PAUL SCHERRER INSTITUT

PSI

Andreas Menzel :: Coherent X-Ray Scattering Group :: Paul Scherrer Institut

Ptychographic Nanotomography at SLS

“Round Beam” Mini-Workshop at SOLEIL
June 14–16, 2017, Saint Aubin, France

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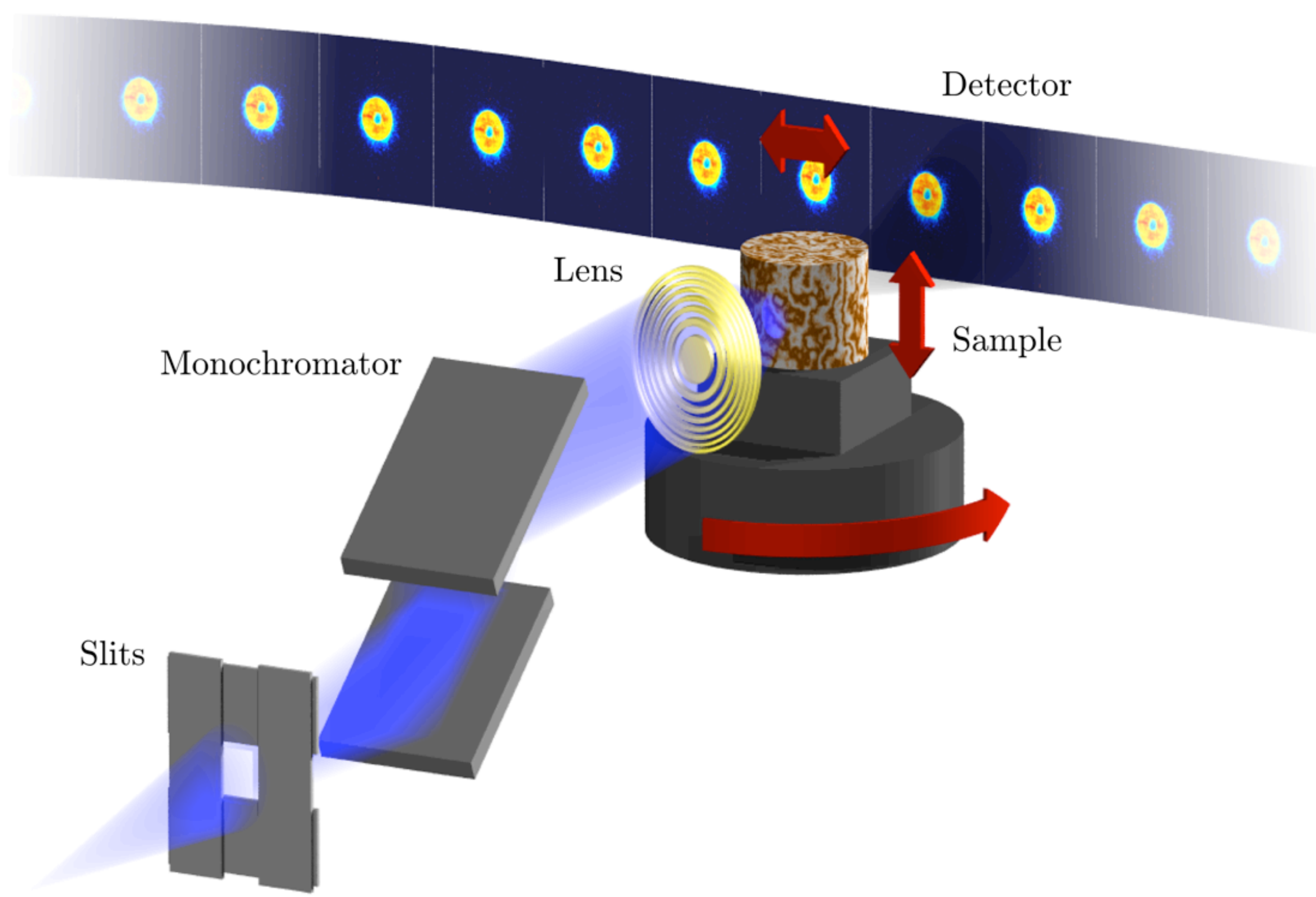
Coherent X-Ray Scattering Group
and Special Thanks to:

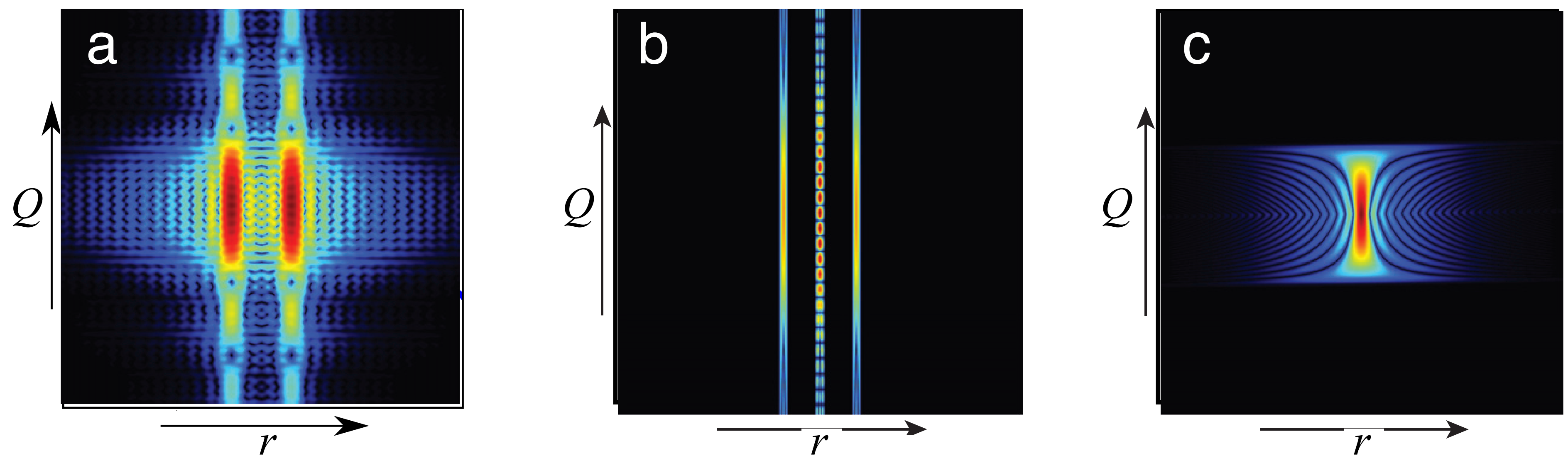
- Mirko Holler, Jörg Raabe, … (OMNY)
- Christian David and his X-Ray Optics Group
- Bernd Schmitt and his Detector Group
- Derek Feichtinger and his Scientific Computing Group
- J.C. da Silva (now ESRF)
- Alessandro Sepe (Adolphe Merkle Institute, Fribourg)
- Sarah Shahmoradian (BIO @ PSI)
- and other users of cSAXS

Pty·chog·ra·phy *noun*

from Greek: πτυξ = to fold (crease)
and: γραφή = writing, drawing



Ptychographic Sampling Ratio

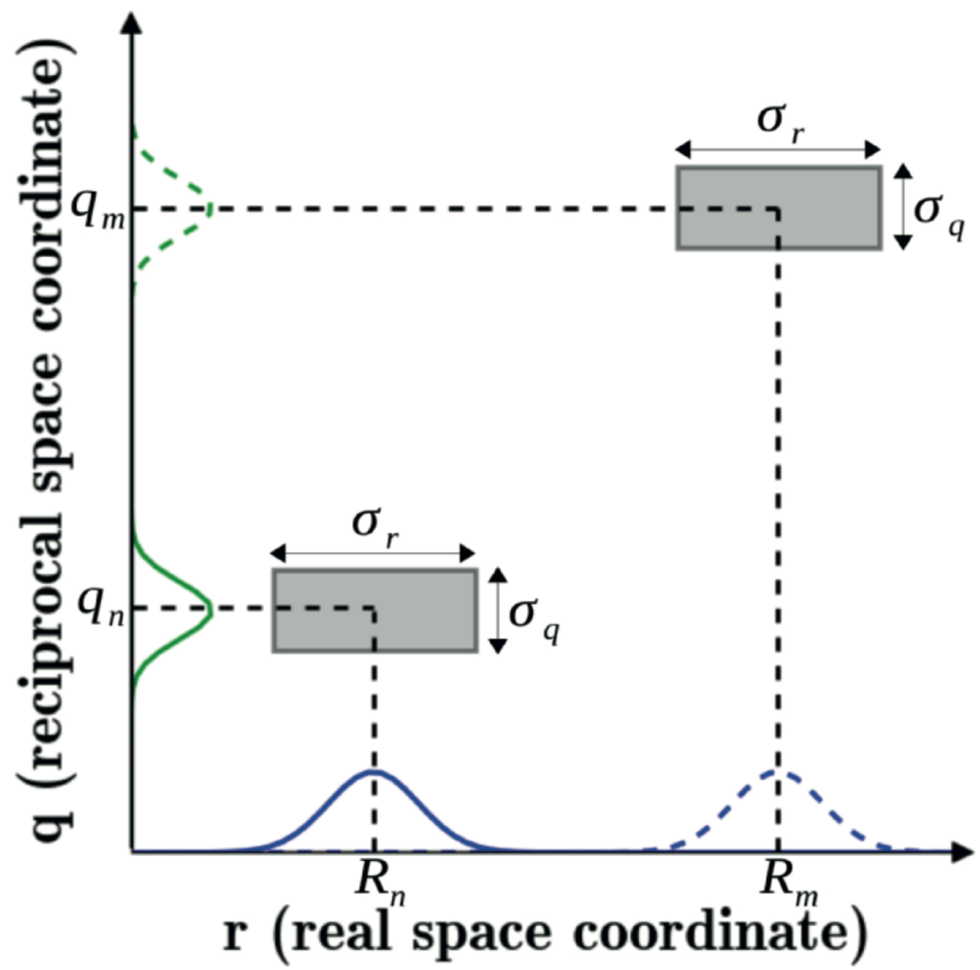


$$I(\mathbf{q};\mathbf{R}) = |\Psi(\mathbf{q};\mathbf{R})|^2 = \left| \int_{-\infty}^{\infty} \mathrm{d}\mathbf{r}\, O(\mathbf{r}) \underbrace{P(\mathbf{r}-\mathbf{R}) \exp(-i\mathbf{q}\cdot\mathbf{r})}_{\equiv P^*_{\mathbf{R},\mathbf{q}}(\mathbf{r})} \right|$$

The measurable quantity $I(\mathbf{q};\mathbf{R})$ is a spectrogram. It represents the energy density of $O(\mathbf{r})$ in the phase space neighborhood of the position $(\mathbf{q};\mathbf{R})$.

J.C. da Silva, A. Menzel, Opt Express **23**(26) (2015) 33812

Ptychographic Sampling Ratio



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J.C. da Silva, A. Menzel, Opt Express **23**(26) (2015) 33812

Ptychographic Sampling Ratio

$$\frac{2\pi}{\Delta q \Delta R} = 1$$

"critical sampling"
poor localization properties of the window functions. Numerical stability will be poor, and the reconstruction may be reduced to phase retrieval on individual, decoupled "views."

$$\frac{2\pi}{\Delta q \Delta R} > 1$$

in real space: "overlap"
in reciprocal space: "oversampling"

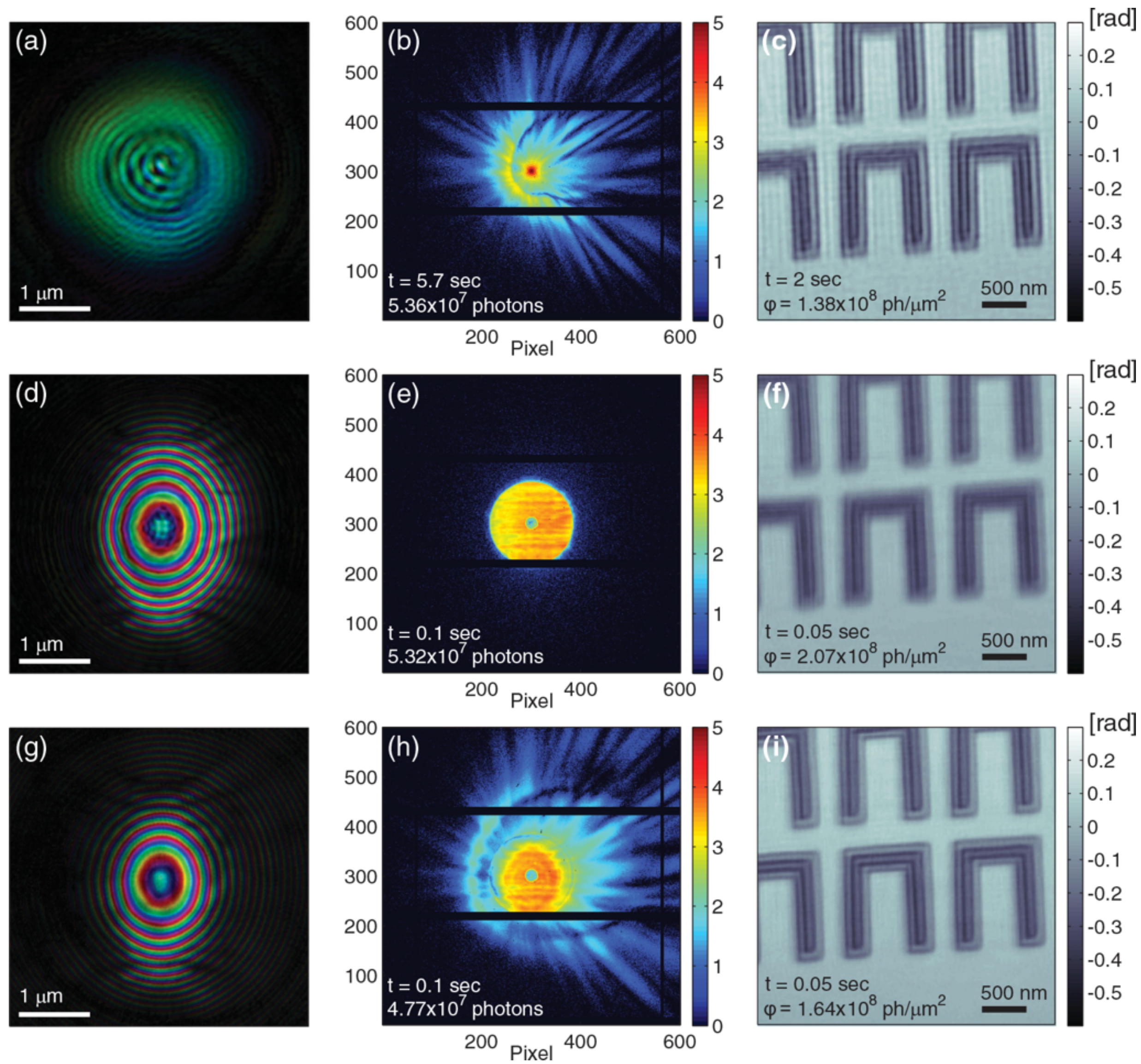
$$\frac{2\pi}{\Delta q \Delta R} < 1$$

the window function may not completely fill 4D phase space

Note that a successful and stable reconstruction with such poor sampling was observed. We speculate that this could be explained by a structured illumination, featuring a larger footprint in phase space than the minimal size.

T.B. Edo *et al.*, Phys Rev A **87**(5) (2013) 053850
J.C. da Silva, A. Menzel, Opt Express **23**(26) (2015) 33812

Illumination Design



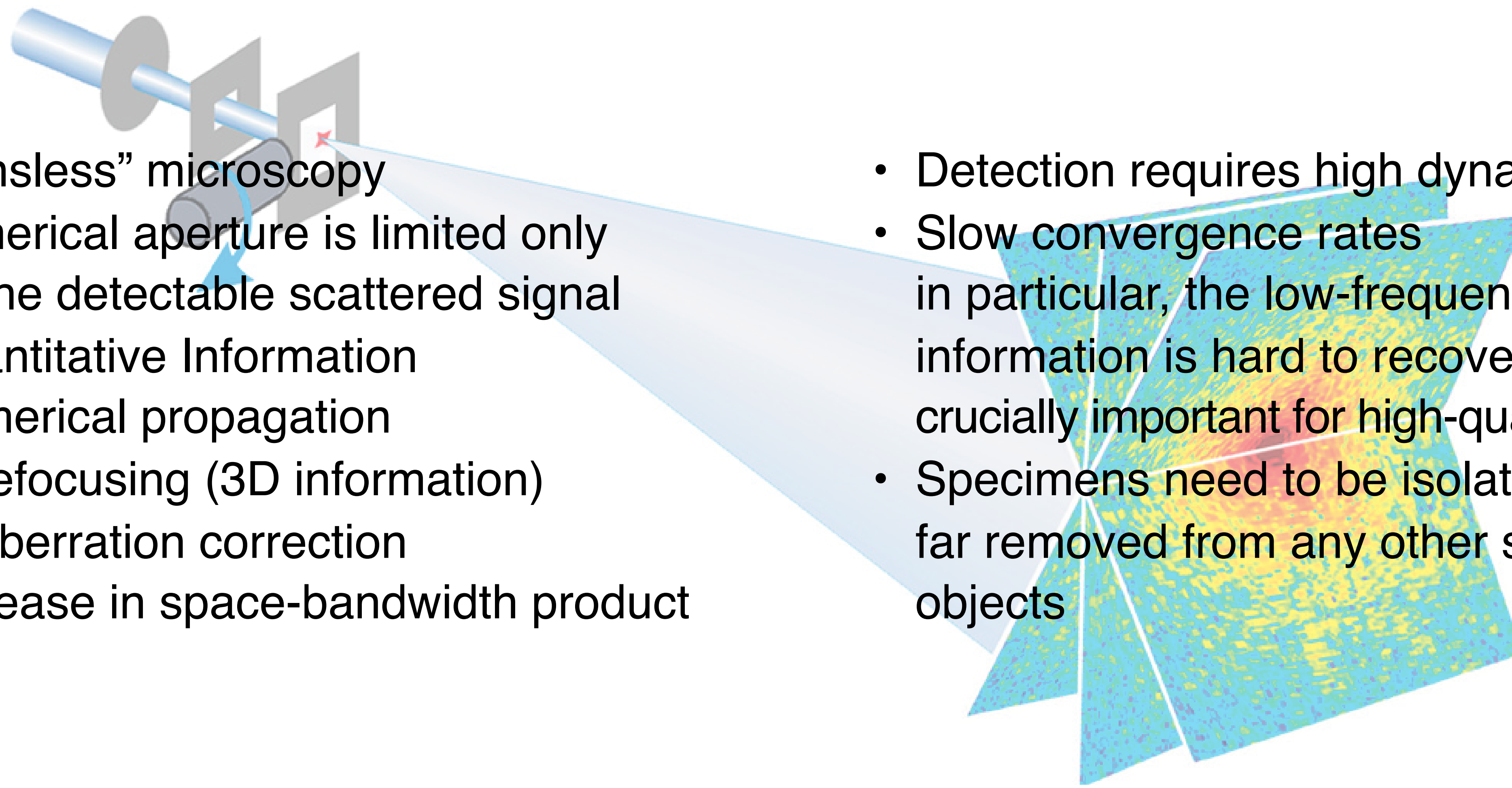
Structured illuminations were found beneficial to reconstruction stability, image resolution, and dose efficiency and allow for “super-resolution.”

A. Maiden *et al.*, JOSAA **28** (2011) 604.

Guizar-Sicairos *et al.*, Phys Rev B **86** (2012) 100103.

Coherent Diffractive Imaging

An Overview

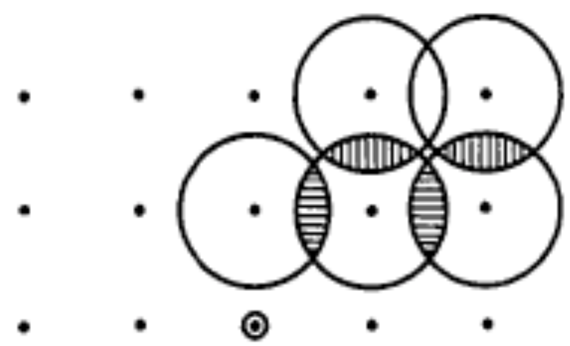


- "Lensless" microscopy
  numerical aperture is limited only
  by the detectable scattered signal
- Quantitative Information
- Numerical propagation
  - refocusing (3D information)
  - aberration correction
- Increase in space-bandwidth product

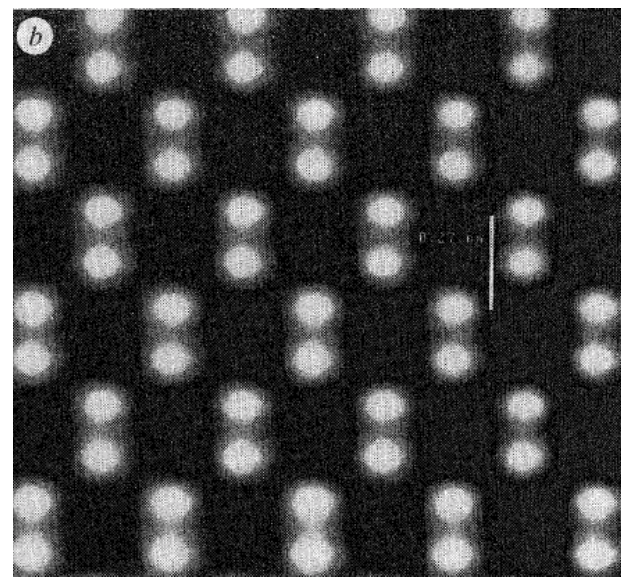
- Detection requires high dynamic range
- Slow convergence rates
  in particular, the low-frequency
  information is hard to recover albeit
  crucially important for high-quality images
- Specimens need to be isolated, i.e.,
  far removed from any other scattering
  objects

image credit: H. Jiang *et al.*, PNAS **107** (2010) 11234

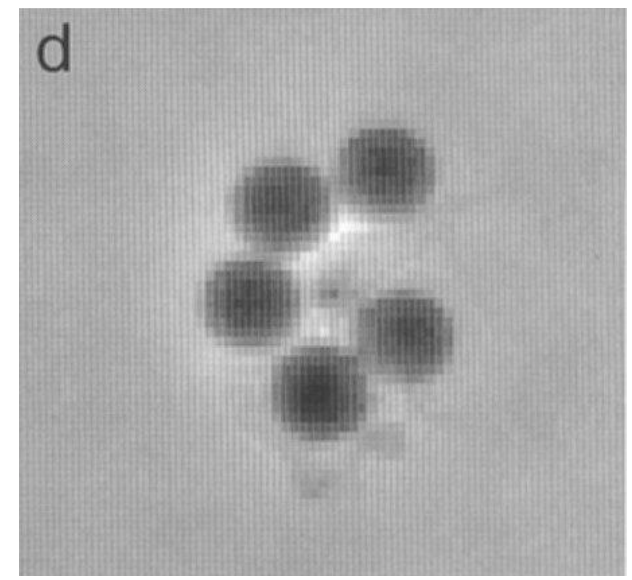
Ptychography
A Brief History…



Hoppe, *Acta Cryst. A* **25** (1969) 508;
Hegerl and Hoppe, *Ber. Physik. Chemie* **74** (1970) 1148

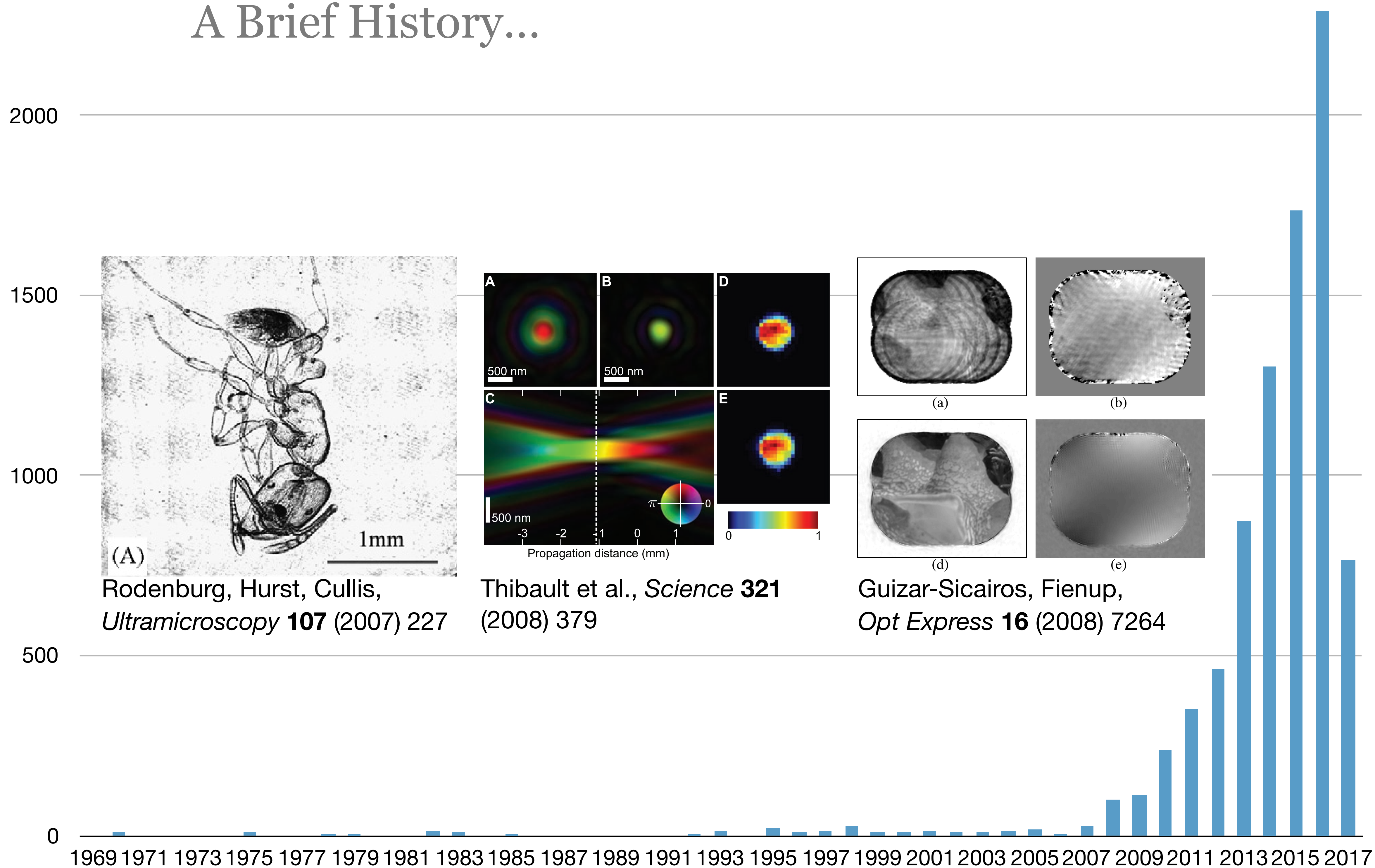


Nellist, McCallum, Rodenburg, *Nature* **374** (1995) 630



Chapman, *Ultramicroscop* 6**6** (1996) 153

Ptychography
A Brief History…



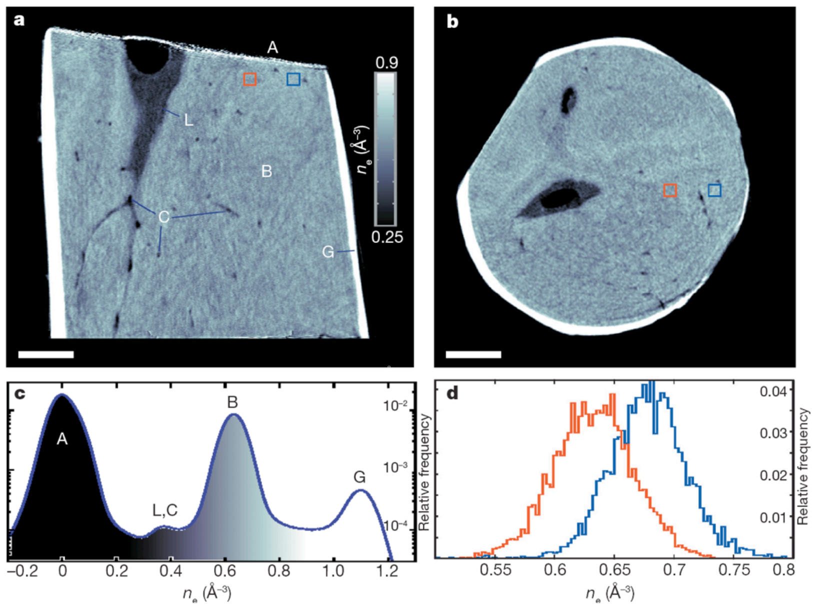
Rodenburg, Hurst, Cullis, *Ultramicroscopy* **107** (2007) 227

Thibault et al., *Science* **321** (2008) 379

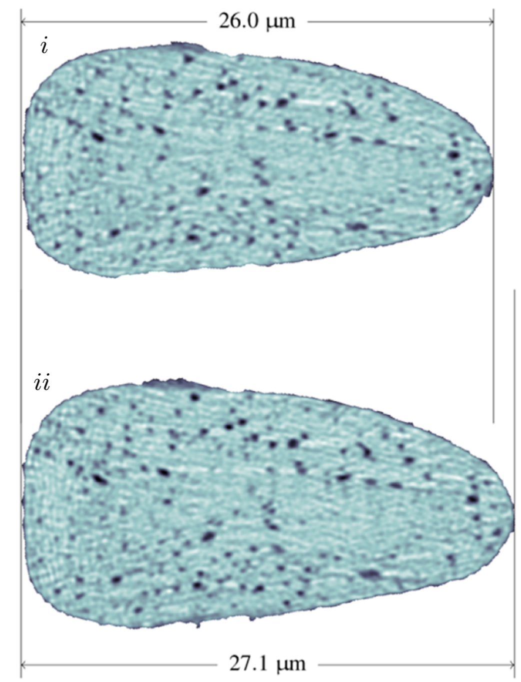
Guizar-Sicairos, Fienup, *Opt Express* **16** (2008) 7264

Number of citations of all preceding publications marked by the keywords "ptychography," "inhomogeneous primary wave," or "Wigner distribution deconvolution."
Data according to Thomson Reuters, Web of Knowledge, accessed Jun 13, 2017.

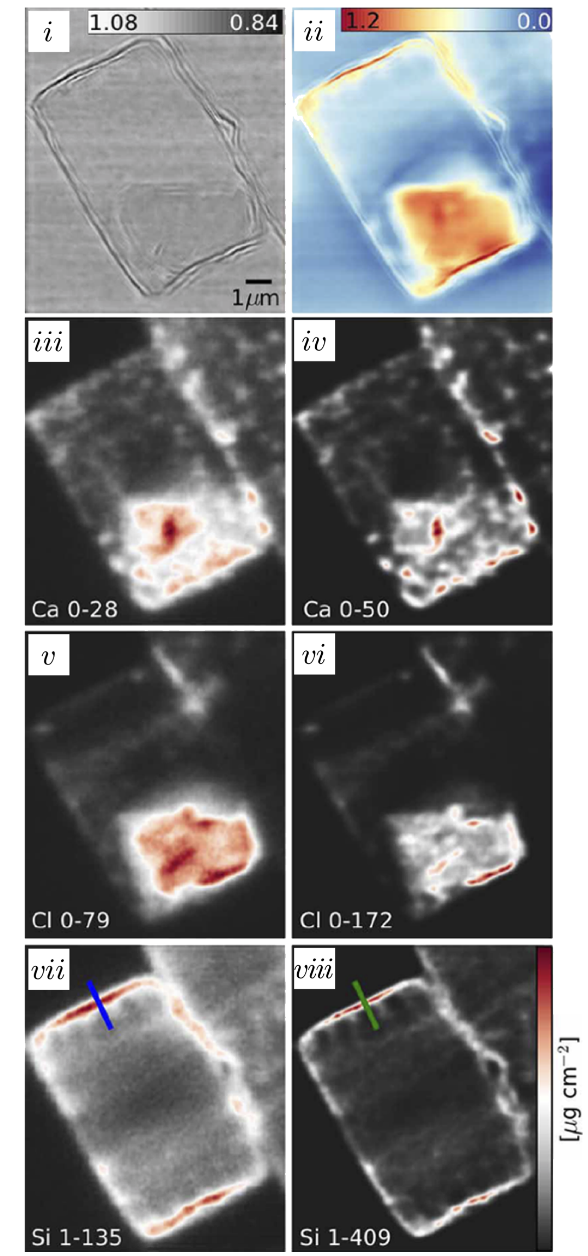
Ptychography
A Brief History…

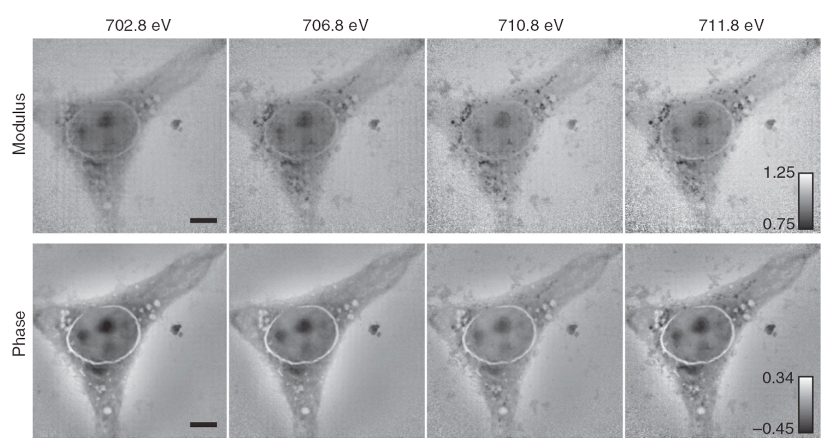


Dierolf *et al.*,
Nature **467** (2010) 436.

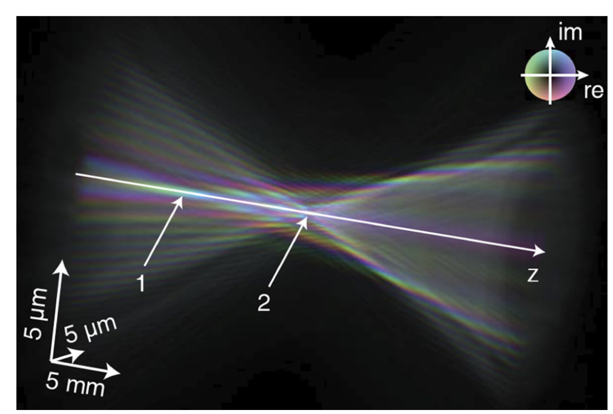


Esmaeili *et al.*,
Macromolecules **46** (2013) 434.





Maiden *et al.*,
Nature Commun **4** (2013) 1669.



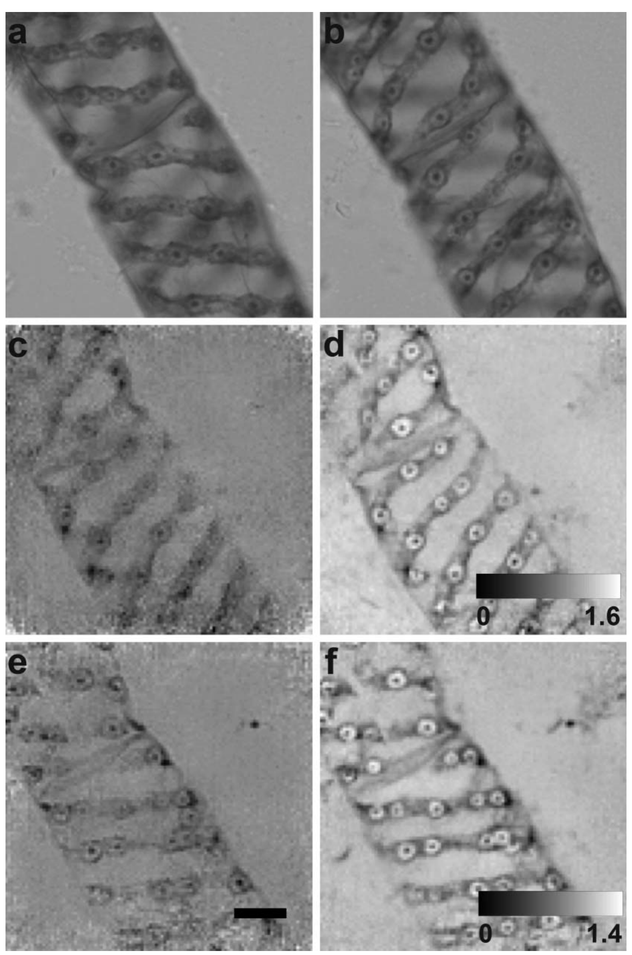
Schropp *et al.*,
Sci. Rep. **3** (2013) 1633.

Vine *et al.*, Rev. Sci. Instrum.
83 (2012) 033703.

Ptychography
Recent Developments

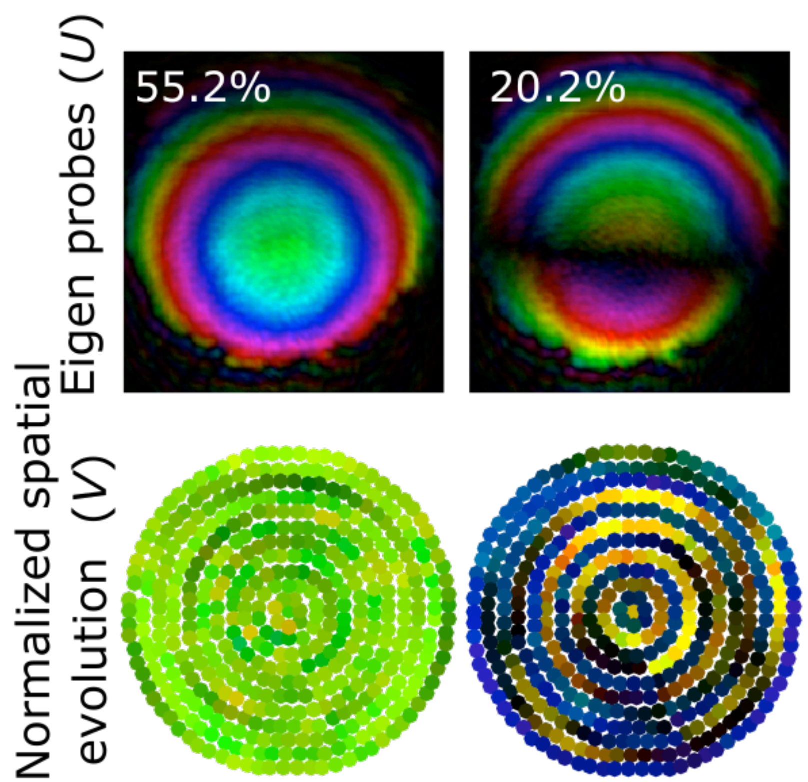
3D reconstruction using a multi-slice approach

Maiden *et al., J Opt Soc Am A* **29** (2012) 1606.
Suzuki *et al.*, *Phys Rev Lett* **112** (2014) 053903.
Shimomura *et al.*, *Phys Rev B* **91** (2015) 214114.



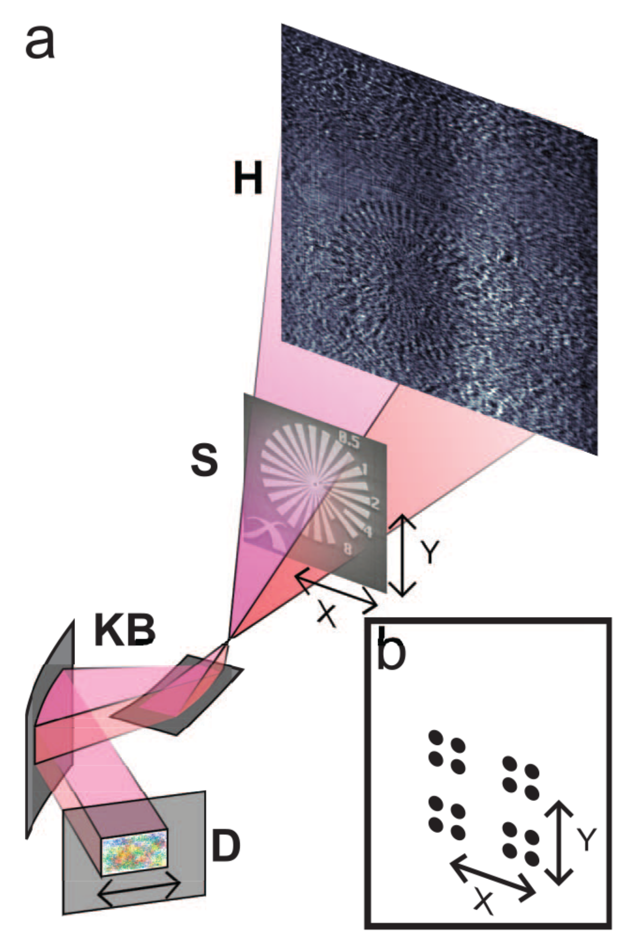
multiple modes, state mixtures and variations, instabilities

Thibault, Menzel, *Nature* **494** (2013) 68
Odstrčil *et al.*, Opt. Express **24** (2016) 8360.



different geometries e.g., near-field ptychography, Fourier ptychography…

Stockmar *et al.*, *Sci. Rep.* **3** (2013) 1927.
Zhen *et al.*, *Nat. Photonics* **7** (2013) 739.



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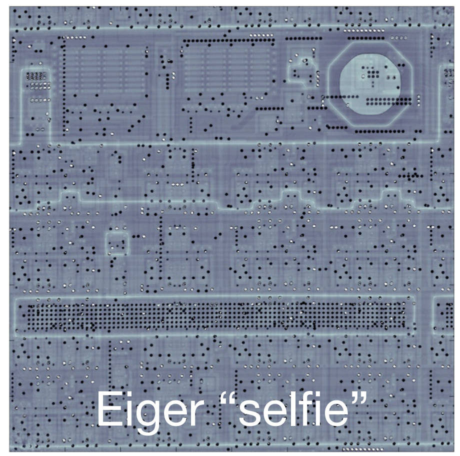
Comprehensive Approach

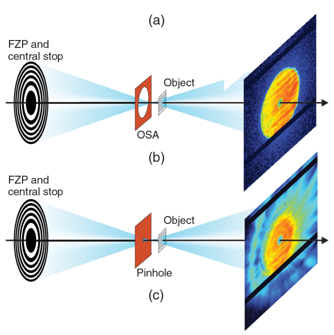
Detector Technology

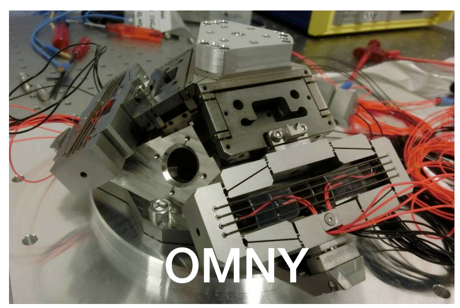
Pilatus is
being replaced
by Eiger



Experimental Design

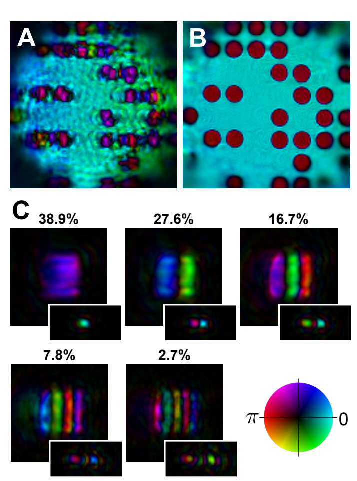
optimizing illumination and sample positioning



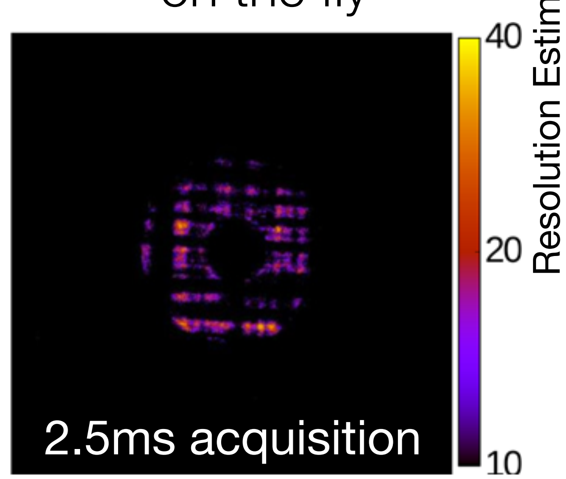


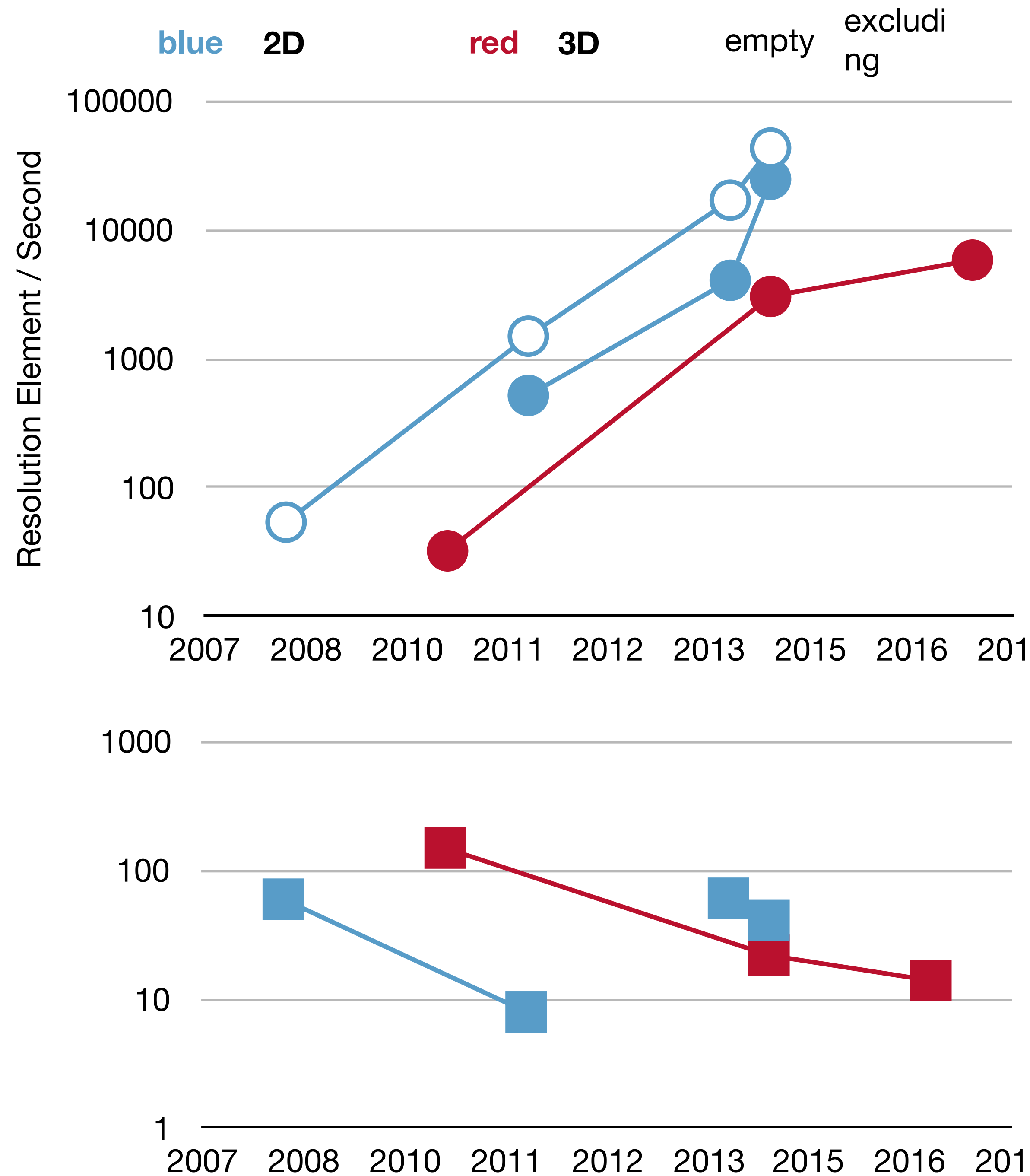
Analysis Development

"multi mode"



"on the fly"





Acquisition rate could be doubled yearly, ,
resolution approaching 10 nm (in 3D) and below (in 2D)

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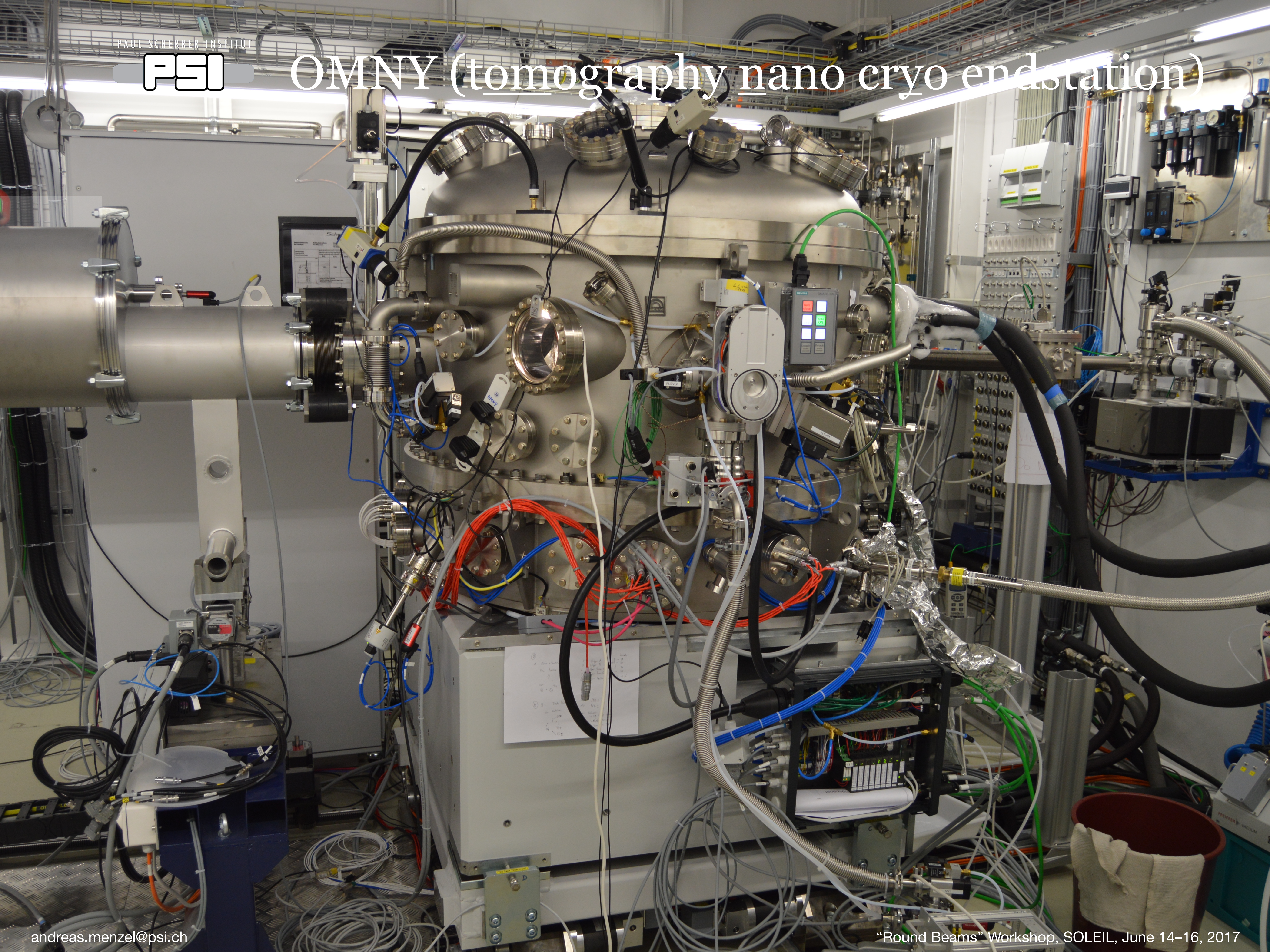
OMNY (tomography nano cryo endstation)



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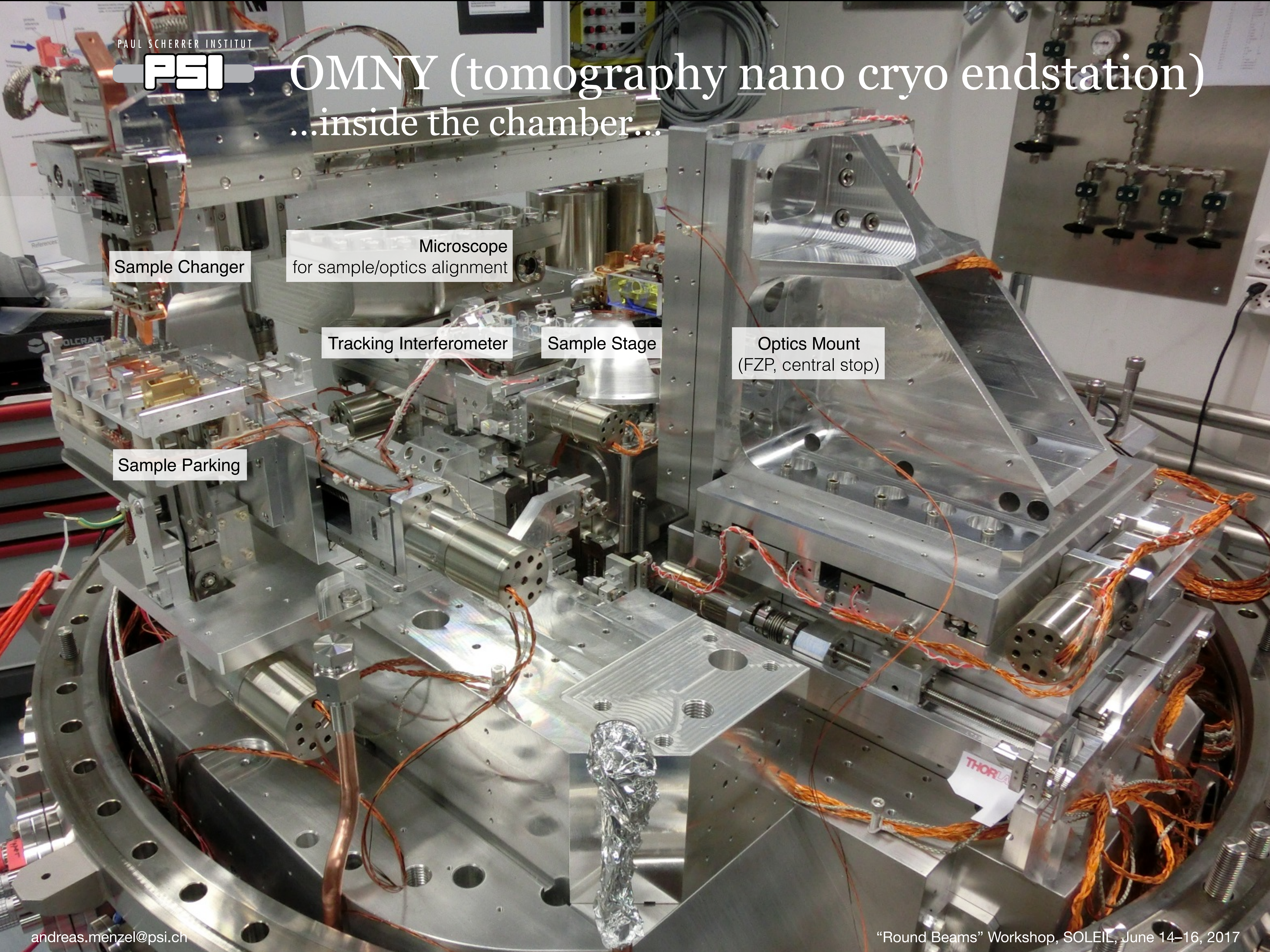
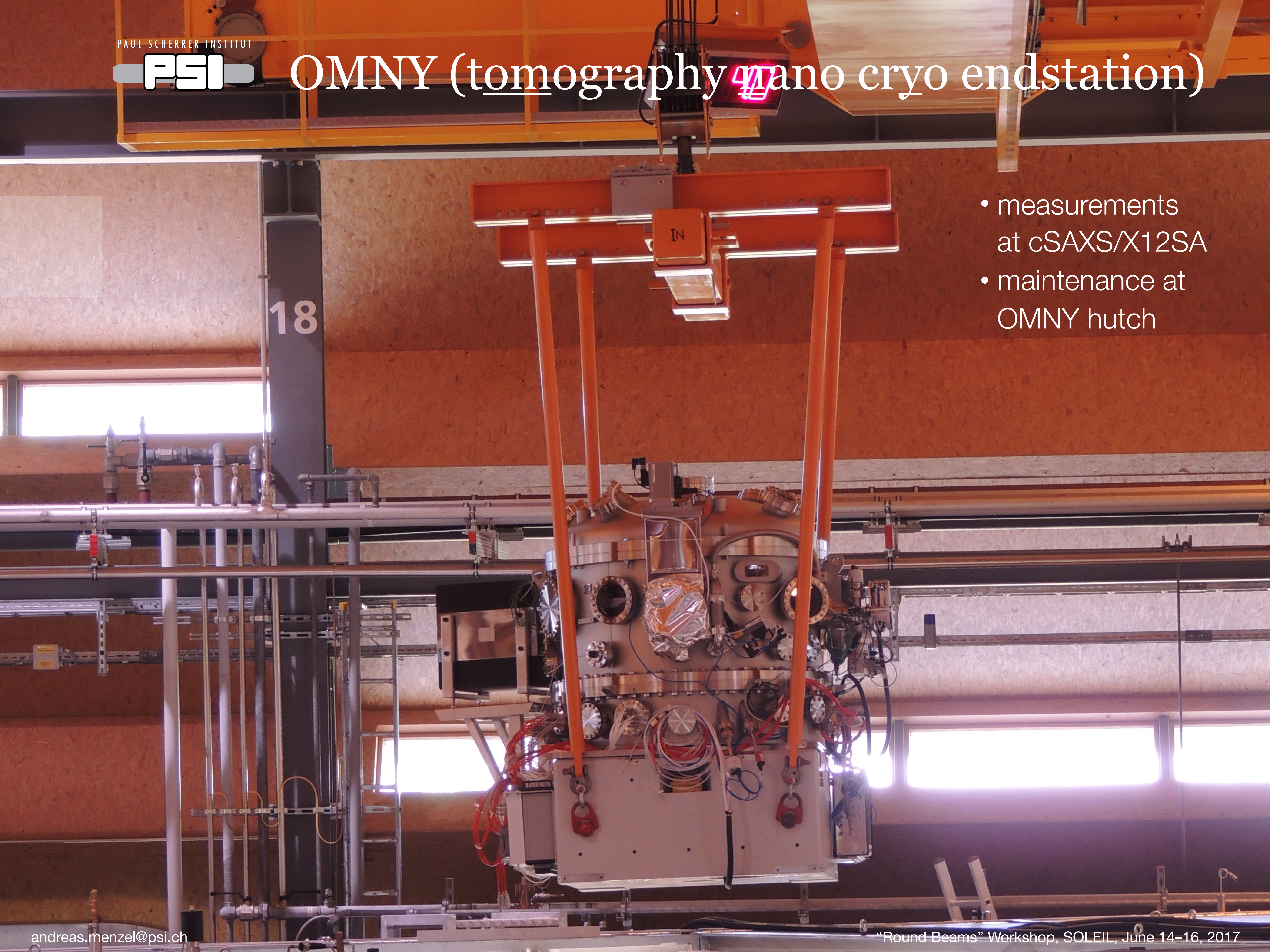
OMNY (tomography nano cryo endstation)

…inside the chamber…

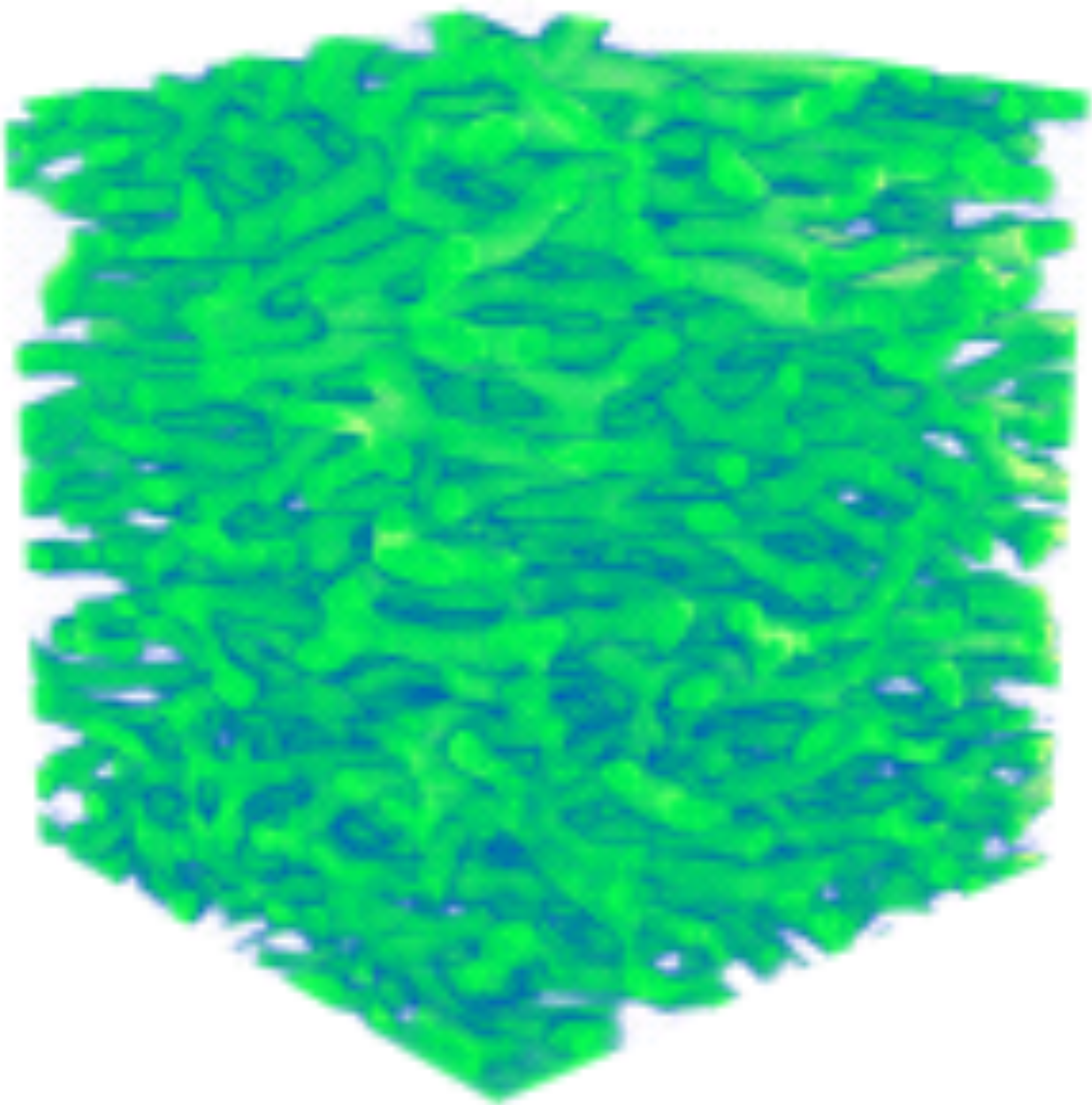


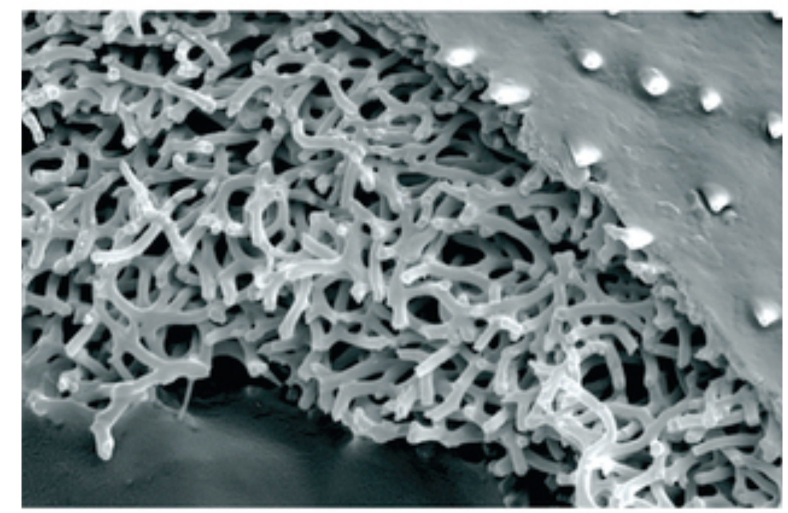
OMNY (tomography nano cryo endstation)



- measurements at cSAXS/X12SA
- maintenance at OMNY hutch

(Very) First Results





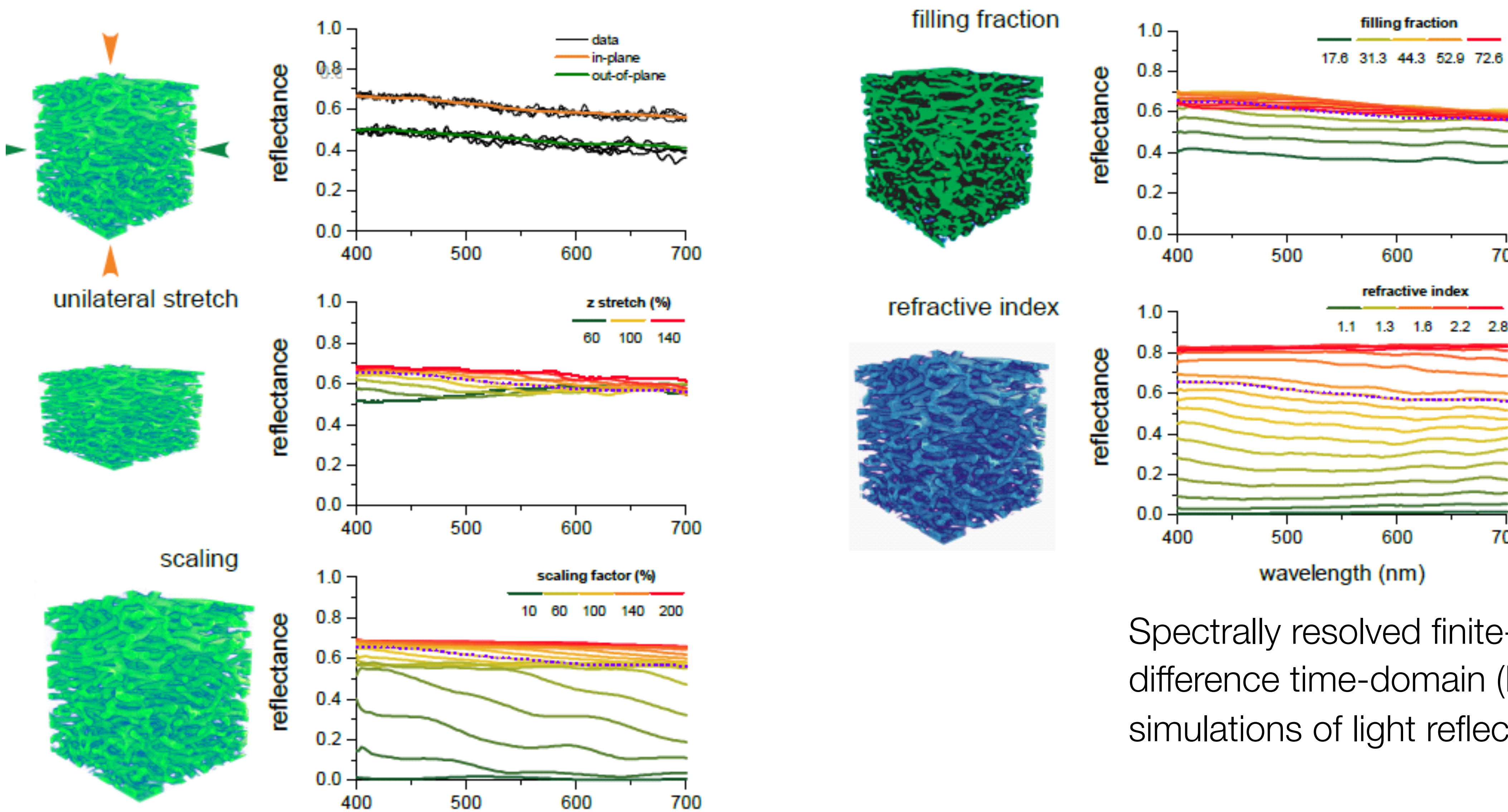
measurement at 92 K in vacuum
3D resolution: 28 nm

B.D. Wilts *et al.*, accepted in *Advanced Materials*

collaboration with A. Sepe, Adolphe Merkle Institute, Fribourg (Switzerland)

(Very) First Results

Evolutionary-Optimised Photonic Network Structure in Beetle Wing Scales Characertised by X-ray Nanotomography

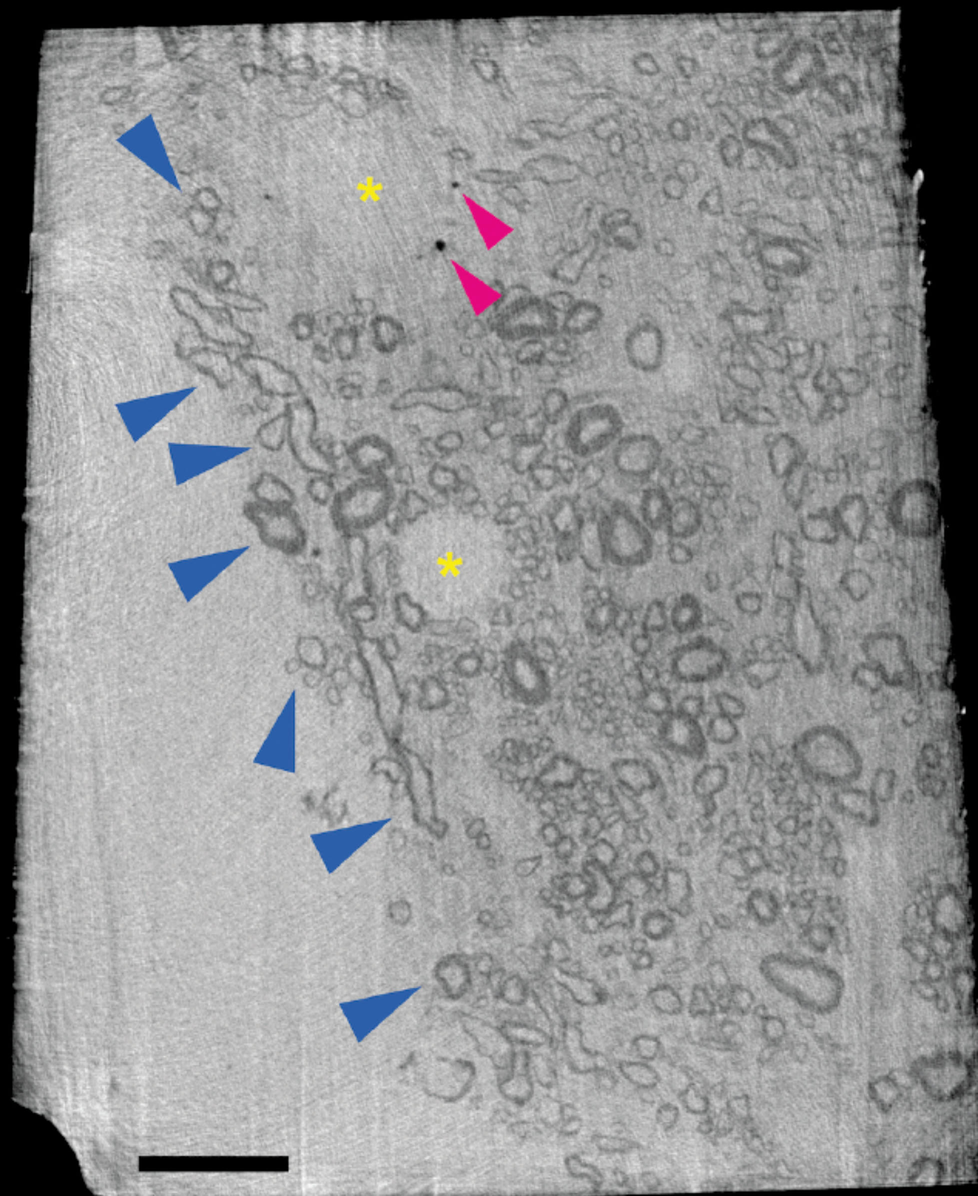


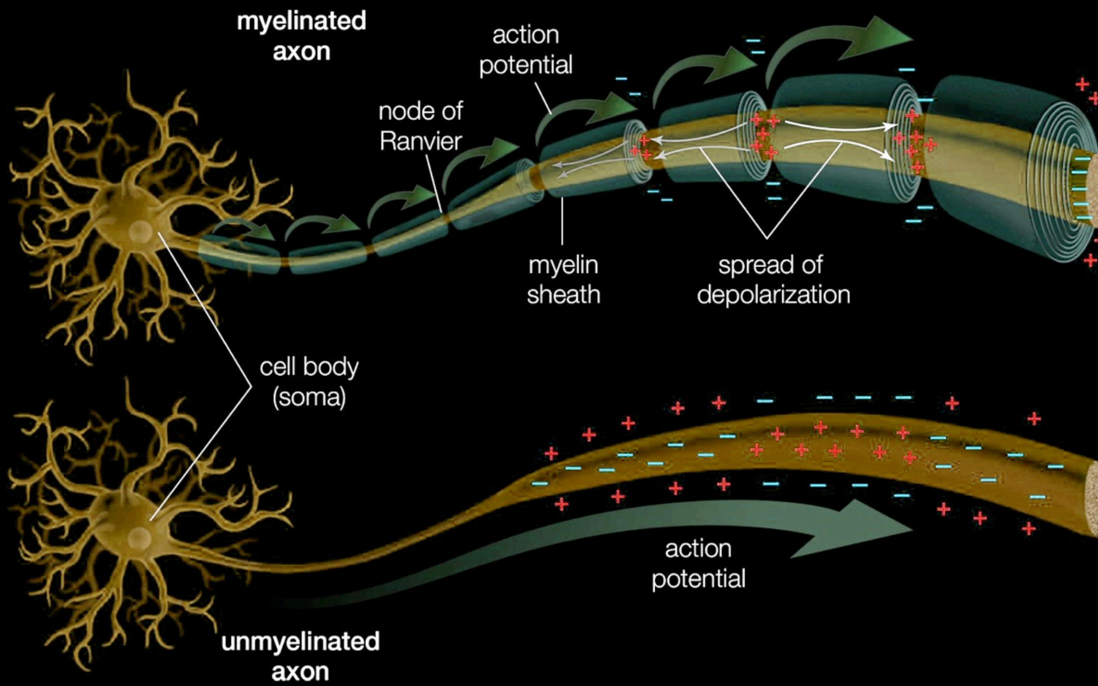
Spectrally resolved finite-difference time-domain (FDTD) simulations of light reflection

B.D. Wilts *et al.*, accepted in *Advanced Materials*

Ptychography

unstained cryo-preserved mouse brain





myelinated axons
nuclei
lysosomal lipofuscin?

unstained cryo-preserved mouse brain

S. Shahmoradian *et al.*, accepted in *Sci. Rep.* in collaboration with Uni Basel and Roche Innovation Center Basel

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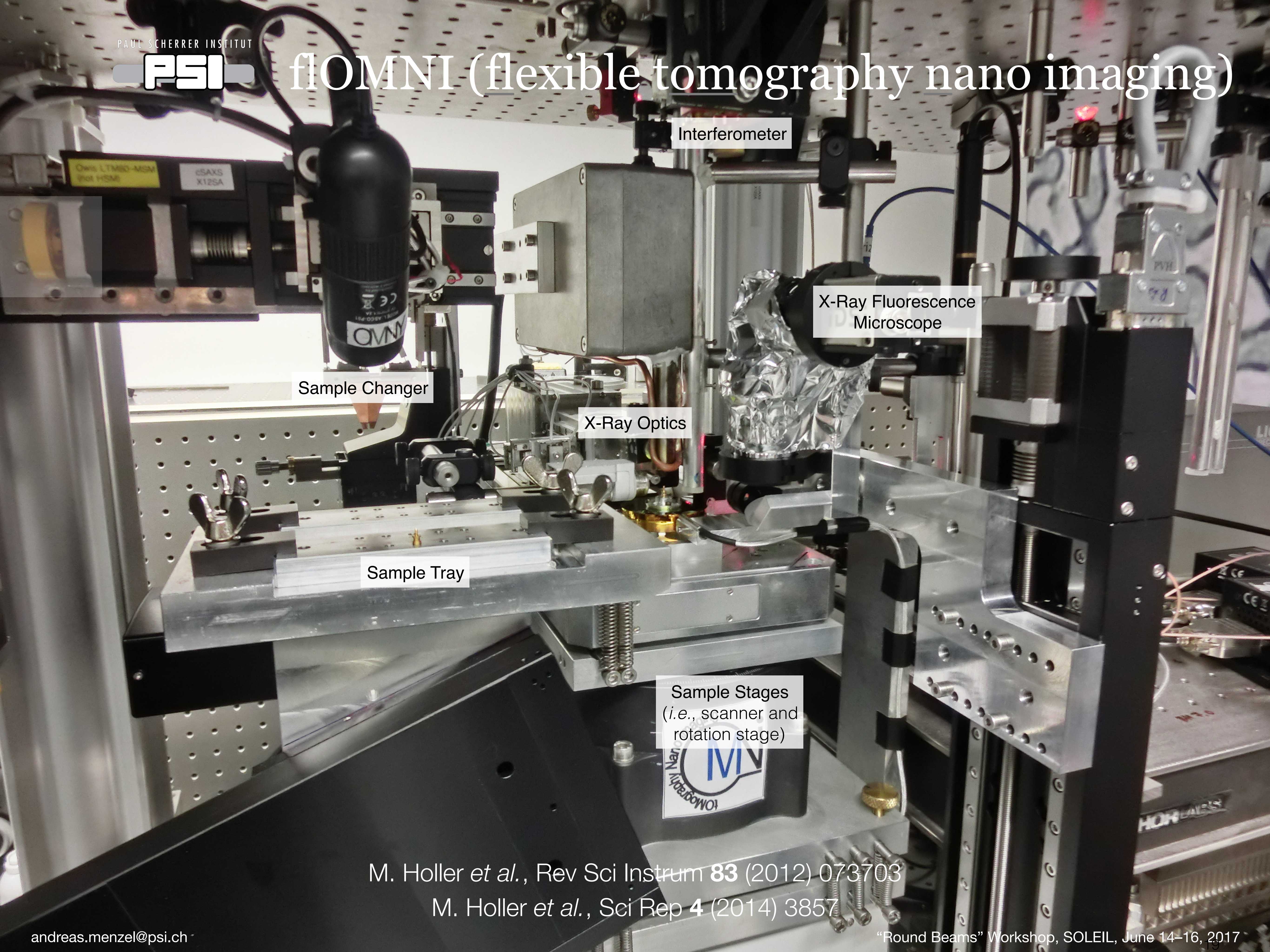
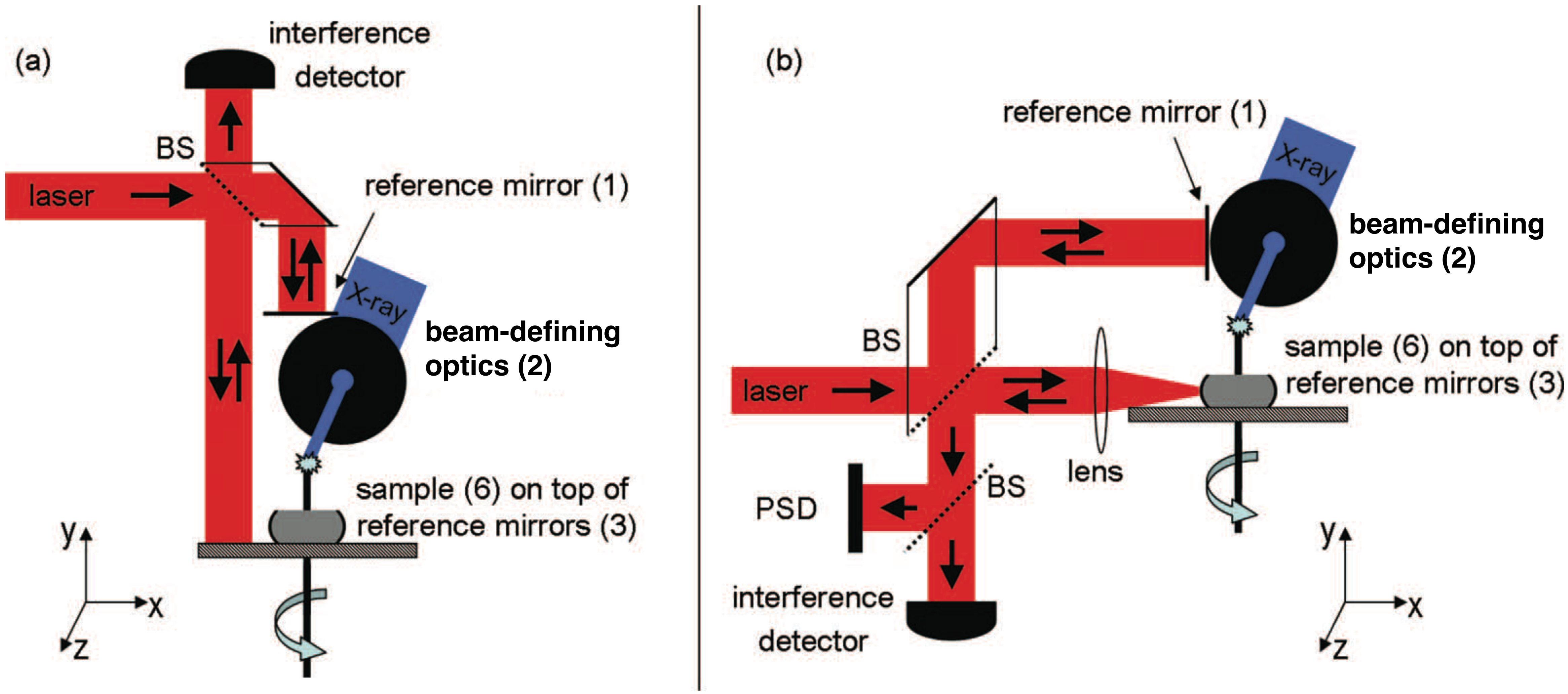
flOMNI (flexible tomography nano imaging)



M. Holler *et al.*, Rev Sci Instrum **83** (2012) 073703
M. Holler *et al.*, Sci Rep **4** (2014) 3857

Positioning Control

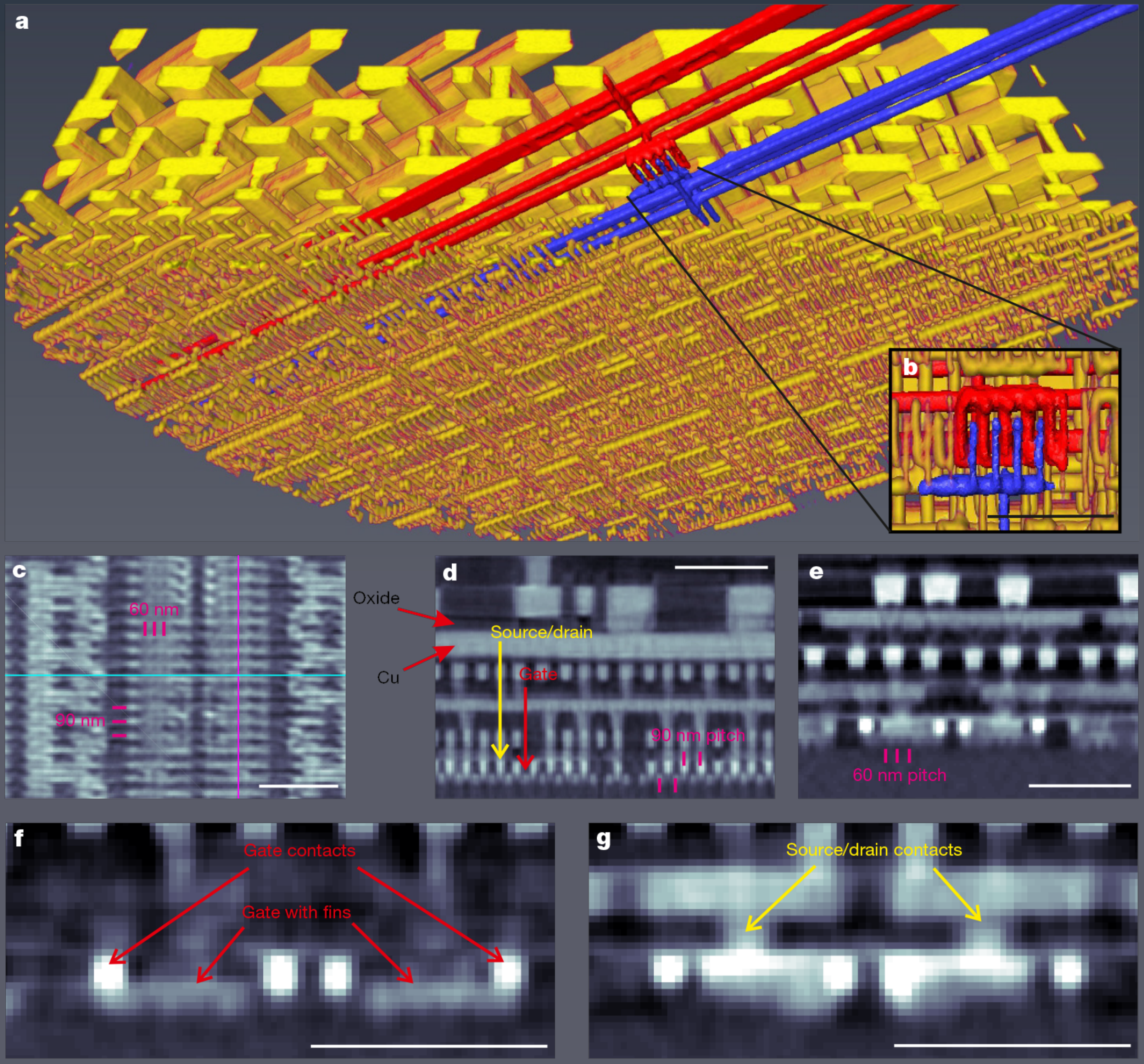
Optics need to allow for interferometrically controlled sample positioning or position measurement in three dimensions (or more). As chosen for the sample, short dead paths, i.e., distances between references and object of interest are highly desirable.



M. Holler *et al.*, Rev Sci Instrum **83** (2012) 073703
M. Holler *et al.*, Sci Rep **4** (2014) 3857

Imaging of Integrated Circuits

Intelprocesser, 22nm Technology



M. Holler *et al.*, Nature **543**(7645) (2017) 402

Imaging of Integrated Circuits

Some Sort of Roadmap

	achieved*	achieved†	demanded#
	2D	3D (tomography)	"3D" (via laminography)
field of view	500 × 288 μm^2	∅ ~ 10µm	10 × 10 mm^2
resolution	~ 40 nm	~ 15 nm	10 nm
measurement time	~ 70 min ~ 4 × 10^3 s	~ 1 day ~ 9 × 10^4 s	25 days ~ 2 × 10^6 s
effective dwell time	~ 40 µs	~ 170 µs	~ 0.1 µs

long-term requirement: increase in coherent flux: ~ 5000

*Guizar-Sicairos *et al.*, Opt. Express **22** (2014) 14859

†M. Holler *et al.*, Nature **543**(7645) (2017) 402

#http://www.iarpa.gov/index.php/research-programs/raven

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Upgrade Plans

Plan:	SLS-2	→ gain in coherent flux: $10^{1.5}$
	optimized undulator	→ gain in flux: $10^{0.5}$
	reduction of longitudinal coherence	→ gain in flux: 10^{1}
	more efficient optics	→ gain in flux: 10^{1}
	total gain in coherent flux	in the order of 10^{4}!
	total gain in flux	close to 10^{3}

This would render these ambitious goals entirely feasible!

Yet: Reduction of longitudinal coherence may be problematic:
While it can be controlled and accounted for, it limits probe size and thus affects already stringent scanning requirements.

Conclusion

While developments are still ongoing, X-ray ptychography has already matured to a reliable imaging technique, sought after by scientists who want to learn about their samples (and have no particular interest in the technique itself).

To satisfy the increasing demand, ptychography needs to become faster and more efficient. This requires new sources and state-of-the-art optics, detectors, positioning and metrology, and computing power.

With upcoming/planned sources, the future looks bright indeed in regard to

- sample-limited resolution,
- high throughput, large sample ensembles, representative volumes etc., and
- increased time-resolution.

However, oftentimes and already now, neither data acquisition nor image reconstruction prove “rate-limiting” in most imaging projects but the subsequent analysis, such as segmentation, parameterization, and quantitative evaluation. User training and IT resources need to be organized accordingly.