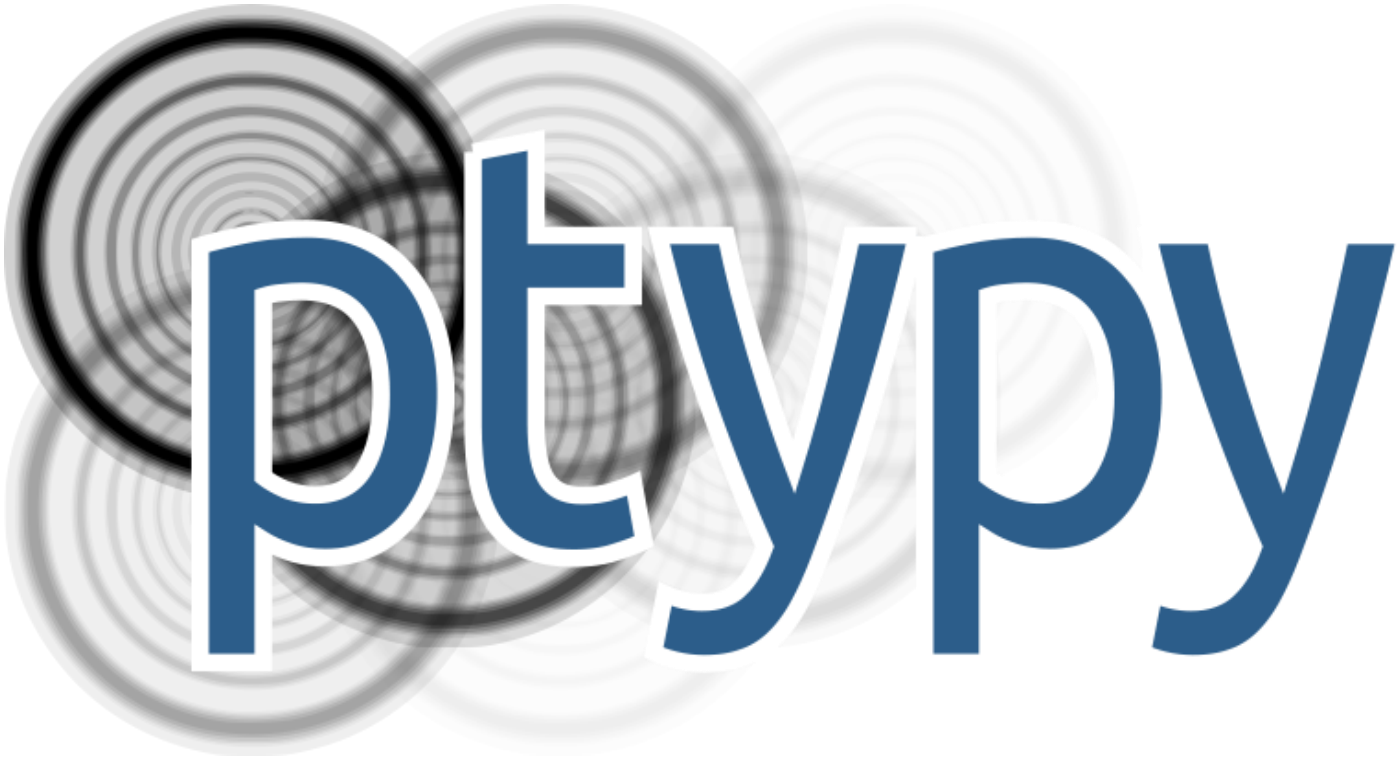
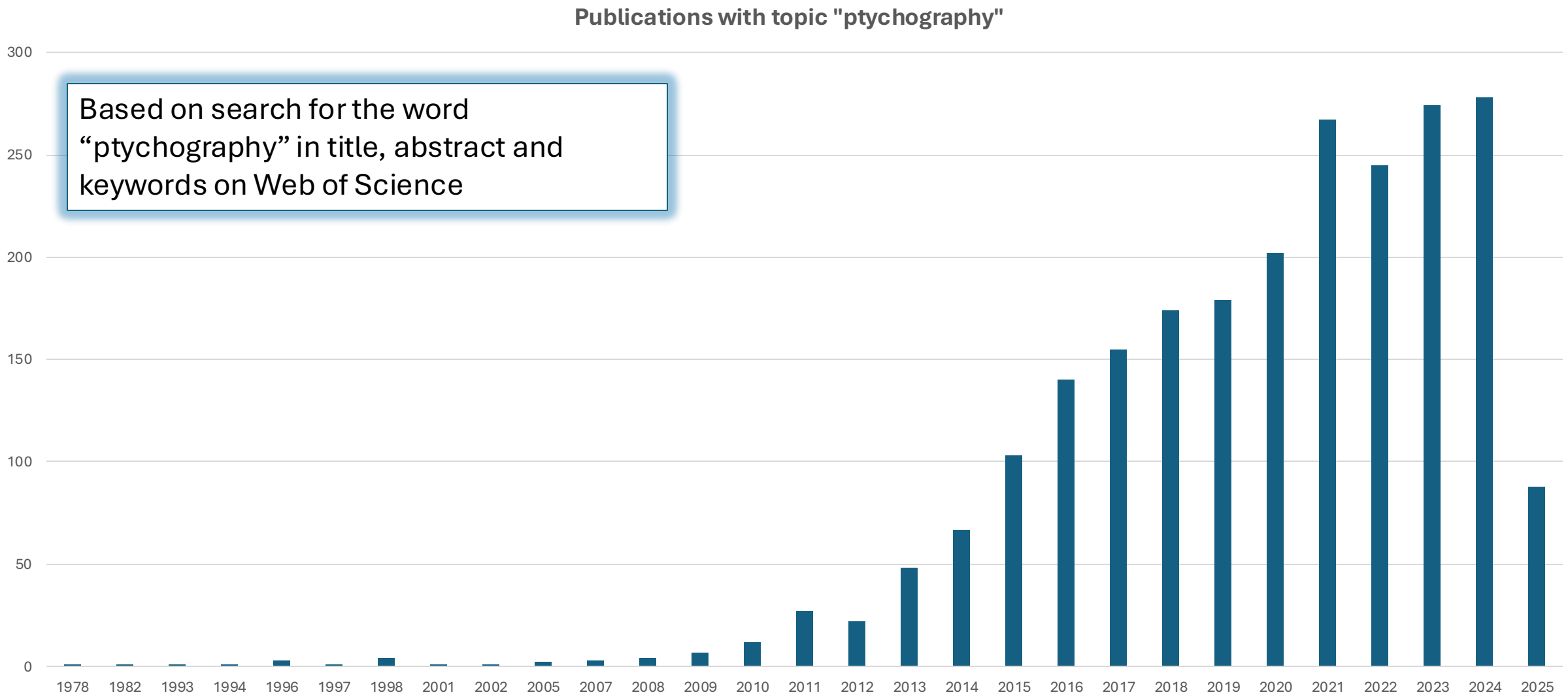


Benedikt Daurer & Pierre Thibault

Current and Future Challenges

PtyPy 2025 @SOLEIL, 12th and 13th May 2025

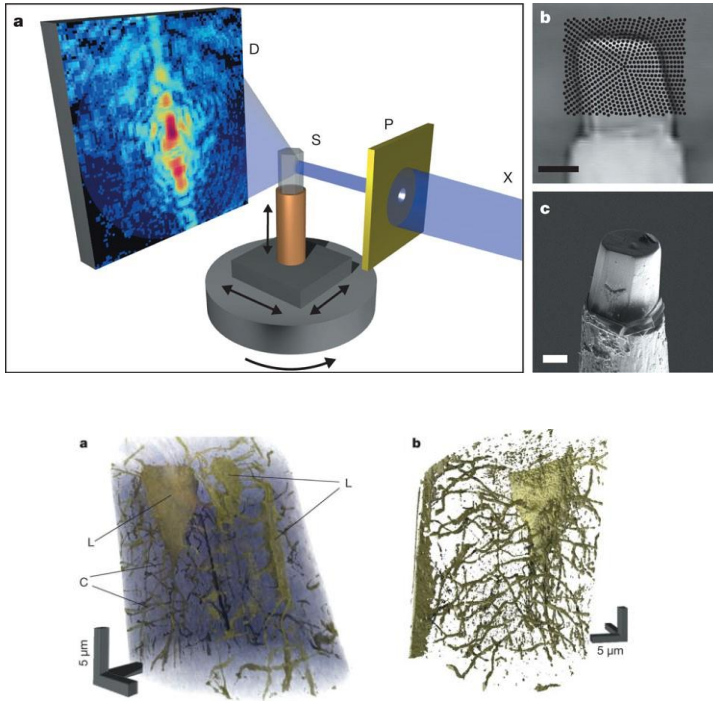
How popular is ptychography as a method?



Based on search for the word “ptychography” in title, abstract and keywords on Web of Science

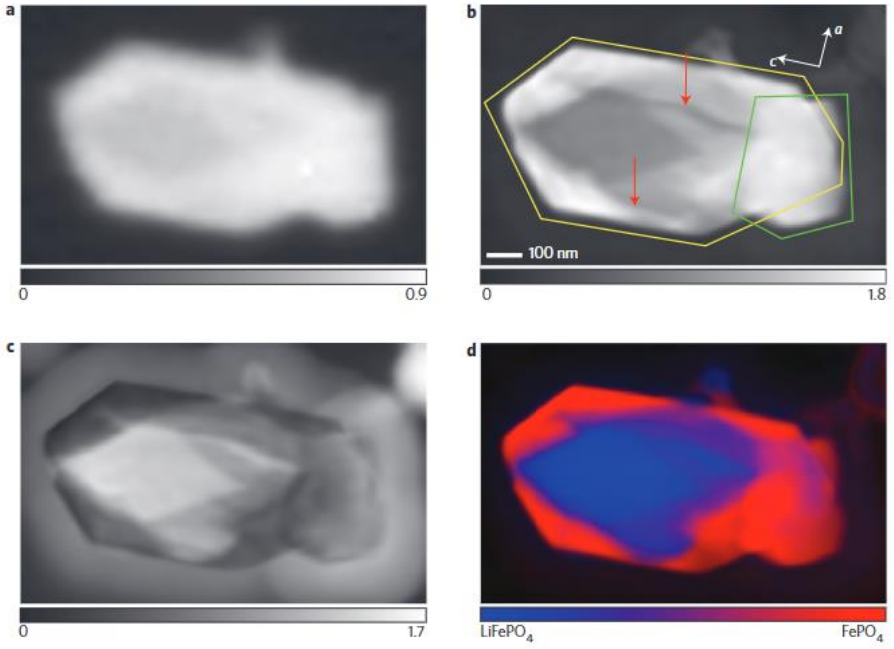
A few ptychography highlights and trends

Ptycho-Tomography
Expanding to Three dimensions



Dierolf, M. *et al*. *Nature*, 467(7314), pp. 436–439 (2010)

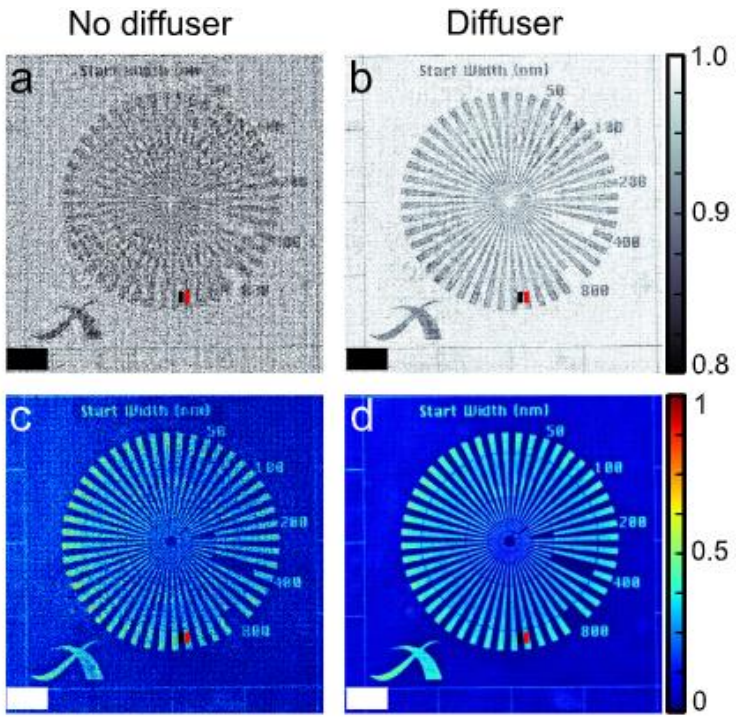
Spectro-Ptychography
Chemical specificity



Shapiro, D.A. *et al.*, *Nature photonics*, 8(10), pp. 765–769 (2014)

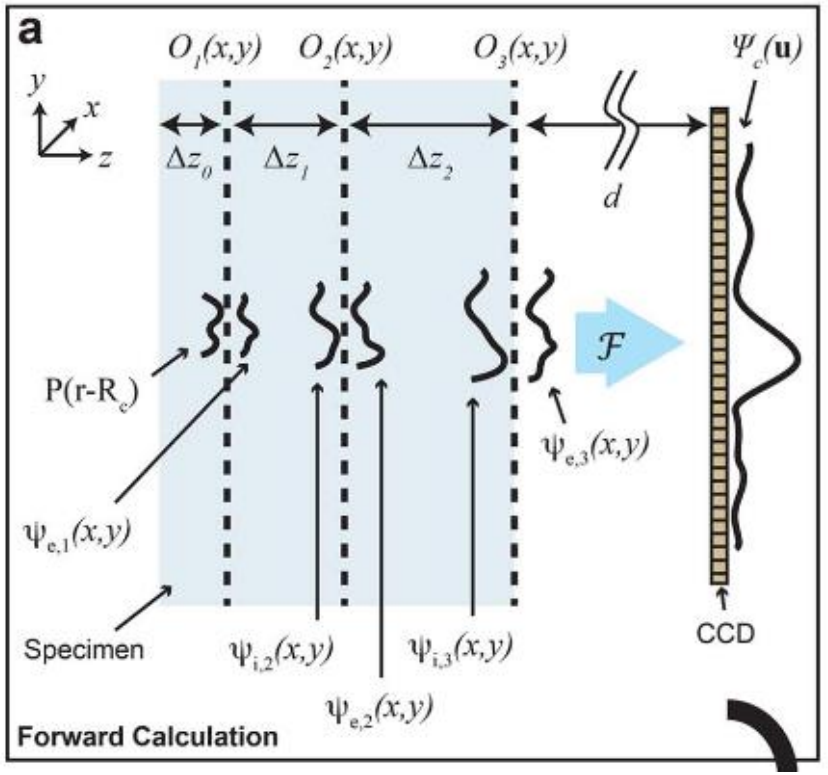
A few ptychography highlights and trends

Ptychography in the nearfield



Stockmar, M. *et al.*, *Scientific reports*, 3, p. 1927 (2013)

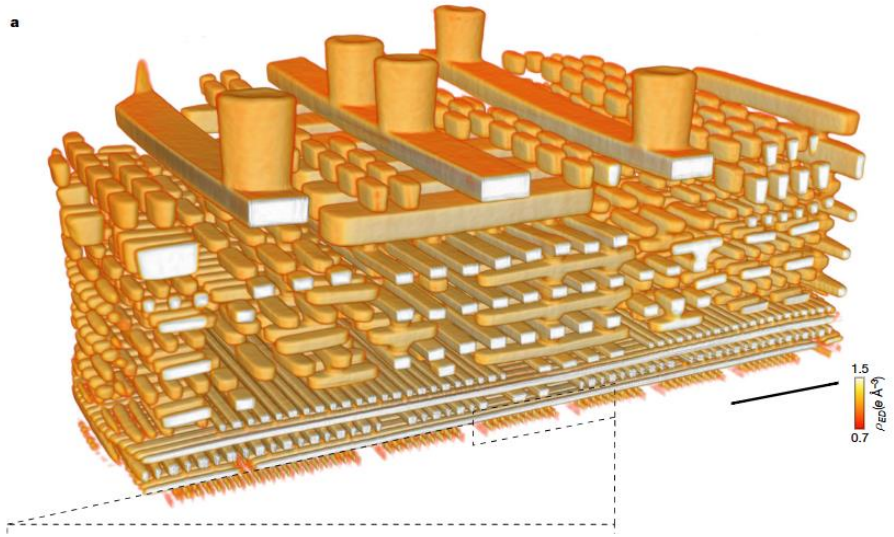
Ptychography with thick samples



Maiden, a. M. *et al.*, *JOSA A,* 29(8), pp. 1606–1614. (2012)

A few ptychography highlights and trends

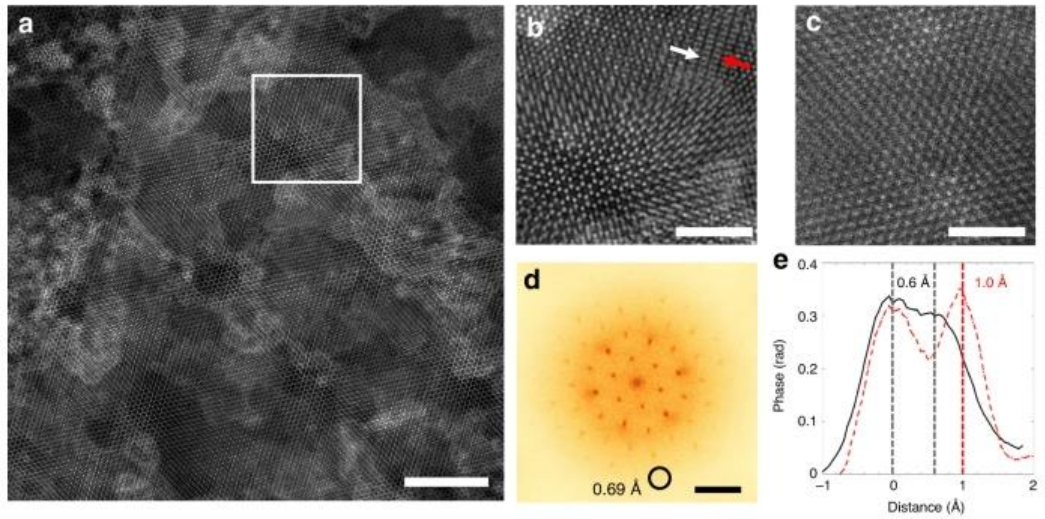
Burst ptychography in Three dimensions



Achieved record in 3D resolution by adding more refinement

Aidukas, T. *et al.*, *Nature*, 632(8023), pp. 81–88. (2024).

Ptychography with electrons

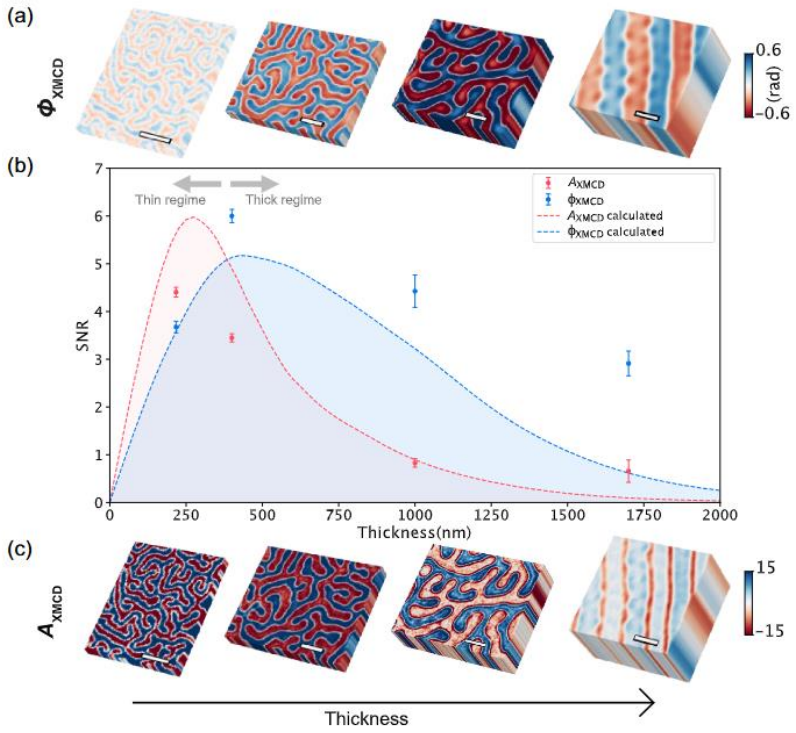


Sub-Angstrom resolution

Chen, Z. *et al, Nature communications*, 11(1), p. 2994. (2020)

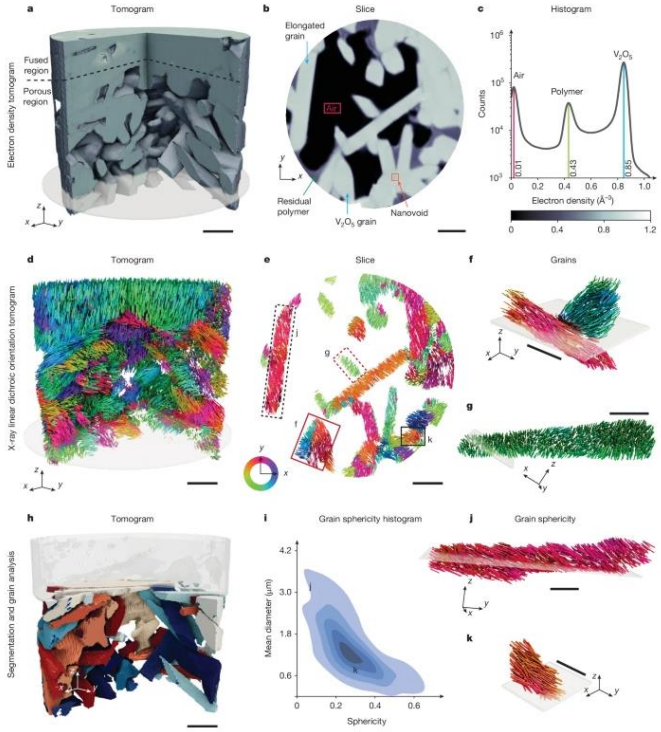
A few ptychography highlights and trends

Magnetic Dichroism with ptychography in Two dimensions



Neethirajan, J. *et al., Physical review. X*, 14(3), p. 031028. (2024)

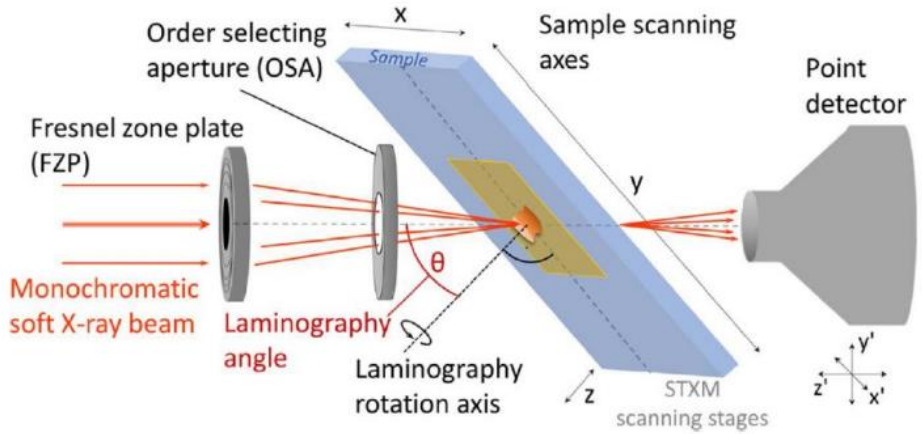
Magnetic Dichroism with ptychography in Three dimensions

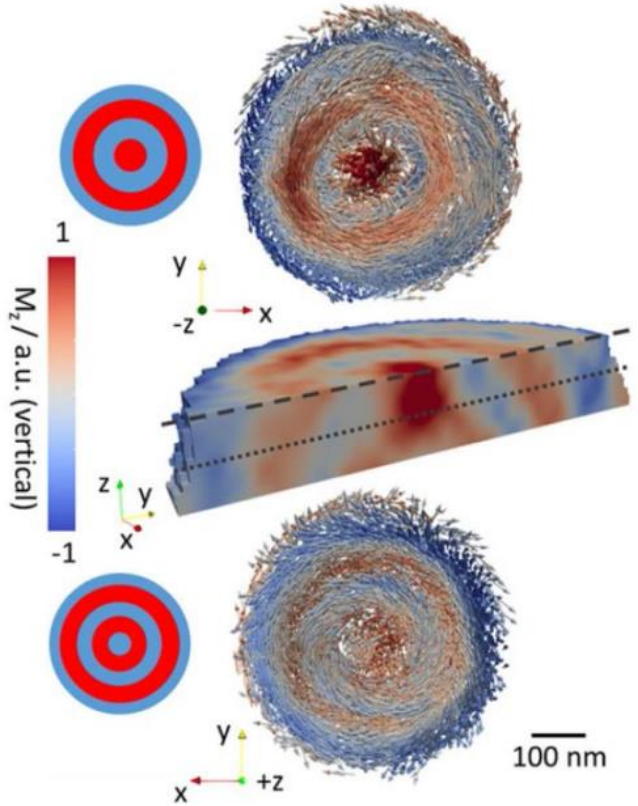


Apseros, A. *et al., Nature*, 636(8042), pp. 354–360. (2024).

A few ptychography highlights and trends

New Diamond-II flagship beamline
CSXID / I17

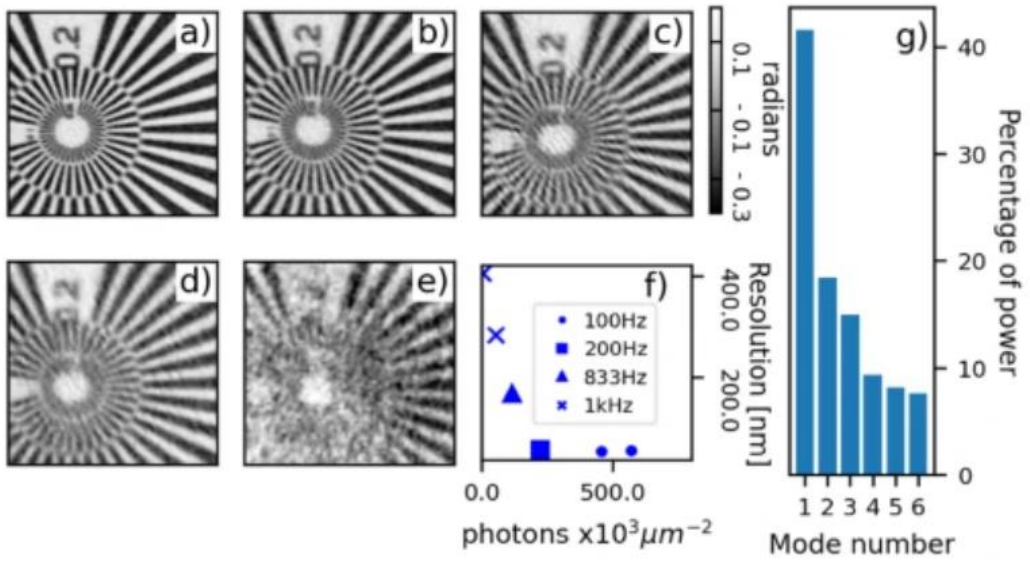




Available to the community in 2030

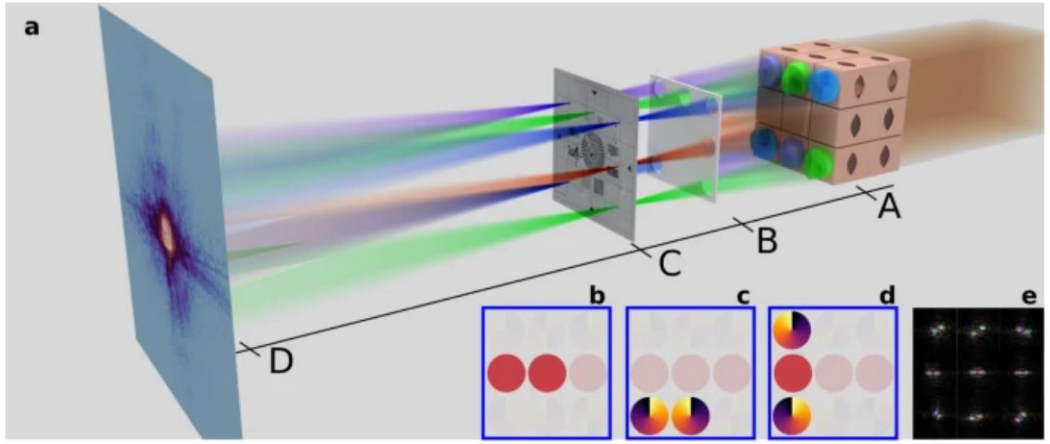
A few ptychography highlights and trends

Ptychography with very fast detectors



Batey, D. *et al., Scientific reports*, 12(1), p. 7846. (2022).

Ptychography with multiple beams

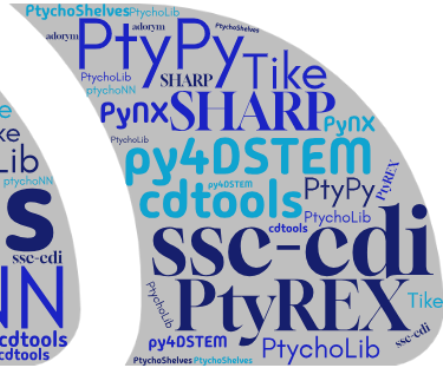


Lyubomirskiy, M. *et al.*,*Scientific reports*, 12(1), p. 6203. (2022).

A non-complete list of other approaches

- Ptychography with a very large field of view
- Correlative imaging with fluorescence and other modalities
- Wavefront sensing with ptychography
- Tele-ptychography
- Single-shot ptychography
- Broadband ptychography
- Ptychography with very low dose
- Etc.

Landscape of ptychography software



How does PtyPy fit into this landscape?

Sources

X-rays ✓ Optical light ✓

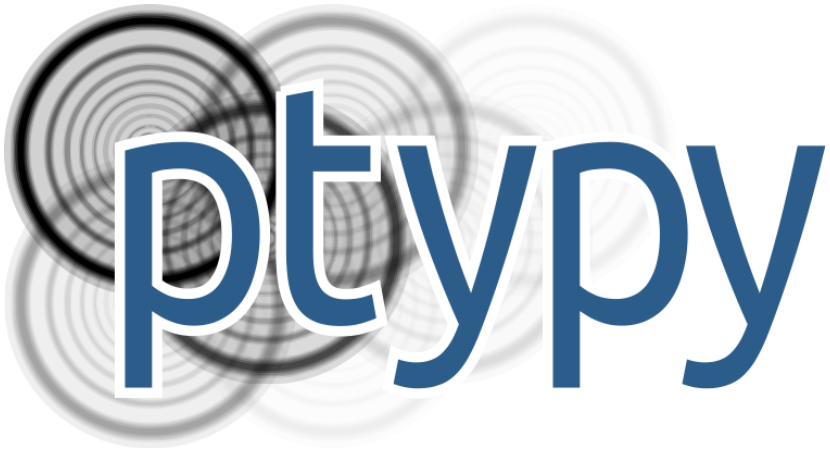
Electrons ✓

High-throughput

GPU acceleration ✓ Scalable ✓

Data streaming ✓

Efficient data loading ✗



Innovative Geometries

Multi-beam ✓ Nearfield ✓

Multi-probe ✓ Multi-wavelength ✓

Multi-slice ⏳ Tele-ptycho ✓

Other features

Mixed states ✓

Refractive index ⏳ Noise models ✓

Validation utils ⏳ Subpixel optimisation ✗

Current core developer priorities

- Better documentation
  - New paper with latest features
  - New documentation page
- High-performance upgrades
  - Identify and fix bottlenecks in data loading and model creation
  - Improve the MPI communicator
  - Distributed object with shared borders
- User experience
  - Redo parameter validation with Pydantic/Dataclass
  - More general overlap metric
  - Improve interaction class to support web front-end more natively

The user community's added priorities

- Multi-slice ptychography
- Refractive index ptychography
- New obscure geometry X
- New favourite phase retrieval algorithm Y
- GPU acceleration for all of the above
- And more, what is your priority?

We – the core developers – cannot implement any of these, but hopefully the wider community can!

15-19 September 2025, Triest ▸ speak to us if interested

Q & A

- What's missing in PtyPy?
- How can we improve the code?
- How can we improve the documentation?
- How can we improve the hands-on tutorials?
- Did we miss anything important during the basic lectures?
- Should we keep organising these user workshops?
- Anything else you would like to ask us?