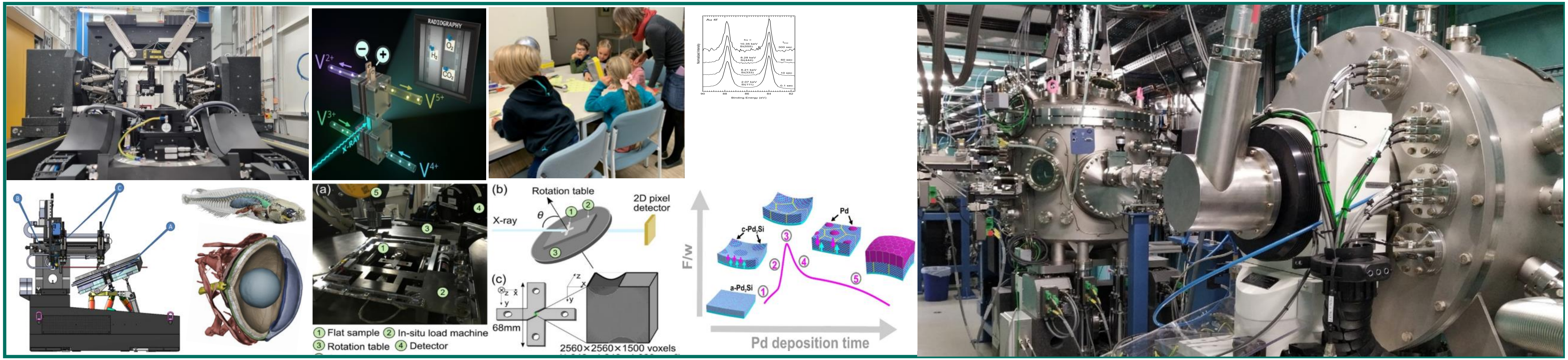
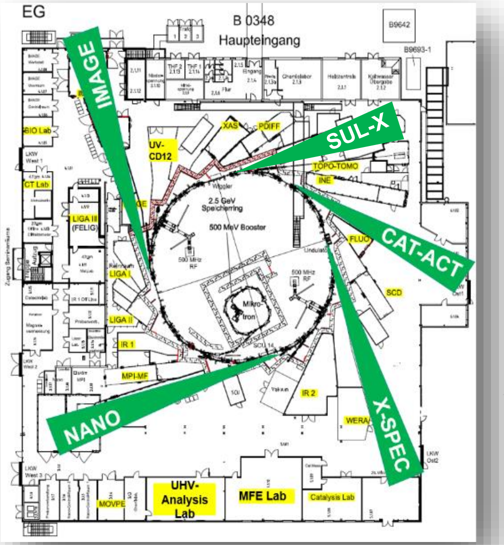
Proposed DTS-ST4 in PoF V – First Draft

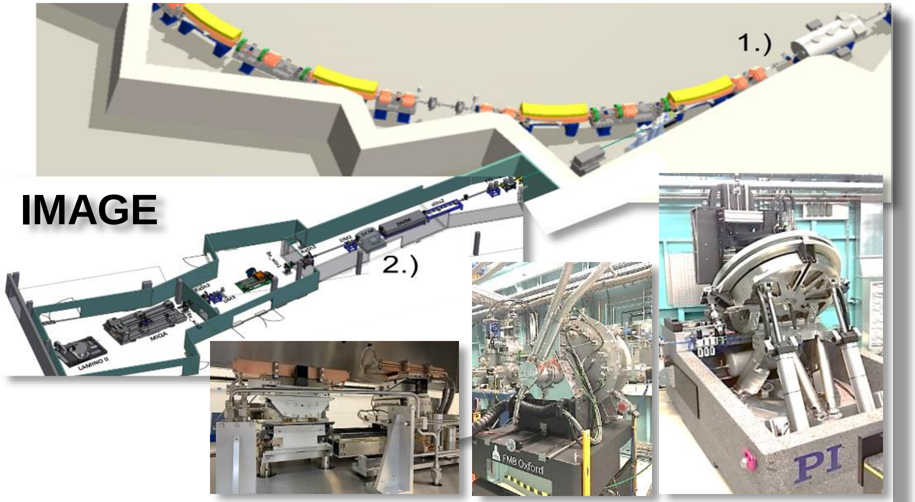
Tilo Baumbach, Clemens Heske

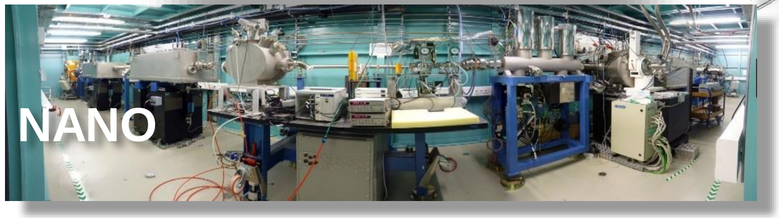


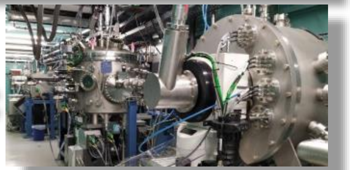
MML@KIT towards PoF V



MML with Unique Instrumentation of its
SPECTROSCOPY, SCATTERING & IMAGING CLUSTERs
at the **KIT Light Source** and beyond







SPECTROSCOPY Cluster, incl.

- X-SPEC, SUL-X, and MFE-Lab
- Next-generation hard and soft X-ray spectrometers (with UNLV)
- *Operando* cells

IMAGING Cluster, incl.

- IMAGE, UFO-station towards Serial CT
- *In situ* LAMINO and X-ray microscopy stations
- Hierarchical, correlated and *in vivo* imaging

SCATTERING Cluster, incl.

- NANO & Heavy duty diffractometers
- Thin-Film-Labs with *in situ* MBE, MOVPE, PLD, sputtering, laser processing etc.

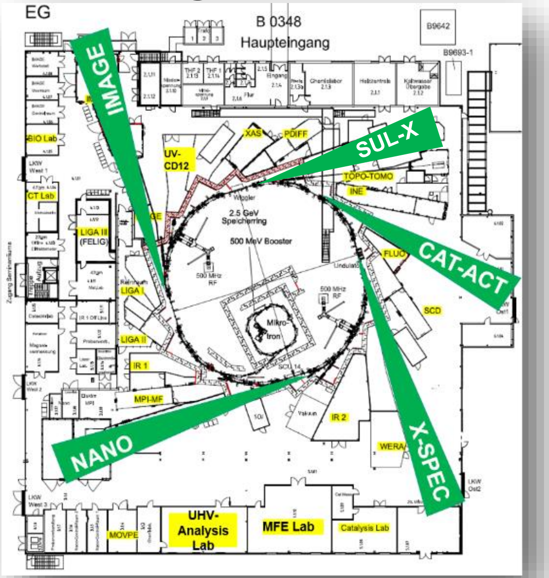
MML@KIT towards PoF V

Photon Science and Synchrotron Radiation Research

enabled by combining the strengths of

- the Beamlines and Labs at the KIT Light Source
- complementary experimental stations at low-emittance photon facilities

KIT Light Source



providing a unique portfolio

- for pioneering method development and fundamental research
- for systematic, large comparative studies
- as a **unique home-court advantage** for KIT Programs and Centers

MML@KIT towards PoF V

Photon Science and Synchrotron Radiation Research

enabled by combining the strengths of

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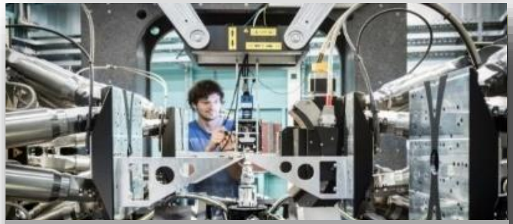
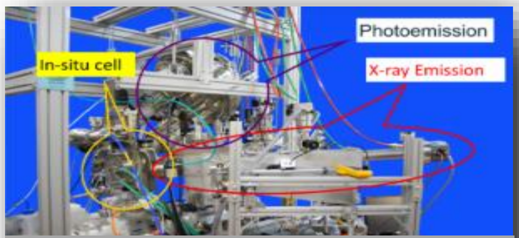
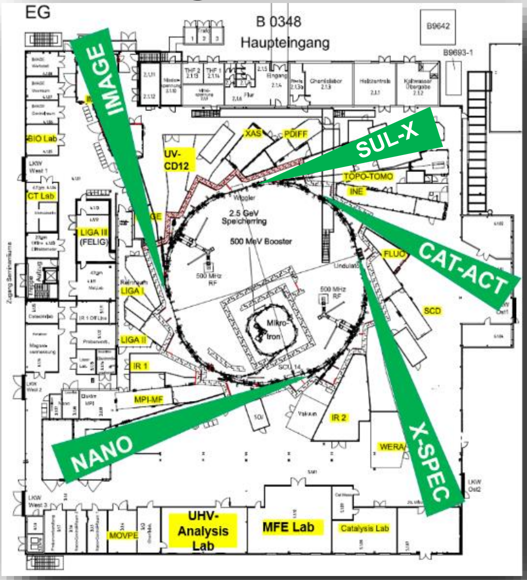
KIT Light Source



HIKA at PETRA III / IV



SALSA at ALS



LAMINO I at ESRF

Surface Science Labs at UNLV

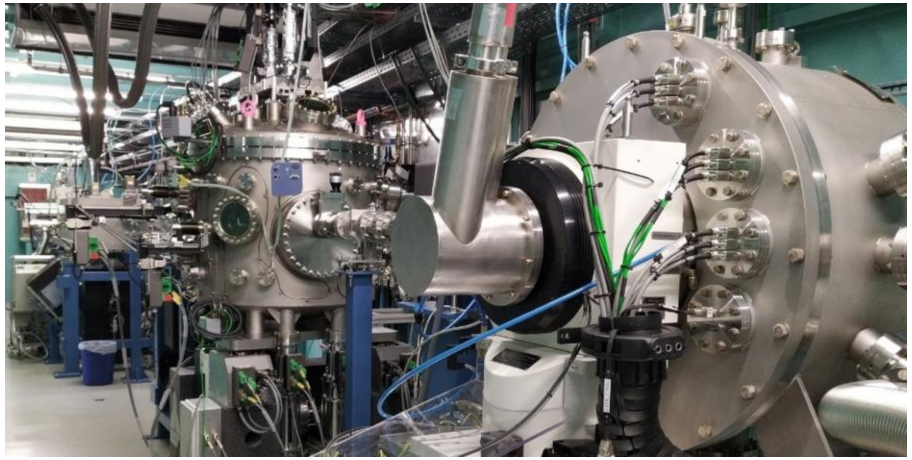
providing a unique portfolio

- for pioneering method development and fundamental research
- for systematic, large comparative studies
- as a **unique home-court advantage** for KIT Programs and Centers

MML@KIT towards PoF V

Method & Instrument Development

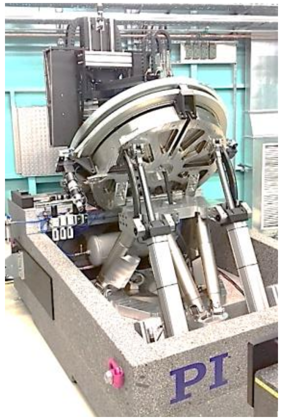
- **Two main thrusts in MML**
  - Development and utilization of **novel characterization approaches and instruments** for the Spectroscopy, Scattering, and Imaging Clusters
  - Develop high-throughput, ***in vacuo*, *in situ*, *in vivo*, *operando*** concepts at large-scale photon facilities as **cross-cutting enabling technologies in MML** and **for other KIT programs** and strategic partners

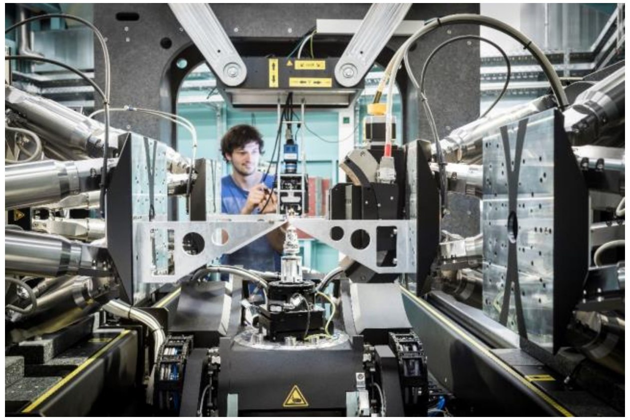


- **Cutting edge methods and instrumentation, in particular at X-SPEC, IMAGE, and soon at HiKA**

→ Worldwide unique combination of soft and hard X-ray spectroscopy for *in situ / operando* applications

→ Worldwide unique CT/Laminography portfolio towards serial tomography and hierarchical *in situ / operando* imaging





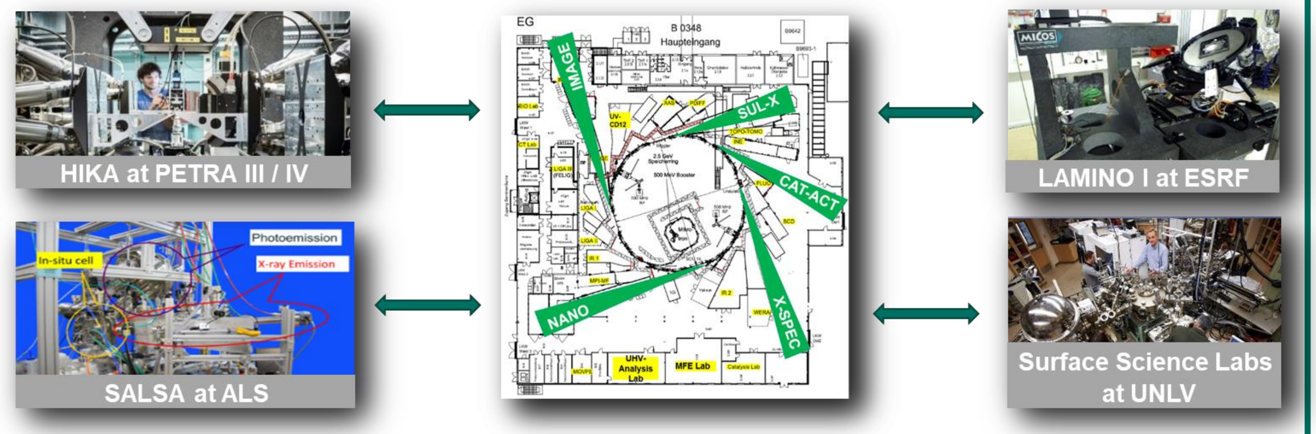
MML@KIT towards PoF V

Cutting-Edge Characterization Methods for

Synchrotron Radiation Research

Cutting-Edge Characterization Methods for

- Biomaterials & bionics, tissues & organoids
- (Bio)Medical diagnostics with compact sources
- Biodiversity & indicator organisms for climate



- Materials & devices in quantum technologies
- Materials & technologies for information
- Energy materials
- Optics & Photonics
- Catalysis

- Artificial intelligence for high-throughput data acquisition
- AI-supported large scale 3D and 4D Image Analysis
- Proprietary and open-source platforms for synchrotron-based scientific data and computing

- Pioneering method development and fundamental research
- Systematic, large comparative studies
- Unique home-court advantage for KIT Programs and Centers

MML@KIT towards PoF V

Initial Situation: PoF IV

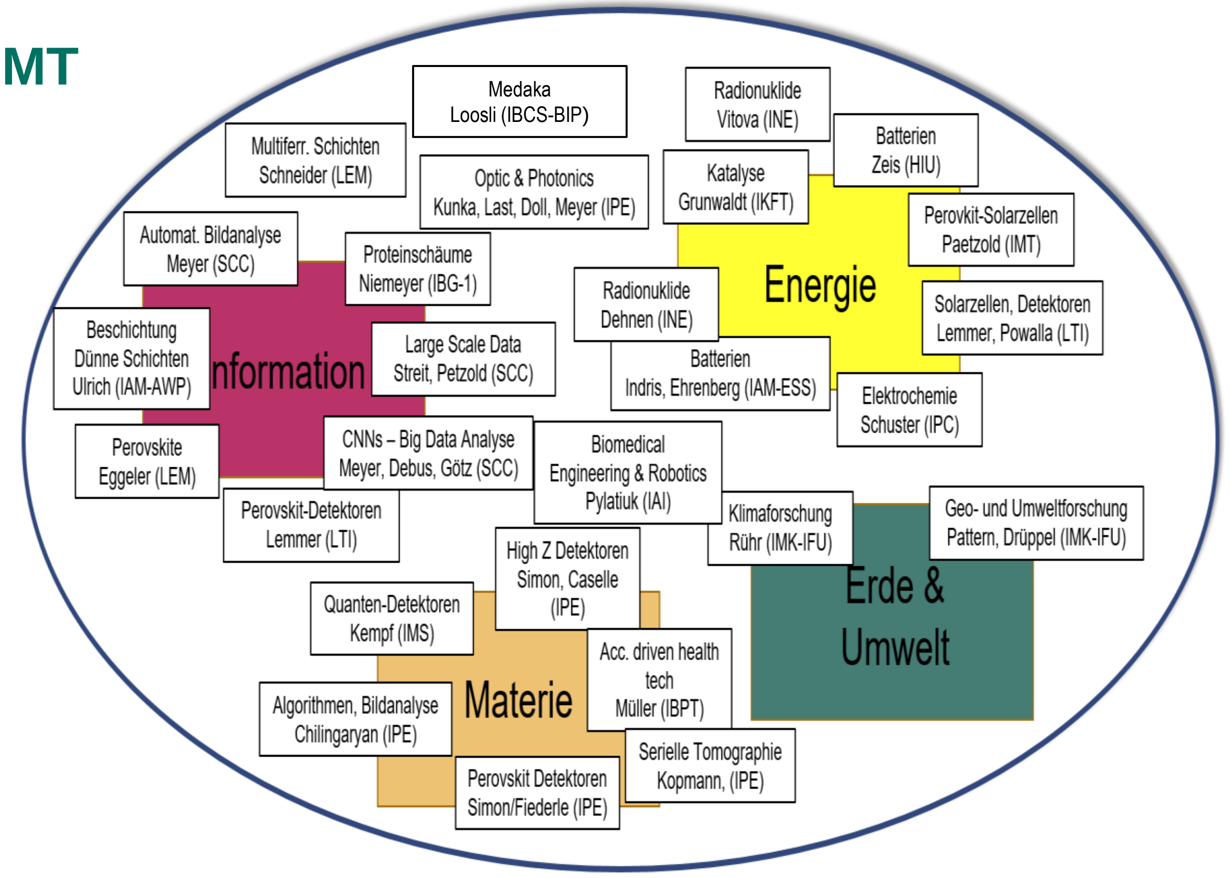
Accelerator Research: Operation of the **KARA** Storage Ring and all accelerator R&D in **Matter - MT**

Research with Synchrotron Radiation at the **KIT Light Source** and beyond:

Matter – MML

- **Operation** of the Imaging, Scattering & Spectroscopy Clusters
- Methodical & instrumental **development**
- Scientific **research** applications, collaborating with leading KIT groups and external partners

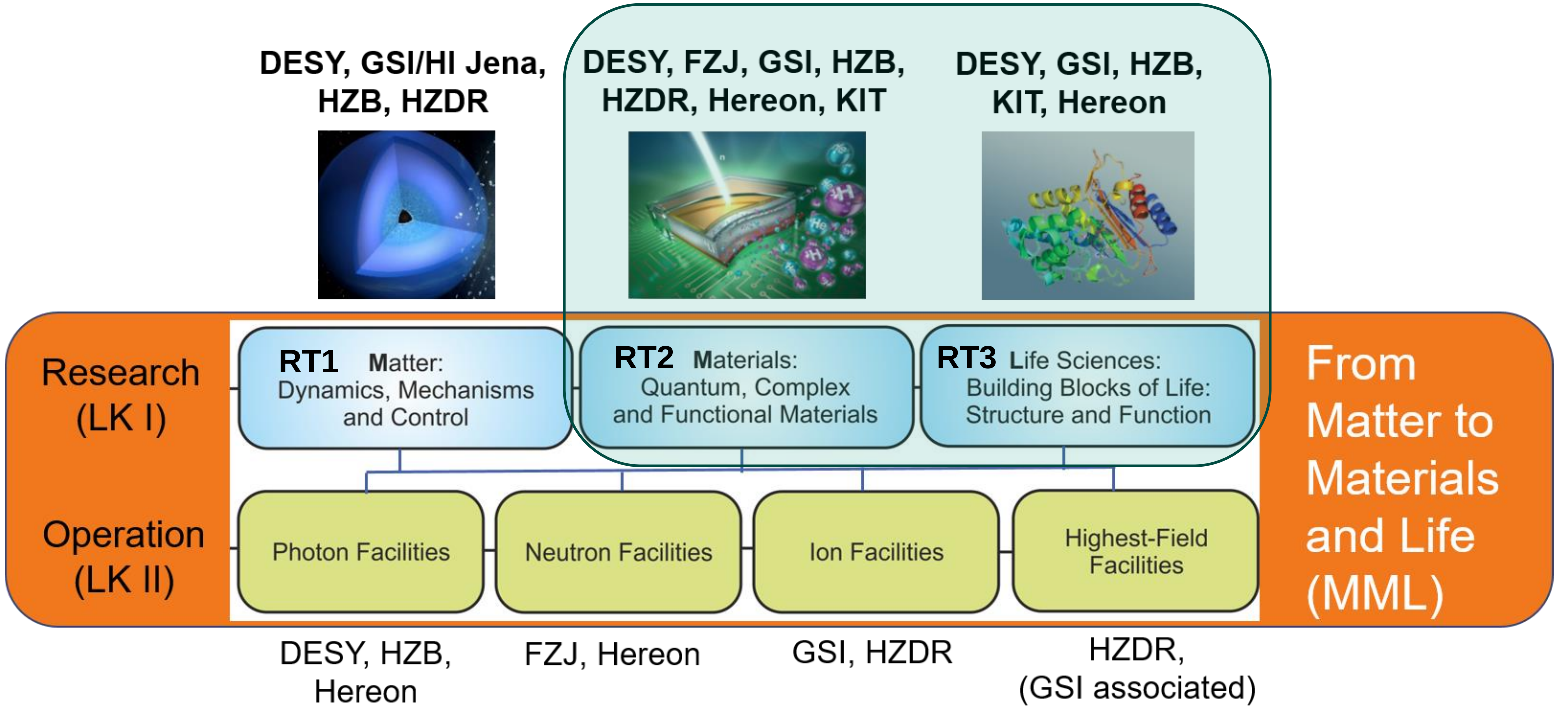
Operation of further beamlines in 4 Programs of the Helmholtz Research Fields Energy (MTET, NUSAFE) and Information (NACIP, MSE)



Examples of KIT@MML collaborations with other Programs

MML research topics PoF V

- Successful restructuring of MML for PoF IV



New in PoF IV

- Transfer of magneto-hydrodynamics (HZDR) from *Energy* to MML
- GSI campus Darmstadt returned to PoF and participates in all 3 MML topics
- Transfer of Biophysics (GSI) from *Health* to MML (from cancer therapy to radiation protection)
- KIT: Operation of the storage ring (KARA) shifted to the MT-Program; Beamline Clusters in MML (LK I)

During PoF IV

- Helmholtz Institute for High Energy Density (HIHED) in Rostock not founded
- Upgrade proposals PETRA IV, BESSY II+/III

- Continuation and sharpening this successful structure in PoF V
  - RT1 (Matter): Creation of a subtopic level
  - RT2 (Materials) and RT3 (Life): Current subtopic structure will be retained

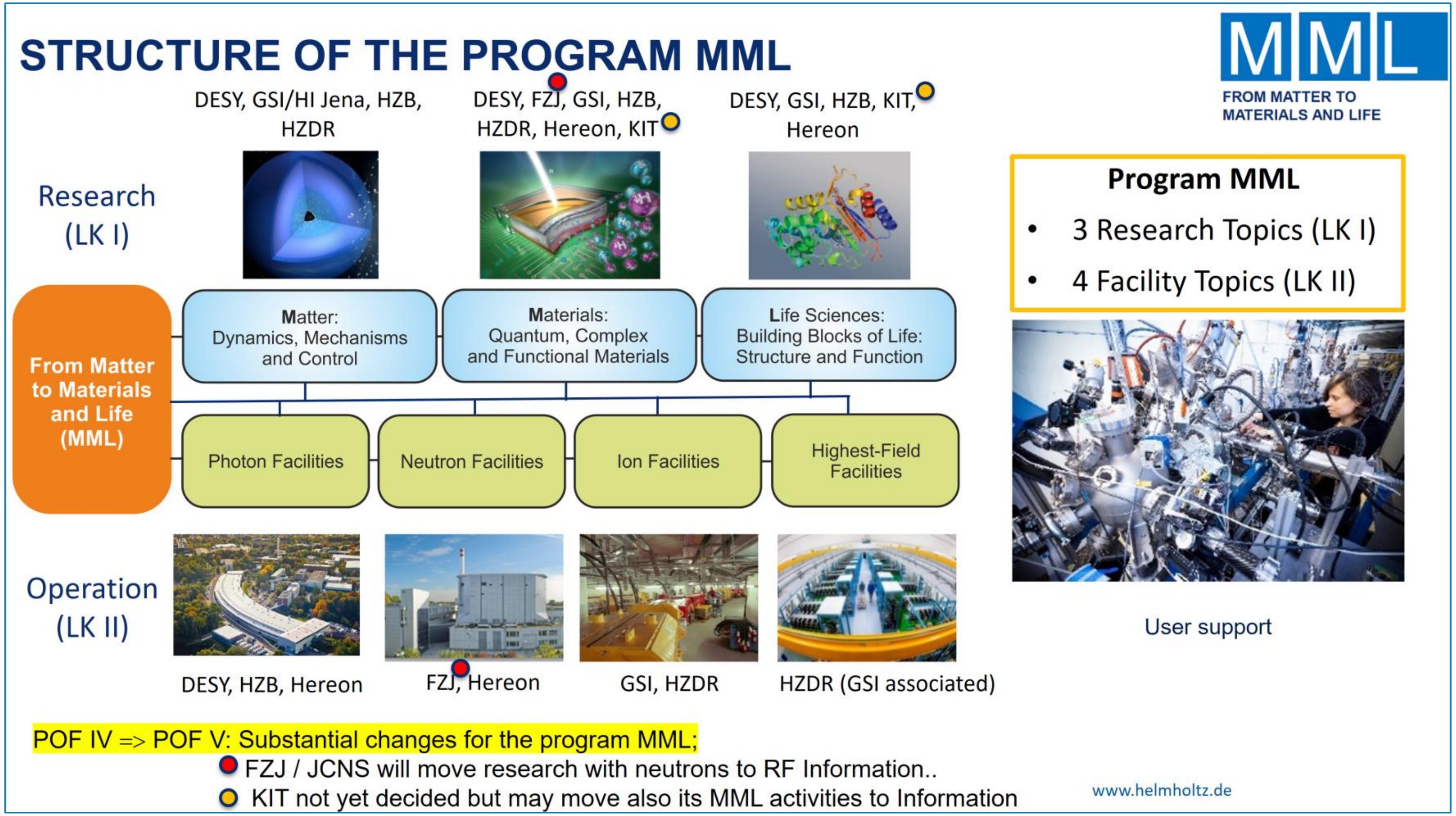
The Vision in PoF V

- Stay at the forefront of the latest synchrotron methods and instruments

- Develop strategies for AI-based automated, high-throughput data acquisition, data analysis, and data management

- Reap the rewards
  - benefit from the **integrated beamline & laboratory infrastructure** at KIT
  - capitalize on our **leading characterization approaches** combining cutting-edge synchrotron radiation and multi-environment sample concepts (*in vacuo*, *in situ*, *in vivo*, *operando*)
  - utilize **the cross-sectional technology portfolio** for networking with other programs and our strategic external partners

MML@KIT towards PoF V



Th. Stöhlker, MML-Presentation, MATTER LA Hamburg, 29.01.2024

LA Matter 26.04.2024: KIT will continue its previous MML activities from the PoF IV funding phase in PoF V, but integrated into other programs

Present Status: Coordination Meetings with Information (P3) and with MT in Matter

The Vision in PoF V

- Stay at the forefront of the latest synchrotron methods and instruments

- Develop strategies for AI-based automated, high-throughput data acquisition, data analysis, and data management

- Reap the rewards
  - Characterization of **real-world materials, devices, and processes** related to **energy**, **information & mobility** technologies
  - **AI-driven high-throughput** imaging and analysis for **large-scale comparative morphological studies** (materials & devices, biomaterials & tissues)

Detector Technology and Systems (DTS)

ST1 — Sensing and Detecting Technologies

- Sensors
- Electrical and Photonic Integrated Circuits (ASICs) and on-detector Intelligence
- 3D and Interposer Interconnection & Packaging

ST2 — Quantum Technologies

- Quantum Sensors and Production Technologies
- Scalable Readout for Superconducting Quantum Devices

ST3 — System Technologies and Applications

- Detector System Concepts & Demonstrators in Research Field "*Matter*" and beyond
- Intelligent Data Acquisition (DAQ) and Real-time Computing
- Novel Engineering Techniques, Advanced Materials, Cooling

Research infrastructures

- Interconnect and Packaging Facilities
- Quantum Sensor Production Facilities
- Detector Test Beams
- Assembly Facilities

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ST4 Multidimensional Imaging Techniques

- Spectroscopy
- Tomography

Research infrastructures

- Interconnect and Packaging Facilities
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Detector Technology and Systems (DTS)

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ST4 Multidimensional Method Development and Applications

- Imaging, Spectroscopy, Scattering – Methods and Systems
- High-throughput, *in situ, in vivo, operando* Applications
- AI-Supported Multidimensional Data Analysis

DetecTABL: Research Infrastructures for Detector Development, Test and Application Beamlines & Labs)

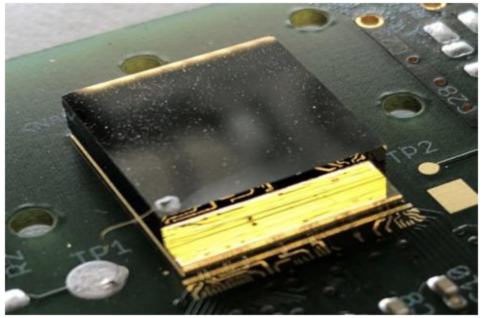
- Interconnect and Packaging Facilities
- Quantum Sensor Production Facilities
- Assembly Facilities
- Test and Application Beamlines & Labs

Contributions to ST1-3

- **High-Z detectors based on CdZnTe/GaAs (collaboration with U-Frei …)**

  Goal: Development of CdZnTe/GaAs sensor technologies from crystal growth towards detector production:

  - **Growth of CdZnTe**
    - Partner in the OptiBeams proposal in the HORIZON-INFRA-2024-TECH-01-01 call - coordinated by DESY Flash
    - Cooperation with PSI for the growth of 75 mm diameter CdZnTe crystals
  - **Technology for pixel detectors**
    - Work on flip-chip bonding in cooperation with IPE
  - **Production of TPX3 (TPX4) and Eiger (PSI) detectors**
    - Production of detector modules with different thicknesses from 0.5 up to 3 mm for covering X-ray energies from 30 keV up to 300 keV
    - Development of large area detectors
- **Application of CdZnTe pixel detectors**
  - **Application at PETRA and XFEL**



Starting point BMBF Project: 05K22VFBA - PERODET

U-Frei – MML – MT Collaboration

Contributions to ST1-3

- **Research on Perovskites**
  - New class of semiconductors: Perovskite semiconductors (promising photovoltaic materials)
  - Perovskite materials are promising as an alternative to conventional high-Z semiconductors regarding availability, toxicity and low production costs compared to conventional high-Z materials like CdZnTe or GaAs
- **Crystal growth from solution and from the melt of $CsAgBiBr_6$ and $CsPbBr_3$ materials**
- **Intensive material characterization**
  - (topography, XDL, SIMS, I-V, DLTS, ...)
- **Detector technology:**
  - Development of planar technology (surface preparation, contacts, bonding)
- **Development of a growth process:**
  - Deposition directly on electronics (solution, 3D printing, ...)
- **Production of detectors:**
  - using Timepix3 and Timepix4 with High-Z sensor based on perovskites semiconductors

Starting point BMBF Project: 05K22VFBA - PERODET

U-Frei – MML – MT Collaboration

ST4 Multidimensional Method Development and Applications

- **Imaging, Spectroscopy, Scattering – Methods and Systems**
- **High-throughput, *in situ, in vivo, operando* Applications**
- **AI-Supported Multidimensional Data Analysis**

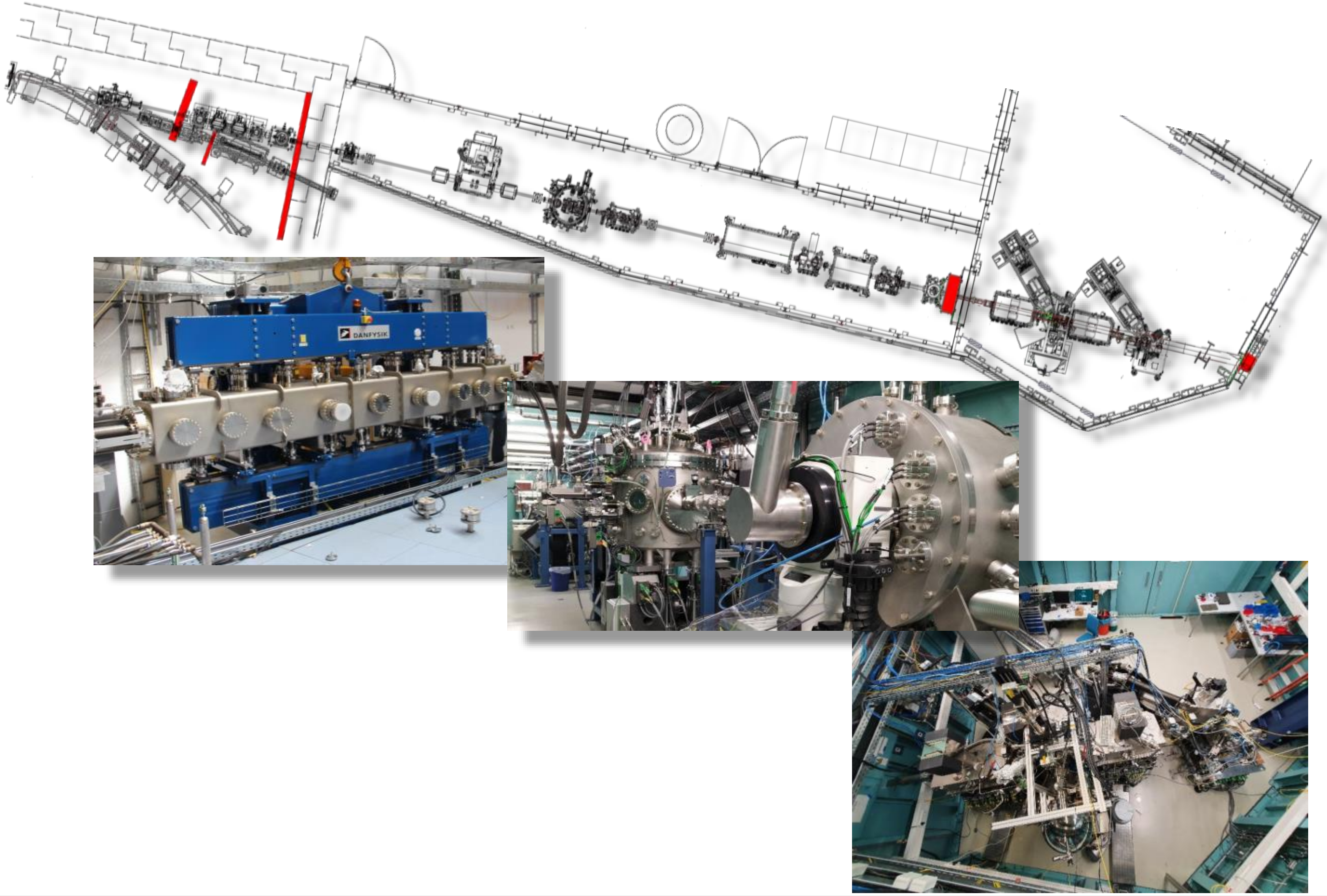
Imaging, Spectroscopy, Scattering

Methods and Systems

Karlsruher Institut für Technologie

Example: The X-SPEC Beamline at the KIT Light Source

- 70 eV – 15 keV!
- XES/RIXS, XAS, (HAX)PES
- *Two undulators (soft, hard),*
  two monochromators (soft, hard),
  two endstations (UHV and ambient)
- Next-generation soft X-ray spectrometers
- *Operando* cells

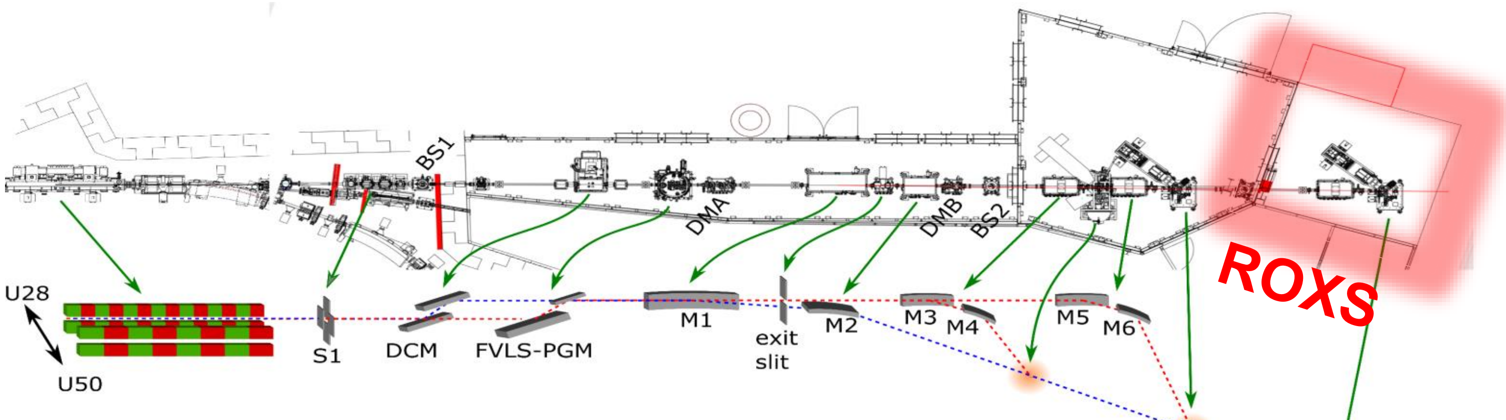


L. Weinhardt *et al.* JSR **28**, 609 (2021)

X-ray spectroscopy of nuclear materials

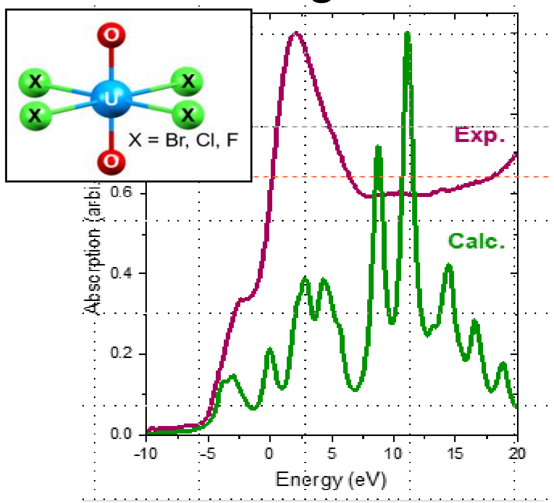
- **Stay at the forefront of the latest synchrotron methods and instruments**

  - High-activity samples
  - Electronic structure
  - Actinide-Ligand bonding
  - Development of *Extremely Fast RIXS Maps (EFRM)*

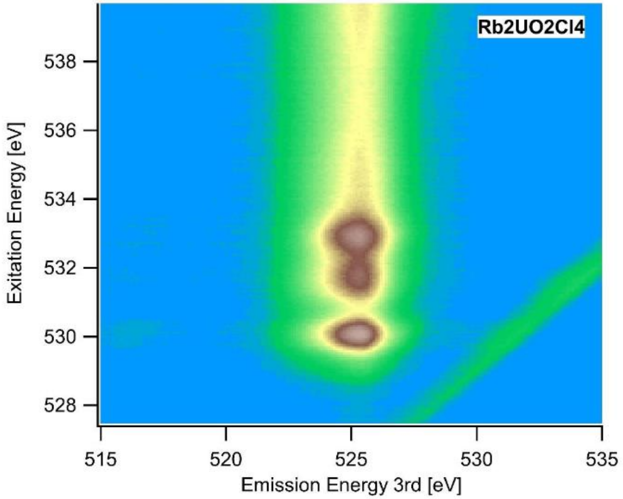


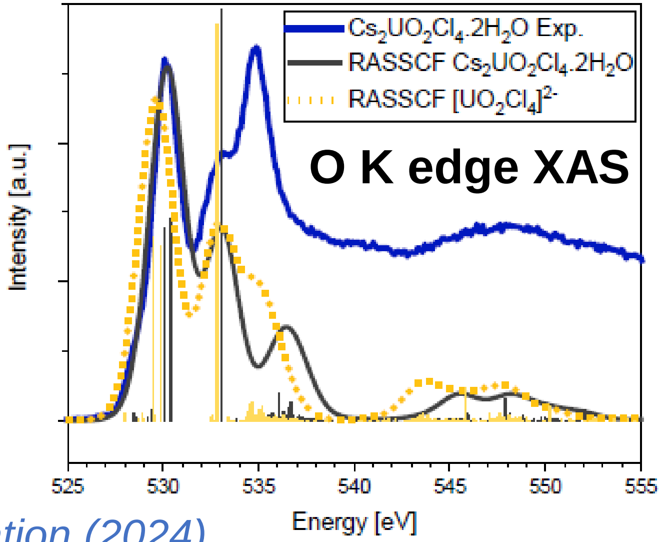
The planned ROXS station @ X-SPEC for PoF V & SFB Bright Light (**R**adionuclide materials **O**bserved with soft **X**-ray **S**pectroscopy)

F K edge XAS



Neill et al., in preparation (2024)

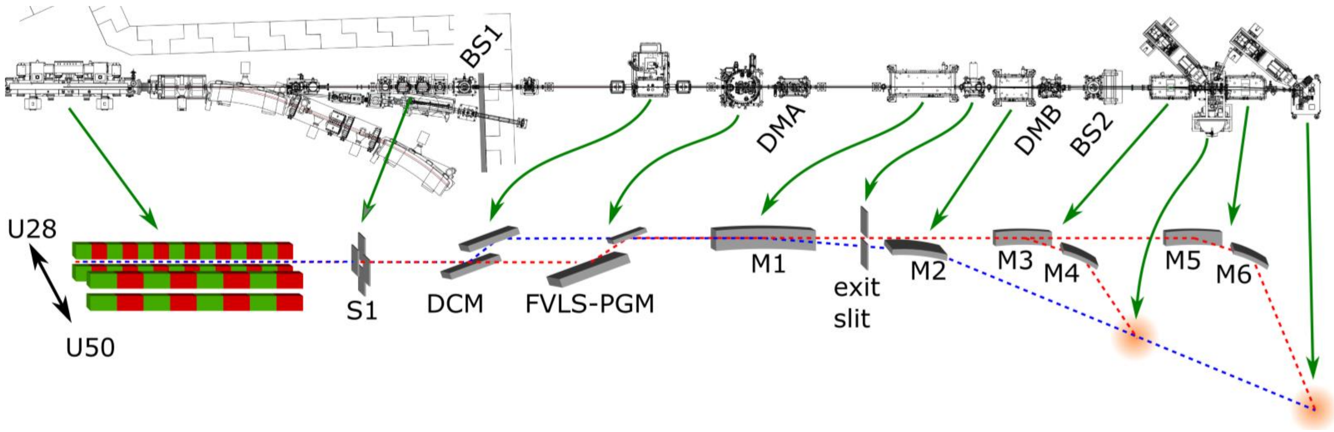




Müller et al., in preparation (2024)

High-throughput, *in situ, in vivo, operando* Applications

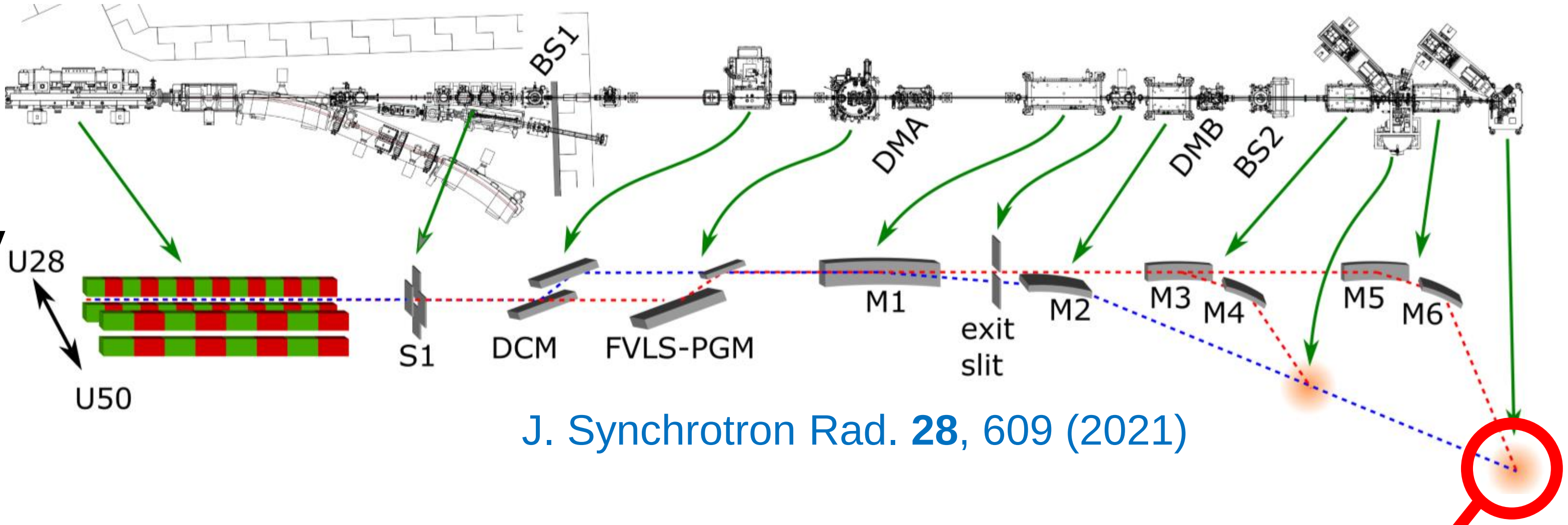
Example: The X-SPEC Beamline



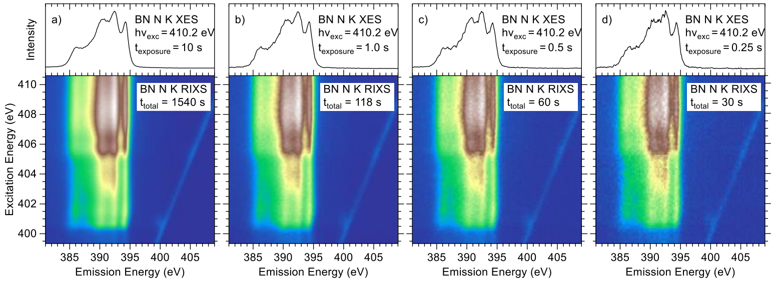
- **High dose efficiency short exposure times towards *operando* soft x-ray detection systems**
- **Combination of powerful optics (e.g., gratings) and pixel array detectors**
- **On-the-fly component integration from source (undulator), monochromator, and focusing optics, to sample, analyzer optics, and soft x-ray photon detection systems**

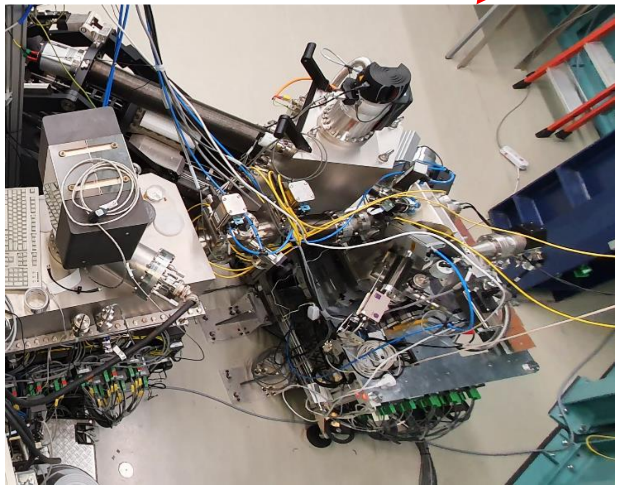
Rapid resonant inelastic soft x-ray scattering (rRIXS) maps at X-SPEC

- Novel high transmission soft x-ray spectrometer detection system
- Reduces time for a RIXS map from tens of minutes to tens of seconds



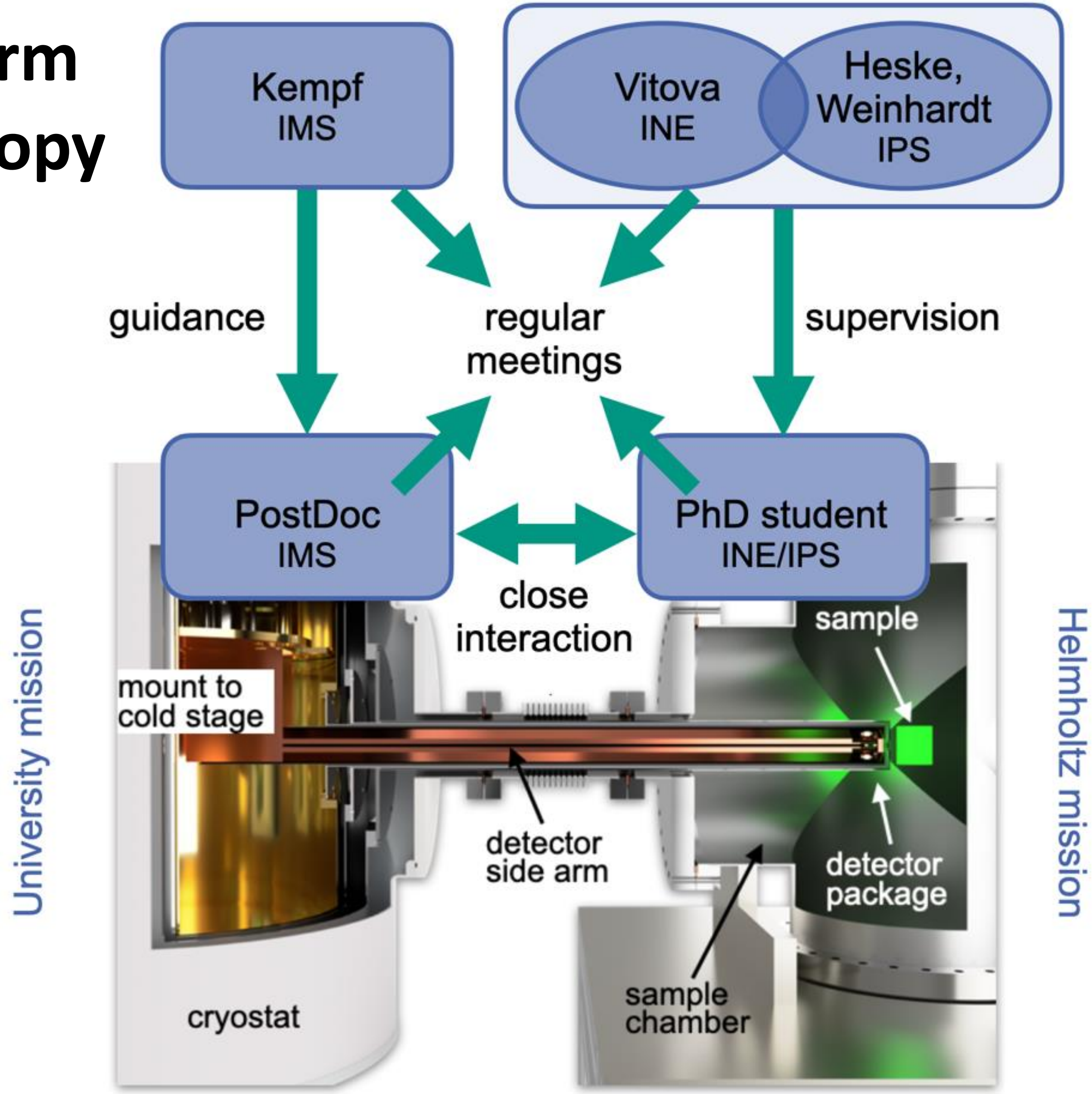
J. Synchrotron Rad. **28**, 609 (2021)





QUASY - Quantum Sensor Platform for Synchrotron X-ray Spectroscopy

- **Magnetic Microcalorimeters – MMCs**
- For various beamlines in the Spectroscopy Cluster
- Energy resolution orders of magnitude better than for conventional EDX detectors

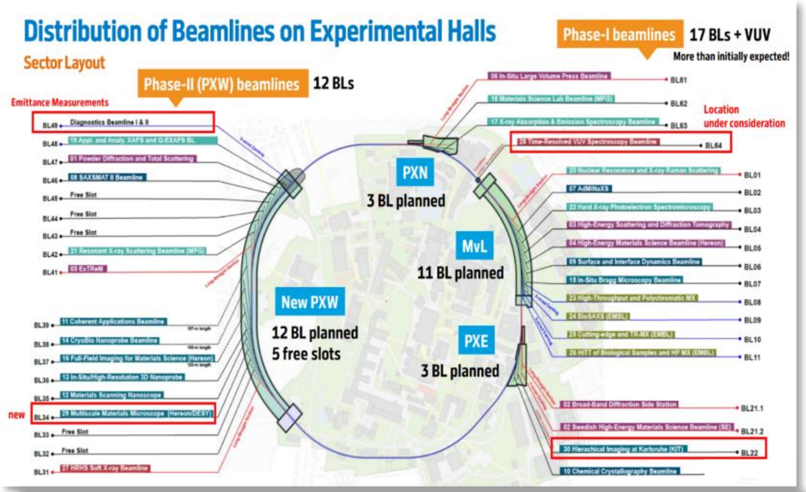


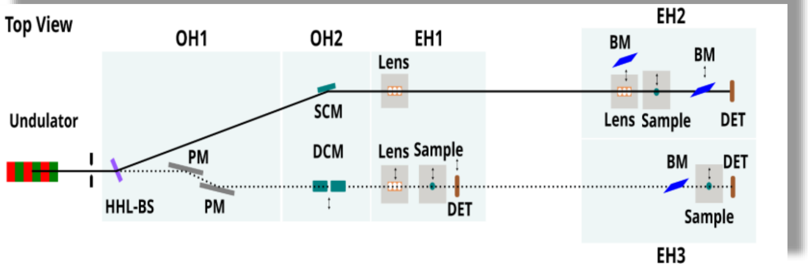
Collaboration with S. Kempf (IMS), T. Vitova (INE)

Imaging, Spectroscopy, Scattering
Methods and Systems

Example: The HIKA Beamline at PETRA III / IV

Hierarchical Imaging and Serial Tomography Methods





PETRA IV Beamline Portfolio

Beamline	Techniques	Energy range
01 Powder Diffraction and Total Scattering	PXRD, TS	15 - 80 keV
02 Swedish High-Energy Mater. Sci. Beamline (SE)	WAXS/3DXRD, SAXS, Imaging	38 - 150 keV
03 High-Energy Scatt. and Diff. Tomography		40 - 120 keV
04 High-Energy Mater. Sci. Beamline (HEREON)		30 - 200 keV
05 ExTReM	XRD, PDF, PCI, CDI	25 - 58 keV
06 *In-situ* Large Volume Press Beamline	AD-/ED-XRD, PXRD, A/PCI	40 - 130 keV
07 AdMiNaXS Beamline	GI/T/SAXS/WAXS, CoGISAXS	7 - 30 keV
08 SAXSMAT II Beamline		5 - 60 keV
09 Surface and Interface Dynamics Beamline		8 - 40 keV
10 Chemical Crystallography Beamline	PXRD, Crystallography	15 - 50 keV
11 Coherent Applications Beamline	XPCS, XCCA, Holotomo.	7 - 25 keV
12 Materials Scanning Nanoscope	XRF, XRD, XBIC, XEOL, Ptycho.	2.4 - 50 keV
13 In-Situ/High-Resolution 3D Nanoprobe	XRF, XRD, XBIC, XANES, Ptycho.	4 - 100 keV
14 CryoBio Nanoprobe Beamline		17 - 60 keV
15 *In-situ* Bragg Microscopy Beamline		7 - 40 keV
16 Full-Field Imaging for Mater. Sci. (HEREON)	Tomography, Radiography	10 - 200 keV
17 Multiscale Mater. Microscope (DESY/HEREON)	Holotomo., Radiography	60 - 200 keV
18 HIKA Beamline (KIT)	Tomography, Laminography	10 - 60 keV
19 X-ray Absorption & Emission Spec. Beamline	HR-XES/XAS, TR-XES/XAS	4 - 25 keV
20 Materials Science Lab Bea…	… Tomography	2 - 100 keV
21 Applied Analytical XAFS and Q-EXAFS Beamline		4 - 45 keV
22 Nuclear Resonance and X-ray Raman Scattering		6.5 - 73 keV
23 Resonant…		2.4 - 14 keV
24 Hard X-ray Photoelectron Spectromicroscopy	HAXPES(…), CDI	2.4 - 15 keV
25 High-Thru. MX	MX, SSX	6 - 30 keV
26 BioSAXS Beamline…		6 - 20 keV
27 High Performance and Microfocus MX (EMBL)	SSX, …	5 - 30 keV
28 Bio Diffraction and Imaging (EMBL)	HT-MX, HiTT	6 - 30 keV
29 HRHS Soft X-ray…		0.25 - 4 keV
30 Time-Resolved VUV Spectroscopy Beamline		…04 - 0.04 keV

High-Energy Beamlines

Scattering and Diffraction

Imaging and Coherence

Spectroscopy Beamlines

MX Beamlines

Soft and VUV Beamlines

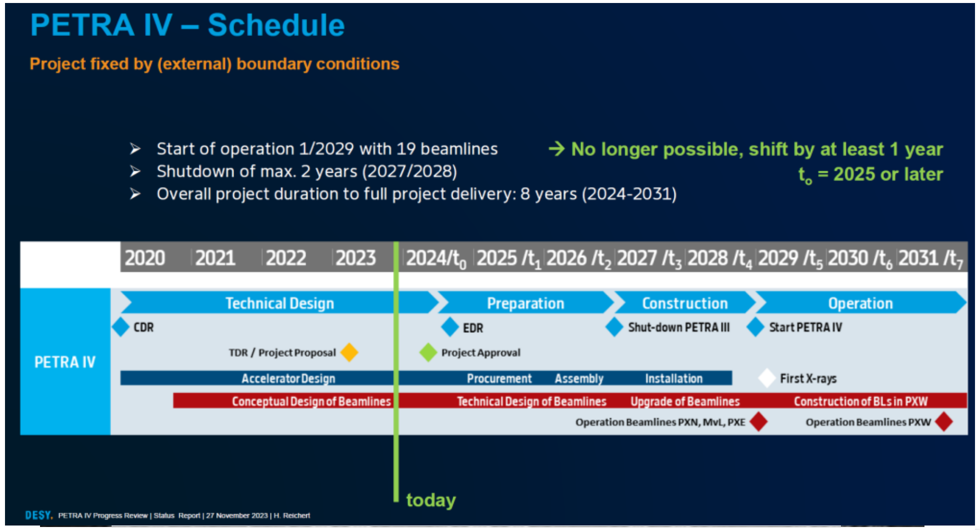
BL-22 – HIKA:
Hierarchical Imaging and Serial Tomography Karlsruhe Beamline

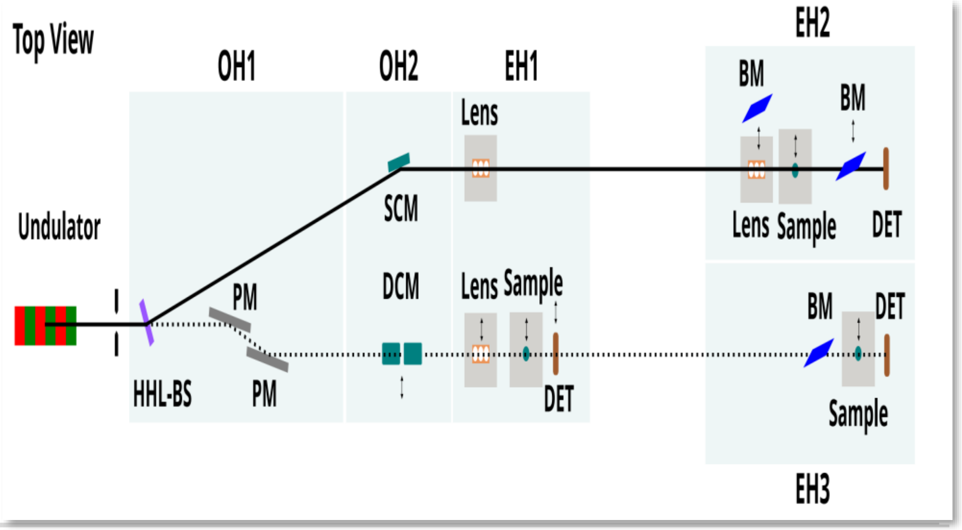
Imaging, Spectroscopy, Scattering

Methods and Systems

BL-22 - Hierarchical Imaging and Serial Tomography Karlsruhe (HIKA) Beamline at PETRA IV

Transfer of the X-ray Microscopy MIQA to Hamburg	Q1/2021
Start of the HIKA construction	Q4/2021
Experimental hutch, preparation and control hutches finalized	Q2/2023
First beam in the hutch	Q3/2023
Implementation of parallel beam CT modes	Q4/2023
Implementation of X-ray microscopy modes	Q4/2024
Implementation of dose-efficient and hierarchical imaging	Q4/2025
Serial CT via BMBF ErUM SMARTMorph; KI-Morph; KI4D4E	Q4/2025
HIKA Adaption & Extension for PETRA IV	2027-31

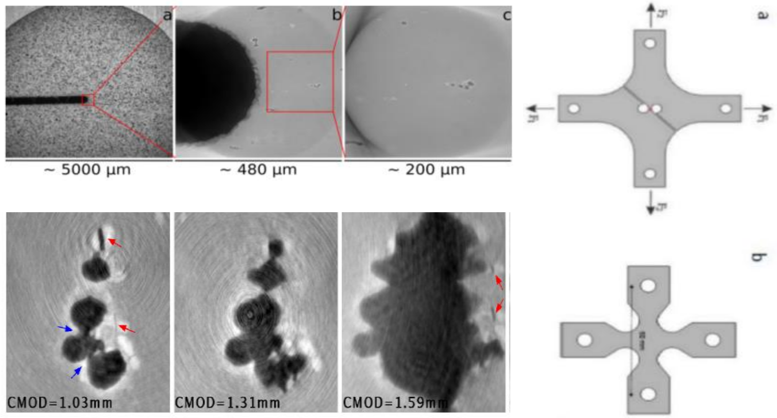




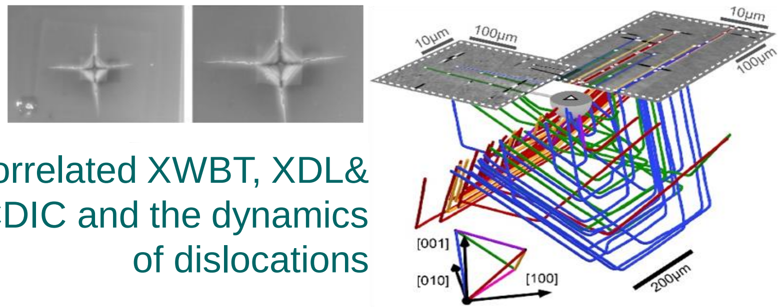
Imaging, Spectroscopy, Scattering
Methods and Systems

Unique portfolio for morphological *full-field* imaging

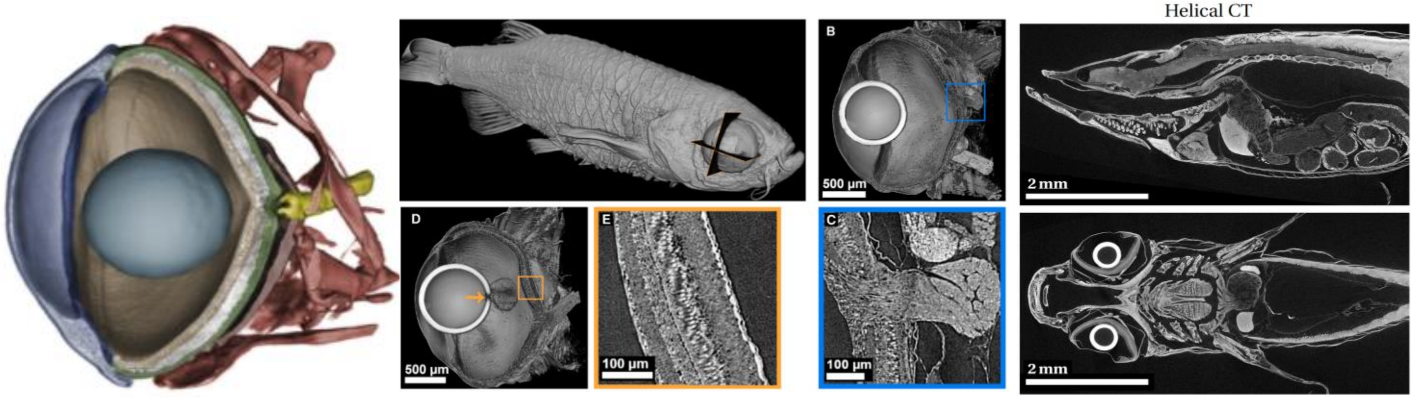
- micro **tomography** & **laminography** → 3D morphology
- high-throughput → large **comparative** studies
- *operando, in situ* and *in vivo* imaging → 4D morpho**dynamics** …
- combined BMI, parallel beam imaging and X-ray microcopy
  → multiscale and **hierarchical** X-ray imaging
- multiple X-ray contrasts, light microscopy → **correlated** imaging



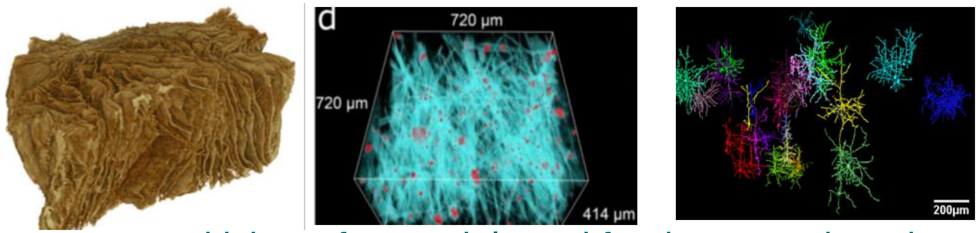
Hierarchical laminography under biaxial load



Correlated XWBT, XDL& CDIC and the dynamics of dislocations



High-throughput and hierarchical tomography of model organisms



Dose-sensitivity soft materials and for tissue engineering

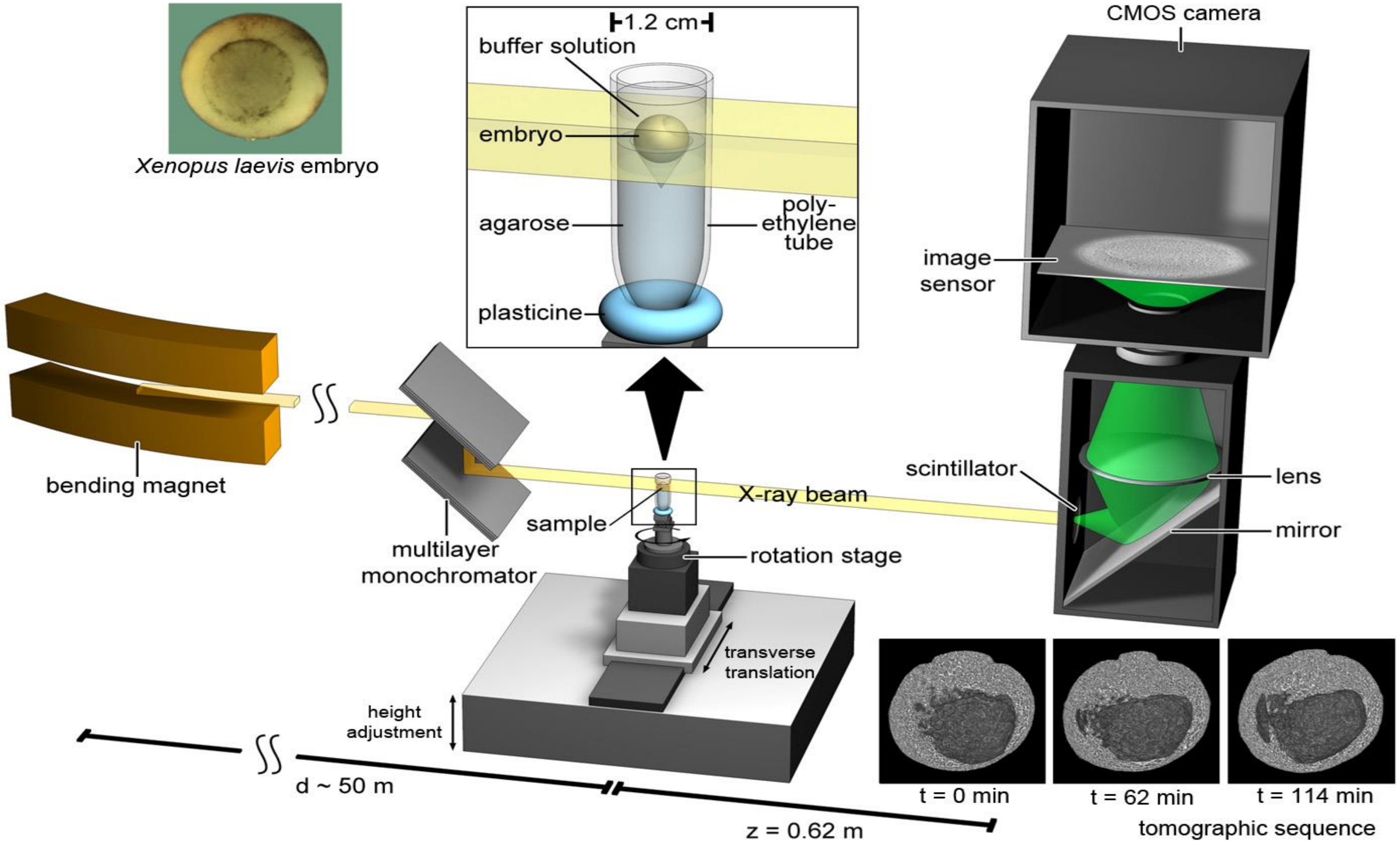
High-throughput, *in situ, in vivo, operando* Applications

Example: The Imaging Cluster

Detector System integration, e.g.,

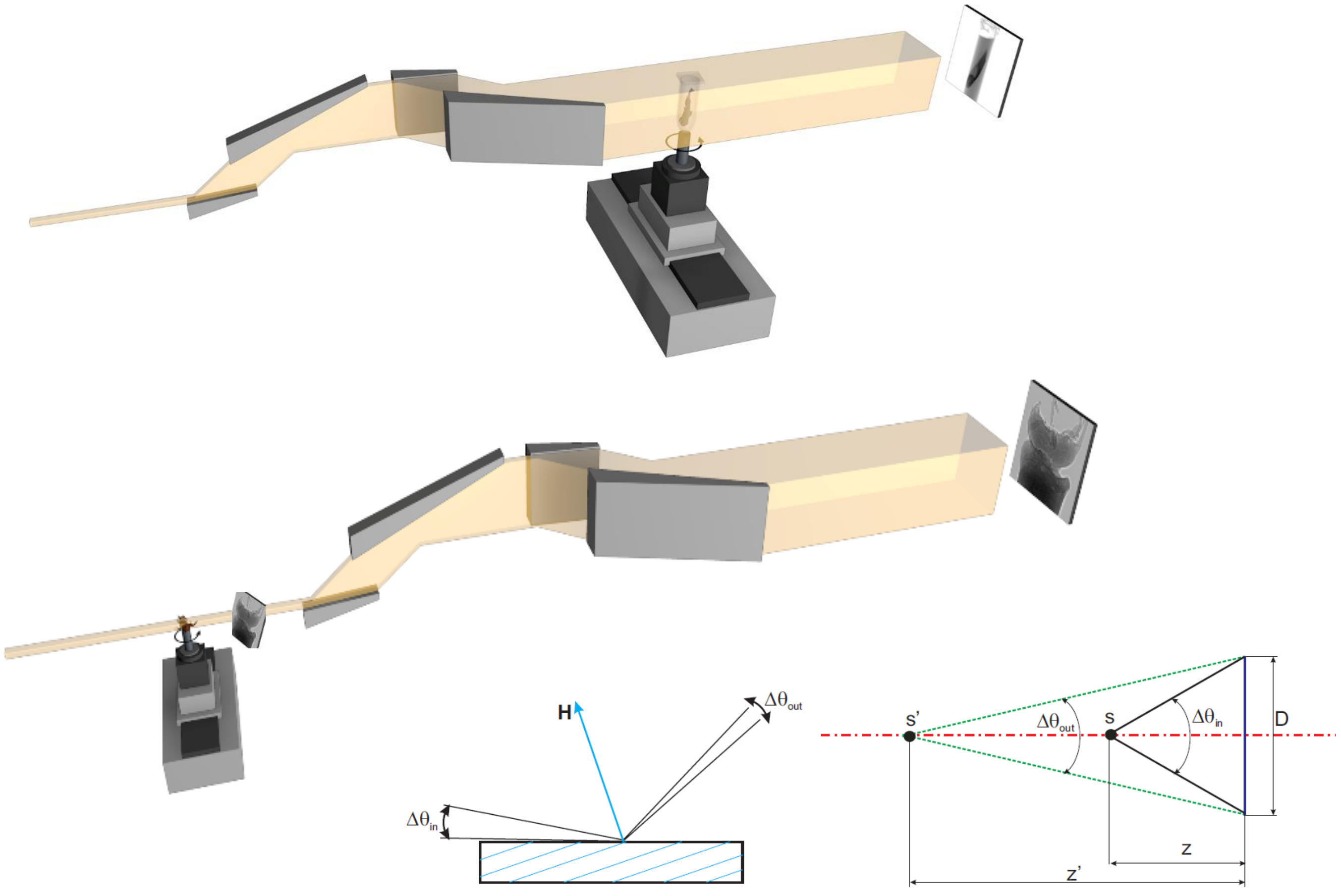
- **SPCDs combined with Bragg-Magnifiers for µm-resolved imaging**
  → Dose-efficiency, noise suppression, higher contrast at 1µm resolution
- **Propagation based imaging with km-long beamlines by combining Bragg-Demagnifier Technology and low Z and high Z SPCDs → drastic contrast amplification → dose-efficient phase contrast at large fields of view**
- **Ultrafast up to MHz Imaging**
- **Spectroscopic Imaging**

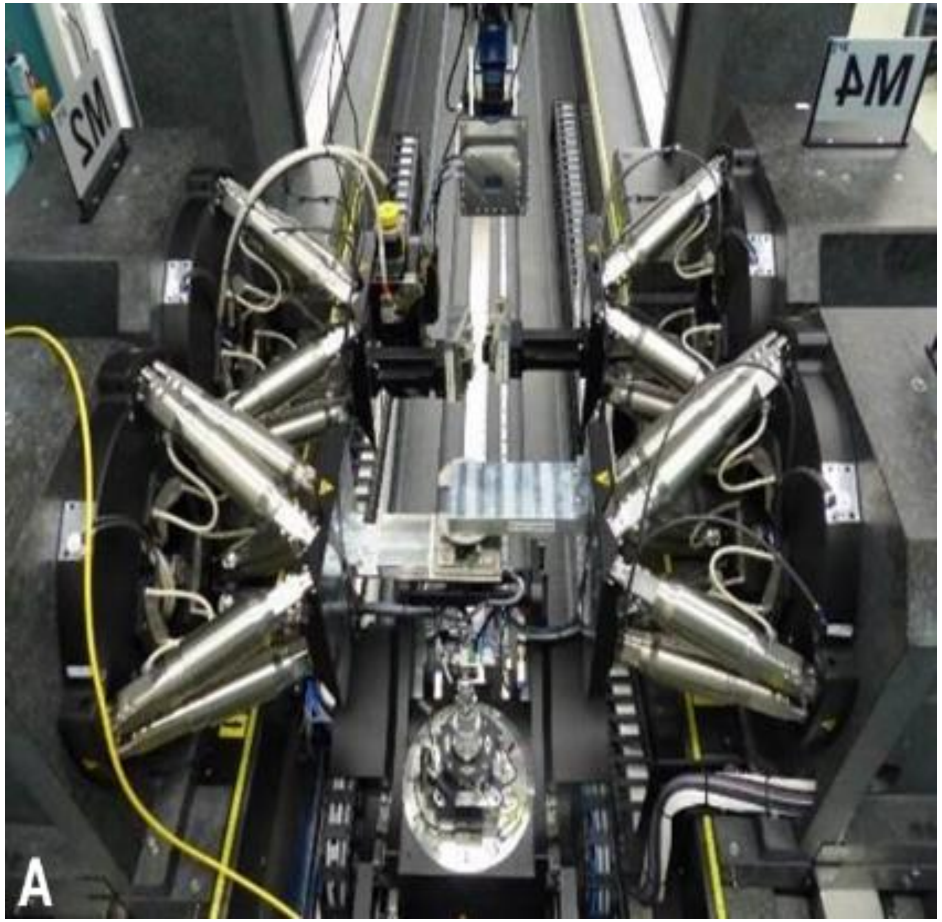
In Vivo Tomography on the Cellular Level



Moosmann et al. NATURE 2013, NATURE Protocols, 2014

Combination of Single Photon Counting Pixel Array Detectors and Magnifying Coherent X-ray Optics

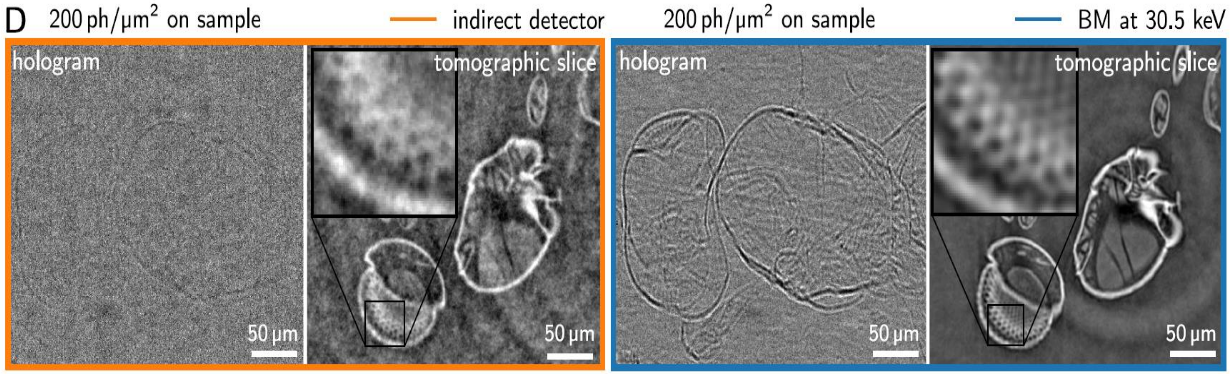


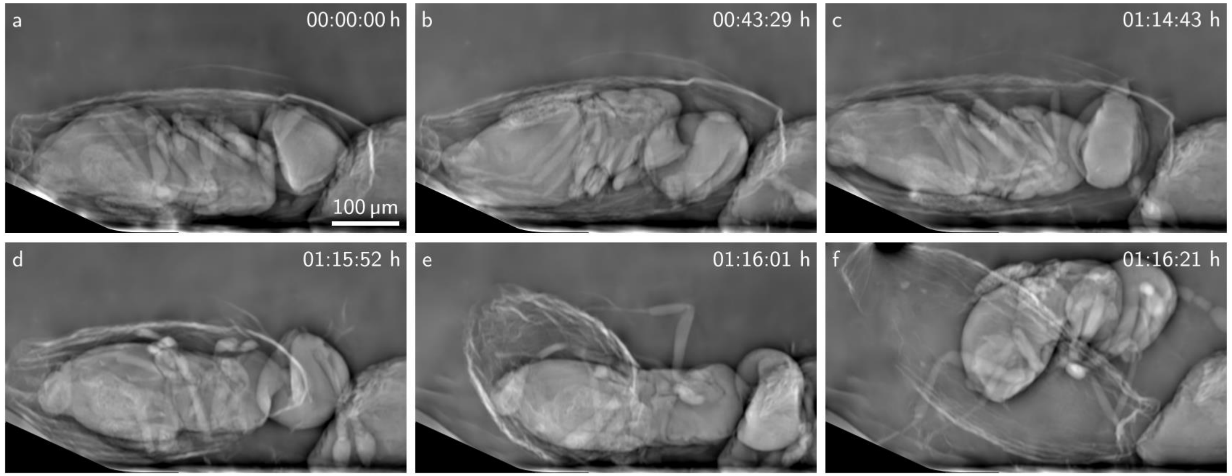


µm-resolution imaging with SPCDs

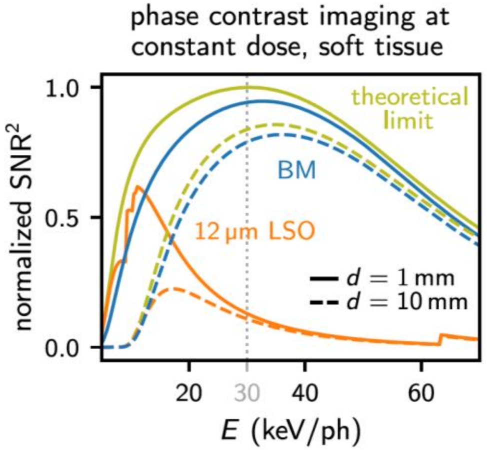
Bragg Magnifier optics as image magnifier combined to GaAs Lambda Detector

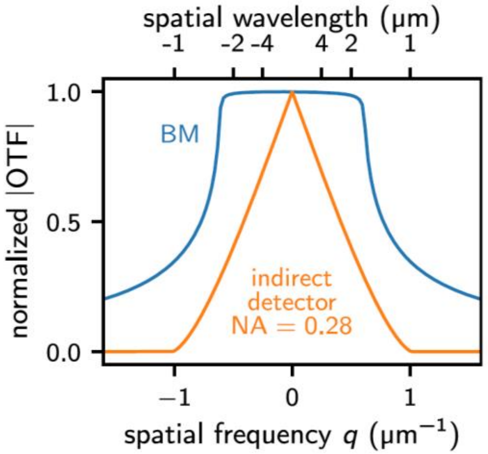
- Magnification up to 200, highly dose-efficient (>93%), up to *in vivo* imaging for µm resolution

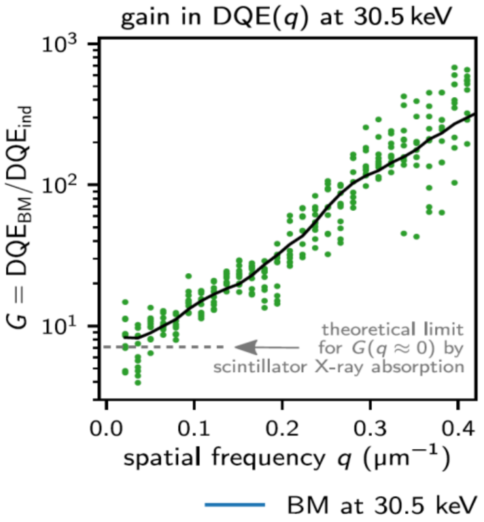




Trichogramma wasp biting through a parasitized moth egg shell







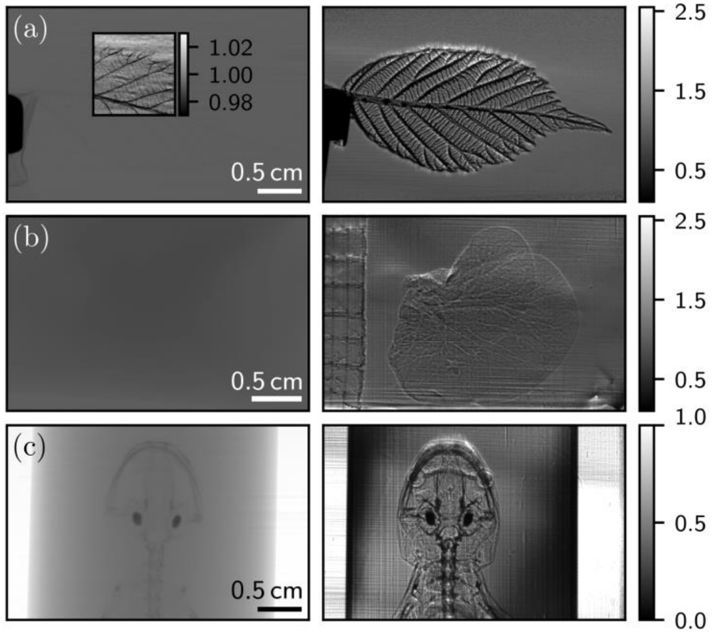
At high spatial frequencies:

gain in DQE about 2 orders of magnitude

R. Spiecker et al., Optica 2023

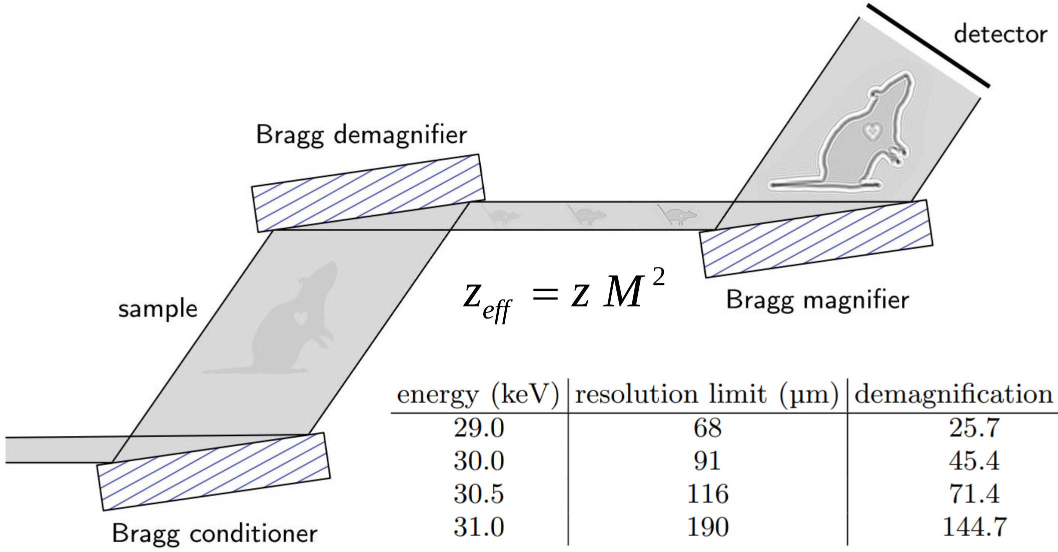
SPCDs combined with coherent X-ray optics realizing kilometers long beamlines

Dose efficient contrast enhancement



blackberry leaf, mouse liver lobe and salamander in ethanol

Proof of principle experiments at KIT`s HIKA station @PETRA III



energy (keV)	resolution limit (µm)	demagnification M	gain factor M^2
29.0	68	25.7	660
30.0	91	45.4	2061
30.5	116	71.4	5098
31.0	190	144.7	20938

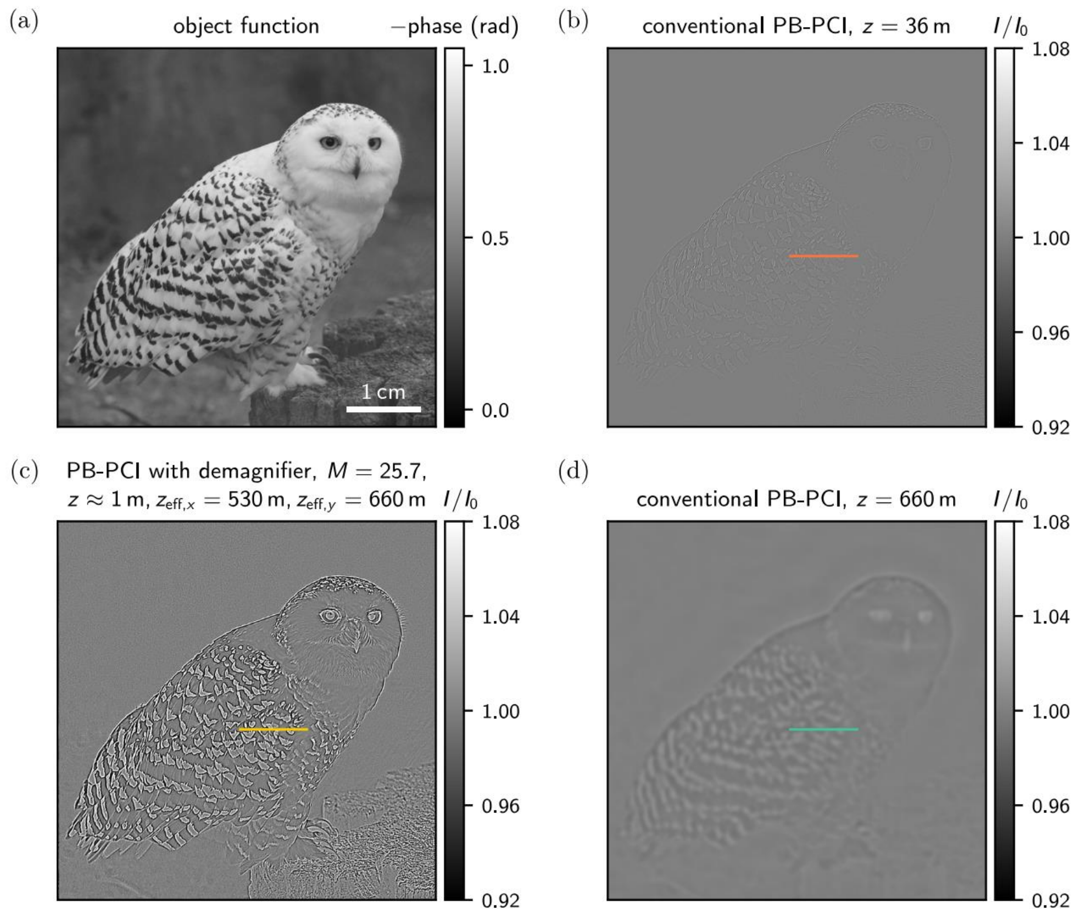
R. Spiecker et al, under review

Patent application file number 10 2023 101 392.0

- **Combination of SPCDs and Coherent Bragg Optics** provides massive **phase contrast amplification**
- Dose-efficient phase-contrast applicable to larger objects → radiation sensitive objects, (bio-)medical diagnostics
- **Combination with novel compact brilliant X-ray sources** → new options for bio-medical imaging

SPCDs combined with coherent X-ray optics even better than **kilometers long beamlines**

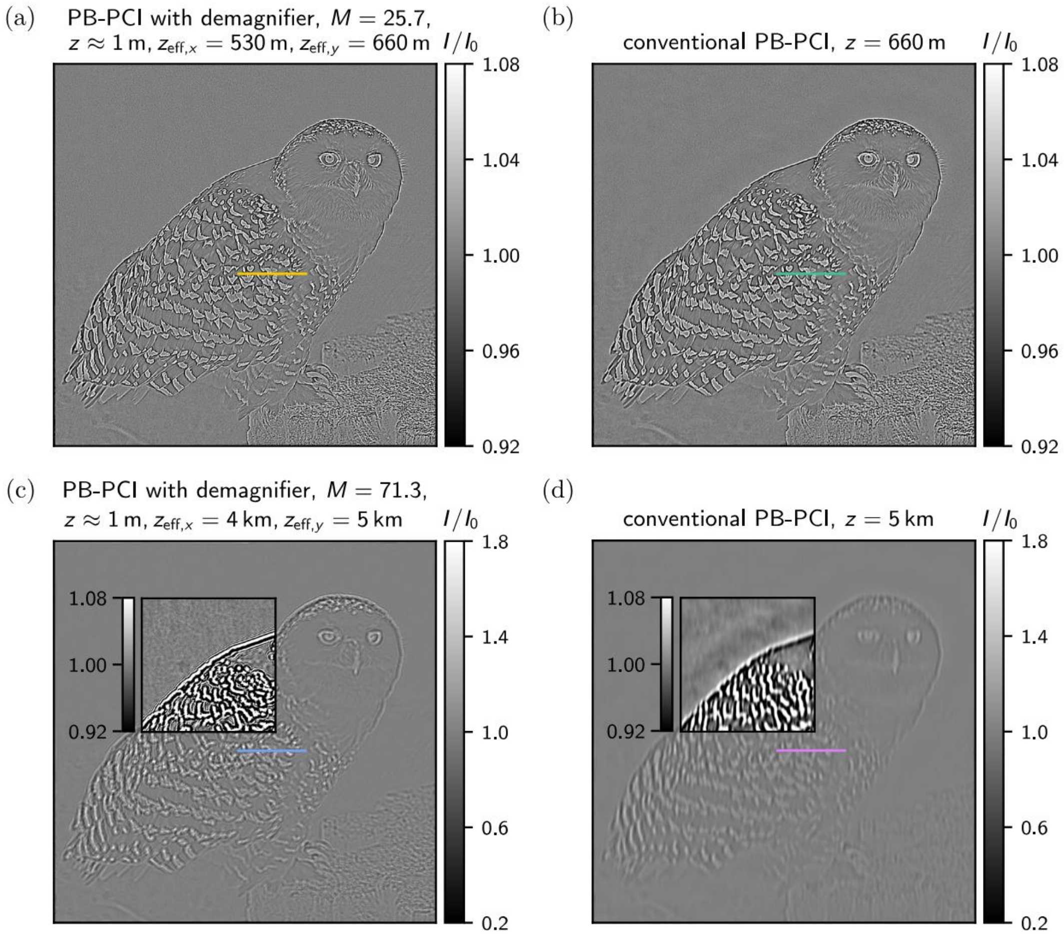
at P23 PETRA III, but assuming symmetrical source



SPCD+BM

SPCD, no BM

Comparison for ESRF EBS conditions at BM18



SPCD+BM

SPCD, no BM

Imaging, Spectroscopy, Scattering

Methods and Systems

Example: Morphological Imaging

Goals

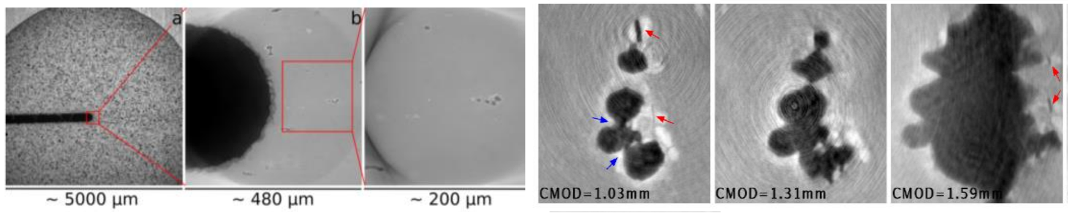
- Material response during fabrication & processing
- Microfluidics, e.g., in injection nozzles, capillaries

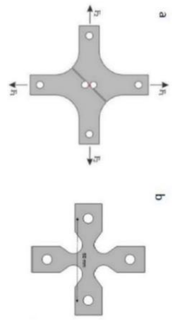
Approaches

- Serial tomography / laminography for large comparative studies
- Hierarchical imaging
- Ultrafast cine-radiography & tomography
- All this *in situ, operando & in vivo*

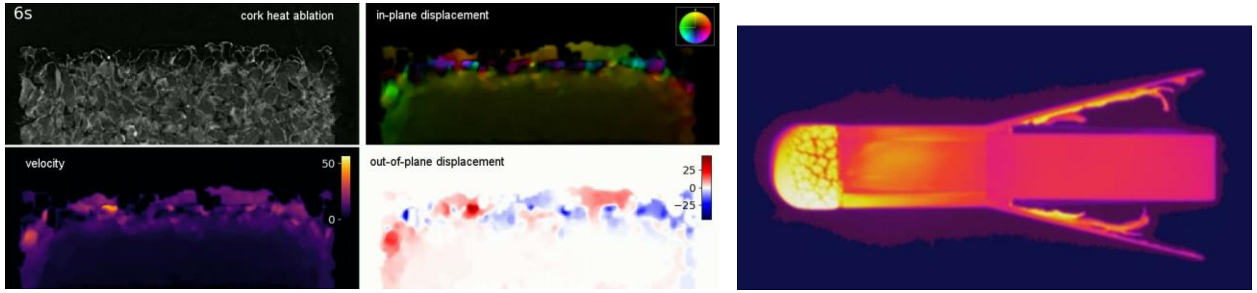
Application fields

- Energy, information, automotive, aerospace, health-tech applications

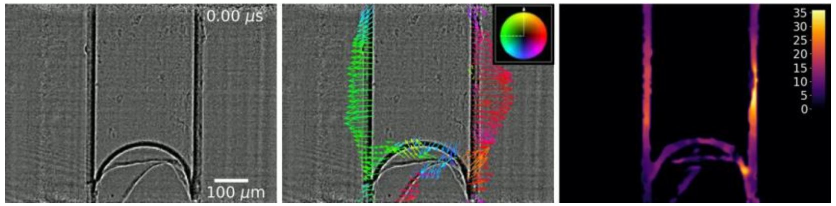


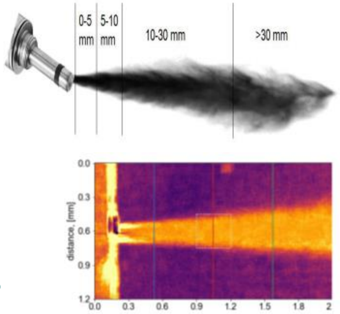


Hierarchical laminography of crack formation



Ultrafast CT of pyrolysis in heat shields for space crafts





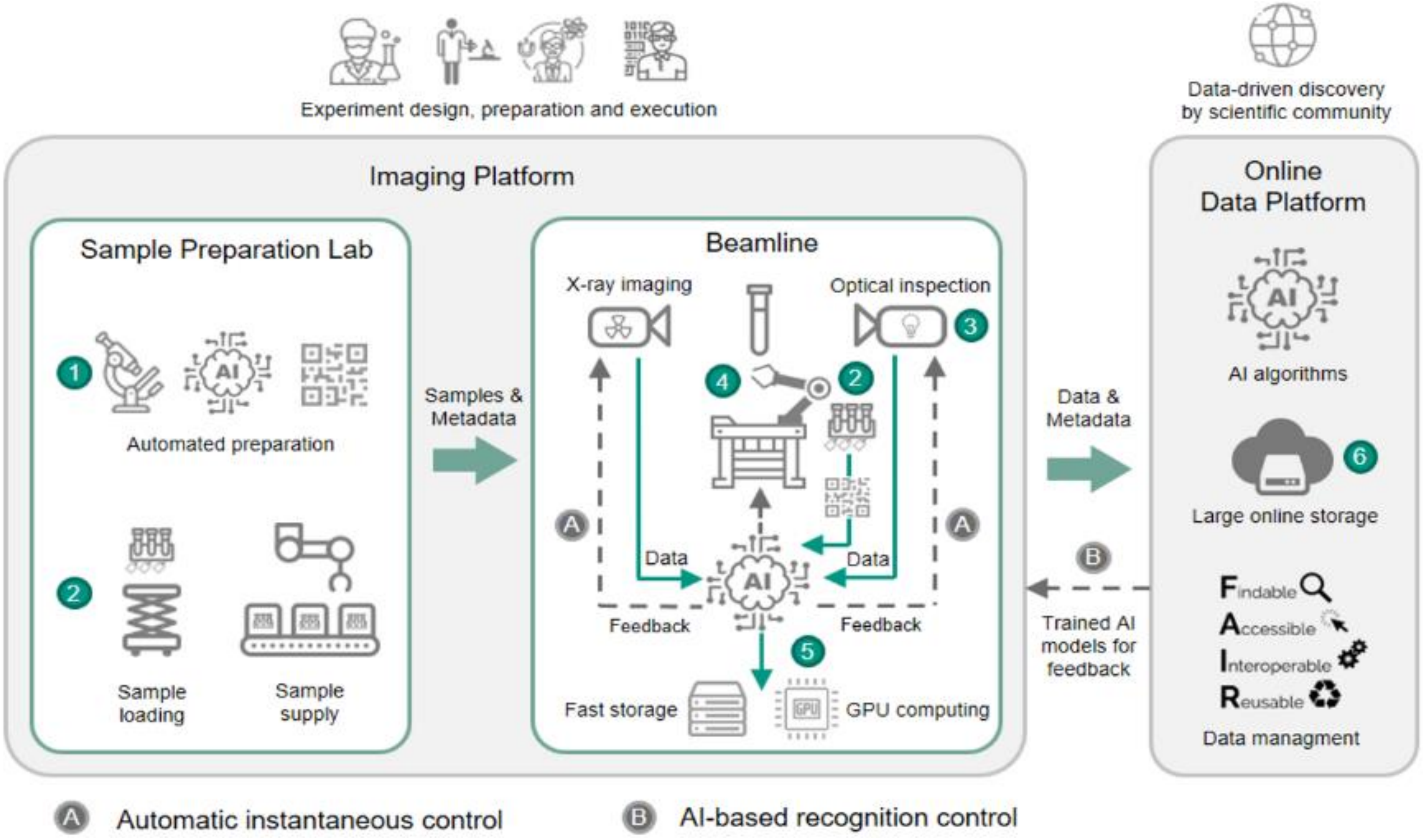
MHz imaging for high speed microfluidics

High-throughput, *in situ, in vivo, operando* Applications

Example:

X-ray Imaging

Intelligent DAQ systems with smart pixel array detectors and in-line algorithms for data analysis



AI-Supported Multidimensional Data Analysis

Develop Strategies for AI-based Big Data Analysis, and Management

MorphoSphere for digitized morphology

LSDF-III Pilot Project

DFG Deutsche Forschungsgemeinschaft

Bundesministerium für Bildung und Forschung

Aktionsplan ErUM-Data
Von Big Data zu Smart Data: Digitalisierung in der naturwissenschaftlichen Grundlagenforschung

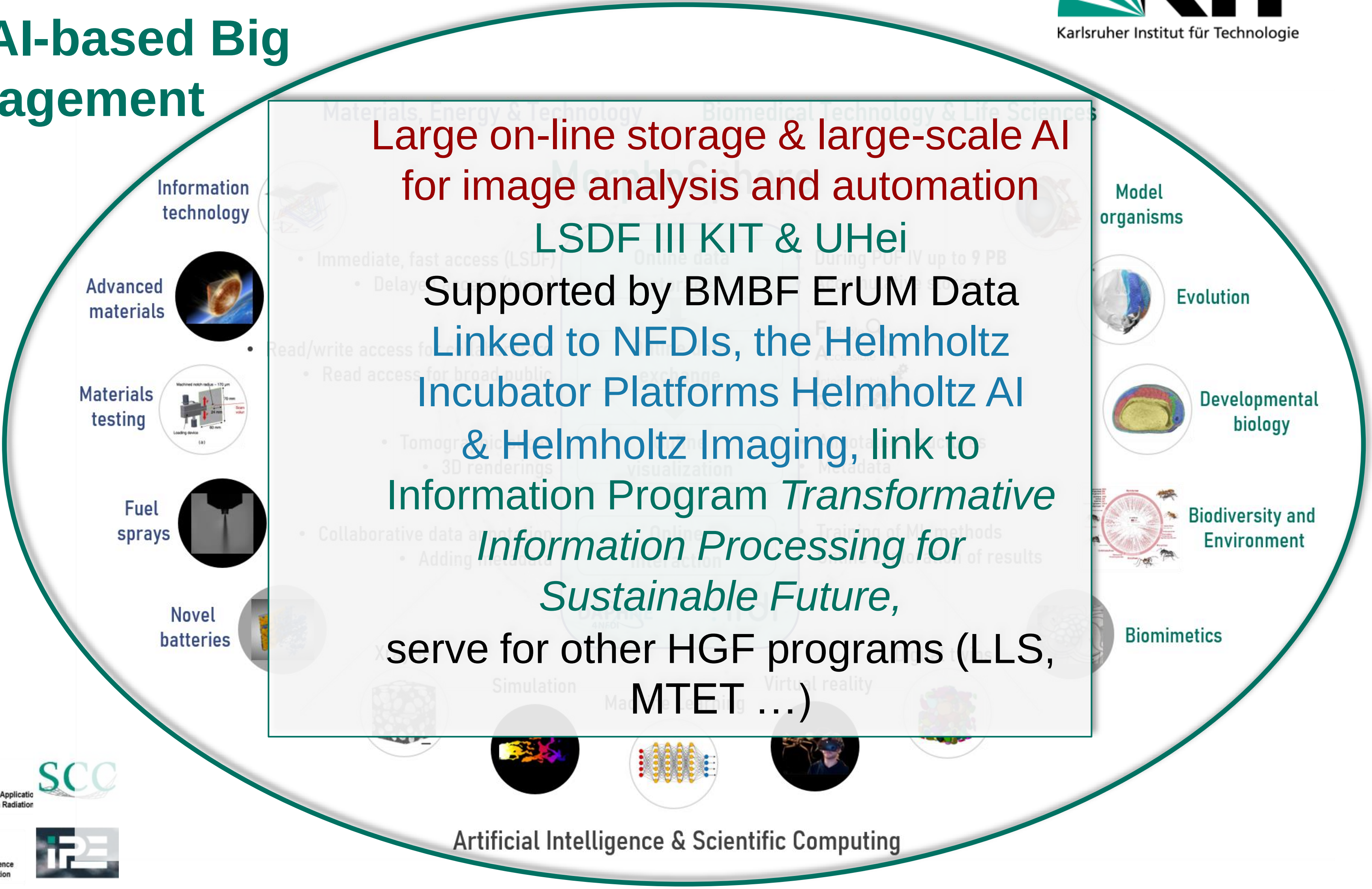
Aktionsplan ErUM-Pro
Projektförderung zur Vernetzung von Hochschulen, Forschungsinfrastrukturen und Gesellschaft

SMART-Morph 2022-2025
Smart modules for AI-supported Serial X-Ray Tomography for Comparative Morphological Studies

KI-Morph 2023-2026
Artificial Intelligence for Automated Segmentation of 3D Image Data for Morphological Structure Analysis

KI4D4E 2023-2026
An AI-based framework for visualizing and evaluating massive amounts of 4D tomography data for beamline end users.

Universität Heidelberg Zukunft seit 1386 · COS Centre for Organismal Studies Heidelberg · KIT Karlsruhe Institute of Technology · LAS Laboratory for Applications of Synchrotron Radiation · SCC · EMCL · URZ Universitäts-Rechenzentrum · IBCS-BIP · IPS Institute for Photon Science and Synchrotron Radiation · IPE



Large on-line storage & large-scale AI for image analysis and automation

LSDF III KIT & UHei

Supported by BMBF ErUM Data

Linked to NFDIs, the Helmholtz Incubator Platforms Helmholtz AI & Helmholtz Imaging, link to Information Program *Transformative Information Processing for Sustainable Future*,

serve for other HGF programs (LLS, MTET …)

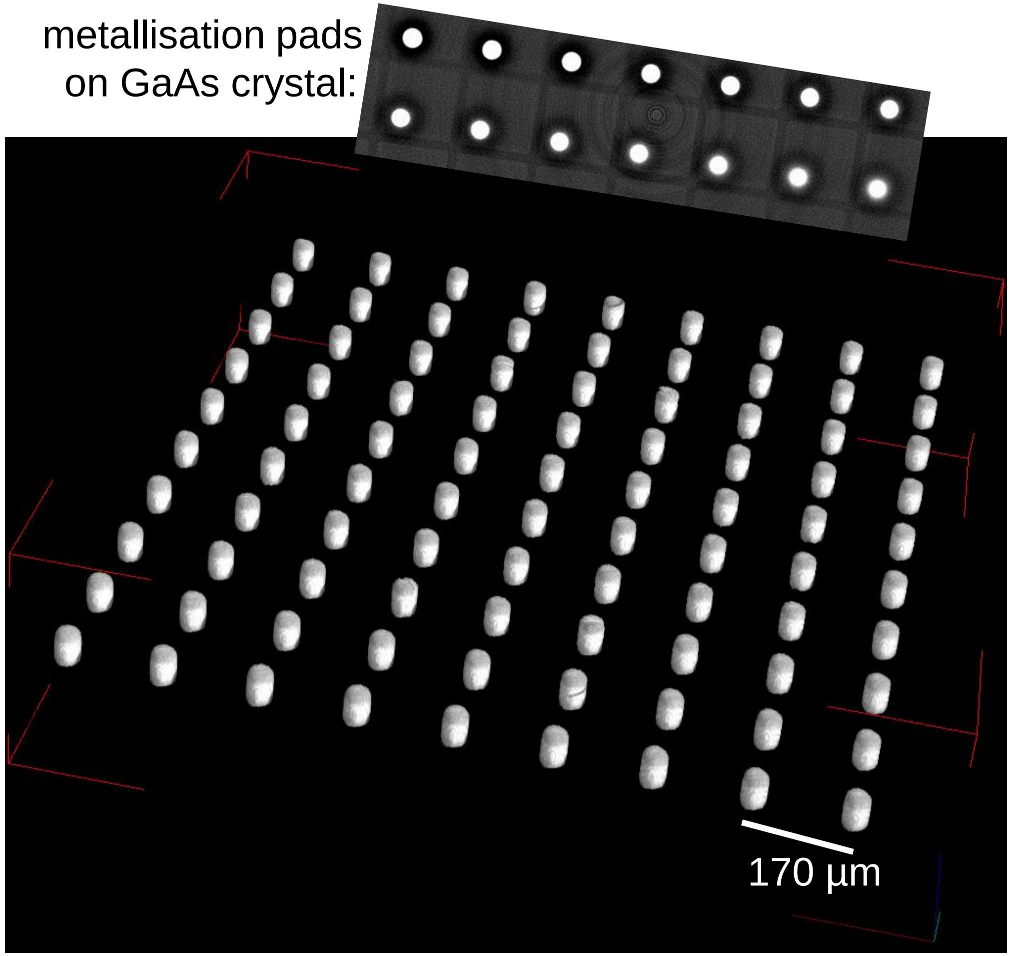
ST4 Contributions to ST1-3

- **Sensor Materials Characterization**
  - Crystal defect characterization of High-Z sensor materials by X-ray topography, rocking curve imaging, 3D diffraction laminography …
- **Non-destructive testing**
  - Testing Flip Chip Interconnections by X-ray absorption Laminography …
- **Characterization of Detector System Performance**
  - key-parameters of full detector assemblies, e.g. energy resolution; spatial resolution, flux-dependent linearity, stability, charge-sharing, …
- **Systems Integration of novel Detectors:** Integration in versatile X-ray imaging pipelines (Hard- and Software) at synchrotron beamlines and X-ray tube-based laboratory setups
- **Dedicated method developments** based on novel detectors and combinations with optics, smart analysis
  - Dose-efficient phase contrast imaging, hierarchical imaging, serial CT, Cine-tomography, MHz-imaging
  - Spectroscopic X-ray imaging with machine learning based material decomposition …
- **Application Tests:** Quality measure for imaging properties evaluating exemplary applicability in life-science, material research, …
- **MT-DTS-ST4 connects to other Programs and Research Fields**

Non-destructive testing
for flip-chip interconnection technology

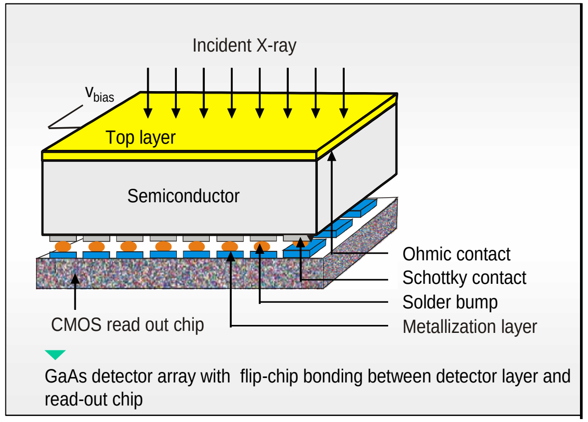
Karlsruher Institut für Technologie

metallisation pads
on GaAs crystal:



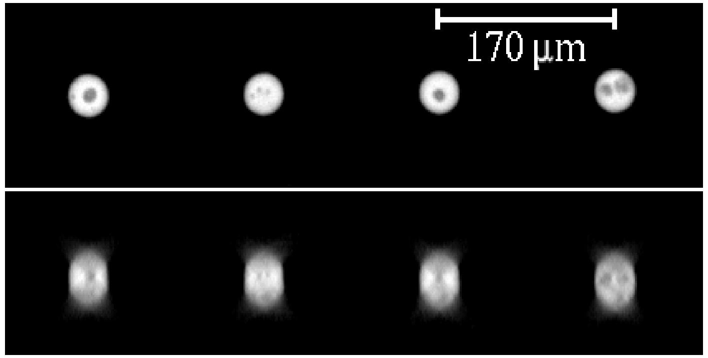
3D rendering of an ROI: central part of
AuSn solder joint array L. Helfen *et al., NIM A* 563,163-166 (2006).

GaAs hybrid x-ray detector



GaAs detector array with flip-chip bonding between detector layer and read-out chip

1800 projections
1.6 µm pixel size
E=40 to 60 keV

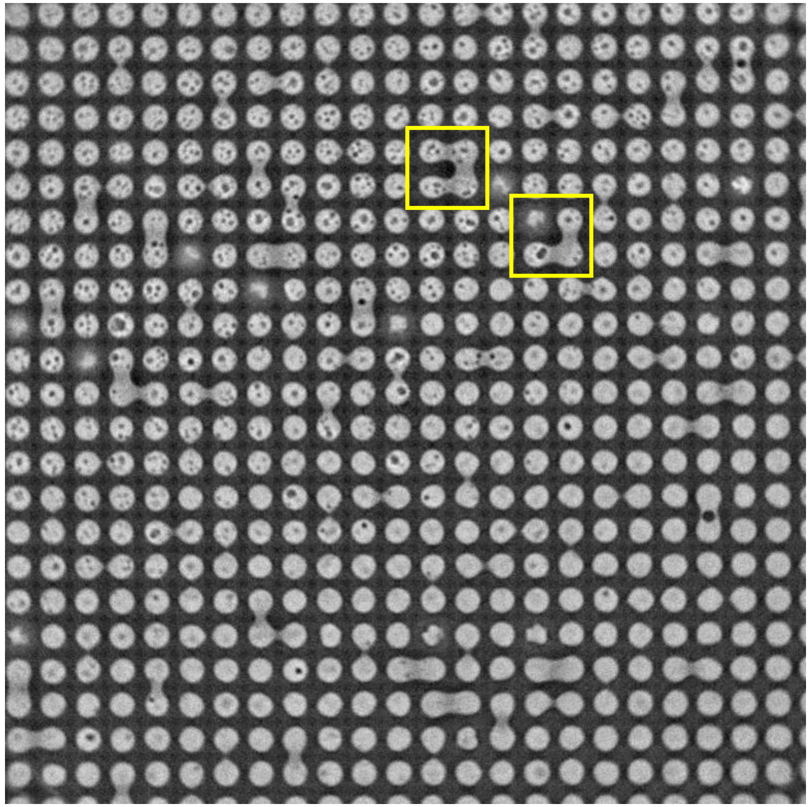


two mutually perpendicular
cross-sectional slices

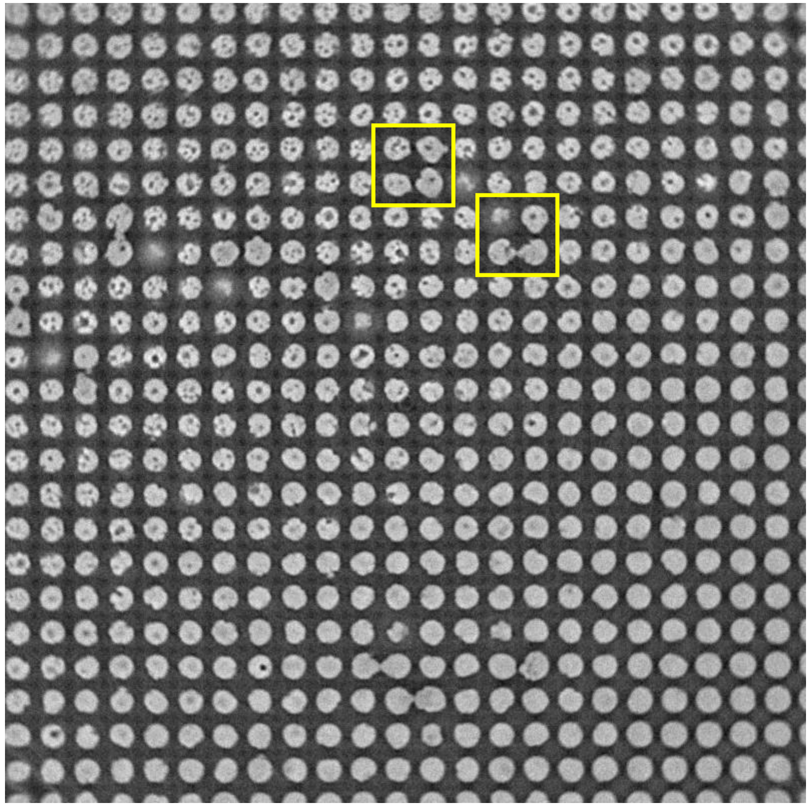
Non-destructive testing
for flip-chip interconnection technology

***In situ* imaging:** AuSn solder flow on Si-GaAs assemblies

Reconstructed slices: AuSn solder joint array (55 µm pitch) under **heat treatment** (T=300°C)



...

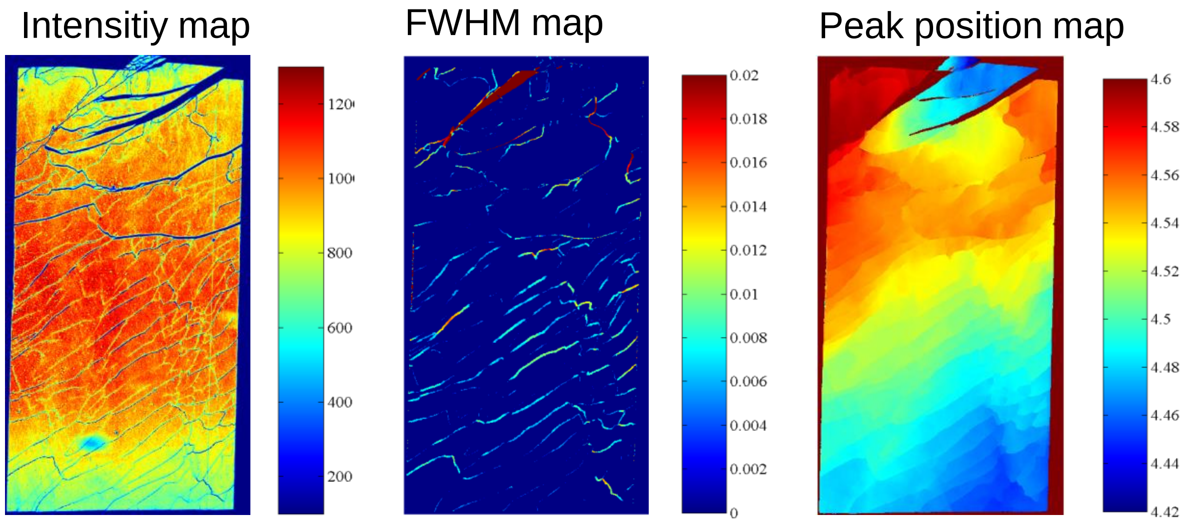


ID15: 30 keV<E<70 keV at 60 mA ring current
600 projections (1.6 µm pixel size)

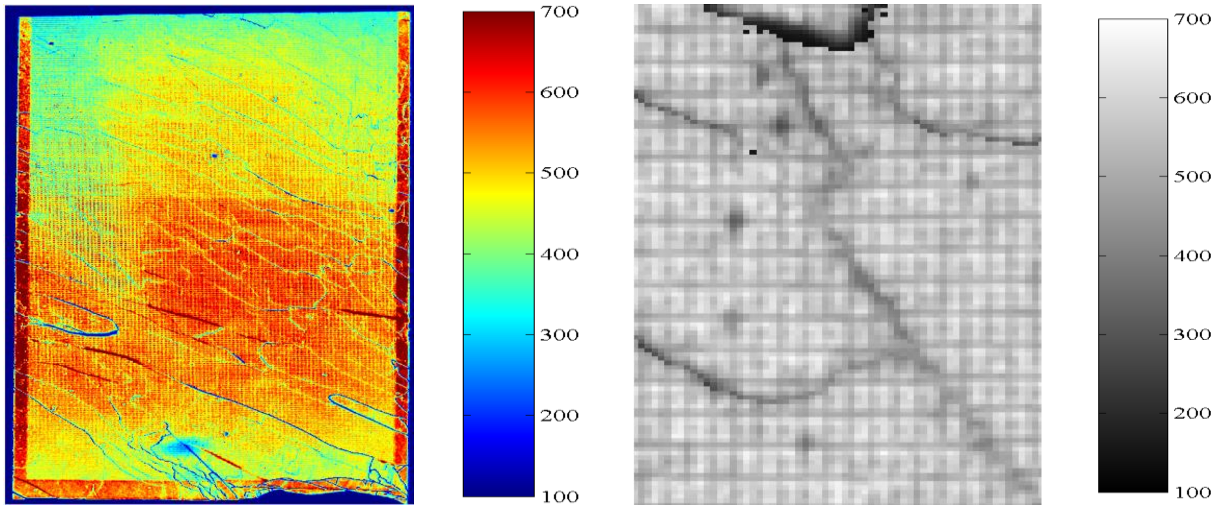
Characterization of Sensor Materials

Karlsruher Institut für Technologie

Rocking curve imaging of CdZnTe sensors



Correlation of Defect structure and detector pixel performance in a CdZnTe-Medipix Detector



(PhD-thesis Elias Hamann)

ST4 contribution to DetecTABL

Karlsruher Institut für Technologie

- **Detector Test X-ray Lab**
- **Imaging Methods for Defect Analysis**
- **Beamlines for Application tests**

- **MT-DTS-ST4 connects to other Programs and Research Fields**

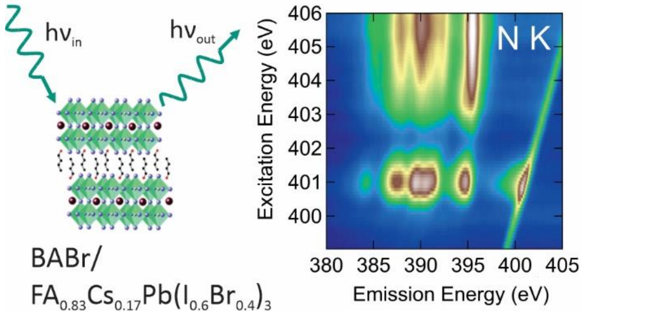
ST4 Multidimensional Method Development and Applications

- **Imaging, Spectroscopy, Scattering – Methods and Systems**
- **High-throughput, *in situ, in vivo, operando* Applications**
- **AI-Supported Multidimensional Data Analysis**

MT-DTS-ST4 connects to other Programs and Research Fields

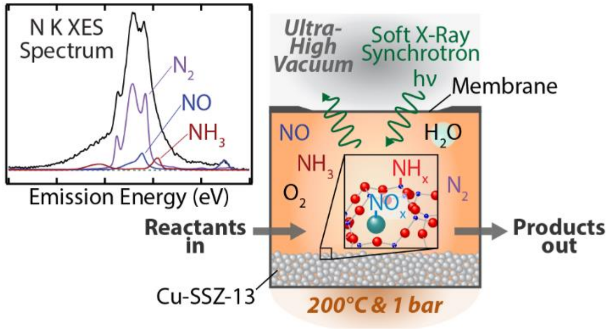
Example: Characterization of Structure and Dynamics of Materials, Devices and Processes

Karlsruher Institut für Technologie

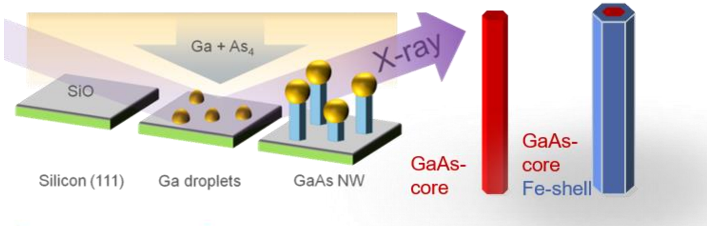


Goals

- Characterize structure and its evolution on micro, nano, and atomic scales
- Correlate structure, dynamics, and properties
- Determine *in situ/operando* changes of electronic and chemical structure during processing/operation

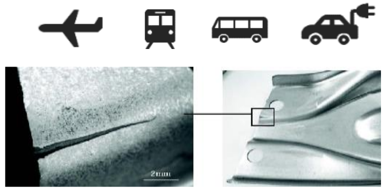


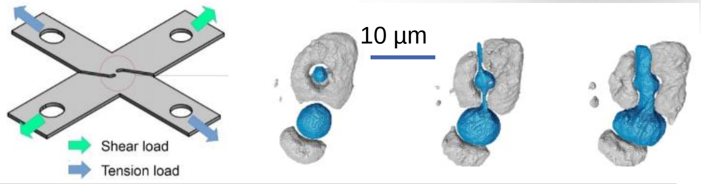
Energy technologies: → characterize processes for **storage, conversion …**
(photovoltaics, solar hydrogen, catalysts, batteries, electrolytes, …), understand degradation



Information technologies: → characterization of **growth and processing** of wafers, thin films, multilayers, nanomaterials, nanostructures → correlate structure and properties to understand multiferroics, photonics, quantum devices, high power electronics, …

Transport technologies → *In situ* and *operando* 3D defect recognition and 4D damage analysis

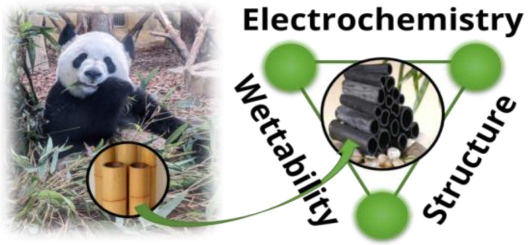




MT-DTS-ST4 connects to other Programs and Research Fields

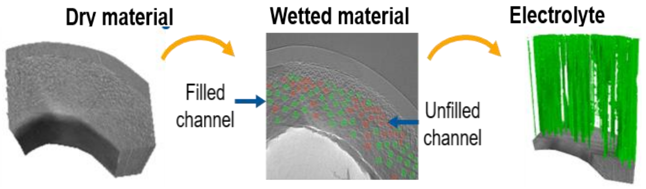
Example: Morphology of biomaterials, biological systems and bio(technological) processes

Bionics



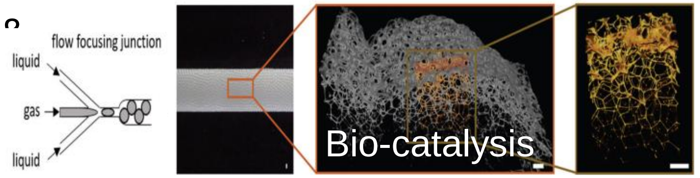
Goals

- Digitize morphology of large sample series
- Determine quantitative morphological / morphometric / morpho-dynamic information



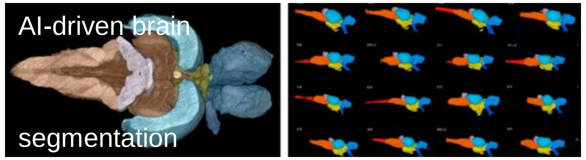
Biomaterials & -technologies: → morphology and bio-compatibility of biomaterials; → tissue engineering, scaffolds, organoids; → bionics, bio-catalysis, food engineering …

Model organisms: → correlate morphology and molecular data; determine gene functions multigenic contributions to **development and disease** → Generate digital twins of biological systems (medaka, zebrafish, xenopus, … brain);



Model organisms

Biodiversity: → Digitize morphological diversity, correlated with molecular & ecological data, including human impact; → Focus on **indicator organisms for climate impact on biodiversity**, and models for environmental change on development; → Identify morphological key features to determine evolutionary key events for diversification.

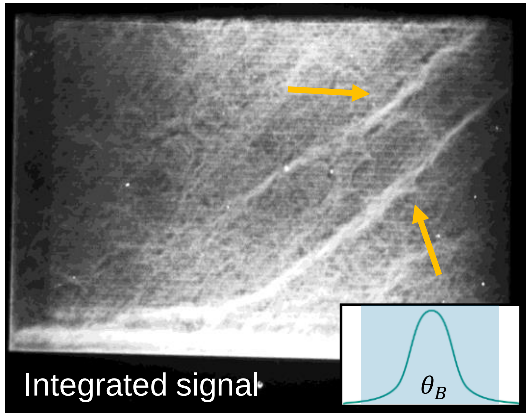


Summary

- Based on the results of MML, KIT proposes to strengthen MT-DTS by a fourth Subtopic
- KIT’s beamlines and labs will strengthen the DTS “Research Infrastructures” → DetecTABL
- ST4 will support the system conception, design, characterization and application
  - Detectors for the use in Multidimensional Characterization of Materials, Devices, and Systems
  - Serial Digitalization of Morphology of materials and organisms …
- MT-DTS-ST4 connects to other Programs and Research Fields

Characterization of Sensor Materials

- Stronger absorption → high X-ray energies required
  → narrow Darwin curves → sufficiently precise instrumentation crucial!

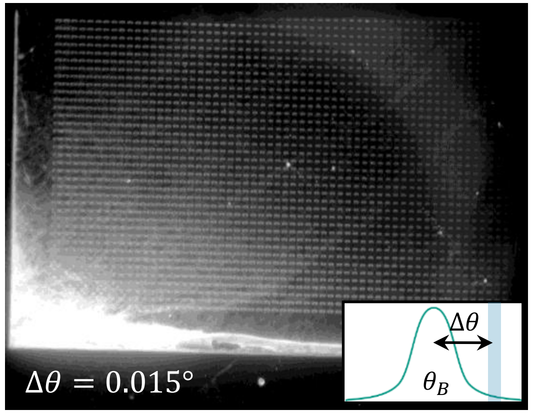


- 68.5 keV @ ID15A
- 004 reflection ($\theta_B = 3.669°$)
- 300 projections

→ Dislocation cell walls visible

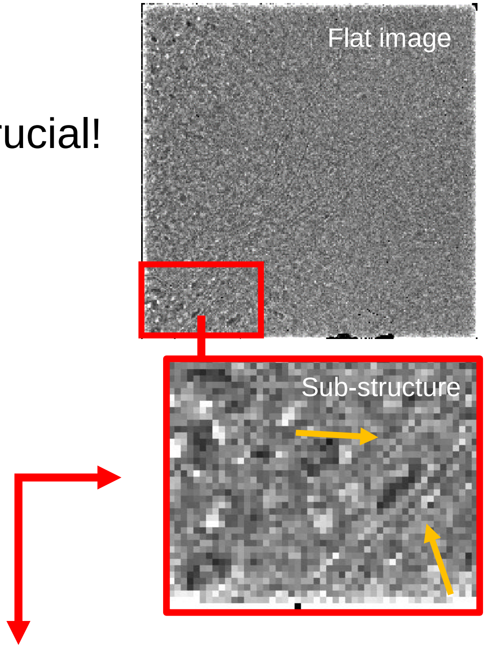
→ Work on 3D reconstruction ongoing (challenging)

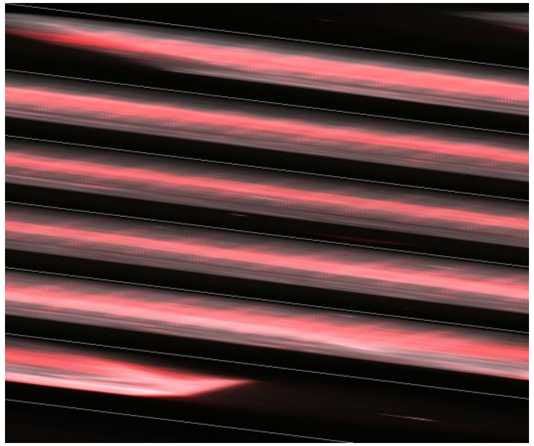
- Changed contrast conditions (weak-beam):



- Pixel positions indicated by strain localizations

→ XDL data can be precisely linked to Medipix flat image contrast!



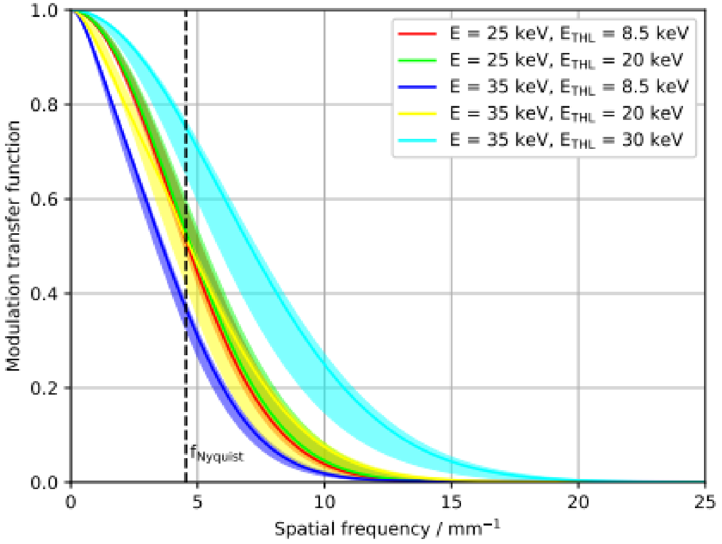


Application of X-ray Diffraction Laminiography to High-Z Sensor Materials

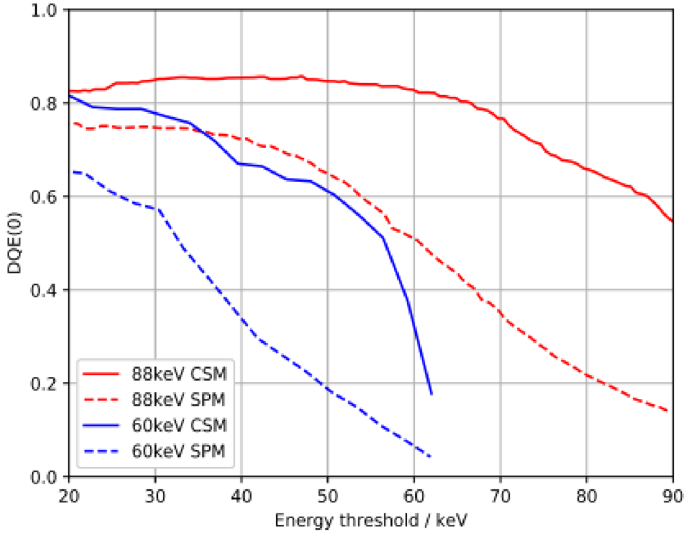
Example: GaAs Medipix Sensor

Contribution of ST4 to the Characterization and Application of Detector-Systems

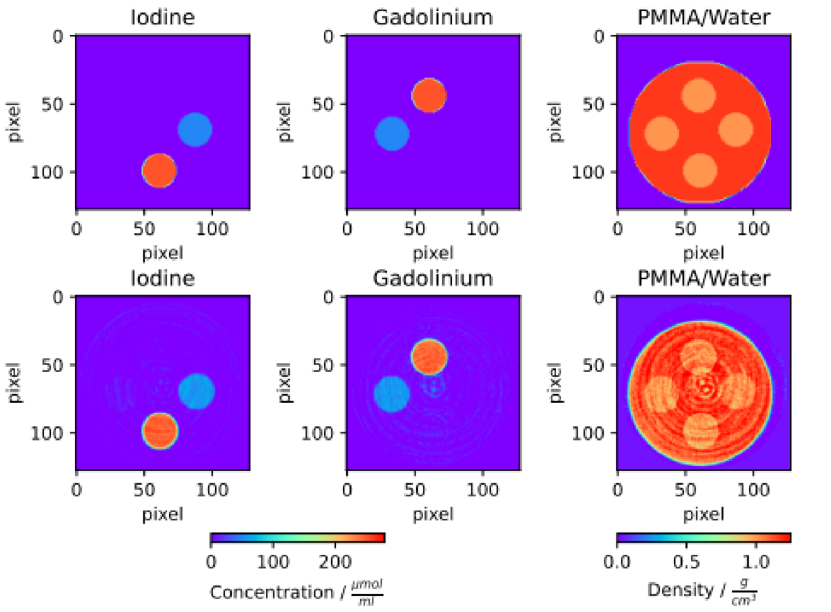
Example: Spectroscopic Imaging



Presampling-MTF measurement of a Medipix3RX detector with a 2mm **CdTe** sensor in **Single-Pixel-Mode**



DQE(0) measurement of a Medipix3RX detector with a 2mm **CdTe sensor** for different photon energies



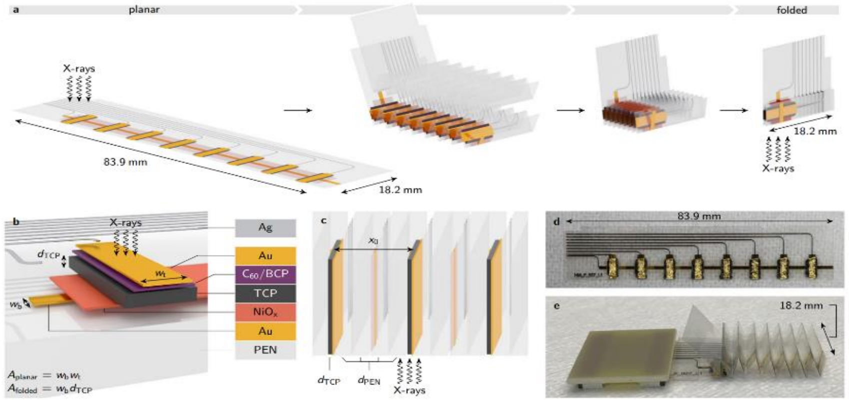
Material specific spectroscopic CT-slices of a test phantom. Top: ground-truth, bottom: measurement, Medipix3RX with 2mm CdTe in charge-summing-mode

PhD-thesis Marcus Zuber

Contribution of ST4 to the Characterization and Application of Detector-Systems

- **Origami-inspired perovskite X-ray quantum detector by printing and folding**

npj H. Mescher et al.
2



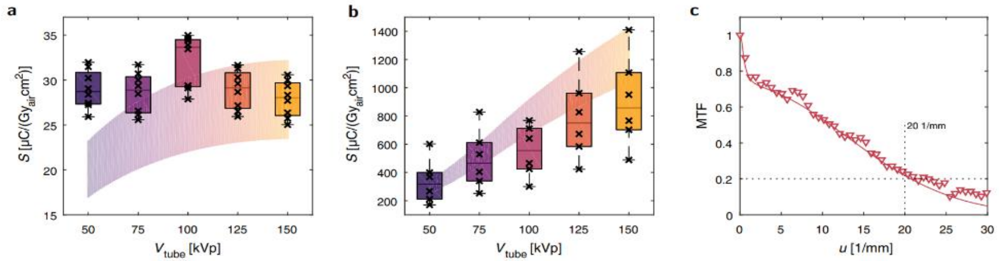


Fig. 3 X-ray sensitivity and spatial resolution. a, b X-ray sensitivities S of the planar (**a**) and the folded (**b**) detector as a function of the utilized X-ray tube voltage V_{tube}. The experimentally determined sensitivities are represented by box plots. The individual pixel sensitivities are also shown as symbols (crossed markers). The theoretical sensitivity prediction is depicted by the coloured areas. **c** Presampled modulation transfer function MTF of the folded detector as a function of the spatial frequency u. The MTF is determined by a numerical (markers) and an analytical (solid lines) approach.

Flexible Inkjet-Printed Triple Cation Perovskite X-ray Detectors

Henning Mescher*, Fabian Schackmar, Helge Eggers, Tobias Abzieher, Marcus Zuber, Elias Hamann, Tilo Baumbach, Ulrich W. Paetzold, and Uli Lemmer*

Nature/npj Flexible Electronics (2023) 7:9 ; https://doi.org/10.1038/s41528-023-00240-9