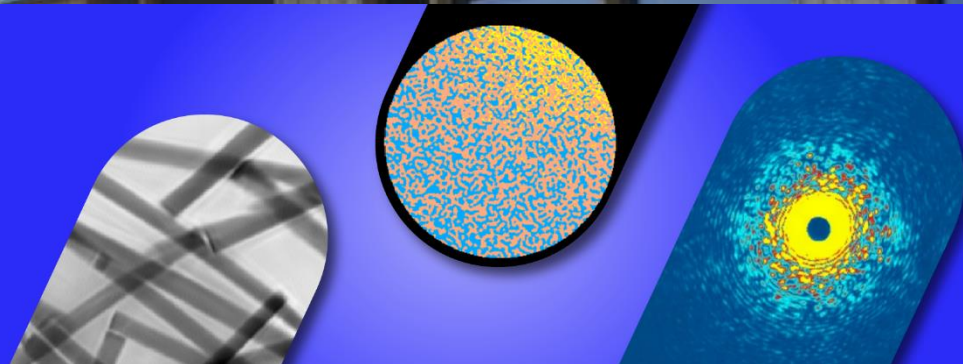


Ptychography (PTYPY) Software Workshop 2025

12th–13th May, 2025 – Synchrotron SOLEIL



A Ptychographic X-ray Computed Tomography set-up on the SWING beamline

Javier Pérez

Christer Engblom, Filipe Alves, Florent Langlois,
Felisa Berenguer, Yves-Marie Abiven, Alain Lestrade

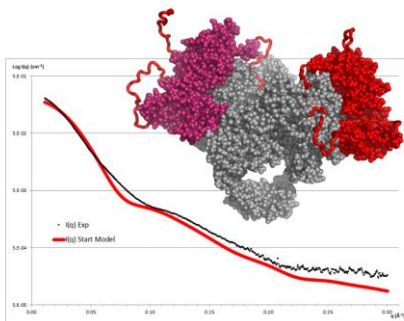
<https://www.synchrotron-soleil.fr/en/beamlines/swing>



Since 2008

« Classical » SAXS
BioSAXS
SAXS Mapping
PXCT (ptycho-tomography)

Protein conformations

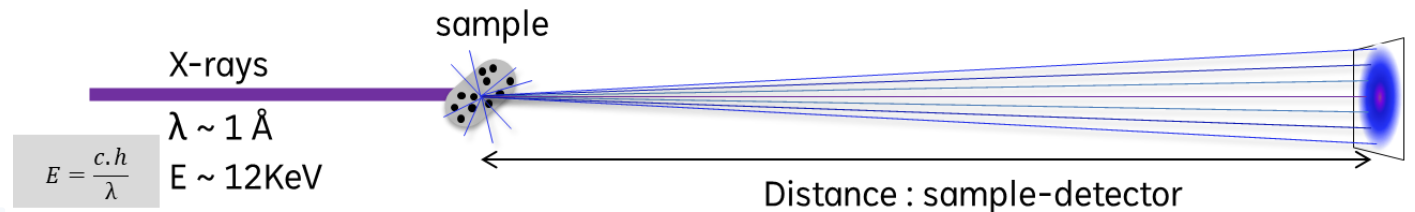


Roudenko O., Thureau A. & Pérez J., March 2018
Petrella, S., et al. (2019). Structure, 27, 579–589.

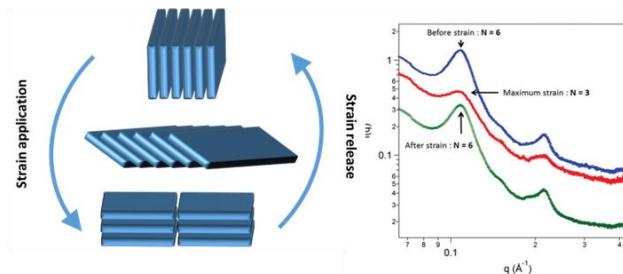
- **S**mall and **W**ide angle X-ray scatter**I**NG

From macromolecule to material.

- Hard X-rays Energy (U20 undulator): 5 keV to 16 keV (wavelength: 2.5 Å to 0.75 Å)
- Usual beam size (FWHM): 25-400 (H) x 25-100 (V) μm²
- Structural information from non-crystalline samples (scale: nm to μm)

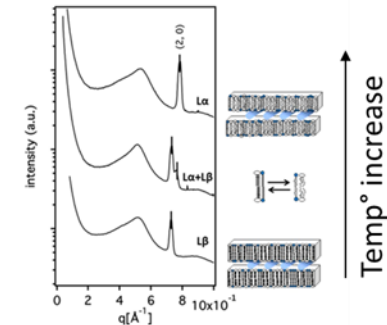


Deformation under strain



Beaudoin, E., et al. (2017), *Nanoscale*, 9(44): 17371-17377

Phase transition of lipids/ liquid crystals

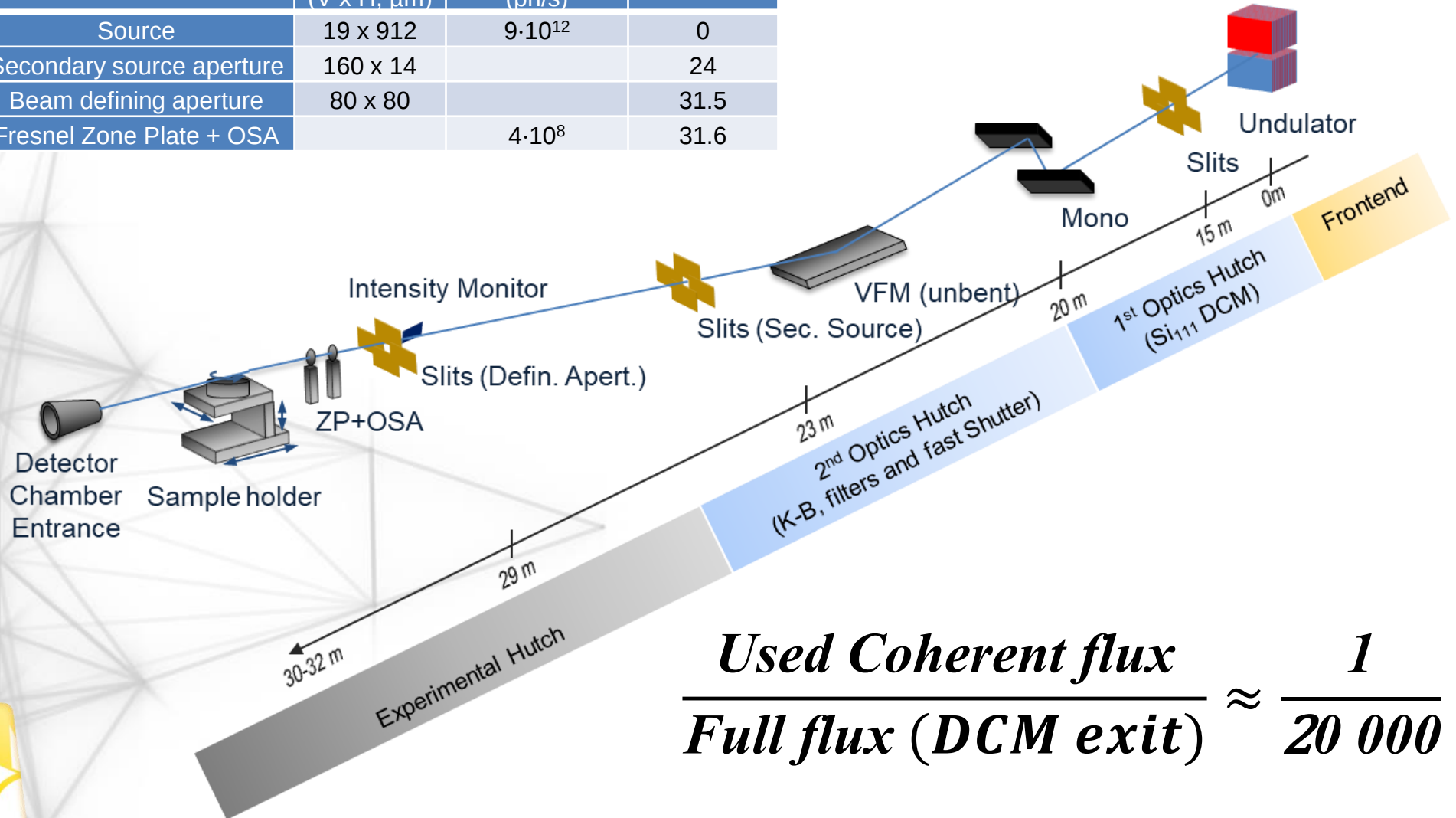


Temp° increase

Bizien, T., et al.
(2015), *Langmuir*,
31(44): 12148–
12154.

SAXS data are usually interpreted *via* mathematical,
physically meaningful, **expert models**

Optical Element	Beam Size (V x H, μm)	Flux @8 keV (ph/s)	Position (m)
Source	19 x 912	$9 \cdot 10^{12}$	0
Secondary source aperture	160 x 14		24
Beam defining aperture	80 x 80		31.5
Fresnel Zone Plate + OSA		$4 \cdot 10^8$	31.6



$$\frac{\text{Used Coherent flux}}{\text{Full flux (DCM exit)}} \approx \frac{1}{20\,000}$$

Current NANOPROBE setup

Interferometric Frame

- With the interferometers heads using fiber-based technology (Resolution <1nm)

Coherent length matching slits

- JJ-Xray

Fresnel Zone Plate Optic (FZP)

- 3x linear stages (Ts, Tx, Tz) using piezowalk technology (Resolution: 50 pm)
- 4x Interferometer heads using fiber-based technology (2 in X axis and 2 in Z axis) (Resolution <1nm)



Engblom, Christer, et al. "euspen's 20th International Conference & Exhibition, Geneva, CH, June 2020."

Order Sorting Aperture positioner (OSA)

- 3x linear stages (Ts, Tx, Tz) using piezowalk technology (Resolution: 50 pm) with Zerodur scale encoder (Resolution: 5 pm)

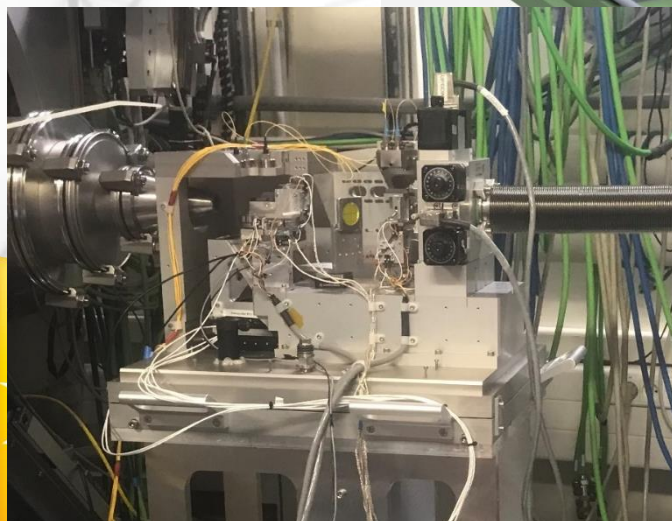


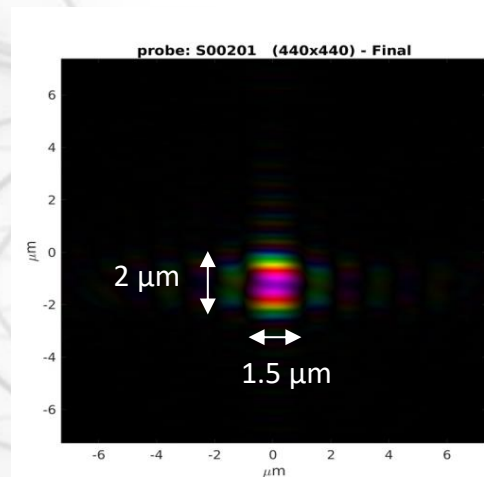
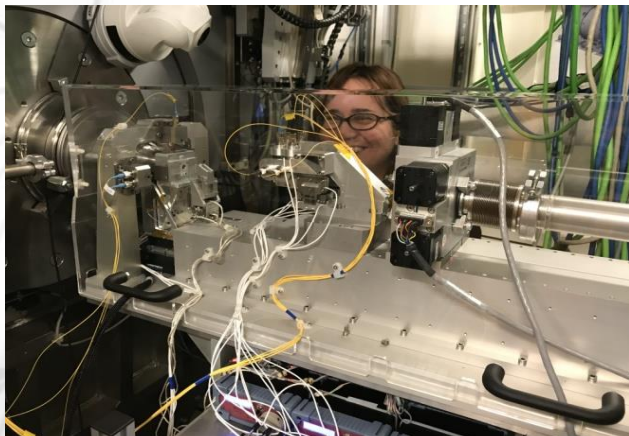
Sample Stage

- 3x linear stages (Ts, Tx, Tz) using piezowalk and linear motor technology
- 1x Rotation Stage (Rz) using piezo Stick&Slip technology
- 1x Rx tilt using a piezo amplifier device
- 1x Reference cylinder (Roughness <5nm)
- 5x Attocube Interferometers heads using fiber-based technology (2 in X axis and 3 in Z axis) (Resolution <1nm)

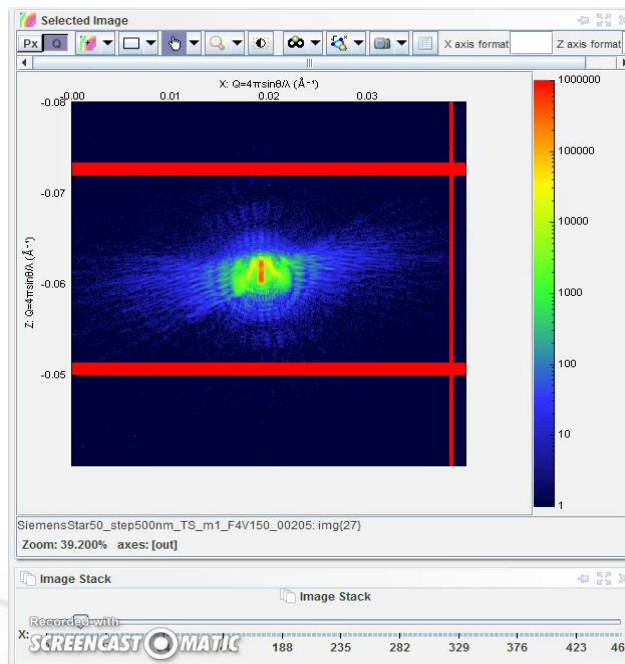


X Beam

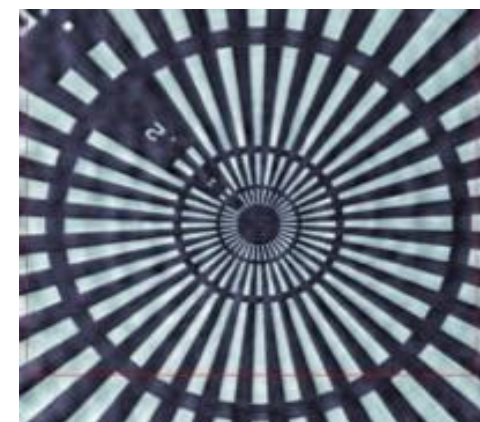
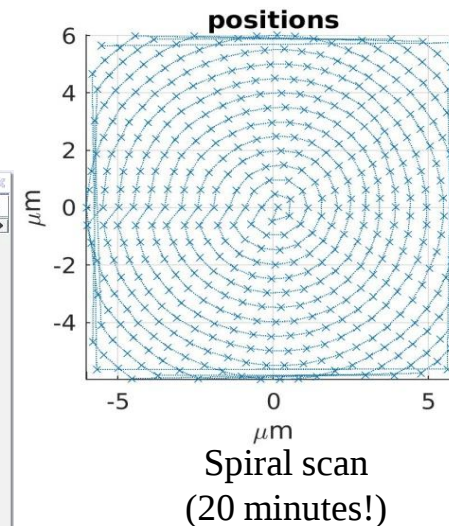




Probe function



*Eiger4M detector,
75 μm pixel size
No beam-Stop*



Siemens Star

Inner spacings : 50 nm

Resolution : 40 nm (Fourier Shell Correlation)

All ptychographic results generated via cSaxs Ptycho-shelves application (PSI)

*K. Wakonig et al., J. Appl. Cryst. (2020). **53**, 574-586*

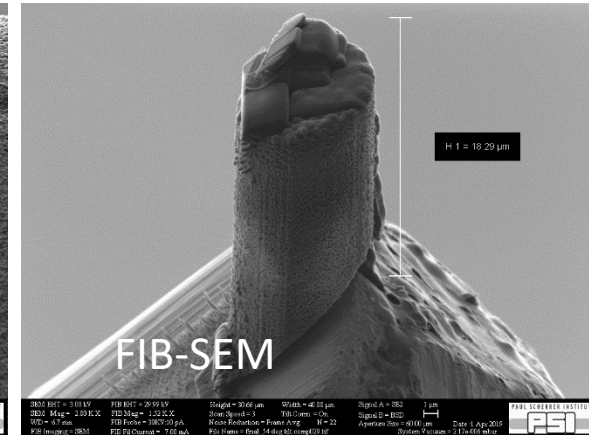
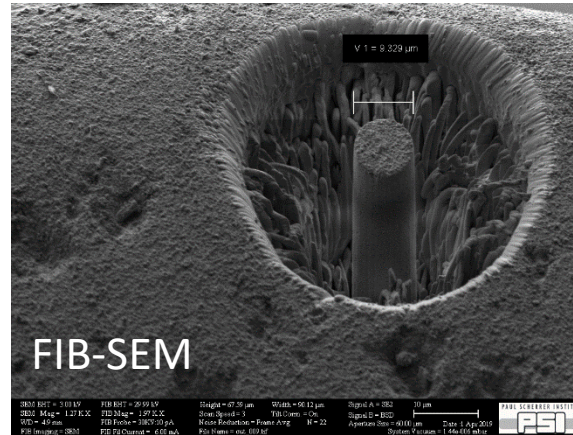
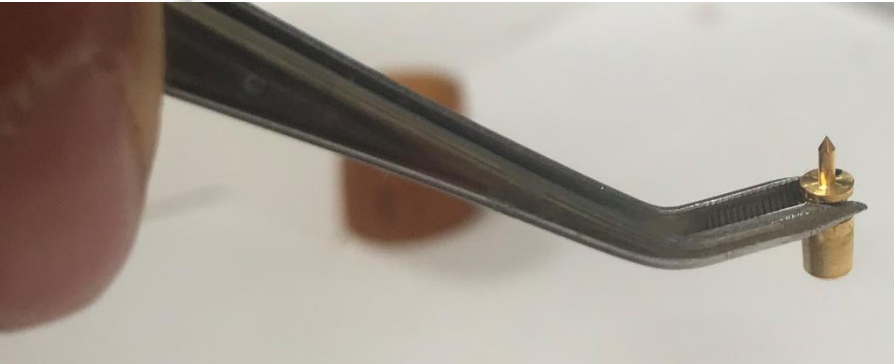
Ultra high resolution Siemens Star (XRESO-20)

- Thickness T_a : 100nm
- Minimum Patern size: 20nm
(radial)

2D Resolution
(Fourier Shell
Correlation) : 19 nm



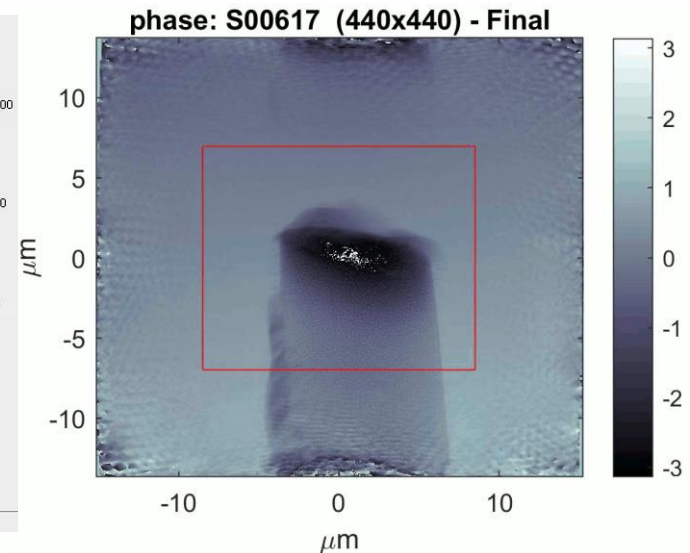
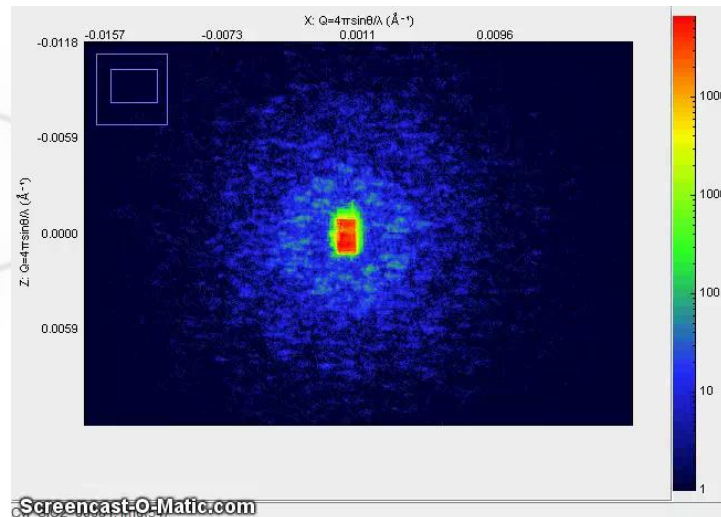
Porous Silica partly coated with Ta₂O₅ (37nm thick) (provided by cSaxs)



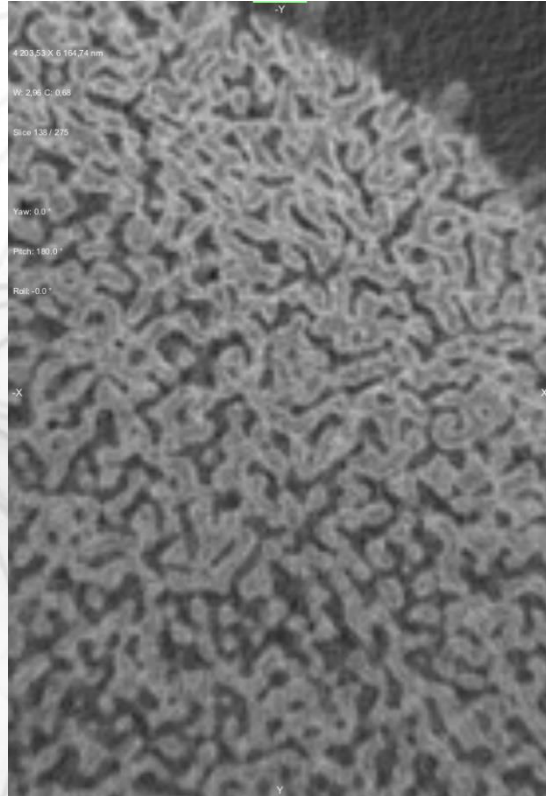
M. Holler *et al.*, Rev. Sci. Instrum. **88**, 113701 (2017)

Collection conditions:

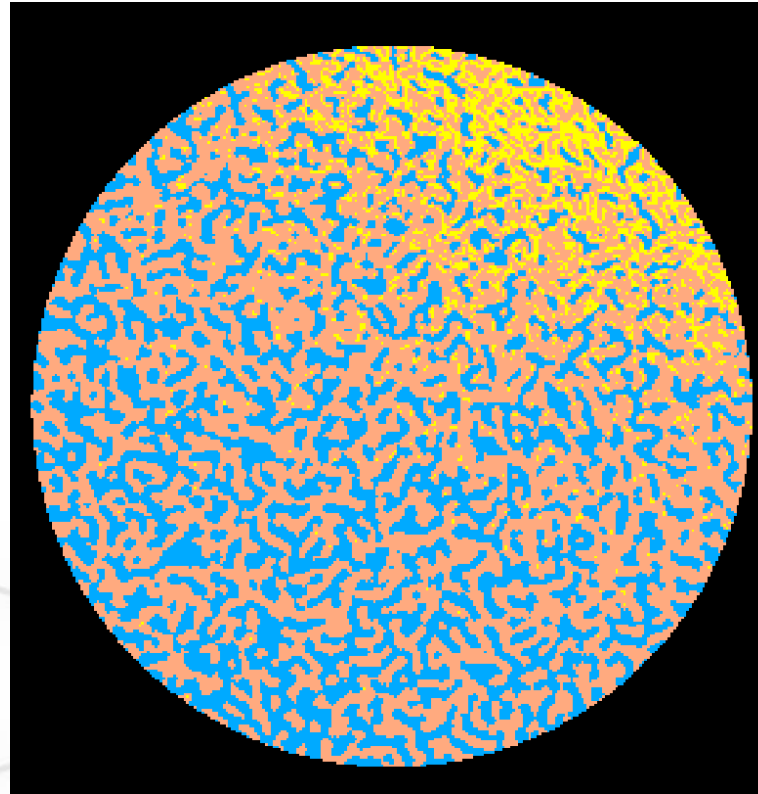
- **Ptychography**
 - $E : 8 \text{ keV}$
 - **Probe size : $1.5 \times 2 \mu\text{m}$**
 - Sample diameter : $10 \mu\text{m}$
 - Steps : $528 \times 0.5 \mu\text{m}$
 - Exposure time per step : 100 ms
- **Tomography**
 - # projections : 272
 - **Total exposure time : 4 h**
 - **Total time : 10 h 40 min**



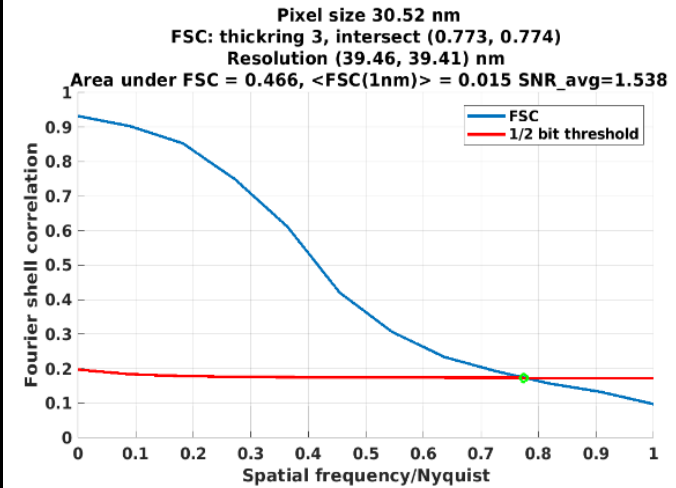
Porous Silica partly coated with Ta₂O₅ (37nm thick) (provided by cSaxs)



*Slice of the raw reconstruction
(visu: ORS Dragonfly)*



*Slice after segmentation
(ORS Dragonfly)*



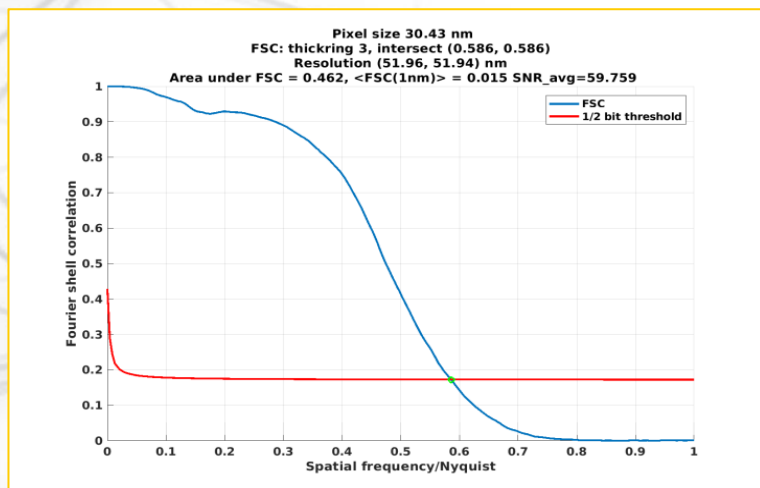
**3D Resolution ~ 40 - 50 nm
(Fourier Shell Correlation)**

*Pore diameter
Actual: 137 nm
From our segmentation: 168 nm*

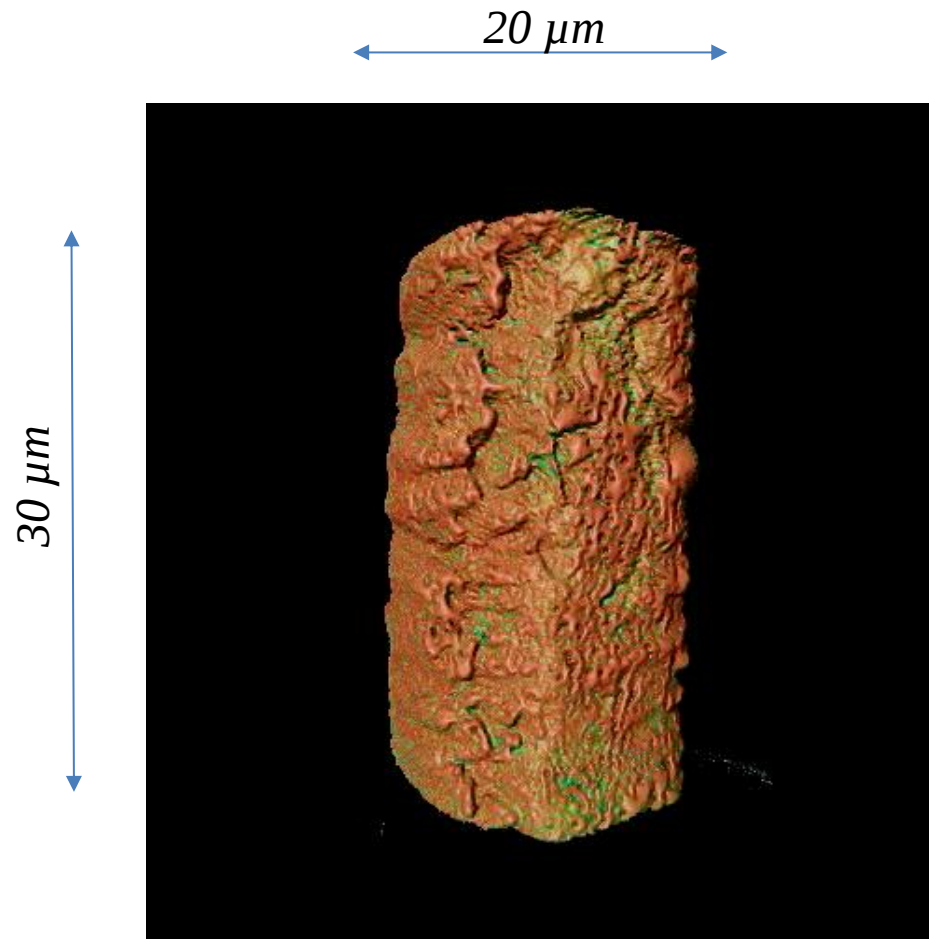
*Tomographic reconstructions generated via cSaxs application (PSI)
Michal Odstrčil et al., Opt. Express 27, 36637-36652 (2019)*

NiMo catalyst (credit : Julio Cesar Da Silva, Inst. Néel, Grenoble)Collection conditions:

- Ptychography
 - E : 8 keV
 - **Probe size : $5 \times 4 \mu\text{m}$**
 - Dist Eiger4M : 6.4 m (max distance)
 - FOV : $26 \times 30 \mu\text{m}$
 - Steps : $314 \times 1.4 \mu\text{m}$
- Tomography
 - # projections : 640
 - **Total exposure Time : 5h35**
 - **Total time : 10h50**
 - Total Nb incoming photons : $\sim 5.10^{12}$ ph, $\sim 4.10^8$ ph/ μm^3



Resolution achieved: $< 52 \text{ nm}$ (3D FSC)



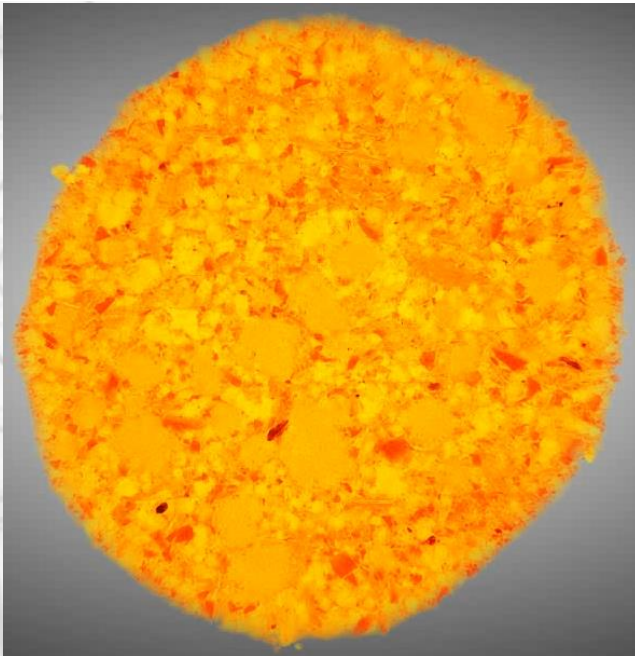
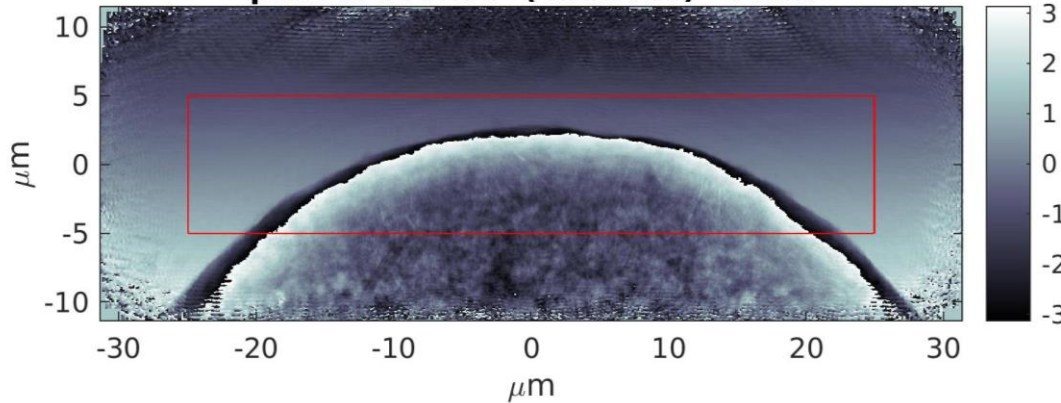
**Global view of the reconstruction
(visu: ORS Dragonfly)**

Fluid catalytic cracking (FCC) catalyst: ACM-101 J. Gascon et al. US Patent App. 17/630,786 (2022)

Collection conditions:

- Ptychography
 - E : 8 keV
 - Dist Eiger4M : 6.4 m (max distance)
 - **FOV : 50 x 12 μm**
 - Steps : 412 x 1.0 μm
- Tomography
 - # projections : 800
 - **Total exposure Time : 9h10**
 - **Total time : 17h30**

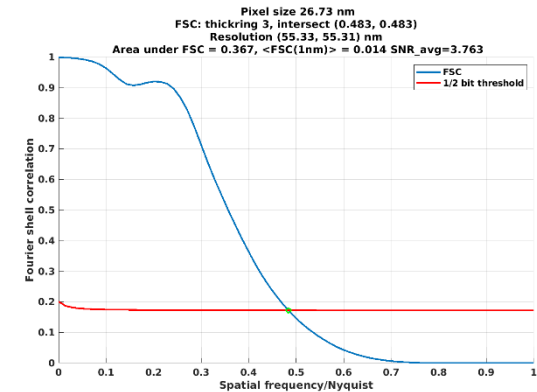
phase: S00100 (480x480) - Final



3D rendering
(visu: ORS Dragonfly)



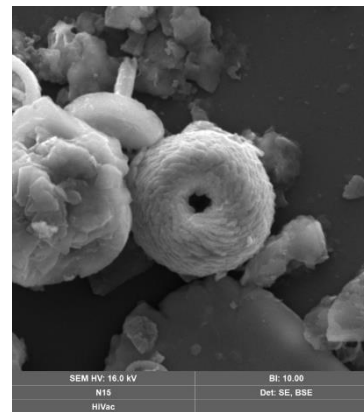
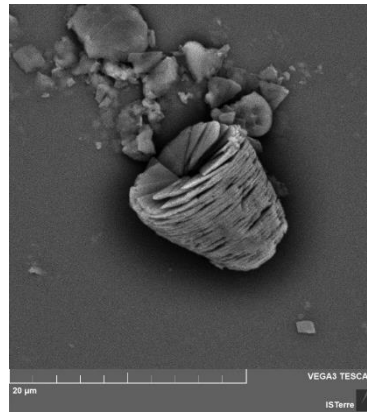
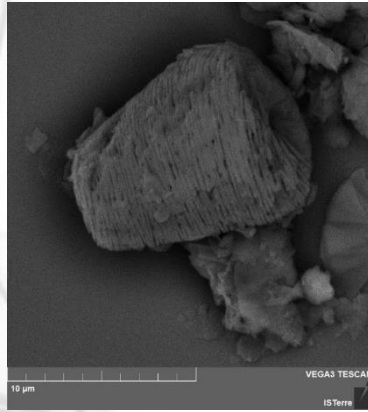
Slice by slice rendering
(visu: ORS Dragonfly)



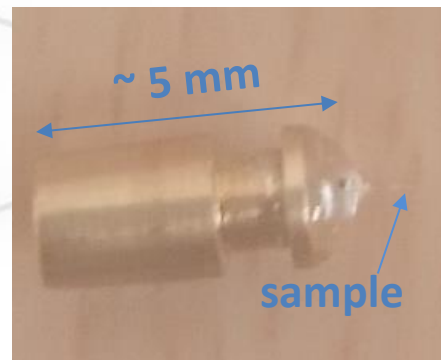
3D Resolution achieved
(FSC): 55 nm

“Nannoconus”

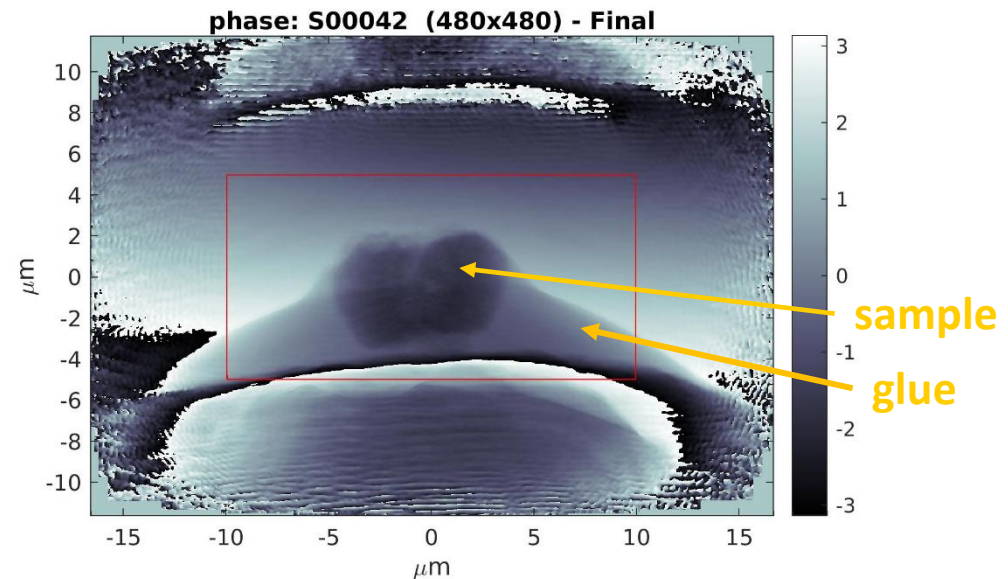
**Major planktonic bio-carbonate producers in
Early Cretaceous (~152 - 100 Ma)**



SEM images of different
species of Nannoconus from
Cape Hatteras, North Carolina.



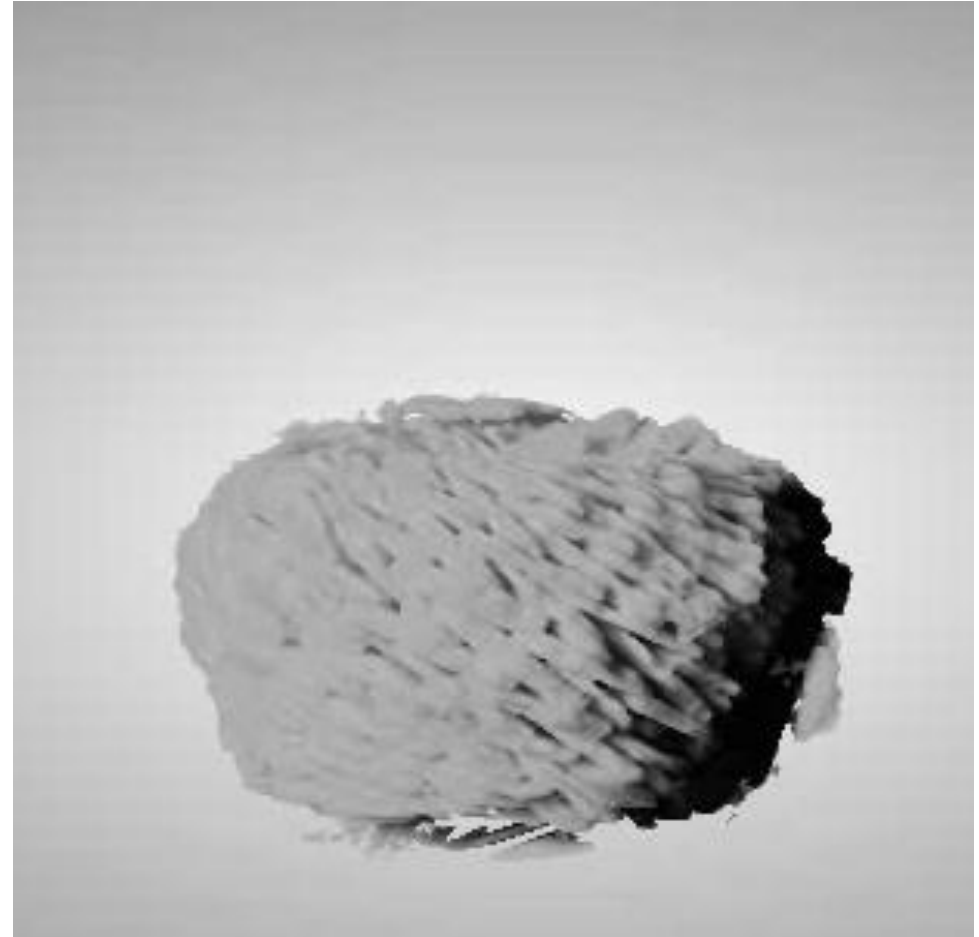
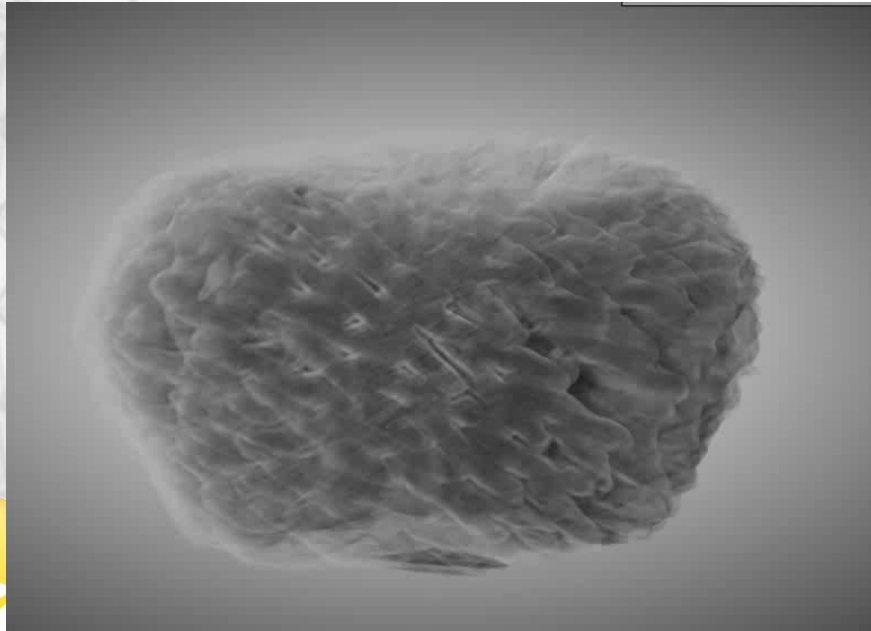
Silica needle passing
through a capillary
holder



Nannoconus globulus subsp. globulus

Collection conditions:

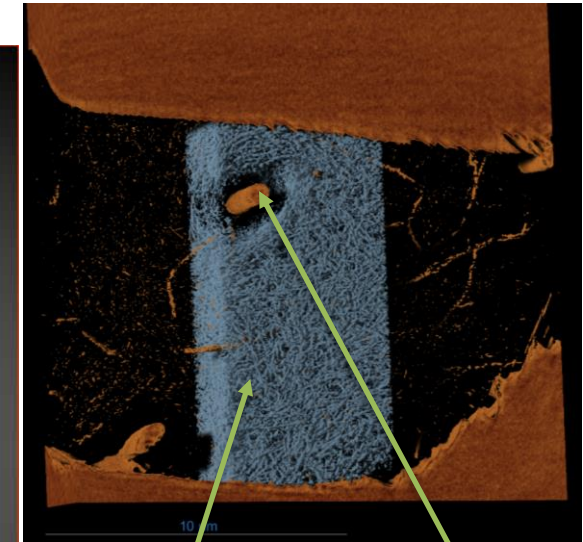
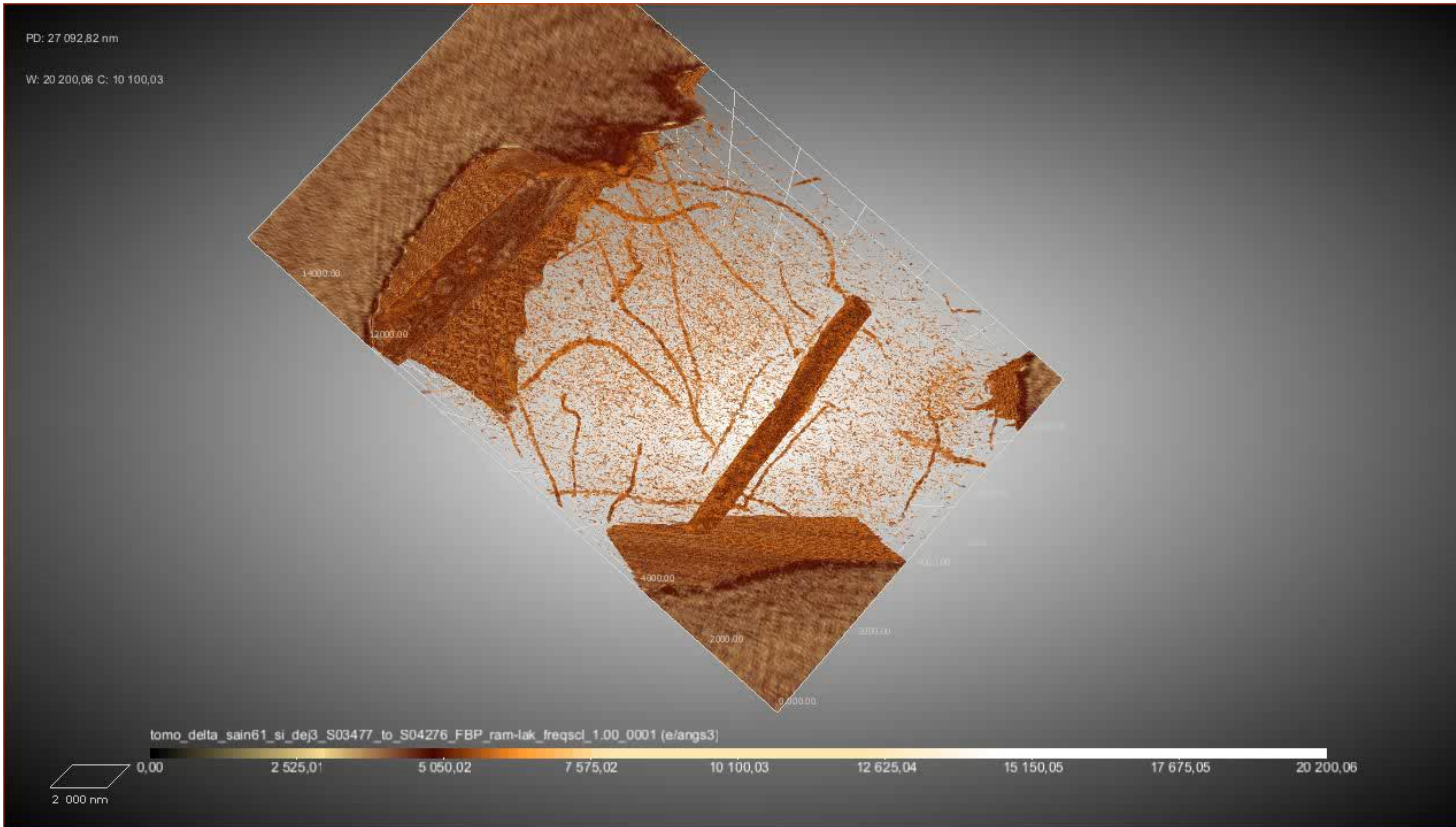
- **Ptychography**
 - $E : 8 \text{ keV}$
 - Dist Eiger4M : 6.4 m (max distance)
 - **FOV : $20 \times 10 \text{ } \mu\text{m}$**
 - Steps : $164 \times 1.0 \text{ } \mu\text{m}$
- **Tomography**
 - # projections : 664
 - **Total exposure Time : 3h00**
 - **Total time : 6h10**



**3D Resolution achieved
(FSC): 60 nm**

R. CHOWDHURY et al. (2025), Submitted to BioGeoSciences

Dentinogenesis Imperfecta study (cyl. Ø 15 µm)



Collagen
network
(blue)

Microtubule
(brown)
diam ~ 1 µm

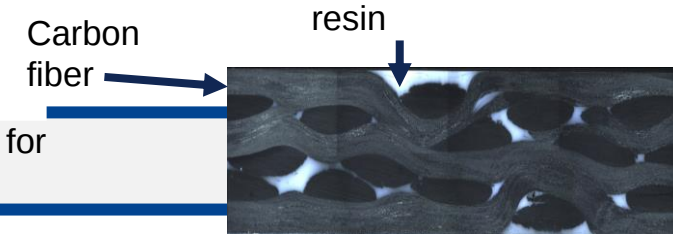
Elsa Vennat
Margot Riou
Muriel De la Dure-Molla

Alexandre Jeetoo
Thomas Reiss
Alexis Nicolay

Ptychography X-ray Computed Tomography of constituents' materials of organic matrix composites materials used in aeronautics

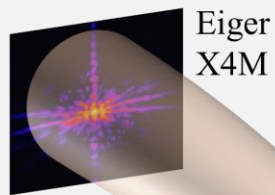
Motivations

- Better knowledge of fundamental properties of carbon fibers and resin materials for better used of organic matrix composites materials

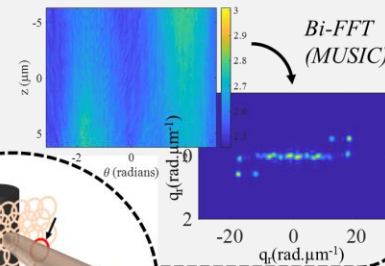


Carbon fibers

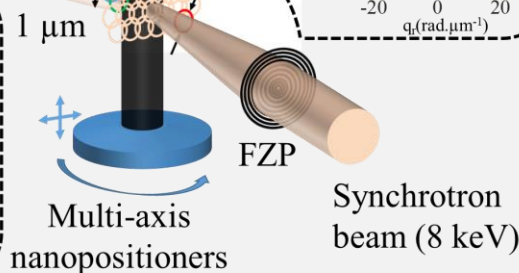
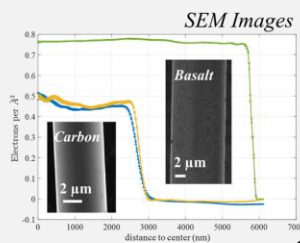
resolutions : 45 nm on 20x20x40 μm^3 imaged volume



Surface profil analysis



Electronic density



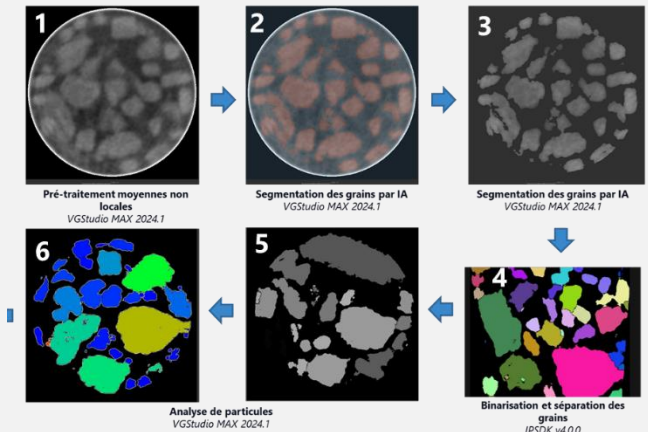
Ducouso et al., Carbon Trends 19 (2025) 100490

Resin

Monitoring of chemical reaction : Imaging of hardeners dissolution in epoxy for different reticulations

Proof of concept : 1 : PXCT acquisition; 2-3 : Hardeners segmentation using AI ; 4 : hardeners differentiation ; 5-6 – data analysis

resolutions :
150 nm on
20x75x75 μm



Next : Same work for different reticulation → chemical model of hardener dissolution

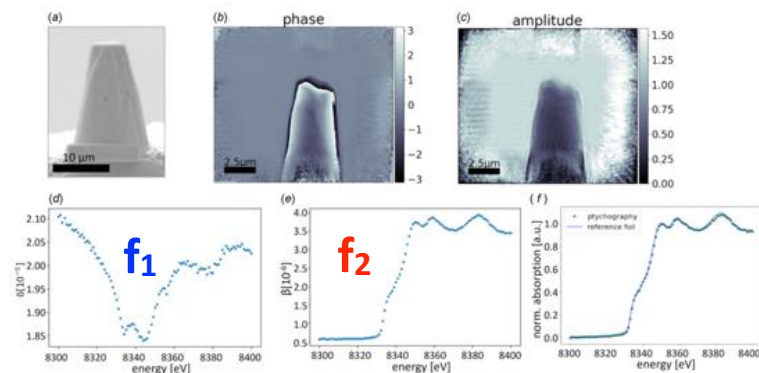
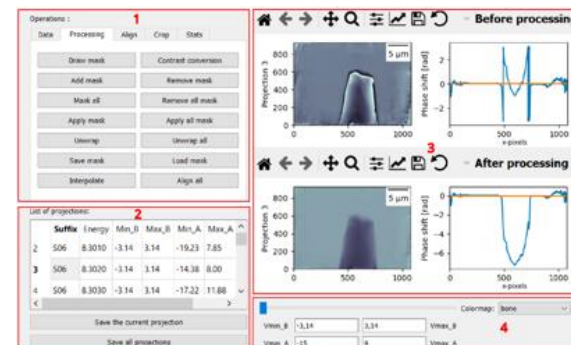


Table 1
Tabulated values (Chantler database) of δ for different elements at different energies.

	δ (8.337 keV)	δ (8.383 keV)
Ni	1.86×10^{-5}	2.08×10^{-5}
Fe	2.11×10^{-5}	2.09×10^{-5}
Pt	4.80×10^{-5}	4.75×10^{-5}
Ga	1.50×10^{-5}	1.48×10^{-5}

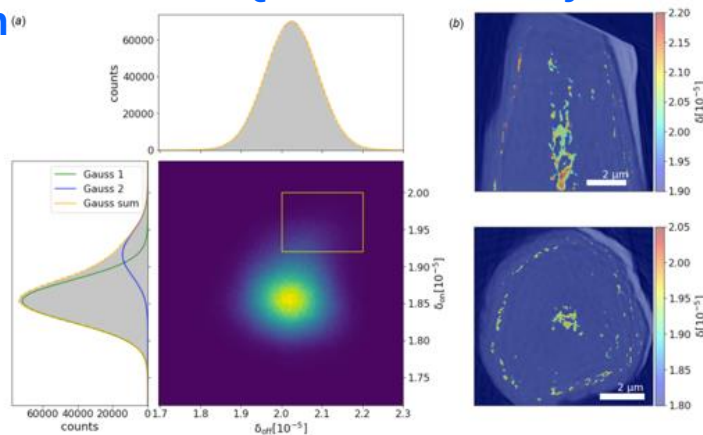
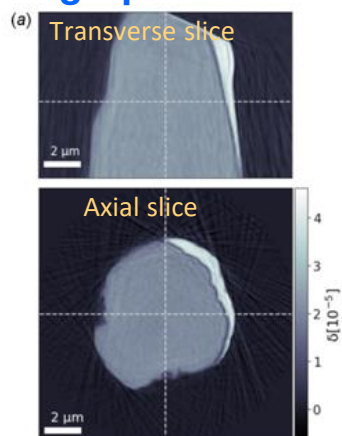
ProSPyX



No needs for Kramers-Kronig

Quantitative analysis

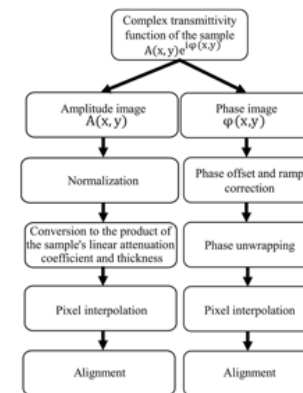
Tomographic reconstruction^(a)



Anico Kulow



Redhouane Boudjehem



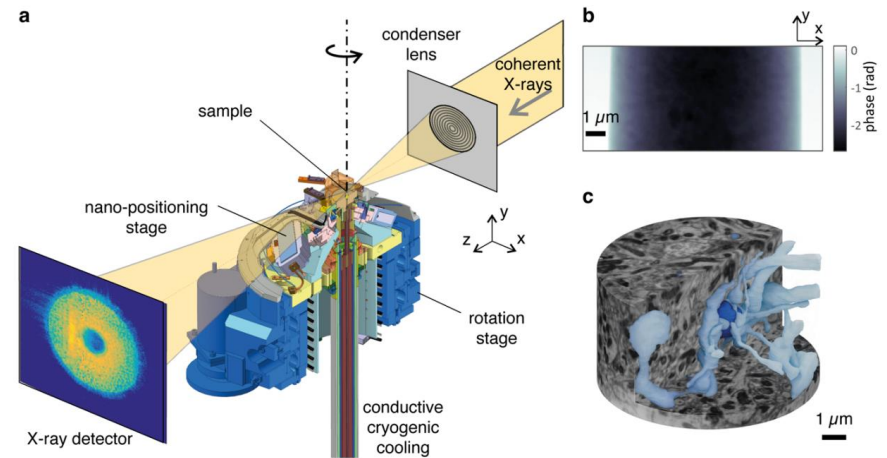
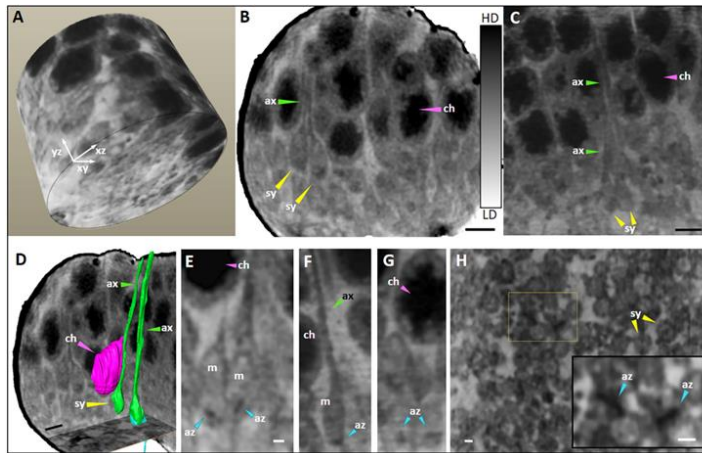
A. Kulow et al., J. Synchrotron Rad., 31, 867-876 (2024)

R. Boudjehem et al., J. Synchrotron Rad., 31, 399-408 (2024)

R. Boudjehem, Thèse de Doctorat, 2024, Univ. de Grenoble Alpes

- PXCT will directly benefit from **upgrade** to SOLEIL II
Decrease collection time from hours to minutes
Increase sample diameter to $> 100 \mu\text{m}$
- Currently Developing a **cryo setup** for hydrated tissues

Black bar: $3 \mu\text{m}$, white bar: 500 nm



Ana Diaz
Manuel Guizar-Sicairos
Mirko Holler
Klaus Wakonig



Florian Meneau
Carla Polo



Stephan Kubsky
Andrea Somogyi
Sébastien Ducourtieux
Cédric Bourgoïn



Julio Da Silva
Anico Kulow



Rajkumar Chowdhury
Fabienne Giraud-Guillot
Alejandro Fernandez-Martinez



Alla Dikhtiarenko
Jorge Gascon Sabate

