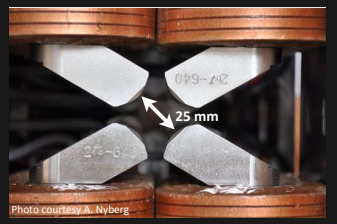
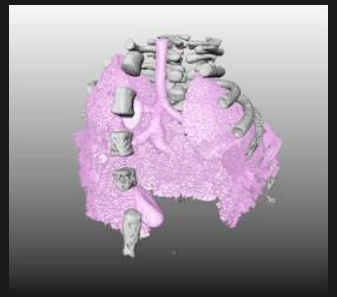
Outline

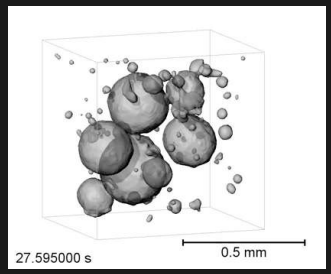


I. Brief introduction into tomographic microscopy
   I. Acquisition and reconstruction

II. Applications
   I. Bio: lungs
   II. Hard matter: Aluminum foams



III. Overview of MAX IV instruments for imaging
   I. Beamlines, techniques



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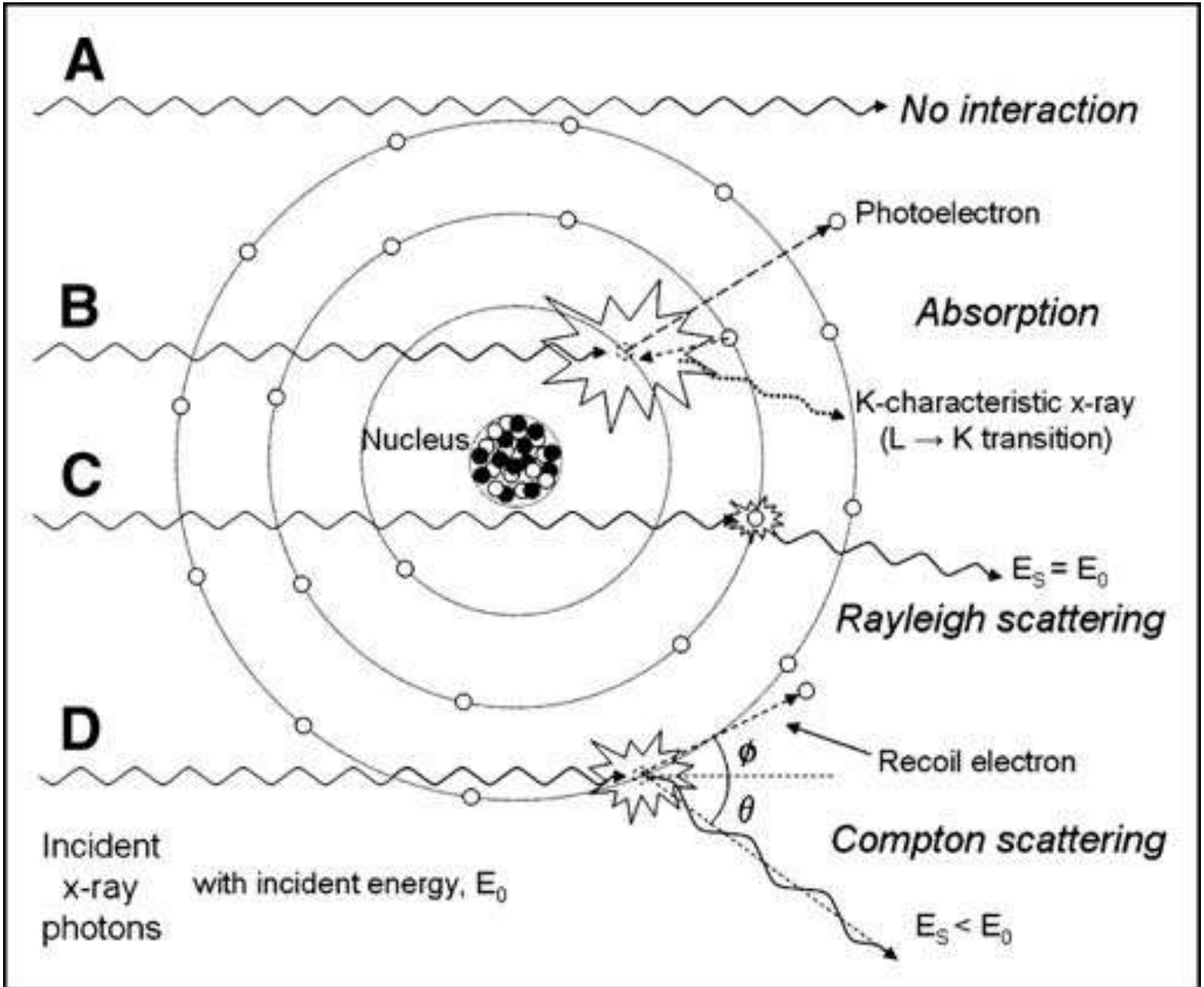
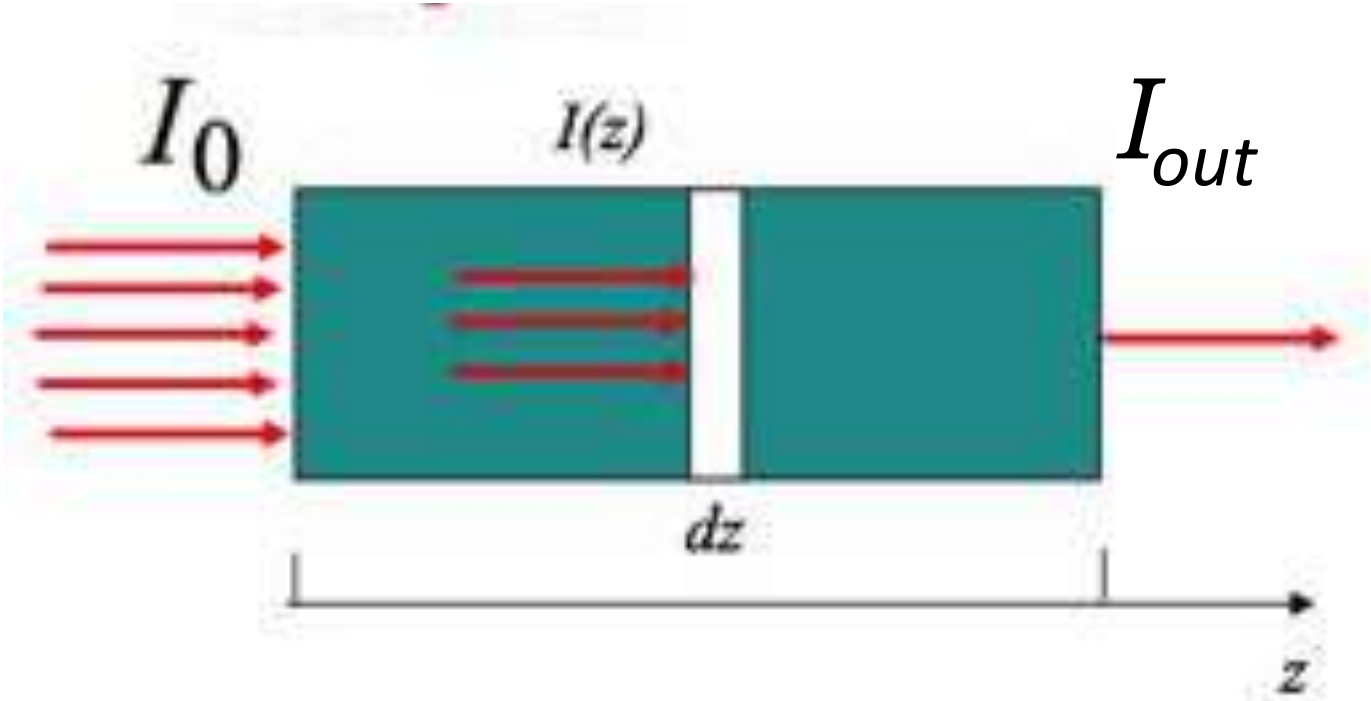
Absorption and scattering



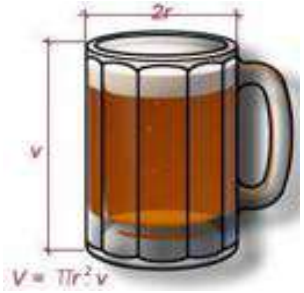
X-ray attenuation in the object



$$-dI = \mu \cdot I(z)dz \quad \Rightarrow \quad I(z) = I_0 \cdot e^{-\mu z}$$

μ^{-1} - the absorption length

Beer-Lambert law



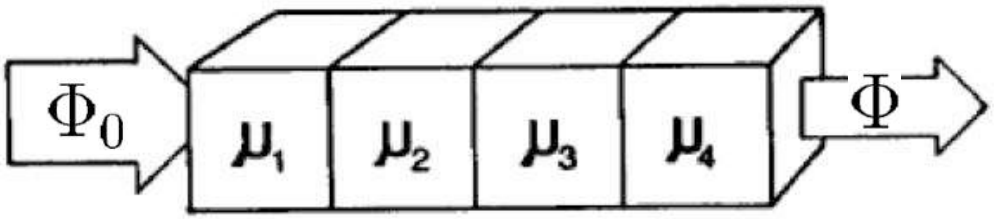
Probing matter with X-rays

polychromatic case

$$\Phi = \int_E \Phi_0(E) e^{-\int_{SD} \mu(l,E) dl} dE$$

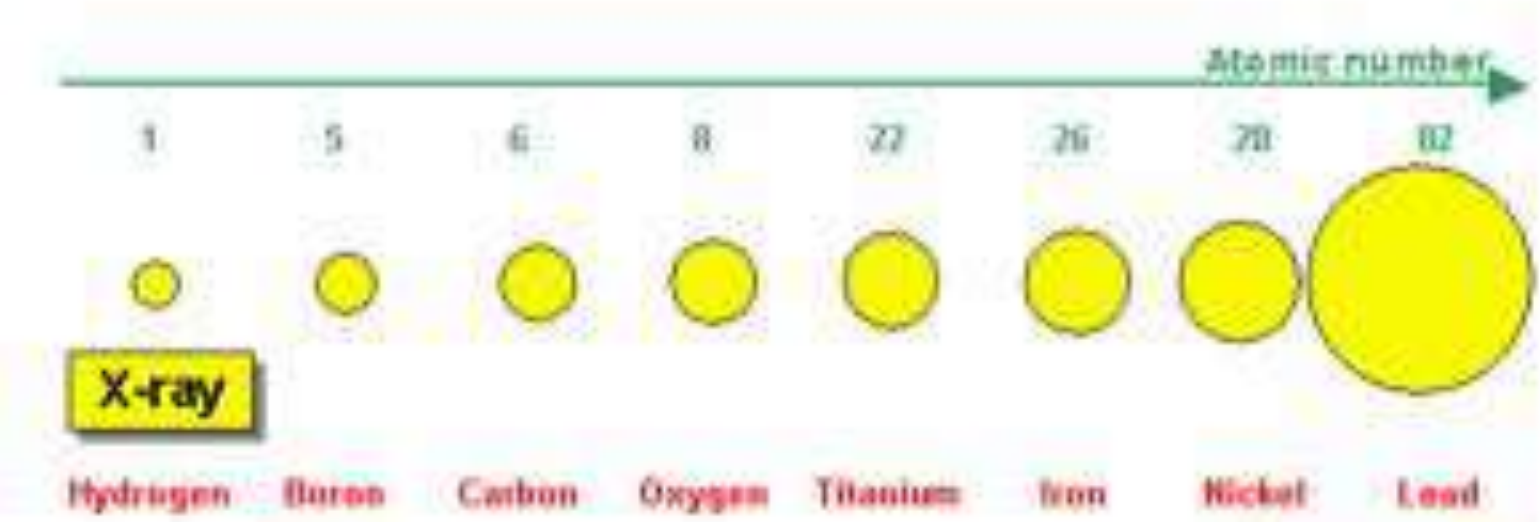
monochromatic case

$$\Phi = \Phi_0(E) e^{-\int_{SD} \mu(l,E) dl}$$



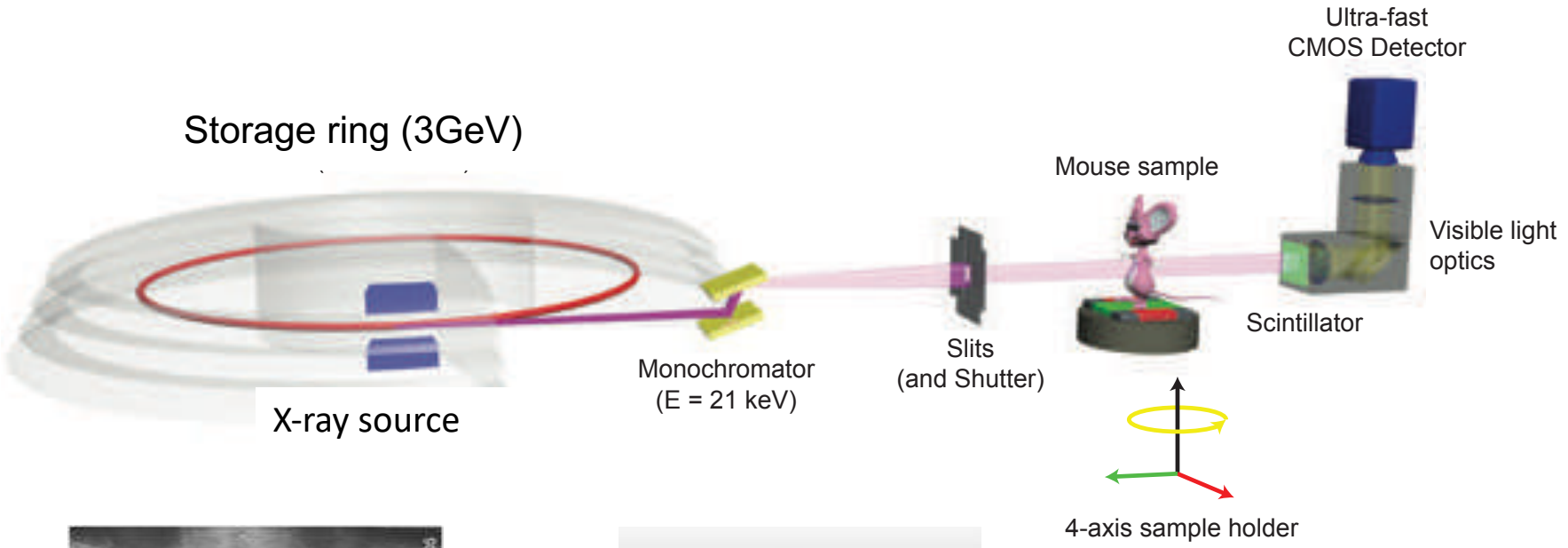
The attenuation is linear and additive
(this is why tomography works!)

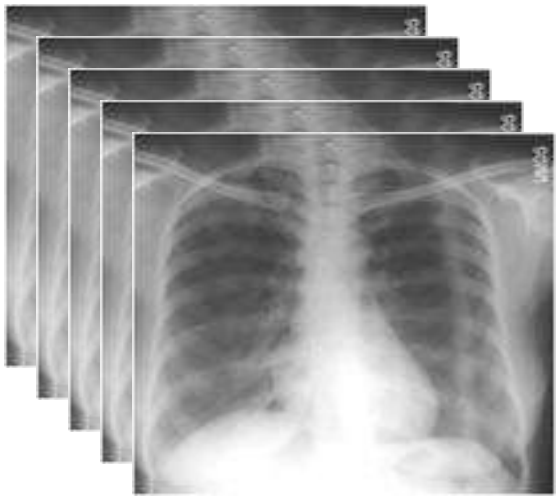
Probing matter with X-rays

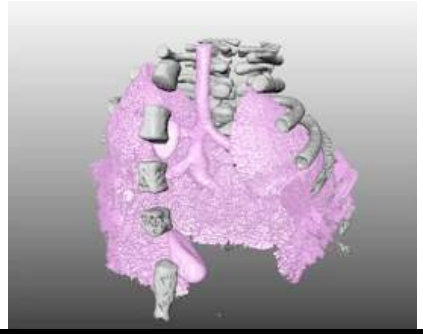


X-rays $\sigma_{abs} \propto Z^4 \cdot (\hbar\omega)^{-3}$

What is imaging?







Tomographic reconstruction
Synchrotron

Pixel size: 11 -> 0.3 µm

FOV: 22 x 22 -> 1 x 1 mm^2

Projections: 300–2000

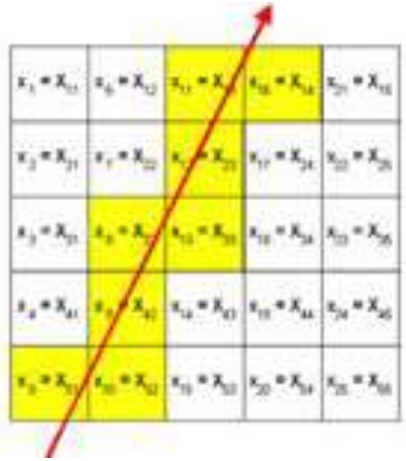
Exposure times: 0.1–300 ms

Total scan time: 0.05 to 500 s

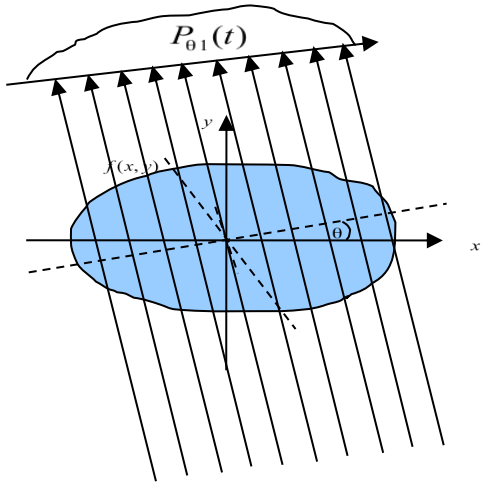
Tomographic reconstruction concepts?

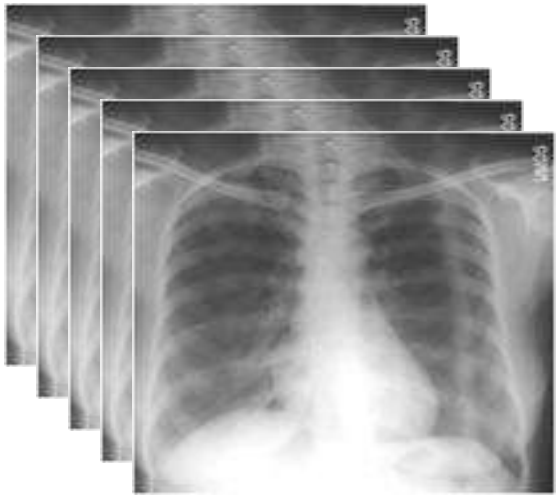
Numerical (algebraic)

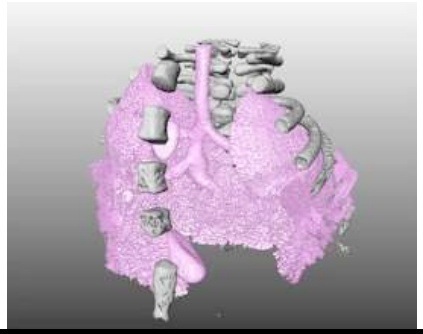
Ax = b



Analytical (backprojection)

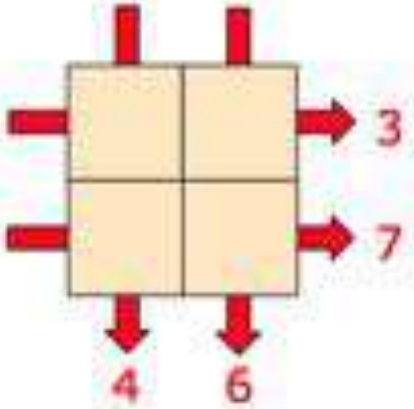






Tomographic reconstruction
Synchrotron

Analogy: the "Sudoku" Problem – 数独



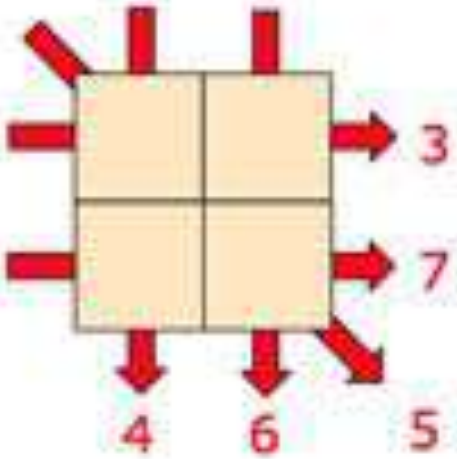
$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 3 \\ 7 \\ 4 \\ 6 \end{pmatrix}$$

0	3
4	3

1	2

With enough rays, the problem has a unique solution.

Here, one more ray is enough to ensure a full-rank matrix:



$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 3 \\ 7 \\ 4 \\ 6 \\ 5 \end{pmatrix}$$

The solution is now unique but it is still sensitive to the noise in the data.

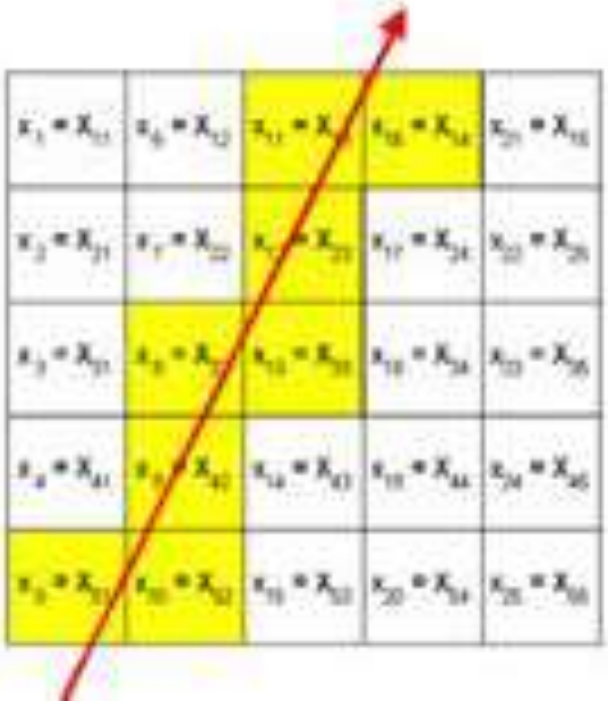
Tomography

Damping of i-th X-ray through domain:

$$b_i = \int_{\text{ray}_i} \chi(\mathbf{s})\, d\ell, \quad \chi(\mathbf{s}) = \text{attenuation coef.}$$

Assume $\chi(\mathbf{s})$ is a constant x_j in pixel j, leading to:

$$b_i = \sum_j a_{ij}\, x_j, \qquad a_{ij} = \text{length of ray } i \text{ in pixel } j.$$



This leads to a large linear system:

$$A\,x = b \qquad b = b^* + e$$

Noise

Projections

Image

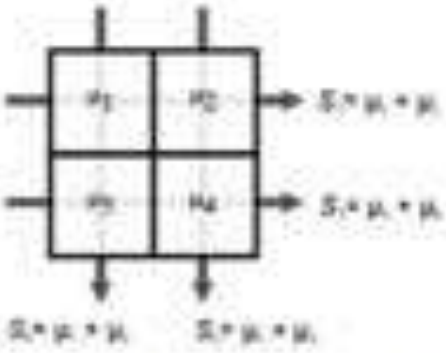
"Geometry"

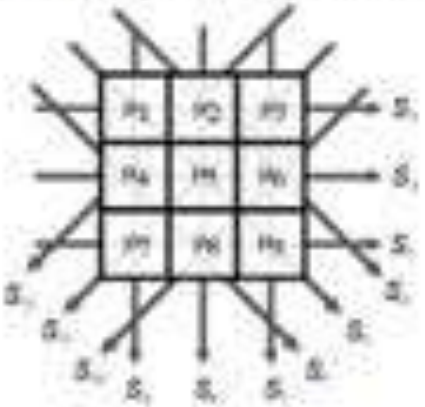
$$b^* = A\,x^*$$

$$x^* = \text{exact image}$$

Tomography

- **Direct inversion** (solving N equations with N unknowns)





- Houndsfield in 1957 solved 28000 equations simultaneously!
- Need more than N^2 measurements to overcome linear independence

NOBELFÖRSAMLINGEN KAROLINSKA INSTITUTET

THE NOBEL ASSEMBLY AT THE KAROLINSKA INSTITUTE

11 October 1979

The Nobel Assembly of Karolinska Institutet has decided today to award the Nobel Prize in Physiology or Medicine for 1979 jointly to

Allan M Cormack and Godfrey Newbold Hounsfield

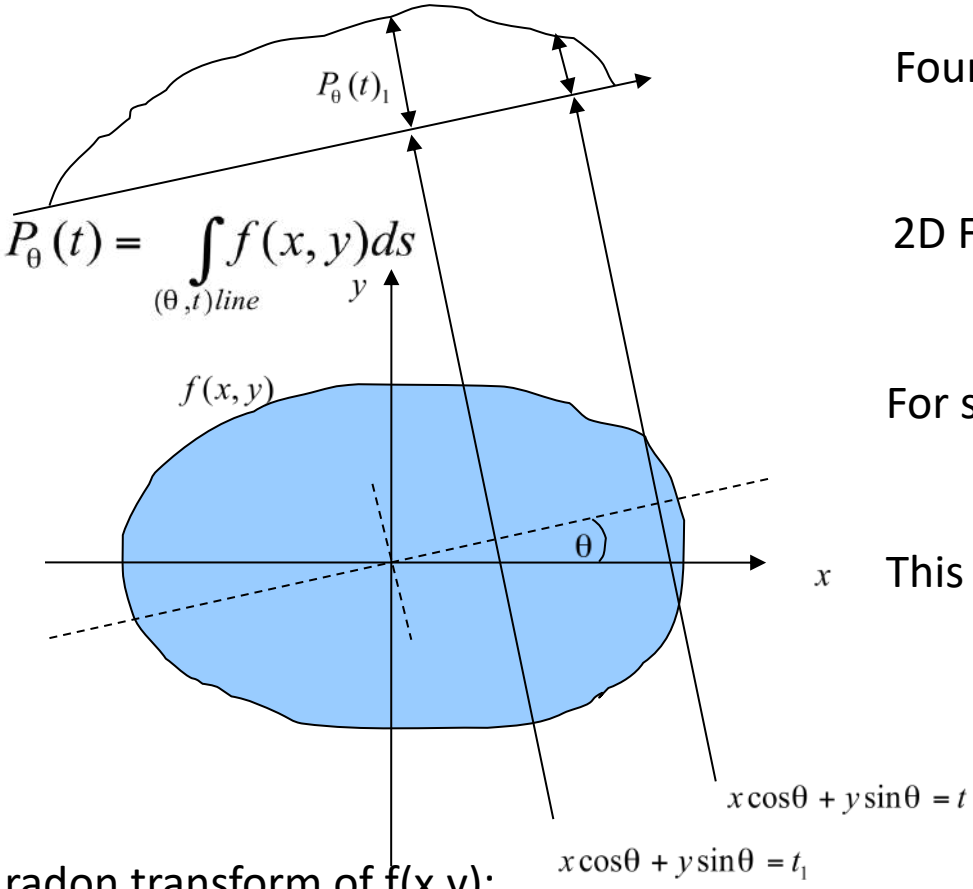
for the "development of computer assisted tomography".

Tomography

Johan Radon, *Über die Bestimmung von Funktionen durch ihre Integralwerte Längs gewisser Mannings-faltigkeiten*, Berichte Sächsische Akadamie der Wissenschaften, Leipzig, Math.-Phys. Kl., 69, pp. 262-277, 1917.

Main result: An object can be perfectly reconstructed from a full set of projections.

Tomography



Fourier transform of the projection

$$S_\theta(w) = \int_{-\infty}^{\infty} P_\theta(t) e^{-j2\pi wt} dt$$

2D Fourier transform of f(x,y):

$$F(u,v) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y) e^{-j2\pi(ux+vy)} dxdy$$

For simplicity v=0 (just a rotation)

$$F(u,0) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y) e^{-j2\pi ux} dxdy$$

This allows to split the integral:

$$F(u,0) = \int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(x,y)dy\right] e^{-j2\pi ux} dx$$

$$P_{\theta=0}(x) = \int_{-\infty}^{\infty} f(x,y)dy$$

$$F(u,0) = \int_{-\infty}^{\infty} P_{\theta=0}(x) e^{-j2\pi ux} dx$$

radon transform of f(x,y):

$$f(x,z) = \int_0^{\pi}\left[\int_{-\infty}^{\infty} S_\theta(w)\,|w|\, e^{i2\pi wt} dw\right] d\theta$$

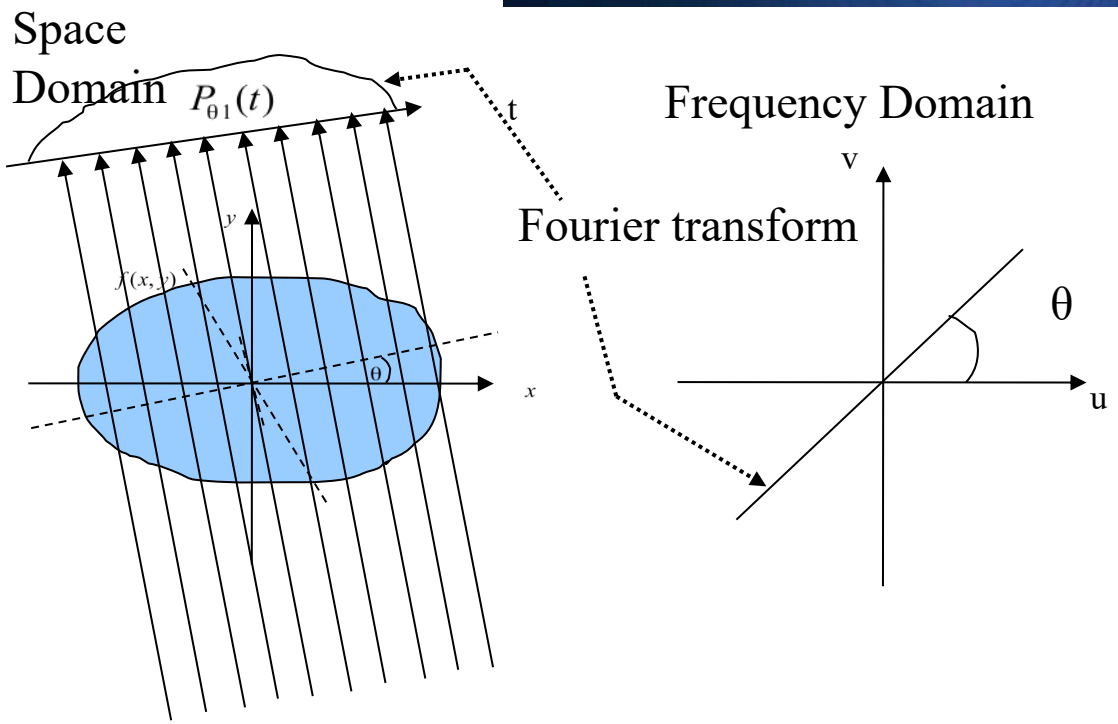
Determinant of Jacobian of the change from cartesian to polar coordinates

FOURIER SLICE THEOREM:

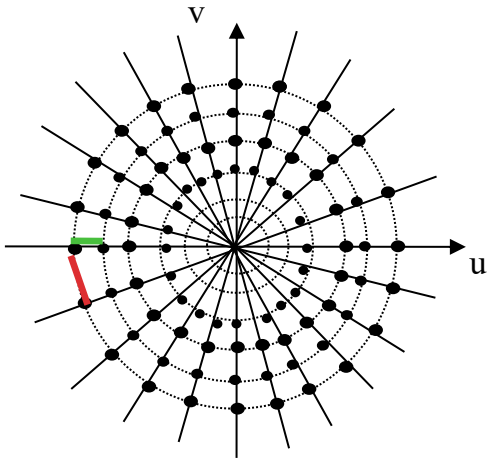
$$F(u,0) = S_{\theta=0}(u)$$

The Fourier transform of the projection gives the value of the 2D Fourier transform of the object function along a line rotated by the tomographic angle.

Tomography



Collection of projections of an object at a number of angles



FILTERED BACKPROJECTION

Sum for each of the K angles between 0 and 180

- Measure the projection, Pθ(t) Fourier transform it to find Sθ(w)
- Multiply it by the weighting function 2.π.|w|/K
- Sum over the image plane the inverse Fourier transforms of the filtered projections

For reconstruction we interpolate onto a square grid, but for high frequencies points are further apart, which results in image degradation

$$- = \frac{1}{pixelSize \times CCDsize}$$

$$\backslash = \frac{1}{2 \times pixelSize} \frac{\pi}{N_{proj}}$$

$$N_{proj} = \frac{\pi}{2}.CCDsize$$

Kak & Slaney, Principles of Tomography, 1999

The classical approach to time-resolved tomography

Dynamic studies in 3D are possible if

the rate of structural changes in the sample $\{V_{EVOL}\}$ < spatial resolution $\{\delta R\}$/scan time $\{t_{SCAN}\}$)

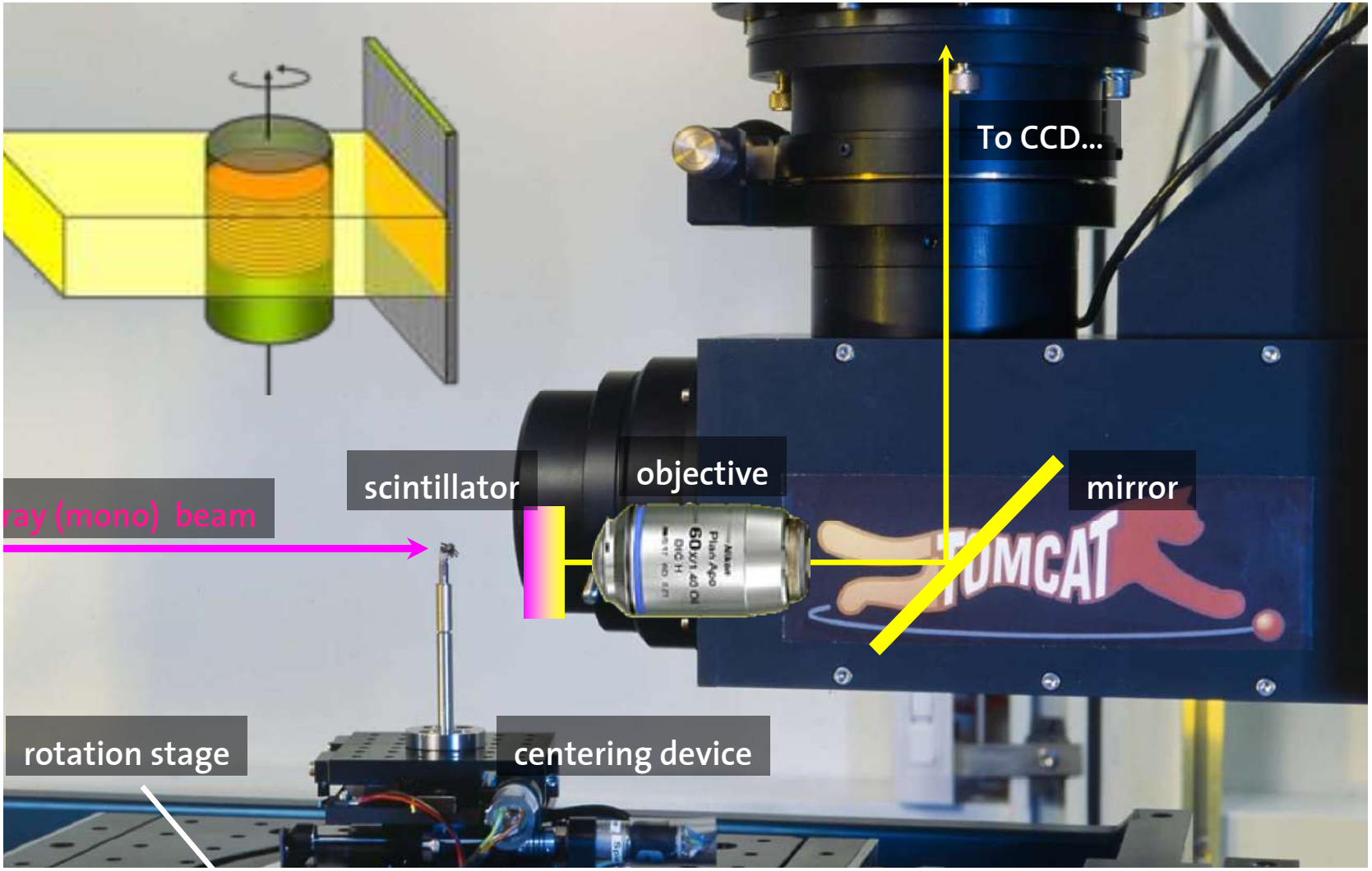
$$t_{SCAN} < \delta R / V_{EVOL}$$

0.5 s 5 µm 10µm/s

Mokso et al, J/ Phys. D. 2013

15

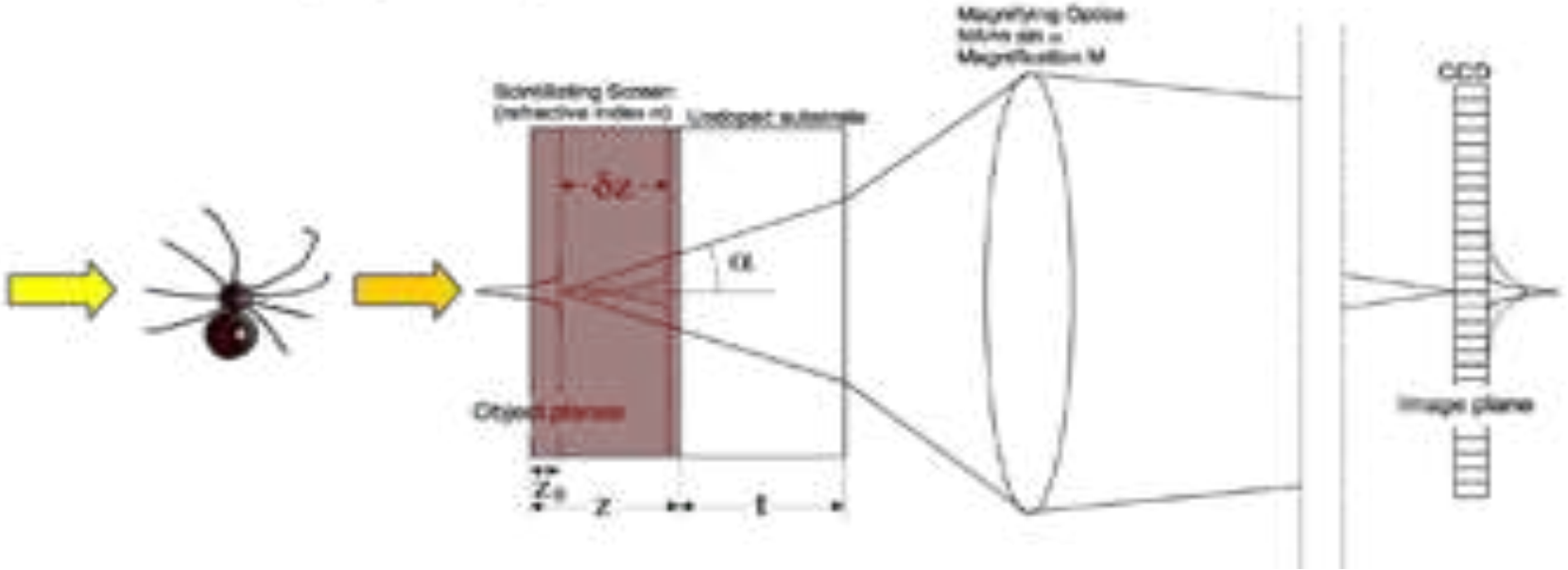
Indirect detectors



Indirect detectors

Indirect 2D X-ray detection

1. X-rays impinge on scintillating screen
2. Scintillator screen/thin powder converts X-rays to visible light
3. Visible light is collected by high efficiency lens
4. Lens magnify image onto CCD chip



Imaging geometries

(i) Parallel beam microscopy

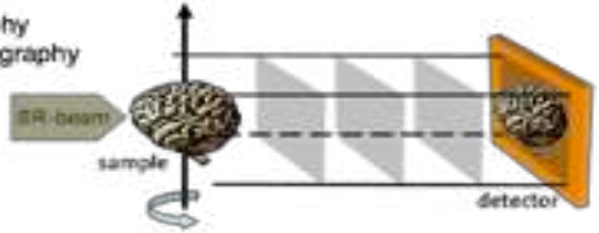
(ii) TXM: Transmission (full-field) microscopy

(iii) SXM: Scanning microscopy

(iv) PXM: Projection microscopy

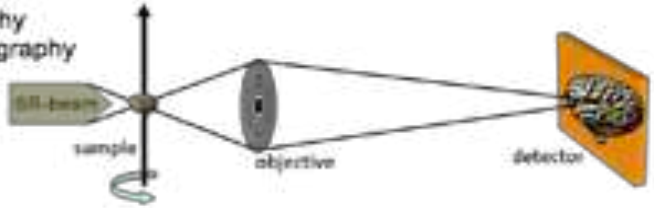
(i) Parallel beam microscopy

- Absorption Radiography / Tomography
- Phase contrast Radiography / Tomography
- Resolution >= 1 micron



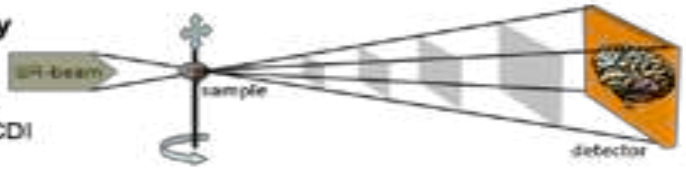
(ii) TXM: Transmission (full field) microscopy

- Absorption Radiography / Tomography
- Phase contrast Radiography / Tomography
- High resolution, down to tens of nm
- Dose inefficient



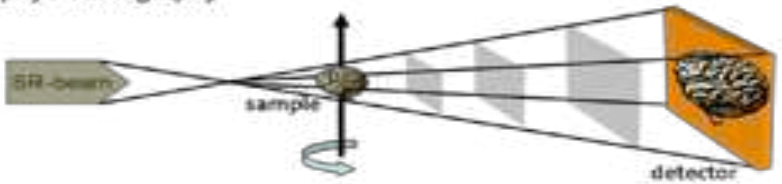
(iii) SXM: Scanning microscopy

- Slow
- Chemical sensitivity / Phase contrast
- For coherent illumination geometry: CDI



(iv) PXM: Projection microscopy

- Phase contrast Radiography / Tomography
- Fast and dose efficient
- High resolution



The radiation dose

Absorbed dose:

$$D = \frac{E_{\text{abs}}}{m} = \frac{\Delta I h\nu}{V\varrho} = \frac{(I_0 - I_1)h\nu}{\varrho A \Delta x}$$

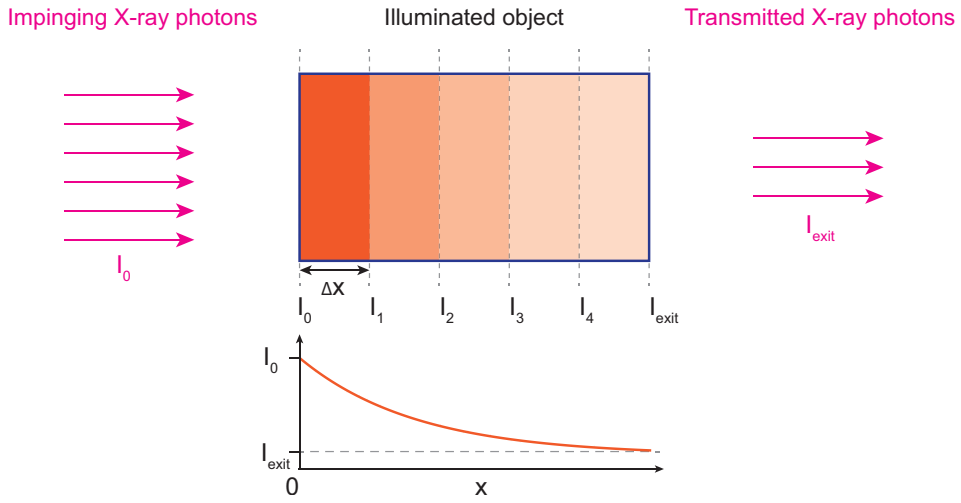
with

$$(I_0 - I_1) = I_0 \cdot \left[1 - e^{-\left(\frac{\mu_{\text{en}}}{\varrho}\right)\varrho\Delta x}\right]$$

Skin (entrance) dose:

$$D = N \cdot \left(\frac{\mu_{\text{en}}}{\varrho}\right) h\nu,$$

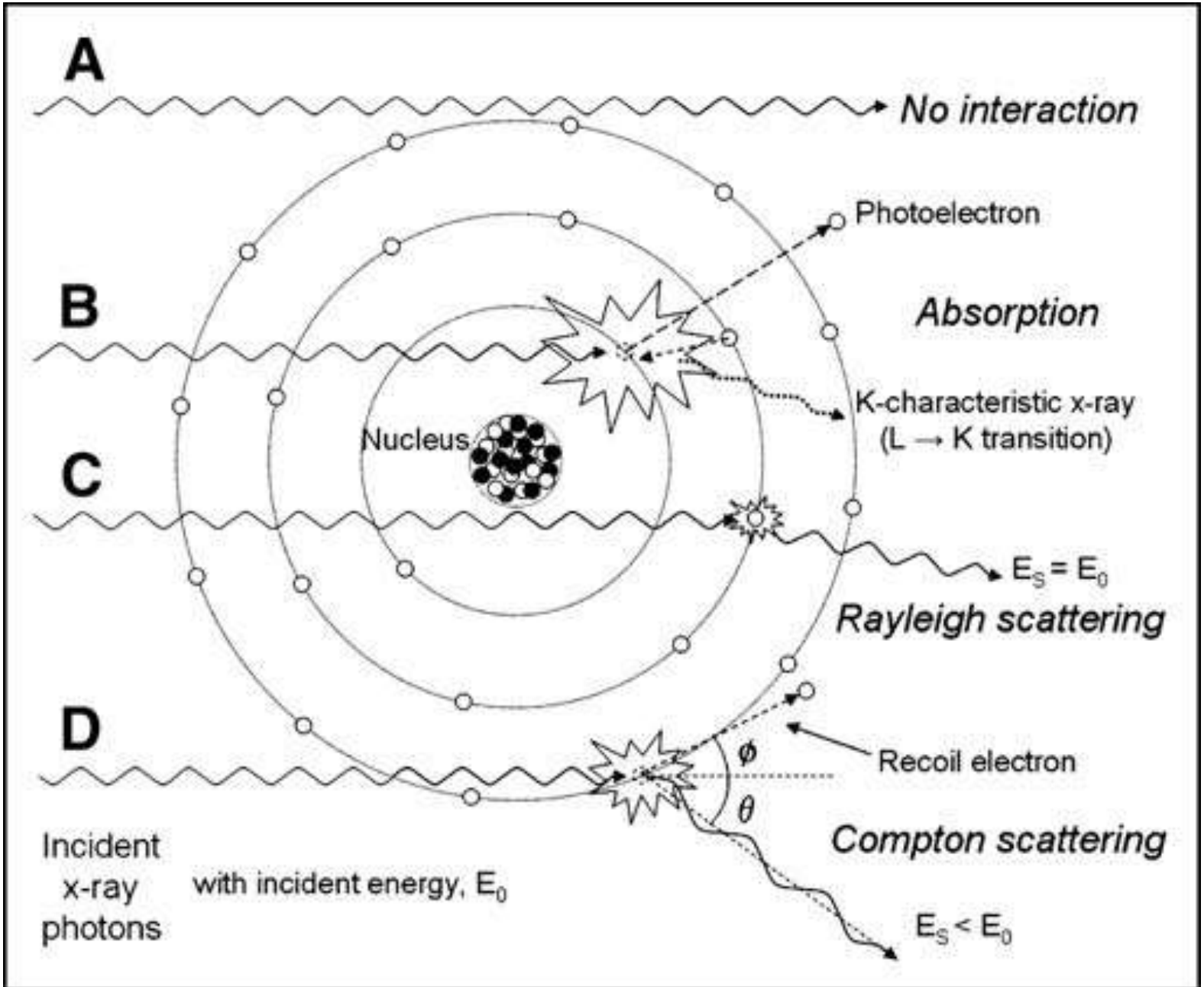
E_{abs}: absorbed energy [J]
m : mass [kg]
ρ : density
ΔI: number of absorbed photons with energy hν
A : cross section area
Δx : slice thickness



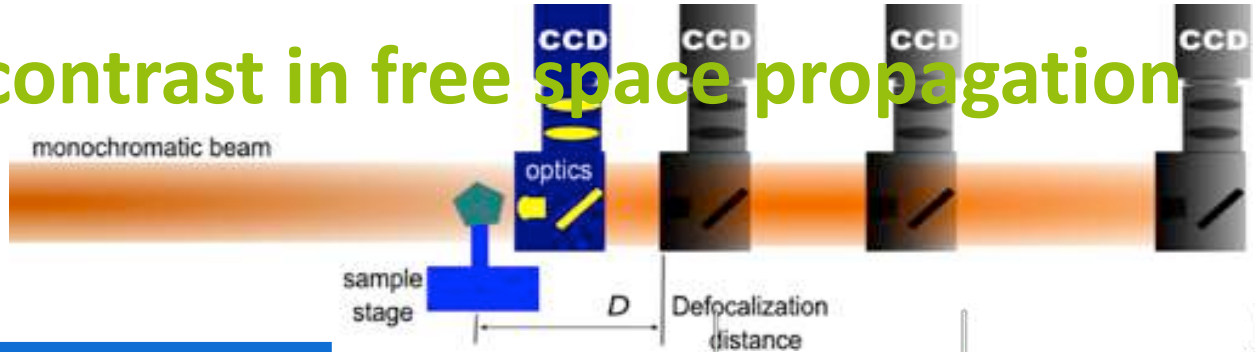
$$D\,[\text{Gy}] = \frac{I_0 h\nu}{\mu^{-1}\rho} \approx 1.602 \times 10^{-4} \cdot \frac{I_0\ [\text{photons}/\mu\text{m}^2] \cdot h\nu\,[\text{eV}]}{\mu^{-1}\ [\mu\text{m}] \cdot \rho\ [\text{g/cm}^3]}.$$

[Howels et al.]

Absorption and scattering



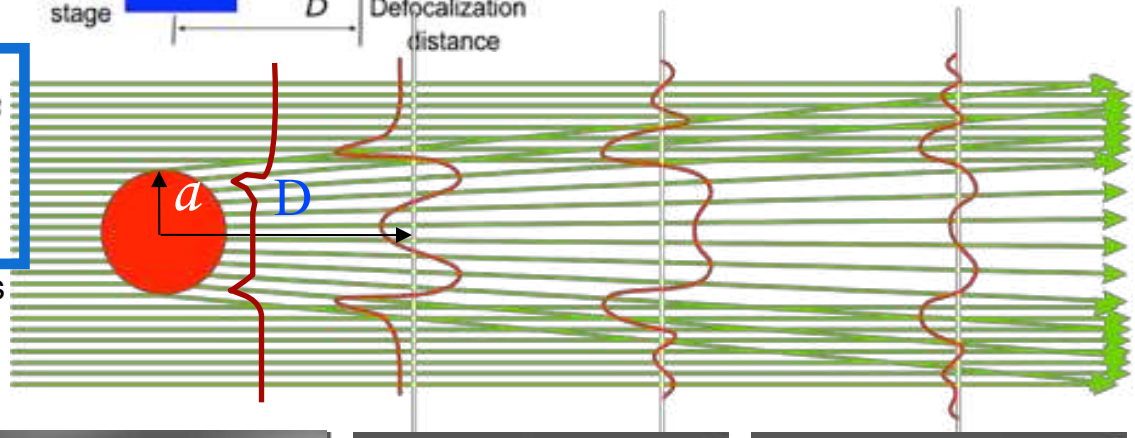
Phase contrast in free space propagation

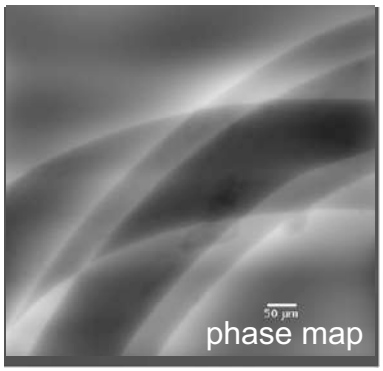


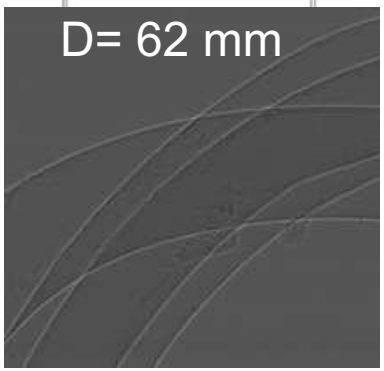
$$U_D(x) = U_0(x) \otimes \sqrt{\frac{-i\pi}{\lambda . D}} . e^{\frac{i\pi}{\lambda . D} . x^2}$$

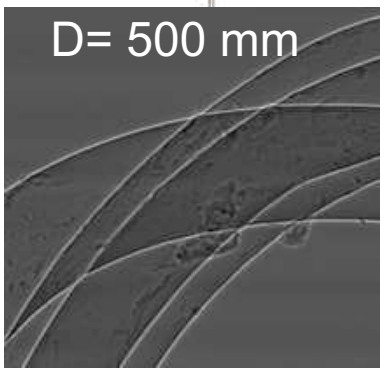
propagator

Born, M., and E. Wolf, 1990, Principles of Optics









Three phase fibers

Fresnel diffraction
Partially coherent illumination

$$\varphi(f) = \frac{\sum_m \sin(\pi \lambda D_m f^2) I_m(f)}{\sum_m 2\sin^2(\pi \lambda D_m f^2)}$$

Cloetens et al. J. Phys. 1999

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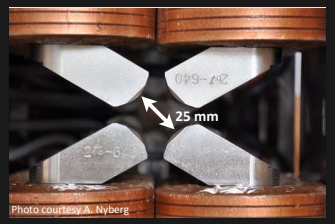

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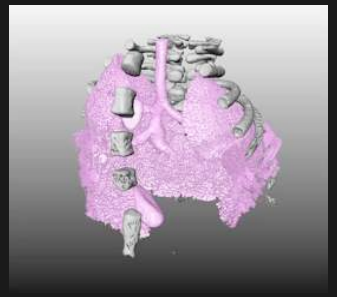

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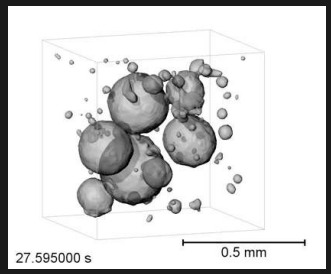

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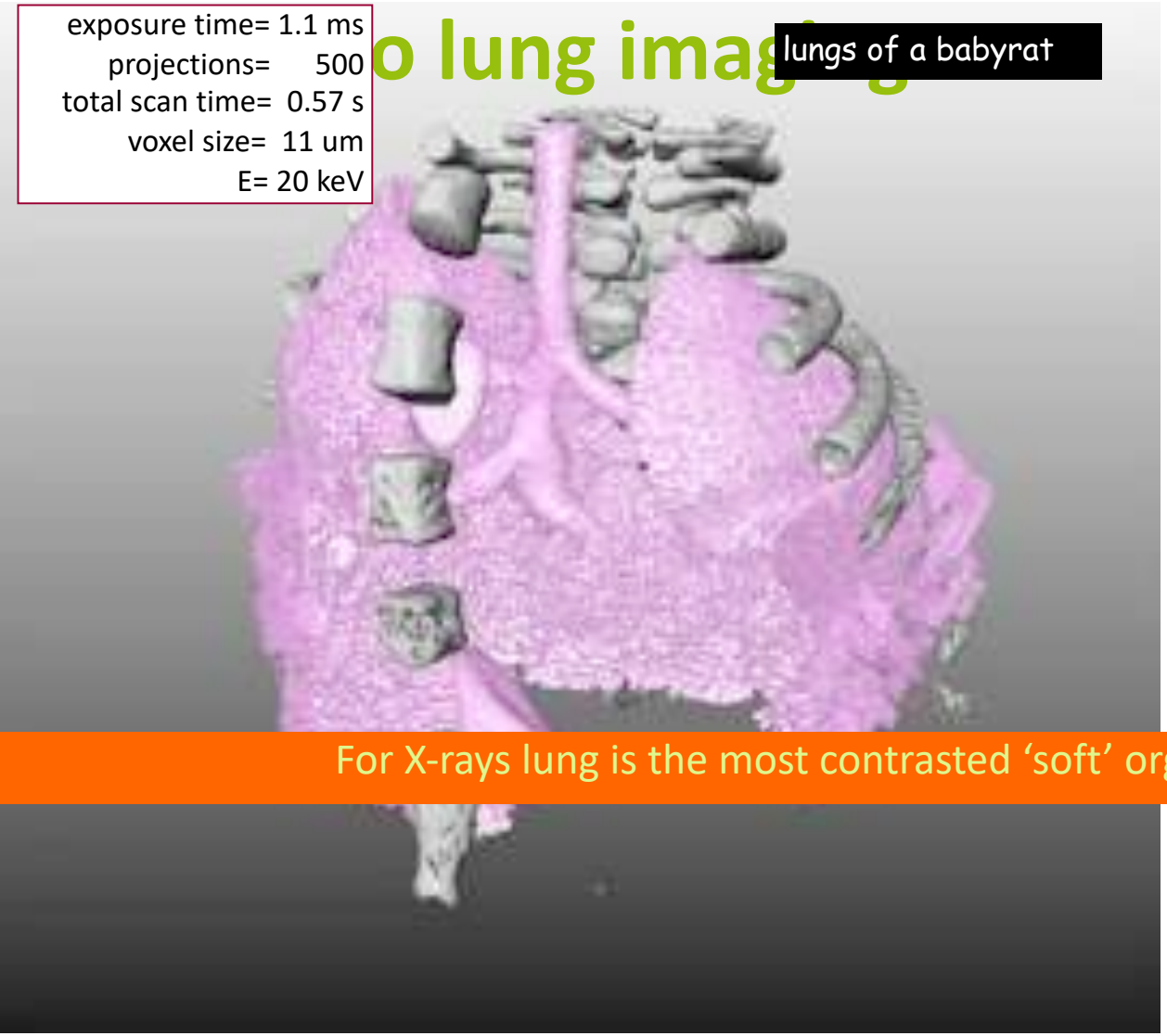
o lung imag

exposure time= 1.1 ms
projections= 500
total scan time= 0.57 s
voxel size= 11 um
E= 20 keV

lungs of a babyrat



For X-rays lung is the most contrasted ‘soft’ organ in the body

G. Lovric Phys Med 2016

R. Mokso et al AIP Conf. Proc. 1365 (2011)

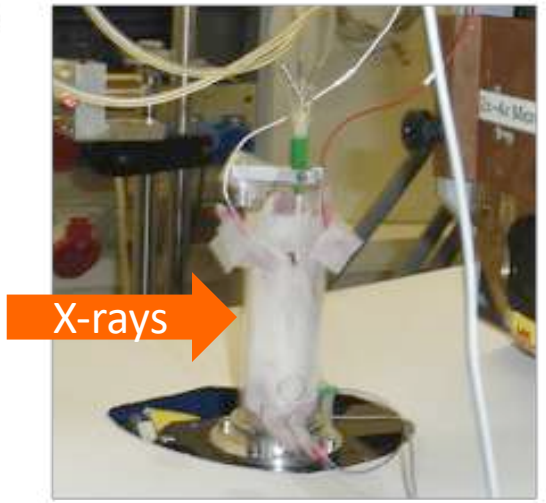
Rajmund.Mokso@maxiv.lu.se

MAXIV

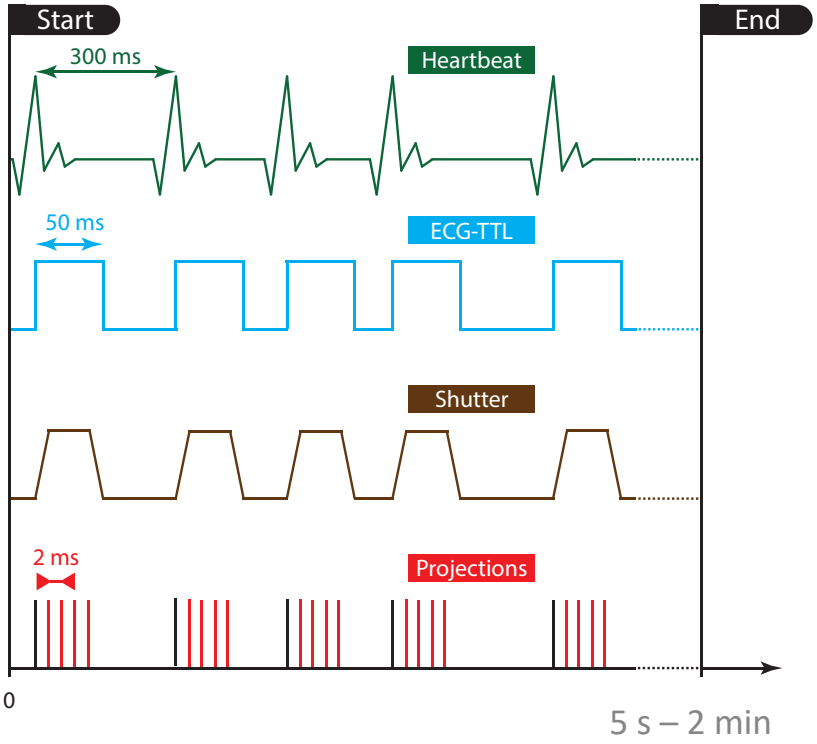
Gated acquisition mode

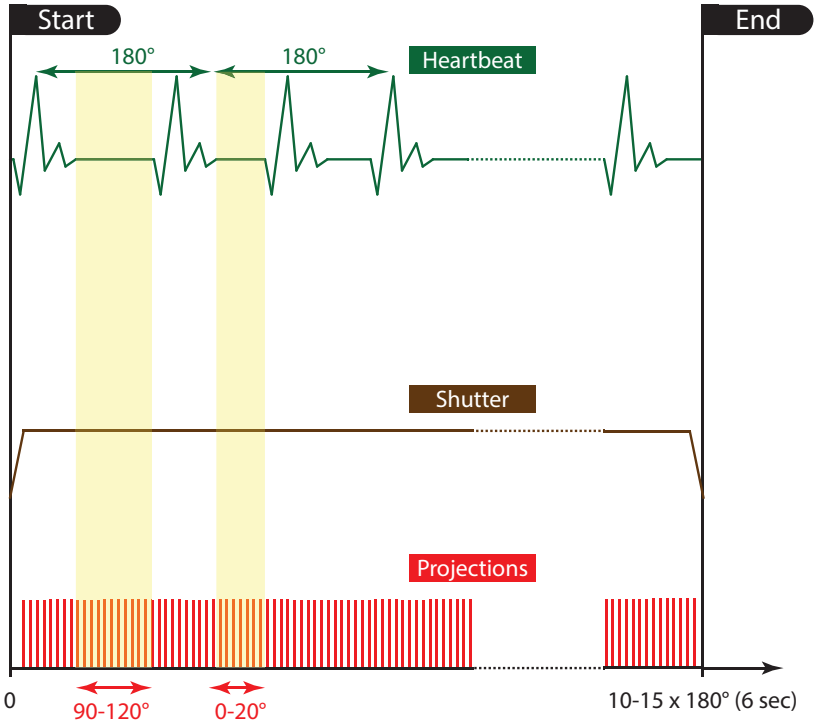
Ventilation and ECG

- Retrospective image guided gating



G. Lovric , PhD thesis





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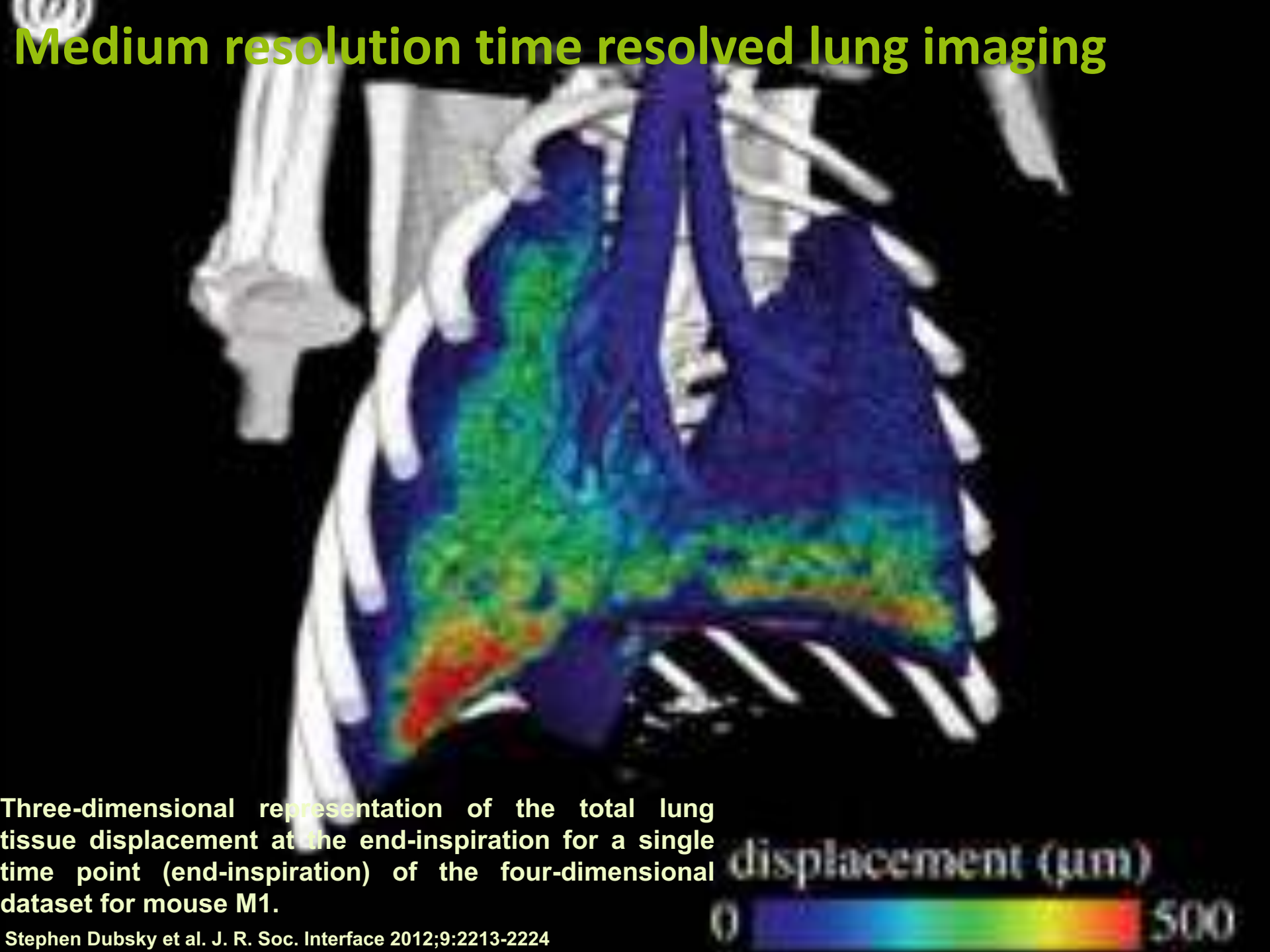
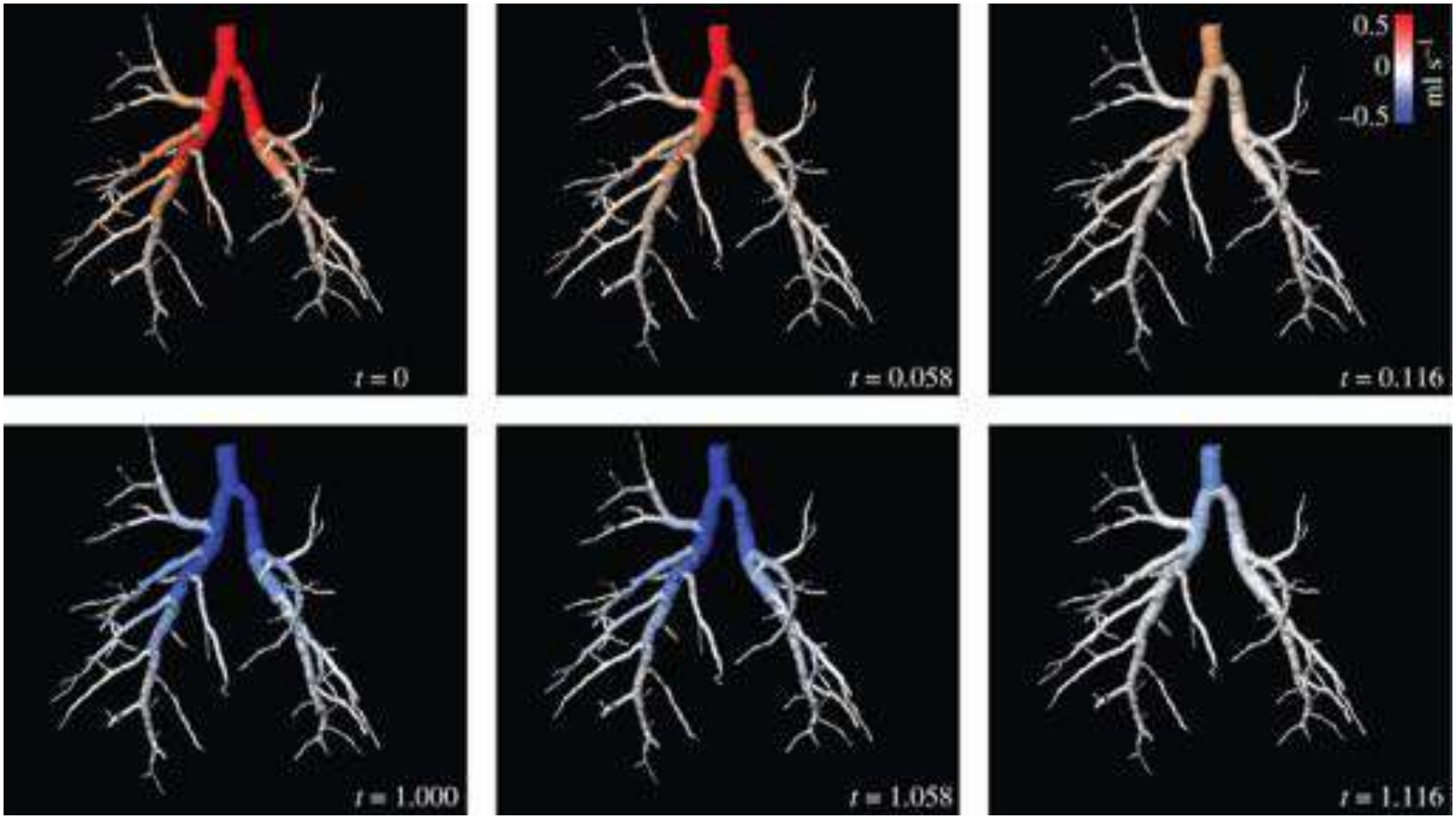
Medium resolution time resolved lung imaging



Three-dimensional representation of the total lung tissue displacement at the end-inspiration for a single time point (end-inspiration) of the four-dimensional dataset for mouse M1.

Stephen Dubsky et al. J. R. Soc. Interface 2012;9:2213-2224

Distribution of air flow through an airway tree in rabbit lungs

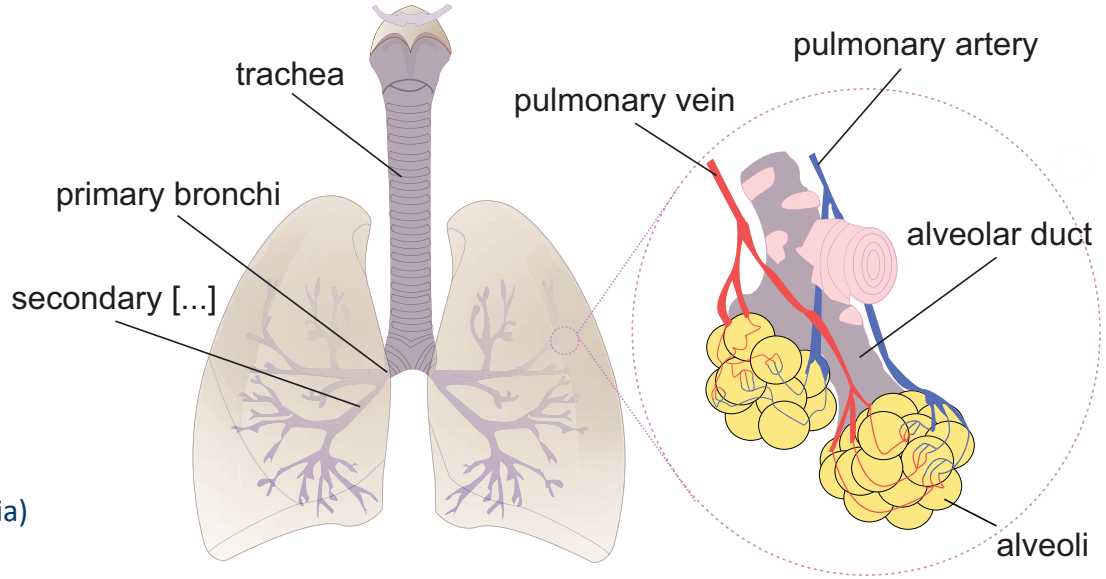


Stephen Dubsky et al. J. R. Soc. Interface 2012;9:2213-2224

Dynamic imaging of lungs: motivation

Ventilator-induced lung injury (VILI)

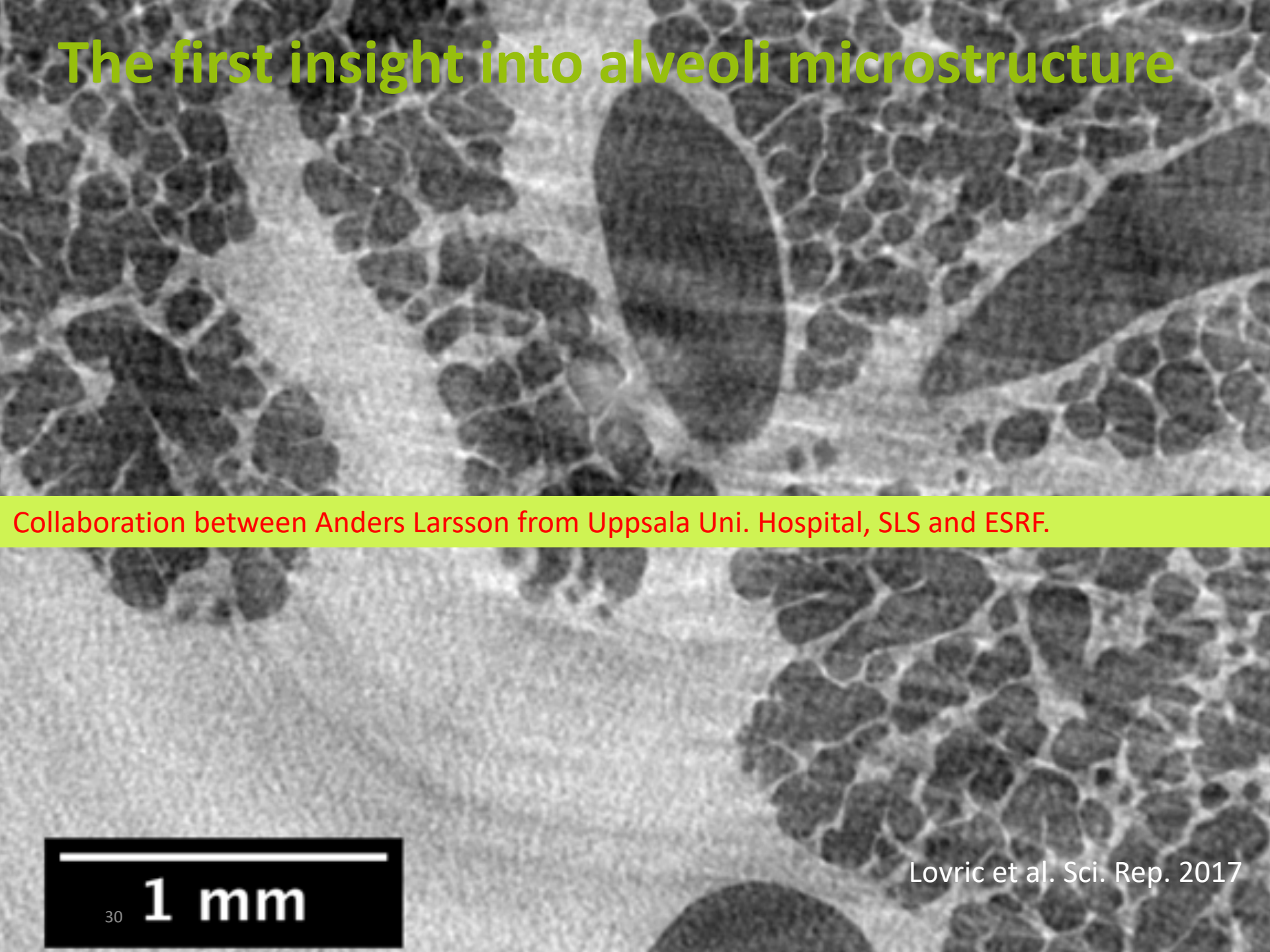
- Overextension of lung tissue in certain lung regions (mechanical damage, biotrauma)
- Still unclear how ventilation induces its deleterious effect [4]
- Hypothesis: local strains in the alveolar wall cause hotspots (overstretching regions)



Human lungs (Source: Wikipedia)

[4] Rausch, S. M. K., Haberthür, D., Stampanoni *et al.*, Ann Biomed Eng **39** (11), 2835 (2011).

The first insight into alveoli microstructure



Collaboration between Anders Larsson from Uppsala Uni. Hospital, SLS and ESRF.

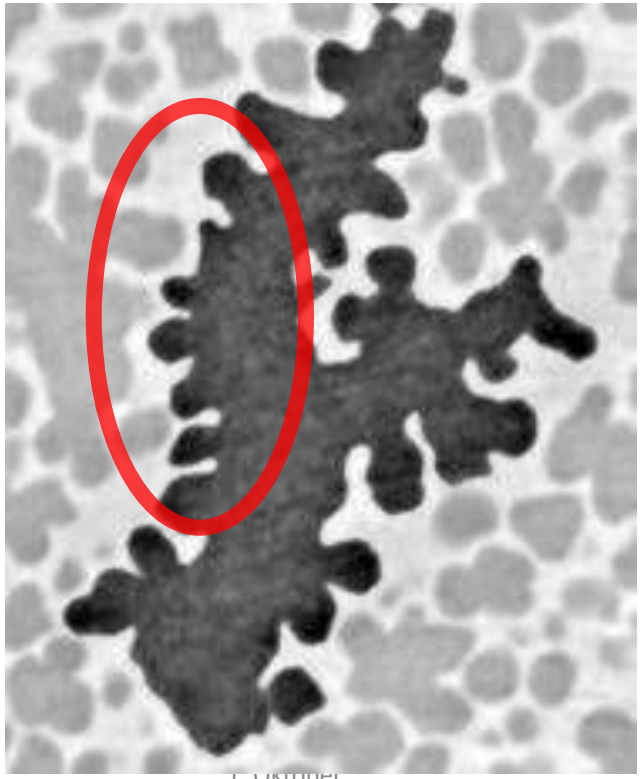
Lovric et al. Sci. Rep. 2017

Lung tissue quantification

Challenges in lung tissue analysis

- How to detect non-linear and regional changes in the lung?
- How to quantify them?

G. Lovric , PhD thesis



$$\Delta p = 5\,\mathrm{cmH_2O}$$

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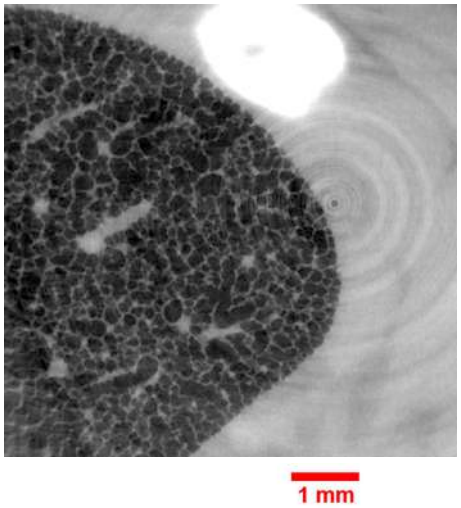
Alveoli dynamics quantification

A detailed insight into the lung

- Apply *quantification* and *labeling* tools, previously used for foam and bone data [14] and dendritic microstructures [15]

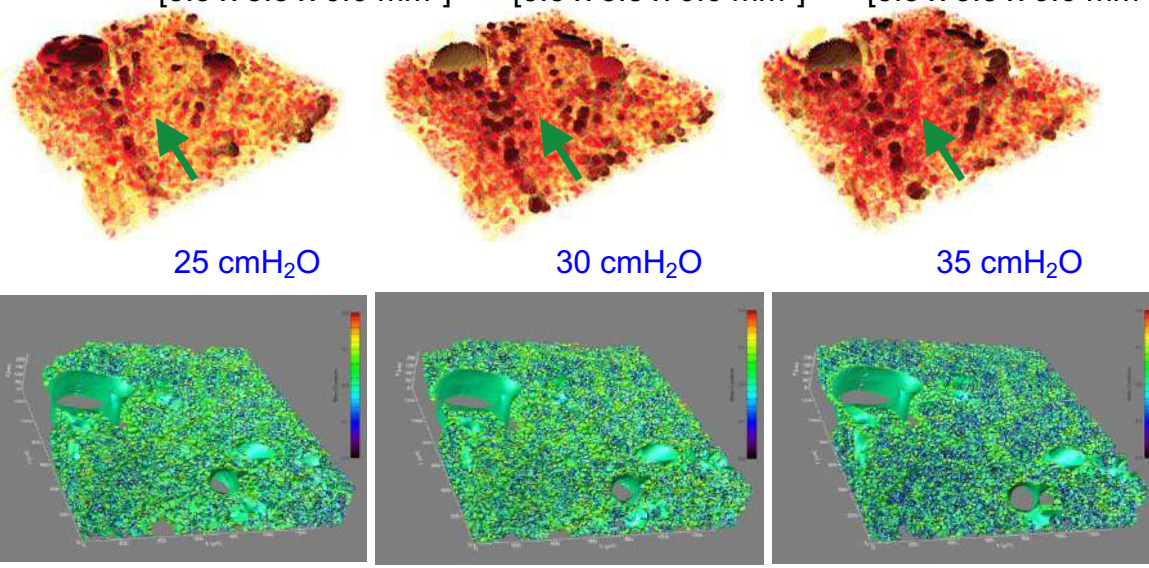
Original tomographic slice



Thickness map

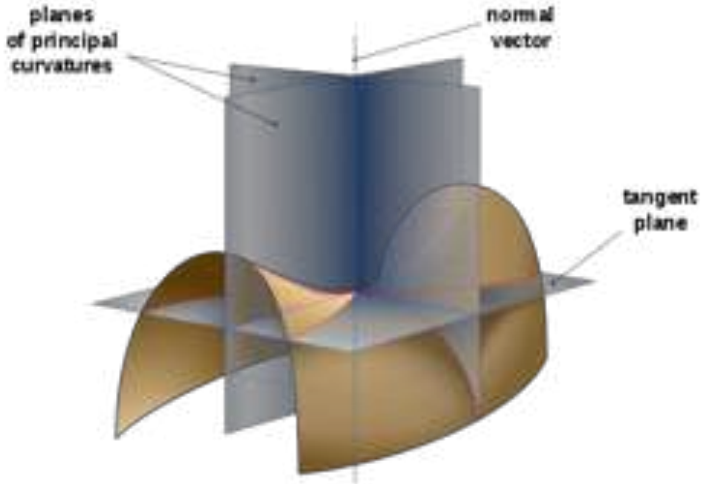
Curvature

[3.5 x 3.5 x 0.6 mm^3] [3.5 x 3.5 x 0.6 mm^3] [3.5 x 3.5 x 0.6 mm^3]

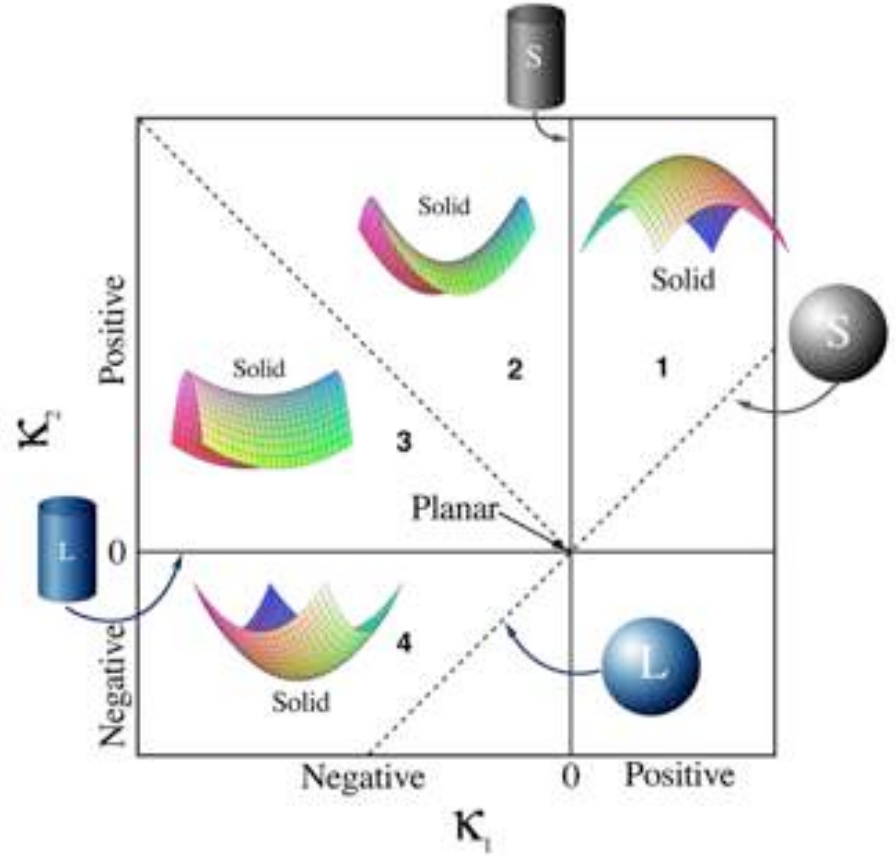


G. Lovric , PhD thesis, Lovric et al. in preparation

Curvature analysis

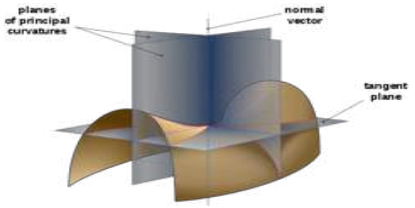


▲ Directions of principal curvatures
(Source: Wikipedia)

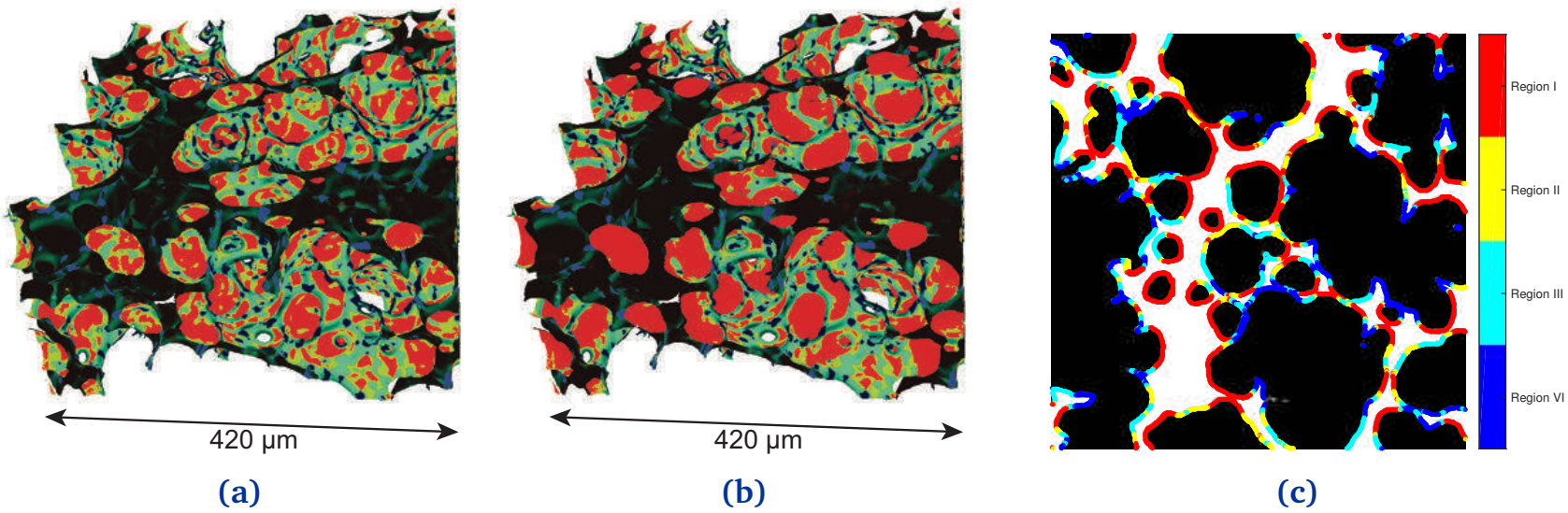


$\kappa_1, \kappa_2 \ldots$ eigenvalues of the shape operator

Shape analysis of lungs alveoli

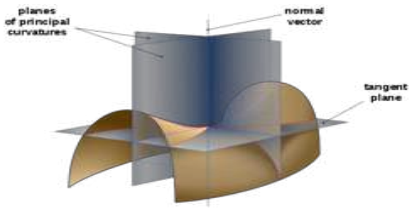


G. Lovric , PhD thesis

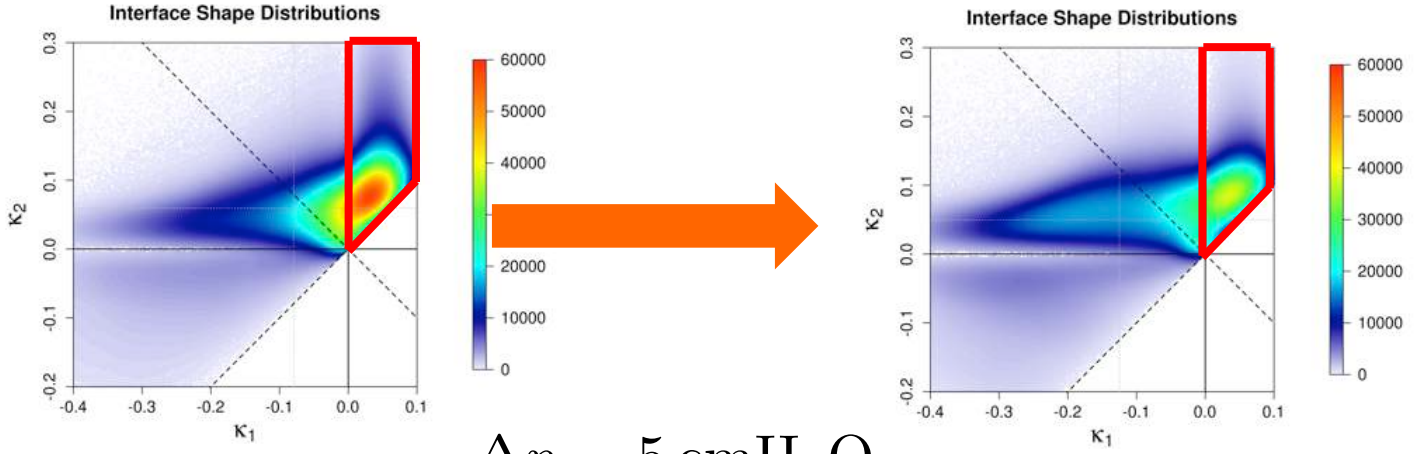


(a) (b) (c)

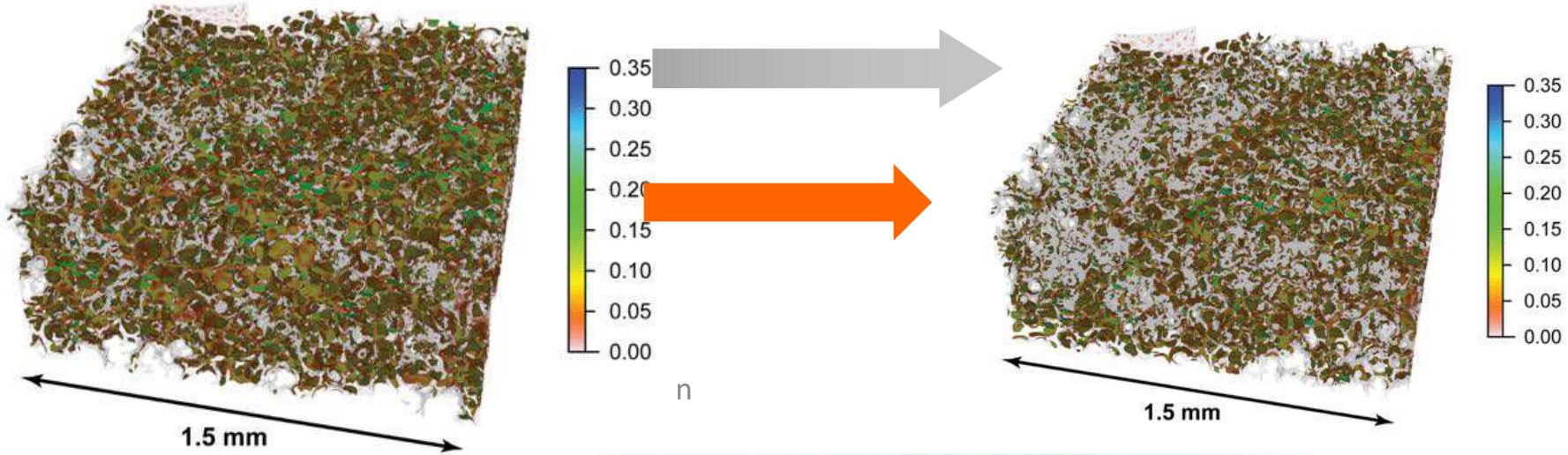
Figure 6.13. 3D visualization of the four regions from the ISD-plot with different geodesic radius: **(a)** depicts the calculation with radius $R = 3.5$ and **(b)** with $R = 15$. In **(c)** a 2D slice is shown from **(b)**.



Gated acquisition mode



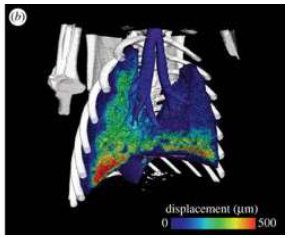
$$\Delta p = 5\,\mathrm{cmH_2O}$$



G. Lovric , PhD thesis, Lovric et al. in preparation

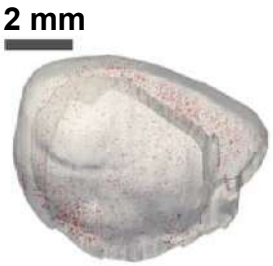
Hierarchical imaging of tissues

Medical imaging and therapy
(in vivo, medium resolution >30 um, low dose, large beam , large FOV)

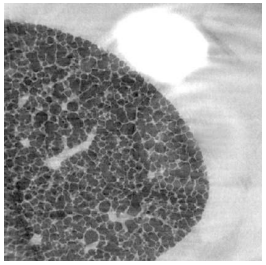


Longitudinal in vivo

The whole organ

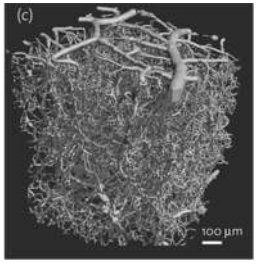


Down to a micrometer resolution
(rarely in vivo, high resolution ~ 1um, higher dose, small FOV)



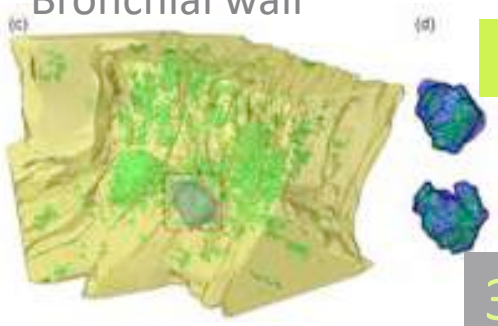
Accute in vivo

Zooming into organs



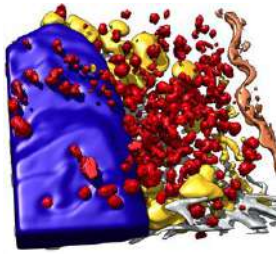
Nano-scale imaging beamlines
(fixed tissue, resolution ~ 100nm, high dose, small samples ~100um)

Bronchial wall



Fixed tissue

Cell level



3 orders of magnitude in spatial resolution

MAX IV

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Al foam – from nucleation to cell wall rupture

Real life system dynamics

The rise of the Aluminum foam:
From nucleation to film rupture
Acquisition speed: 208 tomo / s
TOMCAT beamline, SLS

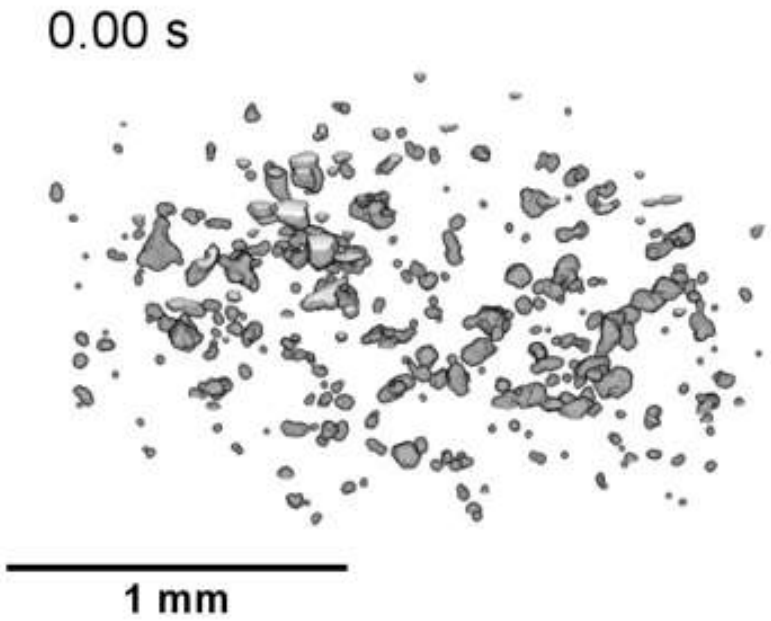
nature COMMUNICATIONS

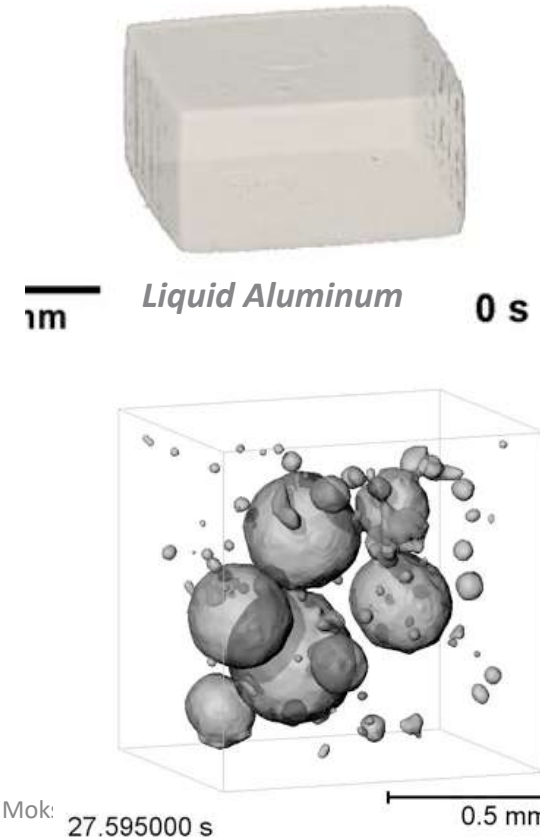
ARTICLE

https://doi.org/10.1038/s41467-019-11521-1 OPEN

Using X-ray tomoscopy to explore the dynamics of foaming metal

Francisco García-Moreno[1,2], Paul Hans Kamm[1,2], Tillmann Robert Neu[1,2], Felix Bülk[1,2], Rajmund Mokso[3], Christian Matthias Schlepütz[4], Marco Stampanoni[4,5] & John Banhart[1,2]



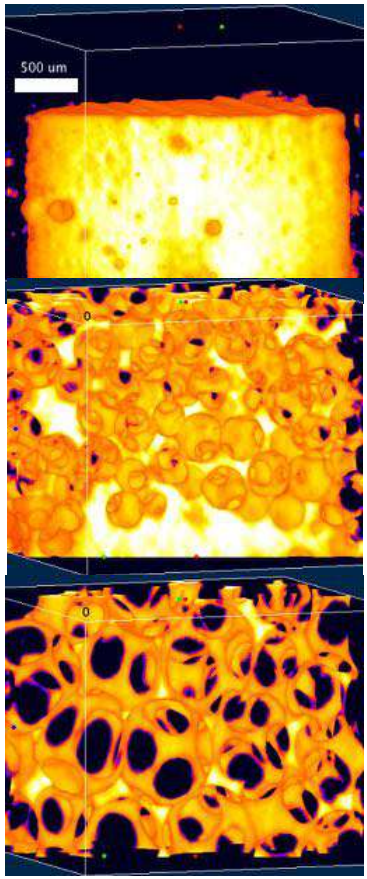


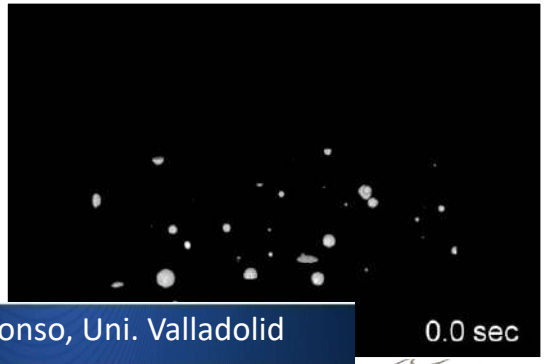
PU foams

Nucleation

”Liquid” foam

Solid foam

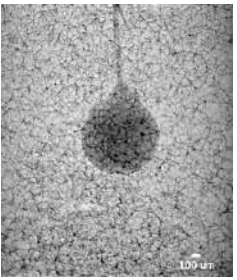
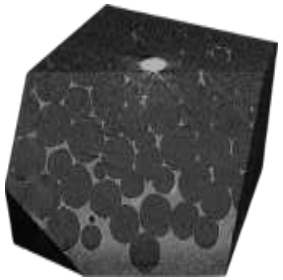
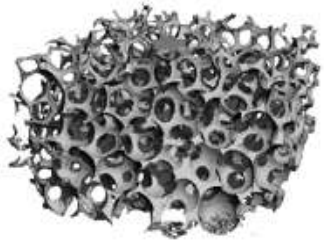
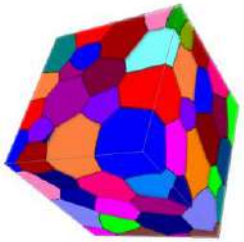
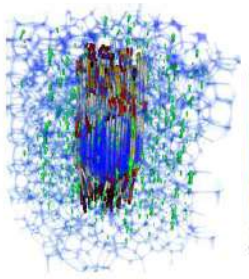
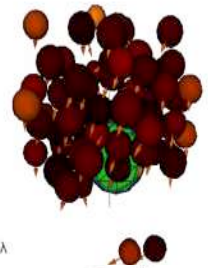




E. Solorzano, S. Alonso, Uni. Valladolid

Data courtesy of E. Solorzano and S. Alonso, Univ. Valladolid

Image-based quantitative information retrieval

acquisition

Scanning
Sample conditioning

reconstruction

segmentation

feedback

1TB / 2 min

robust, simple & universal

labeling

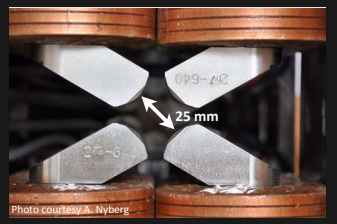
quantification

visualization

Customized & flexible

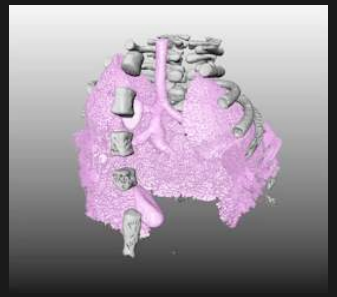
Rajmund.Mokso@maxiv.lu.se

Outline

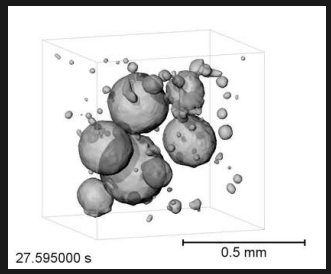


I. Brief introduction into tomographic microscopy
   I. Acquisition and reconstruction

II. Applications
   I. Bio: lungs
   II. Hard matter: Aluminum foams



III. Overview of MAX IV instruments for imaging
   I. Beamlines, techniques

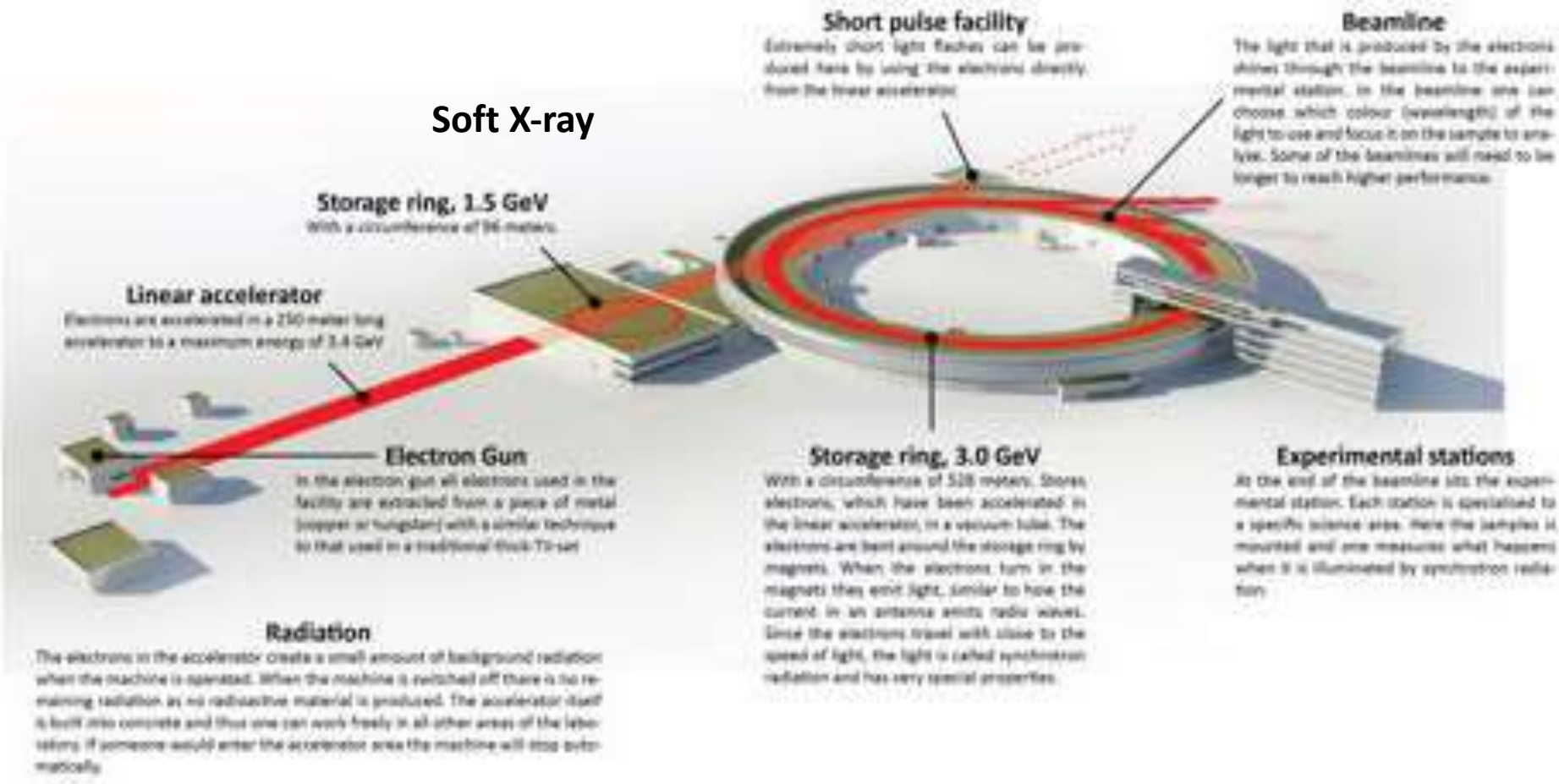


Rajmund.Mokso@maxiv.lu.se

Vetenskapsrådet

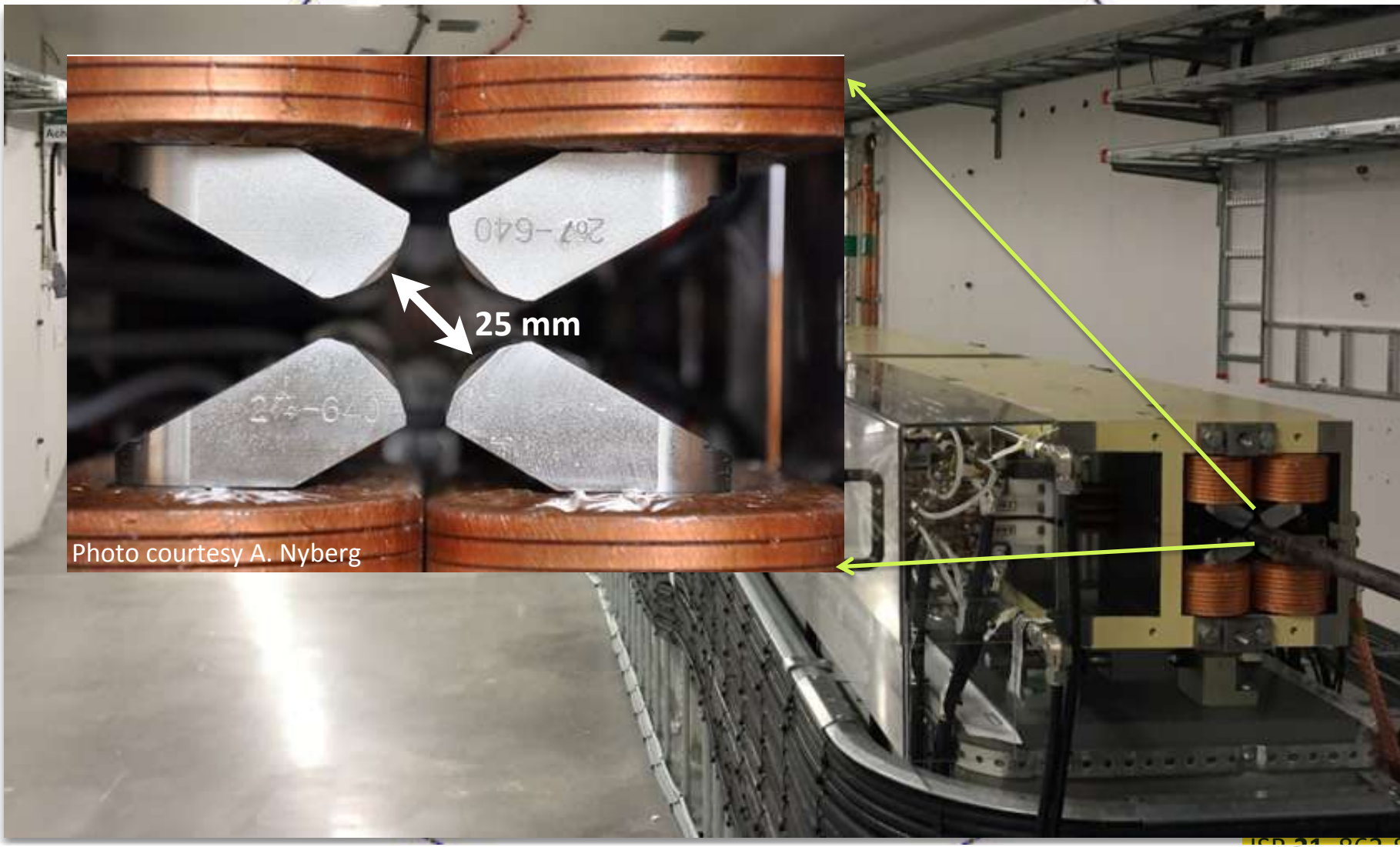
MAX IV

Investment in accelerator ~1150 MSEK
13 initial beamlines ~900 MSEK
+ 3 beamlines



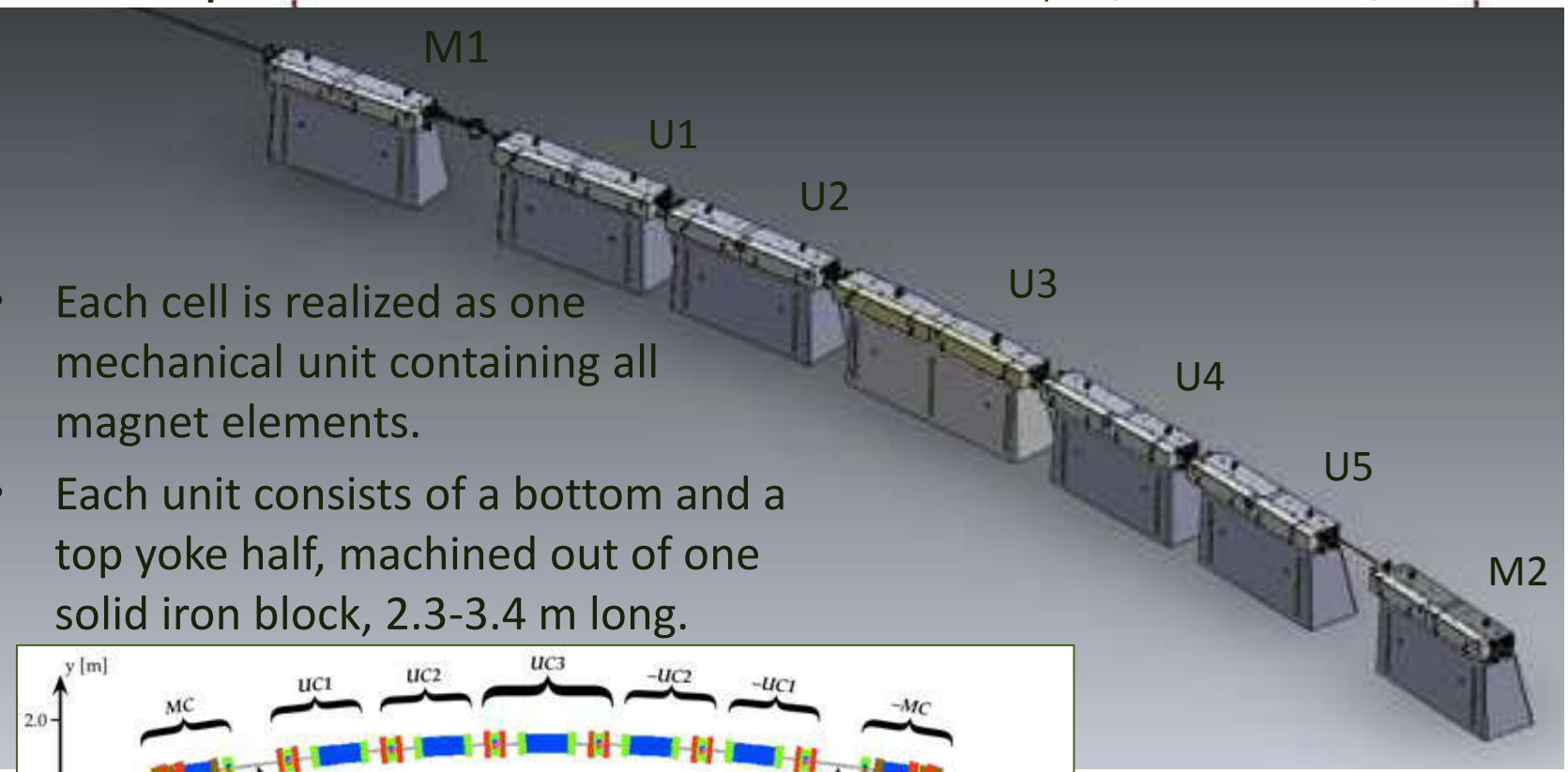
MAX IV storage ring

- 528 m circumference, 500 mA with top-up, 20 achromats

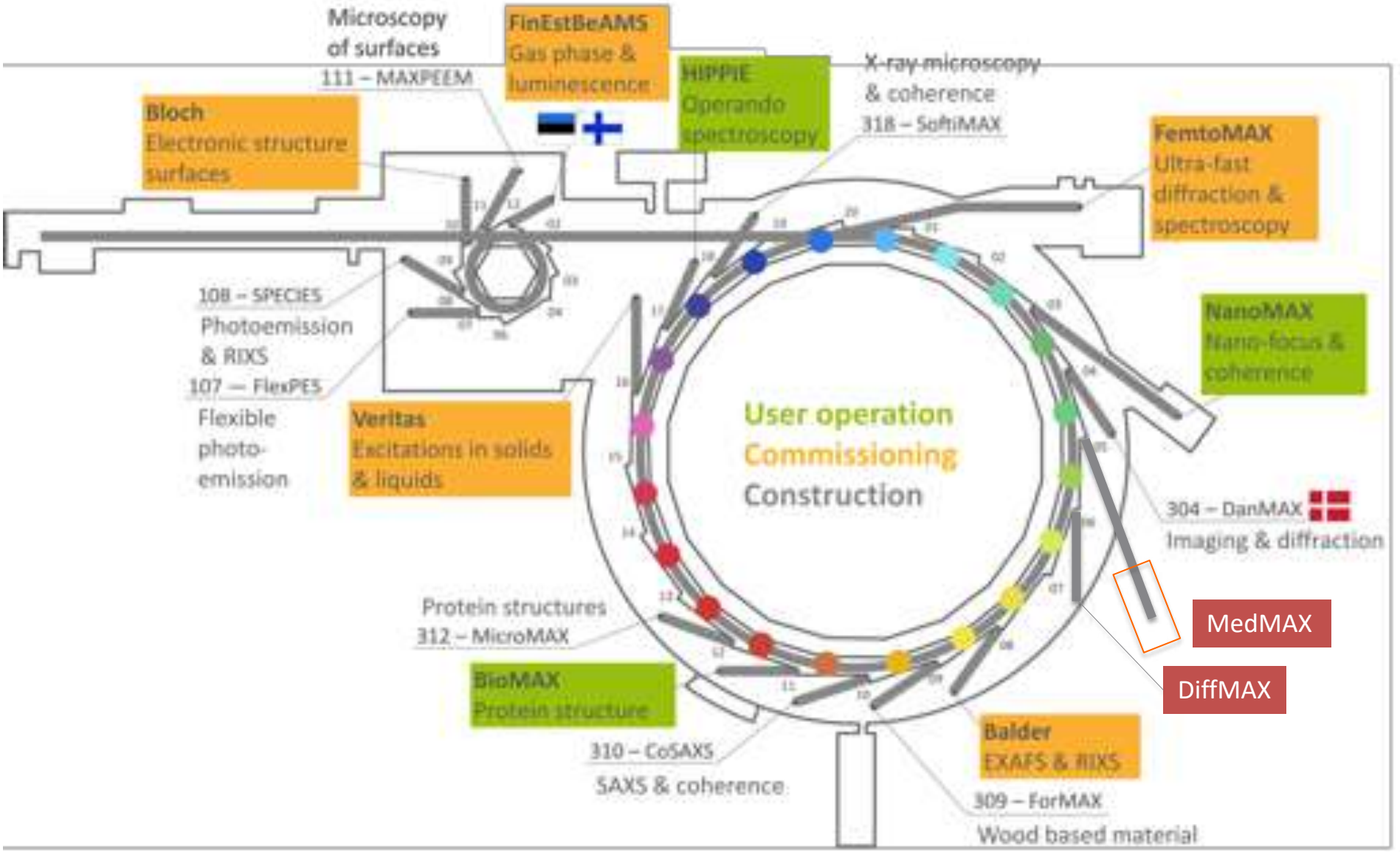


MAX IV magnets

- 528 m circumference, 500 mA with top-up, 20 achromats
- 19 long straights (4.6 m) for users, 1 for injection
- 40 short straights (1.3 m) for RF & diagnostics
- 7-bend achromat: 5 unit cells (3°) & 2 matching cells (1.5° LGB)
- 328 pm rad bare lattice emittance (ε_y adjusted to 2-8 pm rad)



- Each cell is realized as one mechanical unit containing all magnet elements.
- Each unit consists of a bottom and a top yoke half, machined out of one solid iron block, 2.3-3.4 m long.


Microscopy of surfaces
111 – MAXPEEM
FinEstBeAMS
Gas phase & luminescence
HIPPIE
Operando spectroscopy
X-ray microscopy & coherence
318 – SoftiMAX
Bloch
Electronic structure surfaces
FemtoMAX
Ultra-fast diffraction & spectroscopy
108 – SPECIES
Photoemission & RIXS
107 – FlexPES
Flexible photo-emission
Veritas
Excitations in solids & liquids
NanoMAX
Nano-focus & coherence
User operation
Commissioning
Construction
304 – DanMAX
Imaging & diffraction
MedMAX
DiffMAX
Protein structures
312 – MicroMAX
BioMAX
Protein structure
Balder
EXAFS & RIXS
310 – CoSAXS
SAXS & coherence
309 – ForMAX
Wood based material

Tomography in Lund

Zeiss Xradia XRM 520 since 2015
www.solid.lth.se/resources/4d-imaging-lab/

NanoMAX

The nanofocus beamline
(tomography maybe after 2020)

DanMAX

Diffraction & tomography

ForMAX

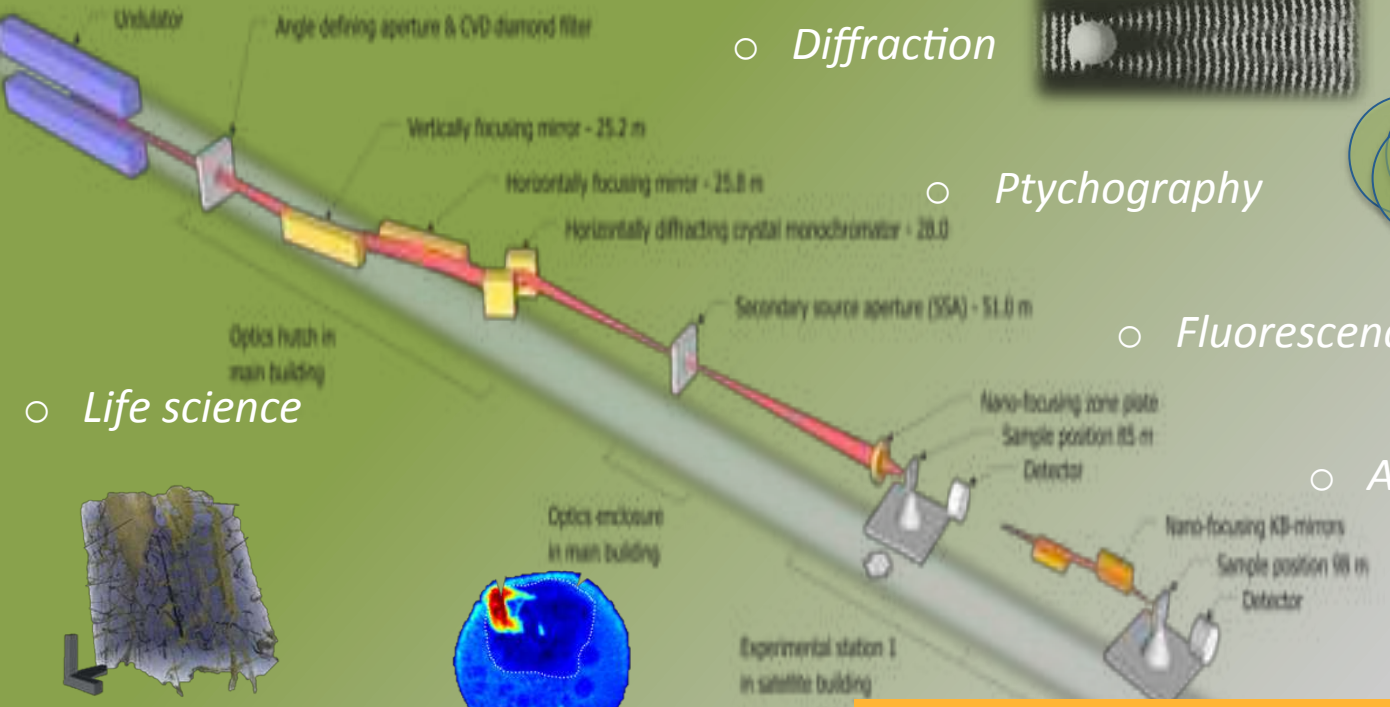
SAXS beamline with
some tomography

2016 2017 2018 2019 2020 2021 2022 2023

Rajmund.Mokso@maxiv.lu.se

NanoMAX: scanning X-ray nano-probe

2D & 3D
Structure & strain
Elemental distribution
Morphology



- *Diffraction*
- *Ptychography*
- *Fluorescence*
- *Absorption*
- *Life science*

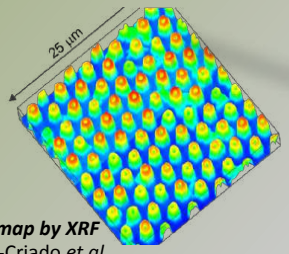
Bone inner structure by Ptychography
M Dierolf *et al. Nature* 2010 467, 436-439

Malaria pigment in red blood cell by XRF
F. Dubasr et al. Chem. Commun 2012 48, 910

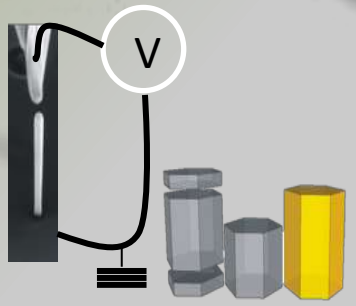
Focusing beam to ~40 nm (10 nm)
Clean and with high degree of coherence

- *Materials science*

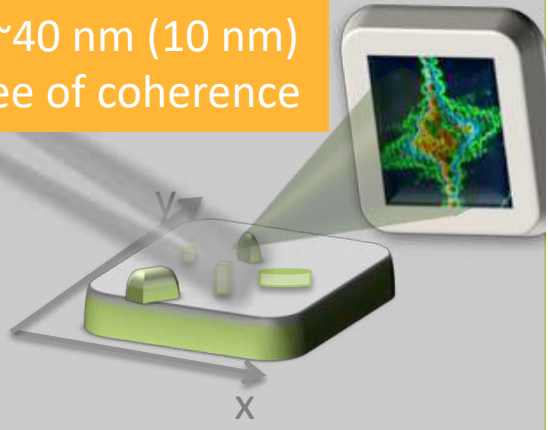
Strain in SiGe device by Bragg ptychography
S. O. Hruszkewycz et al. arXiv:1506.01262v1 [cond-mat.mtrl-sci]



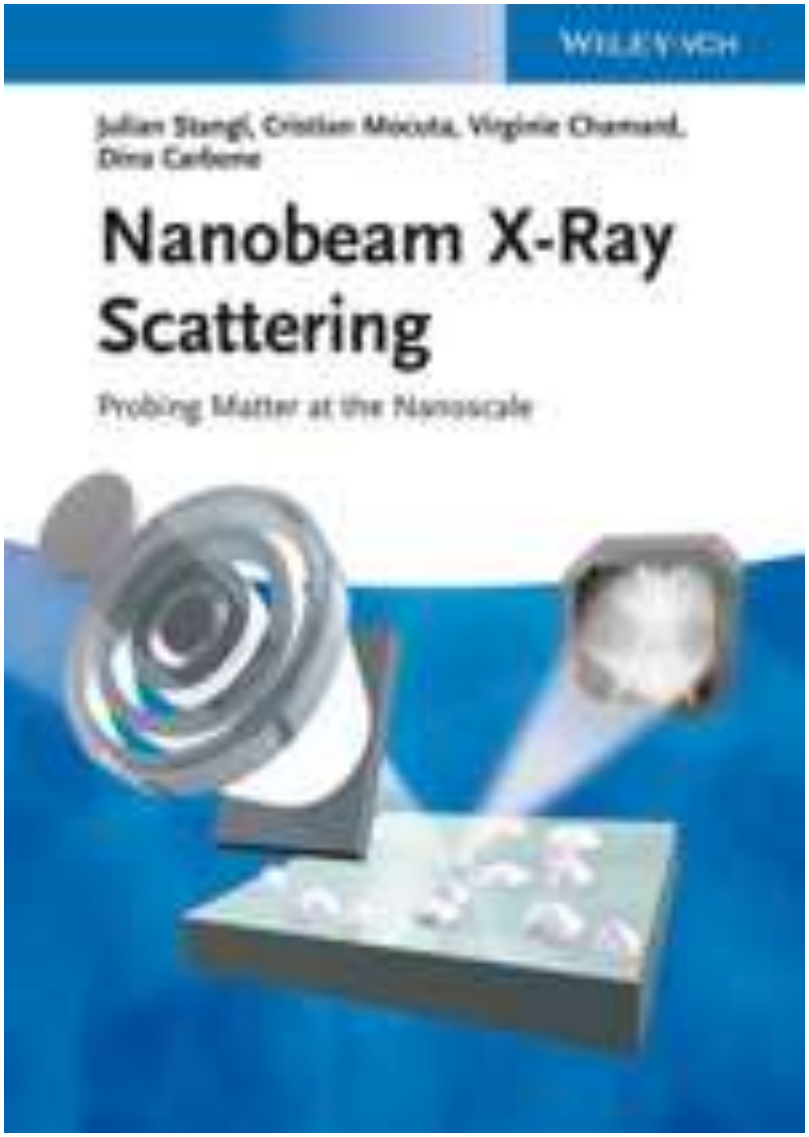
Ga density map by XRF
G. Martinez-Criado *et al*
Nano Lett. (2012) **12**, 5829

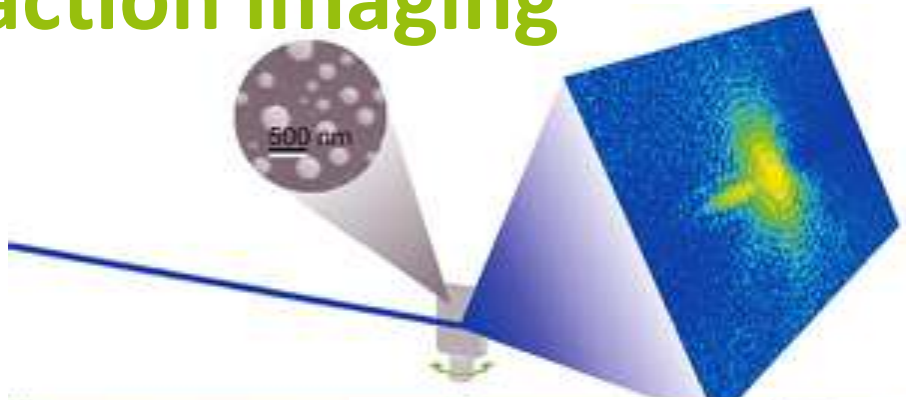


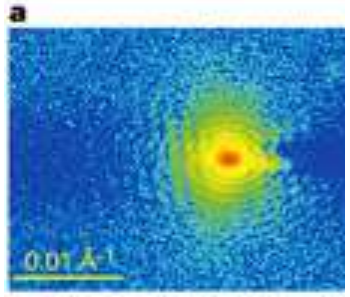
Structure and transport in GaAsby In-Situ XRD
G. Bussone te al. *Nano Lett.* 2015, 15 981

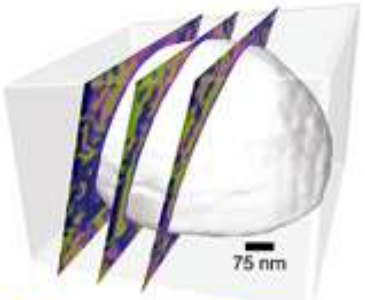


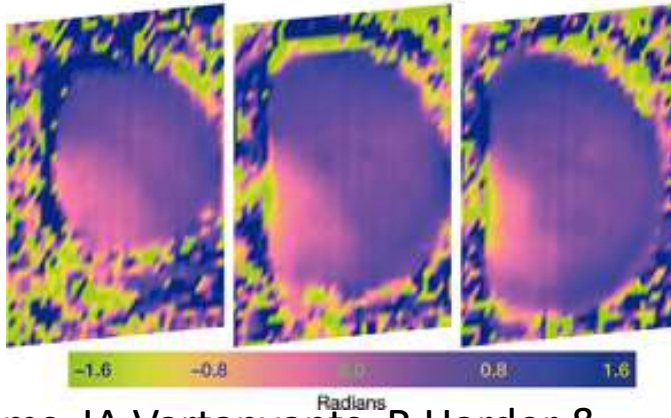
Bragg coherent diffraction imaging









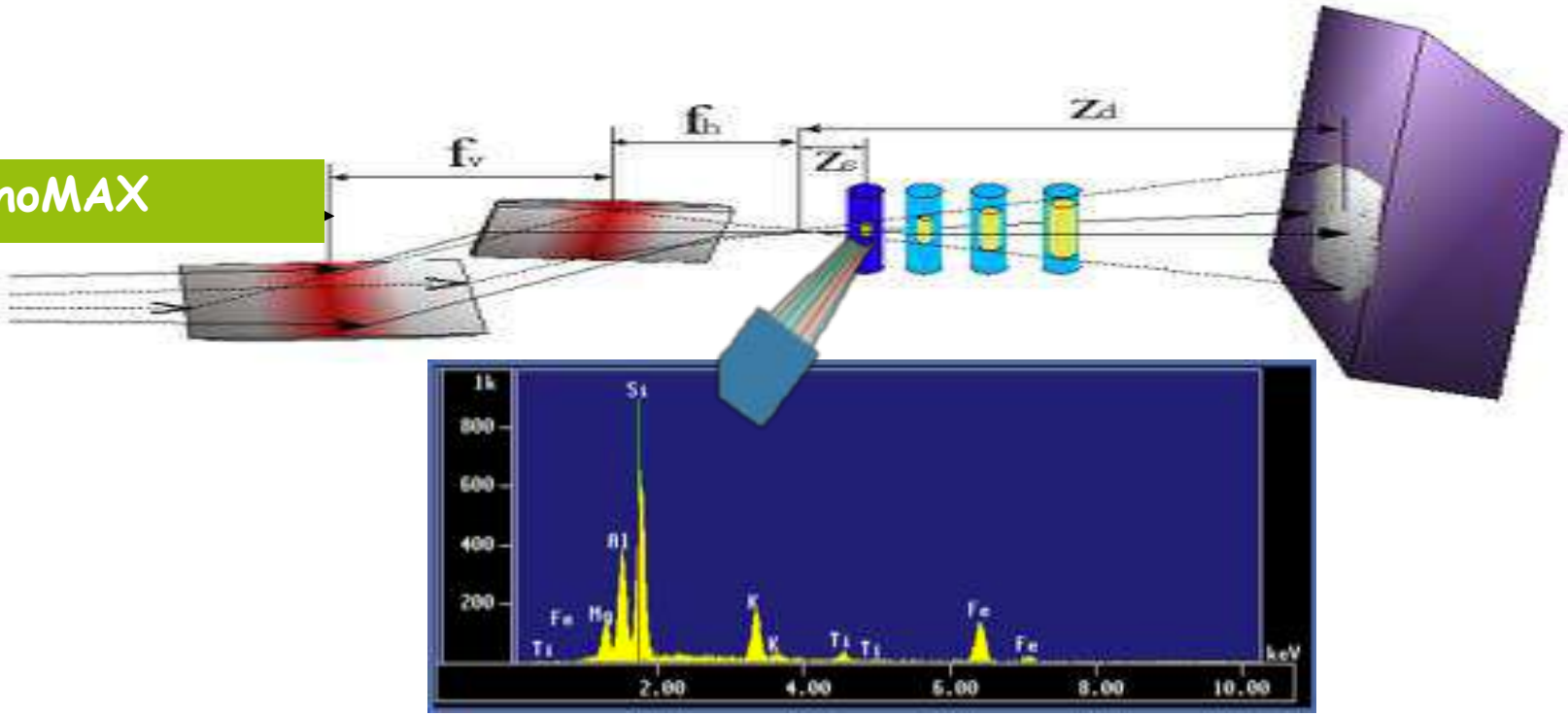


MA Pfeifer, GJ Williams, IA Vartanyants, R Harder & IK Robinson, *Three dimensional mapping of a deformation field inside a nanocrystal*. **Nature 442**, 63-66 (2006)

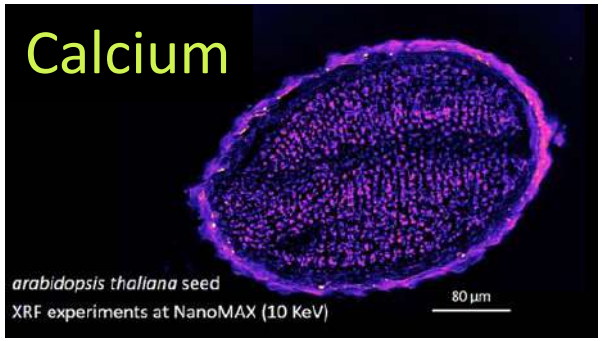
Nanoimaging, Fluorescence spectroscopy

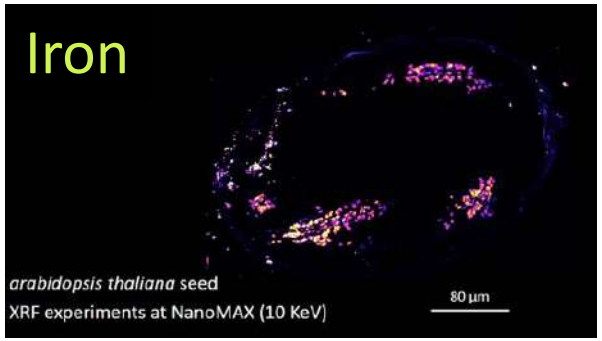
NanoMAX

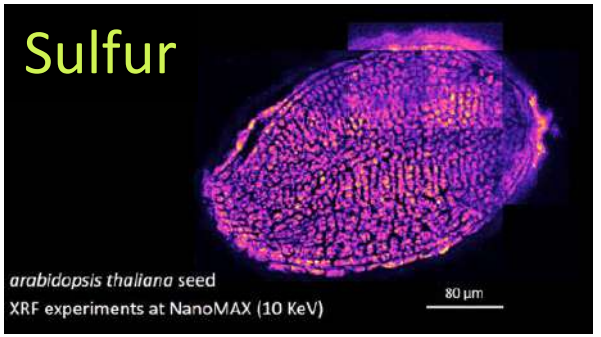
source



Elemental map distribution in arabidopsis seed



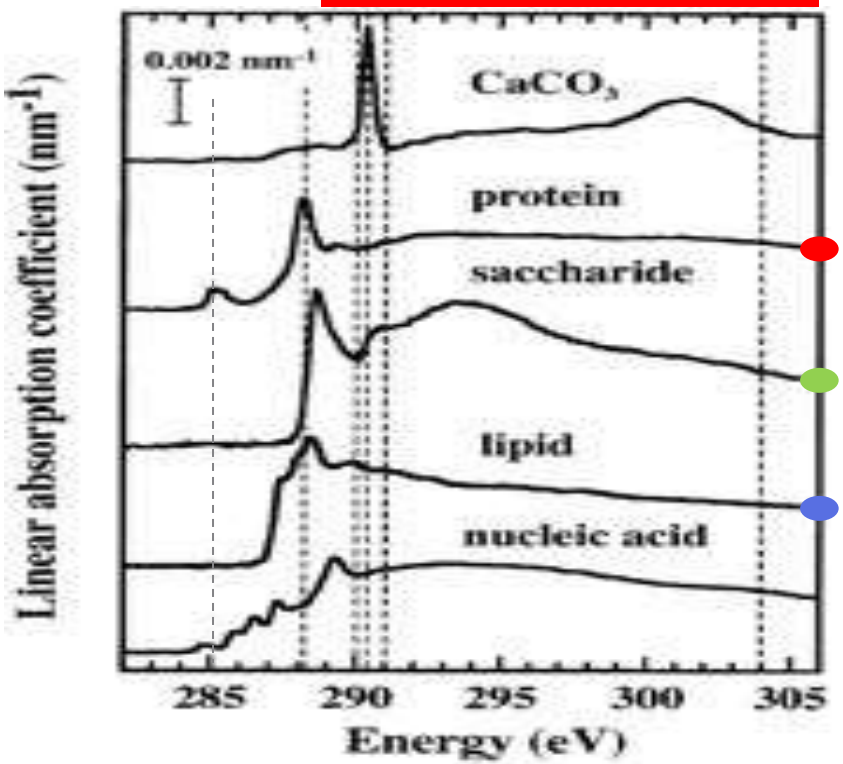




Rajmund.Mokso@maxiv.lu.se

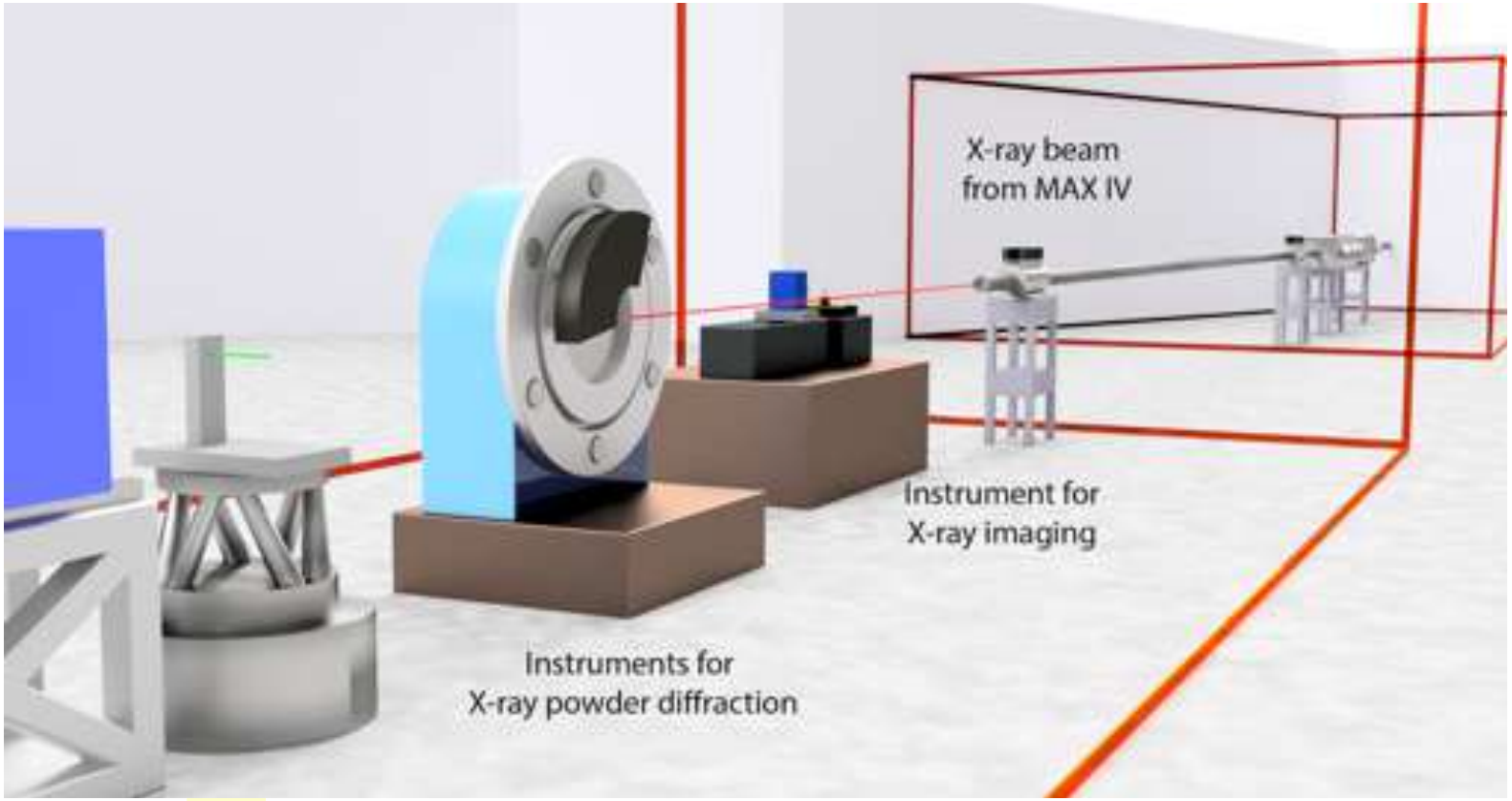
SoftiMAX:
Soft X-ray scanning spectro-microscopy

In operation from 2020

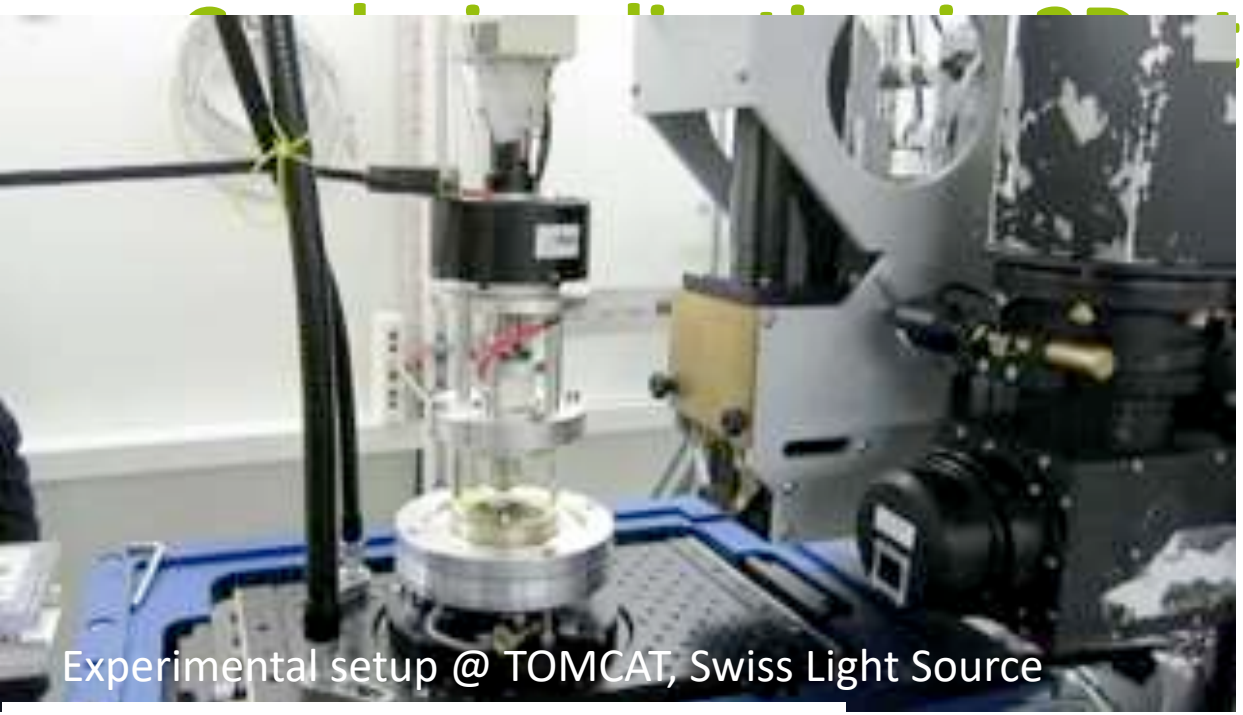


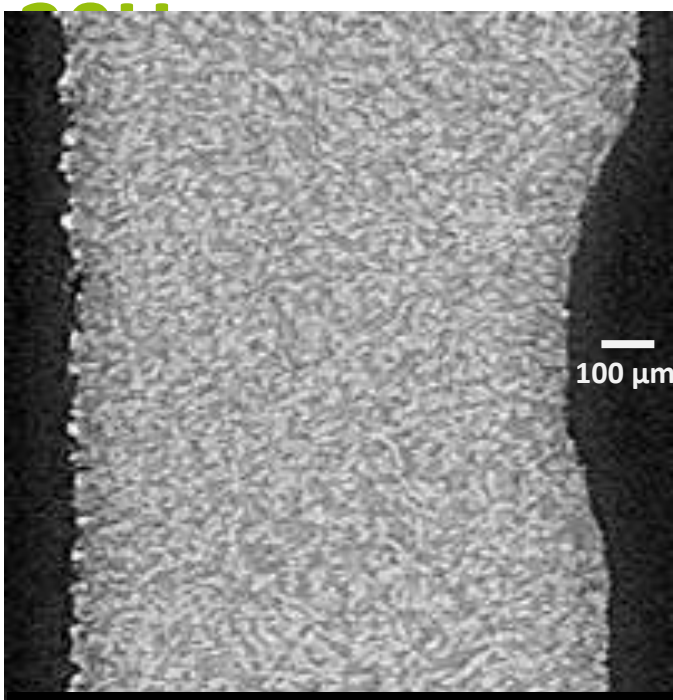
Chemical contrast at the nanoscale

DanMAX: Tomographic microscopy and Powder diffraction

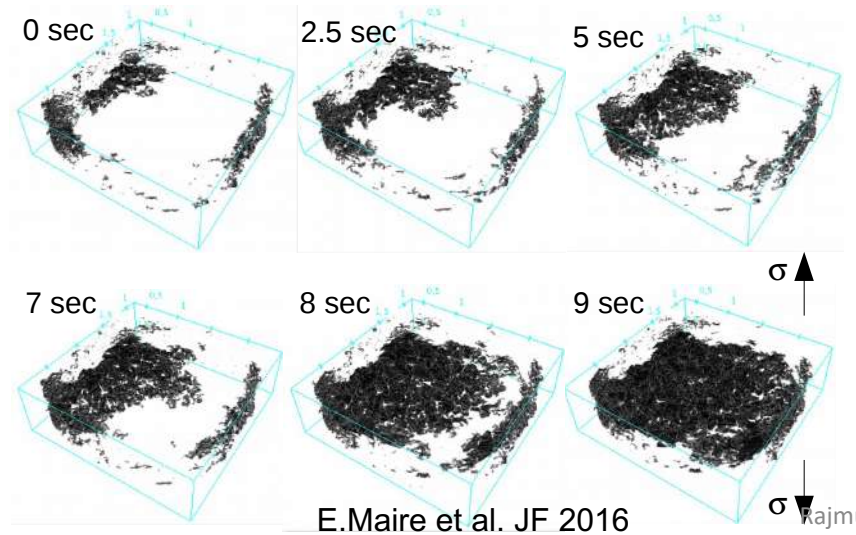


Fast tomography to study in situ materials





Vertical tomographic slice, time separation ~ 50 ms, voxel = 3µm



E.Maire et al. JF 2016

Al – Alumina (Eric Maire, INSA Lyon)

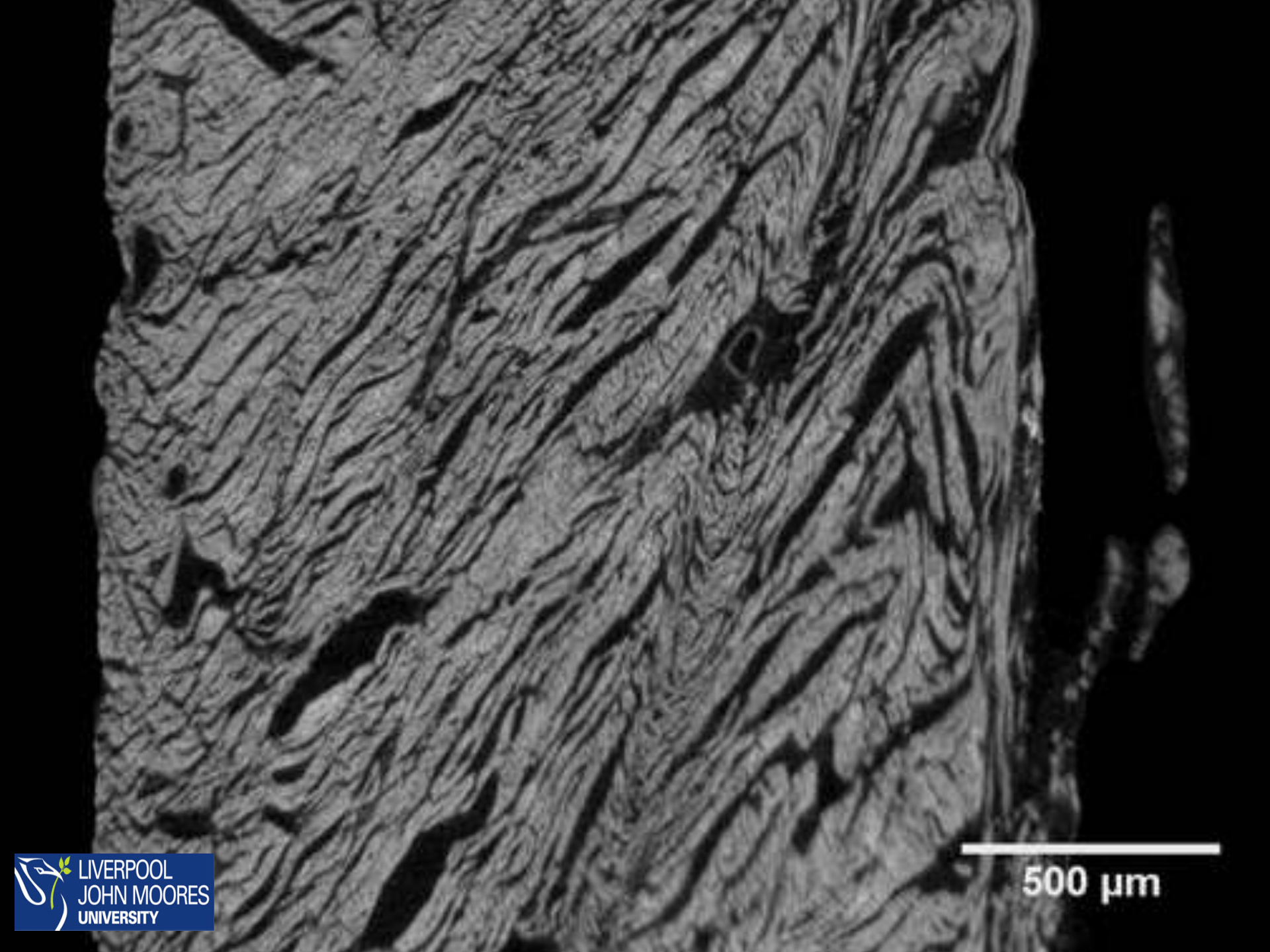
Rajmund.Mokso@maxiv.lu.se

4D IMAGING LAB@LTH

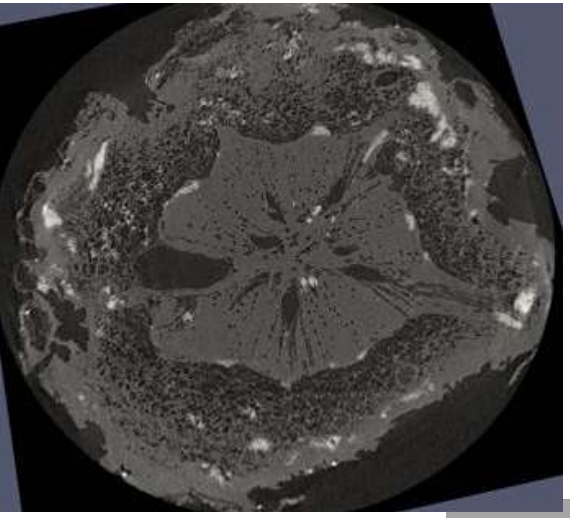
@Division of Solid Mechanics, LTH, Lund

- Installed June 2014 through infrastructure and strategic funding from LTH
- Zeiss Xradia XRM 520 x-ray tomograph
- 3D imaging of bulk objects with resolutions down to < 700 nm
- Focus on “in-situ” and “in-operandi” experiments for “4D imaging”
- Development of software for 3D/4D image analysis and quantification

www.solid.lth.se/resources/4d-imaging-lab/



Lab CT of grape stem



4D imaging Lab in Lund – Zeiss versa 520, 5 µm spatial resolution in 3D

Conclusions

For tomographic reconstruction we use both numerical and analytical tools. Numerical are still slower.

Synchrotron and lab-based tomographic instruments routinely go down to about 1 μm spatial resolution. There is a factor of ~100 in acquisition speed between synchrotron and lab-based tomography

In Lund we can do 3D imaging with in 4Dlab (LTH), in a couple of years also at MAX IV

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