MSE Day

5 November 2024

Materials Information Discovery

Materials Systems Engineering

Jan Korvink, Joachim Mayer

Topic Spokespersons

HELMHOLTZ Information

Topic 5: Materials Information Discovery

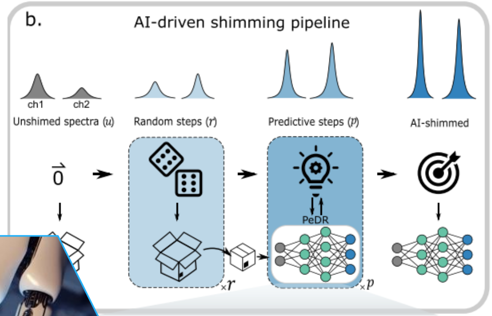
Mission and Goals

What were the goals of the topic?

- Development of digital and correlative characterization platforms which will act as key enablers for future materials engineering
- A generic concept covering *in situ* and *operando* measurements and in-system combinations of methods will be developed
- Broad range of competences in methods and physical/life science applications
- Based on unique infrastructures:
  Ernst Ruska-Centre (ER-C) at FZJ
  Karlsruhe Nano and Micro Facility (KNMF), HiT-NMR, CORREL

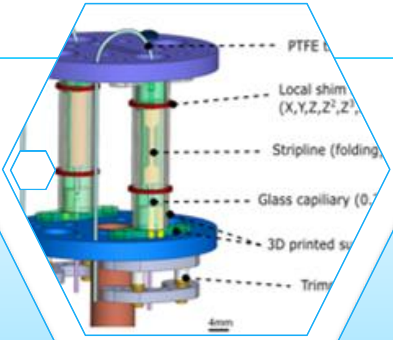
HiT-NMR: high throughput screening

Intelligent calibration and sample preparation



Becker, M. et al., *Sci. Rep.* 13 (2023) 17983.

Increased sample throughput

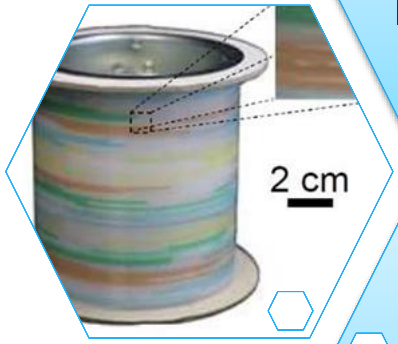


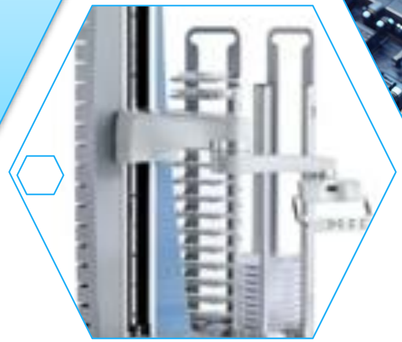
Detector Parallelization

Machine assisted learning

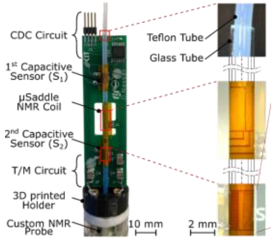
Automation

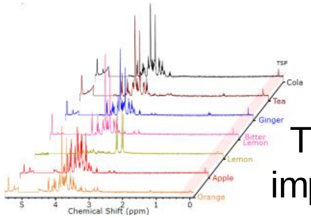
Flow sampling





Accelerated sample handling





Throughput improved x50

Nassar, O. et al., *Microsys. Nanoeng.* 7 (2021).

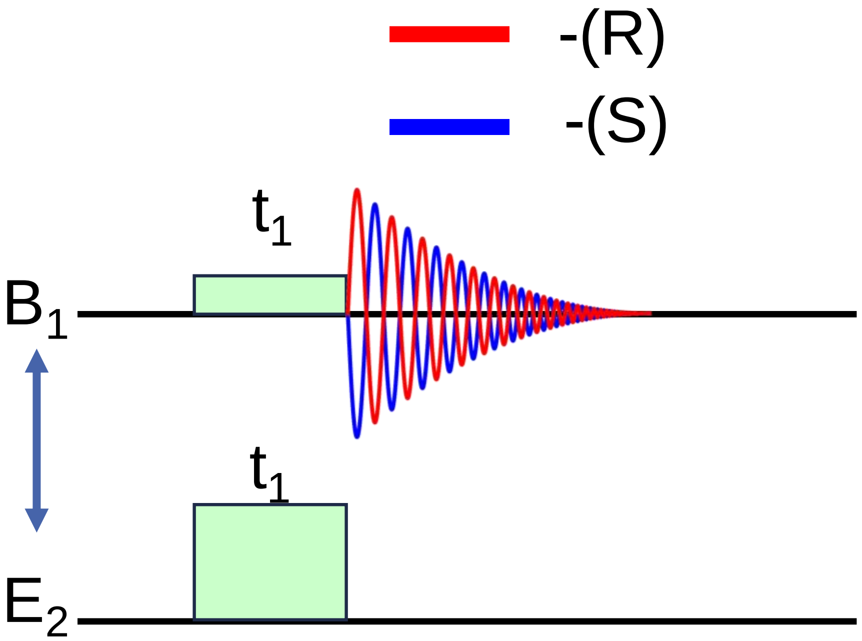
Screening Applications

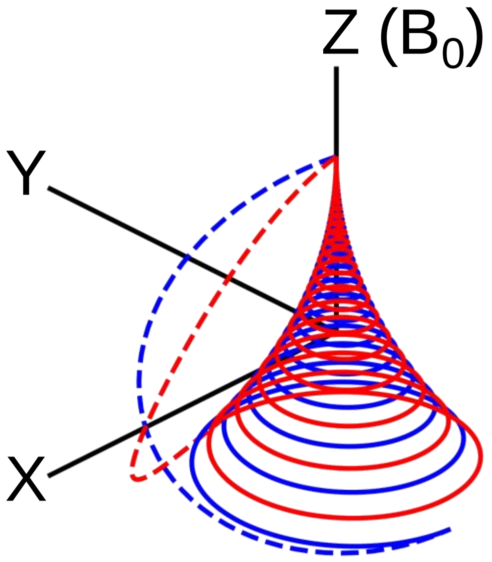
Metabolomics | Drug Discovery | Improved Catalysts

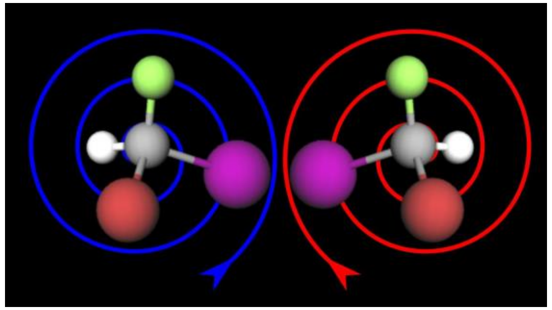
Closed-loop screening platform

MDMC KNMF Karlsruhe NANO MICRO Facility HELMHOLTZ Information

Evolution of the magnetisation with chiral tensor





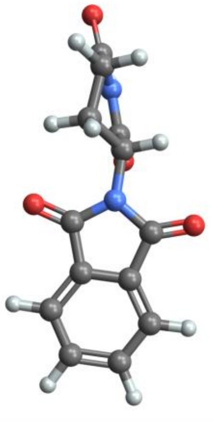


Chiral NMR experiment:

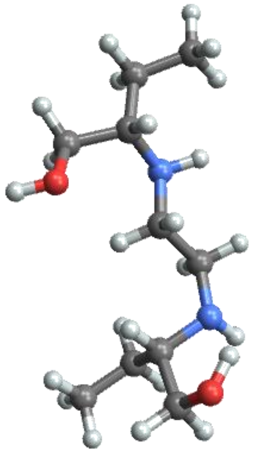
1. Magnetisation in the initial state
2. RF E_2 perturbation [17,18,19]
3. Magnetisation relaxation
4. Intensity/phase difference [19]

[17]: Buckingham, Chem. Phys. Lett., 2004
[19]: Garbacz et. al., Phys. Chem. Chem. Phys., 2015
[19] S Wadhwa, D Buyens, JG Korvink, Advanced Materials, 2024

Chiral drugs are ubiquitous and ordered by enantiomer

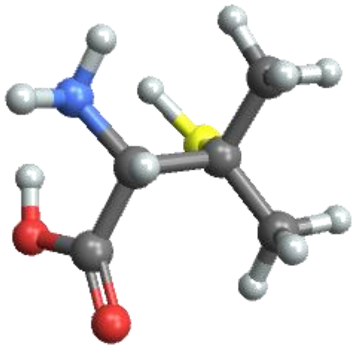


Thalidomide

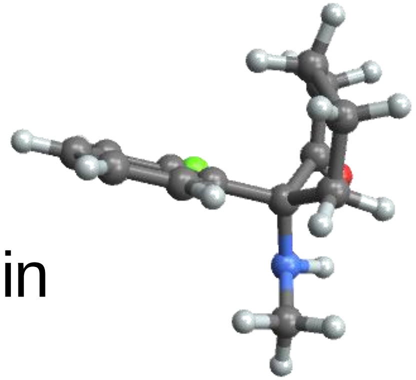


Ethambutol

Enantiomer	Eutomer (Good)	Distomer (Bad)
Thalidomide [5]	Sedative	Teratogenic
Ethambutol [6]	Tuberculosis	Blindness
Penicillamin [7]	Antiarthritic	Mutagen
Ketamin [8]	Anesthatic	Hallucinogen



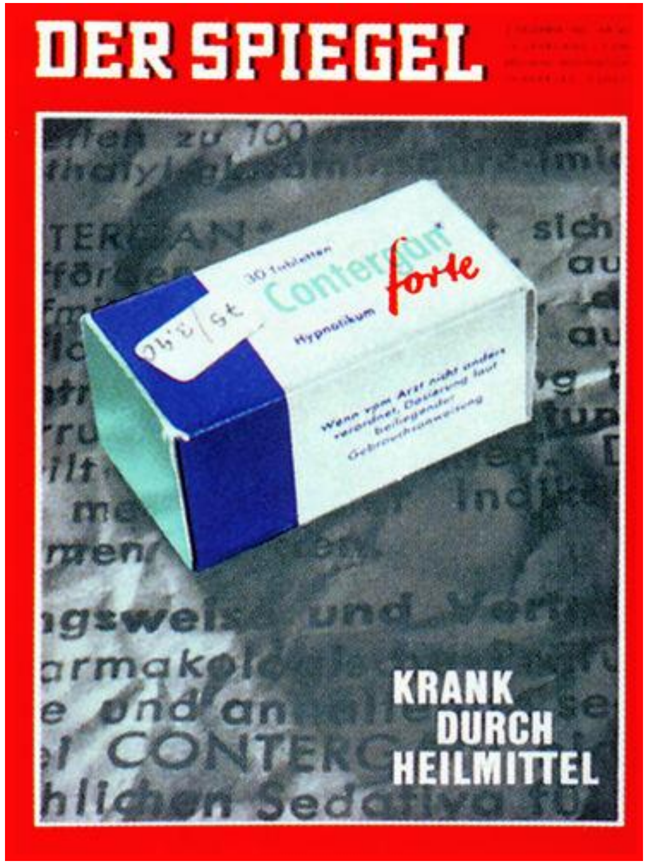
Penicillamin



Ketamin

[5]: Vargesson, Birth Defects Res C Embryo Today, 2015.
[6]: Song et. al., Medicine, 2017.
[7]: Yang et. al., Analytic Chimica Acta, 2021.
[8]: Andrade C. The Journal of clinical psychiatry, 2017.

Thalidomide (Contergan) scandal



1962

Daily Mail

TUESDAY, DECEMBER 21, 1971

3p

IS SANTA VALUE FOR MONEY? Centre Pages

Anger grows over the Mail's disclosures about heartbreak children

SCANDALOUS!

—that's the experts' verdict

By HARRY LONGMUIR

TWO of Britain's leading thalidomide experts yesterday described compensation terms offered to deformed children as 'scandalous.'

The Armitage family—'plagued by letters from solicitors.'

Fight insulting offer urges boy's mother

Shots at soldiers kill girl

1971

Sunday newspaper of the year

THE SUNDAY TIMES

THE LAST DAYS OF SHANE WARNE

MAGAZINE

50 GREAT DRESSES FOR SUMMER

STYLE

Drug scandal that damaged 20,000 babies

Epilepsy pills are still being given to pregnant women in a travesty that recalls thalidomide

COMING A CROPPER?

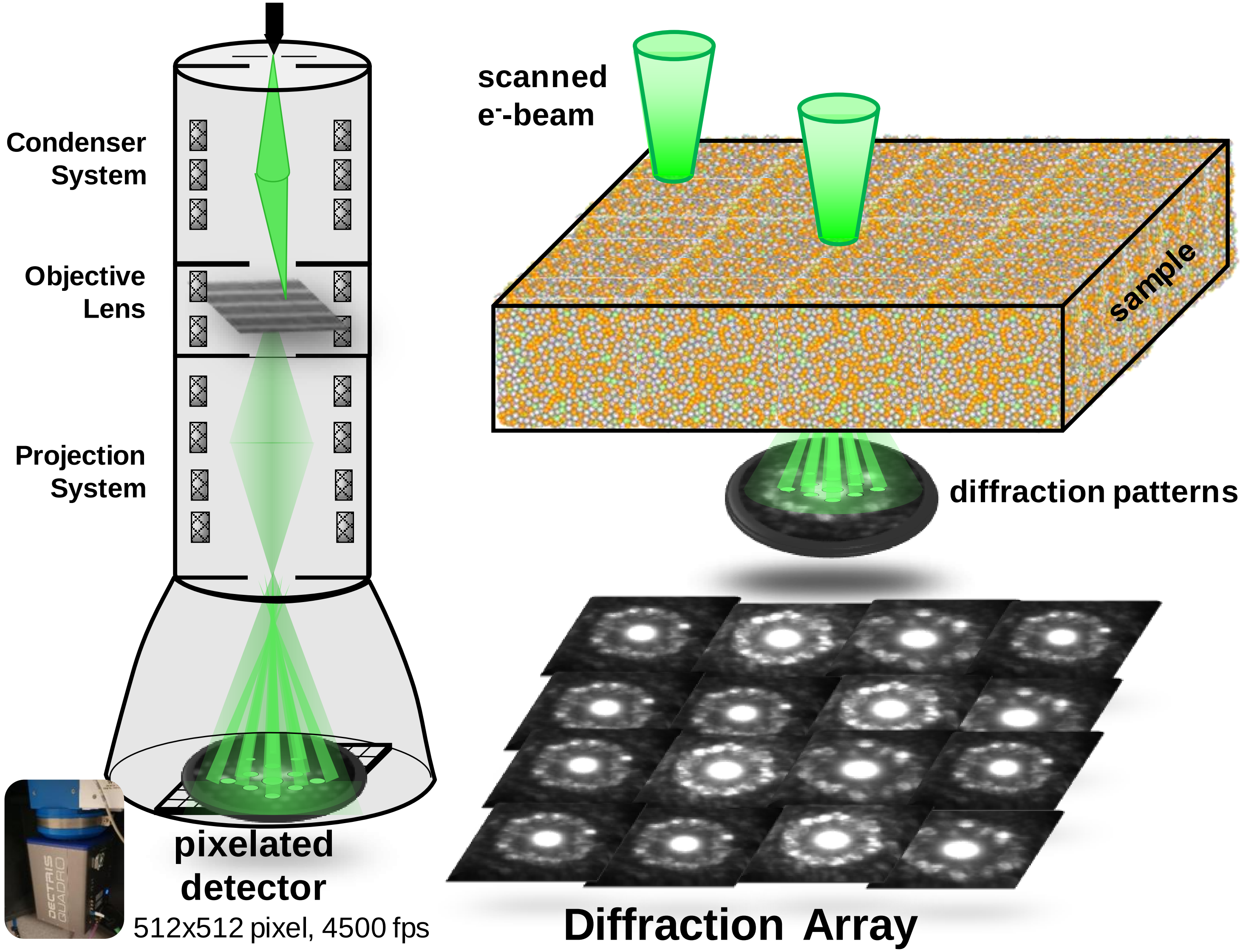
$100m final plea of Isis hostage Cantlie

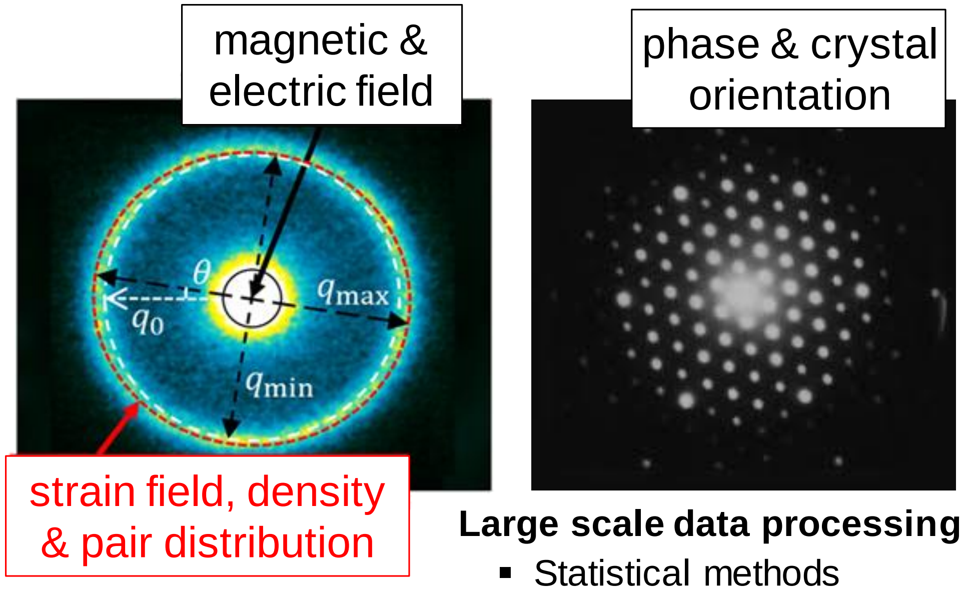
Shipping migrants to Africa is ungodly, Welby tells PM

2022

Methodology

4D-STEM Diffraction Mapping





Large scale data processing

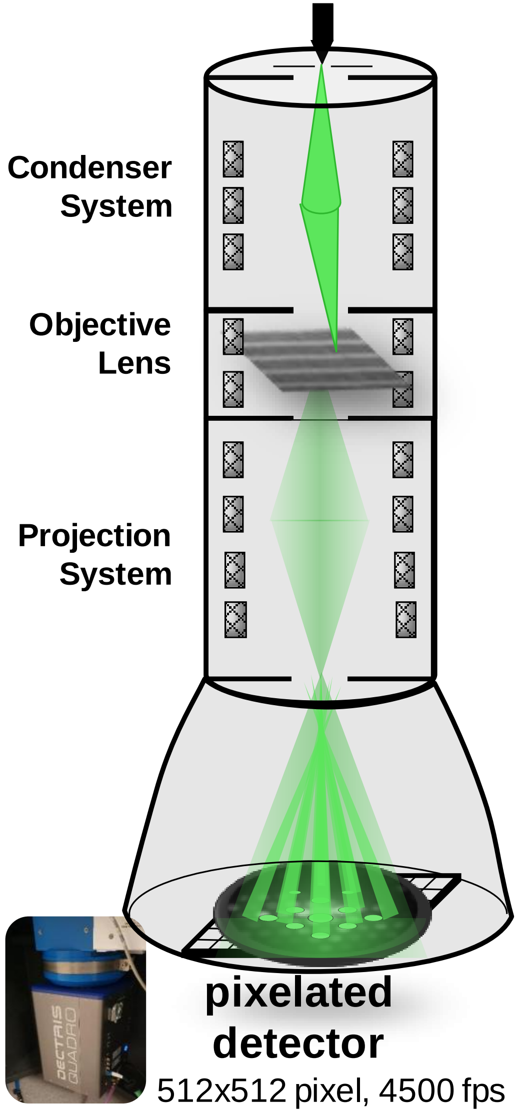
- Statistical methods
- Machine learning

In-situ Electron Microscopy
Institute of Materials Sciences
TU Darmstadt

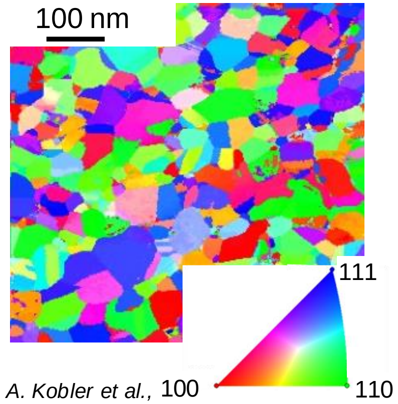
Institute of Nanotechnology
Karlsruhe Nano Micro Facility
Helmholtz Institute Ulm

4D-STEM – Simultaneous Structure & Function Analysis

Karlsruhe Institute of Technology

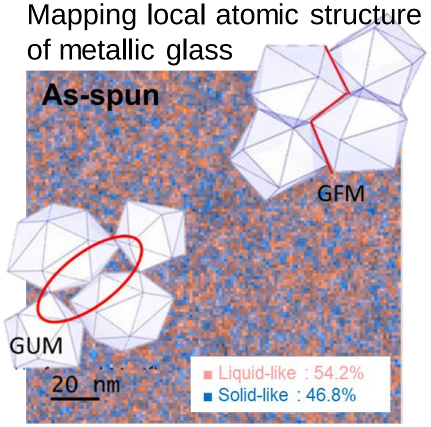


Phase & Crystal Orientation
Crystallographic texture of Nanocrystalline Pd



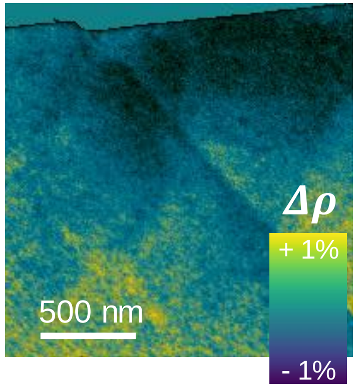
A. Kobler et al., Ultramicroscopy, **2013**, *128*, 68-81

Short/Medium Range Order
Mapping local atomic structure of metallic glass

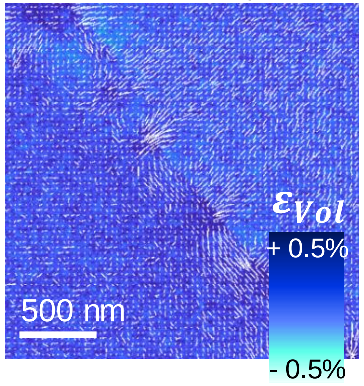


S. Kang et al., *Acta Materialia*, **2024**, *263*, 119495

Atomic Packing Density
Density variations in a deformed metallic glass

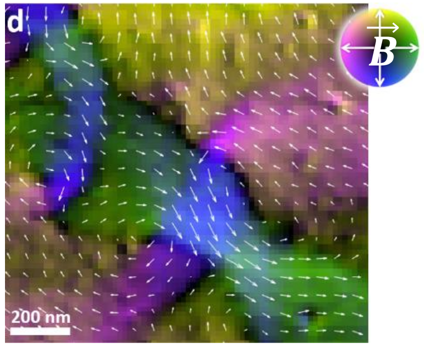


Strain Distribution
Residual strain fields in a deformed metallic glass



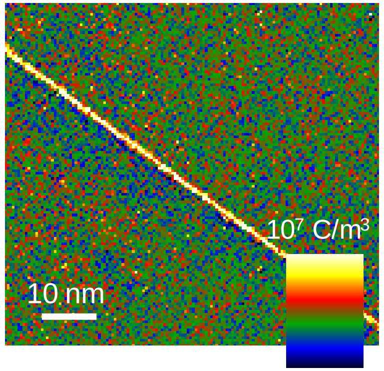
S. Kang et al., *Advanced Materials*, **2023**, *35*, 2212086

Magnetic Field
Ferromagnetic amorphous alloy

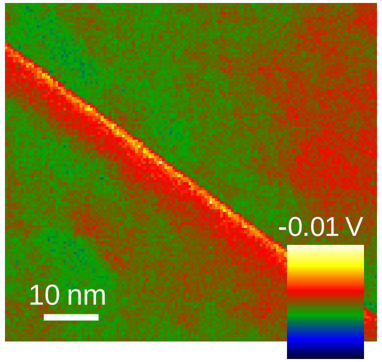


S. Kang et al., **2024**, *in preparation*

Charge Density
GB in ferroelectric ceramic

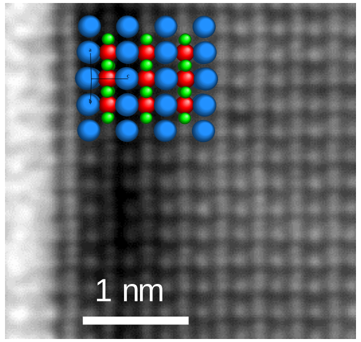


Electric Field
GB in ferroelectric ceramic



S. Kang et al., **2024**, *in preparation*

Mean Inner Potential
GB in BTO



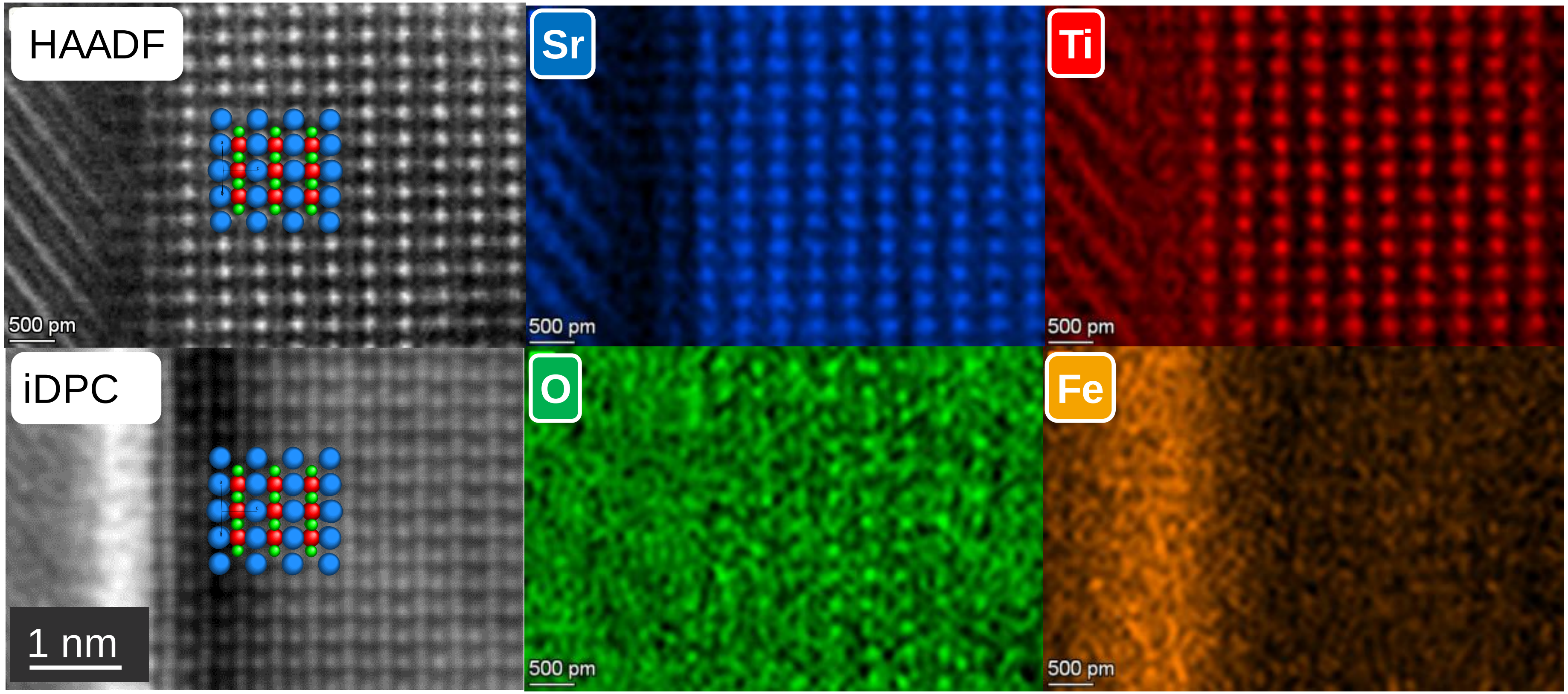
D. Jennings et al., *Acta Materialia*, **2024**, *273*, 119941

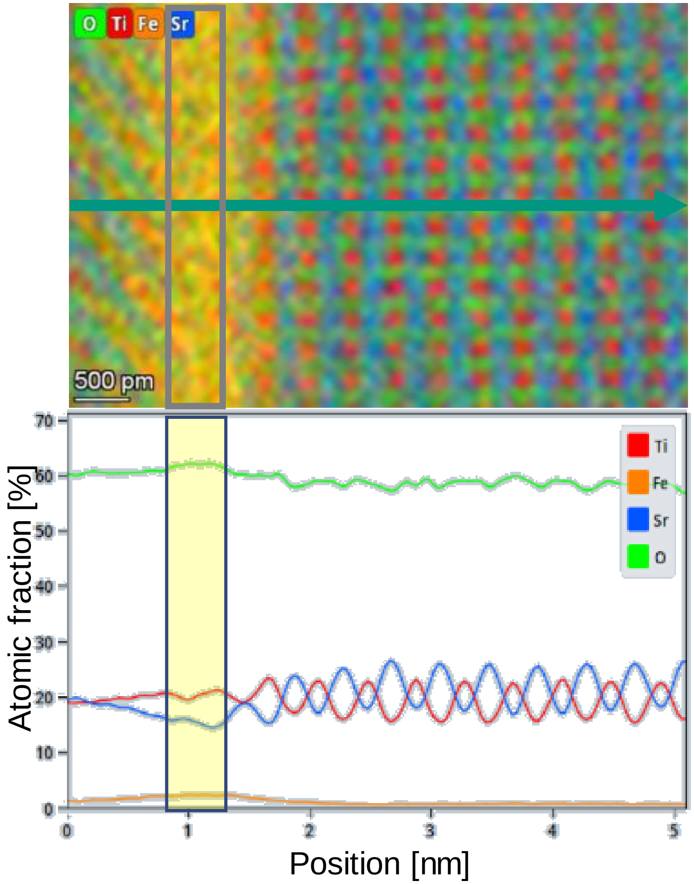
Structure and Segregation at Grain Boundaries

Di Wang

Karlsruhe Institute of Technology

Anisotropic Segregation at Grain Boundary $Sr_{1-x}Fe_xTiO_3$





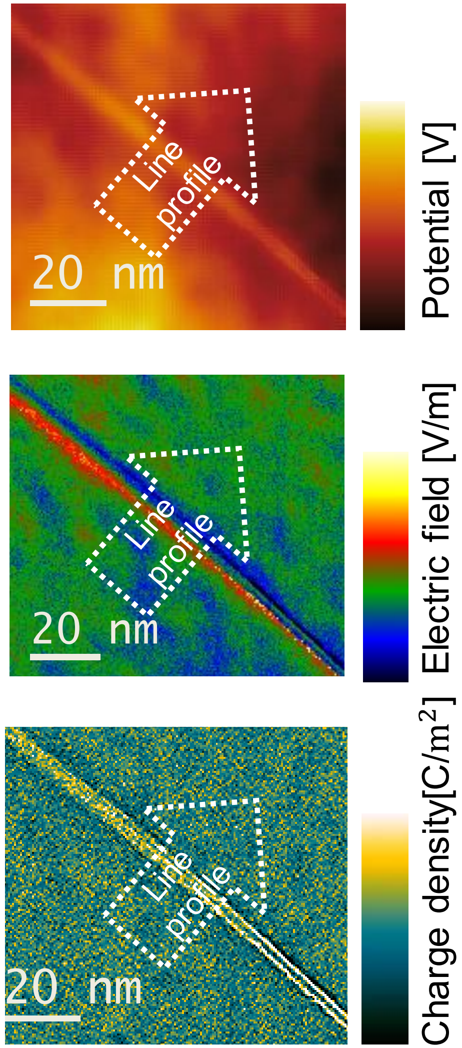
D. Jennings et al., Acta Mat., **2024**, *273*, 119941

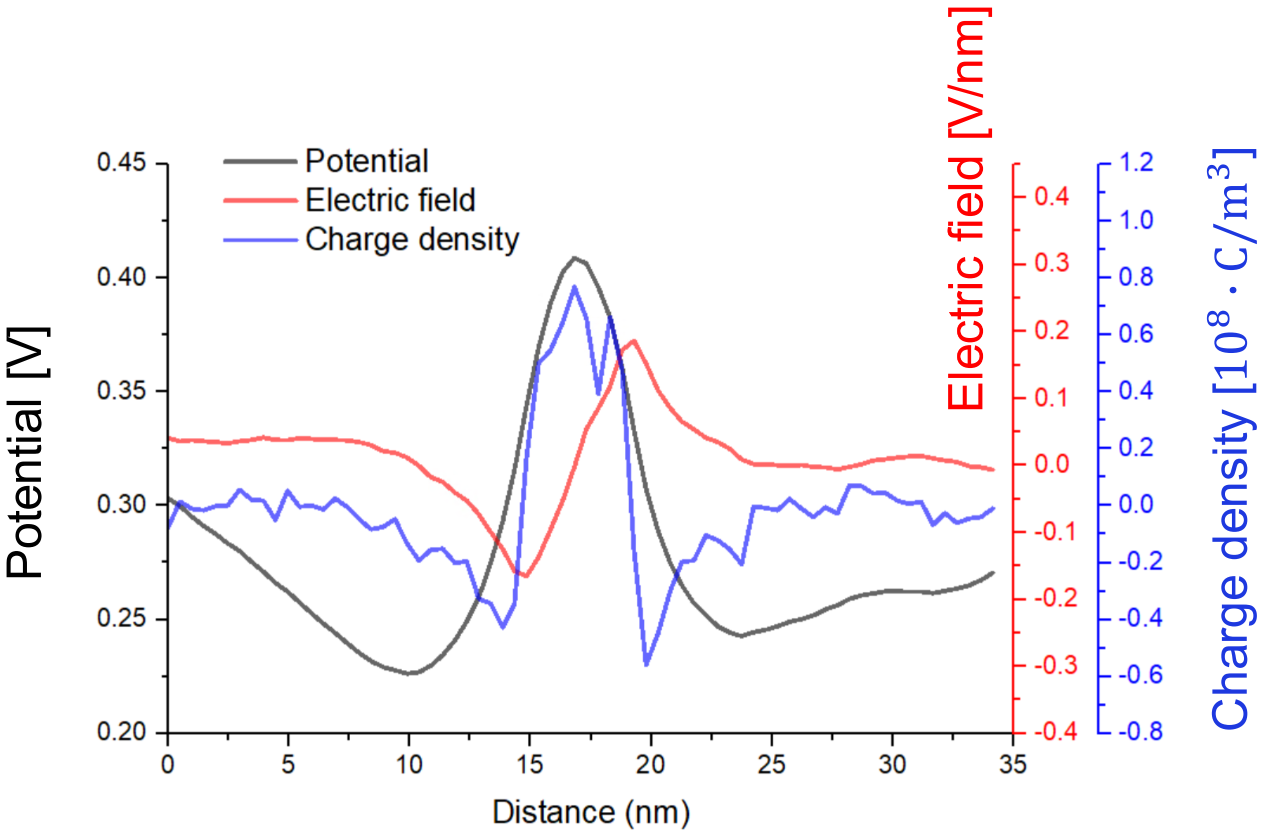
In-situ Electron Microscopy
Institute of Materials Sciences
TU Darmstadt

Institute of Nanotechnology
Karlsruhe Nano Micro Facility
Helmholtz Institute Ulm

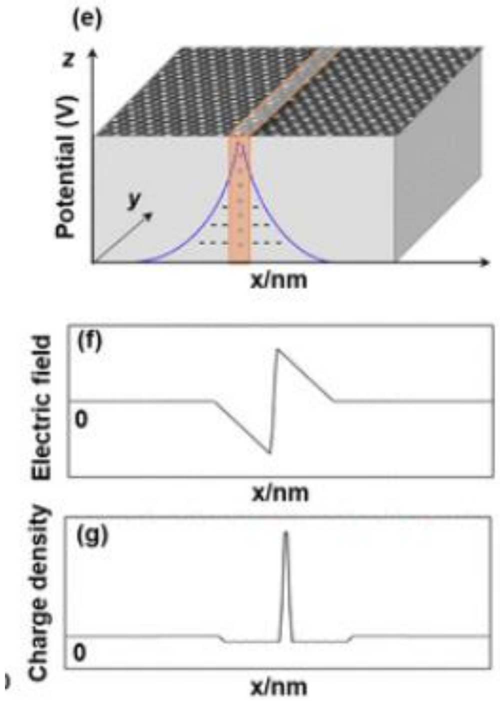
Space Charge Layer at Grain Boundary

Potential, E field, Charges at Grain Boundary $Ba_{1-x}Fe_xTiO_3$





theoretically predicted SCL

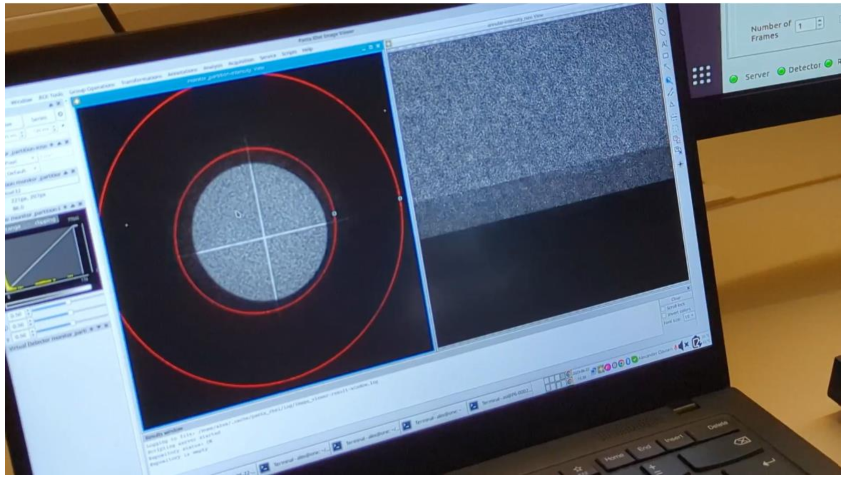


Yang et al. ***Nano Lett***., 21, 9138–9145 (2021)

Direct imaging of space charge layer (SCL) at grain boundary

S. Kang et al., **2024**, in preparation

LiberTEM project

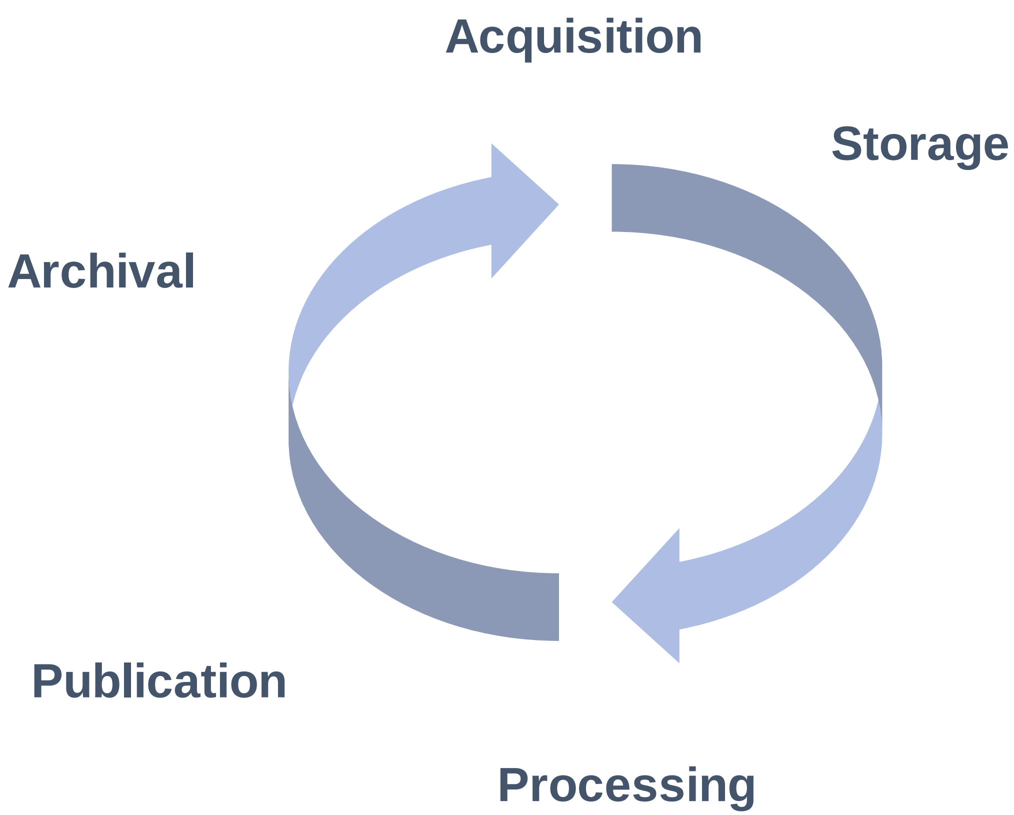


Live and interactive 4D STEM with ***1 mio scan points per second*** *using the event-based CheeTah T3 camera by Amsterdam Scientific Instruments, LiberTEM-live and CEOS' Panta Rhei.*

LiberTEM

- Apply computationally intensive methods like AI to live data and large offline data
- Fast open source stream-oriented processing
- Interactive live processing with some of the fastest detectors currently available
- Decouples data source, user-defined implementation of an algorithm, execution engine and display of results
- Interoperability and re-use in different contexts
- Successful collaboration with many vendors
- https://libertem.github.io/ for more information

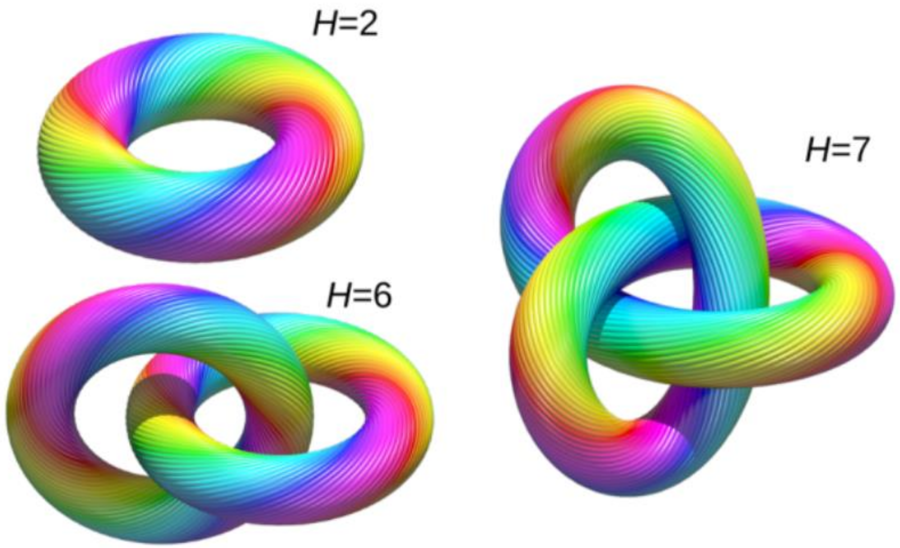
ER-C Data Management



- https://er-c-data.fz-juelich.de
- Use at CEA (Matthew Bryan)
- Versatile, modular, performant data management
- Standards-based interfaces
- User-friendly, familiar
- Easy collaboration
- Link storage with compute, metadata
  - AI!
- Pilot in production use
- EU project EOSC Data Commons

Magnetic hopfions

Hopfions can be considered as closed twisted skyrmion strings that take the shape of a ring in the simplest case.

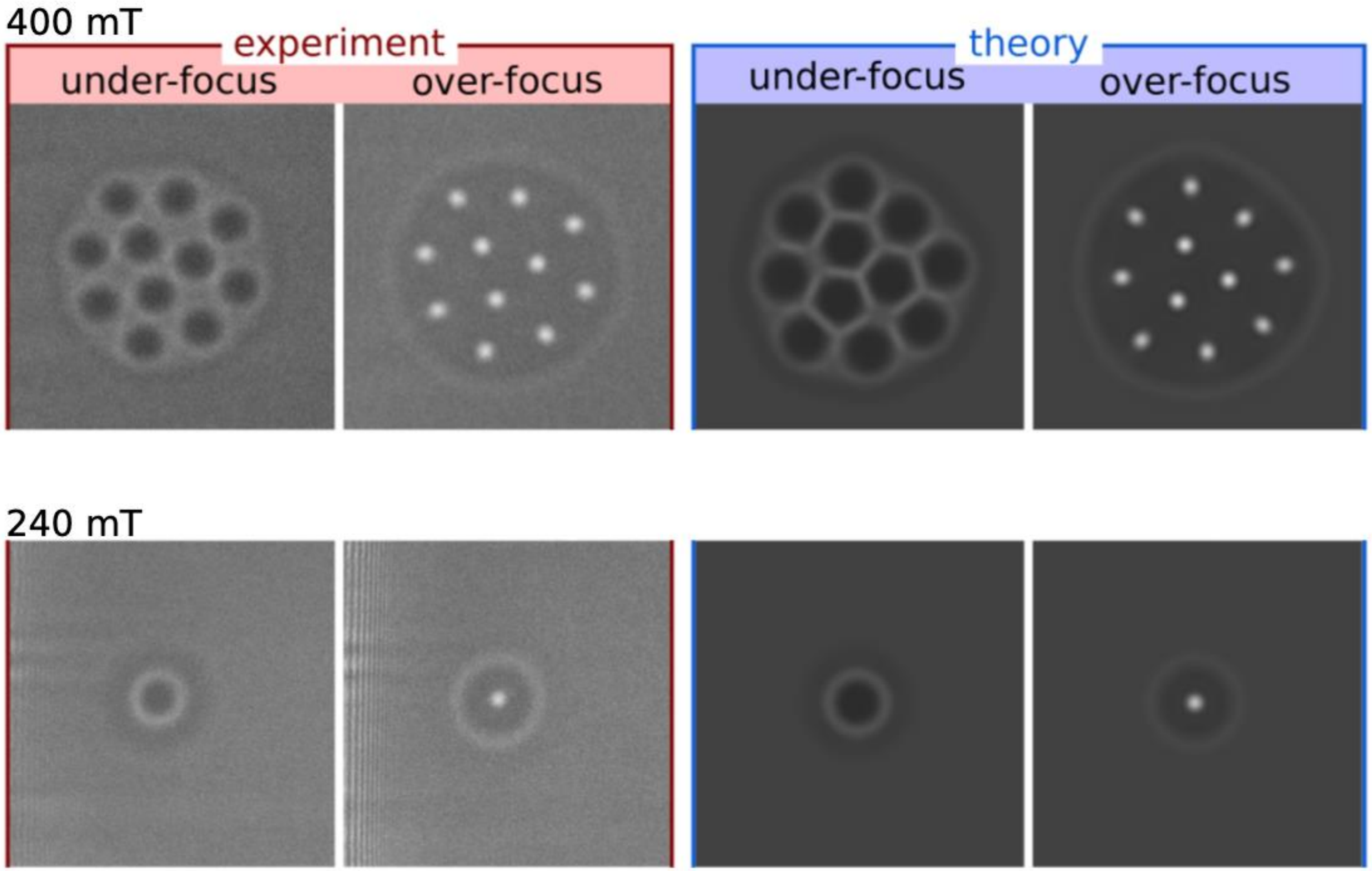


The complexity of the hopfion shape and size increases with the Hopf index *H*.

Magnetic hopfions in solids
F N Rybakov, N S Kiselev, A B Borisov, L Döring, C Melcher, S Blügel
APL Materials 10 (2022), 111113.

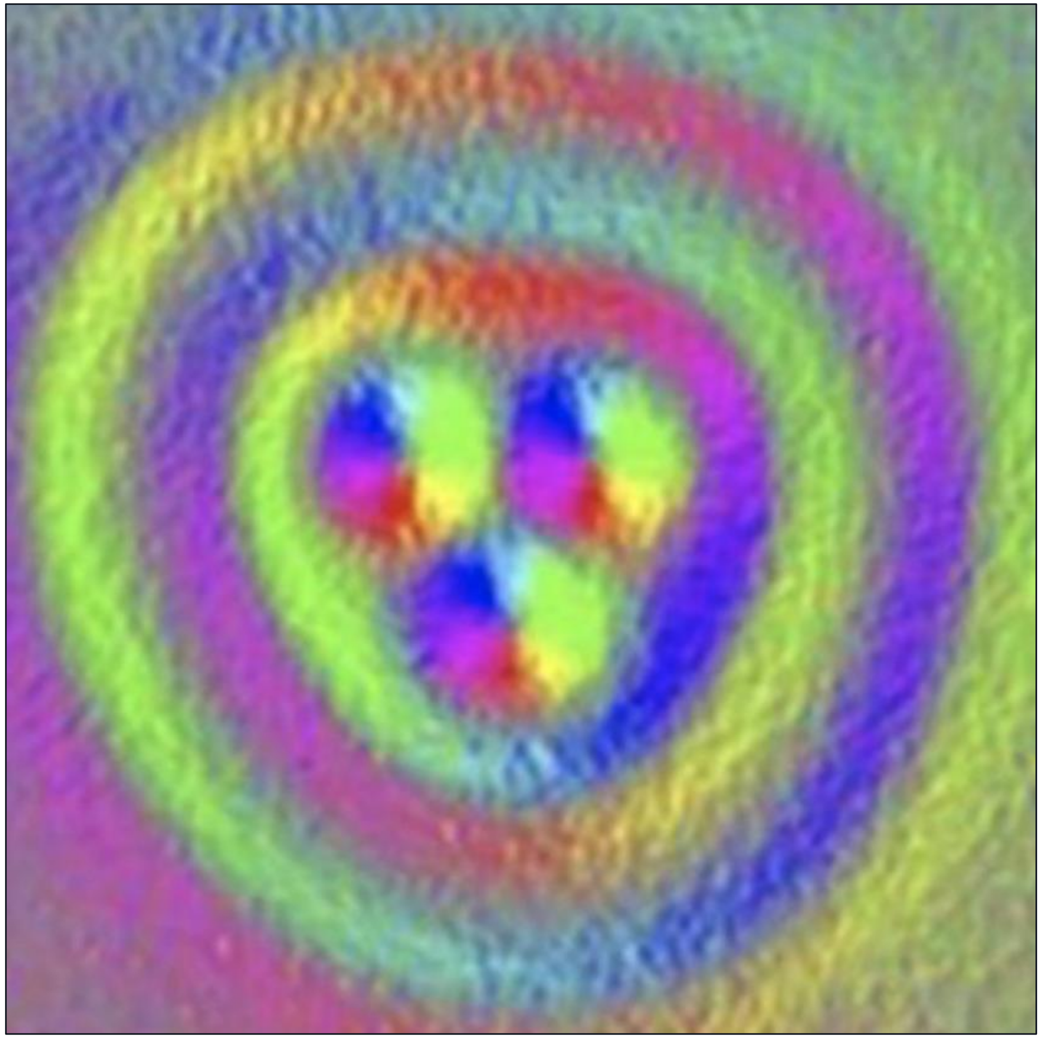
ÜLICH
schungszentrum

Coupled states of skyrmion strings and hopfions in FeGe plates of thickness 180 nm at 95 K



Hopfion rings in a cubic chiral magnet
F Zheng, N S Kiselev, F N Rybakov, L Yang, W Shi, S Blügel and R E Dunin-Borkowski
Nature 623 (2023), 718-723.

Magnetic hopfions



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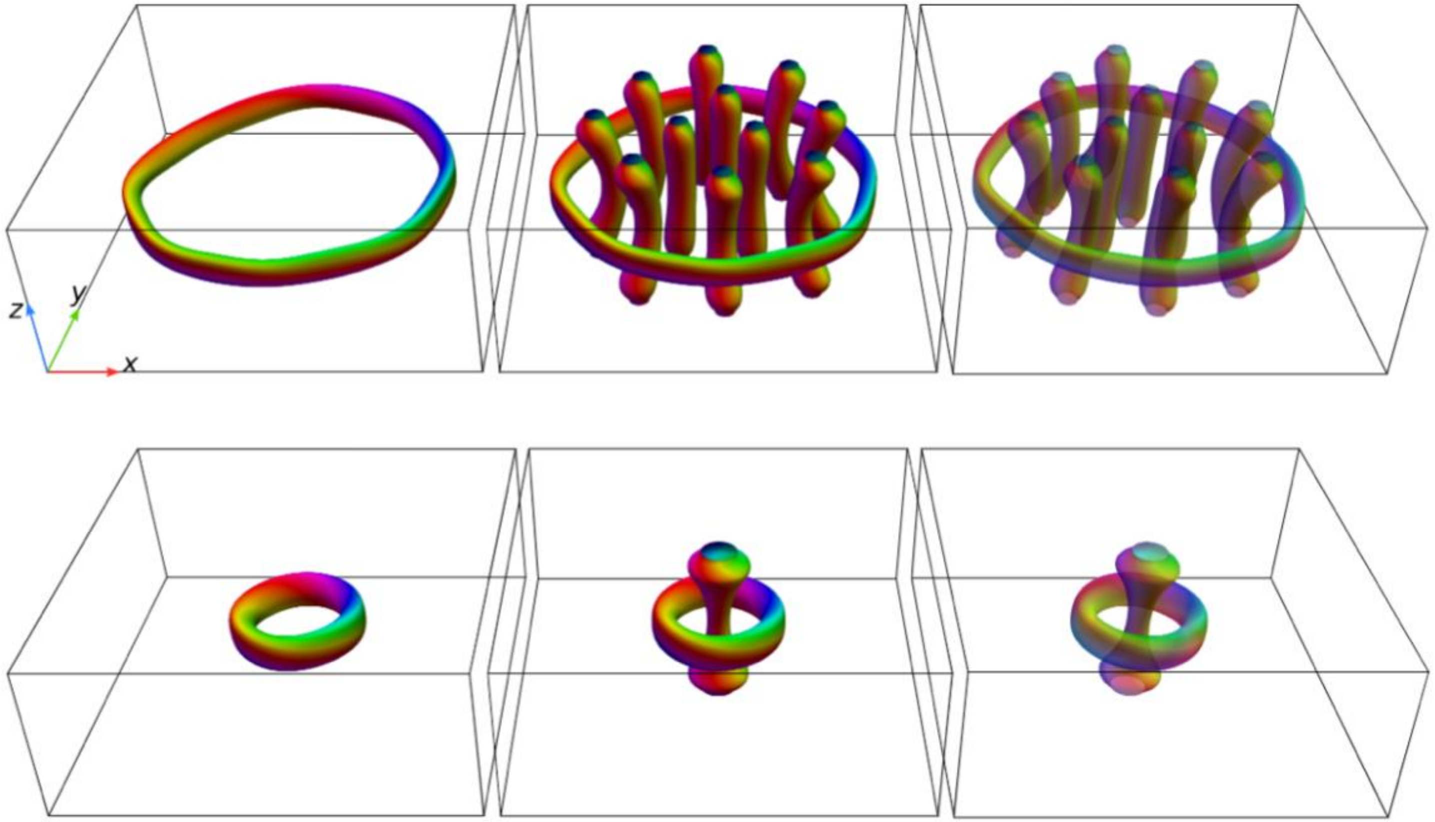
Magnetic hopfions

Simulations of $m_z = 0$ isosurfaces for hopfion rings with Q = −11 and −1.
Left: hopfion ring alone. Right: semitransparent isosurfaces.



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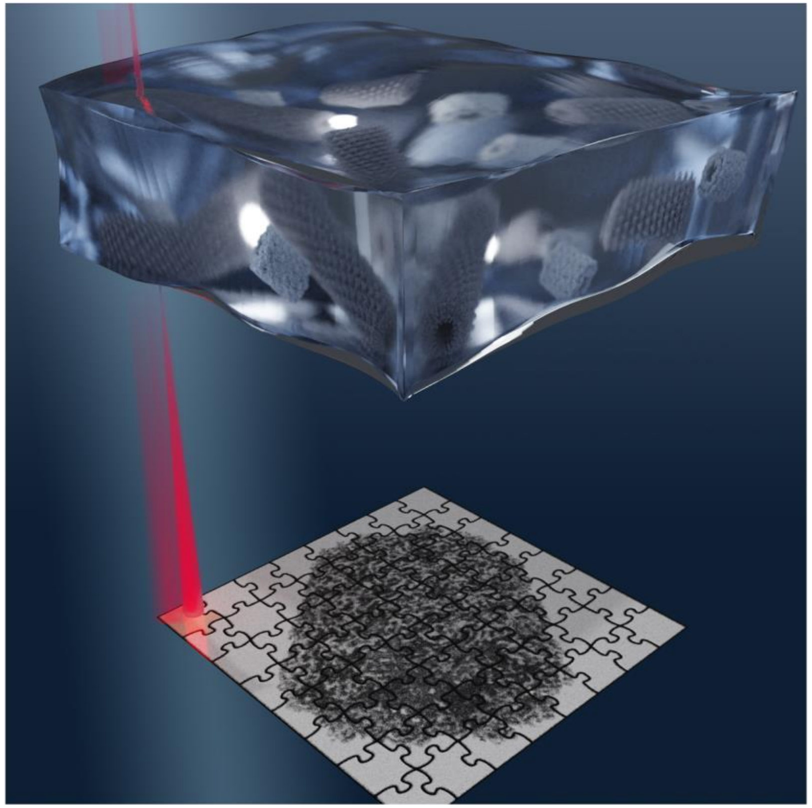
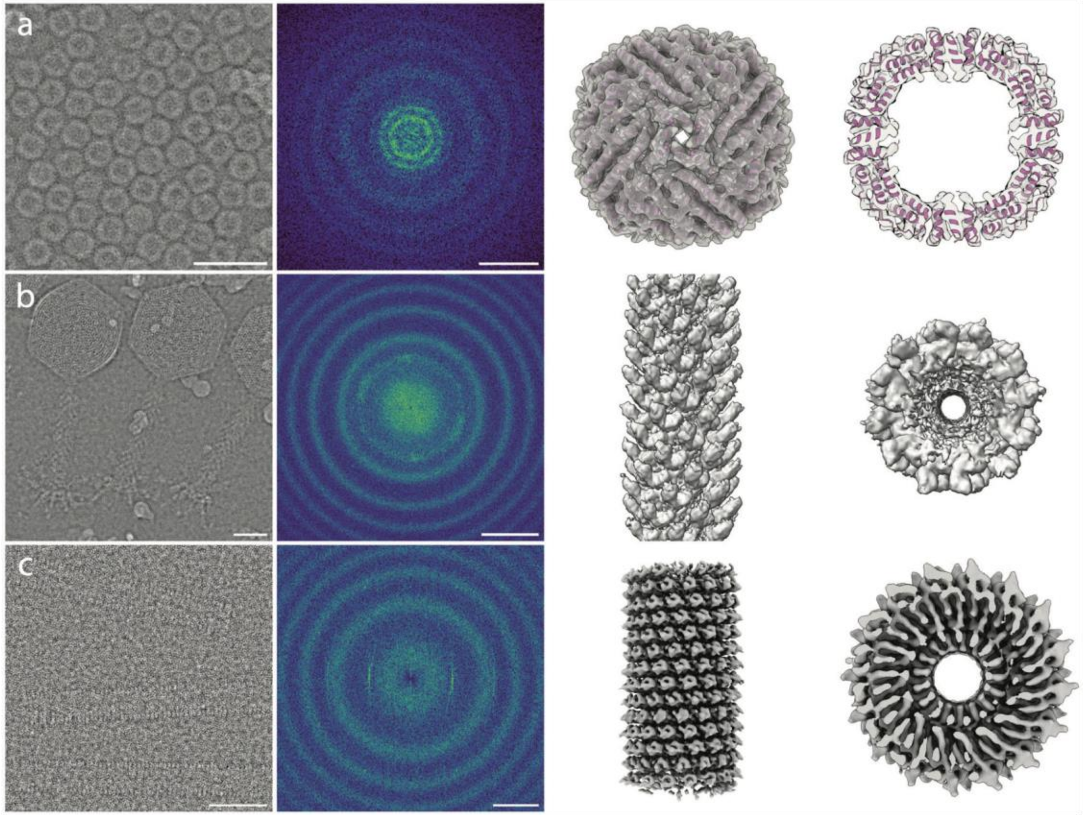
Nature 623 (2023), 718-723.

JÜLICH
Forschungszentrum

Single-particle averaging of cryo-ptychographic images





Küçükoğlu, B., …**Sachse, C.**, Müller-Caspary, K., … Stahlberg, H., *Low-dose cryo-…* (2024)
Nat Commun 15, 8062. https://doi.org/10.1038/s41467-024-52403-5

European Research Council
Established by the European Commission

ERC Synergy grant: 4D-BioSTEM with Knut Müller Caspary and Henning Stahlberg

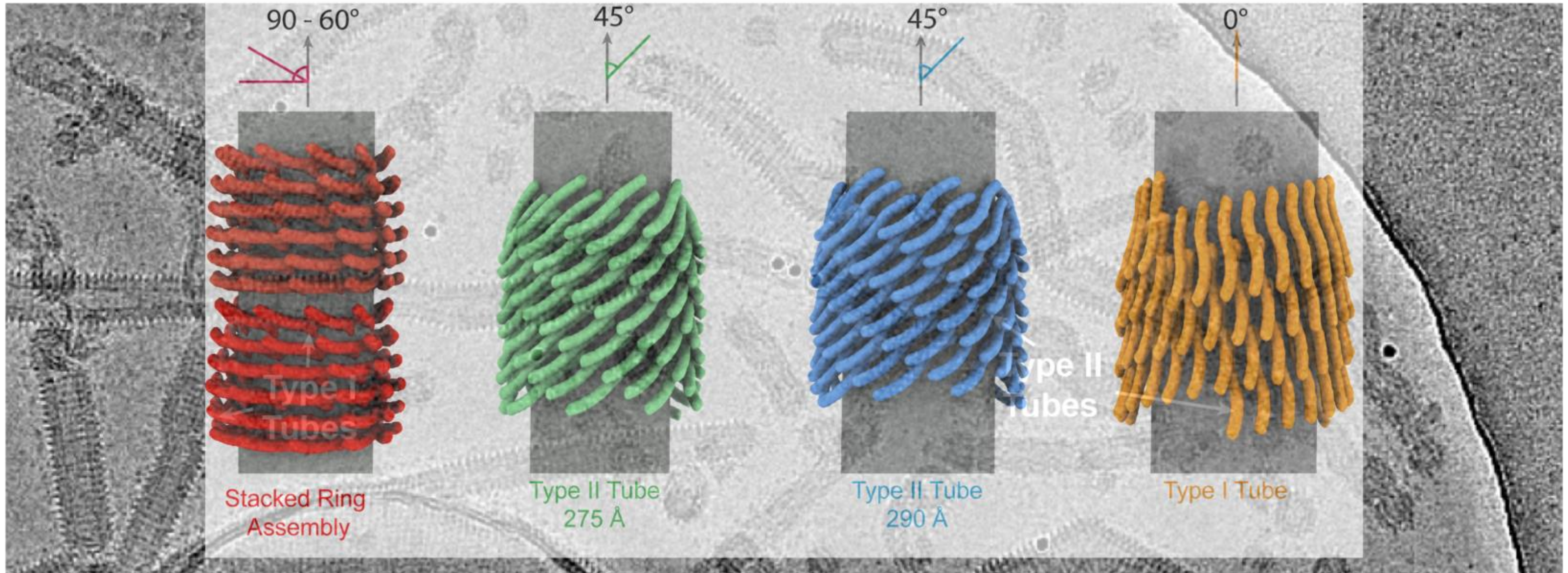
Mechanisms of membrane repair

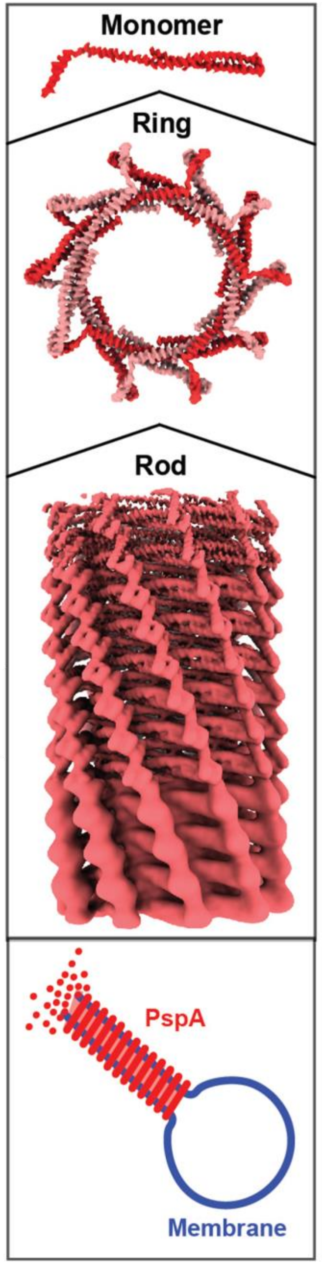
- PspA rods show structural plasticity and remodel membranes

  Junglas, Hudina … **C. Sachse**, *Structural plasticity of… (2024)*
  Nat Struct Mol Biol. https://doi.org/10.1038/s41594-024-01359-7

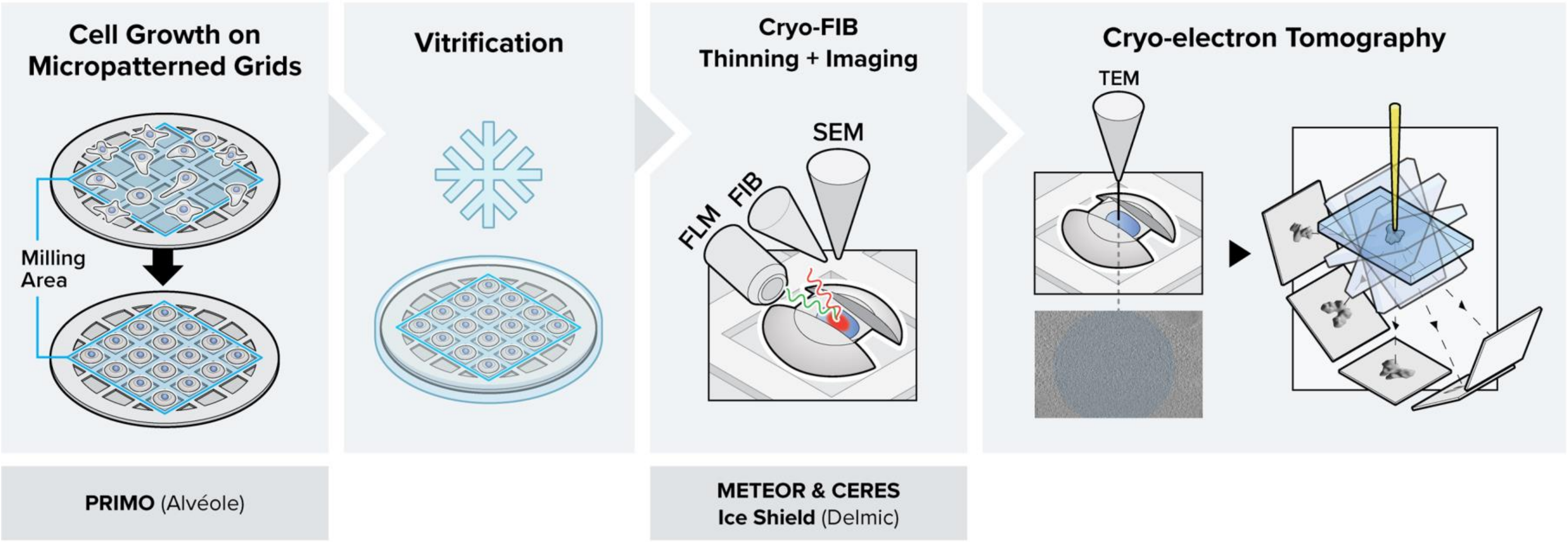
- Vipp1's structural diversity on membranes, from carpets to helical tubes to single/stacked-ring assemblies is critical for membrane remodeling

  Junglas et al., … **C. Sachse,** *Structural basis for Vipp1… (2024)*
  Nat Struct Mol Biol. https://doi.org/10.1038/s41594-024-01399-z





A correlative workflow for cellular cryo-imaging

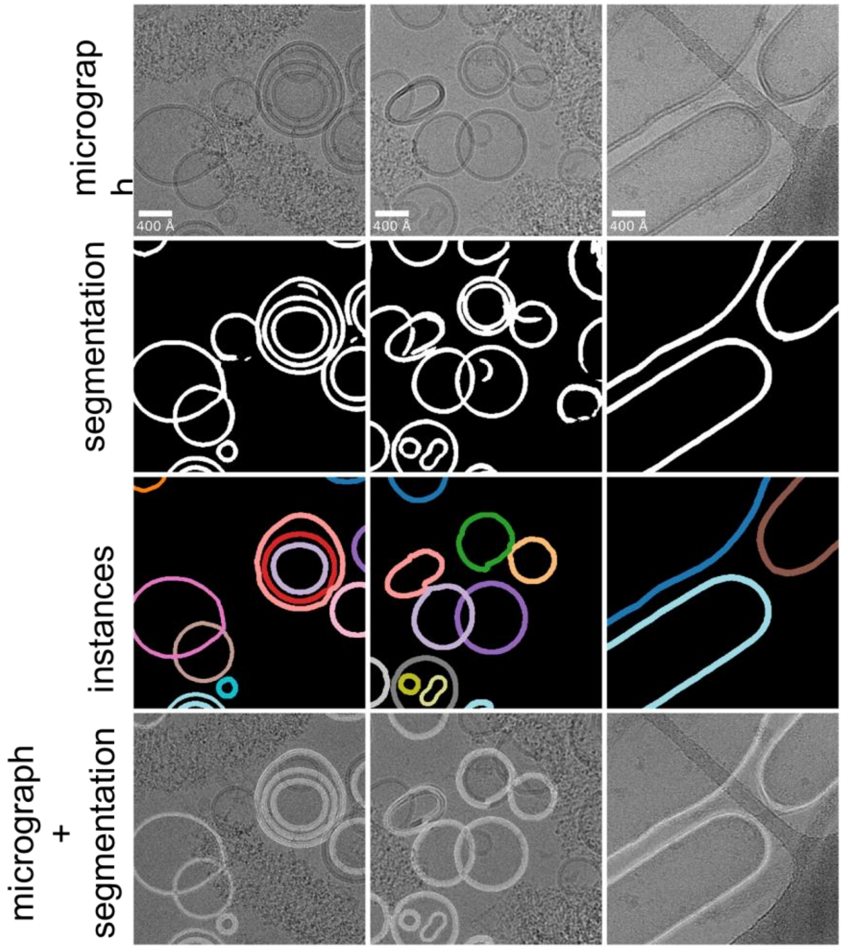


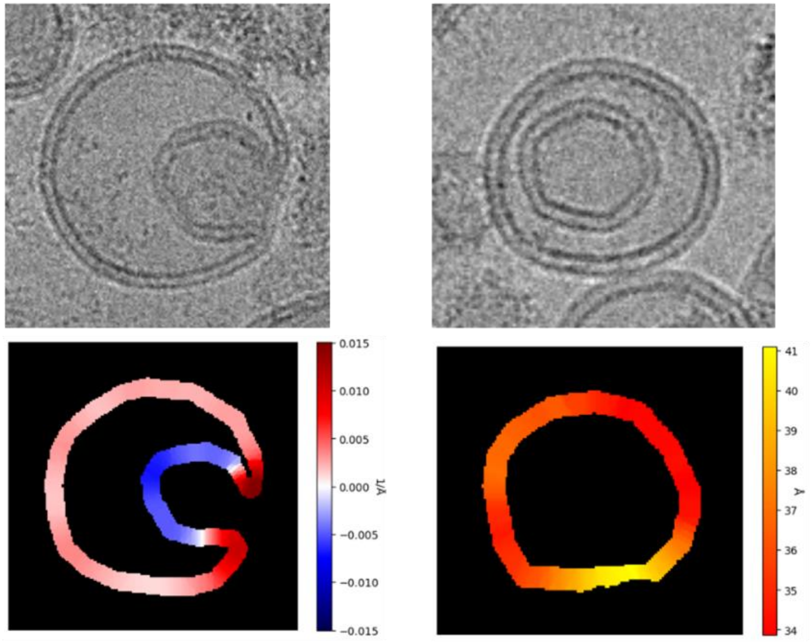
Berkamp, S. … **Sachse, C.**, 2023. *Correlative Light and Electron*… BIO-PROTOCOL 13. https://doi.org/10.21769/BioProtoc.4901

Berkamp: Poster on cryo-ET of biological cells in combination with EDX

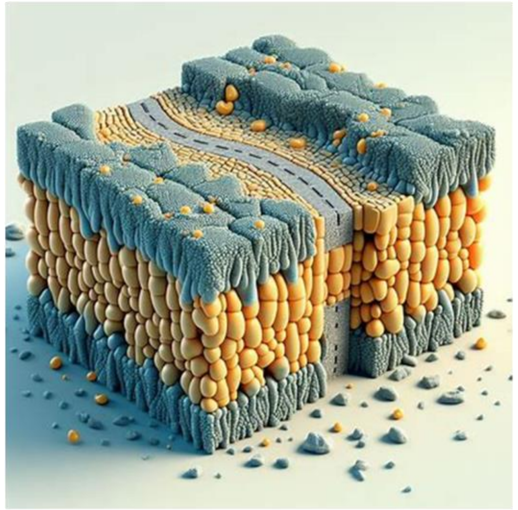
Azad/Sundermeyer: Poster on workflow including PlasmaFIB (TFS Arctis)

CryoVIA - An image analysis toolkit for membrane structures





Schönnenbeck: Poster on CryoVIA



- AI-assisted membrane segmentation
- Feature extraction
- Parameterization of membrane properties
- Shape analysis
- Quantitive automated analysis of 1000s of micrographs

Schönnenbeck, P. … **Sachse, C.**, CryoVIA - An image analysis toolkit for the quantification of membrane structures from cryo-EM micrographs (2024). *under review at Structure*

Call launched in summer of 2015

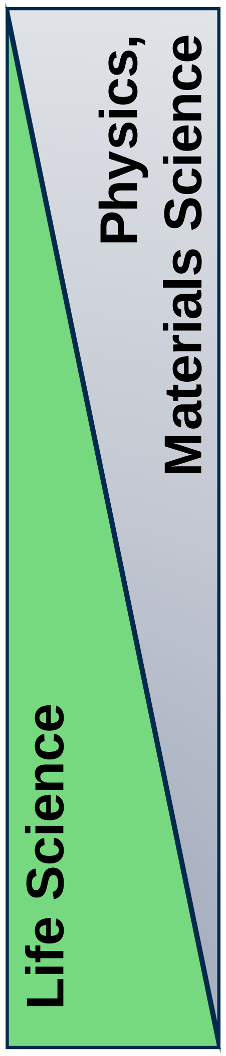
ER-C 2.0

RAFAL E. DUNIN-BORKOWSKI,
JOACHIM MAYER,
AND CARSTEN SACHSE

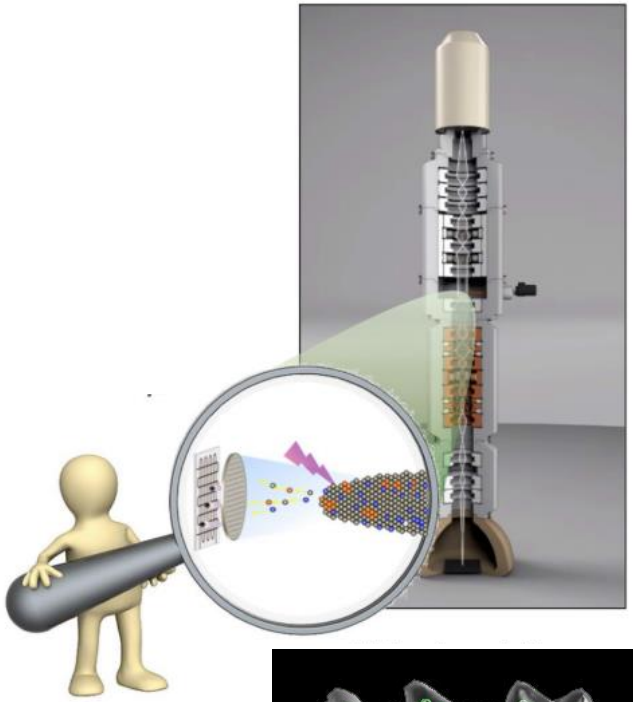
National user facility for high-resolution electron microscopy

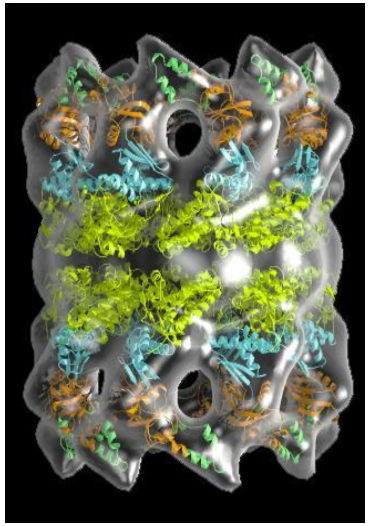
ER-C 2.0

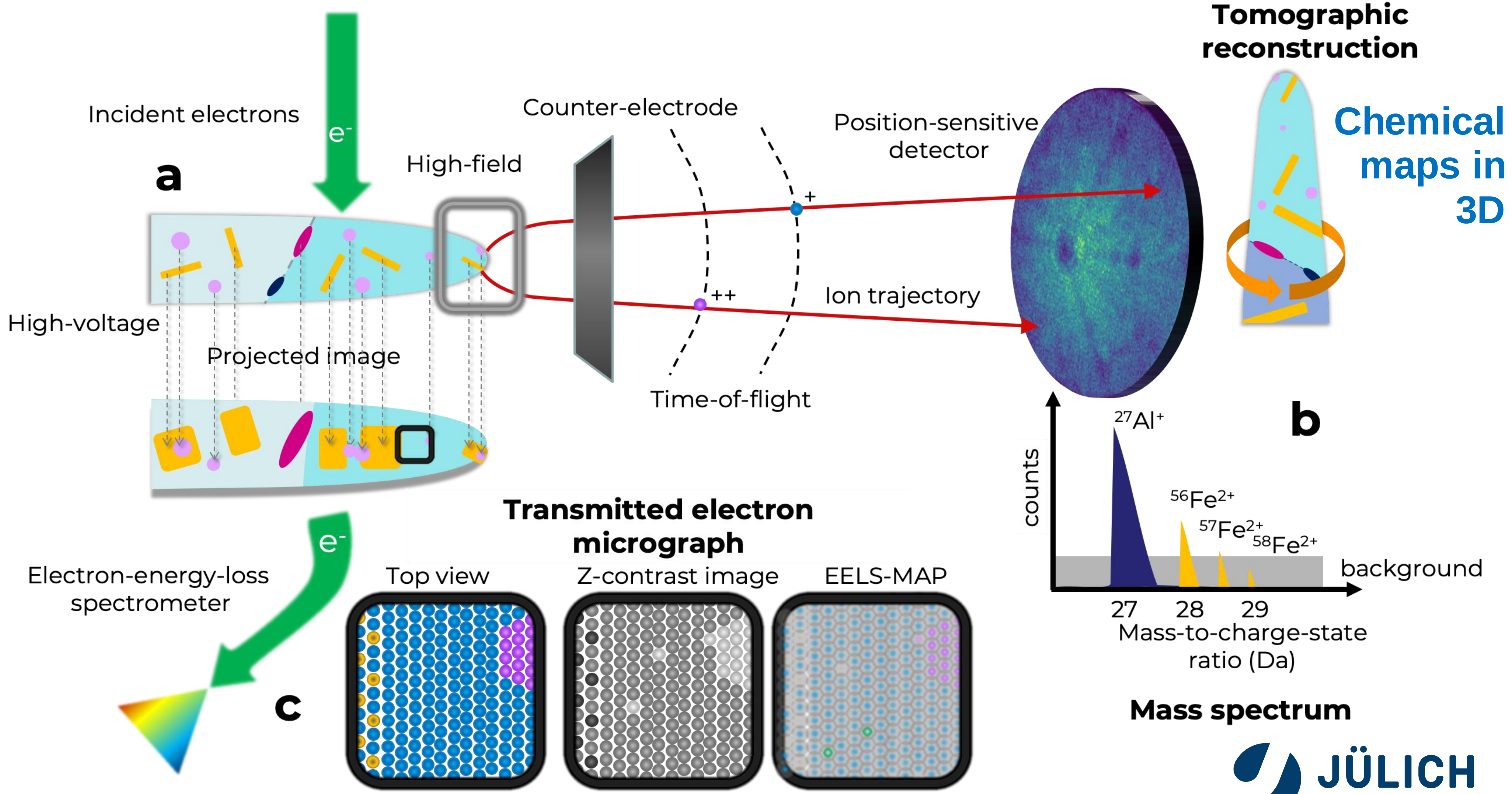
Five Internationally unique Instruments



- **TOMO**:
  TEM combined with an integrated atom probe
- **OPERANDO:**
  Liquid-He cooled UHV-(S)TEM for *in situ* experiments
- **FEMTO:**
  Dynamic *in situ* TEM with ps time resolution
- **SPECTRO**
  Low Voltage (S)TEM with highest spectroscopic resolution
- **BIO:**
  Biological TEM with Cc corrector, phase plate, energy filter, He cooling and single electron detector

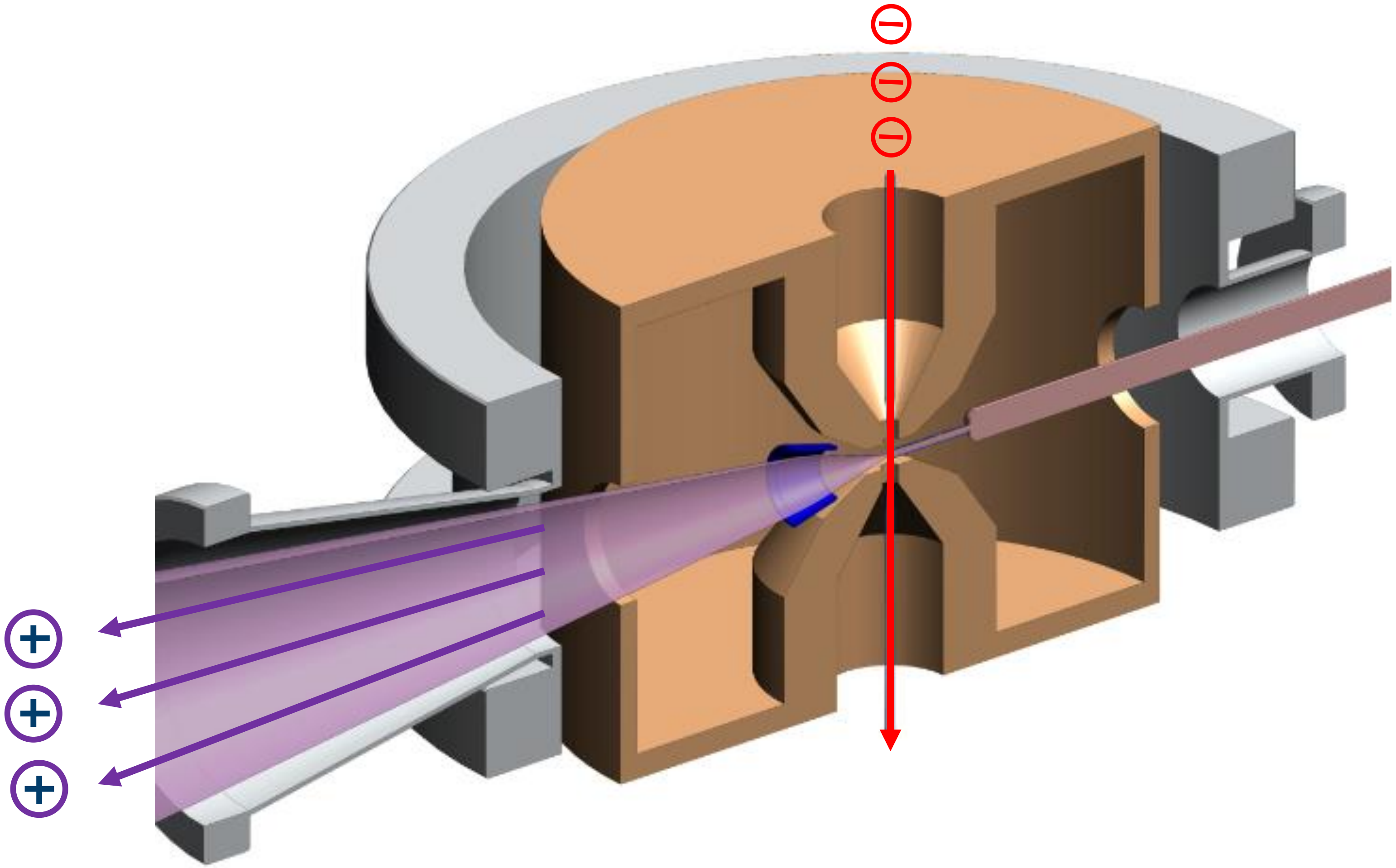




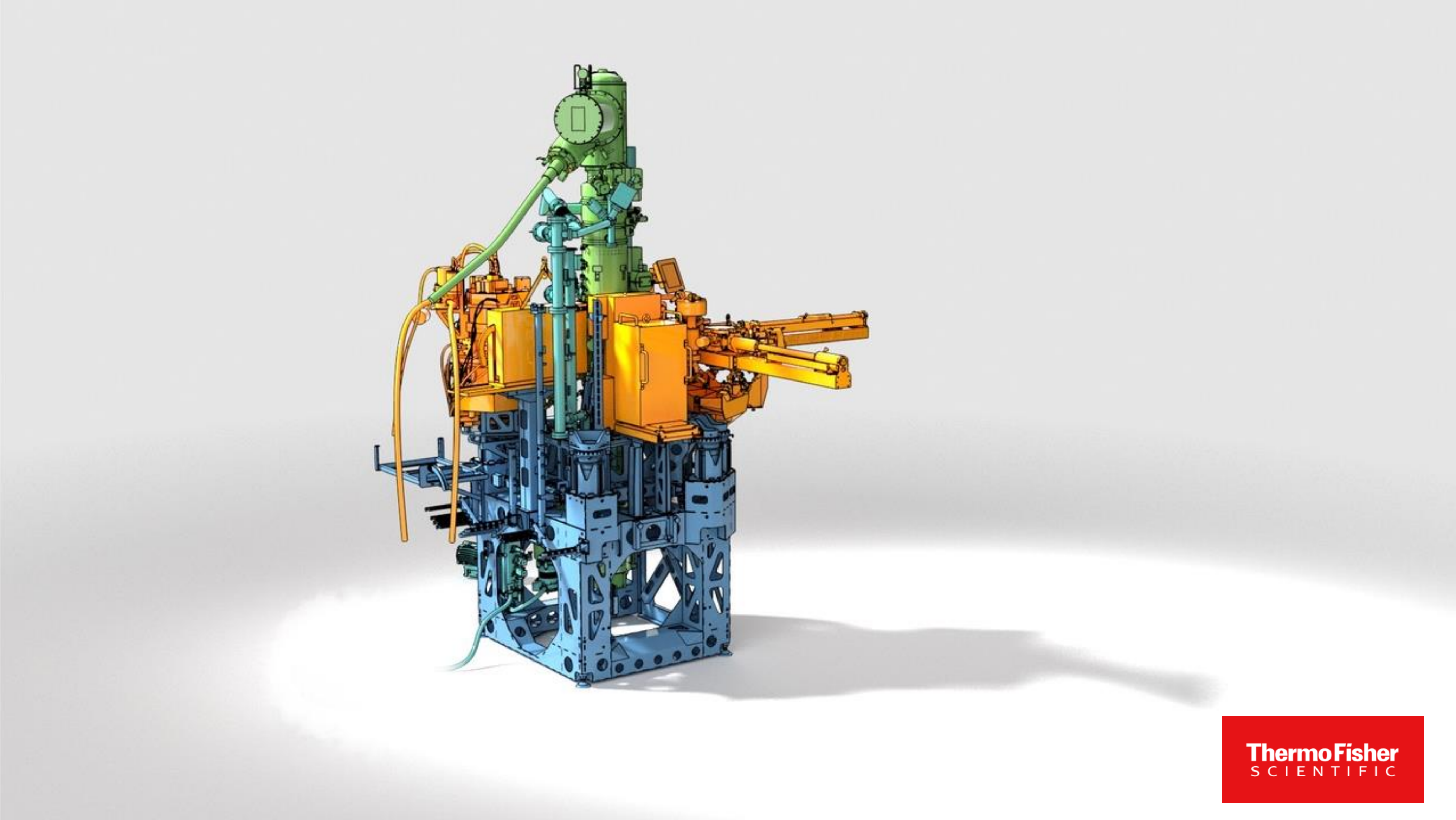


atomic structure, electronic structure

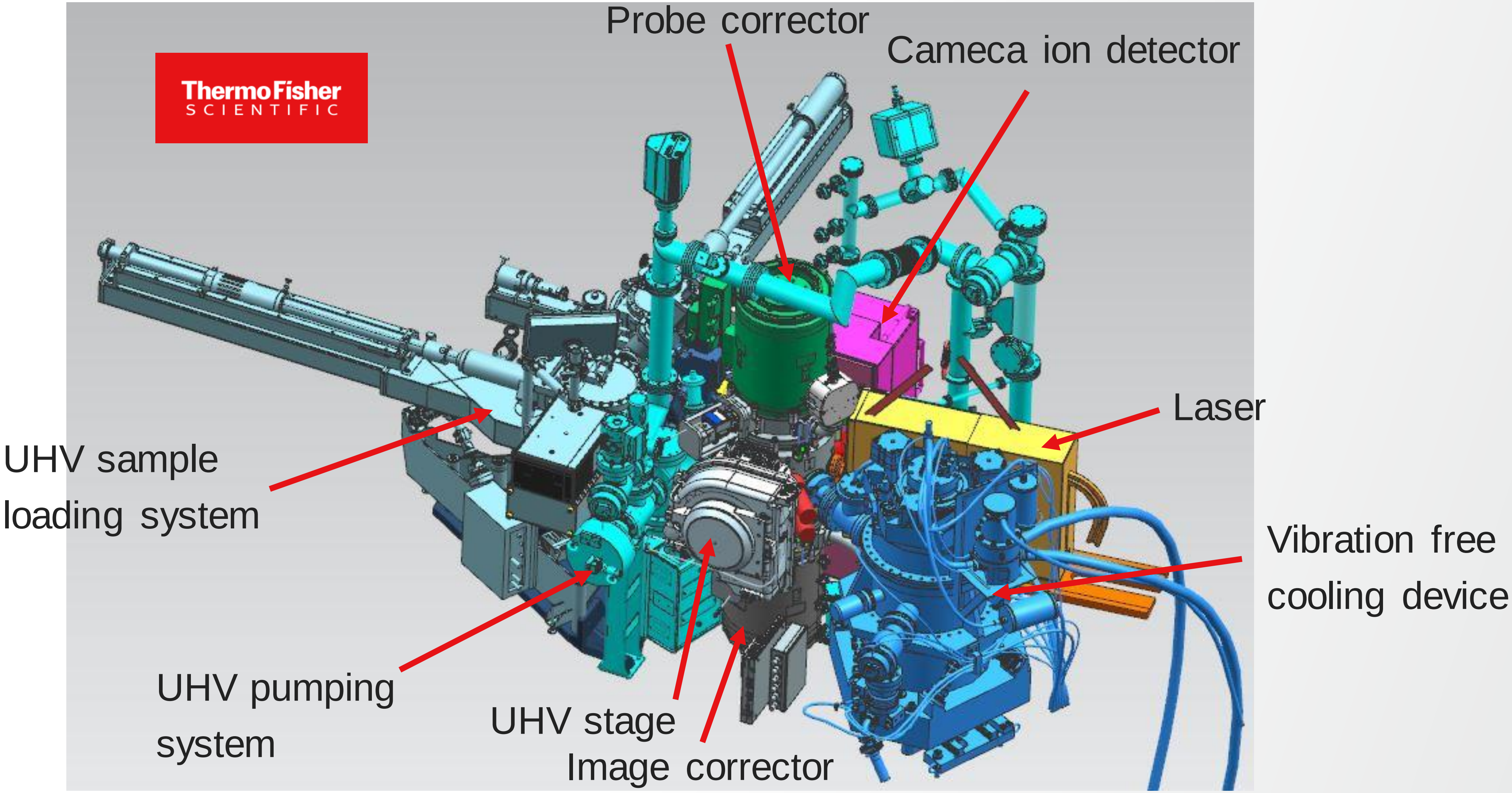
TOMO:
Basic Instrument Design



ER-C 2.0: TOMO instrument - overview

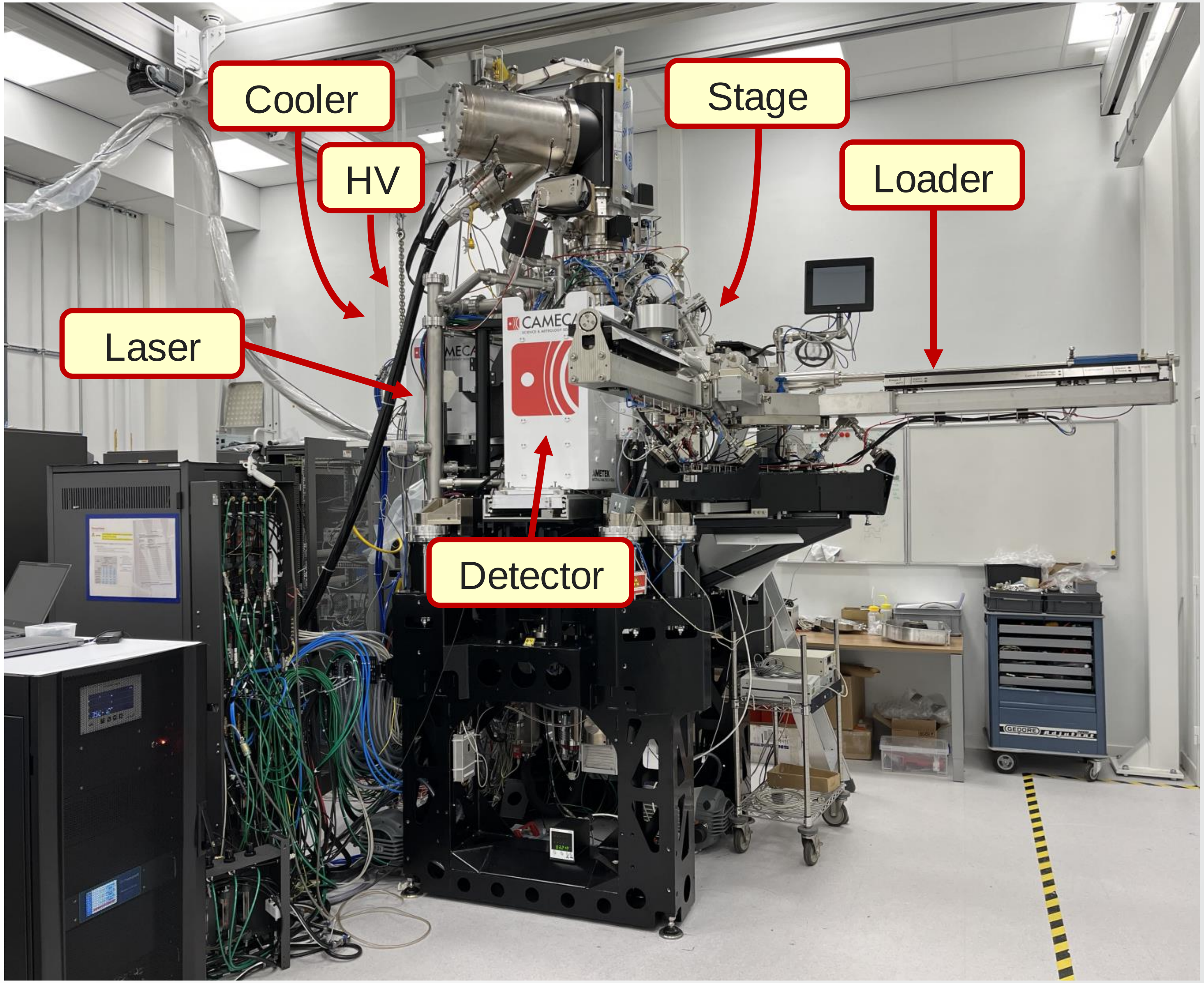


TOMO column with components around octagon



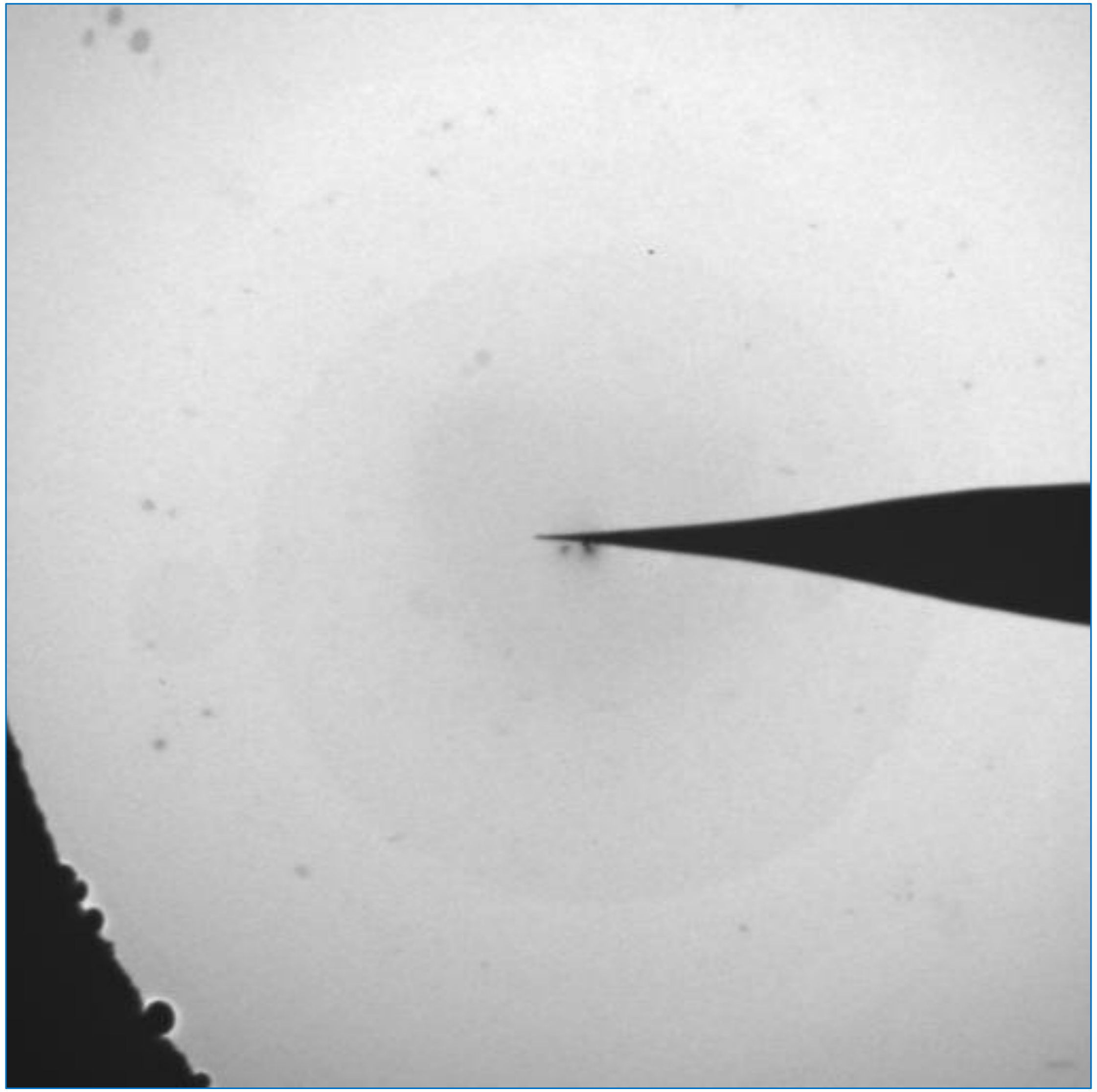
Jülich TOMO prototype

- Integrated APT on TEM
- Uncorrected 300 kV instrument
- Principal system component test
- Experimentation workflow test

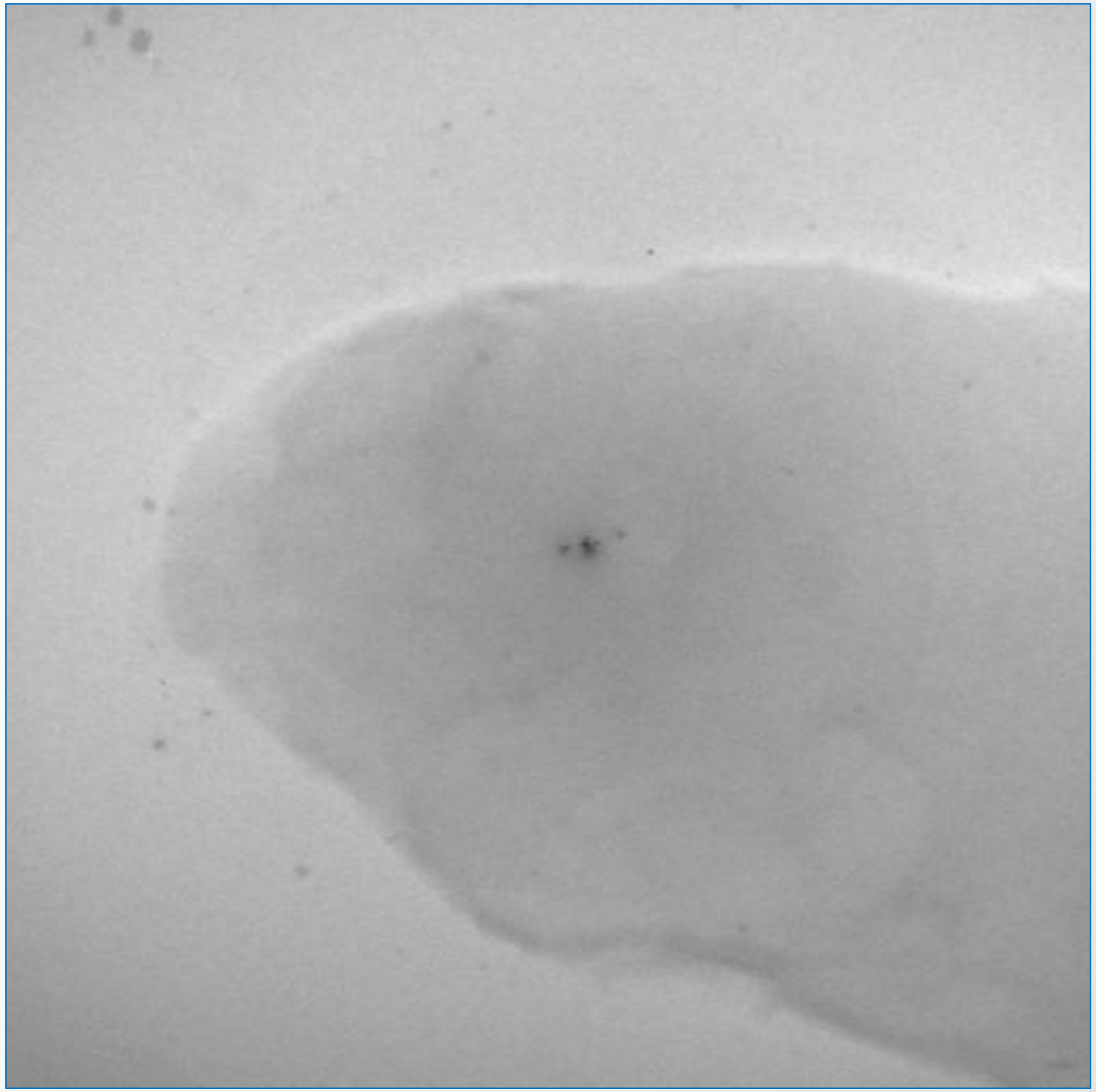


First APT data on TOMO TEM – Aluminium Reference

Field free mode 630 x

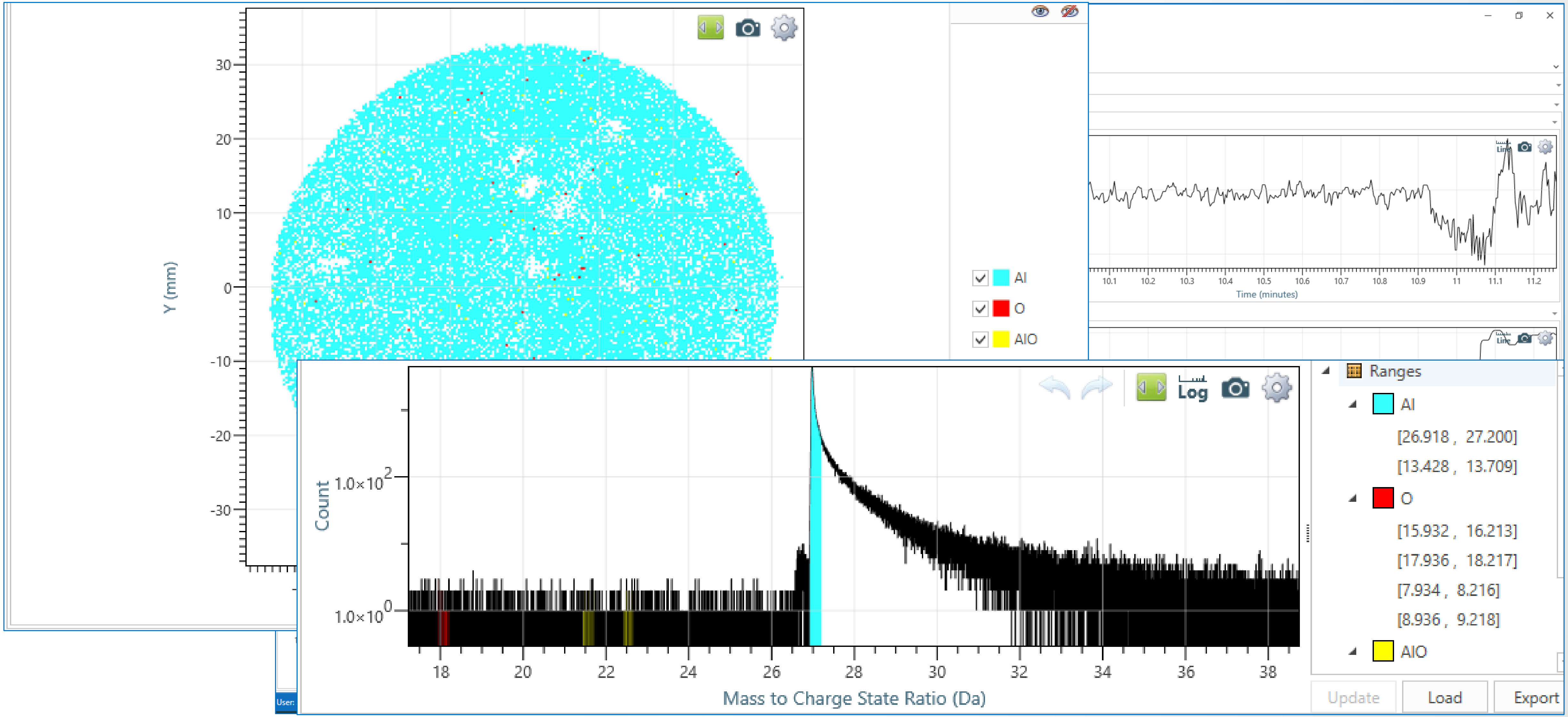


CTEM 57 kx



Intermittently evaporate the needle …

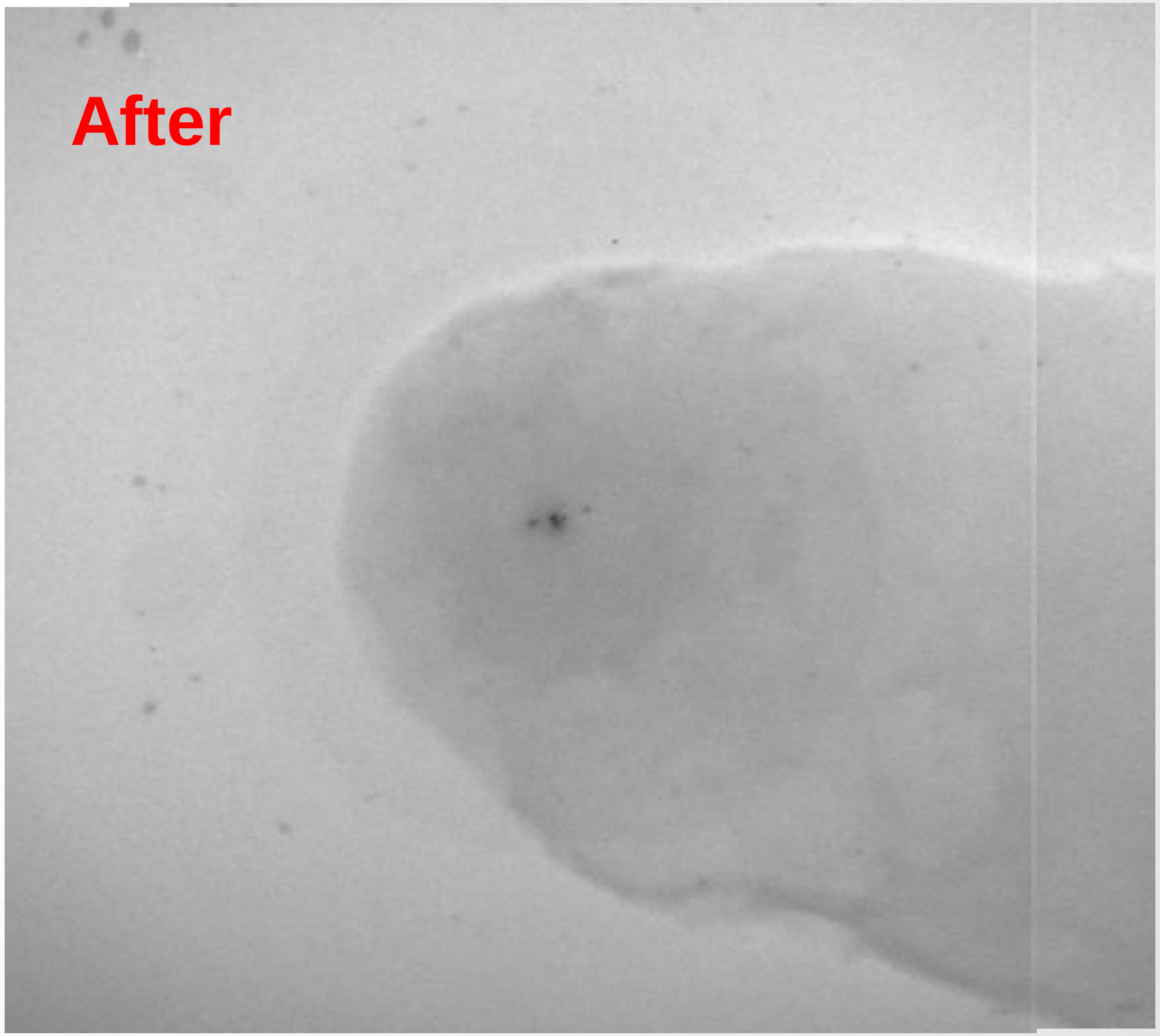
CAMECA atom probe suite



… and observe in TEM mode

Compare to previous state:

- APT needle bias off
- Objective lens field on (constant current mode)



ER-C 2.0 New Building