Workflow for Near Real-Time Processing of Large 4D STEM Experimental Datasets

Daniel G. Stroppa

Quantitative Electron Microscopy

Port Barcares, FR

14.May.2025

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Disclaimer

DECTRIS and beyond

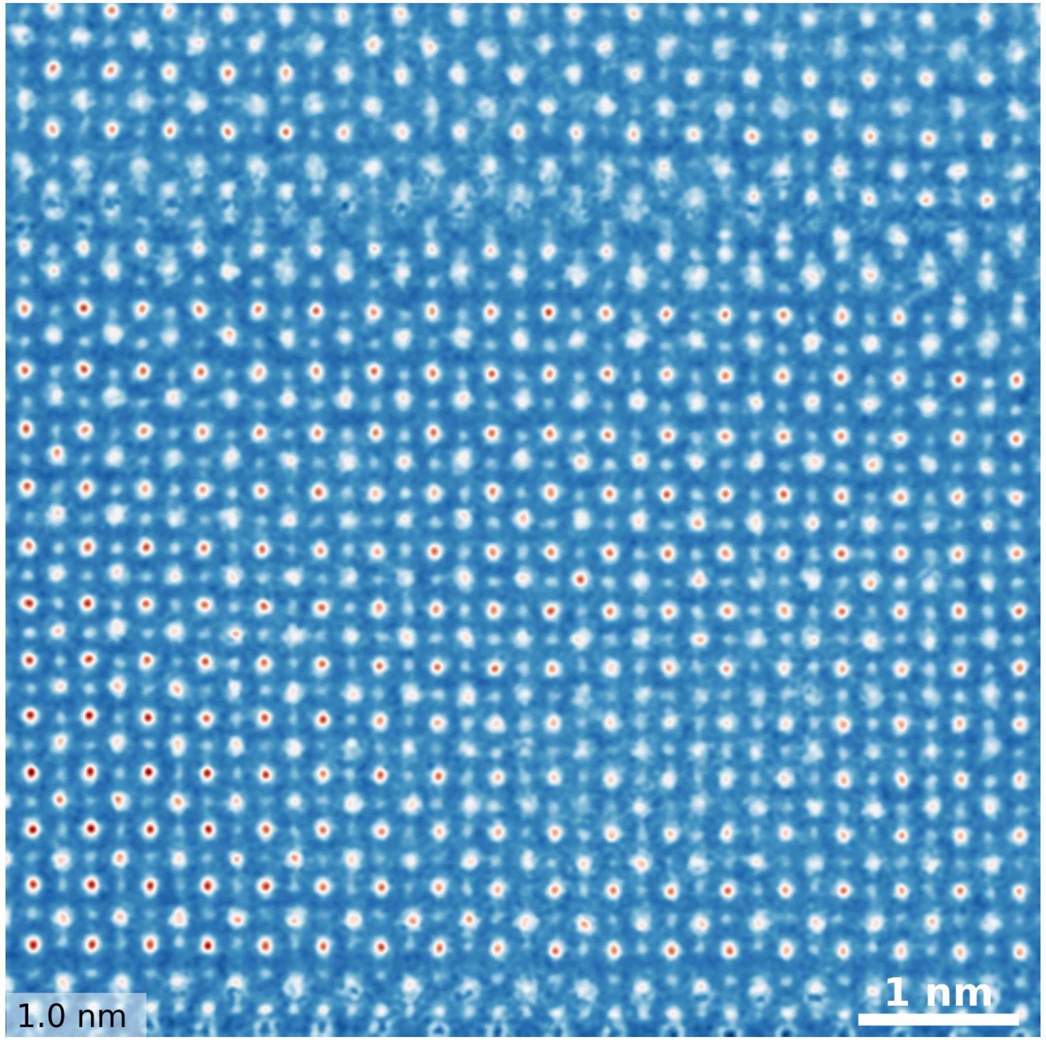
- *ideas that may fit any detector*

4D STEM and beyond

- *ideas that may apply to different applications*

Pace and style

- *after-lunch session*
- *32 slides / 90 min*
- *take it offline*



Have fun!

QEM 2009

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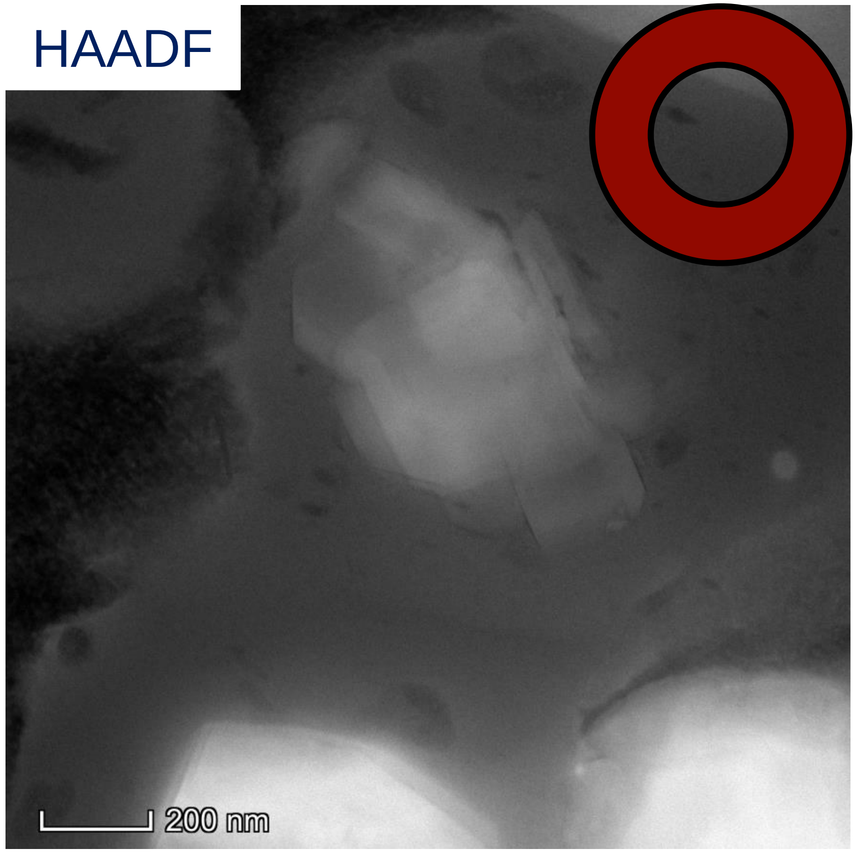
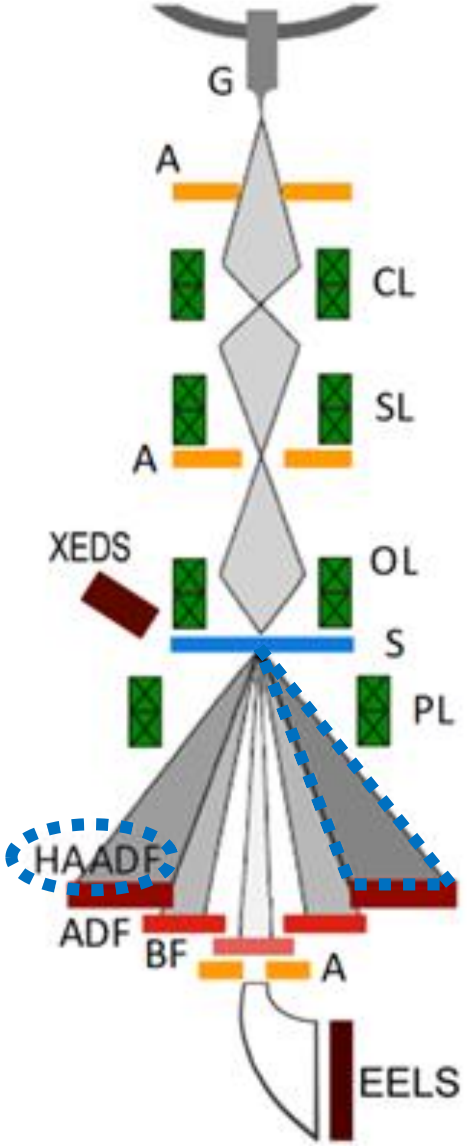
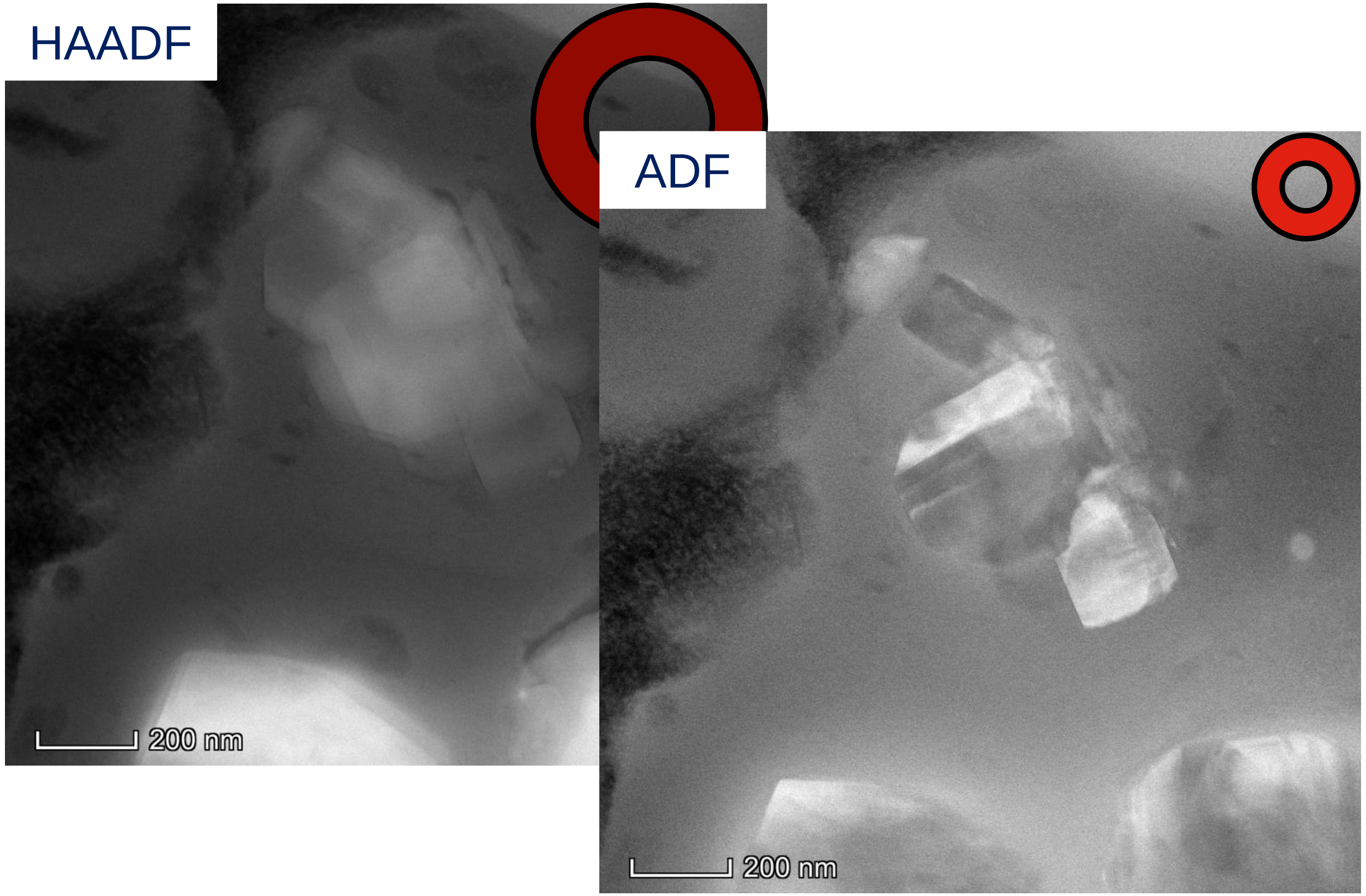
STEM imaging



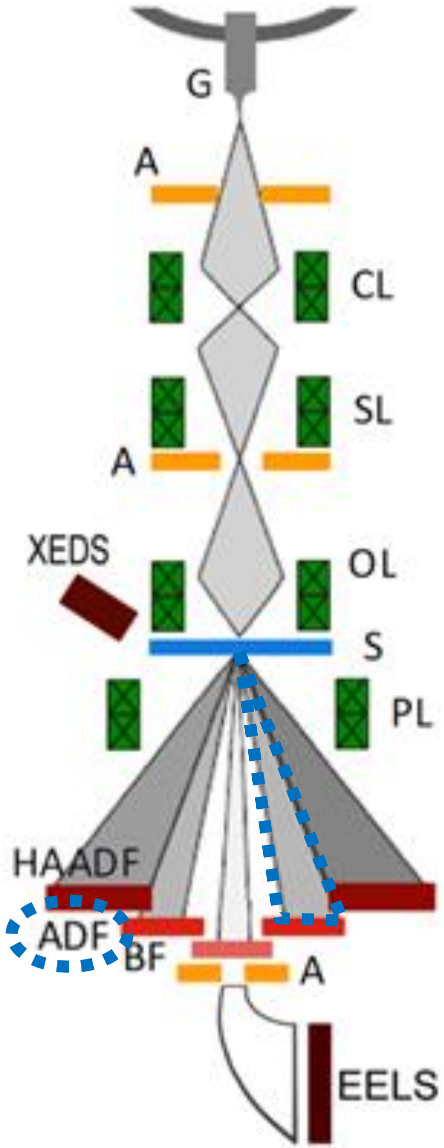


STEM imaging of Al oxide precipitates in rubber

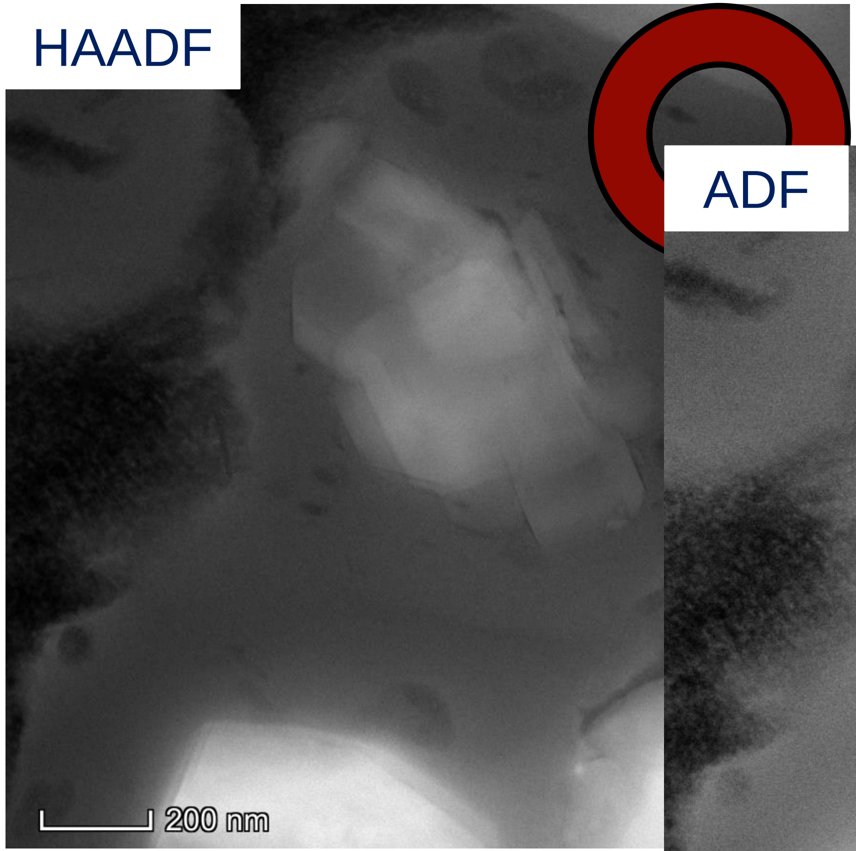
STEM imaging

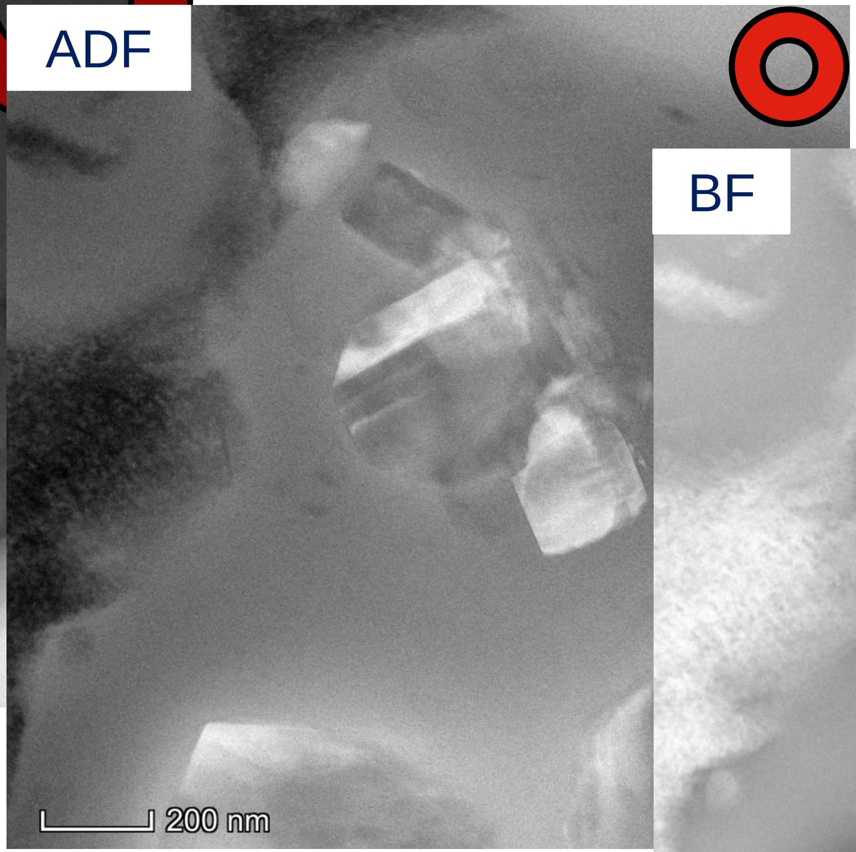


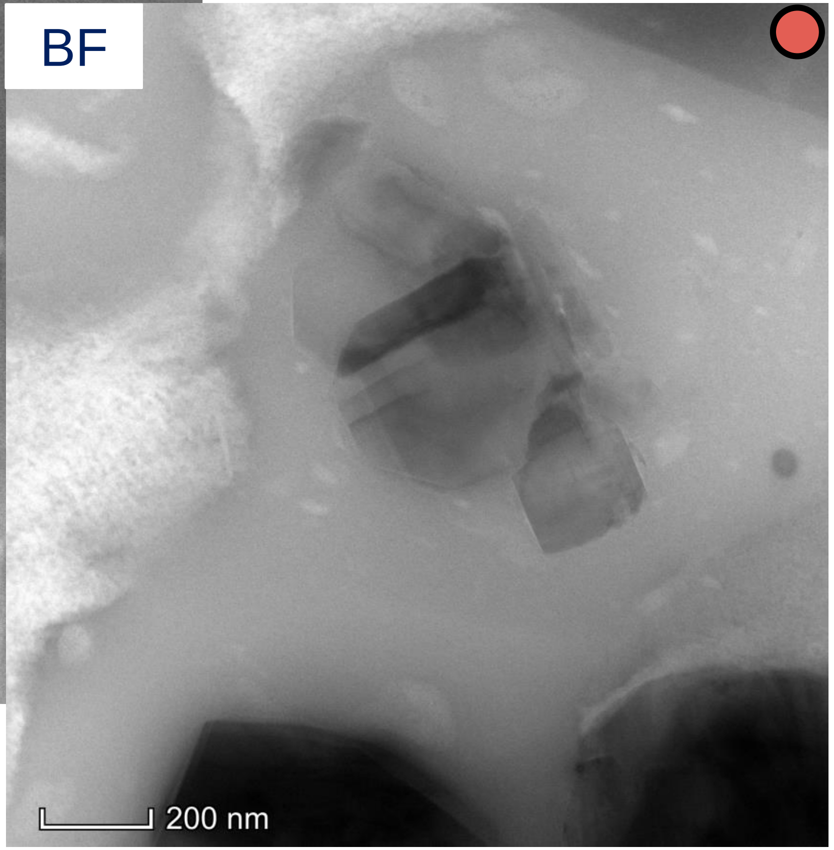
STEM imaging of Al oxide precipitates in rubber



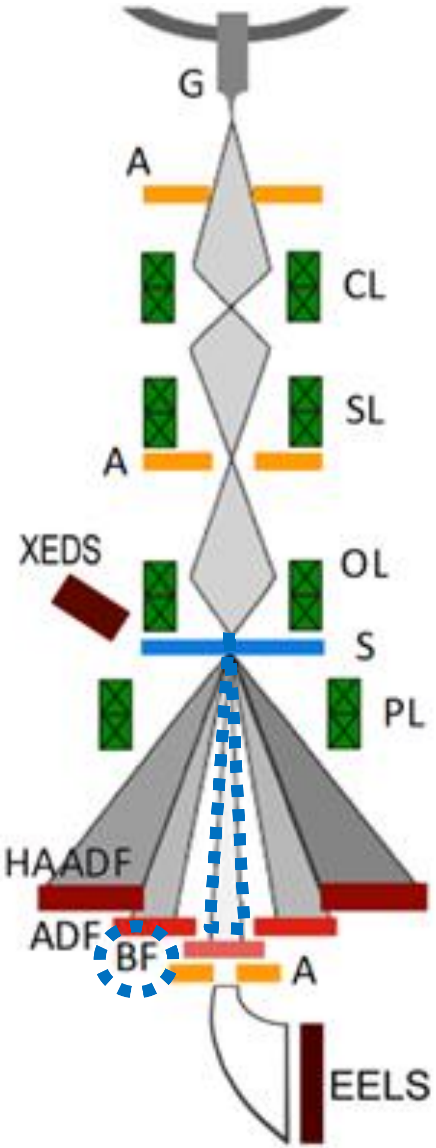
STEM imaging







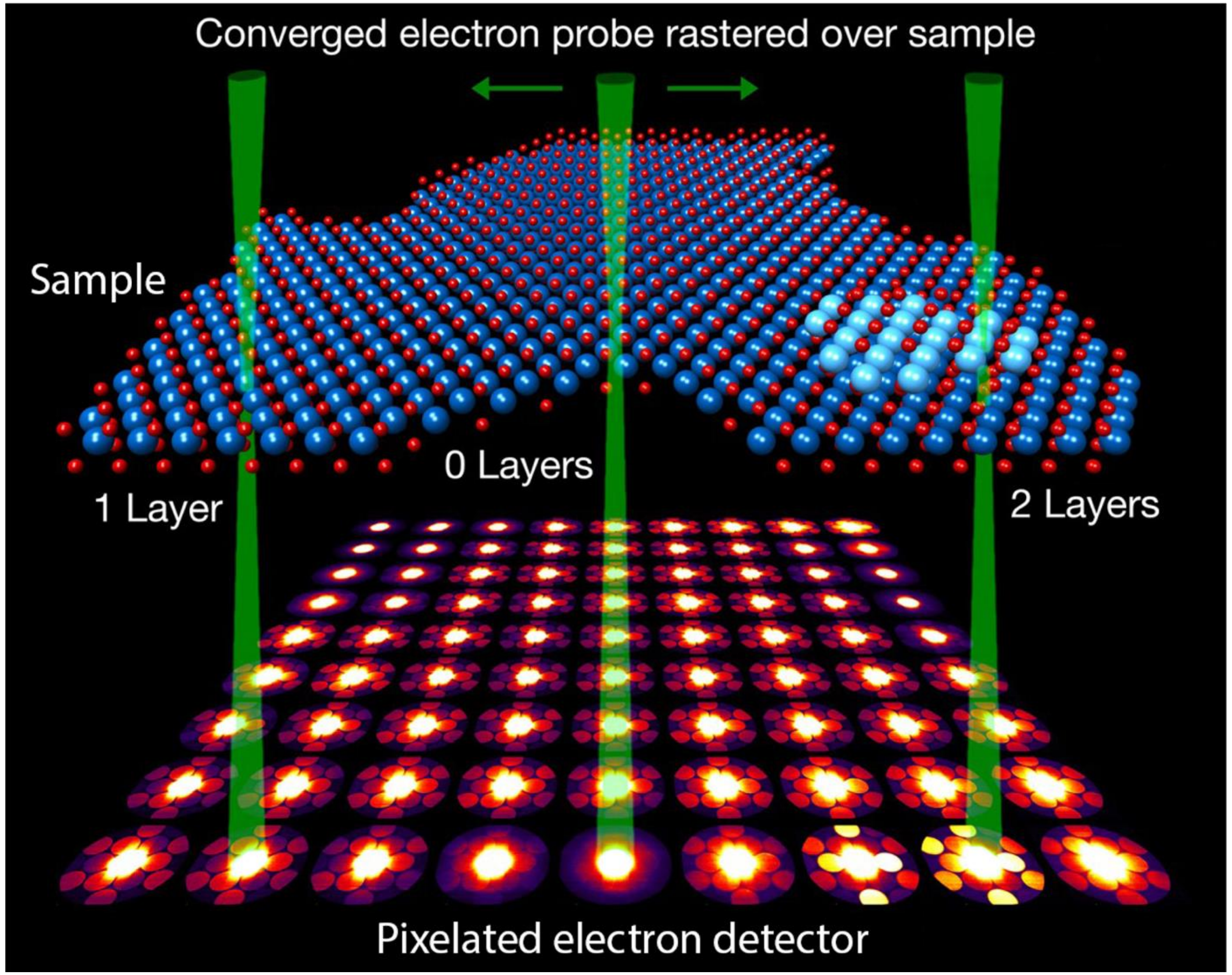
STEM frame (typical)
1024 x 1024
10 µs / pixel
10 s / frame



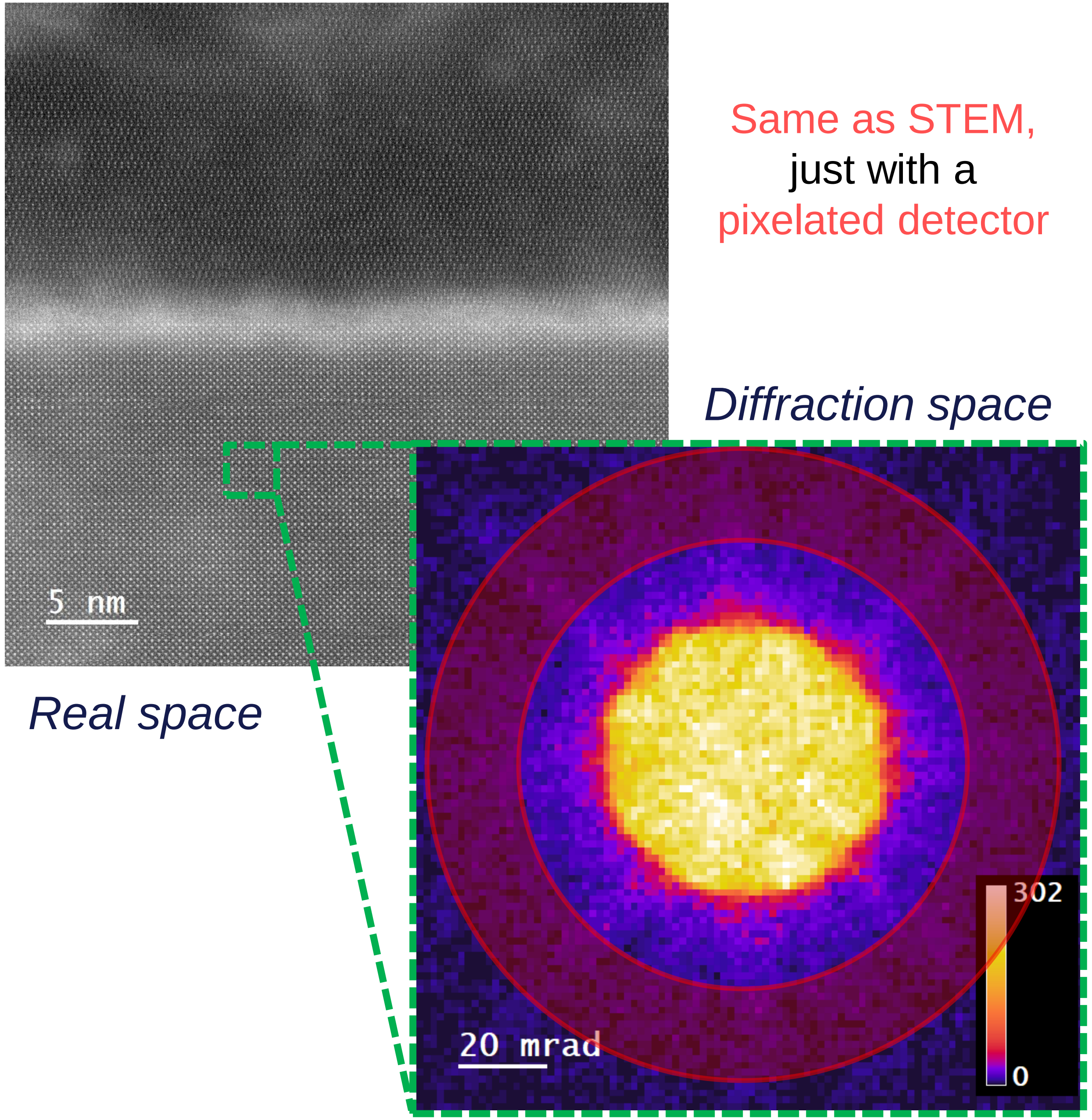
STEM imaging of Al oxide precipitates in rubber

Sample information at different scattering angles

4D STEM setup



Same as STEM, just with a pixelated detector



4D STEM (or diffraction mapping!)

Reference: Ophus C. et al., Microscopy and Microanalysis (2019), 25-3, 563-582.

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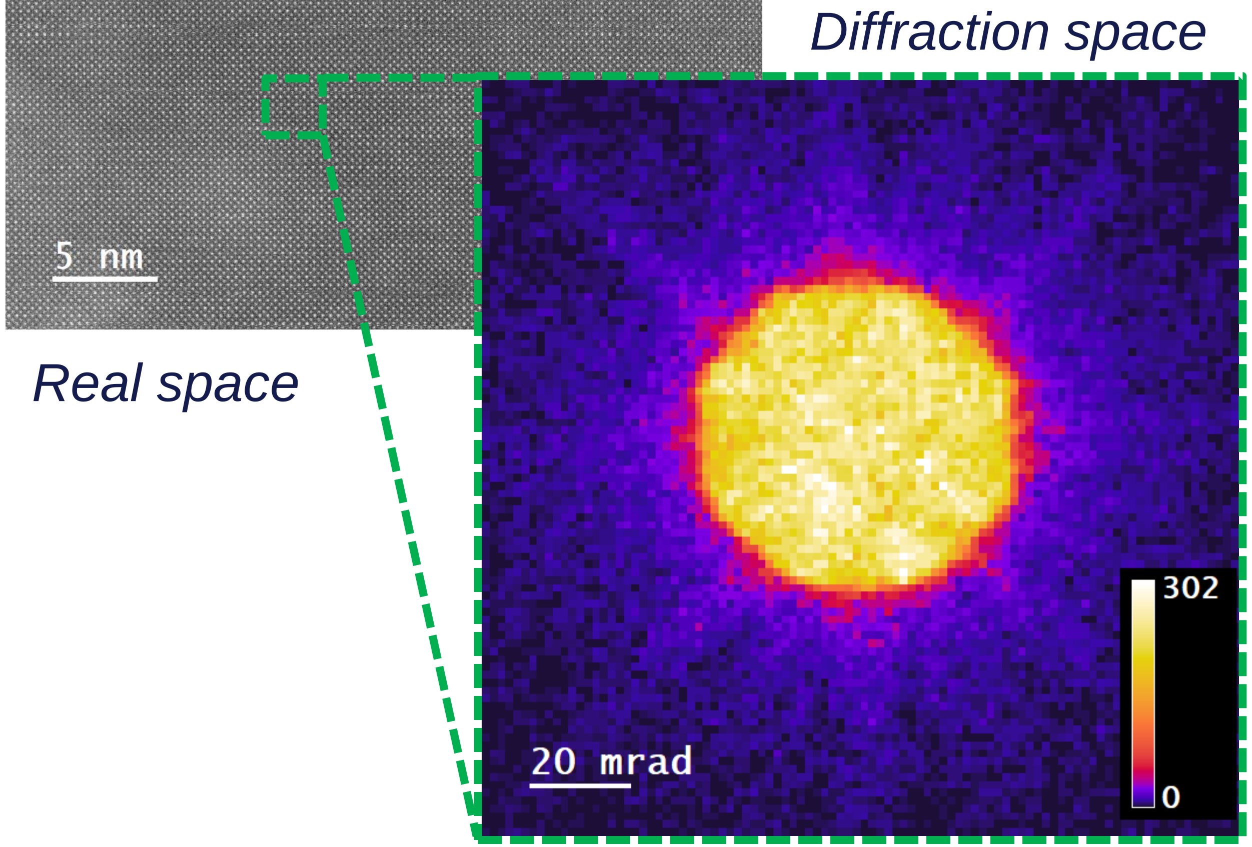
Datasets size



1. **Real Space (x, y)**

   - Scan dimensions: user choice

   - Example: 1024 x 1024

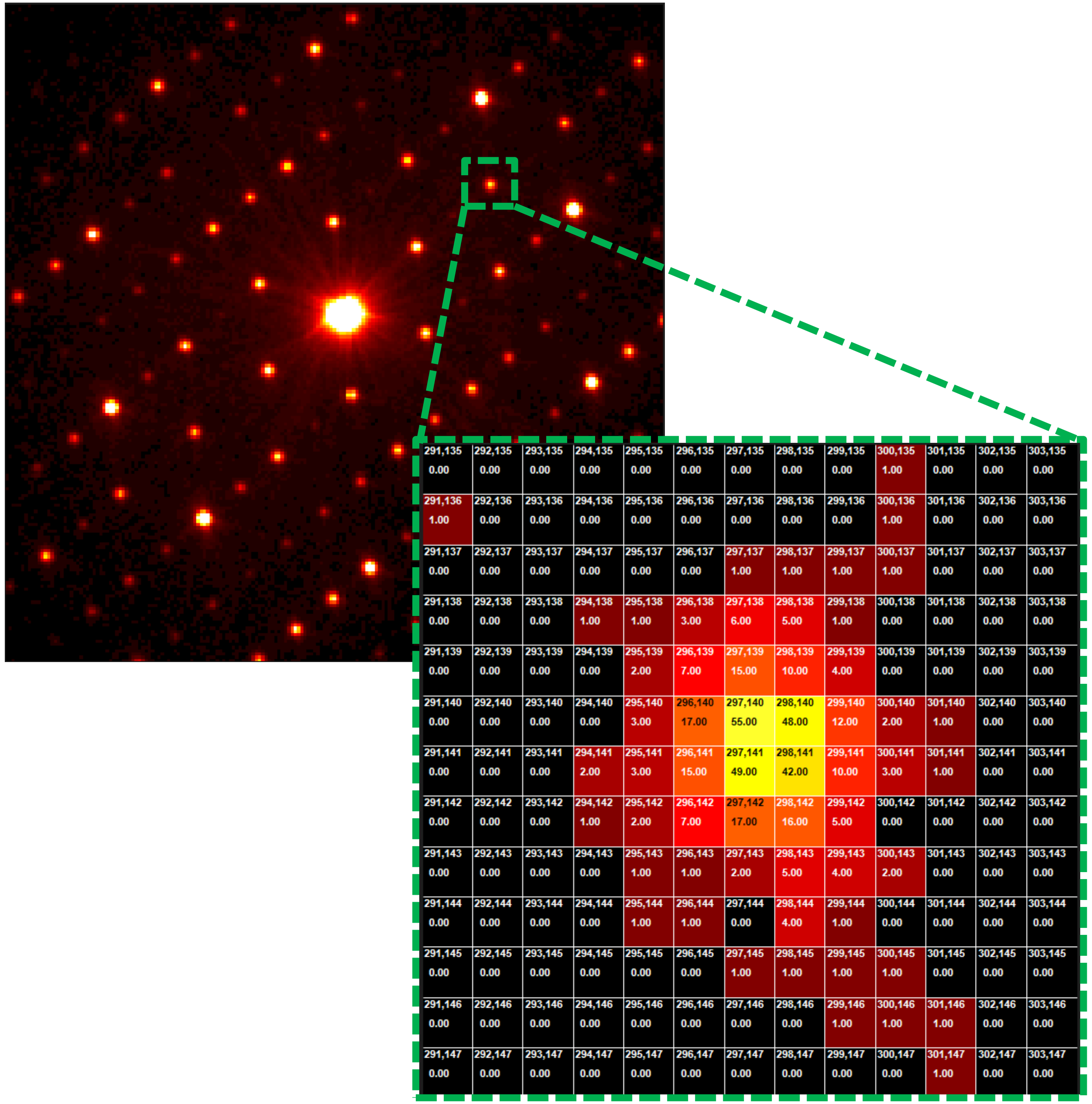
2. **Diffraction space (i, j)**

   - Detector dimensions: hardware

   - Example: 192 x 192

~ 4 . 10^{10} "pixels"

Datasets size



3. **Bit depth (d)**

   - Dynamic range: amount of signal

   - Example: 16 bits

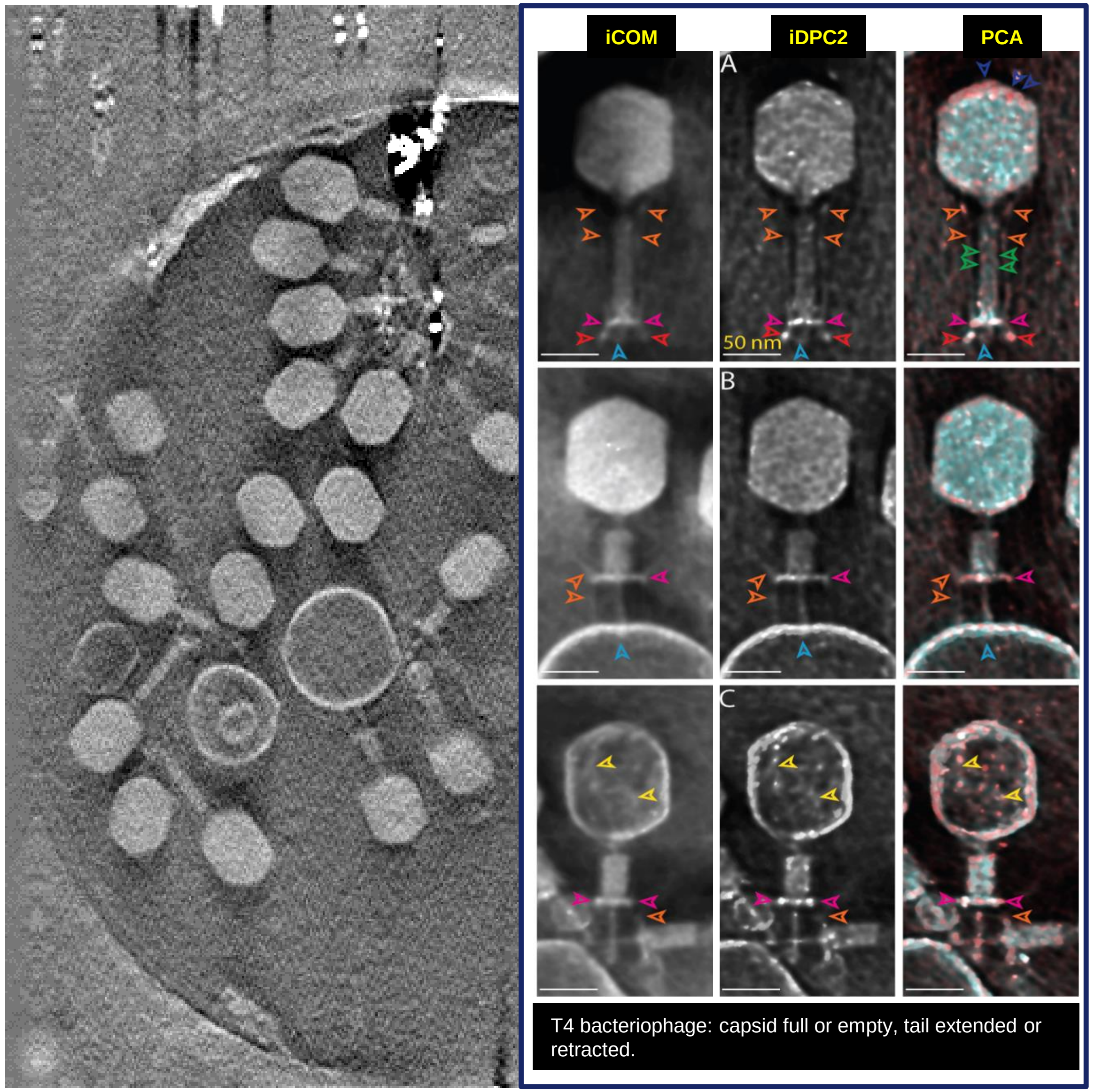
   ~ 80 GB (!)

4. **Compression** *(optional)*

   - Lossless and lossy strategies

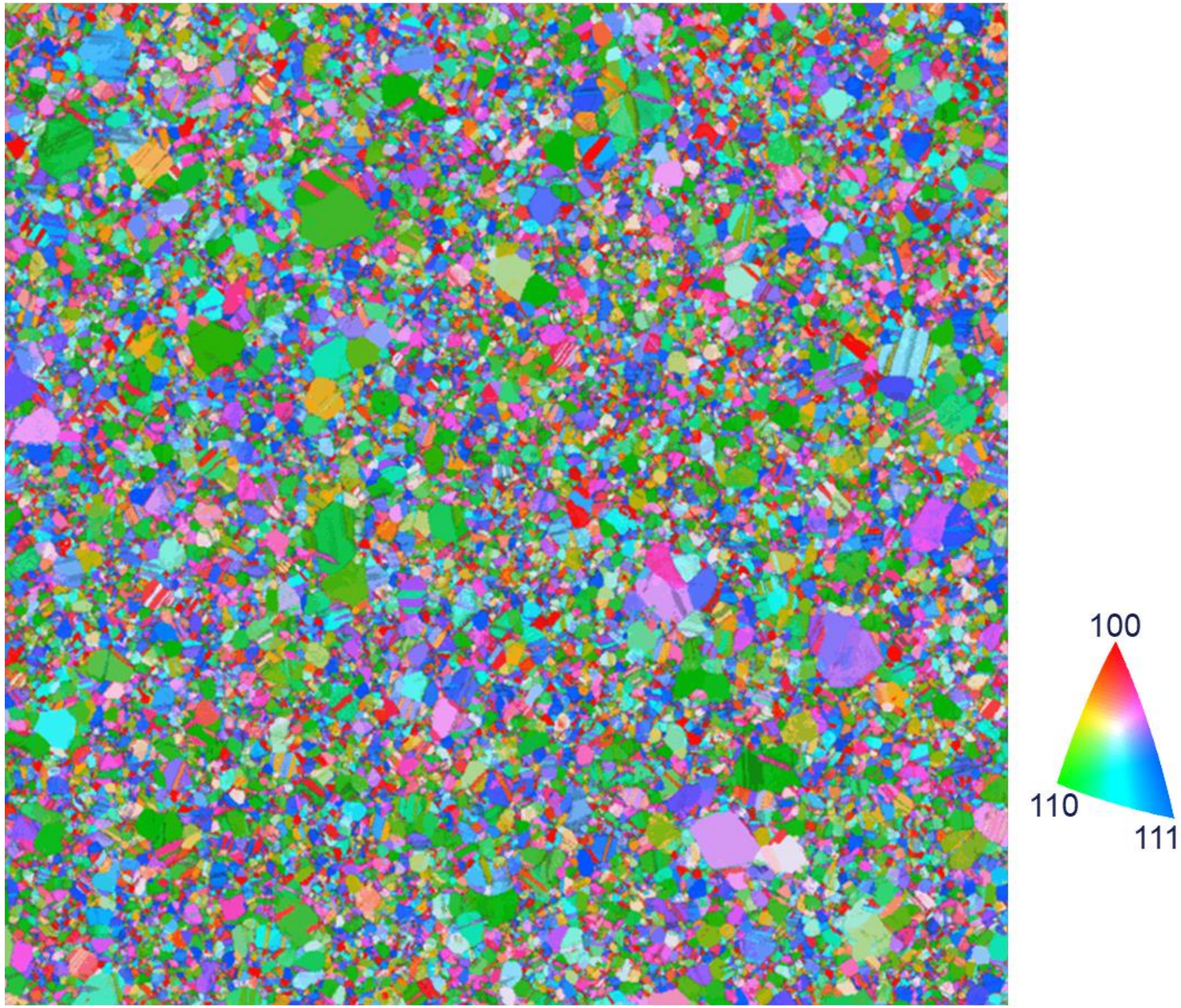
   - Example: HDF5 ~ 80 - 95% reduction

“New wave” of 4D STEM applications



T4 bacteriophage, 4D STEM ***tomography***

41 x 1024 x 1024 datasets, Serial-EM integration



Nanocrystalline gold, ***in situ heating + 4D STEM***

200 kV*, 1024 x 1024 datasets, 100 s per map*

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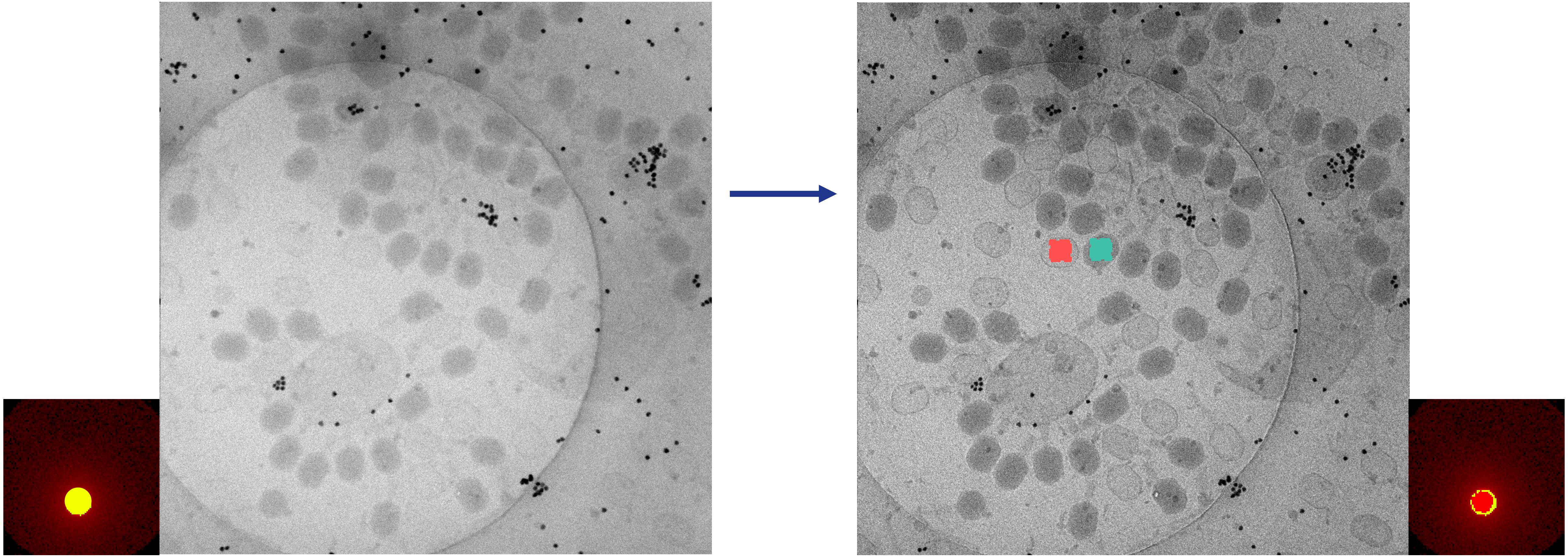
4D STEM applications

a) Virtual STEM detectors

"Flexible imaging with tuneable contrast"



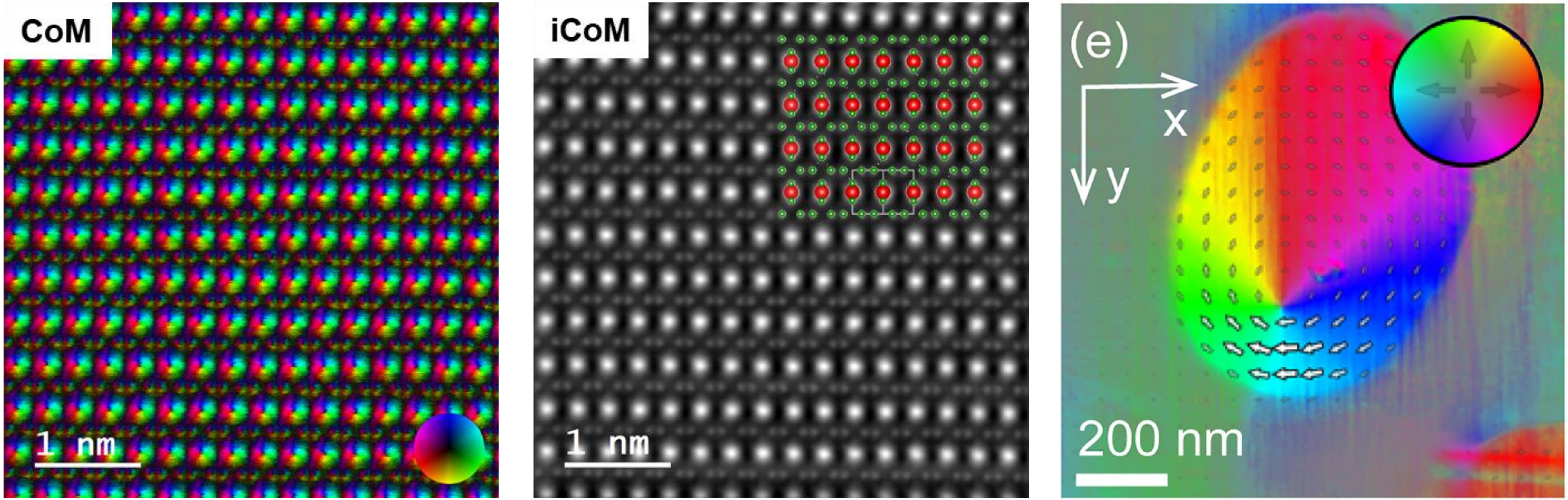
Shahar Seifer, Michael Elbaum, Lothar Houben, Roberto dos Reis

Reference: Microscopy and Microanalysis, 30, 476-488 (2024) - [https://zenodo.org/records/10679006].

4D STEM applications

b) E / B fields imaging

"DPC for EM fields and advanced imaging"



Elisabeth Mueller, Mingjian Wu

Reference: [https://zenodo.org/records/ 8354219]

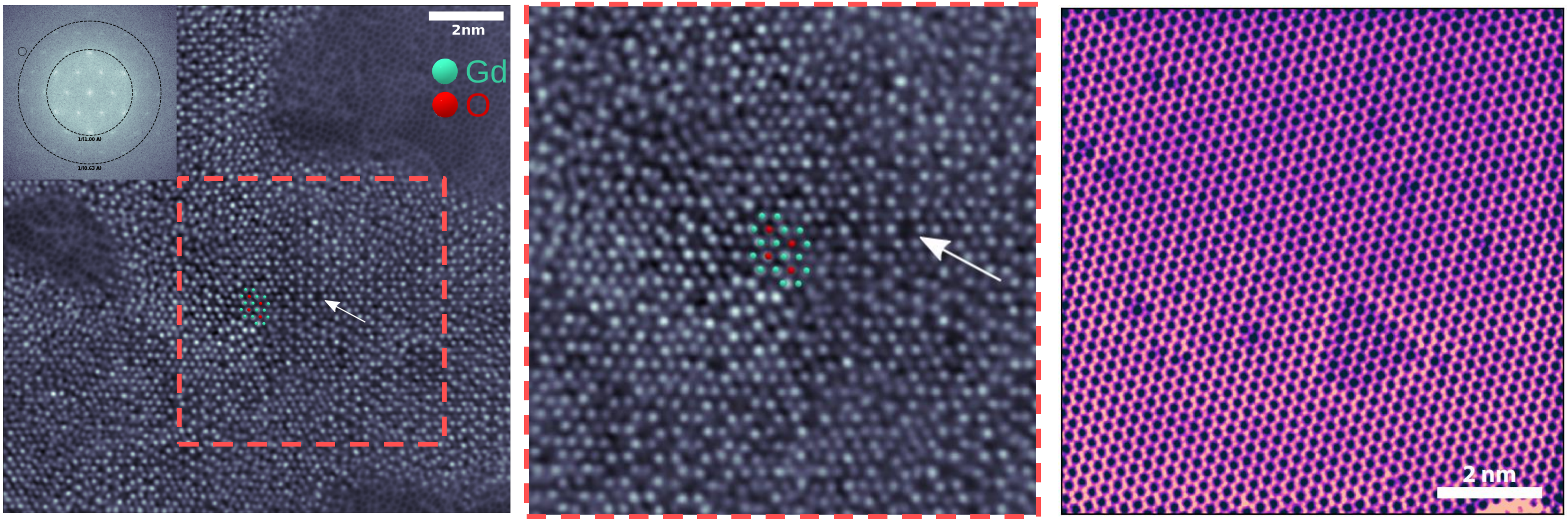
Christian Liebscher

Zhang, X. et al. Scripta Mater. 247 116097 (2024).

4D STEM applications

c) Ptychography

"Image reconstruction for ultimate resolution"



Philipp Pelz, Mingjian Wu

Reference: [https://zenodo.org/records/ 8354219]

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py4DSTEM

BERKELEY LAB

Colin Ophus, Stephanie Ribet, Georgios Varnavides

https://arxiv.org/abs/2309.05250 (2024).

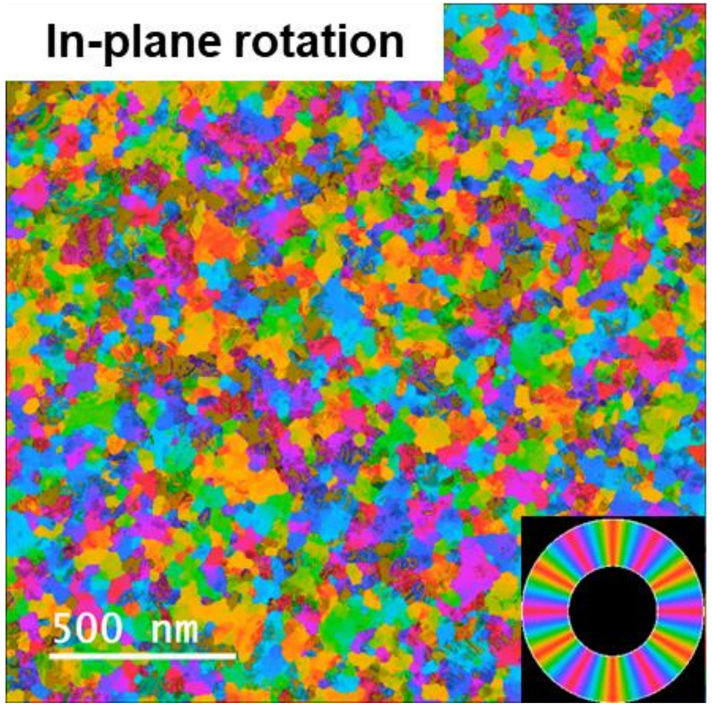
4D STEM applications

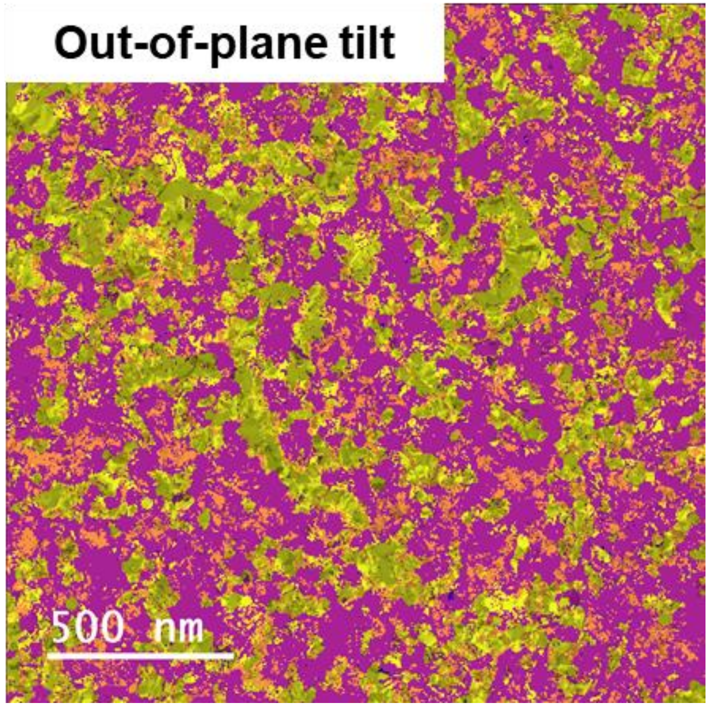
d) Crystal phase / orientation mapping

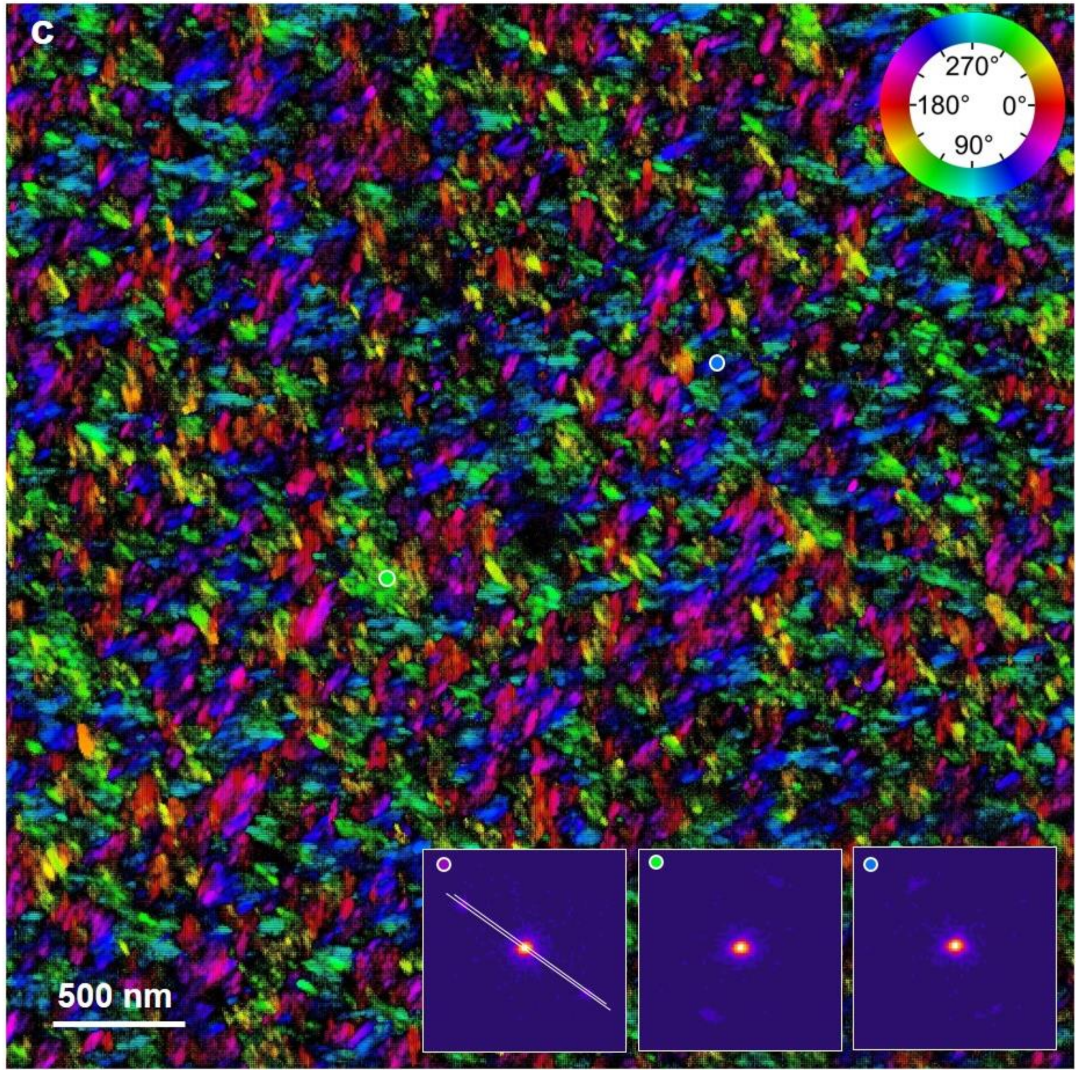
"HR-EBSD with TEM"

e) Strain analysis

"Alternative to complex methods"







Mingjian Wu, Erdmann Spiecker

Reference: Wu, M. et al. J. Phys. Mater. 6 045008 (2023), [https://zenodo.org/records/ 8354219]

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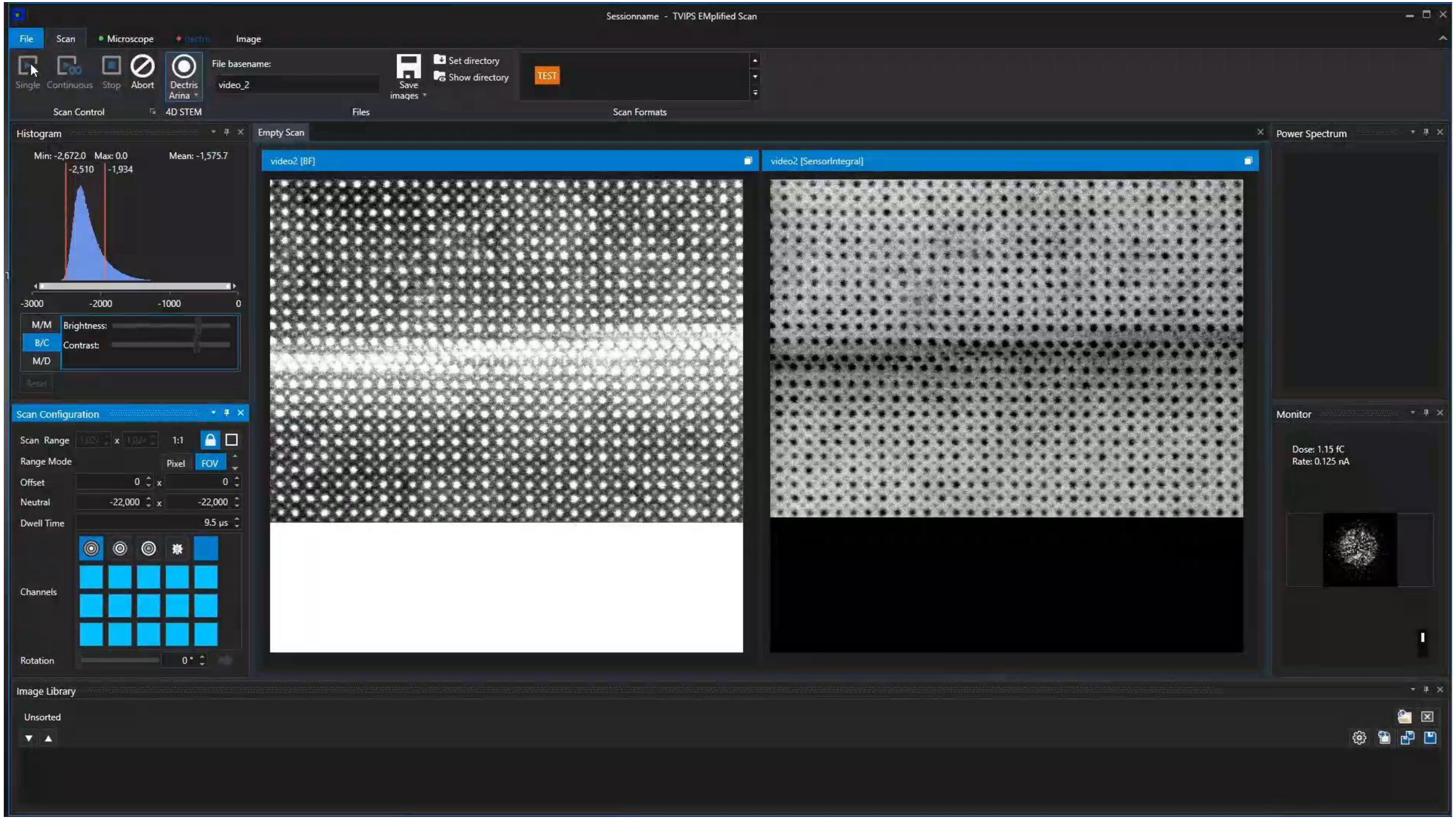
Fast 4D STEM today



ARINA detector at > 100’000 fps

Data rate in numbers

Real Space (x, y): 1024 x 1024

Diffraction space (i, j): 96 x 96 (bin2)

Raw data size (GB): 19 GB

Compressed size (GB): 2 GB

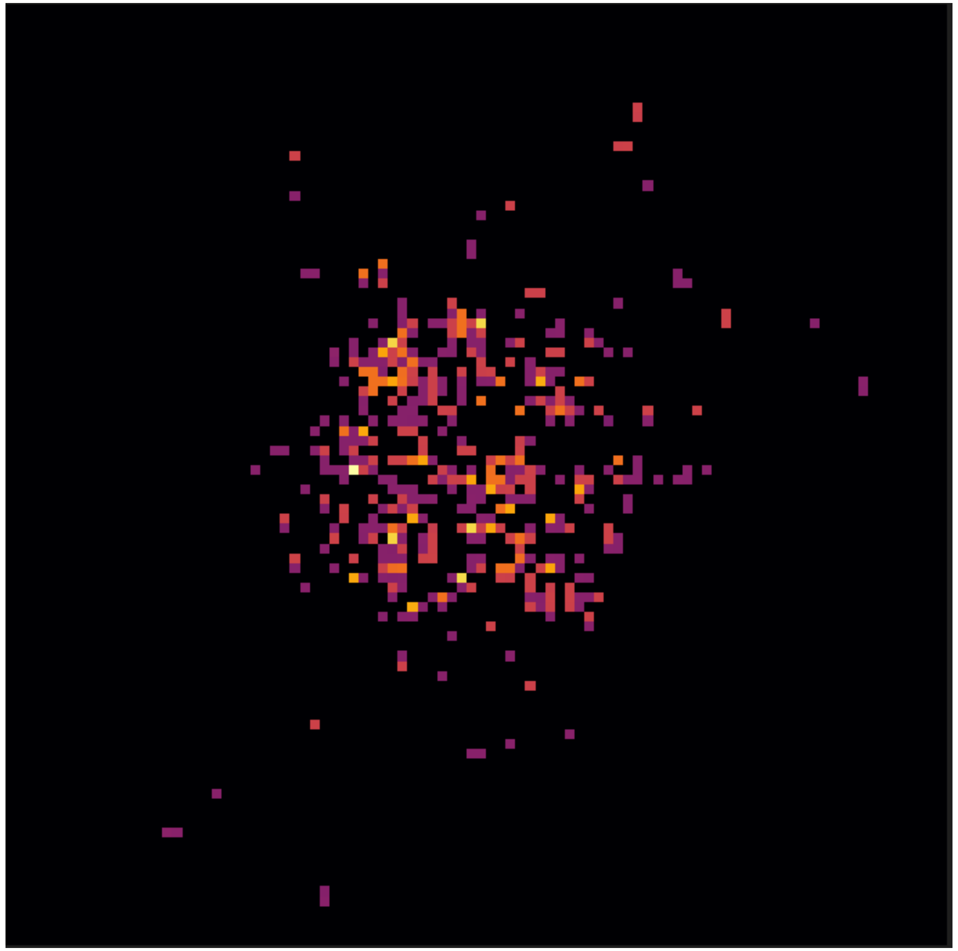
Acquisition time (s): ~ 11 s

ARINA detector at > 100’000 fps

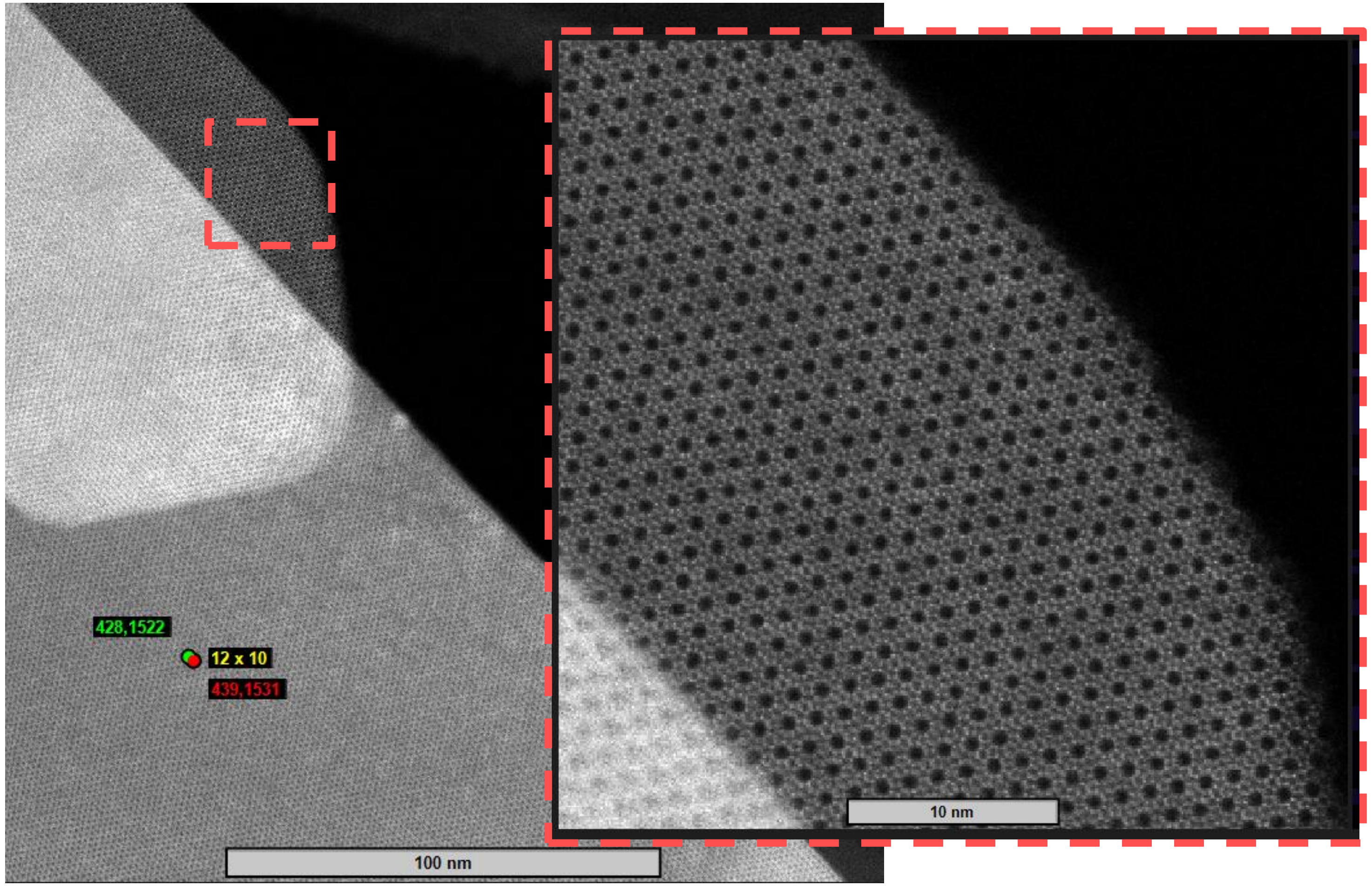
“Bigger, faster, more dynamic range...”

Importance of near real-time processing

"4D STEM is not readily interpretable"

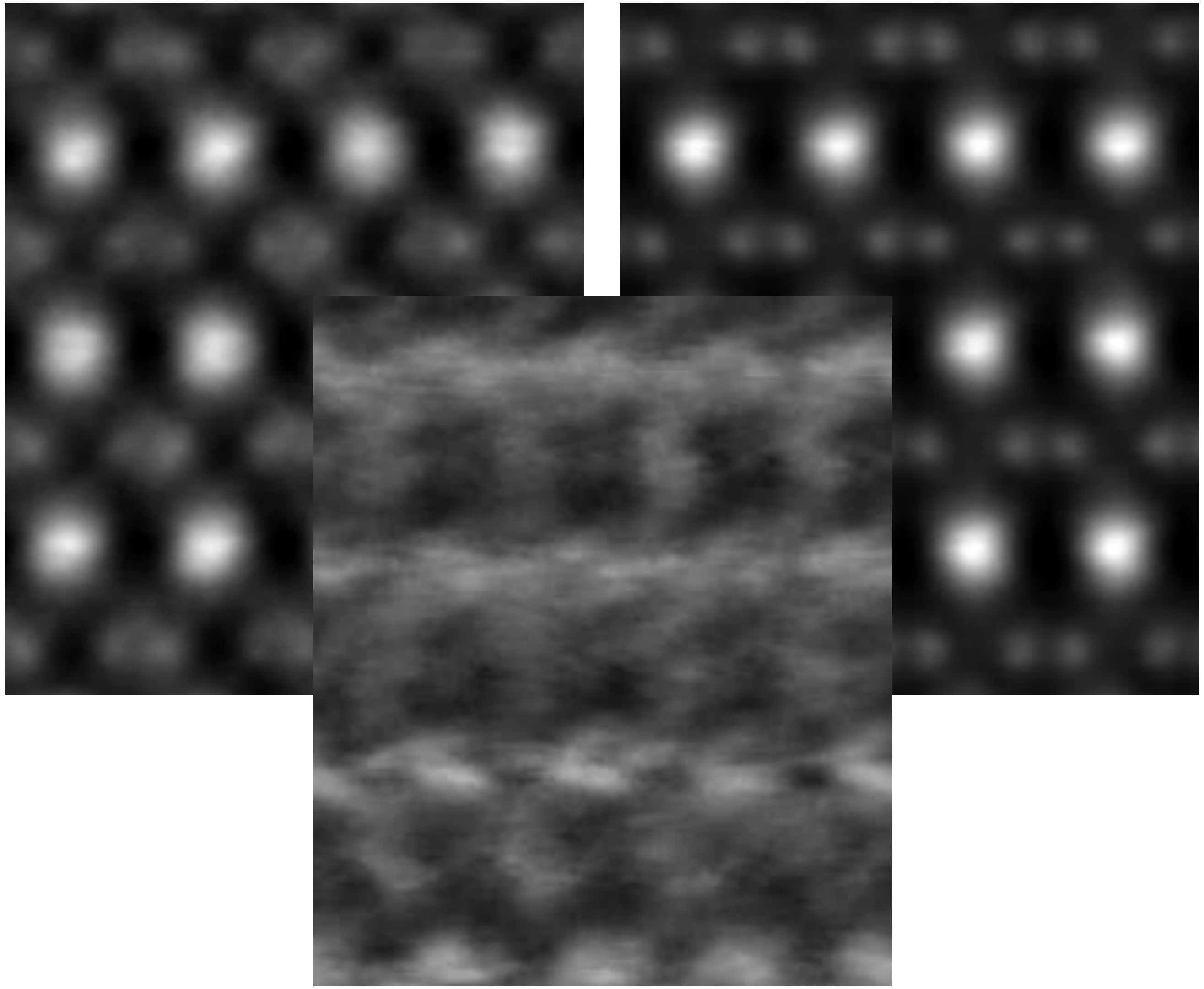


"Region of interest selection"

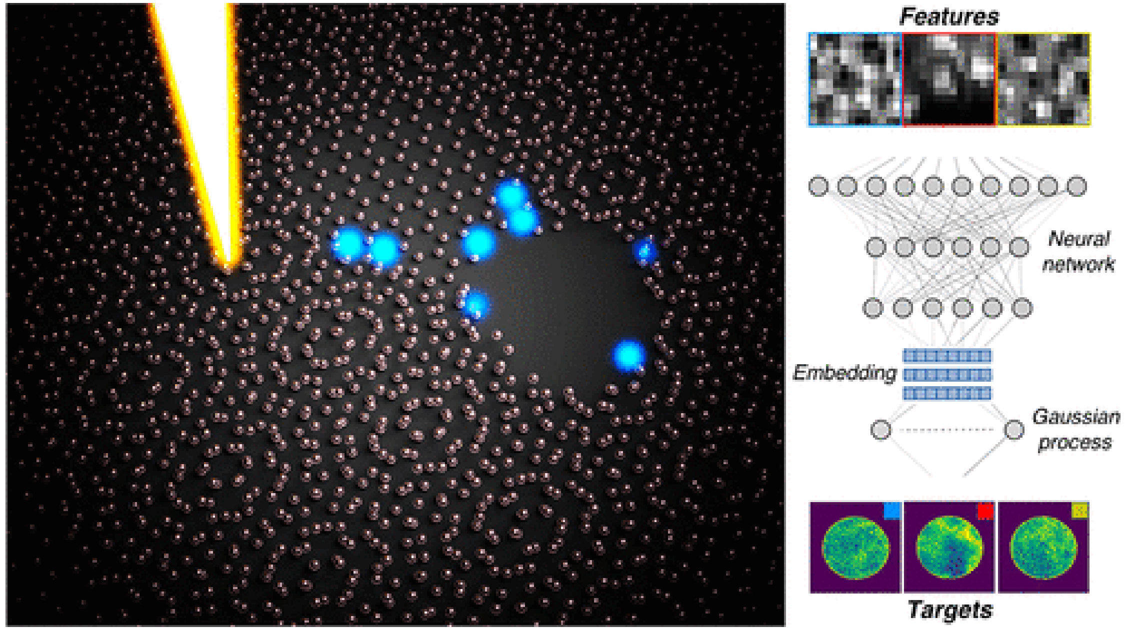


Importance of near real-time processing

“TEM tuning support”

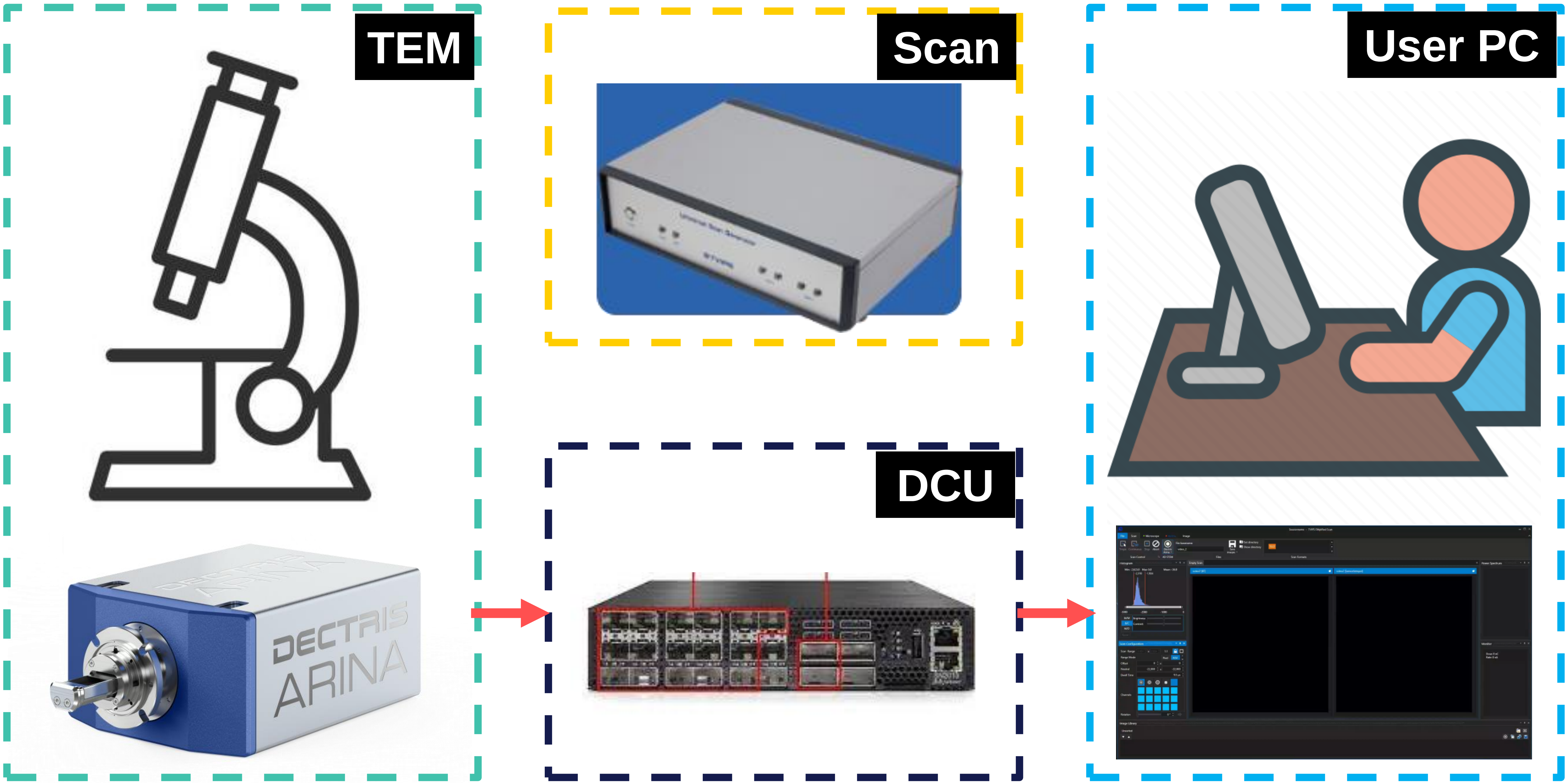


“(No-)Human-in-the-loop”

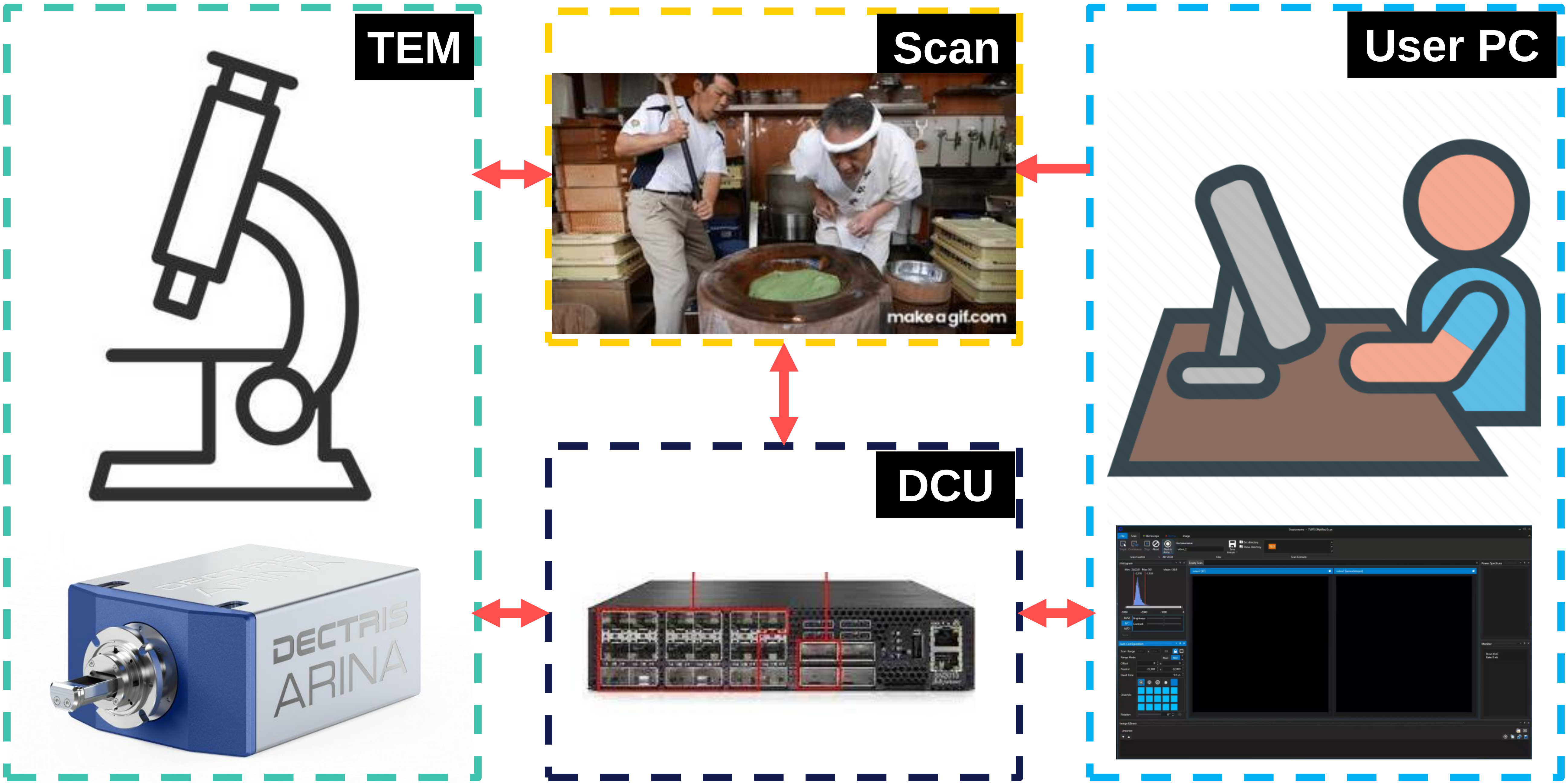


Reference: *Roccapriore, K. et al. ACS Nano 16-5, 7605–7614 (2022)*

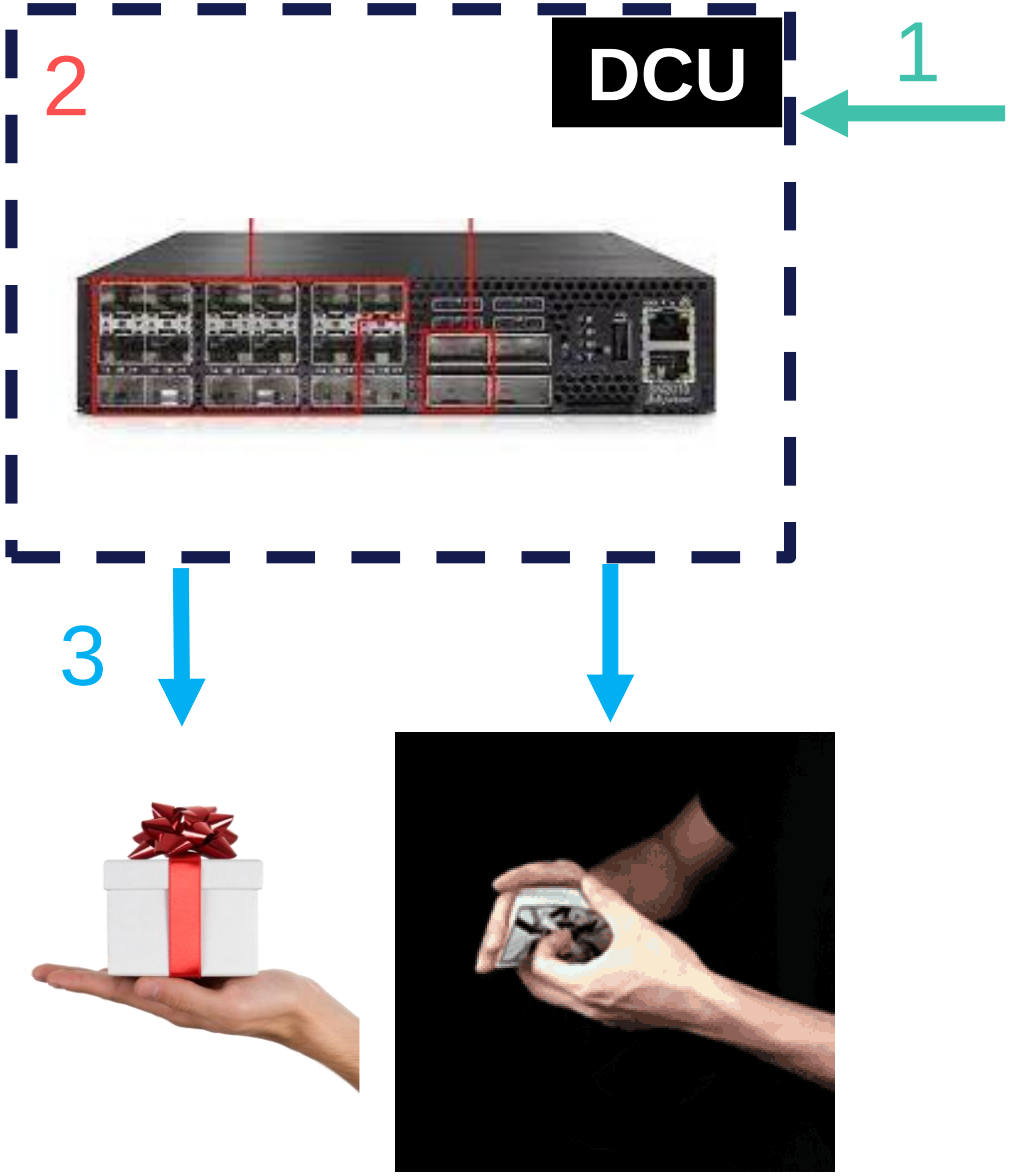
Data path with ARINA



4D STEM data acquisition



Detector Control Unit in details



1. **Communication with ARINA**

   - API interface

   - Open scripting for custom acquisitions

2. **Tasks you probably don't care**

   - Detector frame synthesis, compression

   - Calibrations and adjustments

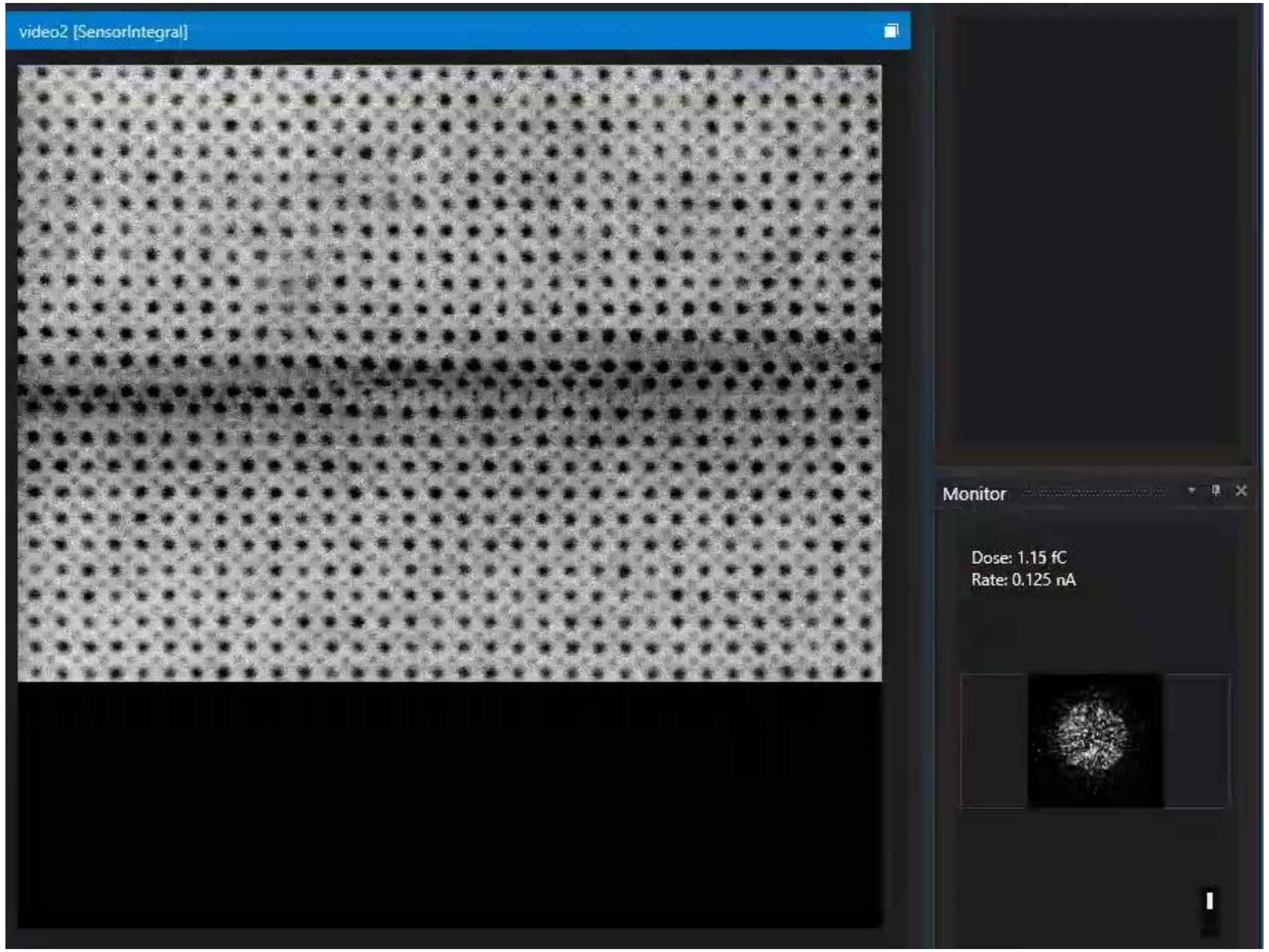
3. **Data output**

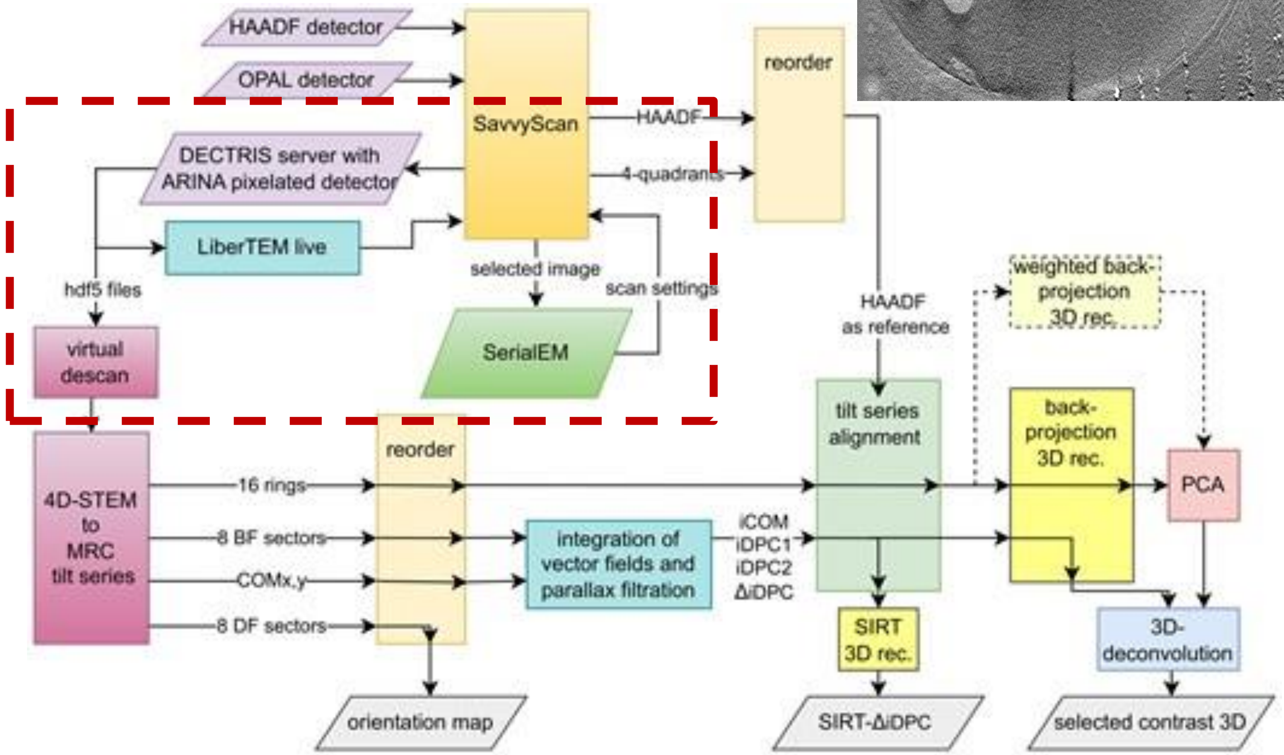
   - 3 simultaneous channels (2 relevant)

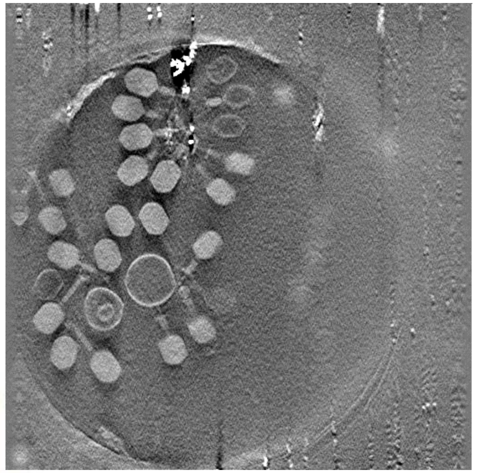
     - Filewriter: "*here is your full data stack*"

     - Stream: "*every frame, ASAP*"

Elementary processing of stream interface

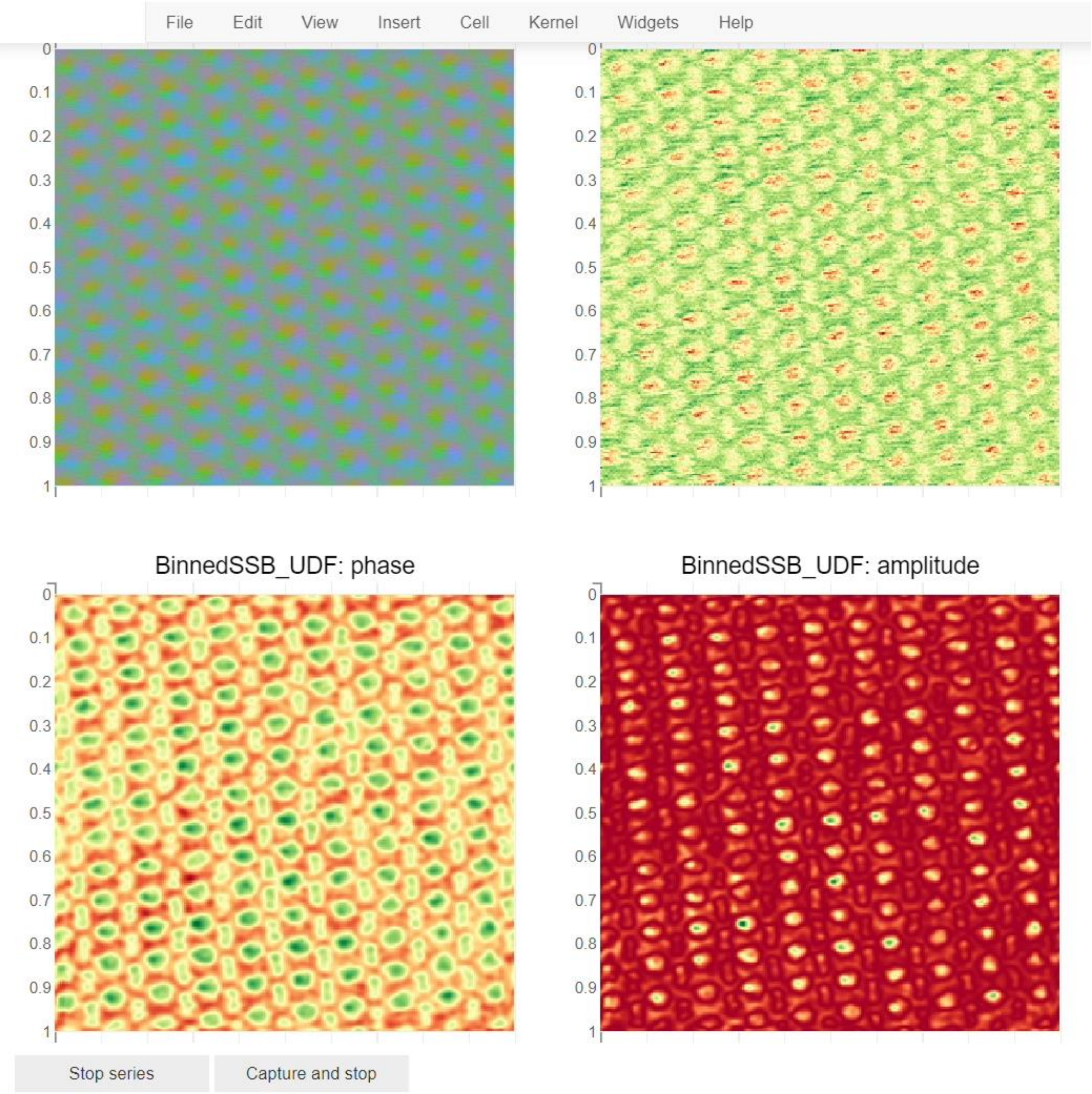


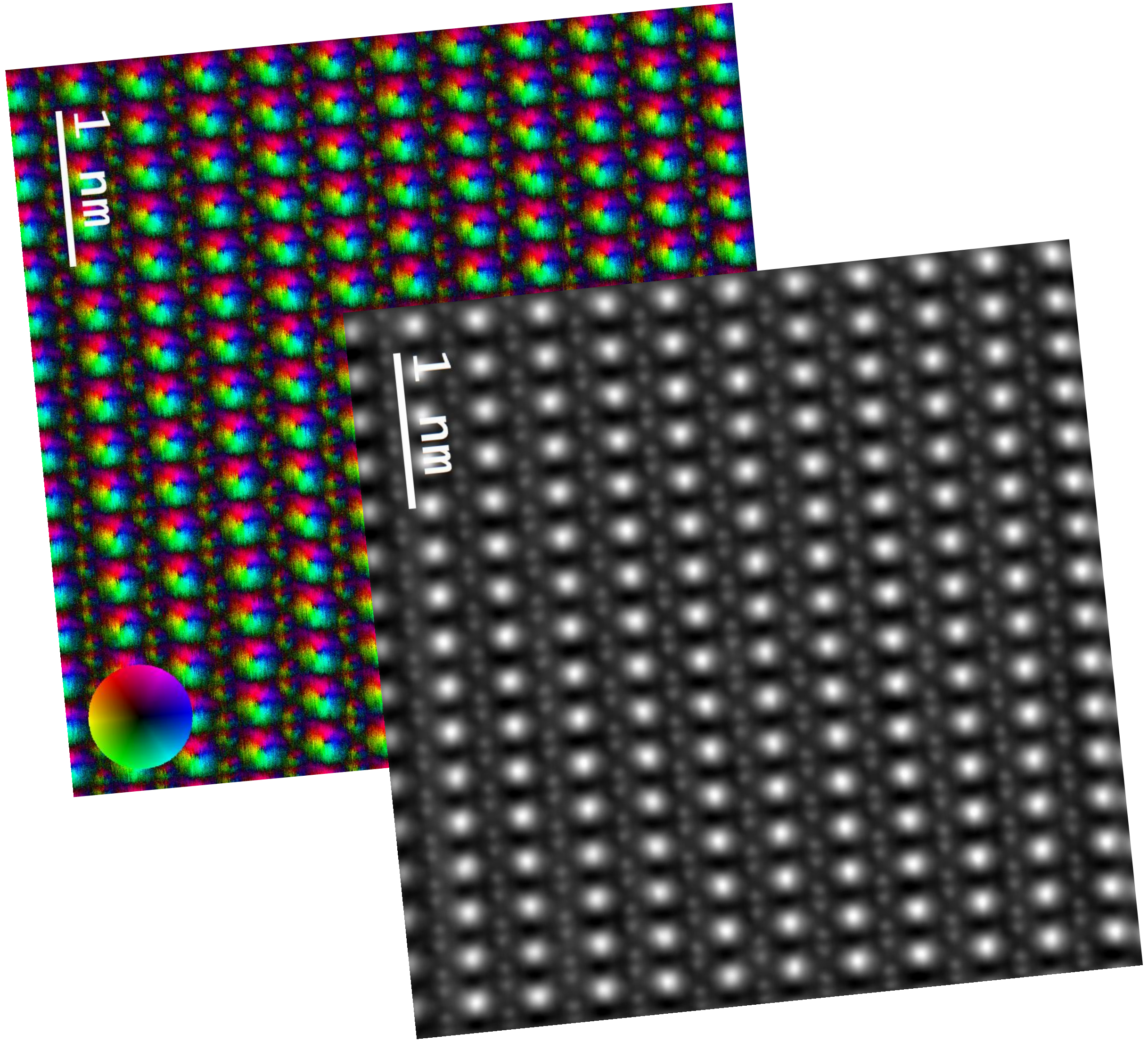




Reference: Seifer, S. et al, Micr. Microanal. 30 (3), 476–488 (2024)

Heavier processing of stream interface

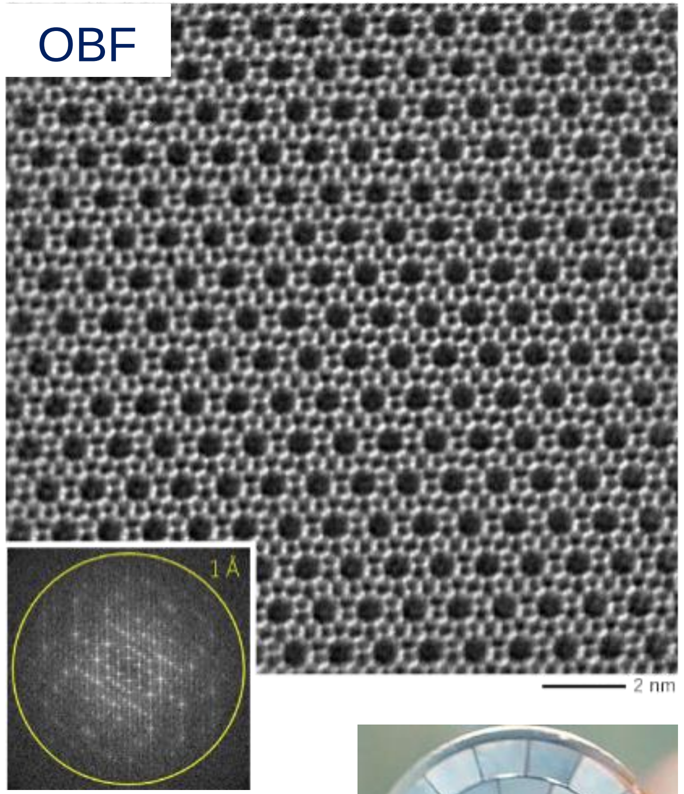


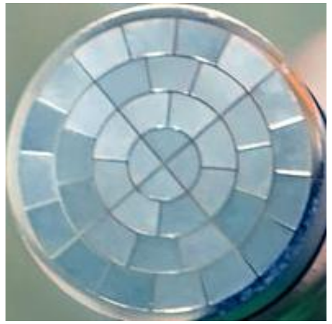


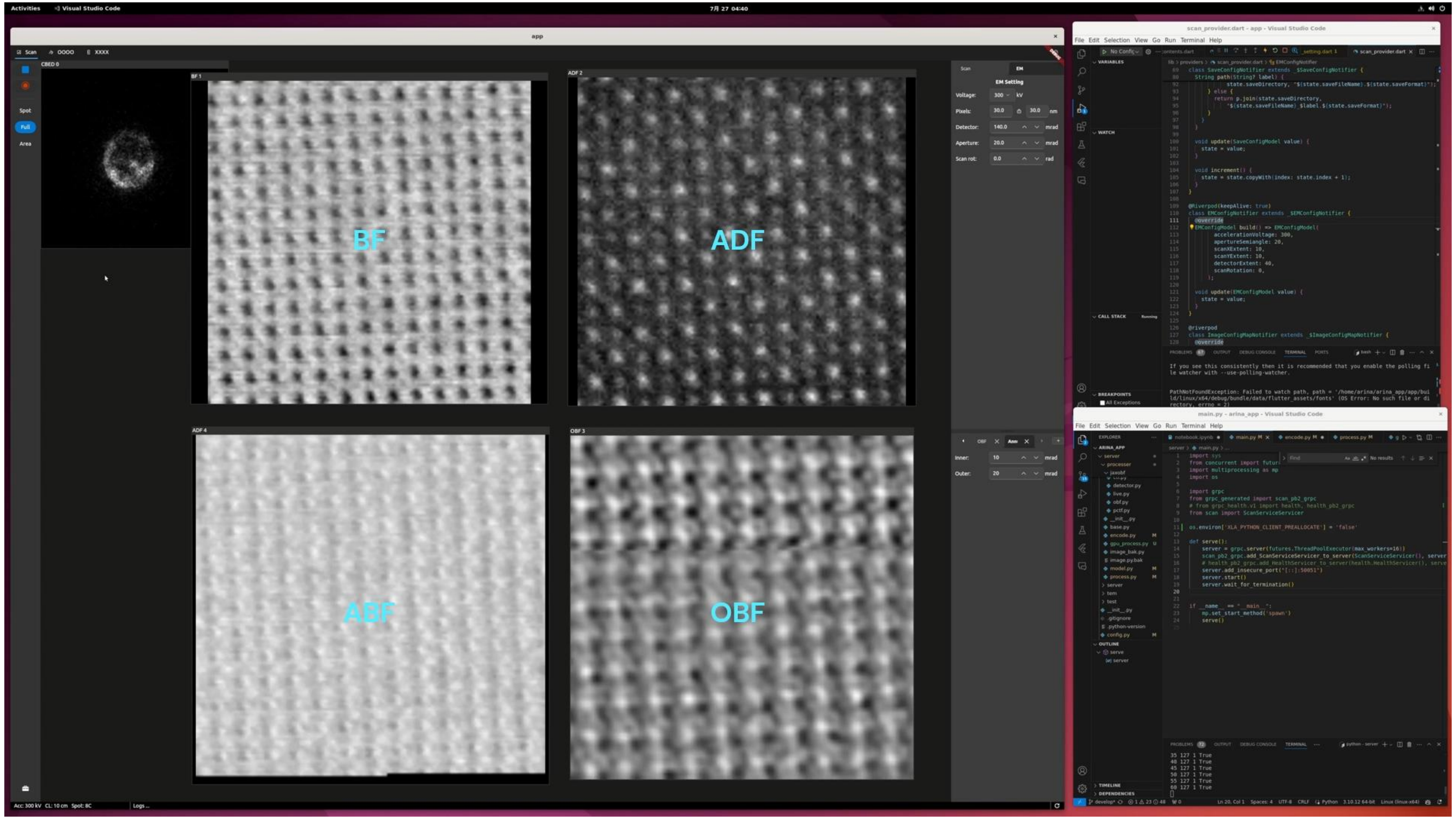
LiberTEM

Reference: Clausen, A. and Weber, D., https://github.com/LiberTEM/LiberTEM-live

Heavier processing of stream interface

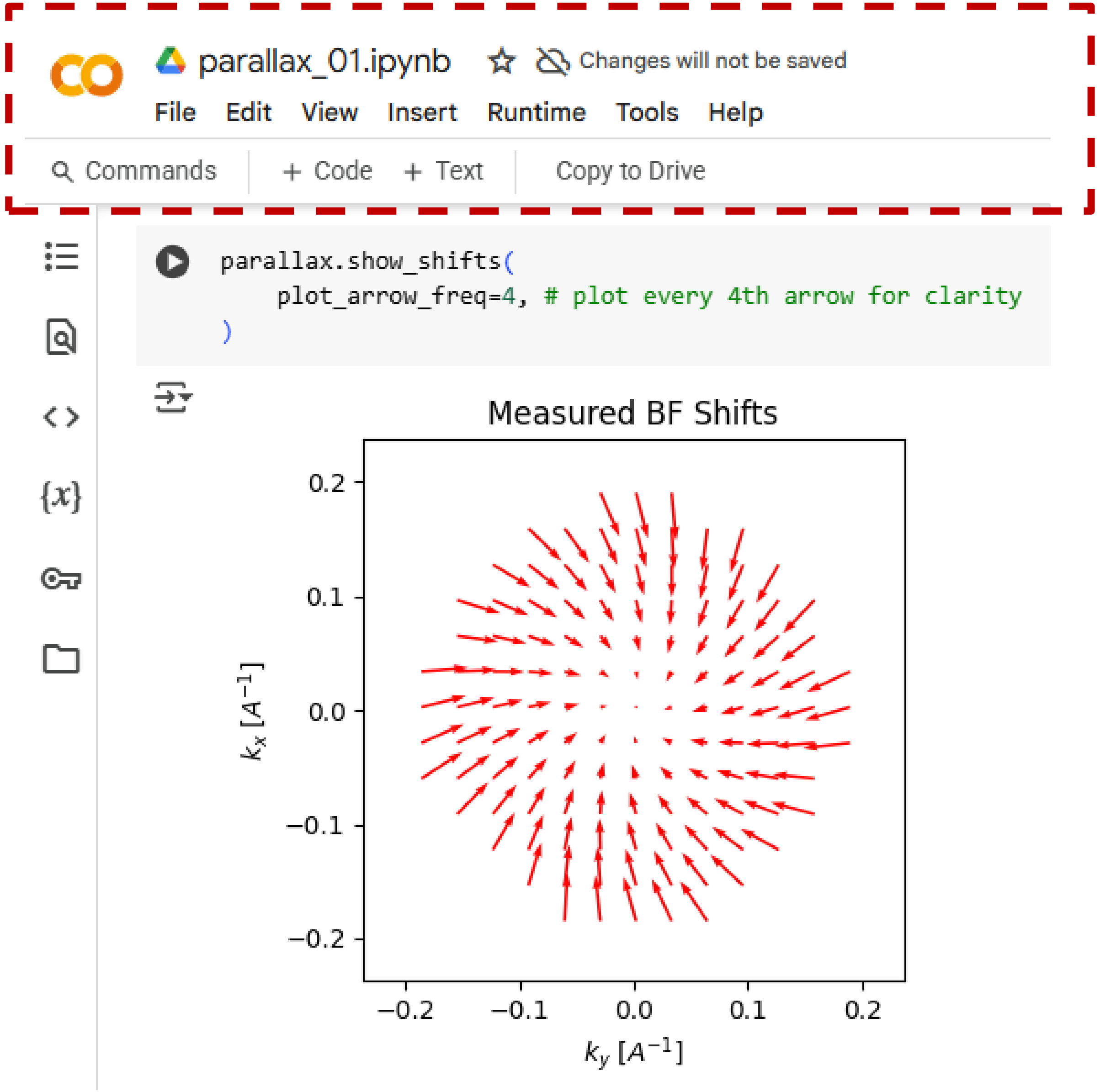


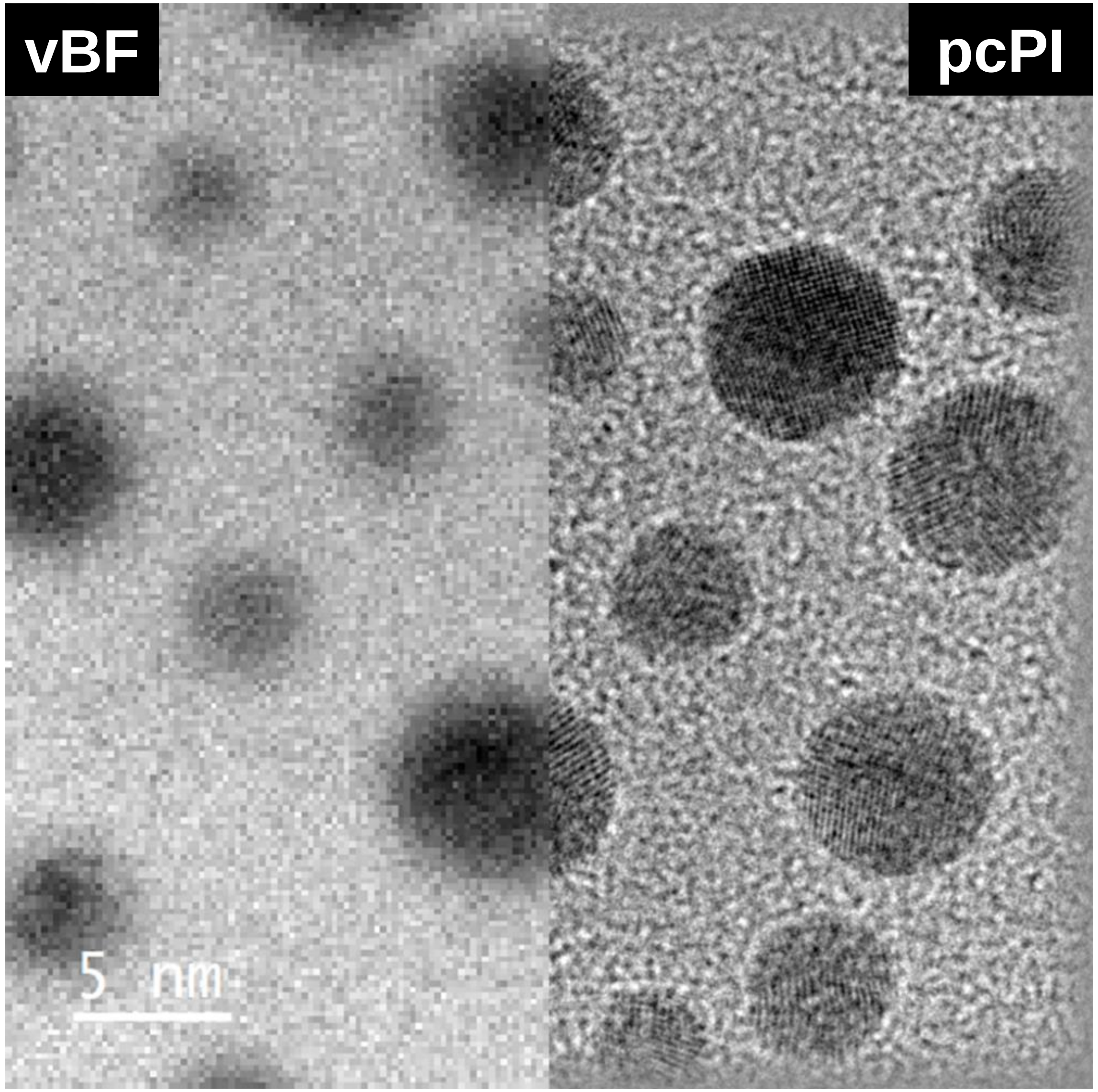




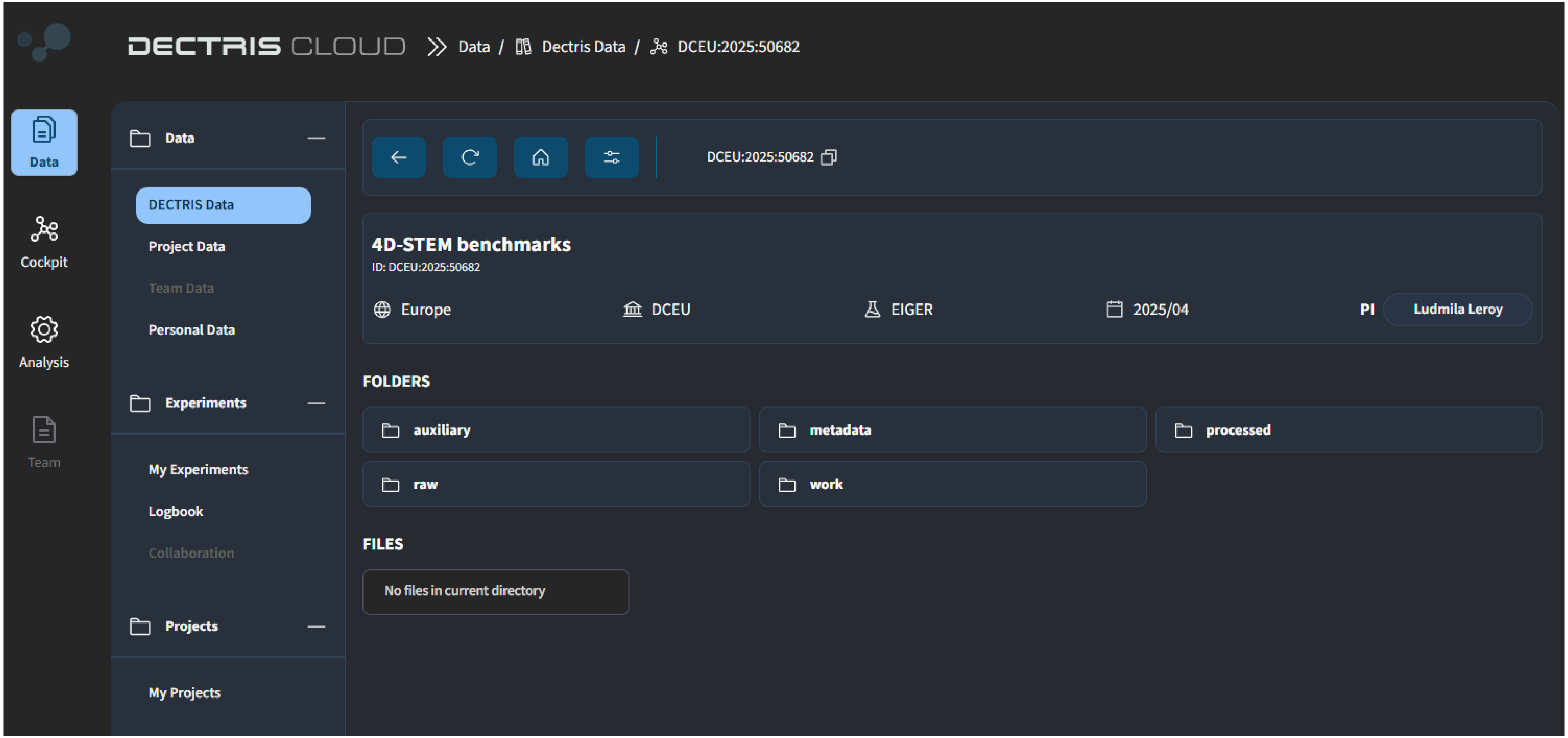
Reference: Ooe K. et al., Ultramicroscopy 220(2021), 113-133.

Next chapter – the Cloud





Next chapter – the DECTRIS Cloud



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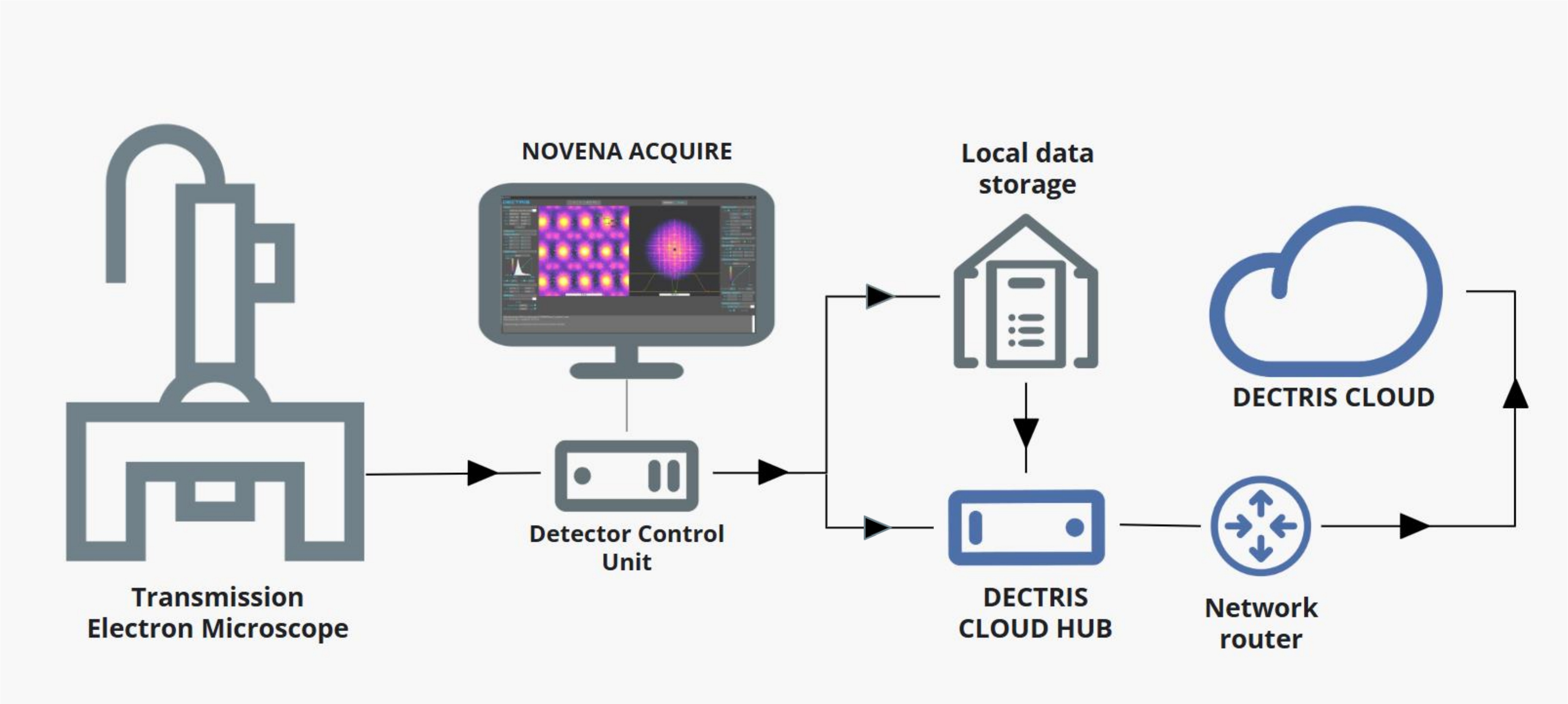

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