XTOP 2026

16th Conference on High-Resolution X-Ray Diffraction and Imaging

21-25 September 2026
Karlsruhe, Germany

BOOK OF ABSTRACTS

Contents

XTOP 2026

16th Conference on High-Resolution X-ray Diffraction and Imaging
21–25 September 2026, Karlsruhe, Germany

XTOP 2026 brings together scientists working in X-ray diffractometry and reflectometry, coherent and conventional X-ray diffraction imaging and topography, as well as 2D and 3D X-ray imaging using phase contrast and complementary contrast mechanisms. The conference is a leading forum for laboratory- and synchrotron-based methods, instrumentation, and applications. A dedicated tutorial supports the training and integration of young researchers into this vibrant international community.

Scientific Topics

X-ray imaging, diffraction and scattering methods

- **Near-field 2D imaging and 3D tomography methods** with various contrasts, such as absorption, phase, extinction, diffraction (e.g. topography), dark-field, and others
- **Far-field methods,** such as X-ray reflectivity (XR), grazing incidence diffraction (GID), grazing incidence small-angle scattering (GISAXS), high-resolution diffraction (HR-XRD), nano diffraction, coherent diffraction imaging (CDI), ptychography, and others
- **X-ray microscopy,** such as full-field transmission microscopy (TXM), scanning microscopy (STXM), dark-field microscopy (DF-XRM), and others
- **Related techniques,** such as standing wave methods, quantum imaging, Compton microscopy

Related topics

- **Theory and algorithms,** such as near field and far field image formation, phase retrieval, volume reconstruction, kinematical / DWBA / dynamical diffraction approaches, diffuse scattering approaches, and others
- **Computing and AI approaches** for simulations, statistical analysis, volume segmentation, high-throughput computing, and others
- **Instrumentation,** such as new beamlines and experimental stations, new possibilities by improved sources, optics, detectors, sample environments and others
- High-throughput, in situ, operando, in vivo approaches
- Crystal defects: theory and experiment
- **Scientific applications** in materials research, nano-sciences, life sciences, natural and cultural heritage, and other fields
- **Industrial applications**
- **Bio-medical applications**

Scientific Rationale

XTOP spans a broad portfolio of high-resolution X-ray diffraction, scattering and imaging approaches, encompassing near-field and far-field regimes as well as laboratory- and large-scale-facility-based instrumentation and applications. In particular, XTOP aims to bridge the various method groups by addressing the concepts and practical challenges they share—often across boundaries that, at first glance, appear to separate: how X-ray wavefields interact with the samples and sophisticated optics;

how optics or propagation shape measurable contrast; how to model refraction, scattering, diffraction of complex samples with or without multiple-scattering effects (the forward problem); and how to achieve robust object volume reconstruction from incomplete and noisy data (the inverse problem). Increasingly, these shared challenges are accompanied by the convergence of reciprocal-space and real-space approaches.

This “bridging the gap” perspective has characterised XTOP since its start in 1992, when questions such as multiple-scattering effects / dynamical diffraction theory were central across X-ray topography and high-resolution diffraction. It remains equally relevant today as coherence-driven and hybrid near and far field strategies develop. Recent advances at modern laboratory sources and at synchrotron/X-FEL facilities, with substantially increased flux and coherence, as well as new optics further accelerate this development and enable multi-contrast, multiscale (hierarchical) studies and high-throughput, in situ, operando or in vivo applications, all supported by advanced computing and AI.

In this spirit, XTOP provides a forum to identify common physical or computational principles and transferable solutions that emerge when experts from seemingly distinct method groups work together.

XTOP Panels

Chair: Tilo Baumbach
Co-Chair: Olaf Baake
Co-Chair: Daniel Hänschke

Local Organization Committee:

Esra Aran
Olaf Baake
Angelica Cecilia
Tomáš Farago
Daniel Hänschke
Mathias Hurst
Merve P. Kabukcuoglu
Bärbel Krause
Jan-Thorsten Reszat
Sandra Richers
Rebecca Spiecker
Svetoslav Stankov
Clément Tavakoli
Thomas van de Kamp
Ekaterina Walter
Marcus Zuber

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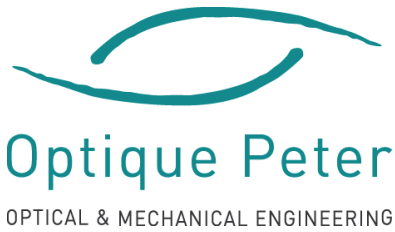

Institutional supporters

XTOP 2026 – Program

Sunday, 20.09.2026

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20:00-20:15		Dinner for Tutorial Participants
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22:00-22:15		Dinner for Tutorial Participants
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22:30-22:45		Dinner for Tutorial Participants
22:45-23:00		Dinner for Tutorial Participants

Monday, 21.09.2026

08:30-08:45	Registration			
08:45-09:00	Registration	Tutorial Opening		
09:00-09:15	Registration	Tutorial (Chair: Tilo Baumbach)	Vincent Favre-Nicolin	*Coherent X-rays and Applications: CDI and Ptychography*
09:15-09:30	Registration	Tutorial (Chair: Tilo Baumbach)	Vincent Favre-Nicolin	*Coherent X-rays and Applications: CDI and Ptychography*
09:30-09:45	Registration	Tutorial (Chair: Tilo Baumbach)	Vincent Favre-Nicolin	*Coherent X-rays and Applications: CDI and Ptychography*
09:45-10:00	Registration	Tutorial (Chair: Tilo Baumbach)	Vincent Favre-Nicolin	*Coherent X-rays and Applications: CDI and Ptychography*
10:00-10:15	Registration	Coffee Break		
10:15-10:30	Registration	Coffee Break		
10:30-10:45		Tutorial (Chair: Tilo Baumbach)	Julia Herzen	*Phase-Contrast and Dark-Field Imaging for Biomedical Applications*
10:45-11:00		Tutorial (Chair: Tilo Baumbach)	Julia Herzen	*Phase-Contrast and Dark-Field Imaging for Biomedical Applications*
11:00-11:15		Tutorial (Chair: Tilo Baumbach)	Julia Herzen	*Phase-Contrast and Dark-Field Imaging for Biomedical Applications*
11:15-11:30		Tutorial (Chair: Tilo Baumbach)	Julia Herzen	*Phase-Contrast and Dark-Field Imaging for Biomedical Applications*
11:30-11:45		Tutorial (Chair: Tilo Baumbach)	Julie Villanova	*X-ray Microscopy Techniques*
11:45-12:00		Tutorial (Chair: Tilo Baumbach)	Julie Villanova	*X-ray Microscopy Techniques*
12:00-12:15		Tutorial (Chair: Tilo Baumbach)	Julie Villanova	*X-ray Microscopy Techniques*
12:15-12:30		Tutorial (Chair: Tilo Baumbach)	Julie Villanova	*X-ray Microscopy Techniques*
12:30-12:45		Tutorial (Chair: Tilo Baumbach)	Julie Villanova	*X-ray Microscopy Techniques*
12:45-13:00		Lunch Break		
13:00-13:15		Lunch Break		
13:15-13:30		Lunch Break		
13:30-13:45		Lunch Break		
13:45-14:00		Lunch Break		
14:00-14:15		Tutorial (Chair: Tilo Baumbach)	Tobias Schülli	*Diffraction Imaging at Synchrotron Light Sources: From Topography to Coherent Nanoprobes*
14:15-14:30		Tutorial (Chair: Tilo Baumbach)	Tobias Schülli	*Diffraction Imaging at Synchrotron Light Sources: From Topography to Coherent Nanoprobes*
14:30-14:45		Tutorial (Chair: Tilo Baumbach)	Tobias Schülli	*Diffraction Imaging at Synchrotron Light Sources: From Topography to Coherent Nanoprobes*
14:45-15:00		Tutorial (Chair: Tilo Baumbach)	Tobias Schülli	*Diffraction Imaging at Synchrotron Light Sources: From Topography to Coherent Nanoprobes*
15:00-15:15	Registration	Tutorial (Chair: Tilo Baumbach)	Stefan Kowarik	*X-ray Scattering by Nanostructure*
15:15-15:30	Registration	Tutorial (Chair: Tilo Baumbach)	Stefan Kowarik	*X-ray Scattering by Nanostructure*
15:30-15:45	Registration	Tutorial (Chair: Tilo Baumbach)	Stefan Kowarik	*X-ray Scattering by Nanostructure*
15:45-16:00	Registration	Tutorial (Chair: Tilo Baumbach)	Stefan Kowarik	*X-ray Scattering by Nanostructure*
16:00-16:15	Registration	Tutorial Closing		
16:15-16:30	Registration			
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19:45-20:00	Registration			
20:00-20:15		Welcome Reception - Finger Food & Drinks		
20:15-20:30		Welcome Reception - Finger Food & Drinks		
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22:15-22:30		Welcome Reception - Finger Food & Drinks		
22:30-22:45		Welcome Reception - Finger Food & Drinks		
22:45-23:00		Welcome Reception - Finger Food & Drinks		

Tuesday, 22.09.2026

08:30-08:45	Registration		**Conference Opening**	
08:45-09:00				
09:00-09:15		**I: Diffraction & Scattering - 1/2** Chairs: Stefan Kowarik & Jörg Grenzer	Ivan Zaluzhnyy	*Nanodiffraction for Spatially-Resolved Studies of Complex Materials*
09:15-09:30				
09:30-09:45			Steffen Tober	*XRR with Nanometre Beams - Characterising Micrometre Surfaces*
09:45-10:00			Martin Zimmermann	*X-ray Reflectivity and Reciprocal Space Mapping with a Micro-Focus Rotating Anode: From Micron-Sized Beams to Fractional-Order Bragg Peaks*
10:00-10:15			Michał Kamiński	*Real-Time Manipulation of Ag Thin Film Growth Studied by GISAXS*
10:15-10:30			Ivan Vartaniants	*Structure of Protein Cage Supercrystals Revealed by Angular X-ray Cross-Correlation Analysis*
10:30-10:45			**Coffee Break**	
10:45-11:00				
11:00-11:15		**II: X-ray Microscopy** Chairs: Julie Villanova & Irina Snigireva	Saša Bajt	*Novel Imaging Modalities Enabled by Multilayer Laue Lenses*
11:15-11:30				
11:30-11:45			Benjamin Apeleo Zubiri	*Electron-Tomography-Informed Super-Resolved Nano X-ray Computed Tomography*
11:45-12:00			Benedikt Rösner	*Supersampling Scanning Transmission Microscopy: Unlocking Sub-10 nm STXM Resolution*
12:00-12:15			Maik Becker	*Crystallographic and Defect Analysis of Colloidal Photonic Supraparticles Using Zone-Axis Wide-Field XRM and NanoCT*
12:15-12:30			Mathias Hurst	*Hard X-ray Holographic Projection Microscopy Using Multilayer Laue Lenses for Hierarchical 3D Imaging*
12:30-12:45			**Lunch Break**	
12:45-13:00				
13:00-13:15				
13:15-13:30				
13:30-13:45				
13:45-14:00				
14:00-14:15		**III: New Instrumentation** Chairs: Tobias Schülli & Cristian Mocuta	Patrik Vagovič	*MHz X-ray Tomoscopy: Rotation-Free 4D Imaging with Diamond Bragg Beam-Splitter Optics at the European XFEL*
14:15-14:30				
14:30-14:45			Angel Rodriguez Fernandez	*Shear Wave Propagation Imaged Inside Crystalline Semiconductors After Below Melting Threshold Using Diffraction Near Field X-ray Microscopy*
14:45-15:00			Julia Rogalinski	*Time-Resolved 3D Imaging Opportunities with XMPI at ForMAX*
15:00-15:15			Simon Bode	*Synchrotron Laminography for Multimodal, Hierarchical, and in Situ 3D Imaging*
15:15-15:30			Tilman Donath	*Advancing Synchrotron Imaging Using Next-Generation Hybrid Photon Counting Detectors*
15:30-15:45			Caori Organista	*FaXToR: The First Fast Hard X-ray Micro-Tomography Beamline at the ALBA Synchrotron*
15:45-16:00			**Coffee Break**	
16:00-16:15				
16:15-16:30		**IV: Appl. & Ind. Res.** Chairs: Mark Goorsky & Lutz Kirste	Tamzin Lafford	*Development of X-ray Metrology for Advanced CFET Logic and 3D-DRAM Devices*
16:30-16:45				
16:45-17:00			Marcello Fonda	*Spectral Photon-Counting Micro-CT for Dental Implant Integrity and Infiltration Analysis*
17:00-17:15		**Poster Session 1**	**Poster Session 1**	
17:15-17:30				
17:30-17:45				
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18:30-18:45			**Dinner**	
18:45-19:00				
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19:30-19:45		**Evening Lecture**	**Lars Krogmann, Director of the Natural History Museum Stuttgart "From Museum Collections to Digital Biodiversity Research"**	
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Wednesday, 23.09.2026

08:30-08:45	**V: Phase-Contrast Imaging** Chairs: Saša Bajt & Mathias Hurst	Marina Eckermann	*Waves for LIfe Sciences: Characterization of Biomedical Structures with a Focus on X-ray Imaging*
08:45-09:00			
09:00-09:15		Oriol Roche	*Multimodal, Multi-Scale Imaging of Human Vagus Nerve at the I13-1 Coherence Beamline*
09:15-09:30		Martin Spiecker	*Dose-Efficient Propagation-Based X-ray Phase Contrast Imaging at High and Low Resolution by Bragg Crystal Optics*
09:30-09:45		Irina Snigireva	*Multilens X-ray Interferometry Based on Si Planar Compound Refractive Lenses*
09:45-10:00		Giovanni Lemma	*Phase-Contrast and Dark-Field Imaging and Tomography at OptImaTo Laboratory: Implementation and Optimization with Modulation-Based Technique*
10:00-10:15		**Coffee Break**	
10:15-10:30			
10:30-10:45	**VI: Diffraction & Scattering - 2/2** Chairs: Ivan Zaluzhnyy & Steffen Tober	Anna Kossoy	*High-Resolution XRD Characterization of Surface Guided Xanthine Derivatives for Optical Metamaterial Application*
10:45-11:00		Sarah Siraj	*Swelling Dynamics in Ultrathin Protein Films*
11:00-11:15		Ritwika Mandal	*Strain Waves as a Symmetry-Breaking Field in Photoexcited V_2O_3*
11:15-11:30		Aleksandra Wierzbicka	*Residual Effects in GaN Nanowires on ZrN Buffer Layers Studied by XRD and Raman Spectroscopy*
11:30-11:45		Berkin Nergis	*In-Situ Synchrotron HRXRD Investigation of Epitaxial YSZ/Ti/Pt/BaFe12O19/Bi3Ti5FeO15 Multiferroic Heterostructures on Si(111) for Non-Volatile Memory Applications*
11:45-12:00		Vladimir Kaganer	*X-ray Diffraction Profiles from Dislocations and Stacking Faults in a-Plane AlN Films*
12:00-12:15		**Official Conference Group Photo**	
12:15-12:30		**Packed Lunch**	
12:30-12:45			
12:45-13:00	**Excursion**	**Excursion** **Heidelberg Castle & Old Town**	
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19:00-19:15		**Dinner**	
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Thursday, 24.09.2026

08:30-08:45	VII: CDI & Ptychography Chairs: Dina Carbone & Felix Wittwer	Oleg Gorobtsov	*Diffractive Imaging of Mesostructure in Disordered Energy Materials*
08:45-09:00			
09:00-09:15		Dmitry Karpov	*Bridging Real and Reciprocal-Space Nanoimaging of Biogenic Calcite: Bragg Coherent Diffraction, Ptychography, and Cryo X-ray Fluorescence*
09:15-09:30		Aksel Mihaylov	*Bragg Coherent Diffraction X-ray Imaging of Nanoparticles with Unknown Orientation*
09:30-09:45		Johannes Ihli	*Dynamic In-Situ Ptychographic X-ray Tomography with Environmental Control*
09:45-10:00		Thomas Sarrazin	*Spectroscopic BCDI: Combined Chemical and Structural 3D Mapping of Bimetallic Nanocatalysts*
10:00-10:15		Anton Plech	*Photodynamics of Gold Nanorod Transformation Studied by Femtosecond Coherent Diffraction Imaging at the European XFEL*
10:15-10:30		Runqing Yang	*Challenges and Solutions of Diffraction Signal Numerical Separation in Multibeam Ptychography*
10:30-10:45		**Coffee Break**	
10:45-11:00			
11:00-11:15	VIII: Theory, AI & Algorithms Chairs: Vladimir Kaganer & Edwin Fohtung	Yuhe Zhang	*Deep Learning for Advanced 3D and 4D X-ray Image Reconstruction*
11:15-11:30			
11:30-11:45		Warre Heylen	*Evolution-Based EUV Scatterometry Fuelled by Machine Learning Diffraction Predictions for 3D Nanoscale Semiconductor Structures*
11:45-12:00		Alexander Mikhalychev	*Sensitivity Maximization in XRR and HRHRD by Fisher Information: Search for the Most Informative Scan Points*
12:00-12:15		Adrien Toulouse	*Development of Algorithms and Modeling Tools for Low-Energy CD-SAXS Measurements*
12:15-12:30		Xiaoying Tan	*Conditional Machine Learning Model for Scalable Landmark Detection in Comparative Morphological Imaging of Medaka Inbred Lines*
12:30-12:45		**Lunch Break**	
12:45-13:00			
13:00-13:15			
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14:00-14:15	IX: Diffraction Contrast Imaging - 1/2 Chairs: Carsten Detlefs & Carsten Richter	Mark Goorsky	*Diffraction Contrast Imaging of Ultra-Wide Bandgap Substrates and Structures for Hetero-Integration*
14:15-14:30			
14:30-14:45		Albert Zelenika	*3D Mapping of Dislocation-Crack Tip Interactions in $SrTiO_3$ by Dark-Field X-ray Microscopy*
14:45-15:00		Ilhem Nadia Rabehi	*Sub-Grain Origin and Dynamics in Cast-Mono Silicon for Photovoltaic Solar Cells Revealed by X-ray Topography and Diffraction Rocking Curve Imaging*
15:00-15:15		Merve Pinar Kabukcuoglu	*Temporal Evolution of 3D Dislocation Structures in Silicon by Correlative X-ray Diffraction Imaging*
15:15-15:30		Lutz Kirste	*Revealing Growth Discontinuities in Ammonothermal GaN by Advanced Bragg Diffraction Imaging Techniques*
15:30-15:45		Tobias Schülli	*Operando Spatio-Temporal Imaging of Devices and Functional Nanostructures by X-ray Nano Diffraction Imaging Methods*
15:45-16:00		**Coffee Break**	
16:00-16:15			
16:15-16:30	X: Related Tech. Chairs: Oleg Gorobtsov & Ivan Vartaniants	Sharon Shwartz	*Quantum X-rays: Emerging Opportunities for Imaging, Spectroscopy, and Metrology*
16:30-16:45			
16:45-17:00		Jesper Wallentin	*In Situ Nanofocused Microsecond XPCS Enables Spatiotemporal Mapping of 8 nm-Diameter Nanoparticle Diffusion During Mesocrystal Assembly*
17:00-17:15	Poster Session 2	**Poster Session 2**	
17:15-17:30			
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18:45-19:00		**Transfer to ZKM**	
19:00-19:15	Conference Dinner	**Conference Dinner at ZKM** **Sponsored by DECTRIS Ltd.**	
19:15-19:30			
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22:45-23:00		**Transfer to GenoHotel**	

Friday, 25.09.2026

08:30-08:45	XI: High-Throughput, In Situ & Operando Chairs: Anton Plech & Christian Schlepütz	Christian Schlepütz	*Imaging Materials in Motion: From Sheared Foams to Human Middle Ear Mechanics*
08:45-09:00			
09:00-09:15		Leonardo Oliveira	*Imaging Pressure-Nucleated and Field-Erased BiFeO3 Domains via In-Situ Nano-XRD*
09:15-09:30		Tomáš Faragó	*Towards Serial Computed Tomography*
09:30-09:45		Thomas Cornelius	*Shape Memory Zirconia-Based Ceramic Micropillars Studied by in Situ Laue Microdiffraction*
09:45-10:00		Aleksandr Goikhman	*Compact PLD Sample Environments for In-Situ X-ray Studies of Thin-Film Growth at Synchrotron Beamlines*
10:00-10:15		Hongjian Wang	*Neuromorphic X-ray Radiographic and Tomographic Imaging*
10:15-10:30		**Coffee Break**	
10:30-10:45			
10:45-11:00		Thomas van de Kamp	*High-Throughput Digitization of Insect Morphological Biodiversity*
11:00-11:15		Guillaume Freychet	*Resonant Tender X-ray Scattering and Diffraction: A Key Tool to Reveal the Location of Counterions in Polymeric Organic Mixed Ionic/Electronic Conductors*
11:15-11:30	XII: Diffr. Contrast Imaging - 2/2 Chairs: Nathalie Mangelinck-Noël & Tamzin Lafford	Konrad Prikoszovich	*Effect of the Initial Strain State on the Evolution of the Average Elastic Strain Tensor for 2000+ Grains in Armco Iron During Elastic Loading*
11:30-11:45		Lucia Puertas Pelaez	*Multimodal 3D X-ray Imaging of Grain Boundary Migration at Triple Junctions*
11:45-12:00		Dina Carbone	*New Insight onto the Metal to Insulator Transition in Ca2RuO4*
12:00-12:15		Carsten Richter	*Evolution of Dislocations Throughout the Seeded Growth of AlN Crystals Investigated by 3D X-ray Diffraction Imaging.*
12:15-12:30		Carsten Detlefs	*From Grain Maps to Dislocation Dynamics: A Multimodal Diffraction Microscopy Framework for Bulk Microstructure Evolution*
12:30-12:45		**Conference Closing**	
12:45-13:00			
13:00-13:15		**Packed Lunch**	
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Status as of 15 September 2026

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Tutorial

Session Chair

Tilo Baumbach

Coherent X-rays and Applications: CDI and Ptychography

Vincent Favre-Nicolin[1]
[1] *ESRF, Grenoble France*

Presentation type: Tutorial Lecture **Presentation time:** 09:00-10:00

In this tutorial we will introduce the notion of coherence for X-rays, starting from the interference of electromagnetic waves. We will distinguish longitudinal coherence, which is set by the monochromaticity of the beam, from transverse coherence, which depends on the source size and distance, and we will see what coherence lengths can be expected at modern synchrotrons and XFELs.

We will then look at what happens when a sample is illuminated coherently: the far-field diffraction pattern becomes the Fourier transform of the object, producing speckle and, in principle, allowing an image to be reconstructed. Since only intensities are measured, we will discuss the phase problem and the iterative algorithms used to solve it.

Finally, we will present Coherent Diffraction Imaging, whose resolution is set by the extent of the measured scattering rather than by the optics, and Ptychography, which extends the approach to large objects.

Phase-contrast and dark-field imaging for biomedical applications

Julia Herzen[1]
[1] *TUM, Munich, Germany*

Presentation type: Tutorial Lecture **Presentation time:** 10:30-11:30

The development of highly coherent X-ray sources from third-generation synchrotrons to today's diffraction-limited storage rings and X-ray free-electron lasers has significantly expanded the capabilities of X-ray imaging. Phase-contrast imaging utilizes the refraction of X-rays rather than their attenuation, offering greatly enhanced sensitivity to soft biological tissues, where traditional absorption contrast falls short. The dark-field imaging method, on the other hand, accesses small-angle scattering and can reveal sub-resolution microstructures, such as the alveolar architecture of lung tissue or microcalcifications in breast tissue.

This tutorial introduces the physical principles underlying both contrast mechanisms, starting with the complex refractive index and explaining how absorption, phase shift, and scattering contribute to three complementary imaging channels. The focus is primarily on imaging at the micrometer scale, specifically micro-CT. We will then survey the main experimental methods used, categorizing them into two groups: optics-free techniques and optics-based methods. The optics-free approach includes pure propagation-based imaging. The optics-based methods are more diverse, employing gratings, apertures, and related wavefront markers. We will discuss the strengths, limitations, and dose considerations associated with each.

Finally, we highlight representative biomedical applications, ranging from high-resolution imaging of soft tissues and biomaterials to preclinical studies, and outline the current challenges in achieving quantitative and dose-efficient imaging.

X-ray Microscopy Techniques

Julie Villanova[1]
[1] *ESRF, Grenoble France*

Presentation type: Tutorial Lecture **Presentation time:** 11:30-12:30

X-ray microscopy covers a range of techniques that enable the imaging of samples in 2D and 3D using X-ray beams, providing information on their microstructure and chemical composition with spatial resolutions ranging from the micrometer to the sub-micrometer scale. This tutorial will introduce the different existing experimental setups and the main techniques used for X-ray microscopy.

The tutorial will focus particularly on synchrotron hard X-ray full-field 3D nano-imaging, including recent developments in the field that are pushing the limits of spatial and temporal resolution, enabling increasingly detailed characterization of complex materials. The principles and specific features of the main approaches used for 3D X-ray nano-imaging, as well as the challenges associated with sample preparation, data acquisition, and image reconstruction will be discussed. A dedicated section will focus on in situ and operando studies. Each case will be illustrated with applications mainly related to materials science.

Finally, particular emphasis will be placed on the correlation of X-ray full-field nano-imaging with complementary 2D and 3D nano-analysis techniques, as combining structural, morphological, and chemical information at different length scales can provide a more comprehensive understanding of heterogeneous and complex materials.

Diffraction Imaging at Synchrotron Light Sources: From Topography to Coherent Nanoprobes

Tobias Schülli[1]
[1] *ESRF, Grenoble France*

Presentation type: Tutorial Lecture **Presentation time:** 14:00-15:00

Diffraction imaging — the class of techniques that combines the structural sensitivity of X-ray diffraction with spatially resolved measurement — has undergone a profound transformation over the past three decades. What began with X-ray topography, a near-field technique exploiting the direct projection of diffraction contrast onto a detector or a film placed close to the sample, has evolved into a rich family of far-field methods that extract structural information from the angular distribution of scattered intensity.

This tutorial introduces the conceptual foundations of diffraction imaging and traces a path from the very idea to most advanced implementations. We begin with X-ray topography as a reference point: a technique requiring no focusing optics, exploiting near-field geometry defects across large crystal volumes with sensitivity to individual dislocations. Its simplicity, directness, and continued relevance at modern synchrotron sources make it the natural starting point for understanding what diffraction imaging fundamentally achieves.

We then examine how the transition to far-field geometry — where the detector records the full diffraction pattern rather than a direct image — opens access to a qualitatively different regime of information. Using X-ray optics, scanning nanobeam X-ray diffraction is a prominent and widely established example. Its full-field counterpart places the optics in the diffracted beam and is referred to as Dark Field X-ray Microscopy (DFXM). Both techniques see a rapid pick-up by different user communities and examples show their relevance in areas ranging from semiconductors to metallurgy.

As the far-field encodes phase as well as amplitude, the family of diffraction imaging methods is completed by Bragg Coherent Diffraction Imaging (BCDI) and Bragg ptychography enabling computational image reconstruction. This shift, made practical by the coherence properties of third- and fourth-generation synchrotron sources is currently further progressing thanks to the improvement of reconstruction algorithms.

For each technique we discuss the resolution-determining factors, and the trade-offs between field of view, spatial and strain resolution. Special attention is given to operando capabilities, which have made diffraction imaging an indispensable tool for studying materials under realistic functional conditions in semiconductors, battery electrodes, and catalytic systems.

Recent experimental results from the ESRF illustrate these capabilities concretely, demonstrating how the new coherent flux delivered by fourth-generation sources is reshaping what is experimentally achievable — and pointing toward the opportunities that other facilities will be able to bring to this field in the coming decade.

X-ray scattering by nanostructure

Stefan Kowarik[1]
[1] *University of Graz, Graz, Austria*

Presentation type: Tutorial Lecture **Presentation time:** 15:00-16:00

X-ray scattering links nanoscale structure to reciprocal-space intensity. The tutorial introduces diffraction, SAXS, GISAXS and GID for layers, nano-wires and -dots, emphasizing finite-size shape, strain and truncation rods. Complementing the microscopy tutorials on individual objects, the focus here is on scattering from statistical ensembles.

I: Diffraction & Scattering - 1/2

Session Chairs

Stefan Kowarik
Jörg Grenzer

Nanodiffraction for spatially-resolved studies of complex materials

Ivan Zaluzhnyy[1]
[1] *Universität Tübingen, Germany*

Presentation type: Invited Talk **Presentation time:** 09:00-09:30

X-ray diffraction has been used to study the structure of well-ordered crystalline materials since its discovery about a century ago. Nowadays, the excellent parameters of the new synchrotron sources allow us to focus the X-ray flux to a nanometer-scale spots. Apart from the obvious advantages of studying nanoscale objects with a focused x-ray beam, it is also possible to perform a raster scan of a larger sample to obtain spatially-resolved information of its structure. This is especially advantageous to characterize the fabricated nanodevices or study the structure of novel non-crystalline materials. Depending on the typical length scale of the non-uniformity of the sample, different size of the x-ray beam should be chosen.

This talk will be focused on spatially resolved studies of superlattices performed at the Coherence beamline P10 of PETRA III. These superlattices are formed from lead-halide perovskite nanoparticles coated with organic ligands. By utilizing the raster scan with an x-ray beam focused to approximately 200 nm, and measuring simultaneously SAXS and WAXS signal with a 2D detector, it is possible to determine the structure of the superlattice and characterize the properties of individual nanoparticles in the superlattice.

References

[1] D. Lapkin, et al., Nat. Commun. 13 (2022) 892
[2] J. Hiller et al., ACS Nano 19 (2025) 26117
[3] J. Hiller et al., Nano Lett. 26 (2026) 2955

XRR with nanometre beams - Characterising micrometre surfaces

Steffen Tober[1], Andreas Stierle[2], Hans-Georg Steinrück[3], Vedran Vonk[4], Jiangtao Zhao[5], Steven Leake[5], Azat Khadiev[1], Wieland Corts[6], Toka Matar[6], Lisa Randolph[6], Breno Rabelo Couthino Saraiva[7]

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Presentation type: Oral **Presentation time:** 09:30-09:45

The use of X-ray reflectivity (XRR), an established method for non-destructive probing of electron density profiles of semiconductor [1], polymer [2] or model catalyst [3] surfaces and interfaces with sub-nm-resolution, so far is limited to flat, mm-sized samples. The large effective footprint of the X-ray beam at relatively small incident angles results in a spillover that significantly reduces the reflected signal and increases the background for smaller samples. To study smaller samples such as dispersed catalyst particles or individual particles of multigrain catalysts, a significant reduction of the footprint is necessary.

As demonstrated for crystal truncation rods by Stubbs et al., the nm-sized X-ray beams of modern synchrotron sources with a correspondingly small footprint can be used for XRR on µm-sized samples [4]. Small sample and beam sizes, however, require a precise positioning procedure of the sample to ensure reliable measurements [5].

We present proof-of-principle studies comparing the nanobeam XRR of mm- and µm-sized thin-film samples (Au/Ti on Si) measured with 400 and 80 nm X-ray beams at ESRF ID01 focused using compound refractive lenses (CRL) or Fresnel zone plates (FZP), respectively [6]. Our results show a reasonable agreement between XRR on mm- and µm-sized parts of the sample and thereby the general feasibility of XRR of µm-sized samples using nm-sized beams. Adjustments to the scan procedure allowed a reliable, precise positioning of the beam on the sample and are expected to enable adapting our method for studies of catalysts under in situ and operando conditions.

References

[1] S. L. Moffitt et al., JPCC 127 23099 (2023)
[2] P. Lakner et al.,Langmuir 36 13448 (2020)
[3] R. Gleißner et al., ACS Appl. Nano Mater. 6 8004 (2023)
[4] J. Stubbs et al., Clays Clay. Miner. 69 688 (2021)
[5] V. Vonk et al. J. Appl. Cryst. 58 1978 (2025)
[6] S. J. Leake et al., J. Synchrotron Rad. 26 571 (2019)

X-Ray Reflectivity and Reciprocal Space Mapping with a Micro-Focus Rotating Anode: From Micon-Sized Beams to Fractional-Order Bragg Peaks

Yorick Alexander Birkholzer[1], Martin Zimmermann[2], Fernando Rinaldi[3]
[1] *Cornell University, Germany*
[2] *BAXS, Germany*
[3] *Bruker AXS SE, Germany*

Presentation type: Oral **Presentation time:** 09:45-10:00

Historically, high beam flux and large detectors were accessible only at synchrotron light sources. Using the latest generation high-brilliance microfocus rotating anode generator and a large area hybrid photon counting detector in a custom-build diffractometer manufactured by Bruker AXS, we now have access to very weakly scattering features, such as non-integer Bragg reflections, that are notoriously hard to capture and were previously inaccessible to laboratory-based XRD tools.

In this talk, we will show some highlights of the research we have performed with this unique tool over the past six years at the MESA+ Institute for Nanotechnology at the University of Twente on epitaxial complex oxide thin films grown by the pulsed laser deposition technique. To showcase the unprecedented scanning and mapping capabilities of the state-of-the-art tool both in real space as well as in reciprocal space, we present three case studies, which all benefit from the availability of an intense, well-collimated, and monochromatic X-ray beam with a small footprint and a 2D detector with high dynamic range (EIGER2 R 500K by Dectris).

Firstly, we demonstrate how microfocus X-ray reflectivity (XRR) allows us to elucidate the lateral thickness gradient in a complex oxide heterostructure (LaAlO3 / SrTiO3) wedge sample of few unit cells thickness and correlate this data with reflection high-energy electron diffraction (RHEED) data – a widely used tool to study the growth dynamics of thin films, in situ and operando [1]. Going beyond reflectivity, we show how microfocus X-ray diffraction (XRD) allows us to systematically study compositional gradients in off-center deposited BaTiO3 thin film wedges [2].

Secondly, we show high-resolution X-ray diffraction (XRD) measurements on lithographically defined ferroelectric thin films (BiFeO3 / DyScO3 and PbZr0.55Ti0.45O3 (PZT) / SrTiO3), using an X-ray beam size of only 20 micrometer to probe individual microcapacitors and reconstruct 3D reciprocal space maps [2, 3]. Thirdly, we show how laboratory-source 3D RSMs can detect off-specular fractional-order Bragg peaks in a coplanar asymmetrical experimental geometry. Showcasing the example of PbZrO3/Pb0.9La0.1Zr0.52Ti0.48O3 multilayers, the analysis of weak superstructure reflections inaccessible to most thin-film diffractometers with line-focus beams and small detectors, revealed the formation of interfacial layers with rotated polarization that greatly enhanced the energy storage density and breakdown strength [5].

References

[1] Smink et al., Physical Review Materials 4 (8), 083806 (2020)
[2] Avila et al., Journal of Crystal Growth 668, 128313 (2025)
[3] Haykal et al., Nature Communications 11, 1704 (2020)
[4] Lucke et al., Advanced Functional Materials 30 (52), 2005397 (2020)

Real-time manipulation of Ag thin film growth studied by GISAXS

Michal Kaminski[1], Bärbel Krause[1], Anny Michel[2], David Babonneau[2], Gregory Abadias[2], Karan Solanki[2], Alessandro Coati[3], Andrea Resta[3], Alina Vlad[3], Yves Garreau[3], Jixing Xu[4]

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[3] *Synchrotron SOLEIL, France*
[4] *Karlsruhe Institute of Technology (KIT), Germany*

Presentation type: Oral **Presentation time:** 10:00-10:15

Silver thin films are used in a number of applications (e.g., transparent and conductive electrodes and plasmonic devices) which require a continuous layer with thickness of a few nanometers. However, Ag films grown by magnetron sputtering have the tendency to form 3D-structures on weakly interacting substrates, what prevents their application as transparent and conductive layers. It is reported that the use of gas additives (particularly N2 [1]) allows for obtaining a continuous layer at earlier deposition stage.

Using a combination of real-time techniques (grazing incidence small-angle x-ray scattering (GISAXS), grazing incidence diffraction (GID), and substrate curvature measurements) [2, 3] we can access the continuous changes in dynamics of the thin film structure formation. It was reported that application of gaseous N2 at the early stages of the growth suffices to achieve faster continuity [1]. We get a deeper insight into the impact of N2 on the growth mechanisms by investigating the growth with N2 flux varying during the deposition and determining a time-dependent evolution of the nano-clusters size and distribution. We supplement these findings by the results provided by laboratory diagnostic tools. For example, x-ray photoelectron spectroscopy (XPS) gives additional information on the chemistry of the substrate (nitradation) and as-grown layer. We will discuss the impact of nitrogen additive on all growth stages (from initial stages of island nucleation, growth, and coalescence, up to formation of percolated and continuous films).Acknowledgements: The work is performed within the frame of the ANR-DFG project IRMA (491224986).

References

[1] A. Jamniget al., ACSAppl. Nano Mater. 3, 4728-4738 (2020)
[2] B. Krause et al., ACSAppl. Mater. Interfaces 15, 11268-11280 (2023)
[3] M. Kaminskiet al., J. Appl. Cryst. 59 (2026)

Structure of Protein Cage Supercrystals Revealed by Angular X-ray Cross-Correlation Analysis

Ivan Vartaniants, Gerard Hinsley[1], Kuan Hoon Ngoi, Laurin Lang, Young Yong Kim, Niclas Mucke, Dongwon Kim, Michael Rütten, Lars Klemeyer, Maximilian Ruffer, Varnika Yadav, Henrike Wagler, Tobias Katenkamp, Markus Perbandt, Azat Khadiev[2], Dmitri Novikov[1], Tobias Beck

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Presentation type: Oral **Presentation time:** 10:15-10:30

Biohybrid supercrystals are highly ordered 3D assemblies of protein nanocages, offering versatile structural designs through the selection of protein nanocages and their ability to encapsulate various cargos within their cavities. By loading nanoparticles into these nanocages, diverse and complex superstructures can be engineered. In this study, individual biohybrid supercrystals are investigated using small-angle X-ray diffraction. As the samples may consist from single to several crystalline grains, angular X-ray cross-correlation analysis is used to analyze the angular correlations within the intensity distribution in 3D reciprocal space, enabling the determination of the unit cell parameters of the superlattice. Encapsulated nanoparticles serve as effective X-ray scattering markers, facilitating precise identification of the nanocage positions within the superlattice. The arrangement of nanoparticles in the unit cell is validated by comparing the experimental and calculated radial intensity profiles. The findings confirm the superlattice structures of unitary protein-nanoparticle composites, binary composites (including homobinary and heterobinary designs), and supercrystals with core-shell morphologies. Furthermore, single-grain and twin-domain structures are identified, demonstrating the capability of this technique for defect characterization and crystal engineering.

II: X-ray Microscopy

Session Chairs

Julie Villanova
Irina Snigireva

Novel imaging modalities enabled by multilayer Laue lenses

Saša Bajt[1]

[1] *Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Germany*

Presentation type: Invited Talk **Presentation time:** 11:00-11:30

Multilayer Laue lenses (MLLs) are the latest addition to the family of high-resolution X-ray optics. A MLL focuses X-rays only in one direction (just like a cylindrical lens or one-dimensional zone plate), so two MLLs with slightly different focal lengths are needed to produce a focused spot. Focusing to nanometer size beams is achievable but it requires structures fabricated to nanometer precision. Thestructures prepared in our lab using magnetron sputtering are typically 100 µm tall (aperture size) with focal lengths of about 1 to 15 mm, fabricated from many thousands of layers, each several nanometers thick [1]. These layers vary in spacing so as to diffract collimated light to a common focus according to the construction of Fresnel zone plates.For high efficiency, the thickness of these lenses must be several microns or even several tens of microns, depending on the multilayer materials and photon energy.The diffraction of such thick structures is governed by Bragg's law,implying that the layers must be tilted so as to reflect rays towards the focus. To obtain a high numerical aperture (NA) lens the layers have to be "wedged", meaning their interfaces must lie normal to a cylinder of radius equal to twice the focal length.

The development of our MLLs is guided by a wavefront characterization method based on a combination of interferometry and ptychography [2-3]. This enabled us to achieve a record focusing to sub-3 nm [4] and 3D imaging with sub-10 nm resolution of complex structures [5]. In this talk, novel imaging modalities enabled by high NA MLLs will be presented. One of them is Compton microscopy at very high photon energies [6-7], which is especially interesting for high resolution imaging of biological samples. However, our MLLs were also used to focus X-ray Free Electron Laser (XFEL) pulses [8] to image sub-micron crystals via convergent beam crystallography [9].

References

[1] Bajt et al.,Light Sci. Appl.7, 17162 (2018).
[2] Morgan et al.,J. Appl. Cryst.53, 927 (2020).
[3] Ivanov et al.,Opt. Express30, 25450 (2022).
[4] Dresselhaus et al.,Opt. Express32, 16004 (2024).
[5] Zhang et al.,Opt. Express32, 30879 (2024).
[6] Villanueva-Perez et al.,Optica 5, 450 (2018).
[7] Li et al.,Light Sci. Appl12, 130 (2023).
[8] Zakharovaet al.,Opt. Express33,31884(2025).
[9] Chapman et al.,Struct. Dyn.12, 014301 (2025).

Electron-tomography-informed super-resolved nano X-ray computed tomography

Benjamin Apeleo Zubiri[1], Umair Sultan[2], Nicolas Vogel[2], Erdmann Spiecker[1], Allison Götz[1], Dominik Drobek[1], Tom Kirstein[3], Niklas Eiermann[3], Volker Schmidt[3], Orkun Furat[4]

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[4] *SDU Applied AI and Data Science Unit, University of Southern Denmark*

Presentation type: Oral **Presentation time:** 11:30-11:45

Tomographic imaging techniques are crucial for establishing process-structure-property relationships. However, individual modalities face a fundamental field-of-view–resolution trade-off and modality-specific challenges that hamper quantification. Electron tomography (ET) provides nanometer to atomic resolution within few-micrometer to sub-micrometer volumes; employing 360°-ET mitigates the missing-wedge artefact. Nano X-ray computed tomography (nanoCT) extends coverage to specimens from a few micrometers up to ~100 µm at tens-of-nanometer resolution, but contrast is often dominated by Zernike phase contrast, where recorded intensities are nonlinearly related to attenuation or thickness and exhibit halo and shade-off artefacts. These effects complicate segmentation and subsequent quantitative analysis. Although phase-retrieval methods exist, solutions tailored specifically to Zernike phase-contrast nanoCT remain limited [1].

We introduce ET-informed nanoCT (ETiCT), a correlative, two-pronged strategy that leverages high-resolution ET to improve lower-resolution, larger-volume nanoCT. A terraced specimen from a porous silica monolith with an average mesopore size of 20 nm and a macropore size of 400 µm is fabricated via laser ablation (coarse shaping) and focused ion beam milling (final shaping) to match modality field-of-view and penetration constraints. Co-registered 360°-ET and nanoCT datasets provide aligned, multimodal inputs.

First, we perform supervised training of a classifier to achieve cross-modal segmentation of nanoCT using ET-derived annotations. This ET-informed classifier learns to discount Zernike halo and shade-off, yielding more accurate pore delineation and more reliable pore-size metrics than uninformed thresholding. Second, we achieve cross-modal super-resolution using a generative adversarial network (GAN) [2] trained on paired data from the same co-registered volumes: high-resolution ET images as targets and grayscale nanoCT images as inputs. The trained GAN generates super-resolved versions of nanoCT images that recover ET-resolved features and edges while retaining nanoCT volume sizes, thereby enhancing downstream segmentation and quantitative analysis.

ETiCT thus bridges scales and mitigates modality-specific limitations, delivering improved segmentation fidelity and enhanced effective resolution without sacrificing volume coverage. The workflow is practical and reproducible, enabling quantitative, scale-bridging 3D characterization of catalysts, battery electrodes, and related porous architectures. By integrating ET guidance into both segmentation and reconstruction via learning-based super-resolution, ETiCT advances correlative microscopy toward robust, artifact-aware analysis of hierarchical microstructures.

Acknowledgements:We gratefully acknowledge financial support by the German Research Foundation (DFG) within project IDs 416229255, 537140136, 431791331, 316992193.

References

[1] C. Zuo et al., Optics and Lasers in Engineering 2020, 135
[2] J. Song et al., Heliyon 2023, 9, e15134

Supersampling Scanning Transmission Microscopy: Unlocking sub-10 nm STXM Resolution

Benedikt Rösner[1], Simone Finizio[1], Markus Weigand[2], Lars Heller[1], Benjamin Watts[1], Sebastian Wintz[2], Tim Butcher[3], Jörg Raabe[1]

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[3] *MBI Berlin, Germany*

Presentation type: Oral **Presentation time:** 11:45-12:00

The SLS 2.0 upgrade comprised an increase in storage-ring energy from 2.4 to 2.7 GeV, and a significant reduction of horizontal emittance, converting the synchrotron to a so-called fourth-generation storage ring [1]. The new machine greatly benefits from an increase in brightness and brilliant flux. This brings major benefits for future experiments, not only for the use of photon-hungry and coherent techniques, but also for routine acquisition of high-resolution imagers in scanning X-ray transmission microscopy (STXM). Within this contribution, we present a newly developed STXM modality that combines this advantage with a paradigm change in how scanning is performed.

The resolution of STXM imaging is fundamentally limited by the size of the focused X-ray beam, usually focused by means of a Fresnel zone plate lens. The resolution cut-off of this method is usually linked to the outermost zone width of the zone plate: the focus size under coherent illumination conditions can be expressed as [2]. The resolution record using direct scanning has been demonstrated as low as 7 nm some years ago [3].

However, we observed already during these experiments that we approach a regime, where the resolution is not merely limited by the beam size, but also by other factors, such as mechanical vibrations. These vibrations, measured as relative positions between the X-ray lens and the sample stage, are typically in the magnitude of three to five nanometers rms on frequencies of several to some hundred Hz. Thus, both pixel-by-pixel and constant velocity line scan modes are inherently limited by these vibrations.

We now present a paradigm change in how we acquire scan images: instead of optimization and avoidance of vibrations, we read out the real sample position with respect to the beam at kHz rates. With this approach, we are not only able to bypass the inherent limitations from mechanical instabilities, but we are also able to reconstruct images using different criteria, such as noise limits, spatial or temporal resolution [4]. Besides, this method also avoids the high overhead times that are common for scanning on the nanometer level. Using experimental data and simulations, we demonstrate imaging resolutions that are half of the outermost zone width of the respective zone plate: with being the diffraction order of the zone plate lens. Future experiments comprise the use of higher diffraction orders to achieve even better imaging resolution, targeting routine resolution below 5 nm.

Crystallographic and Defect Analysis of Colloidal Photonic Supraparticles Using Zone-Axis Wide-Field XRM and NanoCT

Maik Becker[1], Benjamin Apeleo Zubiri[1], Federico Tomazic[2], Michael Engel[2], Nicolas Vogel[3], Erdmann Spiecker[1], Thomas Przybilla[1], Silvan Englisch[1], Johannes Voß[1], Lukas Roemling[3], Junwei Wang[3], Janis Wirth[1]

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Presentation type: Oral **Presentation time:** 12:00-12:15

Self-assembled colloidal supraparticles (SPs) are aggregates of primary particles that exhibit a wide range of structural configurations and associated optical properties [1]. For primary particle sizes on the order of 200–300 nm (e.g., polystyrene spheres), these assemblies can display photonic behavior in the visible spectral range, resulting in structural color. Such optical effects are most pronounced in highly-ordered, crystalline SPs, which can be fabricated, for instance, by ultraslow drying in spherical confinement. Typical structures include icosahedral, decahedral, and fully face-centered cubic (FCC) arrangements with octahedral symmetry. Scanning electron microscopy (SEM) is well suited to reveal surface morphology; however, access to the full internal 3D structure—including crystal defects and disordered regions—is essential to understand the origin and variation of structural color. Transmission-based imaging methods are therefore required. Due to their size, SPs lie at the upper limit of transmission electron microscopy and tomography (TEM/ET) [1], thereby motivating the use of X-ray microscopy (XRM) and tomography (nanoCT) as key techniques for volumetric characterization [2].

In this contribution, we investigate the 3D structure of crystalline SPs and their defects using a combination of electron and X-ray transmission microscopy/tomography. Drawing parallels to crystalline nanoparticles, which are commonly analyzed by high-resolution (S)TEM along low-index zone axes, we establish an analogous approach in XRM to access crystallographic information in larger assemblies. To this end, we employ a dedicated sample holder setup that enables precise and reproducible tilting of individual SPs, allowing controlled alignment along specific crystallographic directions. We demonstrate this capability by orienting a decahedral SP along its five-fold twin axis to analyze internal defect structures and compare them with simulations, as well as by imaging FCC SPs along different low-index zone axes. While high-resolution, 2D projections already allow the identification of planar defects, the detection and quantification of point defects necessitate volumetric imaging.

To further relate structure to optical response, we complement the experimental analysis with optical simulations based on the reconstructed particle configurations. These simulations enable systematic investigation of how structural motifs and defects influence scattering, color formation, and image contrast in optical microscopy. By linking three-dimensional structure, defect distribution, and optical signatures, this work provides deeper insight into structure–property relationships in colloidal supraparticles and supports their targeted design as photonic materials.

Acknowledgements. Financial support by the Deutsche Forschungsgemeinschaft (DFG) (project No. 416229255, 537140136)

References

[1] J. Wang et al., Nat. Comm. (2018) 9, 5259
[2] S. Englisch et. al., Microsc. Microanal. (2022) 28 (Suppl. 1), 306.

Hard X-ray holographic projection microscopy using multilayer Laue lenses for hierarchical 3D imaging

Mathias Hurst[1], Tilo Baumbach[2], Marcus Zuber[2], Saša Bajt[3], Mauro Prasciolu[3], Naufal Ismail Kreshnaviyanto[3], Henry Chapman[3], Daniel Hänschke[1], Elias Hamann[1], Mateusz Czyzycki[1], Jia Chyi Wong[4], Wenhui Zhang[3], Margarita Zakharova[3], Rolf Simon[1], Sven Niese[5]

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Presentation type: Oral **Presentation time:** 12:15-12:30

We introduce nanoimaging capabilities based on multilayer Laue lenses [1] (MLLs) coupled to high-Z single-photon counting detection systems for holographic projection microscopy [2]. This approach enables high sensitivity, fast measurement, outstanding zooming capabilities, and spatial resolutions ≲50 nm. Operating at hard X-ray energies of 30 keV allows penetration of macroscopic specimens while maintaining sufficient contrast for small features close to the resolution limit.

Optimized image quality is achieved through detailed studies of MLL aberrations and their impact on propagation-based phase contrast imaging. In particular, the influence of optical distortions of different MLL geometries, namely flat and wedged designs, is investigated. This analysis enables the selection of optimal multilayer structures and ensures precise alignment conditions for high-quality imaging [2].

The presented development aims to provide nanoscale three-dimensional imaging with zoom functionality at the novel HiKA (Hierarchical Imaging Karlsruhe) end station located at the P23 beamline of the PETRA III storage ring at DESY. The HiKA station is a synchrotron-based X-ray imaging platform dedicated to hierarchical full-field imaging, integrating zoom capabilities from macro- to nanoscale resolution for computed tomography and computed laminography within a single experimental station. The combination of MLL-based cone beam and parallel beam imaging facilitates imaging with fields of view of a few centimetres down to a few tens of micrometres.

This combined approach enables non-destructive zoom imaging of extended specimens and devices by addressing the trade-off between sample size and local high-resolution imaging through optimization across the full imaging pipeline. Key components include highly sensitive detection using high-Z single-photon counting detectors, dedicated tomographic measurement geometries such as computed laminography [3], phase-contrast imaging [4], hierarchical guidance for identification and selection of regions of interest [5], and correlative imaging techniques using visible light.

The instrument is designed to support applications across materials science, engineering, and life sciences, enabling the investigation of complex hierarchical structures and processes over multiple length scales.

References

[1] Bajt et al., Light Sci. Appl.7, 17162 (2018).
[2] Hurst et al., under submission, (2026)
[3] Hurst et al., Int. J. Plast., in press, (2026).
[4] Faragó et al., Opt. Lett.49, 5159–5162 (2024).
[5] Hurst et al.,Sci. Rep.13, 1055 (2023).

III: New Instrumentation

Session Chairs

Tobias Schülli
Cristian Mocuta

MHz X-ray Tomoscopy: rotation-free 4D imaging with diamond Bragg beam-splitter optics at the European XFEL

Patrik Vagovič[1], Wolfgang Voegeli[2], Alexander Korsunsky[3], Jayanath Koliyadu[1], Pascal Kaul[4], Mohammad Shahsavari, Pontus Fischer[1], Daniel Mosko[5], Peter Szeles[6], Sotirios Damianos[7], Manolis Gavaises[8], Tomas Burian[9], Zuzana Kuglerova[10], Jaromir Chalupsky[10], Libor Juha[10], Yashiro Wataru[11], Hitoshi Soyama[11], Liubov Samoylova[12], Rita Graceffa[12], Luigi Adriano, Chan Kim[12], Igli Draci[6], Jozef Ulicny[6], Vid Angrez[13], Jaka Mur[13], Patricia Pfeiffer[14], Claus-Dieter Ohl[14], Egor Sobolev[12], Tomas Popelar[12], Richard Bean[12], Henry Chapman[15], Tokushi Sato[12], Daniel Eakins[16], Alke Meents[1]

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Presentation type: Invited Talk **Presentation time:** 14:00-14:30

Capturing three-dimensional dynamics that evolve faster than a sample can be rotated is a long-standing limitation of time-resolved X-ray tomography. Tomoscopy, volumetric imaging of fast dynamic processes, can be realised by fast sample rotation or, rotation-free, by simultaneous multi-projection imaging, originally proposed using Laue beam splitters. We present a rotation-free X-ray tomoscopy in which a cascade of thin diamond high-pressure high-temperature type-IIa crystals, operated in Bragg geometry, splits a single X-ray pulse into several mutually inclined, monochromatic beamlets and redirects them through a common point at the sample. Each beamlet is recorded simultaneously on its own ultrafast detector, so a complete set of angular projections of one identical sample state is acquired in a single exposure. Because every projection originates from the same pulse, the volumetric frame rate is set by the source repetition rate rather than by mechanical motion.

The crystal optics are central to the method. Operating in the vertical diffraction plane (sigma-polarisation, polarisation factor C = 1) and using diamond for its high reflectivity and thermal stability under the XFEL pulse train, the inline Bragg-splitter cascade is photon-energy tunable and scalable toward about ten projections at hard X-rays. This overcomes the low throughput and lack of photon-energy tunability of earlier Laue-splitter realisations of multi-projection imaging, which limited that approach at large-scale facilities. Here, the (111), (220), (311) and (422) reflections provide four simultaneous views at 10 keV.

We report the first fully functional four-projection MHz tomoscopy system at the SPB/SFX instrument of the European XFEL, developed within the EIC Pathfinder project MHz Tomoscopy, with first feasibility at the European XFEL and a subsequent synchrotron demonstration. At

storage rings the roughly one billion photons per pulse provide only a million to ten million photons per beamlet, so imaging there must integrate over many pulses and is confined to kilohertz rates. Exploiting the high single-pulse flux of the XFEL, tomoscopy reconstructs a full volume from every femtosecond pulse at the 1.128 MHz intra-train rate, two to three orders of magnitude faster. Using inline phase contrast and per-pulse reconstruction, we follow the complete nucleation, expansion and collapse of a laser-induced cavitation bubble in water. Tomoscopy further offers an intrinsic split-and-delay capability, with geometrical inter-beamlet delays of about 50 to 500 picoseconds for single-shot imaging of ultrafast phenomena relevant to fusion research. The apparatus is protected by patent EP4160623A1.

Shear wave propagation imaged inside crystalline semiconductors after below melting threshold using Diffraction Near Field X-ray Microscopy

Angel Rodriguez Fernandez[1], Jan Siegel, Javier Solis, Jan-Etienne Pudell, Roman Shayduk, Joerg Hallmann, Alexey Zozulya, James Wrigley, Anders Madsen, Johannes Moeller, Klaus Sokolowski-Tinten, Thies Albert, Dominik Kaczmarek, Pablo Villanueva-Perez, Zdenek Matej, Ryszard Sobierajski, Oleksi Liubchenko, Jerzy Antonowicz, Belen Valiente Pascual, Alejandro Fraile

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Presentation type: Oral **Presentation time:** 14:30-14:45

Material processing with femtosecond lasers has attracted enormous interest over the past decades due to the countless potential applications in technology and industry. One key aspect of their performance is the reduced thermal load, enabling the fabrication of smaller and sharper feature sizes, as well as enabling surface and sub-surface processing of transparent materials. This advantage can be implemented by using laser pulses that are shorter than the time it takes for the strongly excited electron subsystem to transfer its energy to the lattice (typically a few ps). Such pulses can generate highly non-equilibrium states and trigger structural changes within a few hundred fs. The processes involved are almost instantaneous non-thermal melting of a surface layer of several tens of nm, followed by the inward propagation of a sharp melt-front, as well as shock wave propagation into the material.

Time-resolved X-ray diffraction has been successfully used to study non-thermal melting in semiconductors thin films. But, most “real-world” processing applications deal with bulk materials. We have developed a novel technique for imaging ultrafast deformations along the depth in thick crystalline wafers. The technique is based on the ultrafast dynamical diffraction process observable in perfect crystals and the temporal information encode in the Borrmann fan. To this end, we have recently performed a fs laser pump (800nm) - fs X-ray probe (9 keV) experiment at the European XFEL facility. During the experiment, thin Si wafers (300 µm) were investigated as a function of pump laser fluence and delay time. To understand the experimental data we have extended the dynamical diffraction model in to include the ultrafast distortion generated by a laser pulse following the Thomsen model and applied it to the experimental data. This new single shot wavefront sensing reveals the dynamics of laser-induced processes over a wide temporal window along the entire thickness of the crystal wafers.

First results clearly demonstrate the high sensitivity of the technique to small distortions of the lattice cell along the depth of the semiconductor crystal, revealing a shear strain deformation not expected from previous studies performed using conventional pump-probe XRD techniques at fluences below the melting threshold. This new experimental data contradicts previous models of the strain wave propagation, presenting a possible mechanism of coupling between the elastic and plastic deformation at higher fluencies [1].

References

[1] Orthogonal lattice distortions inside crystalline Si upon sub-threshold femtosecond laser-induced excitation A. Rodriguez-Fernandez et al. arXiv:2503.10420

Time-resolved 3D imaging opportunities with XMPI at ForMAX

Julia Rogalinski[1], Malgorzata Grazyna Makowska[2], Yuhe Zhang[3], Pablo Villanueva Perez[1], Zisheng Yao[1], Zhe Hu[1], Jackson Da Silva, Vahid Haghighat[4], Samuel McDonald, Kim Nygård[4], Andrea Mazzolari, Korneliya Gordeyeva, Tijana Todorovic, Saeed Davoodi, Daniel Söderberg, Tomas Rosén, Lars Witte, Eliot Jermann, Patrick Wegele, Alexander Grötsch, Jonas Tejbo, Elise Van Vlierberghe, Christian Breite, Yentl Swolfs, Jeroen Soete, Eleni Myrto Asimakopoulou, Eva Malmström Jonsson, Linda Fogelström

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[4] *MAX IV Laboratory - Lund University, Sweden*

Presentation type: Oral **Presentation time:** 14:45-15:00

With the advent of fourth-generation diffraction-limited storage rings (DLSRs), the brightness of synchrotron light sources has increased by several orders of magnitude compared to their predecessors, opening new opportunities for time-resolved X-ray imaging. This enables novel X-ray imaging approaches and opens up previously inaccessible temporal and spatial regimes.

X-ray Multi-Projection Imaging (XMPI) [1] is a method that benefits from the increase in photon flux density at DLSRs, i.e., the number of photons per unit of area and time. It enables the acquisition of time-resolved three-dimensional data (4D) without requiring sample rotation by splitting the incident beam into multiple beamlets that illuminate the sample from different angular directions and are detected simultaneously. Thus, key limitations of conventional time-resolved tomography, such as centrifugal forces and constraints on rotation speed, can be circumvented.

This presentation will discuss the implementation of XMPI at the ForMAX beamline at MAX IV [2], the first operational DLSR. We will present experimental results from representative applicationswith acquisition rates up to one order of magnitude higher than the current limit of time-resolved tomography (1 kHz) [3] with micrometer resolution. Particularly, we will show sample dynamics such as in situ tensile loading of cellulose fibers and wood-adhesive joints, multiphase flows, and additive manufacturing. These examples highlight the potential of XMPI for capturing fast dynamics in complex systems, taking into account their respective spatiotemporal regimes.

We further discuss key technical challenges associated with XMPI, including the design and performance requirements of X-ray beamsplitters, the heat load imposed on the beamsplitters and the image reconstruction from a limited number of projections. Finally, we outline future prospects for XMPI at ForMAX, paving the way for insights into dynamic processes in materials and life sciences.

References

[1] Asimakopoulou, Eleni Myrto, et al. ”Development towards high-resolution kHz-speed rotation-free volumetric imaging.”Optics express32.3 (2024): 4413-4426.
[2] Rogalinski, Julia Katharina, et al. ”Time-resolved 3D imaging opportunities with XMPI at ForMAX.”Synchrotron Radiation33.2 (2026).
[3] García-Moreno, Francisco, et al. ”Tomoscopy: time-resolved tomography for dynamic processes in materials.” Advanced Materials 33.45 (2021): 2104659.

Synchrotron Laminography for Multimodal, Hierarchical, and in situ 3D Imaging

Simon Bode[1], Daniel Hänschke[2], Tilo Baumbach[1], Elias Hamann[2], Mathias Hurst[2], Tomáš Faragó[1], Marcus Zuber[1], Lukas Helfen[3]

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Presentation type: Oral **Presentation time:** 15:00-15:15

In collaboration with DESY and ESRF, KIT has substantially expanded its computed laminography (CL) instrument portfolio by refurbishing ID19 beamline's LAMINO I station at ESRF, constructing the new LAMINO II station at the IMAGE beamline at the KIT Light Source, and commissioning the laminography mode at the new HIKA station at PETRA III's P23 beamline. CL enables the three-dimensional imaging of laterally extended specimens that may vastly exceed the detector field of view. The instruments take advantage of the specific properties of their respective storage rings and beamline optics to offer a variety of contrast mechanisms, energy ranges, band-widths, fields of view, and spatial resolutions.

With continuous development driven by new applications, today these instruments enable hierarchical, non-destructive imaging workflows ranging from large-area screening to local high-resolution investigations, extending to nanoscale resolution by combining CL with magnified projection microscopy [1]. Online reconstruction and volume stitching further allow immediate inspection, e.g., for quality assurance or region-of-interest identification. The integration of dedicated sample environments for mechanical loading, stress testing, and operando device characterization, together with correlative techniques like optical microscopy, enable in situ and operando studies of dynamic processes under application-relevant conditions through multimodal approaches across multiple length scales.

Here, we will present our current capabilities of hierarchical large-area CL for the investigation of plate-shaped fossils. Moreover, we will show the recent progress in multimodal and correlative studies of metal-sheet deformation [2], operando investigations of battery degradation during cycling [3], and monitoring battery failure in simulated crash scenarios using a dedicated indentation chamber [4].

References

[1] Hurst et al., Hierarchically guided in situ nanolaminography for the visualisation of damage nucleation in alloy sheets, Sci. Rep. 13, 1055, 2023
[2] Hurst et al., Particle-induced void growth under shear loading revealed by 3D X-ray laminography and finite element modelling, Int. J. Plast., accepted, 2026
[3] Du et al., 3D hierarchical characterisation of degradation and failure in all-solid-state-battery by synchrotron X-ray computed laminography, under review, 2026
[4] Tancogne-Dejean et al., Fracture is not enough: interlayer destabilization drives battery short circuits under mechanical abuse, under review,2026

Advancing Synchrotron Imaging using Next-Generation Hybrid Photon Counting Detectors

Tilman Donath[1], Sascha Grimm[2], Filippo Baruffaldi[2]
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[2] *DECTRIS AG, Germany*

Presentation type: Oral **Presentation time:** 15:15-15:30

The evolution of synchrotron light sources toward diffraction-limited storage rings fundamentally expands the scope of X-ray imaging. Beyond the traditional absorption-based techniques, it opens multidimensional and coherent methods allowing for the characterization of materials with unprecedented spatial and temporal resolution. This progress is going hand in hand with the development of Hybrid Photon Counting (HPC) detectors capable of handling extreme fluxes while maintaining high frame rates and a wide dynamic range.

This work explores four key frontiers in synchrotron imaging enabled by recent detector advancements. First, we discuss high-speed coherent imaging, where new ASIC architectures enable frame rates up to 120 kfps, facilitating ptychographic measurements that resolve the high-intensity gradient between the central beam and diffuse scatter [1,2]. Second, we present a demonstration of soft X-ray ptychography, utilizing LGAD-based sensors as an ongoing development to extend photon-counting capabilities below 1 keV for the study of light elements and magnetic systems [3].

Furthermore, we highlight the rise of scanning-based multidimensional tomography, such as XRD-CT and SAXS tensor CT. By utilizing high-Z sensor materials (CdTe) and high-speed readouts, it is now possible to map chemical phases and nanoscale orientations in 3D during operando processes, such as battery cycling [4,5]. Finally, we demonstrate the clinical potential of propagation-based phase-contrast imaging, showing enhanced soft-tissue visualization in lung phantoms [6]. Together, these applications illustrate how modern detection technology acts as the primary bridge between the increased brilliance of 4th-generation sources and new scientific insights in materials and life sciences.

References

[1] S. Cipiccia et al., “Fast X-Ray Ptychography: Towards Nanoscale Imaging of Large Volume of Brain.” The European Physical Journal Plus 139, 434 (2024).
[2] G. V. Montemurro et al., “SELUN: A High-Speed X-Ray Photon Counting Detector for Coherent Imaging Applications.” Journal of Synchrotron Radiation 33 (2026).
[3] F. Baruffaldi, et al., “Single-Photon Counting Pixel Detector for Soft X-Rays.” Communications Physics 8, 321 (2025).
[4] G. Vaughan, et al., “ID15A at the ESRF – a Beamline for High Speed Operando X-Ray Diffraction, Diffraction Tomography and Total Scattering.” Journal of Synchrotron Radiation 27, 515 (2020).
[5] T. Donath et al. (2025), ”Enhancing high-energy powder X-ray diffraction applications using a PILATUS4 CdTe detector”, J. Synchrotron Rad. 32, 378–384.

FaXToR: The first fast hard X-ray micro-tomography beamline at the ALBA synchrotron

Caori Organista[1], Alessandra Patera, Llibert Ribó Mor[2], Javier García Álvarez, Steven Wohl, Federico Cova, Joaquín Gómez Sánchez
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Presentation type: Oral **Presentation time:** 15:30-15:45

FaXToR (FAst X-ray TOmography and Radioscopy) is the first micro-tomography beamline in the hard X-ray regime at the ALBA synchrotron. The beamline is fed by a short in-vacuum multipole wiggler, providing high flux across an energy range from 8 keV to 70 keV in both monochromatic (8–50 keV) and filtered white beam modes (30–70 keV) and maximum beam size of 35 mm x 12 mm (H x V) at the entrance of the sample. Utilizing a Double Multilayer Monochromator with Ru/C and W/B4C stripes, FaXToR delivers a high photon flux of up to 1011 photons/s/mm² at 15 keV, enabling the rapid acquisition rates necessary for dynamic studies. Downstream, the sample is located at 36.5 m from the source, where a versatile detection system is utilized for multi-scale imaging. It consists of two indirect detection microscopes coupled with a set of four distinct cameras, allowing users to choose the optimal spatial and temporal resolution for their experiments. In quasi-simultaneous mode, operando experiments with acquisition rates up to 5000 fps and a centimeter-scale field of view can be performed, while zooming in on specific regions of interest to achieve sub-micron resolution. Since the start of user operation in early 2025, FaXToR has hosted both academic and industrial users with interests in biomedicine, biomaterials, paleontology, and materials science, among others. This work presents several successful case studies showcasing the capabilities of FaXToR for multi-scale structural characterization, utilizing propagation-based phase-contrast and absorption-based imaging techniques for both standard micro-CT and operando experiments. In particular, we present the workflow that has enabled dynamic imaging for the materials and life sciences at the beamline, including novelties in hardware design, system synchronization, optimization of reconstruction algorithms, and user interface development. Additionally, we present our plan for expanding phase-contrast imaging beyond conventional free-space propagation, as well as dark-field contrast X-ray imaging through the implementation of Talbot grating interferometry technique at the beamline. Finally, in light of the ALBA upgrade plan foreseen in the near future, we discuss our vision for FaXToR within the 4th Generation synchrotron.

IV: Applied & Industrial Research

Session Chairs

Mark Goorsky
Lutz Kirste

Development of X-ray Metrology for Advanced CFET Logic and 3D-DRAM Devices

Tamzin Lafford[1], Jeremiah McCallister[1], Juliette Van Der Meer[2], Matteo Beggiato[3], Janusz Bogdanowicz[3], Roger Loo[3], Matthew Wormington[4]

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Presentation type: Invited Talk **Presentation time:** 16:15-16:45

The semiconductor industry's drive for better power, performance, area, and cost (PPAC), accelerated by AI's insatiable demand for computing and memory is increasingly enabled by 3D device architectures and vertical scaling. In logic, gate-all-around (GAA) is progressing toward complementary FET (CFET) transistors, which vertically stack n- and p-type devices using Si/SiGe multilayers. In memory, emerging 3D-DRAM pushes these multilayers even further, potentially requiring hundreds of Si/SiGe pairs. Both technologies depend on engineered substrates with epitaxial Si/SiGe multilayers on Si wafers, making this a critical and challenging starting point of the fabrication process flow. Layer parameters such as Ge content, thickness, and interface width define the process window for downstream steps such as selective etching.

Defects in blanket wafers can ultimately cause device failure and must be identified before patterning to avoid losing weeks of product. Thick 3D-DRAM stacks are especially prone to strain relaxation, generating dislocations or lattice undulations that propagate through the multilayer and degrade performance or yield. X-ray diffraction imaging (XRDI) provides rapid, non-destructive visualization of crystalline defects and is highly sensitive to early-stage relaxation. Such relaxation can generate linear defects that originate at wafer edges and move inward as Si/SiGe pair count increases. Fully automated XRDI covering wafer handling, measurement, and analysis enables high-throughput characterization of tens of wafers per hour with no operator intervention after setup. We will discuss common semiconductor killer defects and how XRDI enables in-line defect detection at production-level throughputs.

For detailed layer-by-layer characterization, fitting of HRXRD and XRR data yields Ge composition, layer thickness, and inter-layer roughness. Accuracy improves further when HRXRD and XRR are combined in a hybrid analysis, where XRR constrains thickness and HRXRD determines composition, reducing parameter correlations and accelerating fitting, enabling more precise metrology for in-line process control. Reciprocal space maps (RSMs) with modern 2D detectors can measure additional valuable information for characterizing process issues during development and ramp of epitaxial deposition processes. We will show how advances in HRXRD / XRR hybrid analysis and RSM-based characterization support the development and manufacturing of increasingly complex 3D device structures and help leading edge logic and memory suppliers to meet rising production demands in the AI era.

Spectral Photon-Counting Micro-CT for Dental Implant Integrity and Infiltration Analysis

Marcello Fonda[1], Giovanni Lemma[1], Vittorio Di Trapani[1], Pierre Thibault[1], Gianluca Turco[1]
[1] *University of Trieste, Italy*

Presentation type: Oral **Presentation time:** 16:45-17:00

Spectral photon-counting micro-CT (µCT) is an advanced imaging technique that combines micrometric X-ray CT with energy-resolved detection, therefore enabling material-specific analysis based on the energy-dependent attenuation of different materials. These capabilities are particularly convenient for applications making use of high-Z contrast agents, where the spectral K-edge signature of selected elements can be used to separate their signal from other highly absorbing structures and materials.

In this work, we present a gadolinium-enhanced spectral µCT approach for the non-destructive detection and quantification of infiltrations in titanium dental implants. The implants are immersed in a Gd-based contrast-agent solution while undergoing repeated mechanical loading, mimicking mastication conditions. The liquid contrast agent can therefore infiltrate through micro-gaps, possibly generated by the loading process. In this work, gadolinium is used instead of the commonly employed silver-based alternatives [1] because its K-edge lies at a higher energy, enabling spectral µCT through K-edge identification through titanium.

Tomograpgic acquisitions were performed at the OPTIMATO laboratory, a multimodal and multiresolution X-ray imaging facility [2], implementing cutting-edge technologies including a liquid MetalJet microfocus X-raysource (Excillum, Sweden), a Medipix3-based CdTe photon-counting detector (LAMBDA 350k, X-spectrum, Germany), and a six-axis robotic arm as sample stage. The robotic system enables unconventional acquisition trajectories, which are exploited to obtain artefact-free reconstructions of the implant region. To cope with the strong attenuation of the implant, two beam-hardening correction strategies, one based on polynomial fitting and the second on an iterative procedure, are investigated to reduce metal-induced artefacts and improve the stability of the spectral analysis.

The spectral data, analysed using the Minimum-Residual Basis Material Decomposition algorithm (MR-BMD) [3], show an effective identification of the Gd-filled infiltrations from the titanium of the implant. Unlike conventional attenuation-based µCT, where infiltration analysis generally relies on manual or threshold-based segmentation, the MR-BMD Gd map provides a reliable and direct material-based segmentation, allowing a clear distinction between the infiltration and possible spurious high-Z/dense inclusions in the implant.

This approach provides a laboratory-based framework for identifying contrast-agent penetration and assessing the quality of dental implants. The combination of spectral micro-CT, photon-counting detection, beam-hardening correction, and gadolinium-enhanced imaging offers a promising strategy for non-destructive validation of implant performance and integrity.

References

[1] He Y. et al., Clin Implant Dent Relat Res. 21:741–752 (2019).
[2] V. Di Trapani et al., JINST 19 C01018 (2024)
[3] V. Di Trapani et al., Opt. Express 30, 42995-43011 (2022)

V: Phase-Contrast Imaging

Session Chairs

Saša Bajt
Mathias Hurst

Waves for life sciences: Characterization of biomedical structures with a focus on X-ray imaging

Marina Eckermann[1]
[1] *Institute of Applied Physics, University of Bern, Switzerland*

Presentation type: Invited Talk **Presentation time:** 08:30-09:00

Disease and development mechanisms in the field of biomedical sciences emerge in complex patterns. As different experimental methods are sensitive for different contrast mechanisms, their entity is required to unfold this complexity. In the group of Biomedical Photonics at the Institute of Applied Physics (IAP), we develops tool for the characterization of biomedical samples, including laser-based system such as polarimetric imaging or fluorescence lifetime imaging, optoacoustic microscopy, and - since recently - also X-ray based techniques.

With their short wavelength, hard X-rays can penetrate matter such as biological tissues deeply, and provide information about its interior architecture: going below the diffraction limit of visible light, and not necessarily relying on specific stains, but assessing samples based on their electron density. Here, different X-ray techniques such as X-ray fluorescence, X-ray diffraction, or X-ray phase-contrast tomography are used more and more to address biomedical questions. In the case of X-ray phase-contrast tomography, it could be shown to give access to the chromatin packing in cellular nuclei, or also to cells for which no histological stain exists. To further exploit and develop this, we build on the joint exploitation of synchrotron-facility setups and a home-built device for X-ray phase-contrast nanoCT, together with other (established) experimental tools, in close collaborations with biomedical researchers.

This presentation provides an overview of the techniques developed at the BP-IAP, with a focus on the newly introduced X-ray methods: this comprises an introduction into the physical concepts of the methods, followed by examples of their elaboration and applications in biomedical research.

Multimodal, multi-scale imaging of human vagus nerve at the I13-1 Coherence beamline

Oriol Roche[1], Alexander Duncalf[2], Darren Batey[1], Silvia Cipiccia[2], Kirill Aristovich[2], Alessandro Olivo[2], Nicole Thompson[2], María Gutiérrez[2]

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Presentation type: Oral **Presentation time:** 09:00-09:15

Electrical stimulation of the human vagus nerve (HVN) is used to treat epilepsy and depression and shows promise for extension to other disorders such as inflammatory and cardiac diseases. However, the architecture of the nerve (i.e. the organisation of its internal fibres and their functional mapping to different organs) is still poorly understood, which prevents targeted neurostimulation and limits the therapeutic expansion.

X-ray imaging has recently enabled the visualisation and tracing of HVN fascicles across extended nerve segments at the scale of 10s of micrometres. While this is an important first step, tracing individual fibres within the nerve at the sub-micron scale is required for precise, functionally selective neurostimulation. X-ray phase contrast techniques enable this kind of volumetric imaging thanks to their sensitivity to soft tissue contrast and the possibility of sub-micron resolution.

At the I13-1 beamline, we performed multi-scale imaging of HVN using a combination of micro-computed tomography (micro-CT) and ptycho-tomography. Micro-CT was used to image the whole nerve (~2 mm diameter), resolve A and B fibres (2 – 20 µm), and select regions of interest (ROIs) for further scanning. A ~300 µm punch of such an ROI was then imaged with ptychography to resolve the smaller C fibres (0.2 – 1.2 µm). Due to the large size of the samples, ptycho-tomography scans were performed off-axis over 360 degrees, pushing the limits of sample size that can be imaged at the beamline. These results are then used to trace the path of individual fibres within the nerve.

While in micro-CT mode, we also employed beam tracking (BT), another phase contrast imaging technique which relies on modulating the illumination into beamlets and tracking changes to those beamlets to obtain attenuation, phase and scattering (or “dark-field”) contrast. The dark-field images contain information about the presence of sub-pixel features and their rough direction, so they can be used to pinpoint areas which are good candidates for further ptychographic imaging.

Being able to alternate techniques within one instrument is important for efficient imaging of large samples with multi-scale features, such as HVN. With this work, we have improved the understanding of the internal structure of the HVN by enabling individual fibre tracing. Furthermore, we have shown the potential for multi-scale imaging of biological tissue at I13-1, and pushed the boundaries for the size of samples that we can image.

Dose-efficient propagation-based X-ray phase contrast imaging at high and low resolution by Bragg crystal optics

Martin Spiecker[1], Tilo Baumbach[1], Rebecca Spiecker[2], Marcus Zuber[1], Angelica Cecilia[1], Clément Tavakoli[1], Michal Kaminski[2], Nikolay Zagainov[1], Mateusz Czyzycki[2]

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Presentation type: Oral **Presentation time:** 09:15-09:30

X-ray phase contrast imaging techniques can visualize weakly attenuating samples by exploiting the phase shift that the sample imprints on the incident wavefield. Propagation-based phase contrast imaging (PB-PCI) uses the self-interference of the diffracted wavefield behind the sample, which gradually evolves into intensity contrast as the propagation distance between the sample and the detector increases. However, conventional scintillator-based detectors for micrometer resolution suffer from low detection efficiency. In addition, imaging large samples at moderate resolution requires a propagation distance of tens to hundreds of meters to generate sufficient image contrast.

Both above-mentioned limitations can be overcome by employing Bragg crystal optics. For high resolution, a Bragg magnifier allows directly magnifying the X-ray wavefield and using a highly efficient single-photon-counting detector while maintaining micrometer resolution. This results in a superior imaging performance compared to conventional detector systems and yields a substantial increase in dose efficiency for high spatial frequencies that comprise the relevant high-resolution components of the image [1].

For imaging centimeter-sized samples at moderate resolution, the Bragg demagnifier yields strong image contrast within a meter-scale setup, thereby eliminating the need for very long propagation distances [2]. Simultaneously, image blur caused by the finite X-ray source size is reduced. The strong increase in image contrast is demonstrated experimentally [2]. This approach paves the way for low-dose studies of large radiation-sensitive samples, with potential applications ranging from biomedical soft tissue and small animal in vivo imaging up to medical diagnostics.

Progress and ongoing developments regarding the setup stability are also discussed.

References

[1] R. Spiecker et al., ”Dose-efficient in vivo X-ray phase contrast imaging at micrometer resolution by Bragg magnifiers”, Optica 10 (2023)

[2] R. Spiecker et al., ” X-ray phase contrast imaging with kilometer propagation distance within a meter ”, Phys. Rev. Res. 7 (2025)

Multilens X-ray Interferometry Based on Si Planar Compound Refractive Lenses

Irina Snigireva[1], Anatoly Snigirev[2]

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[2] *Helvetec, Switzerland*

Presentation type: Oral **Presentation time:** 09:30-09:45

We report the development and experimental demonstration of a new class of high-energy X-ray interferometers based on silicon planar compound refractive lenses (CRLs). The proposed bilens and multilens systems use coherent X-ray illumination to generate diffraction-limited secondary sources whose overlapping wavefields produce stable and controllable interference patterns. The observed fringe spacings range from the nanometer to micrometer scale, enabling applications in coherence characterization, phase-sensitive imaging, beam shaping, and nanoscale analysis.

The bilens interferometer, consisting of two parallel CRLs, was tested with 12 keV X-rays and produced submicron interference fringes detected using scanning and moiré imaging techniques. The far-field interference patterns were used for characterization of X-ray beam coherence, demonstrating the potential of the method for advanced beam diagnostics at modern synchrotron facilities.

The interferometer was further applied to phase-sensitive imaging of weakly absorbing samples in the hard X-ray regime. Experimental studies performed at ESRF beamlines showed that the technique enables accurate reconstruction of phase-shift profiles with high spatial and phase sensitivity. The experimental observations were in good agreement with theoretical predictions and numerical simulations, confirming the validity of the proposed approach.

To extend the concept, multilens interferometers containing multiple parallel arrays of planar CRLs were developed and tested in the 10–65 keV energy range. The generated interference patterns exhibited strong longitudinal dependence and were successfully described within the Talbot imaging framework. Experimental results obtained at ESRF beamlines demonstrated good agreement with simulations and confirmed the capability of the multilens interferometer as a high-resolution tool for beam diagnostics and coherent X-ray manipulation.

In addition, a coherent X-ray beam expander based on the multilens interferometer concept was experimentally demonstrated. The device enabled efficient generation of highly divergent coherent beams with controllable angular size and photon flux density in both coherent and incoherent operating modes.

These developments establish multilens X-ray interferometry as a promising technique for diffraction-limited synchrotron sources and next-generation X-ray free-electron lasers, opening new opportunities for advanced X-ray imaging and beam control applications.

Phase-Contrast and Dark-Field Imaging and Tomography at OptImaTo laboratory: Implementation and Optimization with Modulation-Based Technique

Giovanni Lemma[1], Vittorio Di Trapani[1], Marcello Fonda[1], Pierre Thibault[1]
[1] *University of Trieste, Italy*

Presentation type: Oral **Presentation time:** 09:45-10:00

Modulation-based imaging is an X-ray phase-contrast technique capable of simultaneously retrieving transmission, differential phase-contrast, and dark-field signals.The method exploits a structured illumination generated by a modulator, avoiding the need for complex optical components.However, achieving stable reconstructions generally requires the acquisition of multiple images of both the modulator alone and the modulator together with the sample, making tomographic applications demanding in terms of acquisition time and radiation dose.

To address these limitations, a systematic experimental campaign was carried out at the OptImaTo Laboratory(Trieste, Italy) [1], where the setup consists of a liquid-metal-jet X-ray source (MetalJet D2+, Excillum) and a photon-counting detector (Lambda350k, X-Spectrum) featuring a cadmium telluride sensor. Planar radiographs were acquired while varying several experimental parameters, including the type of diffuser (sandpaper was compared with a Vogel-spiral membrane*), the propagation distance, and the number of diffuser stepping positions.

Different image-quality metrics and statistical analyses were employed to assess the influence of these parameters on the reconstructed signals and to identify an optimal trade-off between image quality and acquisition time.The resulting optimized configuration enabled the acquisition of the first modulation-based tomographic scans performed at the OptImaTo laboratory. In addition to the well-established UMPA algorithm [2], reconstruction was implemented in the Fourier domain, using a forward model like the one proposed in [3]. The noise spectrum for a photon-counting detector was included in this reconstruction algorithm to further improve the quality of the results.

* We thank Dr. Emmanuel Brun (STROBE Laboratory, Grenoble, France) for providing the Vogel spiral membrane. More details can be found in [4].

References

[1] Vittorio Di Trapani et al., “Speckle-based imaging (SBI) applications with spectral photon counting detectors at the newly established OPTIMATO (OPTimal IMAging and TOmography) laboratory,” Journal of Instrumentation, vol. 19, no. 1, p. C01018, Jan. 2024.
[2] Fabio De Marco et al., “High-speed processing of X-ray wavefront marking data with the Unified Modulated Pattern Analysis (UMPA) model,” Optics Express, vol. 31, pp. 635–650, 2022
[3] Ginevra Lautizi et al. Universal reconstruction method for x-ray scattering tensor tomography based on wavefront modulation. Phys Rev Appl. 2024;22(2):024031.
[4] Clara Magnin et al. On the optimisation of the geometric pattern for structured illumination based X-ray phase contrast and dark field imaging: A simulation study and its experimental validation. arXiv:2504.10665

VI: Diffraction & Scattering - 2/2

Session Chairs

Ivan Zaluzhnyy
Steffen Tober

High-resolution XRD characterization of surface guided Xanthine derivatives for optical metamaterial application

Anna Kossoy[1], Yishay Feldman[1], Angelica Niazov-Elkan[2], Dan Oron[1]

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[2] *Tel Aviv University, Israel*

Presentation type: Oral **Presentation time:** 10:30-10:45

Numerous biological organisms employ template-assisted crystallization of molecular solids to produce crystal morphologies with unique optical properties that are difficult to reproduce synthetically. Here, we report the growth of large, bio-inspired, birefringent, and defect-free crystalline sheets of a xanthine derivative (theophylline), reaching several millimeters in length, on a single-crystal (11–20) quartz template. Structural mismatch between the hexagonal quartz substrate and the orthorhombic theophylline layer leads to distinctive form of heteroepitaxy.

The surface-guided growth of theophylline crystalline sheets is characterized by a well-defined orientation both in-plane and out-of-plane with respect to the substrate, resulting in pronounced optical anisotropy parallel to the quartz surface.

A combination of out-of-plane and in-plane X-ray diffraction measurements, performed using a Rigaku SmartLab diffractometer, reveals lattice matching between the planes perpendicular to substrate surface, namely (−2204) of quartz and the (017) of theophylline. Molecular-level simulations of interfacial bonding highlight the critical role of hydrogen bonds in establishing coherence between the quartz substrate and the theophylline layer. High-resolution in-plane measurements also confirm the angular relationship between the slow optical axis of the film, [002], and slow optical axis of quartz, [1-100].

This study demonstrates an unusual heteroepitaxial relationship between quartz and an organic dielectric film and highlights the power of combining in-plane and out-of-plane high-resolution X-ray diffraction techniques to elucidate structural features of optically anisotropic materials.

A. Niazov-Elkan, M. Shepelenko, L. Alus, M. Kazes, L. Houben, K. Rechav, G. Leitus, A. Kossoy, Y. Feldman, L. Kronik, P. G. Vekilov, D. Oron. Advanced Materials (2024) 36, 2306996

Swelling Dynamics in Ultrathin Protein Films

Sarah Siraj[1], Dillip Satapathy, Yohko Yano, Wolfgang Voegeli[2], Etsuo Arakawa, Wada Haruto, Aniruddha Barman

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[2] *Tokyo Gakugei University, Japan*

Presentation type: Oral **Presentation time:** 10:45-11:00

Understanding early-time swelling in protein thin films is critical for designing responsive soft actuators. We have demonstrated protein-based actuators with tunable mesoscale structure, where controlled crystallinity enables precise regulation of actuation speed and magnitude under vapor exposure [1]. To uncover the underlying mechanisms, we employ time-resolved synchrotron X-ray reflectivity (XRR) with simultaneous angle- and energy-dispersion to quantitatively probe the swelling dynamics of ultrathin protein films upon exposure to controlled humidity. The ultra-fast XRR at the PF-AR Beamline NE-7A, Photon Factory, Japan, provides sub-second temporal resolution of the evolving film structure during early exposure times. The measurements reveal an interplay between solvent diffusion and polymer relaxation. Interestingly, as relative humidity increases, the system undergoes a transition analogous to a glass transition at ambient temperature, driven by water-induced softening rather than thermal activation. Importantly, it is also found that the protein's intrinsic secondary structure preferentially affects diffusion, suggesting that molecular-scale organization controls macroscopic transport. Additionally, spectroscopic ellipsometry studies track the swelling pathway of protein films dependent on thickness and refractive index to further elucidate diffusion pathways. These findings provide new insight into the mechanisms governing moisture-induced swelling in protein thin films and demonstrate the capability of time-resolved XRR for probing ultrafast structural evolution. These findings and their implications will be discussed in detail.

References

[1] Siraj, S. A., Kumar, V., & Satapathy, D. K. (2025). Langmuir, 41(32), 21553-21561.

Strain Waves as a Symmetry-Breaking Field in Photoexcited V O

Ritwika Mandal[1], Celine Mariette[2], Etienne Janod[3], Maciej Lorenc[4]
[1] *Jean Rouxel Institute of Materials in Nantes, France*
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Presentation type: Oral **Presentation time:** 11:00-11:15

Control of light-matter interaction in quantum materials offers a pathway to access non-equilibrium states with emergent functionalities beyond thermal equilibrium [1, 2]. In strongly correlated systems, particularly those involving large volume changes associated or not to a symmetry breaking, ultrafast laser excitation can drive phase transitions [3, 4]. Recent work [5] further highlights the effect of nanoscopic morphology on the mechanism of macroscopic transformation as well as relaxation dynamics.

In this work, we investigate a geometry controlled strain wave dynamics during photoinduced phase transition in morphologically tailored single crystals of V2O3, a prototypical strongly correlated system. Using time-resolved X-ray diffraction and ultrafast optical reflectivity, we track the coupled structural and electronic dynamics during such a transition.

We identify a multistep process after laser excitation, starting with an initial monoclinic-to-hexagonal inverse ferroelastic transition, within ~ 10 ps. At several tens of ps, the propagation of a unidirectional and coherent strain wave perpendicular to the large surface hit by the ultrafast laser induces a symmetry-lowered state with intermediate volume, stabilising a transient monoclinic metallic phase - a long sought missing link in the V2O3 phase diagram. At longer delays, additional strain waves propagating in-plane drive the system towards the hexagonal phase, with a dynamics governed by the speed of acoustic propagation and the crystal lateral size. These results demonstrate that the strain wave mechanism can act as a dynamical symmetry-breaking field enabling control of photoinduced transition pathway and access to emergent phases.

References

[1] Koshihara, S. et al. Physics Reports 942, 1 (2022).
[2] Zhang, J. & Averitt, R. D. Annual Review of Materials Research 44, 19 (2014).
[3] Amano, T. et al. Nature Physics 20, 1778 (2024)
[4] Mariette, C. et al. Nature communications 12, 1239 (2021)
[5] Mandal, R. et. al. Communications Materials 6, 209 (2025)

Residual effects in GaN nanowires on ZrN buffer layers studied by XRD and Raman spectroscopy

Aleksandra Wierzbicka[1], Radoslaw Szymon[2], Eunika Zielony[2], Zbigniew R Zytkiewicz[1], Marta Sobanska Hab.[1]

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Presentation type: Oral **Presentation time:** 11:15-11:30

GaN nanowires (NWs) grown on conductive transition-metal nitride buffer layers are promising for optoelectronic and electronic applications, where structural perfection and crystalline alignment are crucial for device performance. In this work, we investigate the structural properties of GaN NW ensembles grown on two different substrates: 40 nm ZrN on Si (111) and 100 nm ZrN on Al2O3 (0001). The study combines scanning electron microscopy (SEM), high-resolution X-ray diffraction (HRXRD), reciprocal space mapping (RSM), Williamson–Hall plots (W–H) analysis, and Raman spectroscopy.

The structural characterization was performed using symmetrical GaN 0002, 0004, and 0006 reflections measured in ω scans, 2θ/ω scans, and reciprocal space maps [1]. Rocking curve analysis of the GaN 0002 reflection revealed unexpectedly large tilt values for both nanowire ensembles. However, these values were not fully consistent with the morphology observed by SEM, where the nanowires appeared significantly better aligned. The Williamson–Hall analysis [2] was used to distinguish between factors related to the widening caused by microstrain and those related to the effects of orientation distribution.The W–H plot approach produced substantially lower tilt values than those obtained from rocking curves directly, suggesting that residual broadening effects significantly impact the conventional HRXRD analysis of GaN NW ensembles.

Complementary Raman spectroscopy [3] performed with green laser excitation revealed the presence of the non-polar E2(high) phonon mode together with the polar A1(LO) mode. The Raman spectra also show the presence of the forbidden A1/E1(TO) modes together with quasi-transverse phonon modes. This indicates symmetry breaking and supports the conclusions derived from the X-ray diffraction analysis.

The results presented demonstrate that, when used alone, conventional rocking curve analysis may overestimate the orientational disorder of GaN nanowires due to contributions from residual broadening. Using a combination of HRXRD, Williamson–Hall plots and Raman spectroscopy allows for a more reliable evaluation of nanowire tilt and structural quality in complex nitride heterostructures.

Acknowledgments: This work was supported in part by the Polish National Science Center, Grants No. 2022/04/Y/ST7/00043 (Weave-Unisono), 2021/43/D/ST7/01936, 2025/09/X/ST11/01089 and Foundation for Polish Science (START 088.2025). The authors are grateful to M. Guziewicz for deposition of ZrN layers and A. Reszka for SEM measurements.

References

[1] A. Wierzbicka, et al., Nanotechnology 24 (2013) 035703.
[2] V.P. Klado, et al., J. Cryst. Growth 401 (2014) 347-350.
[3] E. Zielony, et al., Appl. Surf. Sci. 588 (2022) 152901.

In-situ synchrotron HRXRD investigation of epitaxial YSZ/Ti/Pt/BaFe12O19/ Bi3Ti5FeO15 multiferroic heterostructures on Si(111) for non-volatile memory applications

Berkin Nergis[1], Sondes Bauer

[1] *IPS, Germany*

Presentation type: Oral **Presentation time:** 11:30-11:45

We present a comprehensive in-situ synchrotron high-resolution X-ray diffraction study of a five-layer heterostructure — YSZ/Ti/Pt/BaFe12O19(BaM)/Bi3Ti5FeO15(BTFO) — grown by pulsed laser deposition (PLD), performed at the NANO beamline of the KARA synchrotron facility at KIT. At each growth step, rocking curves are recorded while a Pilatus 2M area detector simultaneously captures the full large-angle two-dimensional diffraction pattern. Maximum intensity extraction along detector lines yields a comprehensive diffraction profile in which symmetric coplanar reflections, parasitic phases, polycrystallinity, and the textured nature of BTFO are all monitored in a single scan, drastically reducing acquisition time and demonstrating the capability of in-situ synchrotron HRXRD as a uniquely efficient diagnostic for complex multiferroic heterostructure growth. Multiferroic heterostructures combining ferromagnetic and ferroelectric layers are promising candidates for high-temperature non-volatile memory (NVM) devices exploiting magnetoelectric coupling. Translating such architectures from single-crystal oxide substrates to industry-standard Si(111) wafers requires a complex multilayer buffer strategy whose structural evolution must be understood at every deposition step. The sequential in-situ approach enables direct identification of how each template constrains the texture and phase purity of the subsequent layer. The yttria-stabilized zirconia buffer establishes (111)-oriented epitaxy on Si(111), while the Ti and Pt interlayers provide the adhesion and lattice mismatch template required for growth of the functional oxide bilayer. The ferromagnetic BaM layer grows c-axis oriented on Pt(111), leveraging the hexagonal symmetry match, as confirmed by the evolution of (00l) reflections in the in-situ RSMs. The Aurivillius-phase BTFO presents the principal crystallographic challenge, being inherently prone to polycrystalline nucleation and thus requiring precise control of both deposition parameters and template quality to achieve preferential orientation. Through systematic optimization of PLD parameters for each layer on its respective template, we demonstrate near-single-oriented BTFO films with suppressed polycrystalline grain orientations. In-situ RSMs and rocking curve analysis identify the deposition parameters that favor oriented over polycrystalline BTFO nucleation. These results represent a significant step toward integrating Aurivillius-phase multiferroic heterostructures on silicon platforms for scalable, high-temperature NVM technology.

X-ray diffraction profiles from dislocations and stacking faults in a-plane AlN films

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Presentation type: Oral **Presentation time:** 11:45-12:00

The as-grown a-plane AlN films grown by MOVPE on r-plane sapphire contain basal stacking faults, predominantly I_1 type, bounded by partial dislocations. The plane of the basal stacking faults is perpendicular to the film plane and the dislocations bounding them are threading dislocations. After high-temperature annealing at 1680 °C, stacking faults shrink,some of partial dislocations merge into full dislocations or annihilate. This transformation of the real structure is revealed by transmission electron microscopy.

We characterise types and densities of dislocations and stacking faults before and after high-temperature annealing in more detail by combining laboratory X-ray diffraction measurements (rocking curves in skew diffraction geometry and reciprocal space maps) and Monte Carlo simulations of X-ray diffraction from these defects. The extension of our previous Monte Carlo simulations for full dislocations to stacking faults is straightforward and requires to take care of the directions of the cuts in the dislocation displacement fields: the cuts have to be directed along the line connecting the partial dislocations.

The I_1 type basal stacking faults with displacement vectors f=1/6<20-23> are visible (the scalar product g.f is not multiple of 2*pi) in reflections g=(10-10) and (20-20), and invisible in other available reflections. We observe the ~q^-2 intensity decay in these reflections due to stacking faults, and find a stacking fault density of 6x10^5 cm^-1 by Monte Carlo simulations. Further reflections, insensitive to stacking faults, reveal the q^-3 intensity decay due to partial dislocations bounding stacking faults. Monte Carlo modelling of these reflections provides the density of partial dislocations of 6x10^10 cm^-2 and shows that one third of these dislocations are a+c type dislocations dissociated into partials, while the remaining stacking faults are bounded by partials with the opposite Burgers vectors.

Measurements and simulations of the X-ray diffraction curves after high-temperature annealing reveal only full threading dislocations of a+c type with the density of 1x10^10 cm^-2. Hence, the stacking faults bounded by partial dislocations with opposite Burgers vectors shrink and vanish, while the ones bounded by the dissociated a+c dislocations shrink to full a+c dislocations. The measurement and simulations of the reciprocal space maps complement characterisation of the real structure of the as-grown samples by revealing the misfit dislocations of an effective density (taking into account their positional correlations) in the as-gown sample of 1.5x10^6 cm^-1, which reduces on annealing by a factor of 2, by developing stronger correlations.

VII: CDI & Ptychography

Session Chairs

Dina Carbone
Felix Wittwer

Diffractive Imaging of Mesostructure in Disordered Energy Materials

Oleg Gorobtsov[1], Andrej Singer[2]

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Presentation type: Invited Talk **Presentation time:** 08:30-09:00

Materials for energy applications, such as in batteries and fuel cells, are by nature out of equilibrium during operation. Defects and changes in the material morphology dynamically evolve and affect kinetics and reversibility of function. The changes in the crystal lattice must then be detected operando or in-situ to understand underlying physical processes. Imaging methods have demonstrated that transient dislocations briefly appear in intercalation hosts during ion diffusion in various environments. Here, we summarize several of our findings obtained by operando Bragg Coherent Diffractive Imaging (BCDI) in energy materials, demonstrating how BCDI captures stages of formation of metastable defects, cracking, and layer delamination in various perovskite materials for battery cathodes and fuel cell proton conductors.

Bridging real and reciprocal-space nanoimaging of biogenic calcite: Bragg coherent diffraction, ptychography, and cryo X-ray fluorescence

Dmitry Karpov[1]

[1] *Université Grenoble Alpes, France*

Presentation type: Oral **Presentation time:** 09:00-09:15

Synthetic approaches to strain engineering struggle to control internal lattice distortions reproducibly: morphologically identical nanocrystals exhibit heterogeneous strain. Coccolithophores (unicellular algae) biomineralize calcite with long-recognized morphological consistency and, we now find, equally consistent internal strain. Holococcoliths, the calcite scales produced by cells in haploid phase, show spherically symmetric strain fields across biological replicates; heterococcoliths, produced in the diploid phase, exhibit strain complexity that scales with chiral morphology. The cell controls both crystallographic orientation and impurity distribution beyond what morphological templating alone explains. Resolving the mechanism requires reading both the lattice distortions and the chemical perturbations that drive them.

We approach the question by combining real- and reciprocal-space X-ray nanoimaging on the same single coccolith crystals. Bragg coherent diffractive imaging (BCDI) at ID01 of the ESRF-EBS resolves three-dimensional lattice strain at sub-10 nm resolution and 10 strain sensitivity. Ptychographic X-ray computed tomography (PXCT) at ID16A maps quantitative electron density at similar resolution, exposing intracrystalline density variations. Cryogenic X-ray fluorescence computed tomography (cryo-XRF-CT) on intact, plunge-frozen coccolithophore cells localizes the chemical origin of the measured strain at 35 nm voxel resolution with single-element sensitivity down to tens of atoms per voxel. The workflow builds on our recent implementations of cryo-correlative X-ray microscopy and self-supervised denoising for multi-element XRF detectors.

Applied to both life-cycle phases, the approach exposes two regimes of impurity-strain coupling. In holococcoliths the Sr enrichment toward the crystal rim results in transition from compressive to tensile lattice strain, leading to self-limited growth. In heterococcoliths the strain field becomes strongly anisotropic and follows the broken morphological symmetry, co-localized with asymmetric Sr distributions. At substitutional levels around 0.25 atomic percent (Sr/Ca), strain and impurity co-evolve with a non-linear, anisotropic lattice response that deviates from Vegard's law, corroborated by density functional theory.

By resolving both the lattice signature and the chemical origin of symmetry breaking at the single-nanocrystal level, our tri-modal workflow turns biogenic calcite into a quantitative testbed for impurity-driven strain engineering. The same correlative approach extends to other complex materials in which composition and lattice strain are entangled at the nanoscale. Probing them requires complementary techniques operated at their current limits, where the methods and the understanding of the phenomena they reveal are co-developed.

Bragg Coherent Diffraction X-ray Imaging of Nanoparticles with Unknown Orientation

Aksel Mihaylov[1], Huaiyu Chen[2], Jesper Wallentin[1], Jose Solla Gullon[3], Alexander Björling

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[3] *University of Alicante, Spain*

Presentation type: Oral **Presentation time:** 09:15-09:30

Bragg coherent diffraction imaging (BCDI) is a non-intrusive technique which enables mapping the internal strain fields of crystalline nanoparticles[1]. During BCDI experiments, the sample is oriented to a Bragg anglewith respect to an incoming X-ray beam, fulfilling Bragg's law. A detector measures the resulting Bragg peak and by controlled rotation of the sample along a rocking curve, the entire 3D diffraction volume can be reconstructed. The internal structure of the sample can be recovered by treatment of the diffraction volume via phase-retrieval algorithms.

Uncertainty in the sample's angular orientation during measurements, for example due to radiation pressure[2]or serial imaging schemes, can limit the applicability of BCDI. Methods proposed to overcome this limitation, such as ones based on the Expand-Maximize-Compress (EMC) algorithm, have shown success for angular deviations more than an order of magnitude of the nominal step size[3]. Even so, EMC is based on correlations between diffraction frames, complicating its extension to serial imaging methods where several single diffraction frames are measured from many identical but randomly oriented particles.

In this work, we propose a neural network (NN) which can predict the rocking angleof the sample based on individual diffraction frames, foregoing the need for continuity. Training the NN required no prior knowledge of internal strain and only an approximative shape of the measured particle. The network was tested on a merged dataset, containing diffraction frames (of unknown rocking angles) from three separate but similar~60 nm gold particles. The results showed that the NN was able to reconstruct a coarse sorting of the dataset, introducing continuity that the EMC algorithm could further refine to reconstruct the 3D diffraction volume. By enabling the treatment of datasets with unknown angular orientations and different particles, the proposed network helps bridge the gap toward serial imaging schemes in BCDI.

References

[1] G. J. Williams, M. A. Pfeifer, I. A. Vartanyants, and I. K. Robinson, "Three-Dimensional Imaging of Microstructure in Au Nanocrystals,"Physical Review Letters,vol. 90, no. 17, p. 175501, 04/29/ 2003.
[2] J. W. Kimet al., "Observation of x-ray radiation pressure effects on nanocrystals,"Journal of Applied Physics,vol. 120, no. 16, 2016.
[3] H. Chenet al., "Correcting angular distortions in Bragg coherent X-ray diffraction imaging,"Journal of Synchrotron Radiation,vol. 31, no. 5, pp. 1308–1316, 2024.

Dynamic in-situ ptychographic X-ray tomography with environmental control

Johannes Ihli[1], Arik Malte Beck[2], Zhao Jiang[3], Zirui Gao[4], Tomas Aidukas[5], Christian Appel[5], Yi-Yeoun Kim[6], Andreas Menzel[5], Jeroen Anton Van Bokhoven[7], Manuel Guizar-Sicairos[8], Fiona Meldrum[9], Mirko Holler[10]

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Presentation type: Oral **Presentation time:** 09:30-09:45

Dynamic material transformations such as crystallisation, sintering and phase separation underpin the performance and failure of functional materials, yet remain difficult to visualise in three dimensions under realistic operating conditions. We present an integrated platform for in-situ ptychographic X-ray tomography that combines X-ray ptychography, angularly sparse tomogram acquisition, dynamic 4D reconstruction and a custom environmental control and nano-positioning instrument. This setup enables the acquisition of quantitative electron-density tomograms of 100 um wide samples with 10s of nanometre spatial and minute-scale temporal resolution, continuously across broad temperature ranges and gas atmospheres over extended periods. The approach is dose-efficient and compatible with complex sample geometries, allowing repeated imaging of the same volume throughout a transformation, and yields quantitative 4D datasets that are directly amenable to advanced analysis and multimodal workflows.We demonstrate these capabilities on two case studies. First, we follow the crystallisation of amorphous calcium carbonate from room temperature to 500°C, acquiring hundreds of tomograms that reveal discrete dehydration steps, heterogeneous nucleation pathways, and rare metastable phases, alongside defect-mediated Ostwald ripening in individual crystals. Second, we track the activation, mobility and deactivation of a supported catalyst under methane oxidation conditions from 25°C to 830°C, tracking the formation and evolution of over 100,000 nanoparticles within a hierarchically porous support, uncovering two concurrent catalyst deactivation modes.

Spectroscopic BCDI: combined chemical and structural 3D mapping of bimetallic nanocatalysts

Thomas Sarrazin[1], Marie-Ingird Richard[2], Vincent Favre-Nicolin[1]
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Presentation type: Oral **Presentation time:** 09:45-10:00

Strain, composition, and defects are difficult to disentangle in heterogeneous catalysts. Bragg coherent diffraction imaging (BCDI) [1] retrieves three-dimensional displacement fields and morphology with ~10 nm resolution from a single nanocrystal, but composition and strain produce overlapping contrast in the reconstructed phase. The ambiguity is acute in chemically heterogeneous bimetallics such as Ni-Fe and Pt-Pd, alloys used in CO hydrogenation catalysis, where composition and structure rearrange together under reaction conditions. We are developing nano-focused 3D spectroscopic Bragg coherent imaging (spectro-BCDI) at the ID01-EBS nanoprobe of the European Synchrotron (ESRF). The method combines BCDI with multiwavelength anomalous diffraction (MAD) [2].

Scanning the incident energy across an absorption edge modulates f and f of one element. This adds chemical contrast (composition, oxidation state, local bonding) to the same Bragg reflection that already reports lattice strain, displacement, and defects. Simultaneous nano-focused fluorescence provides element-specific concentration and edge-step calibration. Reconstruction proceeds in two stages. We first fit the diffraction intensities across the energy scan at each point in reciprocal space, using the known f and f , to separate the anomalous and non-anomalous structure factors. Each is then phase-retrieved separately, and the voxel-wise ratio of the two reconstructed densities gives the local composition.

We validate the method on simulated diffraction data with realistic photon statistics and recover composition maps across the particle volume. We demonstrate the technique on two systems: Ni Fe nanocrystals at the Ni K-edge (8.333 keV) and PtPd nanocrystals at the Pt L - edge (11.564 keV). The two cases differ in morphology, fluorescence background and anomalous contrast. We aim to extend the method to in-situ CO hydrogenation, where we can follow how composition and strain evolve together in single nanocrystals during reaction and relate structure to catalytic selectivity.

References

[1] I. Robinson and R. Harder, Coherent X-ray diffraction imaging of strain at the nanoscale, Nat. Mater. 8, 291 (2009).
[2] V. Favre-Nicolin, M. G. Proietti, C. Leclere, N. A. Katcho, M.-I. Richard, and H. Renevier, MAD and DAFS for studying Semiconductor Nanostructures, Eur. Phys. J. Spec. Top. 208, 189 (2012).

Photodynamics of gold nanorod transformation studied by femtosecond coherent diffraction imaging at the European X-FEL

Anton Plech[1], Juan Hidalgo Lopez, Andres Guerrero Martinez, Omkar Rambadey, Ovidio Pena-Rodriguez, Kartik Ayyer, Zhou Shen, Wojciech Gawelda, Guillermo Gonzalez-Rubio
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Presentation type: Oral **Presentation time:** 10:00-10:15

Functional properties in nanomaterials depend critically on size and shapes, as for instance in photonically active gold nanorods for catalysis and molecular sensing [1]. Laser modification has shown to induce rich product morphologies by laser reshaping [1] or fragmentation [2]. In order to visualize the mechanisms that lead to nanorod reshaping we have performed an ultrafast pump-probe experiment at the EU-XFEL (beamline SPB) [3] to reconstruct the 2D projection of photoexcited single gold nanorods in water as function of delay and laser fluence. By taking advantage of massive sampling at the 500 kHz repetition rate of the XFEL operation it was possible to both derive structural models for the transformation dynamics as well as separate model-independent classes of transformations. The relevance of thermally induced melting-relaxation pathway versus solid-state transformation is discussed.

References

[1] G. González-Rubioet al., Acc. Chem. Res. 49, 678–686 (2016)
[2] A. Plech et al., ACS Nano 18, 10527-10541 (2024)
[3] K. Ayyer et al., Optica 8, 15-23 (2021)

Challenges and solutions of diffraction signal numerical separation in multibeam ptychography.

Runqing Yang[1], Pablo Villanueva Perez[1], Maik Kahnt[2], Giovanni Fevola[3], Ken Vidar Falch[3], Mikhail Lyubomirskiy[2], Tang Li[3], Manfred Burghammer[4], Michael Sztucki[4]

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Presentation type: Oral **Presentation time:** 10:15-10:30

Ptychography has become a key technique for high-resolution coherent X-ray imaging[1], but as a scanning-based method, it is limited in acquisition speed and scalability for large-field and high-throughput measurements. Multibeam Ptychography (MBP) addresses these limitations by simultaneously illuminating multiple sample regions, enabling a scalable approach for high-throughput coherent X-ray imaging while maintaining quantitative phase sensitivity and high spatial resolution[2,3].

A central challenge in MBP is that increasing the number of beams also increases the mixing and superposition of the diffraction information, making reconstruction strongly dependent on information separability between beams[4,5]. As more diffraction information from different beams becomes superimposed, separating the contributions from individual beams during reconstruction becomes increasingly difficult, raising fundamental questions regarding the scalability, achievable throughput, and reconstruction quality of MBP.

This presentation addresses the issues causing challenges in numerical separation of diffraction signal from an increasing number of beams in MBP, particularly the role of probe design in improving information separability from different beams. Recent results demonstrate that stable MBP reconstruction requires probe sets that are not only individually suitable for ptychography but also sufficiently separable and uniform when used together under multi-beam conditions[6]. To evaluate these requirements, probe sets are assessed using three key criteria: separability, uniformity, and experimental feasibility. The presentation will further discuss MBP throughput scaling with the number of beams used. Particularly, the relationship between beam number, achievable throughput gain, and the number of diffraction measurements required to maintain stable reconstruction quality.

These observations suggest that the scalability of MBP depends not only on the number of beams but also on how effectively diffraction information from different beams can be separated during reconstruction. Achieving robust and scalable MBP, therefore, requires efficient numerical separation of the diffraction signal from different beams.

References

[1] Pfeiffer, Franz. ”X-ray ptychography.” Nature Photonics 12.1 (2018): 9-17.
[2] Bevis, Charles, et al. ”Multiple beam ptychography for large field-of-view, high throughput, quantitative phase contrast imaging.” Ultramicroscopy 184 (2018): 164-171.
[3] Li, Tang, et al. ”X-Ray Multibeam Ptychography at up to 20 keV: Nano-Lithography Enhances X-Ray Nano-Imaging.”Advanced Science11.30 (2024): 2310075.
[4] Lyubomirskiy, Mikhail, et al. ”Multi-beam x-ray ptychography using coded probes for rapid non-destructive high resolution imaging of extended samples.” Scientific Reports 12.1 (2022): 6203.
[5] Penagos Molina, Daniel S., et al. ”Multiplexing information limits in multi-beam ptychography.”Optics Express33.6 (2025): 12925-12938.[6] Yang, Runqing, et al. ”Optimizing probes for multi-beam ptychography.” Optics Express 34.7 (2026): 12463-12478.

VIII: Theory, AI & Algorithms

Session Chairs

Vladimir Kaganer
Edwin Fohtung

Deep learning for advanced 3D and 4D X-ray image reconstruction

Yuhe Zhang[1], Pablo Villanueva Perez[2], Zisheng Yao[2], Zhe Hu[2], Tobias Ritschel[3]

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[2] *Lund University, Sweden*
[3] *University College London, United Kingdom*

Presentation type: Invited Talk **Presentation time:** 11:00-11:30

The rapid development of high-brilliance X-ray sources, including diffraction-limited storage rings and X-ray free-electron lasers, is enabling X-ray imaging at unprecedented spatial and temporal resolution. At the same time, these facilities generate increasingly large, high-dimensional, and often highly undersampled datasets, creating major challenges for image reconstruction, analysis, and real-time data processing. Recent advances in artificial intelligence and deep learning are opening new opportunities to address these challenges and to fully exploit the capabilities of next-generation X-ray sources.

In this talk, I will provide an introduction to deep learning and its growing role in X-ray imaging, with a special focus on 3D/4D X-ray image reconstruction. I will first present an overview of modern neural network architectures, ranging from simple multilayer perceptrons and convolutional neural networks to advanced frameworks for 3D and 4D image reconstruction, and outline how these approaches address imaging problems across different spatial and temporal dimensions. Then, I will focus on physics-informed and self-supervised learning methods developed for sparse-view 3D/4D reconstruction in X-ray Multi-Projection Imaging (XMPI) [1–5]. By integrating physical imaging models with data-driven priors, these methods enable high-quality reconstructions from sparse, noisy, and limited-angle measurements while reducing acquisition requirements. We will also discuss the practical trade-offs encountered in real-world implementations and demonstrate how learning-based methods offer the potential to explore and understand the structure and dynamics of various samples.

References

[1] P. Villanueva-Perez et al., Optica 5, 1521–1524 (2018).
[2] Y. Zhang et al., Appl. Res. 2, e202300016 (2023).
[3] Y. Zhang et al., Commun. Eng. 4, 54 (2025).
[4] Z. Yao et al., Meas. Sci. Technol. 36, 085403 (2025).
[5] Z. Hu et al., Adv. Sci. 13, e11933 (2026).

Evolution-based EUV Scatterometry fuelled by Machine Learning Diffraction Predictions for 3D Nanoscale Semiconductor Structures

Warre Heylen[1], Vitaly Krasnov[2], Len Pasic, Esben Witting Larsen, Kevin Dorney, Claudia Fleischmann

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Presentation type: Oral **Presentation time:** 11:30-11:45

Extreme ultraviolet (EUV) scatterometry is a promising candidate for in-line dimensional metrology of advanced nanoscale 3D semiconductor devices. A key challenge for deploying EUV scatterometry in practice is the solution of the inverse problem: reconstructing device geometries from measured diffraction signatures. Although machine-learning methods have shown strong potential for scatterometric reconstruction, most published approaches have focused on relatively simple structures described by only a few parameters. In contrast, realistic 3D device architectures are represented by many more parameters, making robust reconstruction substantially more challenging.

In this work, we present a reconstruction framework that combines a neural-network surrogate model with differential evolution for geometry retrieval. The surrogate is trained to emulate finite element method (FEM) simulations and rapidly predict diffraction intensities from geometric parameters, thereby greatly reducing the computational cost of repeated forward evaluations. Differential evolution then uses this fast forward model to efficiently explore the high-dimensional geometric parameter space and identify geometries that best reproduce the measured signature

Compared with both direct inverse neural networks and earlier hybrid approaches based on surrogate forward models with fitting algorithms, the proposed method provides greater robustness for complex experimental reconstructions. Direct inverse models often misinterpret measurement data because real experimental data differ from training simulations due to process-induced variations, simplified geometric representations, and measurement noise. In contrast, hybrid methods based on other fitting schemes such as Levenberg–Marquardt are more susceptible to becoming trapped in local minima in high-dimensional parameter spaces. By combining a neural-network surrogate with differential evolution, our approach addresses both challenges, enabling robust and efficient reconstruction of complex geometries from experimental data.

We demonstrate the method performance on an EUV photomask sample whose geometry is described by 11 parameters. To the best of our knowledge, this exceeds the geometric complexity previously reported for successful reconstruction using either conventional optimization-based approaches or machine-learning-based methods. This result highlights the ability of the proposed framework to handle significantly more realistic and challenging structures than those considered in earlier studies.

By coupling the speed and accuracy of neural-network surrogates with the global search capability of evolutionary optimization, the proposed framework provides a scalable and robust route to accurate reconstruction of complex 3D device geometries, supporting EUV scatterometry as a viable in-line metrology technique for current and future semiconductor technologies.

Sensitivity maximization in XRR and HRHRD by Fisher information: search for the most informative scan points

Alexander Mikhalychev[1], Alexander Schekochihin[1], Alex Ulyanenkov[2]

[1] *Atomicus Sp. z o.o., Poland*
[2] *Atomicus LLC, USA*

Presentation type: Oral **Presentation time:** 11:45-12:00

Measurement of an XRR or HRXRD profile is a time-consuming procedure when a laboratory diffractometer is used. It can represent a bottleneck for a production pipeline in semiconductor industry or overextend the sample processing time in investigation of challenging samples with complicated interference patterns, when high-SNR dataset is required. Typically, an XRR or HRXRD profile is acquired by scanning over certain range of angles with the total acquisition time divided equally between all the scan points [1-3]. However, not all the points are equally valuable for retrieval of the information about the investigated sample. For example, the vicinity of the layer's Bragg peak in an HRXRD profile is likely to contain most of the information about the lattice cell of that layer. In an XRR profile, smaller angles correspond to electron density and surface roughness of the topmost layer, while higher angles with interference fringes are useful for analysis of layer thicknesses [1-4]. Intuitively, a time-efficient approach consists in selecting a small number of the most informative scan points and allocating the available measurement time for them.

From that perspective, a number of practical questions arise. How can one quantify the informativity of a particular measurement scenario? How many scan points (and which ones) are optimal for a specific sample model? How the measurement time should be split between the points? Does inaccurate prior information about the sample hinder the measurement optimization? To give systematic and algorithmizable answers to those questions, we use Fisher information – a powerful mathematical tool suitable for quantification of data informativity and optimization of measurements [5]. First, we illustrate the idea by comparing informativity of individual profile points for single-parameter estimation problems and reproduce the known relation between the sample layers' parameters and the XRR or HRXRD profile parts mostly influenced by them. Next, we develop the measurement optimization methodology for simultaneous inference of multiple sample parameters and apply it to several XRR and HRXRD problems with complex interference patterns. Finally, the influence of the inaccurate prior knowledge about the sample on the appropriateness of the optimized measurement angles is analyzed and the methodology is modified accordingly.

References

[1] Pietsch, U., Holy, V., Baumbach, T. (2004). High-Resolution X-Ray Scattering.
[2] Bowen, D.K., Tanner, B.K. (2018). X-ray metrology in semiconductor manufacturing.
[3] Als-Nielsen, J., McMorrow, D. (2001). Elements of Modern X-ray Physics.
[4] Benediktovitch, A., Feranchuk, I., Ulyanenkov, A. (2013). Theoretical Concepts of X-ray Nanoscale Analysis.
[5] Mikhalychev, A. et al. (2021). Journal of Applied Crystallography, 54, p.1676.

Development of algorithms and modeling tools for low-energy CD-SAXS measurements

Adrien Toulouse[1], Guillaume Freychet[2], Patrice Gergaud[2]
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[2] *Univ. Grenoble Alpes, Cea, Leti, France*

Presentation type: Oral **Presentation time:** 12:00-12:15

With the continued miniaturization of electronic components over the last few decades, there is a rising need for new in-line metrology techniques capable of characterizing component with sub-nanometric resolution. While microscopies such as SEM or AFM are widely spread and used for such measurements, they are reaching their resolution limit. CD-SAXS has been developed over the last decade and shows promising results [1]. However, it is currently not available in lab-based settings (except for High Aspect ratio structures) and requires a synchrotron to go across a 750 µm-thick Si wafer.

Based on the progress of low energy x-ray sources and more precisely High Harmonic Generation sources in recent years, measurements with such source could be in reflection geometry [2]. The use of low energy X-rays allows the use of a relatively high incident angle (>15°). Therefore, the footprint of the beam on the sample is viable for measurements on small patterned area (50x50 µm2).

Promising results were obtained with HHG sources [3, 4]. However, the different interaction between soft x-rays and matter requires us to rethink all the simulation mechanisms. Indeed, hard x-rays approximations like the Born Approximation (BA) and the Distorted Waves BA (DWBA), neglecting absorption phenomena, are not valid anymore. To illustrate those limitations, we propose to compare simulations obtained with BA and DWBA with the results yielded by a Maxwell solver that's used to solve the electromagnetics equations directly.

We will present the results of CD-SAXS and GISAXS simulations obtained with JCM [5] software. JCM enables us to illustrate what's hapenning in both near field and far-field. Then, we will compare the results obtained with the BA and DWBA with the Maxwell solver and discuss the limit of validity of the BA and DWBA approximation with x-ray energies.

Finally, we will illustrate the role of the refraction and absorption phenomena in near field results to explain the final difference between the simulations and discuss the conditions in which the CD-SAXS and GISAXS simulations required maxwell solver.

References

[1] D. F. Sunday, et al., Three-dimensional x-ray metrology for block copolymer lithography line-space patterns, J. Micro. Nanolithogr. MEMS MOEMS 12, 12 (2013)
[2] J. Seres et al., « Source of coherent kiloelectronvolt X-rays ».
[3] V. Soltwisch et al., « Reconstructing detailed line profiles of lamellar gratings from GISAXS patterns with a Maxwell solver ».
[4] C. Porter et al., "Soft x-ray: novel metrology for 3D profilometry and device pitch overlay"
[5] JCMwave

Conditional Machine Learning Model for Scalable Landmark Detection in Comparative Morphological Imaging of Medaka Inbred Lines

Xiaoying Tan[1], Tilo Baumbach[2], Sofiia Syrota[3], Alexey Ershov[3]

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Presentation type: Oral **Presentation time:** 12:15-12:30

Genotype–phenotype mapping relies on precise quantification of anatomical shape. The Medaka Inbred Kiyosu–Karlsruhe (MIKK) panel of 80 fully sequenced isogenic inbred lines offers a powerful resource for systematic genetic studies. High-throughput synchrotron microtomography generates high-resolution 3D volumes of hundreds of medaka fish specimens, but converting these multi-gigabyte volumes into quantitative morphological traits remains challenging. Traditional dense 3D convolutional networks demand excessive GPU memory and scale poorly with image size and target landmark count, limiting large-scale comparative studies across inbred lines.

We propose a hybrid conditional framework that combines reinforcement learning for efficient coarse landmark localization with a convolutional network for high-precision refinement. A conditional reinforcement learning agent navigates large volumes using local 3D observations and learns a landmark-conditioned policy with a single shared model across all landmarks, ensuring a small memory footprint. This agent produces coarse landmark positions, which are subsequently refined by a conditional 3D convolutional network operating on a high-resolution region of interest. The refinement network outputs localized heatmaps, enabling subvoxel accuracy. The conditional design allows the framework to scale to an arbitrary number of landmarks and naturally leverage partially annotated training data.

We applied our model to 3D volumes of medaka fish with up to 49 anatomical landmarks per specimen. The method achieves localization accuracy comparable to inter-annotator variability while drastically reducing GPU memory consumption relative to dense 3D baselines. This efficiency makes large-scale processing of the hundreds of specimens within the MIKK panel feasible on standard hardware. The automatically detected landmarks enable systematic cross-line comparisons of morphological distances, angles, and shape configurations, supporting the design of targeted F2 crosses guided by trait patterns.

IX: Diffraction Contrast Imaging - 1/2

Session Chairs

Carsten Detlefs
Carsten Richter

Diffraction contrast imaging of ultra-wide bandgap substrates and structures for hetero-integration

Mark Goorsky[1], Michael Liao[2]

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[2] *UCLA, USA*

Presentation type: Invited Talk **Presentation time:** 14:00-14:30

Ultra-wide bandgap materials such as b-Ga2O3 and diamond enable advances in optoelectronic and electronic performance.However, the growth of these substrates differs significantly from growth of previous generations of semiconductors such as silicon, InP and GaAs.Diffraction contrast based imaging is described to relate substrate-based defects with subsequent epitaxial growth for b-Ga2O3 –based systems (thick b-Ga2O3 and b-(AlxGa1-x)2O3 with the formation of extended defects particularly important for vertical transport devices.Cracks forming in b-(AlxGa1-x)2O are also studied using these imaging techniques with major cracks forming along different orientations due to the low symmetry of the b-Ga2O3 lattice.

Bulk diamond growth is achieved via vapor phase techniques and can be separated into homoepitaxial and heteroepitaxial processes.While the crystallinity of the homoepitaxial structures is better than for the heteroepitaxial cases, the heteroepitaxial approach provides a more direct route to large diameters for hetero-integration.Using a series of diffraction images based on different orientations, localized areas of strain and misorientation are clearly resolved and the overall relationship between lattice curvature and wafer curvature are clearly elucidated.

Parts of this research were performed on APS beam time from the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

3D Mapping of Dislocation-Crack Tip Interactions in SrTiO by Dark-Field X-ray Microscopy

Albert Zelenika[1], Christoph Kirchlechner[1], Xufei Fang[1], Can Yildirim[2], Oliver Preuss[1], Yaozhu Li[3]

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Presentation type: Oral **Presentation time:** 14:30-14:45

Crack formation and propagation remain major limitations for the reliability of structural and functional ceramics. Dislocation-based toughening, highly effective in metals, could in principle compensate for the intrinsically poor fracture toughness of ceramics, yet its role remains poorly understood because conventional techniques such as TEM and chemical etching cannot access the three-dimensional defect structures around cracks in bulk material.

Dark-Field X-ray Microscopy (DFXM) [1-3] addresses this challenge through non-destructive 3D imaging of dislocations, strain fields and orientation gradients in bulk single crystals, with spatial resolution down to ~100 nm, angular resolution down to ~10-3 ° and strain sensitivity of ~10-5. Here, we apply DFXM at the ID03 beamline of the ESRF to investigate dislocation arrangements around crack-tips in mm-sized single-crystal SrTiO as a model perovskite oxide. Recent advances in room-temperature dislocation engineering enable tailoring of dislocation density across five orders of magnitude (~1010 to ~1015 m-2) in this oxide [4], yet the resulting increase in fracture toughness remains marginal (~20%) [5], contrary to analytical models that predict crack-tip shielding by dislocations [6,7,8].

Specimens with (001) surface orientation were prepared by cyclic Brinell scratching [4], producing dislocation-rich tracks (~1012 m-2) embedded in the pristine material (~1010 m-2), with cracks pre-induced on {110} planes that traverse both regions. DFXM resolved individual dislocations and their associated strain fields around the crack-tip in 3D from layer-by-layer rocking and mosaicity scans, allowing for direct comparison of crack-tip behaviour with/without pre-engineered dislocations.

The result provides the first 3D experimental view of dislocation-crack tip interactions in a bulk perovskite oxide and clarifies why pre-engineered dislocations confer only limited crack shielding in SrTiO3. Beyond this material, the DFXM workflow demonstrated here offers a transferable framework for the quantitative mesoscale characterisation of defect-crack interactions in other semi-brittle crystals [9] in a 3D manner.

References

[1] H. Simons et al., Nat. Commun., 2015, 6, 6098.
[2] H.F. Poulsen et al., J. Appl. Crystallogr., 2017, 50(5), 1441-1456.
[3] C. Yildirim et al., Sci. Rep., 2023, 13, 3834.
[4] X. Fang et al., J. Am. Ceram. Soc., 2024, 107, 1425-1447.
[5] M.N. Salem et al., J. Am. Ceram. Soc., 2023, 106, 1344-1355.
[6] J. Rice and R. Thomson, Philos. Mag., 1974, 29(1), 73-97.
[7] H. Gao, J. Mech. Phys. Solids, 1991, 39(2), 157-172.
[8] A. Hartmaier and P. Gumbsch, Phys. Rev. B, 2005, 71(2), 024108.
[9] A. Frisch et al., J. Am. Ceram. Soc., 2025, 108(9), e20575.

Sub-grain origin and dynamics in cast-mono silicon for photovoltaic solar cells revealed by X-ray topography and diffraction rocking curve imaging

Nathalie Mangelinck-Noël[1], Ilhem Nadia Rabehi[1], Sirine Houam[2], Etienne Pihan[3], Mickaël Albaric[3], Benoit Marie[3], Gabrielle Regula[2], Loïc Patout[2], Guillaume Reinhart[2], Fabrice Guittonneau[4], Laurent Barrallier[4], Thu Nhi Tran-Caliste[5], José Baruchel[5]

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Presentation type: Oral **Presentation time:** 14:45-15:00

In silicon for photovoltaic solar cells, as-grown dislocations, dislocation clusters and sub-grain boundaries (SGBs) can degrade the material electrical properties. In previous works, the origin and/or termination of these clusters were analysed post-growth by tracing downwards the defects in the ingot. It was found that special grain orientations and boundaries affect their evolution. However, open and key questions regarding the origin and dynamics of SGBs remain.

This review summarizes a series of studies using synchrotron X-ray imaging to investigate defect formation and propagation in cast-mono silicon. The cast-mono solidification process combines the cost advantages of directional solidification with the crystalline quality by using monocrystalline seeds. However, its performance can be limited by structural defects, particularly SGBs, which can originate near seed junctions or from the initial seed.

Crystal growth experiments are performed using the GaTSBI furnace — Growth at High Temperature observed by Synchrotron Beam Imaging — a dedicated setup that allows silicon seeds and samples to be heated, partially melted and then, resolidified under controlled thermal conditions. Coupled with synchrotron radiation, this setup enables simultaneous X-ray radiography and topography to reveal in-situ and time resolved evolution of crystallographic defects. Complementary diffraction rocking curve imaging provides quantitative maps giving access to local crystal distortion and lattice misorientation with high angular sensitivity. The characterization by EBSD (Electron Backscatter Diffraction) and by X-ray diffraction (XRD) complete this extensive structural and crystalline defect study and demonstrates the importance of such high angular sensitivity to understand the first stages of sub-grain formation. At a later growth stage, EBSD and XRD results allow to better understand the evolution of SGBs and the interaction of higher misorientation sub-grains with grain boundaries.

Unlike float-zone silicon seeds, where mobile dislocations glide on {111} during heating, cast-mono seeds are mainly characterized by an immobile cellular dislocation network up to temperatures close to the silicon melting point at which dislocations gliding on {111} are also observed. After regrowth from such seeds, sub-grain boundaries oriented along the growth direction are observed in the cast-mono-seeded sample, but not in float-zone-seeded references. Cellular dislocation networks are also associated with long-range crystal orientation gradients, suggesting that background dislocations may impose an organized lattice-rotation field that contributes to the formation and extension of electrically active SGBs.

Synchrotron X-ray imaging is a powerful approach for understanding defect inheritance, rearrangement, and multiplication in cast-mono silicon, providing guidance for improving seed quality and controlling defect formation during silicon crystallization.

Temporal Evolution of 3D Dislocation Structures in Silicon by Correlative X-ray Diffraction Imaging

Merve Pinar Kabukcuoglu[1], Tilo Baumbach[2], Elias Hamann[3], Marcus Zuber[2], Simon Bode[2], Daniel Hänschke[3], Carsten Richter[4], Kaspars Dadzis[4], Nikolaos Sagias[4]

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Presentation type: Oral **Presentation time:** 15:00-15:15

To track the temporal evolution and 3D behavior of individual dislocations in bulk semiconductor wafers under semiconductor-processing-relevant conditions, we bring together X-ray white-beam topography, X-ray diffraction laminography (XDL) [1], and controlled sample annealing environments. In addition to recent developments in 3D XDL methodology, we recently developed and simulated a compact induction heating system with integrated infrared thermography for real-time and quasi in situ synchrotron experiments [2].

In the presented study, this correlative approach is applied to silicon (Si), which remains one of the most important semiconductor materials for modern micro- and nanoelectronic technologies. Thermally activated dislocation slip during wafer processing can critically influence fabrication yield and device performance, particularly with the ongoing miniaturization of electronic devices toward nanometer dimensions.

Here, mechanically damaged Si wafers were subjected to repeated thermal annealing cycles above the brittle-to-ductile transition temperature while the spatio-temporal temperature distribution was monitored by infrared thermography. Between successive annealing stages, quasi in situ 3D X-ray diffraction laminography (XDL) measurements were performed to follow the temporal evolution of thermally activated dislocation structures within the same crystal volume. Complementary X-ray white-beam topography (XWBT) measurements further enabled Burgers vector identification of the evolving dislocation structures.

In this study, more than 100 individual dislocations were identified, labeled, traced across successive annealing stages, and correlated with their corresponding Burgers vectors, enabling quantitative 3D analysis of dislocation propagation during thermal annealing. Furthermore, complex mechanisms including cross-slip, interaction of dislocations, and the early formation of single-ended Frank–Read-like multiplication sources were directly observed in 3D. Correlation of the experimentally observed dislocation propagation, distributions among different {111}<110> glide systems, and multiplication mechanisms with resolved shear stress distributions provides new insight into the interplay between thermally driven dislocation dynamics and crystallographic glide behavior in Si wafers.

References

[1] D. Hänschke et al., Physics review Letters, 119, 215504 (2017)
[2] M. Kabukcuoglu et al., J. Synchrot. Rad., in press (2026)

Revealing Growth Discontinuities in Ammonothermal GaN by Advanced Bragg Diffraction Imaging Techniques

Lutz Kirste[1], Thu Nhi Tran-Caliste[2], José Baruchel[2], Tomasz Sochacki[3], Robert Kucharski[3], Patrik Straňák[1], Karolina Grabianska[3], Jan L Weyher[3], Michal Bockowski[3]

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Presentation type: Oral **Presentation time:** 15:15-15:30

Ammonothermal growth is a key technique for producing high-quality GaN substrates with low dislocation densities, yet repeated regrowth steps during seed enlargement and bulk crystal fabrication inevitably introduce growth discontinuities and associated defects [1]. In this work, we investigate such defect structures in ammonothermal GaN using complementary Bragg diffraction imaging techniques, namely laboratory Lang X-ray topography (L-XRT) and synchrotron-based rocking curve imaging (RCI).

Growth discontinuities manifest predominantly as chains of dislocation bundles forming along specific crystallographic facets, as well as tiling seams originating from seed coalescence. These features appear as extended contrast lines in L-XRT topographs and can be chronologically linked to individual regrowth steps. Quantitative RCI analysis reveals that these defect regions are associated with local lattice tilts of up to ~13 arcsec and alternating strain fields on the order of ±3 arcsec.

A central result of this study is that, despite the presence of such pronounced defect structures, dynamic diffraction effects can still be clearly observed [2]. This is attributed to the remarkably high structural quality of the GaN crystal in the immediate vicinity of the defects. Regions adjacent to dislocation bundle chains exhibit ultra-low dislocation densities and minimal lattice distortion, providing sufficiently perfect volumes for the formation of coherent wavefields required for dynamical diffraction. As a consequence, the diffraction contrast cannot be interpreted solely within a kinematical framework but requires consideration of dynamical scattering processes. These findings highlight the coexistence of localized defect-induced lattice perturbations and extended regions of outstanding crystalline perfection within ammonothermal GaN substrates. The results further demonstrate that Bragg diffraction imaging is highly sensitive not only to defect structures but also to subtle variations in crystal quality that govern the transition between kinematical and dynamical diffraction regimes. In addition to lateral growth discontinuities, vertical discontinuities along the growth direction are considered to provide a comprehensive understanding of defect formation mechanisms in ammonothermal GaN.

This work contributes to the optimization of crystal growth processes by linking specific growth conditions to defect formation while simultaneously emphasizing the preservation of excellent crystal quality necessary for advanced device applications.

References

[1] T. Sochacki, et al., Growth of bulk GaN crystals for the production of substrates, in Comprehensive Semiconductor Science and Technology, second edition, Elsevier, 2025.
[2] L. Kirste et al., Progress in Crystal Growth and Characterization of Materials, vol. 71, no. 3, p. 100668, 2025.

Operando spatio-temporal imaging of devices and functional nanostructures by X-ray nano diffraction imaging methods

Tobias Schülli[1], Cedric Corley-Wiciak, Agnieszka Corley-Wiciak, Nikita Vostrov, Ugwumsinachi Oji, Juan-Manuel Carrillo Larrea, Jiangtao Zhao[1], Steven Leake[1], Marie-Ingrid Richard[2]
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Presentation type: Oral **Presentation time:** 15:30-15:45

With the start of the 1st hard X-ray 4th generation synchrotron source ESRF/EBS flux and brilliance hungry methods typically exploiting nanobeams and coherence are gaining momentum in the community of material science. Spatially resolving X-ray diffraction-based tools are of relevance for the characterization of most emerging nanomaterials or electronic devices. While typical samples for these techniques are microelectronic structures, the resolving power has proven to reach down to length scales relevant for catalysis and basic solid state chemistry as encountered in most electrochemical systems. With worldwide efforts in the upgrading or new conception of synchrotron sources, improvements of several orders of magnitude in the throughput of these methods are now at reach and required dedicated beamline design to exploit the significant improvements in spatial resolution but also in the time domain. At the same time, enabling technologies such as X-ray optics and detectors are closing previously existing gaps, further boosting the use of X-ray nano imaging in new fields of science and engineering. Beamline ID01 at the ESRF is specialized on the imaging of strain and structure under Bragg diffraction conditions. Our results following sample evolution either in real time or in stroboscopic mode show the relevance of such new tools in complex experimental environments as encountered in nanotechnology or semiconductor devices where (time-resolved) nano-imaging of strain and structure are of highest relevance.High resolution in reciprocal and real space is now obtained on time scales allowing to follow operando in areas and on timescales ranging from Batteries (seconds to hours) down to sub nanosecond time resolved imaging of functioning electronic devices. Such high time resolution is reached by exploiting the time structure of the synchrotron X-ray beam itself. The talk will present most recent examples covering these areas. These range from surface acoustic wave devices to high performance microelectronic devices as currently developed by our collaborators from industry and academia.

X: Related Techniques

Session Chairs

Oleg Gorobtsov
Ivan Vartaniants

Quantum X-rays: Emerging Opportunities for Imaging, Spectroscopy, and Metrology

Sharon Shwartz[1]
[1] *Bar Ilan University, Israel*

Presentation type: Invited Talk **Presentation time:** 16:15-16:45

X-rays have revolutionized our ability to probe matter, enabling breakthroughs ranging from protein structure determination and nanoscale imaging to ultrafast studies of chemical and quantum dynamics. These advances have been driven by continuous improvements in x-ray sources, optics, and detectors.

In parallel, quantum optics has transformed the visible and infrared domains by introducing powerful new concepts such as quantum-enhanced imaging, correlation spectroscopy, and nonclassical interference. Bringing these ideas to x-ray energies could open entirely new possibilities for imaging, spectroscopy, and precision metrology.

Recent advances are beginning to bring quantum concepts into the x-ray domain. In particular, time-energy correlations generated through x-ray spontaneous parametric down-conversion (SPDC) have been shown to improve visibility and signal-to-noise ratio in challenging high-background environments, even at low photon flux. More recently, proposals for x-ray SU(1,1) interferometers and quantum magnification schemes have suggested new approaches for enhancing measurement sensitivity and extracting spatial information beyond the limits of conventional x-ray optics. Together, these developments demonstrate that quantum correlations can be exploited to access information that would otherwise be obscured by noise or lost in classical measurements.

Looking further ahead, quantum correlations may enable entirely new approaches to x-ray imaging and spectroscopy. Potential opportunities include sub-shot-noise imaging, correlation-based imaging and spectroscopy, quantum-enhanced phase retrieval, and novel reconstruction techniques capable of suppressing noise and mitigating image degradation caused by scattering or finite source size-induced blurring. Such methods could ultimately address challenges that remain difficult for classical x-ray techniques, opening new routes toward low-dose imaging, enhanced contrast, improved sensitivity, and new forms of image formation.

In Situ Nanofocused Microsecond XPCS Enables Spatiotemporal Mapping of 8 nm-diameter Nanoparticle Diffusion During Mesocrystal Assembly

Leonardo Oliveira[1], Maik Kahnt[2], Jesper Wallentin[3], Klara Suchan[3], Matheus Ferreira[3], Simon Liedtke[3], Iason Andronis[4], Jake Hardy[3], Martin Trulsson[3], Petter Persson[3], Foivos Perakis[4], Dmitry Baranov[3]

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Presentation type: Oral **Presentation time:** 16:45-17:00

Nanoparticles (NPs) can self-assemble into highly ordered mesocrystals, in which long-range interparticle correlations give rise to collective phenomena such as superfluorescence. The degree of ordering critically determines the extent of these collective effects. NP diffusivity is decisive for whether ordered assembly or kinetic disordered arrest occurs but has remained challenging to study experimentally. X-ray photon correlation spectroscopy (XPCS) correlates coherent speckles between rapidly acquired frames to quantify particle diffusion. However, applying XPCS to studies of small NPs, in our case 8 nm CsPbBr , has been out of reach due to the fast dynamics and weak scattering.

We address this with in situ XPCS combining three recent advances: a fourth-generation synchrotron (MAX IV) providing ~100× higher coherent flux than third-generation sources, a nanofocused beam (70 nm) enabling spatially resolved measurements and enhanced contrast, and a prototype detector operating at 120 kHz frame rate giving access to microsecond dynamics. Together, these enable direct, spatiotemporally resolved quantification of NP diffusivity simultaneously with the evolving SAXS signal and local volume fraction throughout evaporation.

We observe a 30-fold slowdown of collective dynamics from 3 µs to 80 µs at volume fractions ~8%, far below geometric close-packing, driven primarily by hydrodynamic suppression rather than thermodynamic clustering. Spatial mapping reveals two distinct pathways. Regions up to 100 µm below the evaporation front maintain sufficient diffusive mobility for ordered mesocrystal formation, while regions further down undergo premature agglomeration and kinetic arrest. Our results establish hydrodynamic interactions as the decisive factor governing pathway selection in evaporative self-assembly and provide direct design criteria for improving mesocrystal yield through tailored solvent and ligand choice. More broadly, they demonstrate nanofocused XPCS as a powerful spatially resolved probe of sub-10 nm NP dynamics in complex, evolving colloidal environments.

XI: High-Throughput, In Situ & Operando

Session Chairs

Anton Plech
Christian Schlepütz

Imaging materials in motion: From sheared foams to human middle ear mechanics

Christian Schlepütz[1]

[1] *Paul Scherrer Institute, Switzerland*

Presentation type: Invited Talk **Presentation time:** 08:30-09:00

Seeing is believing. Yet, when it comes to the investigation of interacting microscopic objects and structures, it is even more: Seeing is understanding! This is particularly true when trying to unravel the nature of dynamic processes at length and time scales that are naturally inaccessible to the bare human eye.

Understanding dynamic processes in materials and biomechanical systems requires direct observation of their internal structural evolution at microscopic length and time scales. Since the properties and performance of both engineered and natural materials are fundamentally governed by their internal microstructure, transient phenomena occurring during formation, processing, or operation often determine their ultimate behavior. Most such processes typically occur within opaque materials or complex environments, rendering them inaccessible to conventional optical characterization techniques.

X-ray tomographic microscopy provides non-destructive three-dimensional visualization of internal structures with micrometer-scale resolution. By rapidly acquiring successive tomographic volumes, dynamic phenomena can be captured as time-resolved three-dimensional image sequences, effectively creating quantitative “4D movies” (3D space plus time). These datasets not only provide intuitive visualization of complex processes but also enable rigorous quantitative analysis of structural evolution, transport phenomena, deformation mechanisms, and dynamic interactions within materials and biological systems.

Realizing such experiments presents several key challenges: (i) matching imaging speed to the characteristic and often hierarchical time scales of the investigated processes, (ii) designing, controlling, and synchronizing experimental environments compatible with high-speed tomography, and (iii) processing and extracting meaningful information from the resulting large-scale 4D datasets.

This presentation will highlight recent advances in synchrotron-based dynamic X-ray tomography and showcase representative applications across materials science and biomechanics. Case studies include bubble rearrangements and stress relaxation in sheared liquid foams, transient flow dynamics in porous media, and motion analysis of auditory structures in fish and the human middle ear. Together, these examples demonstrate how high-speed tomographic microscopy enables unprecedented insight into dynamic processes, transforming visualization into quantitative understanding.

Imaging pressure-nucleated and field-erased BiFeO3 domains via in-situ nano-XRD

Leonardo Oliveira[1], Jesper Wallentin[2], Megan Landberg[3], Aksel Mihaylov[2], Bixin Yan[4], Morgan Trassin[4]

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Presentation type: Oral **Presentation time:** 09:00-09:15

Domains and their walls are functional units that play a central role in energy storage and electromechanical switching. Imaging these nanoscale units and tracking their dynamic response remains a major experimental challenge. Specifically, domains in thin-film device geometries are typically smaller than 100 nm and buried beneath metallic electrodes,making them inaccessible to conventional surface probes.

Nano-focused XRD offers sub-100 nm spatial resolution imaging of buried domains with both lattice strain and tilt sensitivity. We have recently exploited this capability to image ferroelastic-ferroelectric domains in BiFeO -based thin films in a capacitor geometry, uncovering how the mere electrode deposition introduces internal stress and domain reorientation [1]. The long penetration depth of the hard X-rays makes this method ideal for in-situ and operando experiments.

Here, we use in situ nano-indentation to locally transform the crystal structure of La-substituted BiFeO from pseudocubic to orthorhombic, corresponding to a dipolar transition from ferroelectric-to-antiferroelectric state through stress-driven redistribution of La cations [2,3]. Furthermore, we use in-situ electric field applications to erase the transformed regions, tracking the evolution at the single-domain level.

Using scanning nano-XRD at the NanoMAX beamline, we map the evolution of strain and tilt heterogeneities across both stimuli, capturing in real space the nucleation and annihilation of ferroic order under competing mechanical and electrical drives. We discuss our recent finding on how the strain field impact the microscopic mechanisms of the phase transition and its reversal, offering new insight into the interplay between stress, lattice distortion, and polarization in oxide thin films for electronic applications.

References

[1] Hill Landberg, M.O.; Yan, B.; Chen, H.; et al. Direct Imaging of Nanoscale Ferroelectric Domains and Polarization Reversal in Ferroelectric Capacitors. Nano Lett. 25, 16304–16310, 2025.
[2] Mundy, J.A.; Grosso, B.F.; Heikes, C.A.; et al. Liberating a Hidden Antiferroelectric Phase with Interfacial Electrostatic Engineering. Sci. Adv. 8, eabg5860, 2022.
[3] Müller, M.; Yan, B.; Ko, H.; et al. Reversible Control over the Distribution of Chemical Inhomogeneities in Multiferroic BiFeO3. Nat Commun 16, 3951, 2025.

Towards Serial Computed Tomography

Tomáš Faragó[1], Tilo Baumbach[1], Thomas Van De Kamp[1], Marcus Zuber[1], Chandan Sarkar[1], Angelica Cecilia[1], Clément Tavakoli[1], Elias Hamann[2], Nikolay Zagainov[1], Mateusz Czyzycki[2]
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Presentation type: Oral **Presentation time:** 09:15-09:30

Synchrotron-based X-ray microtomography has become an indispensable technique for non-invasive 3D morphological analysis of materials, tissues, small devices and organisms. The growing demand for high-throughput measurements of large specimen collections, e.g., for applications in paleontology (1), linking ecology and morphology (2, 3), genotype-phenotype correlations (4), and even the large-scale digitization of morphological biodiversity (5), is driving the development of increasingly automated X-ray imaging workflows for large comparative morphological studies. However, current high-throughput experiments remain technically demanding and labor-intensive, with existing robotic systems typically limited to scanning only around 50 specimens in a single unattended run.

Future workflows will require substantially increased automation beyond the scanning process itself to encompass the entire pipeline, including sample preparation, data acquisition, image reconstruction, data analysis, and comprehensive data management for measuring campaigns with hundreds and thousands of specimens. We summarize this integrated workflow under the term “Serial CT”. This presentation highlights major recent advances and key technological developments needed for fully automated Serial CT workflows for large-scale morphological research.

We report about two Serial CT systems: one at the HIKA experimental station at the P23 beamline of PETRA III and another at the IMAGE beamline of the KIT Light Source. They are both capable of processing more than 1000 samples at a time. The UFO-II system at IMAGE presently allows Serial CT scanning of such large sample series with a throughput of 60 samples/hour in the filtered white-beam mode. At HIKA, the system can measure 15 samples/hour in the holographic imaging mode with monochromatic beam. Our workflow includes automated CT scanning based on AI sample detection, parallelized data streams, GPU-accelerated 3D reconstruction for quality assurance, automatic metadata collection and compression. First examples studying the morphology of large series of vertebrate model organisms and arthropods demonstrate the potential of Serial CT for life science applications and beyond.

References

van de Kamp, T., et al. (2018): Parasitoid biology preserved in mineralized fossils. Nature Communications 9: 3325.
Rühr, P.T., et al. (2021): Juvenile ecology drives adult morphology in two insect orders. Proceedings of the Royal Society B 288: 20210616.
Edel, C., et al. (2024): Bite force transmission and mandible shape in grasshoppers, crickets, and allies is not driven by dietary niches. Evolution 78: 1958-1968.
van de Kamp, T., et al. (2022): Evolution of flexible biting in hyperdiverse parasitoid wasps. Proceedings of the Royal Society B 289: 20212086.
Katzke, J., et al. (2026): High-throughput phenomics of global ant biodiversity. Nature Methods 23: 663-672.

Shape memory zirconia-based ceramic micropillars studied by in situ Laue microdiffraction

Thomas Cornelius[1], Olivier Thomas, Solène Comby-Dassonneville, Jérôme Chevalier, Helen Reveron, Michael Texier[2], Marcelo Demetrio Magalhaes, Sylvain Meille, Thierry Douillard, David Rodney

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Presentation type: Oral **Presentation time:** 09:30-09:45

Thanks to a stress-induced martensitic phase transformation from tetragonal to monoclinic (t-m), zirconia-based ceramics can exhibit plasticity at room temperature, overcoming the limited ductility and toughness of ceramics. This is a consequence of the traditional trade-off between the strength and ductility of hard-to-deform materials. More recently, it was shown that zirconia-based ceramics stabilised by ceria (CSTZ) undergo transformation at lower stresses and prior to crack initiation [1] than yttria-stabilised tetragonal zirconia [2-4], leading to greater ductility. This transformation-induced plasticity (TRIP) deformation process is analogous to the martensitic transformation in metallic shape-memory alloys (SMAs). As with SMAs, a transformed CSTZ ceramic can transform back from the monoclinic to the tetragonal phase when heated above a critical temperature. Nevertheless, predicting and optimising the macroscopic ductility and phase-memory behaviour of bulk ceramics requires a multiscale approach to understand (1) the transformation at the grain level and (2) its propagation across grain boundaries.

Here, we present in situ Laue microdiffraction studies of the shape memory behaviour of CSTZ micropillars. The tetragonal-monoclinic phase transformation was examined by in situ microcompression, while the reverse transformation was monitored during annealing. The critical stress for the t-m transformation was found to depend on the crystal orientation of the micropillar, with the highest stress occurring in (001)-oriented pillars [5]. This critical stress decreases with the number of compression-heating cycles, likely due to the nucleation of defects such as dislocations and antiphase boundaries. The reverse transformation occurs at a critical temperature on the order of 350 °C, which seems to also be dependent on the number of transformation cycles.

References

[1] J. Chevalier et al., J. Am. Cer. Soc. 103, 1482 (2020)
[2] J. Chevalier et al., J. Am. Cer. Soc. 92, 1901 (2009)
[3] X. Zeng et al., Acta Mater. 116, 124 (2016)
[4] N. Zhang et al., Acta Mater. 120, 337 (2016)
[5] M.D. de Magalhães et al., J. Eur. Cer. Soc. 45, 116794 (2025)

Compact PLD Sample Environments for In-Situ X-Ray Studies of Thin-Film Growth at Synchrotron Beamlines

Aleksandr Goikhman[1]
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Presentation type: Oral **Presentation time:** 09:45-10:00

In-situ studies of thin-film growth are important for understanding how interfaces, strain, defects and functional properties appear during deposition. For X-ray methods this is especially attractive, because diffraction, scattering and photoemission can follow the structure and electronic state of a film before the sample is removed from the growth environment. At the same time, this creates a practical problem: the deposition system must fit into the beamline geometry, provide optical and X-ray access, work under UHV or controlled gas atmosphere, and keep the sample position stable enough for precise X-ray measurements.

In this contribution we present compact pulsed laser deposition (cPLD) systems developed as sample environments for synchrotron beamlines. The main advantage of PLD for this task is that the laser is located outside the vacuum chamber. Therefore, the chamber can be made small, light and beamline-adapted, while still keeping the flexibility of PLD for oxides, metals and multilayer structures.

A representative example is the portable cPLD chamber used at the P23 beamline of PETRA III for in-situ X-ray diffraction studies of oxide thin-film growth. The system had a total weight of about 12 kg, allowed growth at temperatures up to 800 °C in oxygen atmosphere, and was compatible with laser wavelengths of 266 and 532 nm. During BaTiO3 deposition on different substrates, diffraction curves of the BaTiO3 (001) reflection were recorded after defined numbers of laser pulses. This made it possible to follow the evolution of the film during growth and to correlate thickness, strain state, substrate material, temperature and cooling conditions. In a related NiO study, growth oscillations and post-growth analysis were used to identify defect formation and tune the properties of the film.

We also discuss the extension of the same approach to in-vacuo PLD–HAXPES workflows at PETRA III, where thin films grown by PLD can be transferred and studied without exposure to air. Such experiments are especially useful for oxide/metal interfaces and magnetic heterostructures, where the photoelectron spectra depend on magnetization, X-ray polarization and emission geometry.

The examples show that compact PLD can work not only as a preparation tool, but as a real X-ray sample environment. It enables direct feedback between synthesis and characterization, reduces uncertainty caused by ex-situ handling, and opens a practical route to operando studies of thin-film formation at synchrotron facilities.

Fig. 1. Compact PLD sample environment for in-situ X-ray studies at PETRA III.The system enables pulsed-laser deposition directly in the synchrotron beamline with in-situ X-ray diffraction monitoring

Neuromorphic X-ray radiographic and tomographic imaging

Hongjian Wang[1], Benjamin Bejar Haro[2], Goran Lovric[3], Marco Stampanoni[4], Matias Kagias[5]

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Presentation type: Oral **Presentation time:** 10:00-10:15

Synchrotron-based X-ray micro-computed tomography has been a reference technique for many studies investigating fundamental properties and functions of materials and organisms. However, the increased use of imaging technologies is becoming more challenging, as high-speed dynamic imaging experiments either produce exorbitant amounts of data or remain limited in temporal resolution. Recently, bio-inspired neuromorphic event cameras have been introduced as an alternative approach to conventional frame-based cameras, in the sense that they detect per-pixel brightness changes asynchronously and generate a stream of events encoding the triggering time, location, and polarity of each pixel [1]. With the encoded high-frequency information in the events, event-based vision has recently gained popularity in various applications; however, its realization in X-ray imaging remains largelyunexplored.

At the TOMCAT beamline of the Swiss Light Source, Paul Scherrer Institute, we have recently demonstrated an inline dual-camera X-ray imaging setup combining a high-speed frame-based CMOS detector [2] with a neuromorphic event camera, Prophesee Metavision Evaluation Kit 4. Both cameras were coupled to magnifying visible-light optics with an effective pixel size of approximately 1.1 µm and synchronized by an external 1 MHz TTL signal using a PandABox. The setup enables simultaneous acquisition of conventional X-ray projection frames and asynchronous event streams under the same imaging conditions.

Here, we report the first characterization of the system by imaging a live sandclock in radiographic mode and present the necessary post-processing steps for achieving more than fivefold temporal super-resolution [3]. We further showfirst results from our ongoing work in extending the framework to CT acquisitions, which are often limited to sparse angular views. A data-acquisition and reconstruction pipeline based on implicit neural represented is designed to complement the fine-grained angular information from events to enhance tomographic reconstruction. The result is demonstrated both in simulation and real-world validation, showcasing the potential of using only 5 views and events for a CT reconstruction as a future potential measurement protocol. Overall, this work represents an early exploration of neuromorphic sensing for X-ray radiography and computed tomography, with potential benefits for data-rate reduction, improved temporal resolution, and real-time processing in future ultrafast time-resolved synchrotron X-ray imaging experiments.

References

[1] G. Gallego et al., “Event-based Vision: A Survey,” IEEE Transactions on Pattern Analysis and Machine Intelligence, 44, 154–180, 2022.
[2] R. Mokso et al., “GigaFRoST: the gigabit fast readout system for tomography,” Journal of Synchrotron Radiation, 24, 1250–1259, 2017.
[3] H. Wang et al., “Event-guided temporally super-resolved synchrotron X-ray imaging,” Communications Physics, 8, 2025.

High-throughput digitization of insect morphological biodiversity

Thomas Van De Kamp[1], Tilo Baumbach[1], Rebecca Spiecker[2], Elias Hamann[2], Tomáš Faragó[1], Marcus Zuber[1], Chandan Sarkar[1], Angelica Cecilia[1], Clément Tavakoli[1], Cristina Lupaşcu-Vasiliţa[1], Nikolay Zagainov[1], Jenny Hein[1]

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Presentation type: Oral **Presentation time:** 10:45-11:00

Insects are the most diverse group of animals on Earth. They are essential to ecosystems, agriculture, and human livelihoods, yet they are declining at alarming rates. More than one billion insect specimens are preserved in scientific collections worldwide, representing an immense but largely untapped research resource.

X-ray microtomography provides entirely new insights into internal and external morphology, with far-reaching implications for biodiversity research, biomimetics, and paleontology. Such fields will greatly benefit from the “Serial CT” for automatic routine scanning of large number of samples that is being developed at KIT. High-throughput capabilities at the KIT Light Source (1) and PETRA III have already demonstrated the potential for digitizing and performing 3D analysis of both important specimens and extensive scientific collections, including extant and fossil insects.

We present recent results, including the discovery of fossil parasites (2), the identification and evolutionary analysis of a unique flexible biting mechanism in chalcid wasps (3), and our most ambitious large-scale project to date: the ANTSCAN initiative (4, 5), a collaboration between KIT and the Okinawa Institute of Science and Technology (OIST), together with partners from museums worldwide. The resulting dataset contains more than 2200 digitized ants which are available to the broad public via Biomedisa (6). Each ant has its own digital object identifier with associated metadata accessible via RADAR4KIT (7). By enabling rapid acquisition of phenotypic data across the ant tree of life, ANTSCAN has paved the way for unprecedented large-scale comparative studies on ant morphology, diversity and evolution (8).

Furthermore, we will highlight recent advances in large-scale data analysis, including semi-automated segmentation of anatomical structures, body regions, and internal organs from volumetric datasets. We will also discuss the growing potential of computer vision and artificial intelligence approaches for fully automated extraction, classification, and quantitative analysis of morphological traits.

References

[1] Cecilia, A., et al. (2025): Journal of Synchrotron Radiation 32: 1036-1051.
[2] van de Kamp, T., et al. (2018): Nature Communications 9: 3325.
[3] van de Kamp, T., et al. (2022): Proceedings of the Royal Society B 289: 20212086.
[4] Katzke, J., et al. (2026): Nature Methods 23: 663-672.
[5] van de Kamp, T. & Economo, E.P. (2026): Nature Methods 23: 505-506.
[6] Lösel, P.D., et al. (2020: Nature Communications 11: 5577.
[7] RADAR4KIT
[8] Matte, A., et al. (2025): Science Advances 11: eadx8068.

Resonant Tender X-ray Scattering and Diffraction: a key tool to reveal the location of counterions in polymeric organic mixed ionic/electronic conductors

Guillaume Freychet[1]

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Presentation type: Oral **Presentation time:** 11:00-11:15

Resonant x-ray scattering and diffraction is an emerging technique for the nanostructure characterization of soft matter. While these approaches are widely spread for highly ordered material, the amorphous or paracrystalline nature of most of the soft matter systems limits the use of currently developed method such as diffraction anomalous fine structure technique.

In this presentation, we will illustrate the use of resonant x-ray scattering on conjugated polymers used for optoelectronic devices [1, 2]. The performance of such devices are highly dependent upon the molecular packing however. The presence of sulfur atoms in common conjugated polymer such as P3HT or N2200 enable the use of tender x-rays (sulfur K-edge is around 2.47 keV) to probe and enhance signals from the sulfur atoms. Tracking the intensity variation across the sulfur K-edge and comparing with theoretical calculation enable to discriminate between different packing geometries and to extract important new microstructural information. We will both present results in the transmission geometry, on thin films deposited on Si3N4 membranes, as well as in the grazing-incidence (GI) geometry on thin film on Si substrate. Especially for the GI geometry, we will discuss the importance of x-ray absorption and its impact/distortion on the collected signal [3].

Then, we will show how resonant X-ray scattering and diffraction enable to gain unique insight into the behavior of charge balancing counterions within mixed conducting systems. Indeed, with the first operando measurement at the Cl-edge (2.8 keV), we found that instead of counterion size, polymer charge state and associated ion and water interactions dictate counterion location. Specifically, ions reside far away from the electronic charge transporting polymer backbone at low doping and migrate to positions near the backbone with increased charging [4].

References

[1] G. Freychet, et al., J. Am. Chem. Soc. 143, 1409 (2021).
[2] G. Freychet, et al., Mater. Horiz. 9, 1649 (2022).
[3] LQ. Flagg, et al., Chem. Mater. 35, 10, (2023).
[4] D Meli, et al.,Mater. Horiz. 9, 1649 (2025).

XII: Diffraction Contrast Imaging - 2/2

Session Chairs

Nathalie Mangelinck-Noël
Tamzin Lafford

Effect of the initial strain state on the evolution of the average elastic strain tensor for 2000+ grains in Armco iron during elastic loading

Konrad Prikoszovich[1], Patric Gruber[1], Angelica Medina[1], Subin Lee[1], Christoph Kirchlechner[1], Jean-Sébastien Micha[2], Robin Fréville[2], Jonathan Wright, Wolfgang Ludwig, Reinhard Pippan

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Presentation type: Oral **Presentation time:** 11:15-11:30

Strain heterogeneities in a polycrystal can be detrimental to the lifetime of a material. Understanding the complex behaviour between the initial strain state of a grain and its evolution during mechanical loading is essential to predict strain localizations leading to crack initiation and failure.

We combine Diffraction Contrast Tomography (DCT), Far-field 3DXRD (FF-3DXRD), and Phase Contrast Tomography (PCT) measurements at beamline ID11 of the European Synchrotron Radiation Facility (ESRF) to capture the shape, arrangement, orientation, and average elastic strain tensor of a representative ensemble of grains during mechanical loading. The finalized dataset encompasses the relevant information for each grain within the investigated volume throughout the entire loading sequence. Our analysis follows two distinct approaches: (1) statistical analysis of the strain distribution evolution during loading across all grains, correlating mechanical grain behaviour with microstructural properties such as size, orientation and neighbourhood; and (2) focused investigation of individual grains and their local neighbourhood and how the local properties affect the strain level in individual grains.

In this talk, our latest findings on the evolution of strain heterogeneities in bcc Armco iron are presented. We investigated more than 2000 grains present in the entire gauge section of a micro tensile sample during deformation. The initial eigenstrain distributions in the undeformed state were extensively analysed, which allowed us to identify mechanisms based on i) reduction of free volume during recovery and recrystallization as well as ii) shear-coupled grain boundary migration as possible origins of the unexpectedly very broad strain distributions.

The deformation sequence predominantly focused on the elastic regime, with only the final two steps exceeding the macroscopic yield strength. This experimental design allowed us to follow the transition from elastic to plastic deformation on the microstructural level for a large number of grains, providing relevant insights into micromechanical deformation behaviour. By investigating grains with different initial strain levels, we can observe the effect of the strain state on the formation and dissipation of strain hotspots during loading.

Our results present a significant step forward in understanding the evolution of individual grains in polycrystalline materials during elastic tensile deformation in addition to providing key insights into the phenomenon of microplasticity.

Multimodal 3D X-Ray Imaging of Grain Boundary Migration at Triple Junctions

Lucia Puertas Pelaez[1], Can Yildirim[1], Marylin Sarkis[1], Wolfgang Ludwig, Virginia Sanna, Yubin Zhang, Louis Lesage, Aditya Shukla
[1] *ESRF, France*

Presentation type: Oral **Presentation time:** 11:30-11:45

Classic grain growth (GG) models are unable to reproduce the complexity observed experimentally, as they rely on oversimplified assumptions such as purely curvature-driven mechanisms or evolution governed solely by topology. As a result, standard GG models offer limited predictive capability, with numerical simulations being strongly constrained by the experimental data available.

Aiming to overcome these limitations, we have implemented a non-destructivein situdiffraction techniques capable of capturing the involved phenomena with high sensitivity and nanometer-scale spatial resolution in a three-dimensional microstructural context. The process has been characterized by combining general mapping methods for the bulk matrix and neighbors (Diffraction Contrast Tomography (DCT), Phase-Contrast Tomography (PCT) or 3D X-ray Diffraction (3DXRD)), with Dark-Field X-ray Microscopy (DFXM). The latter technique allows magnifying the identified regions of interest and provides strain sensitivity on the order of 5×10 with ~100 nm spatial resolution, thereby enabling a multiscale characterization framework.

In this study, we investigate a polycrystalline AA1050 alloy subjected to multiple annealing steps at temperatures close to its melting point (0.96 T). Following volumetric mapping of the sample using DCT and 3DXRD, the analysis focuses on three neighboring grains forming a triple junction (TJ). For each grain within the selected region of interest, the evolution of local intragranular strain, grain boundary energies and boundary migration at the TJ are tracked. In addition, the presence of second-phase particles is identified and the constraints they impose on the observed boundary motion are assessed. Finally, a direct link between intragranular dislocation structures and grain boundary migration is established, enabling an evaluation of the persistence of these mechanisms at high homologous temperatures (Figure 1). In this way, this work brings us closer to establishing the experimental foundation needed to validate and improve physically based GG models.

New insight onto the metal to insulator transition in Ca2RuO4

Dina Carbone[1], Oier Bikondoa[2], Anita Guarino[3], Antonio Vecchione[3], Rosalba Fittipaldi[3], Roman Hartmann[4], Mario Cuoco[3], Angelo Di Bernardo[5]

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Presentation type: Oral **Presentation time:** 11:45-12:00

Heavy transition metal oxides are model systems for investigating emergent electronic phases generated by the strong coupling between electron correlations, spin–orbit interaction, and lattice distortions. This interplay can produce unconventional Mott physics, spin and orbital ordering, and unusual collective excitations, while offering several routes to tune the electronic ground state. Ca RuO (CRO) is a compelling example, as its electronic properties are intimately linked to its crystal structure. At T=357 K, CRO undergoes an insulator-to-metal transition [1] accompanied by a structural transformation from an orthorhombic insulating phase to a tetragonal metallic phase. This transition can also be induced by pressure or doping [2], electric gating or applied electric current [3].

Conventional x-ray diffraction measurements on bulk crystals provide valuable information on the average structural changes associated with the transition. However, this approach is intrinsically limited in systems where multiple structural phases may coexist, as averaged diffraction signals can obscure the microscopic picture. This limitation is particularly relevant for CRO, where current-driven experiments indicate metastable regimes and phase coexistence over a wide range of applied currents [3].

Here, we use scanning x-ray diffraction microscopy with sub-micron beams [4] to investigate the current- and temperature-induced structural evolution of thin CRO flakes. This scanning approach provides both local structural details and global sample-scale trends, while thin-flake measurements aim to access the intrinsic material response away from bulk complexity, where large volumes, strain fields, defects, and percolative pathways may mask the fundamental behaviour under external fields.

By mapping diffraction signals as a function of applied current or temperature, we attain the visualisation of distinct domains characterized by different c-axis lattice parameters and their distribution within the samples. We observe that the current-driven transition proceeds through a highly inhomogeneous mechanism, with structurally inequivalent regions nucleating, expanding, coexisting, and partially reversing upon current cycling. In contrast, temperature-induced switching shows a more uniform structural evolution, demonstrating unequivocally that that different physical mechanisms drive the transition. These results cast a new light on the phase transition of CRO.

References

[1] M. Braden et al. (1998). Crystal and magnetic structure of Ca2RuO4.... Phys. Rev. B,58(847)
[2] J. Zhanget al. (2019). Nano-Resolved Current-Induced Insulator-Metal Transition. Phys. Rev. X9(0110302); Bertinshaw, J. et al., (2019). Unique Crystal Structure of Ca2RuO4. Phys. Rev. Lett.123(137204)
[3] C. Cirillo et al. (2019). Emergence of a metallic metastable phase .... Phys. Rev. B100(235142)
[4] D. Carbone and O. Bikondoa, (2023). Focused and coherent X-ray beams ....Nuclear Inst. and Methods in Physics Research, B539 (127)

Evolution of dislocations throughout the seeded growth of AlN crystals investigated by 3D X-ray diffraction imaging.

Carsten Richter[1], Merve Pinar Kabukcuoglu[2], Carsten Hartmann[1], Thomas Straubinger[1], Elias Hamann[3], Mathias Hurst[3], Simon Bode[4], Daniel Hänschke[3]

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Presentation type: Oral **Presentation time:** 12:00-12:15

Aluminum nitride (AlN) is a critical substrate material for deep ultraviolet optoelectronics, high-power electronics, and sensor applications. Next to challenges related to n-type doping of AlN, the lack of high-quality crystals with diameter of 4 inches or more is currently hindering a widespread exploitation of this material in semiconductor industry. In the development of crystals with larger diameters and volume, maintaining a sufficient supply of source material and low thermal gradients becomes increasingly challenging. However, controlling these parameters is crucial to limit the formation of crystal defects, such as grain boundaries and dislocations, thereby preserving high crystal quality.

Our work aims at understanding the evolution of defects, in particularly dislocations, during seeded growth of AlN crystals and their diameter-increase by growth on different crystallographic surfaces. We investigated the behavior of dislocations during regrowth on the seed using 2D and 3D X-ray diffraction imaging and complementary techniques, enabling us to determine the direction and sense of the Burgers vectors, as well as dislocation line trajectories in 3D.

While parts of the dislocations are inherited from the seed, they typically exhibit a strong lateral displacement at the seed to bulk interface.

In crystals grown at a relatively small lateral temperature gradient, dislocations bend near the seed interface, with their movement governed by a climb process. The absence of slip was inferred from the Burgers vector orientation in relation to the movement direction and can be explained by a low resolved shear stress that is insufficient to activate glide. In contrast, the climb process is facilitated by a significant level of oxygen impurities, and becomes the dominating mechanism of motion during growth at low temperature gradients (0.1K/mm) [1].

When growing at larger temperature gradients, the crystals diameter increases rapidly [2], entailing enhanced nucleation of dislocations at the <1-100> corners that glide towards the center of the crystal [3]. Dislocations from the seed, however, are partially deflected at the regrowth interface and cannot penetrate into the bulk as shown by 3D imaging data.

These findings demonstrate how the temperature field can be used to control defect formation in AlN substrates and how 3D X-ray diffraction imaging enables insights into the history of dislocation formation, which can be related to the growth processes in these crystals.

References

[1] Straubinger, T. et al. (2023), Crystal Growth & Design, 23(3), pp. 1538–1546.
[2] Hartmann, C. et al. (2023), Applied Physics Express, 16(7), p. 075502.
[3] Herms, M. et al. (2025), physica status solidi (a), 222(19), p. 2400787.

From Grain Maps to Dislocation Dynamics: A Multimodal Diffraction Microscopy Framework for Bulk Microstructure Evolution

Can Yildirim[1], Carsten Detlefs[1], Nils Axel Henningsson, Henning Friis Poulsen[2], Steffen Staeck[2], Marylin Sarkis[1], Wolfgang Ludwig, Lucia Puertas Pelaez[1], Virginia Sanna, Michela La Bella, Yubin Zhang, Louis Lesage, James Ball, Aditya Shukla

[1] *ESRF, France*
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Presentation type: Oral **Presentation time:** 12:15-12:30

Quantifying the evolution of complex and highly deformed microstructures requires access to internal grain structures and defect fields across multiple length and time scales. We present a multiscale diffraction microscopy approach that combines monochromatic and pink-beam Dark-Field X-ray Microscopy (DFXM) with 3D X-ray Diffraction (3DXRD) and Diffraction Contrast Tomography (DCT), all integrated on a single instrument. This configuration enables true 3D and time-resolved 4D characterization of bulk materials, bridging millimeter-scale grain networks and nanoscale defect fields within the same experimental setup.

Monochromatic DFXM provides high angular resolution mapping of crystallographic orientation and elastic strain, while pink-beam operation increases diffracted intensity by more than an order of magnitude, extending access to weakly diffracting and highly deformed microstructures and enabling time-resolved imaging at several hertz. Together, these modes deliver full-field mapping of embedded grains at ~100–150 nm spatial resolution with high strain sensitivity, even under severe peak broadening. Complementary 3DXRD and DCT provide three-dimensional grain morphology, orientation, and boundary networks at the mesoscale. An automated grain indexing workflow integrates orientation data from 3DXRD, DCT, and LabDCT, and maps reconstructed grain positions and orientations directly onto DFXM goniometer motor settings. This enables deterministic navigation from bulk polycrystalline volumes to selected intragranular regions without sample repositioning, while preserving the surrounding grain neighbourhood context.

We demonstrate the framework on complex and highly deformed microstructures. In cold-rolled ferritic alloys, we resolve dislocation cell structures, orientation gradients, and stored energy variations within individual grains. In polycrystalline AA1050 at high temperature, we perform time-resolved imaging of dislocation rearrangements and grain boundary migration during grain growth, directly correlating intragranular defect dynamics with mesoscale grain evolution. The approach enables quantitative characterization of deformation, recovery, recrystallization, phase transformation, and grain growth in bulk materials under realistic conditions, providing a robust basis for physically grounded microstructural modelling.

XTOP 2026 - Poster Sessions

Poster Session 1: Tuesday, 22.09. (17:00-18:30)

Poster ID	Presenter	Title
1.1	Angelica Cecilia	Hierarchical X-ray Imaging P23.2 HIKA Beamline at DESY, PETRA III
1.2	Nischal Dhungana	Characterisation of Sub-Nanometric Line Edge Roughness Using SAXS
1.3	Marek Duchaň	Structural Signatures of Spin Reorientation in Altermagnetic MnTe
1.4	Fabian Gasser	Chirality Determination in Thin Films by Resonant Grazing-Incidence X-ray Diffraction
1.5	Mark Goorsky	Ion Implantation Strain Modelling of 4H-SiC Using X-ray Diffraction
1.6	Jörg Grenzer	Design of a Single Reflection Analyzer-Polarimeter for Light-by-Light Scattering Experiments at the HiBEF-HED Station at the European XFEL
1.7	Warre Heylen	Non-Destructive Structural Investigation of Multilayer Nanostructures with Uncertainty Analysis at 92 eV Using a Tabletop High Harmonic Generation Source
1.8	Warre Heylen	Investigation of Sensitivity of Tabletop HHG 92eV EUV Scatterometry for Laterally Etched SiGe Multilayer Grating Structures
1.9	Vladimir Kaganer	Dislocation Correlations in GaN Epitaxial Films Revealed by XRD and EBSD
1.10	Sebastian Kalbfleisch	The Nano-Diffraction Instrument of the NanoMAX Beamline at MAX IV
1.11	Azat Khadiev	New Experimental Possibilities at the P23 In Situ X-ray Diffraction and Imaging Beamline at PETRA III
1.12	Stefan Kowarik	ORSO – the Open Reflectometry Standards Organisation
1.13	Adam Kubec	Utility Fresnel Zone Plates: Blazed, Hybrid, Spiral, and Aberrated Designs Optimized for Performance and Use-Case-Specific X-ray Optics
1.14	Christian Neemann	3D Laue Microdiffraction Investigation of Deformation and Defect Evolution in Bicrystalline Copper Micropillars During Cyclic Loading
1.15	Petr Pazourek	Temperature-Dependent X-ray Diffraction of Ferroelectric Topological Insulators
1.16	Mario Prescher	Non-Destructive Laboratory Micro X-ray Computed Tomography of Processed AlGaN/GaN RF Power Amplifier Chips
1.17	Nico Scheidegger	GelatoX – a New in-House Setup for Propagation-Based Phase-Contrast Nano-CT of Biomedical Samples
1.18	Johanna Seidel	In Situ X-ray Diffraction During Ice Formation on Alkali Feldspar
1.19	Rolf Simon	PB32/HIKA Beamline at PETRA IV for Hierarchical Imaging, Laminography, and Serial CT with High Coherence and Dose-Efficiency
1.20	Mira Viljanen	Multiscale and Modal Characterisation of Soft Materials at ForMAX
1.21	Luisa Wartner	Increasing Sinter Stability of Pd/(CeO2)/alpha-Al2O3 Model Catalysts Under Methane Oxidation
1.22	Aleksandra Wierzbicka	Influence of Au Catalyst Size on the Structural Properties of CdO Nanowires Grown by Molecular Beam Epitaxy

Poster Session 2: Thursday, 24.09. (17:00-18:30)

Poster ID	Presenter	Title
2.1	Benjamin Apeleo Zubiri	Multiscale Characterization of Hierarchical Particle–pore Systems Using Correlative X-ray and Electron Tomography
2.2	Maik Becker	CNN-Based Mitigation of Zernike Phase-Contrast Artifacts in High-Resolution XRM and NanoCT
2.3	Huaiyu Chen	High-Resolution X-ray Ptychographic Computed Tomography of Brain Tissue Samples
2.4	Carsten Detlefs	Oblique Diffraction Geometry for the Observation of Several Non-Coplanar Bragg Reflections Under Identical Illumination
2.5	Martin Fisk	Precipitation-Induced Strain Field in Ni-Based Superalloys
2.6	Edwin Fohtung	On X-ray Orbital Angular Momentum–Dependent Coherence-Based Imaging
2.7	Luca Franzoni	X-ray Tomography of 3D Printed Hydrogel Based Tissue Scaffolds
2.8	Patrice Gergaud	In Situ µLaue and Dark-Field X-ray Microscopy Investigation of Strain Relaxation Mechanisms in Patterned InGaN Pseudo-Substrates for Red Micro-LED Applications
2.9	Jenny Hein	Evolution and Functional Morphology of Hip Joint Systems in Beetles
2.10	Koei Kadoi	Non-Reconstructive Prior-β Grain Estimation by Synchrotron X-ray Diffraction Spot Distribution Analysis in Ti-6Al-4V with TiC
2.11	Nathan Leubner	Probing Ferroelectric Switching in $BaMgF_4$ via Quasi In Situ Dark-Field X-ray Microscopy
2.12	Cristina Lupaşcu-Vasiliţa	From Pixels to Bases: Integrating Synchrotron X-ray Imaging and DNA Sequencing of Insects
2.13	Wenjie Mei	A Standardized Workflow for Cross-Beamline Data Harmonization and Analysis of Cement Hydration in X-ray Tomography
2.14	Cristian Mocuta	Artificial Laminar Oxide Multiferroic Magnetoelectric Thin Film Structures – Elaboration and Characterization
2.15	Reihaneh Pashminehazar	In Situ Synchrotron X-ray Micro-Tomography and Machine-Learning-Assisted Segmentation of Low-Density Hydrocarbon Phases in Powdered Catalysts
2.16	Ilhem Nadia Rabehi	Crystal Defect Dynamics at the Solid-Liquid Interface in Silicon – Investigation by X-ray Topography and Rocking Curve Imaging.
2.17	Angel Rodriguez Fernandez	I13-1 Coherence: The Multiscale, Multimodal, Ptycho-Tomographic End Station at DLS.
2.18	Veronika Schon	Contrast Engineering in NanoCT of Porous Silica Through Tailored Intrusion Media
2.19	Steffen Staeck	Improving Spatial Resolution for Dark-Field X-ray Microscopy
2.20	Felix Wittwer	X-ray Strain and Stress Tensor Tomography
2.21	Felix Wittwer	Protein Denaturation in Heated Egg Yolk Studied with In Situ X-ray Holotomography
2.22	André Wählisch	Reference-Free Nano-XRF Analysis of TaOx Memristive Devices
2.23	Maria-Iulia Zai	Computational Methods Applied in Materials Studies

Status as of 15 September 2026

Poster Session 1

Hierarchical X-ray imaging P23.2 HIKA beamline at DESY, PETRA III

Mateusz Czyzycki[1], Tilo Baumbach[2], Rebecca Spiecker[1], Elias Hamann[1], Mathias Hurst[1], Tomáš Faragó[2], Marcus Zuber[2], Chandan Sarkar[2], Jan-Thorsten Reszat[2], Angelica Cecilia[2], Clément Tavakoli[2], Martin Spiecker[2], Rolf Simon[1], Nikolay Zagainov[2]

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Presentation type: Poster

HIKa (Hierarchical Imaging Karlsruhe) is a new experimental station at the P23 beamline in the Ada Yonath hall at PETRA III, developed in collaboration between the Karlsruhe Institute of Technology and DESY. Designed as a versatile platform for full-field X-ray imaging, the station has a particular focus on hierarchical imaging and high-throughput 3D microtomography for both materials research and life sciences.

Its main instrumentation consists of a 20-tons multi-purpose optical X-ray table with six modules that can be moved along the optical axis: four hexapod modules for holding X-ray optics such as gratings, lenses, or crystal optics; a high-precision sample module for micro-CT and computed laminography; and a detector module. The modular design of HIKa supports a broad range of advanced X-ray imaging techniques, including parallel beam holographic imaging, 3D microtomography with a multi-magnification X-ray camera, and cone-beam in-line holography. The station enables switching between parallel-beam phase contrast and Bragg optics to achieve magnified fields of view ranging from 1 mm² to 2500 mm², as well as focused-beam holographic projection microscopy using multilayer Laue lenses. This facilitates hierarchical 3D imaging across spatial resolutions ranging from 100 µm down to below 80 nm.

Automated specimen handling and storage of up to 1000 samples, combined with robotics for serial computed tomography and AI-supported pipelines for sample exchange, acquisition, and quality assurance, will facilitate thousands of scans per day. HIKa will also enable SXFM (Scanning X-ray Fluorescence Microscopy), as well as experiments employing versatile Bragg Magnifier (BM) optics for field of view extension and dose-efficient BM-based microscopy. Thanks to the implementation of these advanced, complementary X-ray imaging approaches, HIKa will support both life sciences and materials research through operando and multi-scale investigations, representing a major step toward autonomous, dose-efficient imaging at PETRA III and providing the technological basis for PETRA IV.

Characterisation of Sub-nanometric Line Edge Roughness using SAXS

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Presentation type: Poster

Whilst the roughness characterisation of planar surfaces and interfaces is well established using X-ray reflectivity, extending these principles to study roughness in contour of periodic nanostructures remains a trickier prospect. In particular, the study of line edge roughness is of significant interest for both fundamental scattering studies and advanced nanoscale metrology. As critical dimensions continue to shrink in semiconductor industry, conventional techniques like Atomic Force Microscopy(AFM) and Scanning Electron Microscopy(SEM) are becoming increasingly limited when it comes to nondestructive and statistically reliable characterisation. Small angle X-ray scattering (SAXS) provides a non-destructive alternative for probing periodic nanostructures over large sample areas. SAXS offers an access to buried structures that remain beyond the reach of surface sensitive techniques. Drawing inspiration from the formalism of Sinha et al., we have investigated the possibility of extracting roughness information from periodic line gratings using SAXS. We have established a mathematical framework demonstrating that roughness in these repeating structures gives rise to measurable diffuse scattering features around diffraction peaks, allowing us to access line edge roughness information. To validate this approach, we combined analytical modelling, voxel-based numerical simulations, and synchrotron-based experimental measurements. Our simulations confirm that these roughness induced scattering signatures are indeed observable and provide quantitative insight into how sensitive the method is to various roughness parameters. Experimental results show strong agreement with both the simulations and scanning electron microscopy (SEM) measurements, demonstrating that the extracted parameters are consistent with established metrology techniques. Beyond ideal rectangular gratings, we also examined more realistic trapezoidal line profiles and analysed how the profile shape modifies the scattering response, and in turn, influences roughness extraction. Furthermore, we investigated periodically arranged contact structures modelled as cuboid arrays to examine how structural imperfections and deviations from ideal periodicity affect the diffuse scattering signal. Finally, we assessed the feasibility of transferring this methodology from synchrotron measurements to laboratory-based X-ray instruments. By systematically addressing all these factors we bridge the gap between theoretical modeling and practical implementation. We demonstrate that T-SAXS can be utilised as a quantitative tool for the roughness characterisation of realistic periodic nanostructures. It establishes a route towards advanced, non-destructive metrology for next-generation semiconductor devices, with significant potential for future implementation on laboratory-scale X-ray platforms.

Structural Signatures of Spin Reorientation in Altermagnetic MnTe

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Presentation type: Poster

Manganese telluride (MnTe) is a prototypical antiferromagnet with a spin-polarised electronic structure, recently classified as an altermagnet, with a critical temperature TC≈310 K. In this work, we investigate the structural changes associated with magnetic moment reorientation in the altermagnetic phase using high-resolution X-ray diffraction (HR-XRD). Temperature-dependent diffraction patterns were measured from helium/nitrogen temperatures up to room temperature, enabling precise determination of the lattice parameters a and c.

The extracted temperature dependences a(T), c(T) and the ratio c/a(T) reveal a distinct change in slope at approximately 260 K. This anomaly coincides with the spin reorientation transition, during which the magnetic moments rotate by approximately 30° from alignment along the a*-axis (below 260 K) toward the a-direction (above 260 K).

Our results demonstrate a coupling between the crystal lattice and the magnetic subsystem, providing evidence of magnetoelastic effects in MnTe. The observed structural signatures offer complementary insight to microscopic magnetic probes and contribute to a more complete understanding of the spin reorientation mechanism in this material.

Chirality determination in thin films by resonant grazing-incidence X-ray diffraction

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Presentation type: Poster

Chiral molecules exist as two non-superimposable mirror-image forms, called enantiomers, that share identical chemical composition but can differ dramatically in biological activity, optical response, and spin-transport properties. Distinguishing between different enantiomers by determination of their absolute configuration is therefore essential for any application involving chiral compounds.

For crystalline materials, single crystal X-ray diffraction is the established method for absolute structure determination. Conventionally, assignment of absolute structure relies on the analysis of small intensity differences between Friedel pairs caused by resonant scattering contributions via the Flack parameter or related approaches. While grazing-incidence X-ray diffraction (GIXD) can provide comparable structural information to single crystal diffraction, the systematic inaccessibility of one reflection in each Friedel pair due to substrate shadowing renders their intensity evaluation via any of the conventional approaches impossible. Consequently, to date no direct diffraction-based method for chirality determination in thin films has been developed.

This contribution introduces resonant grazing-incidence X-ray diffraction (GIXD) as a new approach to determine the absolute configuration of chiral organic thin films. The method exploits the energy dependence of diffracted intensities near an absorption edge, where resonant scattering contributions lead to significant variations of peak intensities. As a proof of concept, a 2-(3-bromophenyl)-N,N-diisopropyl-2-oxoacetamide single crystal was investigated using energy-dependent single-crystal X-ray diffraction near the bromine K-edge. By monitoring the intensity of a single Bragg reflection as a function of the incident X-ray energy and comparing it to its calculated energy-dependent structure factor, the absolute configuration of the crystal was reliably determined.

Extended to chiral thin films with varying texture and prepared by different deposition methods, resonant GIXD offers a non-destructive, substrate-independent route to study chirality at surfaces and in thin films.

Ion Implantation Strain Modelling of 4H-SiC Using X-ray Diffraction

Brandon Carson[1], Mark Goorsky[1], Michael Liao[2]

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[2] *Apex Microdevices, USA*

Presentation type: Poster

Wafer bonding and ion exfoliation have provided pathways towards heterogeneous integration of novel semiconductor stack-ups, such as 4H-silicon-carbide-on-insulator (SiCOI) for high-Q microresonators and optical frequency comb generators. Ion implantation typically results in an out-of-plane strain distribution in a shallow, near-surface region of the substrate material, induced by light-atom intercalation and self-interstitials distorting the substrate lattice. To understand the fundamental relationships between this underlying strain profile and X-ray diffraction data, (0001) 4H-SiC implanted with hydrogen ions was characterized using 2θ:ω scans of the (0008) plane using Cu Kα1 radiation. X-ray diffraction allows for characterization of strain induced by ion implantation across a wide range of materials. Typical diffraction measurements performed on ion-implanted materials yield feature-rich scans containing fringes of various widths and amplitudes. Structure-factor considerations show that fringes result from interference effects related to the breadth of the strain distribution or from coherence-length effects, with a fringe contrast related to the skewness of the distribution. These principles are applied to allow for manual strain-profile extraction from a layered model with an arbitrary initial seed. Manual extraction sequentially tailors the layer thicknesses in the strain model to match fringe widths in the diffraction data, then distribution skewness to match fringe contrast, and lastly near-surface thickness and damage adjustments to match the overall intensity envelope. Manual profile extraction shows agreement with both the experimentally obtained implant profile and the experimental diffraction data, using log10 mean absolute error as a goodness-of-fit metric. The method has some limitations, such as difficulty in applying the principles to co-implanted materials or box-profile implants. Commercial and open-source software-based solutions for automated strain-profile extraction are scrutinized, showing that software struggles to produce reasonable strain profiles with small goodness-of-fit metrics, even when provided with an initial seed model close to the desired solution. These strain-extraction techniques can be used to improve software-based fitting algorithms and more accurately determine the extent and magnitude of implantation-induced strain in ion-implanted substrates.

Design of a single reflection analyzer-polarimeter for light-by-light Scattering experiments at the HIBEF-HED station at the European-XFEL

Jörg Grenzer[1], Thomas E Cowan[2], Edgar Weckert[3], Hans-Peter Schlenvoigt[2], Michal Šmíd[2], Robert Lötzsch[4], Willi Hippler[4], Matt Zepf[4]

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Presentation type: Poster

In the presence of strong electromagnetic fields, the quantum vacuum behaves as a nonlinear, polarizable medium, as described in QED theory. If a photon (probe beam) passes through a region with a strong field, its direction or polarization state may change as a result of the vacuum birefringence effect.

However, the cross section of this process is extremely small, i.e. any detectable signal must be distinguished from the majority of the unaltered probe beam. The response of the quantum vacuum can result in signals that differ from the probe beam in terms of polarization, angular distribution, and photon energy. Of particular interest are configurations that allow both, the parallel and perpendicular polarized components to be measured independently.

This can be achieved using an analyzer-polarimeter crystal, in which the two diffracting planes are oriented at 120° to each other, with each plane reflecting one of the two perpendicular polarizations in different directions. This was demonstrated for hexagonal quartz [1], and later for diamond and zincblende structures.

We show that lowering the incidence angle to the surface the crystals bandwidth can be increased and closer matched with the one of the seeded X-ray pulse. Choosing the Ge(440) reflection, results in an energy of 8766eV. The calculation were verified through experiments conducted at the HED station at EuXFEL in the framework of the BIREF@HIBEF collaboration [2]. We tested three crystals with different surface cuts and incidence angles of 54.74° (standard case), 24.74° and 13.27°, resulting in a calculated increase in the crystal's bandwidth of 0.15eV, 0.3eV and 0.4eV.

Two significant parameters were measured: The polarization purity (P, the ratio of signals measured after the analyzer between perpendicular and parallel polarization) and the integral reflectivity (R). We found a value of P in the order of (6+/-1)10 for all three crystals, R for the standard case was ~8%, and for shallower incidence angles, about 23%.

Our results suggest that we have measured the natural polarization purity of the SASE 2 undulator at the EuXFEL, since theoretical studies for the same geometry including the effects of neighbouring multi-beam reflections indicate a better purity of at least 1-2 orders of magnitude. Furthermore, the bandwidth of the seeded pulse has been determined to be greater than 0.3eV, in agreement with the value from the single-shot HIREX spectrometer, which estimated a bandwidth of less than 0.7eV.

References

[1] E.O. Baronova and M.M. Stepanenko, Plasma Phys. Control. Fusion 45, 1113 (2003).
[2] M. Smid et al., Phys. Rev. A 112, 063512 (2025).

Non-destructive structural investigation of multilayer nanostructures with uncertainty analysis at 92 eV using a table-top high harmonic generation source

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Presentation type: Poster

Extreme ultraviolet (EUV) scatterometry and reflectometry are powerful techniques enabling contactless non-destructive structural characterization of blanket and patterned nano-stacks with down to sub-nanometre precision. With increasing availability of lab-scale, high harmonic generation (HHG) EUV sources, these techniques become more accessible and enable more use cases and faster learning cycles, with prospects of becoming in-FAB metrologies.

EUV light offers a number of physical and metrological advantages over X rays for reflectometry and scatterometry. At EUV wavelengths, light–matter interaction is governed by the complex refractive index, whose dispersive and absorptive components exhibit strong material and energy dependence, providing significantly enhanced contrast compared to X ray scattering dominated by electron density. Consequently, EUV measurements are highly sensitive to compositional variations, chemical states, and subtle interface modifications. The longer wavelength also enhances sensitivity to nanometre scale surface and near surface features. In reflectometry, small changes in interface abruptness, intermixing, or ultra thin overlayers produce pronounced changes in reflectance and phase, while EUV scatterometry offers stronger coupling to surface roughness, sidewall features, and profile asymmetries. Moreover, EUV based measurements impose wavelength specific optical constraints that reduce parameter degeneracy in inverse modelling, improving robustness in the retrieval of structural and optical parameters.

In this work we present results of applying EUV scatterometry and reflectometry — powered by a linearly polarized, coherent, 92 eV HHG source— to structural characterization of multilayer grating-type and blanket EUV mask samples highly relevant for the semiconductor industry. We utilized machine learning and evolution algorithm coupled with neural network forward propagator for fast and accurate scatterometry reconstructions on two grating-type samples. We demonstrate successful and accurate reconstruction via simultaneous fitting of up to 11 structural parameters. We show how Markov Chain Monte Carlo (MCMC) algorithm can be efficiently used for performing thorough analysis of reconstruction uncertainties in multidimensional parameter spaces. Coupling MCMC with a neural network forward propagator allows to perform extensive uncertainty analysis in case of EUV scatterometry where it would not be normally possible due to immense computational costs of Maxwell-solver-based propagators. The results demonstrate sub-nanometre precision and are in good agreement with reference TEM measurements.

Investigation of sensitivity of tabletop HHG 92eV EUV scatterometry for laterally etched SiGe multilayer grating structures

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Presentation type: Poster

The continued scaling of semiconductor devices into the sub-10 nm regime, alongside the adoption of complex three-dimensional architectures, is driving unprecedented challenges for process control and metrology. As feature sizes shrink and material stacks become more intricate, conventional metrology techniques struggle to maintain the required accuracy and robustness. Optical critical dimension (OCD) metrology, a long-standing industry standard, is increasingly limited by its reliance on longer wavelengths, leading to reduced sensitivity to nanoscale features and strong parameter correlations in model-based reconstruction.

These limitations become particularly severe for advanced patterning schemes such as EUV lithography, where reduced optical contrast, stochastic effects, and buried or high-aspect-ratio features complicate profile extraction. In contrast, the EUV spectral range offers significantly enhanced material contrast due to stronger variations in optical constants between materials. This contrast is higher than in the visible range—where many materials appear optically similar—and more structured than in the X-ray regime, where interactions become less sensitive to fine compositional differences relevant for pattern fidelity.

As a result, EUV scatterometry is emerging as a promising alternative, providing improved sensitivity to nanoscale features and complex multilayer stacks. It enables more accurate and robust profile reconstruction, addressing key limitations of traditional OCD and supporting next-generation semiconductor manufacturing.

In this work we present the results of sensitivity analysis of EUV scatterometry at 92eV powered by coherent tabletop high harmonic generation (HHG) source applied to laterally etched multilayer SiGe grating-type structures featuring 3 Si-SiGe bilayers where each layer is ~10 nm thick and Ge concentration is 20%. Recesses values range from 5 to 25 nm. Simulations were performed using finite element method (FEM) light propagation implemented in JCMsuite software. The created sample model is characterized by 11 parameters and was based on transmission electron microscopy images of real samples fabricated at IMEC.

We show the impact of different model parameters on EUV diffraction responses, identify regions of sensitivity (angular ranges and diffraction orders) and evaluate reconstruction sensitivities. Furthermore, we present the results of cross-parameter correlation analysis.

We demonstrate that lateral recesses in multilayer SiGe structures create measurable variability in higher diffraction orders formed by EUV light. This highlights the strong potential of EUV diffraction as a lab-scale, non-destructive technique for critical dimension metrology, addressing the increasing precision demands of the semiconductor industry.

Dislocation correlations in GaN epitaxial films revealed by XRD and EBSD

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Presentation type: Poster

The elastic energy of a single straight dislocation per unit length ~ln(L/a) diverges as the lateral crystal size L is increased to infinity. To reduce the elastic energy, dislocations are correlated such that the long-range strain field of a dislocation is screened by surrounding dislocations. The screening distance R is accessed in XRD as a transition from the Gaussian central part of the diffraction line to its tails, which show an intensity decay proportional to q^−3. In many XRD studies, the dislocation density is of primary interest, while the screening distance is an auxiliary fit parameter required for accurately determining the dislocation density.

High-resolution electron backscatter diffraction (HR-EBSD) provides maps of the spatial distribution of all components of strain and rotation tensors at the crystal surface. Since the dislocation strain depends on the distance from the dislocation line by a universal law (~1/r), the correlation functions of the strains and rotations decrease proportionally to the logarithm of the distance for distances smaller than R, and becomes zero at larger distances. Plotting the correlation function against the logarithm of the distance yields a hook-shaped curve. The kink in this curve provides the screening distance without the need for any fitting or assumptions about the dislocation correlations.

We study GaN(0001) epitaxial films with threading dislocation densities differing by orders of magnitude, from 6x10^5 to 2x10^10 cm^-2. We carry out both laboratory XRD and HR-EBSD measurements on the same samples and also perform Monte Carlo simulations of the XRD line profiles and HR-EBSD strain maps, using one and the same model of dislocation distributions for both experimental techniques and the same computing program.

The dislocation densities and the screening distances obtained by XRD and HR-EBSD are compared with those directly accessible by visual examination of cathodoluminescence maps and scanning electron micrographs. We find that XRD overestimates the dislocation densities, presumably due to contributions from the strained region near the film-substrate interface. The screening distances obtained by XRD from different reflections exhibit a larger scattering, but are consistent with those obtained by HR-EBSD within a factor of two. The screening distances obtained for the GaN films with threading dislocation densities 5x10^8 and 2x10^10 cm^-2 show that the dislocation strain is screened by only four neighboring dislocations in both samples.

The Nano-Diffraction Instrument of the NanoMAX Beamline at MAX IV

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Presentation type: Poster

The nano-diffraction instrument is based ondiffraction-limited KB focusing mirrors with a long working distance of 100 mm. The focusing optics produce a highly coherent nano-focused beam down to 40-200 nm, depending on the photon energy [2,3]. With its two-circle goniometer, a set of custom-built, long-stroke XYZ positioners, and a high-load XYZ piezo scanner the instrument can accommodate sample environments weighing of up to 1000 g.In-situ optical microscopes, providing both on-axis and top-view perspectives, assist in pre-aligning samples within the X-ray focus. A pixel detector inside an evacuated flight tube measures the forward-scattered signal. A robotic arm allows for the flexible positioning of a state of the art pixel detector in 3D for coherent diffractive imaging or Bragg ptychography [4].Wide-angle scattering experiments can utilize a large-area detector positioned near the sample. The fluorescence signal emitted by the samples is captured by an energy-dispersive detector. The instrument's long working distance and flexibility make it suitable for experiments involving various sample environments such as nano-indenters [5], electro-chemistry cells [6], XBIC setups [7], heaters, high-pressure cells [8], or other user-supplied setups [9]. We will present its capabilities, recent instrument improvements and upgrades, current sample environments, and results of selected user experiments.

References

[1] D. Carbone, et al., Journal of Synchrotron Radiation, 29 (2022), 876–887.
[2] U. Johansson, et al., Journal of Synchrotron Radiation, 28 (2021), 1935–1947.
[3] A. Björling, et al., Opt. Express, 28 (2020), 5069–5076.
[4] L. Peng, et al., Light: Science & Applications, 11 (2022), 73.
[5] G. Lotze, et al., Journal of Synchrotron Radiation, 31 (2024), 42–54.
[6] A. Björling, et al., Journal of Synchrotron Radiation, 26 (2019), 1830–1834.
[7] J. Keller, et al., Solar RRL, 8 (2024), 2301018.
[8] J. Cheng, et al., Matter and Radiation at Extremes, 5 (2020), 038401.
[9] S. Das, et al., Catal. Sci. Technol., 14 (2024), 5885–5898.

New experimental possibilities at the P23 In-Situ X-ray Diffraction and Imaging Beamline at PETRA III

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Presentation type: Poster

The in situ X-ray diffraction and imaging beamline P23 at PETRA III (DESY, Hamburg) focuses on the crystallography, physics, and chemistry of systems dominated by low dimensionality and confinement effects, with a strong emphasis on in situ and operando techniques. Currently, the beamline operates with one experimental hutch; a second hutch, established through a joint KIT/DESY collaboration and dedicated to advanced hard X-ray microscopy techniques, will become available to users in 2026.

The spectroscopic undulator source and X-ray optics deliver up to 10^{13} photons/s in the 5–32 keV energy range, providing tunable X-ray energies and beam sizes down to the sub-micrometer scale. The experimental hutch is equipped with a heavy-load HUBER diffractometer capable of supporting sample environments up to 150 kg in four-circle geometry and up to 15 kg on the Eulerian cradle in a 5+2-circle configuration. The instrumentation pool is designed for multi-scale analysis of bulk and nanostructured materials and devices. Available sample environments include heating chambers, a flow liquid-helium cryostat, a source-measure unit, and piezo-based positioning stages. An in situ pulsed laser deposition chamber can be provided upon request. The beamline accommodates a wide variety of user-supplied sample environments and laser systems and is certified for operation with hazardous gases.

The beamline offers a broad range of X-ray diffraction methods, with a primary focus on reciprocal space mapping, X-ray reflectivity, grazing-incidence diffraction, and X-ray standing wave techniques, including time-resolved measurements and sub-micrometer spatial resolution. Complementary scattering and spectroscopic techniques, such as powder diffraction and X-ray absorption near-edge spectroscopy (XANES), are also available. Secondary emission methods include X-ray fluorescence, optical luminescence detection, and Raman spectroscopy.

The beamline enables multimodal experimental approaches and supports anomalous X-ray scattering across the full accessible energy range.

We will present new beamline capabilities and highlight recent results from in-house research and user experiments.

ORSO – The Open Reflectometry Standards Organisation

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Presentation type: Poster

ORSO is an international, open initiative dedicated to advancing X-ray and neutron reflectometry. Here, we introduce our working groups and highlight recent achievements in standardising data formats and developing artificial-intelligence- and fit-based approaches to data analysis. ORSO also works to improve experimental reproducibility, share best practices for sample environments, and develop educational and outreach materials for the reflectometry community.

Utility Fresnel zone plates: blazed, hybrid, spiral, and aberrated designs optimized for performance and use-case-specific X-ray optics

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Presentation type: Poster

Fresnel zone plates are key optical components for high-resolution X-ray microscopy, nanofocusing, and coherent imaging. While conventional binary zone plates remain widely used, many current applications require more than small focal spots alone. Higher diffraction efficiency, controlled illumination, tailored wavefronts, and robustness against experimental constraints increasingly call for application-specific zone plate designs.

In this contribution, we present an overview of Fresnel zone plate concepts and their connection to practical fabrication routes. Blazed, hybrid, and stacked zone plate geometries are discussed as strategies to increase diffraction efficiency. As examples Spiral zone plates are considered as beam-shaping optics that generate vortex-like or donut-shaped intensity distributions for specialized microscopy and coherent imaging applications. We also discuss deliberately designed non-ideal zone plate designs, also referred to as “dirty” zone plates, where local zone positions are intentionally modified to tailor the illumination function and improve performance or robustness in iterative imaging methods such as ptychography.

XRnanotech’s fabrication toolbox includes high-resolution electron-beam lithography, X-ray LIGA, electroplating of high-density absorber materials such as Au and Ni, and ALD deposition of Ir and Pt for harder X-ray energies. Etching-based approaches using materials such as Si, SiO , SiN, Mo, and Ru are particularly relevant for softer X-ray energies down to the EUV range. SiO can also serve as a template material for line-doubled zone plate concepts. In addition, metal-assisted chemical etching is well suited for high-aspect-ratio silicon structures and enables aspect ratios above 100. The flexibility of lithographic patterning allows different combinations of resolution, aspect ratio, absorber material, and optical geometry to address a broad range of X-ray energies and imaging architectures.

By connecting design strategy, fabrication route, and intended application, we show how next-generation Fresnel zone plates can be selected and optimized for synchrotron and laboratory-based X-ray systems, including full-field transmission X-ray microscopy and illumination optics for high-resolution ptychography.

3D Laue microdiffraction investigation of deformation and defect evolution in bicrystalline copper micropillars during cyclic loading

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Presentation type: Poster

Mechanical fatigue is one of the most important failure mechanisms in metallic materials and is strongly influenced by microstructural features. Localized microplasticity, including dislocation motion on specific slip systems and the formation of dislocation structures, initiates fatigue damage at the microscale. Interactions between dislocations and grain boundaries play a crucial role in the evolution of fatigue damage, although these processes are not yet fully understood. Advanced synchrotron-based characterization techniques such as depth-resolved 3D Laue microdiffraction provide new opportunities to investigate these mechanisms in bulk crystalline materials with high angular and spatial resolution.

In this work, bicrystalline copper micropillars (10 x 10 x 25 µm3), each containing a predefined grain boundary (including Σ3 and impenetrable grain boundaries), were fabricated by femtosecond-laser ablation and focused ion beam milling. Cyclic bending experiments were conducted at the European Synchrotron Radiation Facility (ESRF, Grenoble) using a polychromatic X-ray microbeam (5-27 keV) to probe the samples after different stages of cyclic loading. Three-dimensional micro-Laue diffraction experiments based on the Differential Aperture X-ray Microscopy (DAXM) technique, employing tungsten wires as apertures, were conducted to obtain depth-resolved information on crystal orientation, lattice parameters, and deviatoric strain tensor components.

Three-dimensional strain distributions and lattice misorientation were analyzed after several stages of cyclic deformation. Localized lattice misorientations associated with crystal defects were observed, and Kernel Average Misorientation (KAM) analysis provided insight into the distribution of geometrically necessary dislocations generated during cyclic loading. The results reveal heterogeneous deformation behavior near grain boundaries and help to explain the interaction between dislocations and different grain boundary types.

These results demonstrate the potential of depth-resolved 3D Laue microdiffraction for investigating microstructural evolution during mechanical deformation and improving the understanding of early-stage fatigue mechanisms in metallic materials.

Temperature-dependent X-ray diffraction of ferroelectric topological insulators

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Presentation type: Poster

Topological insulators are characterised by a unique band structure with surface states exhibiting linear dispersion of a Dirac cone and spin-momentum locking. Moreover, the combination of ferroelectric properties with the Rashba effect – spin splitting of the band structure – enables control of spin polarisation by an external electric field. This makes chalcogenide compounds, such as Pb1-xSnxTe, promising candidates for the realisation of next-generation spintronic devices.

In the present work, we employed temperature-dependent X-ray diffraction to investigate the ferroelectric phase transitions of the aforementioned chalcogenide compounds deposited on a BaF2 (111) substrate. The goal of this work was to observe the ferroelectric phase transition from the NaCl phase Fm-3m to the rhombohedral phase R3m, and to determine the transition temperature. X-ray structural analysis was performed over the temperature range of 10 K to 300 K and included 2θ scans and reciprocal space map (RSM) measurements.

Non-destructive Laboratory Micro X-ray Computed Tomography of Processed AlGaN/GaN RF Power Amplifier Chips

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Presentation type: Poster

For next-generation GaN-based RF power amplifiers, reliable failure analysis and process monitoring of fully processed devices are crucial [1]. Conventional approaches often rely on destructive cross-sectioning or synchrotron-based X-ray tomography to access buried features such as metallization and die-attach interfaces. Recently, advanced micro X-ray computed tomography (microCT) and deep-learning-based reconstruction workflows have been demonstrated to provide detailed information of complex electronic devices, enabling improved failure analysis and quality inspection [2]. In this work we demonstrate that lab-based microCT using a ZEISS Xradia Versa 520 system enables non-destructive, in-house 3D imaging of processed GaN-on-4H-SiC RF power amplifier chips.

The devices under test are diced 3 mm × 4 mm high-frequency power amplifier chips based on a 100 nm AlGaN/GaN HEMT technology on a s.i. 4H-SiC substrate. MicroCT is used to assess the 3D integrity of the processed chips after fabrication.

X-ray tomography is performed at 30 kV tube voltage and 2 W power with a 4× optical objective and 1601 projections at 1×1 binning. Overview scans with a voxel size of 2.46 µm cover the entire chip, and local high-resolution scans achieve voxel sizes down to 1.00 µm in selected regions of interest. The reconstructed volumes allow virtual slicing through the devices and visualization of frontside and backside metallization, deliberately implemented via structures used for backside contacting, and the die-attach region. Furthermore, machine-learning-assisted segmentation of the measurements enables extraction of quantitative volume fractions (e.g. void content in percent), which provides additional information, especially on voids in the metallization and soldering.

We discuss the achievable contrast between metallization, solder and the surrounding semiconductor, and evaluate the detectability of critical defects such as cracks, voids, and incorrectly processed vias that can degrade RF performance or lead to early device failure. Our results show that lab-based microCT provides sufficient spatial resolution and contrast to support routine process control and failure analysis of GaN RF power amplifier chips, significantly reducing the need for destructive analysis and access to synchrotron radiation facilities.

References

[1] M. Bakowski et al., Advances in Technology Innovation, vol. 3, no. 4, 2018
[2] H. Villarraga-Gómez et al., Journal of Failure Analysis and Prevention, vol 24, 2024

GelatoX - A New In-House Setup for Propagation-Based Phase-Contrast Nano-CT of Biomedical Samples

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Presentation type: Poster

Propagation-based X-ray phase-contrast CT (PB-CT) at the sub-micron scale has largely been limited to synchrotron facilities, where high spatial coherence is readily available. Bringing this into a local laboratory requires careful combination of a stable, spatially coherent X-ray source with precise mechanics and high-dynamic-range detection. We present GelatoX, a newly commissioned home-built lab-based nano-CT system designed for high-resolution PB-CT of biological and biomedical samples.

The system is build around an Excillum Nanotube N3 transmission-target source with a LaB6 emitter, a tungsten-on-diamond target, a minimum focal spot size of 150 nm, and long-term spot stability below 100nm, at up to 160 kV acceleration voltage. Further downstream, a SmarAct nano-positioning stage is integrated for precise and reproducible alignment, as well as a matched detector system. Home-built systems come with the decisive advantage of controlling and optimizing the experimental parameters according to the scientific question: As such, we operate the system primarily at 60 kV, which is suitable for soft tissues, and choose between two X-ray detectors with distinct properties, namely a Ximea sCMOS for the low-energy part of the spectrum and a single-photon counting X-spectrum for high energies. With a Fresnel number and geometric magnification tuned to operate in the edge enhancement regime, we optimize the X-ray phase-contrast for the sample under investigation. Our own python-based control software allows for optimized data acquisition schemes. Full experimental control is not limited to data acquisition but comprises also the full data accessibility for data processing, for which we use the HoToPy-toolbox. The system is designed to achieve sub-micron voxel resolution and is well-suited to investigate a broad range of biological and biomedical samples.

With GelatoX being located in close proximity to the hospital of the University of Bern, our approach gives medical researchers access to novel X-ray technologies and allows us to develop the technique in close collaboration with the user community. As a first application, we image formalin-fixed, paraffin-embedded biopsy punches of human glioma tissue. Our goal is to characterize the three-dimensional organization of tumor and peritumoral structures, including fibre orientation and degree of fibrosity, and to assess the architecture of the tumor microenvironment in a label-free, non-destructive manner. The commissioning is ongoing, and we will present the system design, current performance characterization, and imaging results available at the time of the conference.

In situ X-ray diffraction during ice formation on alkali feldspar

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Presentation type: Poster

Alkali feldspar is a highly ice nucleation active constituent of mineral dust aerosol [1]which can influence precipitation formation and cloud optical properties by initiating heterogeneous ice formation in clouds. The extraordinary high ice nucleation ability of natural alkali feldspar was attributed to its complex microstructure exhibiting chemical phase separation (perthitic structure) [2] and a variety of surface defects like step edges, cracks or pores [2]. From microscopic observations, it is known that ice crystals grow with a preferential orientation on such feature-rich alkali feldspar surfaces [3,4,5]. However, a molecular understanding of the observed epitaxial orientation relationship and the fundamental ice nucleation mechanism is still missing.

In this project, we conducted in situ X-ray diffraction (XRD) experiments at the beamline P08 of Petra III (DESY, Hamburg) using a newly developed environmental cell setup to study ice crystal formation from water vapor on cleaved surfaces of natural alkali feldspars. Our substrates were pre-characterized using a laboratory diffractometer and the MPI beamline at KARA (KIT, Karlsruhe) to optimize the in situ ice experiments at DESY. The high-resolution XRD information allows us to quantify the local and the average ice crystal orientation with respect to the substrate. We studied alkali feldspar surfaces with increasing complexity to identify the influence of certain defects on the ice activity. Our first results obtained at DESY confirm the epitaxial relationship between vapor-grown ice and the K-rich phase of natural perthitic alkali feldspar under atmospherically relevant conditions. We will present and discuss further insights into ice formation on alkali feldspar regarding the surface complexity.

References

[1] Atkinson et al., Nature (2013) 498(7454), 355-358.
[2] Whale et al. Phys. Chem. Chem. Phys. (2017) 19, 31186—31193.
[3] Kiselev et al., Science (2017) 355, 367-371.
[4] Kiselev et al., Atmos. Chem. Phys. (2021) 21, 11801-11814.
[5] Keinert et al., Faraday Discussions (2022) 235, 148-161.

PB32/HIKA Beamline at PETRA IV for hierarchical imaging, laminography, and serial CT with high coherence and dose-efficiency

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Presentation type: Poster

Presently the P23 beamline in the Ada Yonath Hall (PXE) at PETRA III hosts the experimental station HIKA (Hierarchical Imaging Karlsruhe) which was developed in collaboration between the Karlsruhe Institute of Technology (KIT) and DESY as a versatile platform for full-field X-ray imaging. The station has a particular focus on hierarchical imaging from the macro to the nanoscale (spatial resolution between ~100 µm and ~ 50 nm) and high-throughput 3D microtomography for both materials research and life sciences.

PB32/HIKA will belong to the first phase beamlines of the PETRA IV project. It will be refurbished at its current location with new insertion device, optical elements and dedicated instrumentation for full-field imaging, especially hierarchical imaging, including parallel beam imaging and microscopy modes, serial micro-computed tomography (SµCT) and laminography (CL) for morphological imaging studies. Coherent Bragg optics (combining magnifying and de-magnifying optics) will provide dose-efficient holographic imaging options for both 1 µm resolution and large field of views whereas Multilayer Laue Lenses will be used for hard-x-ray nanoimaging. All these techniques will exploit the unique brilliance and coherence of PETRA IV for exceptional holographic phase contrast and highest holographic dose efficiency.

Main applications are high-throughput studies like large comparative morphological studies in materials (e.g. batteries) and life sciences (e.g. biodiversity studies), studies of a wide range of flat samples, e.g. by scanning volumes along large sample areas and zooming into high resolution ROIs, 4D in situ and operando studies, biomedical applications and in vivo studies (e.g. during embryogenesis for developmental biology). The proposed beamline optics, instrumentation, beam properties, performance parameters, and applications will be presented.

Multiscale and -modal Characterisation of Soft Materials at ForMAX

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Presentation type: Poster

The increasing complexity of hierarchical and functional materials requires characterisation approaches capable of resolving structure and dynamics across multiple length scales and modalities in parallel. The ForMAX beamline at MAX IV [1] combines full-field X-ray imaging with small- and wide-angle X-ray scattering (SWAXS), enabling correlative structural characterisation from the nanometre to millimetre scale within one instrument. Here, we highlight the multimodal and multiscale imaging opportunities available at ForMAX for operando and time-resolved studies of hierarchical materials. The beamline combines high-flux synchrotron microtomography, radioscopy, and scanning SWAXS imaging methods with fast transitions between measurement modalities. These methods together enable access to local morphology, porosity, fibre orientation, phase distribution, and nanoscale ordering during dynamic processes such as deformation, flow, drying, or material transformation. We will present how the combined imaging and scattering modalities at ForMAX can bridge real-space and reciprocal-space characterisation, enabling quantitative correlations between microscale morphology and nanoscale organisation. The presented capabilities are relevant for a broad range of applications, including bio-based and fibrous materials, soft matter, multiphase systems, food science, and biomedical imaging.

References

[1] Nygård K. et al. (2024). ForMAX–a beamline for multiscale and multimodal structural characterization of hierarchical materials. Synchrotron Radiation, 31(2), 363-377.

Increasing sinter stability of Pd/(CeO2)/alpha-Al2O3 model catalysts under methane oxidation

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Presentation type: Poster

Methane with the highest hydrogen-to-carbon ratio of all hydrocarbons, is a promising alternative for conventional (diesel) fuel. However, highly active, long lifetime exhaust gas catalysts are required to prevent methane slip due to its more than 20 times higher greenhouse gas potential compared to CO2.Pd is the most active material for catalytic driven complete methane oxidation at relatively low temperatures and lean (oxygen-rich) reaction gases. Nevertheless, nanoparticle sintering during the catalytic reaction is the major cause for catalytic activity loss due to a decreasing active surface.

Here we present two different approaches based on tailored metal-support interactions for increased sinter stability of Pd nanoparticles during methane oxidation under operando conditions. On the one hand, we altered the α-Al2O3surface modifications by Ar+-ion bombardment with different sputter energies. Generated vacancies induced the growth of Pd nanoparticles close to their thermodynamic equilibrium shape which displayed a higher sinter resistance during one cycle of methane oxidation. On the other hand, we use epitaxial ceria (CeO2) nano-islands on α-Al2O3as a heterogeneous support for Pd nanoparticles. Ceria is characterized by strong metal-support interactions, high oxygen storage capacity, and unique redox properties based on the facile and reversible change in oxidation state between Ce4+ and Ce3+. These properties make it especially interesting for applications in heterogeneous catalysis where it is used as active support material for noble metals acting as oxygen buffer during oxidation processes.

To obtain detailed information about the sintering mechanism and material transport during the catalytic reaction, we investigate well-defined model systems by (high-energy) grazing incidence X-ray diffraction at Petra 3 (DESY) and ESRF, combined with X-ray reflectivity and atomic force microscopy. This approach enables the identification of atomic-scale details of the catalyst structure and their correlation with catalytic activity changes determined by mass spectrometry.

Influence of Au Catalyst Size on the Structural Properties of CdO Nanowires Grown by Molecular Beam Epitaxy

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Presentation type: Poster

Cadmium oxide nanowires were grown by molecular beam epitaxy (MBE) using Au catalyst droplets with different diameters in order to investigate the influence of the catalyst size on the morphology and crystalline properties of the nanowires. CdO is a transparent conductive oxide with promising applications in optoelectronics, transparent electronics, gas sensors and nanoscale electronic devices, making the control fabrication of high-quality CdO nanowires particularly important [1]. The variation of the Au droplet dimensions resulted in significant changes in the nanowire geometry, including their length, width, and packing density. A comprehensive structural characterization was performed

Scanning electron microscopy (SEM) investigations confirmed a strong correlation between the catalyst size and the nanowire morphology. Larger catalyst droplets led to noticeable changes in nanowire density and diameter distribution. TEM and scanning transmission electron microscopy analyses revealed a high crystalline quality of the CdO nanowires together with a well-defined growth orientation and high structural uniformity along the nanowire axis. The nanowires exhibited low defect density and homogeneous morphology over large sample areas.

Energy-dispersive X-ray spectroscopy (EDX) measurements confirmed the presence of Au catalyst droplets at the nanowire tips and demonstrated the compositional homogeneity of the CdO nanostructures. The combined electron microscopy studies provided detailed information about the nanowire dimensions, alignment, and structural uniformity for samples prepared with different catalyst sizes.

X-ray diffraction (XRD) and Grazing incidence XRD (GIXRD) measurements demonstrated very good crystalline quality of all investigated samples. Additionally, systematic shifts of the diffraction peaks were observed as a function of the Au catalyst size. The observed changes suggest modifications of the microstrain relations in the CdO nanowires as well as variations in the tilt and twist distributions associated with the nanowire ensemble. The results indicate that the catalyst dimensions play an important role not only in determining the nanowire morphology but also in influencing their structural coherence and strain relaxation mechanisms.

The presented study demonstrates that precise control of the Au catalyst size provides an effective route for tuning both the morphological and structural properties of CdO nanowires grown by MBE, which is important for their future application in nanoscale electronic and optoelectronic devices.

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References

[1] A. Sekkat, et al., J. Mater. Chem. A, 12 (2024) 25600-25621.

Poster Session 2

Multiscale characterization of hierarchical particle–pore systems using correlative X-ray and electron tomography

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Presentation type: Poster

Hierarchical porous, particulate materials underpin catalysts, batteries, electrolyzers, and separation media, with performance governed by coupled intra- and interparticle pore networks spanning multiple length scales. Precise multiscale characterization is therefore essential and requires correlative 3D microscopy to bridge the field-of-view–resolution trade-off of single modalities.

We present a lab-based, scale-bridging workflow that integrates electron tomography (ET), nano X-ray computed tomography (nanoCT), and micro X-ray computed tomography (microCT) to quantify particle and pore statistics from nanometers to millimeters. [1] A central challenge – simultaneously resolving fine internal structures and acquiring statistically robust particle populations – is addressed by coordinated sample design, multimodal imaging, and identical-location analysis.

As a model system, we study porous silica particles produced by polymerization-induced phase separation, featuring hierarchical meso- and macroporosity. [2] A customized tapered pillar of embedded particles is prepared by mechanical grinding and polishing to optimize the field of view (FOV) for each imaging technique. This geometry enables millimeter-scale microCT surveys for statistics on thousands of particles while preserving regions for high-resolution investigation by nanoCT at identical locations. MicroCT using a ZEISS Xradia 620 Versa captures ensembles and packed assemblies at down to 500 nm resolution on mm-scale specimens. Individual particles and their intraparticulate pore networks are imaged by nanoCT using a ZEISS Xradia 810 Ultra with 50 nm resolution at a (16 µm)² FOV and 150 nm at (64 µm)² FOV. Therein, Zernike phase contrast enhances structural details in weakly absorbing silica. To access smaller mesopores, we perform 360°-ET on a pillar extracted from a representative particle, mitigating the missing wedge and providing nanometer-scale ground truth. Cross-modal registration of corresponding regions of interest enables direct data correlation. Reconstructed volumes are segmented using supervised, neural-network–based methods to robustly delineate solid and pore space under phase-contrast conditions. The unified pipeline yields quantitative descriptors across scales, including particle size, pore size distributions (meso- to macropores), and porosity.

This work underscores the value of cross-scale, correlative 3D microscopy for a comprehensive understanding of hierarchical materials. Complementary imaging modalities, accurate registration, and machine-learning segmentation enable robust process–structure–property correlations and guide the optimization of functional porous architectures.

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References

[1] A. Götz et al., JTMS2025, 9, 100069.
[2] U. Sultan et al., JACS 2025, 147(23), 19841.

CNN-Based Mitigation of Zernike Phase-Contrast Artifacts in high-resolution XRM and NanoCT

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Presentation type: Poster

Zernike phase contrast (PC) X-ray microscopy (XRM) is widely used to image weakly absorbing materials, but it introduces characteristic halo and shade-off artifacts that propagate into tomographic reconstructions. If not properly addressed, these artifacts can compromise quantitative analysis, particularly in nano-computed X-ray tomography (nanoCT). Developing robust strategies to mitigate such effects is therefore essential for reliable 3D characterization. Phase retrieval techniques offer a route to recover phase information from intensity images [1], using approaches such as iterative, analytical, and data-driven methods. However, most of these methods are developed for propagation-based phase contrast, corresponding solutions for Zernike PC nanoCT remain limited.

In this work, we introduce a workflow that integrates experimental Zernike PC XRM/nanoCT with physics-based phase-contrast modeling and convolutional neural networks (CNNs) to enhance 3D reconstruction quality. A Fourier optics model is used to simulate PC image formation, with parameters adjusted to replicate the ZEISS Xradia 810 Ultra system. This approach enables the creation of paired datasets: (i) simulated PC images and (ii) corresponding mass-thickness images. A CNN trained on these data is subsequently applied to experimental tilt series to predict mass-thickness projections before reconstruction. Reconstructions based on CNN-corrected projections exhibit improved contrast compared to conventional Zernike PC reconstructions.

We demonstrate the approach on colloidal supraparticles, which are self-assembled, highly-ordered particle aggregates that form discrete crystalline structures [2]. In practice, they rarely crystallize perfectly: amorphous regions and defects are common and can strongly affect optical properties. Establishing reliable correlations between processing, structure, and function therefore requires 3D characterization of defects at the single-particle scale. XRM provides an excellent match to the relevant length scales for this purpose [3]. While high-resolution 2D projections already allow the identification of planar defects such as stacking faults, the detection and quantification of point defects (e.g. vacancies) necessitate volumetric imaging.

In addition, we investigate the adaptation of the sparse sphere reconstruction method [4] to Zernike PC nanoCT. By representing the volume as a collection of homogeneous, monodisperse spheres with known size, this approach aims to recover particle-level information even under limited-angle or low-dose acquisition conditions, offering a promising strategy for more robust defect identification in functional colloidal assemblies.

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References

[1] C. Zuo et al., Optics and Lasers in Engineering. 2020, 135
[2] J. Wang et al., Adv. Funct.Mater. 2020, 30, 19907730.

[3] S. Englisch et al., Microsc. Microanal. 2019, 25, 392.
[4] D. Zanaga et al., Nanoscale. 2016, 8, 292

High-Resolution X-ray Ptychographic Computed Tomography of Brain Tissue Samples

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Presentation type: Poster

Mapping the brain connectome at high resolution is essential for understanding neural circuit organization and function. Electron microscopy (EM) provides sufficient resolution, but it requires cutting the sample in thin slices, which is prone to artefacts and hinders automatic segmentation of large brain volumes. X-ray imaging, in particular X-ray ptychographic computed tomography (PXCT), offers a promising complementary approach by enabling non-destructive 3D imaging of intact samples. However, radiation damage and the high dose required during data acquisition remain major challenges when pursuing high spatial resolution.

Previous studies have used resin-embedded samples to mitigate radiation damage, achieving a 3D Fourier shell correlation (FSC) resolution of around 38 nm under cryogenic conditions1. In this work, we explore critical-point drying (CPD) as an alternative sample preparation method. CPD-prepared brain tissue has been proven to provide higher phase contrast in phase-contrast X-ray microscopy at a spatial resolution of around 100 nm2.

Here, we investigate the combination of CPD sample preparation with advanced reconstruction strategies to balance dose reduction and resolution. High-resolution PXCT measurements were performed on CPD brain tissue samples at the NanoMAX beamline at MAX IV. To mitigate radiation damage from the high-flux nanobeam, we optimized the incident flux during acquisition. We then applied advanced reconstruction algorithms to recover image quality under these dose-limited conditions. In addition to conventional projection alignment3, this includes deformation compensation using non-rigid tomographic reconstruction4 to correct sample motion and structural changes during acquisition, as well as denoising based on the Noise2Noise framework5 to improve contrast while preserving structural details.

Using this workflow, we achieve a 3D Fourier shell correlation (FSC) resolution of approximately 27 nm at a relatively low dose of 3.0 × 10 Gy, notably without the use of cryogenic conditions, demonstrating the potential for high-resolution PXCT under more accessible experimental setups.

References

[1] Bosch, C. et al. Nondestructive X-ray tomography of brain tissue ultrastructure. Nature Methods22, 2631–2638 (2025).
[2] Khan, S. et al. Critical point drying of brain tissue for X-ray phase-contrast imaging. J Synchrotron Rad33, 759–768 (2026).
[3] Odstrčil, M. et al. & Guizar-Sicairos, M. Alignment methods for nanotomography with deep subpixel accuracy. Opt. Express27, 36637 (2019).
[4] Odstrcil, M. et al. Ab initio nonrigid X-ray nanotomography. Nat Commun10, 2600 (2019).

[5] Laugros, A. et al. Self-supervised image restoration in coherent X-ray neuronal microscopy. Preprint (2025).

Oblique diffraction geometry for the observation of several non-coplanar Bragg reflections under identical illumination

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Presentation type: Poster

We present a method to determine the strain tensor and local lattice rotation with Dark Field X-ray Microscopy. Using a set of at least 3 non-coplanar, symmetry-equivalent Bragg reflections, the illuminated volume of the sample can be kept constant for all reflections, facilitating easy registration of the measured lattice variations.

This requires an oblique diffraction geometry, i.e. the diffraction plane is neither horizontal nor vertical. We derive a closed, analytical expression that allows determination of the strain and lattice rotation from the deviation of experimental observables (e.g. goniometer angles) from their nominal position for an unstrained lattice.

Precipitation-induced strain field in Ni-based superalloys

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Presentation type: Poster

Strain-age cracking (SAC) is a major failure mode in precipitate-hardening Ni-based alloys. It occurs during post-weld heat treatments or multi-pass welding and is particularly severe in alloys that precipitate rapidly and develop a high volume fraction of precipitates. Some alloys are even classified as “non-weldable.” Despite decades of research, the mechanisms behind SAC remain debated. Several theories have been proposed, one of which focuses on the role of negative misfit strains between the precipitates and the matrix.

This project investigates how precipitation-induced misfit strains and alloy composition influence strain evolution. In this work, we investigate the strain fields associated with embedded γ precipitates within the γ matrix of two superalloys: Haynes 282 and Allvac 718Plus. Scanning transmission X-ray diffraction (STXRD), using a focused beam size of 60 × 60 nm², was employed to spatially resolve the strain fields in both the matrix and the precipitates. The results provide direct insight into the elastic interactions between the two phases at the nanoscale.

STXRD with a focused nano-beam enables the strain field of individual precipitates to be resolved. However, SAC occurs primarily at grain boundaries. To investigate how precipitation-induced strain fields generate stresses and strains at grain boundaries during ageing, the strain evolution of individual grains during ageing has been studied using dark-field X-ray microscopy (DFXM).

Understanding strain fields caused by precipitation across both nanometre and micrometre length scales in Ni-based superalloys is critical for elucidating degradation mechanisms that limit structural integrity at elevated temperatures. In these alloys, lattice-parameter mismatch between the γ matrix and coherent γ′ precipitates generates internal stress fields that can promote crack initiation through strain-age cracking during thermal exposure.

On X-ray Orbital Angular Momentum–Dependent Coherence-Based Imaging

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Presentation type: Poster

Structured X-ray beams carrying orbital angular momentum (OAM) provide a new degree of freedom for coherent scattering experiments. Here, we investigate how twisted X-ray illumination modifies coherent Bragg diffraction and explore extending coherent Bragg diffraction imaging (BCDI) to OAM-resolved measurements. Experiments were performed at the ID01 beamline of the ESRF using a fabricated spiral zone plate to generate X-ray beams with well-defined OAM states.

We studied model systems with distinct structural symmetries, including an achiral Pt nanocrystal, an intrinsically chiral Te nanocrystal, and chiral ferroelectric polarization domain textures in a quasi-2D BaTiO membrane. Coherent X-ray Bragg diffraction measurements were carried out for multiple OAM modes ($\ell = -3, -1, 0, +1, +3$) from small isolated nanocrystals.

The resulting 3D Bragg diffraction intensities exhibit systematic OAM-dependent contrast variation in a helical dichroic mode, indicating that the beam has access to an OAM-resolved scattering form factor arising from higher-order multipole interactions. Such OAM-resolved Bragg electron densities may provide access to new physics, including symmetry-selective scattering, chiral lattice distortions, orbital-current contributions to the structure factor, and other angular-momentum–dependent scattering channels. These results establish a framework for orbital-angular-momentum–dependent coherent Bragg diffraction imaging and highlight the potential of structured X-ray illumination for probing symmetry, chirality, and lattice distortions in complex materials.

X-ray Tomography of 3D printed hydrogel based tissue scaffolds

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Presentation type: Poster

Hydrogel-based 3D tissue cultures offer new opportunities to model human disease and to support the development of novel therapies. The usage of stereolithography 3D printing, combined with computer-aided design (CAD), enables precise control over scaffold geometry. X-ray micro-tomography is a quick and powerful tool to assess print quality, detect structural defects, and even in-operando quantify shape changes induced by cultured tissues. In this project we develop phase-contrast based X-ray metrology of hydrogel scaffolds. The polymer used in this work is poly(ethylene glycol) diacrylate (PEGDA). It consists of a PEG chain terminated by two acrylate groups. This two elements are, respectively, hydrophilic and hydrophobic; the balance between these two components determines the bulk hydrophilicity of the final polymer. The two polymers under examination have distinct molecular weights and distinct ratio between hydrophobic and hyrophilic component concentrations: PEGDA 250, who has hydrophobic characteristics; and PEGDA 700, which forms the hydrogel. As a first step, scaffolds printed with PEGDA 250 were scanned by X-ray tomography in both dry and wet conditions. Working with the hydrophobic material simplifies the imaging problem. Thus, these measurements serve as a bench-mark for the future analysis of PEGDA 700 hydrogel samples. Imaging a water-filled hydrogel scaffold at sub-micron resolution is considerably more demanding. For this purpose we develop advanced laboratory based X-ray phase contrast microscopy with a liquid metal jet X-ray source. Also complementary strategies will be pursued, such as contrast agents to locally enhanch electron density at the scaffold-water interface. Together, these approaches are expected to provide the sensitivity needed to characterize PEGDA 700 scaffolds quantitatively and to detect subtle shape changes relevant to tissue culture applications in operando.

In-situ µLaue and Dark-Field X-ray Microscopy Investigation of Strain Relaxation Mechanisms in Patterned InGaN Pseudo-Substrates for Red Micro-LED Applications

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Presentation type: Poster

The development of high-resolution micro-displays is strongly limited by the difficulty of fabricating efficient red micro-light emitting diodes (micro-LEDs) with pixel pitches below 10 µm. Red emission from InGaN-based active layers requires indium concentrations above 35%, while conventional growth on GaN-on-sapphire substrates limits In incorporation to ~25% due to the large lattice mismatch between GaN and InGaN. To overcome this limitation, CEA-Leti is developing a relaxed InGaN pseudo-substrate based on the patterning of a two-dimensional InGaN layer into micrometric mesas, enabling partial strain relaxation while preserving crystalline quality [1].

Recent in-situ laboratory measurements of the in-plane lattice parameter versus temperature, combined with reciprocal space mapping after annealing, revealed an unexpected additional relaxation of the patterned InGaN layer occurring at relatively low temperatures without indium exodiffusion. This relaxation is temperature dependent, takes approximately three hours at 150°C, and no further relaxation occurs after a second annealing cycle. We hypothesize that this mechanism originates at the InGaN/GaN interface and is driven by the glide of mixed dislocations near mesa edges due to stress anisotropy induced by dry etching. Although beneficial for strain accommodation, this process may also introduce crystalline defects detrimental to the optical performance of red LEDs.

The objective of this work is to investigate locally the relaxation mechanisms occurring during annealing and to evaluate the resulting structural homogeneity of patterned InGaN layers. In-situ µLaue diffraction experiments have been performed at the BM32 beamline at ESRF [2] using a focused X-ray beam of approximately 0.3 µm. Local strain maps were acquired across individual 5 µm mesas during thermal cycles from room temperature up to 600°C, as well as during isothermal annealing experiments between to study relaxation kinetics (Fig. 1.a). Particular attention have been paid to the comparison between mesa center and edges in order to determine where relaxation initiates and how it propagates spatially.

Complementary Dark-Field X-ray Microscopy measurements performed at ID01 and ID03 [3, 4] provide statistical maps of strain, tilt, mosaicity, and defect distributions over hundreds of mesas with sub-100 nm spatial resolution (Fig. 1.b). Previous cathodoluminescence and scanning X-ray diffraction measurements revealed strong mesa-to-mesa variability, likely related to structural inhomogeneities such as dislocations and domain misorientation. Correlating diffraction imaging with luminescence measurements will allow us to identify the structural origins of this variability and assess whether relaxed InGaN pseudo-substrates provide the homogeneity required for the epitaxy of efficient red quantum wells for next-generation micro-display applications.

Evolution and Functional Morphology of Hip Joint Systems in Beetles

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Presentation type: Poster

Beetles (Coleoptera) combine exceptional taxonomic diversity with a wide range of locomotory, postural and behavioural adaptations. Yet the internal architecture of their leg joints has received comparatively little attention. The coxa–trochanteral joint, functionally comparable to a hip joint, connects the leg to the body and is often treated as a simple hinge in insects. High-resolution three-dimensional studies, however, have shown that beetles can possess more complex rotational and screw-like articulations, including screw-and-nut systems in which helical structures of the trochanter engage with corresponding structures of the body-side joint cavity.

Here, beetle hip-joint morphology is examined with a particular focus on weevils (Curculionoidea), the group in which true biological screw-and-nut joints were first described. High-Throughput synchrotron X-ray microtomography, three-dimensional reconstruction, landmark-free geometric morphometrics and phylogenetic comparative analyses are combined to quantify internal joint morphology across a phylogenetically broad sample. Atlas-based shape analysis makes it possible to compare highly derived joint structures without relying on dense sets of predefined homologous landmarks. In addition, geometric descriptors such as winding angle, axial span and pitch are used to characterize screw-like components of the articulation.

This approach links internal morphology, mechanical architecture and evolutionary history in a joint system that is difficult to access with conventional methods. The results show that beetle hip joints are not adequately described as simple hinges, but include a range of mechanically specialized configurations. They also illustrate how three-dimensional imaging and landmark-free morphometrics can be used to study small, enclosed and morphologically complex biological structures. More generally, beetle leg joints provide a useful system for investigating how mechanical function and evolutionary diversification interact in arthropod morphology.

Non-Reconstructive Prior-β Grain Estimation by Synchrotron X-ray Diffraction Spot Distribution Analysis in Ti-6Al-4V with TiC

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Presentation type: Poster

Introduction

TiC heterogeneous nucleation site particles added to Ti-6Al-4V promote equiaxed grain refinement. The electrostatic levitation furnace in the International Space Station (ISS-ELF) eliminates container contact and suppresses convection, enabling independent evaluation of TiC-driven nucleation. Because TiC acts on the primary βphase, prior-βgrain number is essential. Techniques such as diffraction contrast tomography enable full three-dimensional (3D) grain reconstruction but are computationally expensive for prior-βgrain estimation. The objective of this study was to propose a method for estimating prior-βgrain number from synchrotron X-ray diffraction (XRD) spot statistics without full 3D reconstruction.

Procedures

Ti-6Al-4V samples with 5 mass% TiC were solidified in ISS-ELF under a condition promoting prior-βgrain coarsening (Coarse Condition) and refining (Refine Condition). Synchrotron XRD was performed at BL20XU of SPring-8 while rotating the sample through 360° in 0.5° steps. Diffraction signals were extracted as the logarithm of intensity relative to the per-pixel median across all frames. Theα-phase {1 0 -1 0} ring was selected for its high intensity and separation from neighboring diffraction spots. Continuously observed spots were grouped, and the maximum projected areaA_maxper group was taken as a characteristic value. Geometrically paired spots from the rotating-stage geometry were integrated to avoid double counting. The Kneedle algorithm for detecting discrete curves was applied to theA_maxhistograms after 5-bin movingaverage smoothing, with the analysis range bounded where the count gradient fell below 1% of its maximum.

Results

TheA_max histogram of theCoarse Conditionshowed a pronounced drop with increasingA_max, approximately four times steeper than the gradual monotonic decrease of theRefine Condition.

Discussion

The drop reflects the size contrast between grain-boundary α and intragranular α colonies, which is amplified by the large prior-βgrains characteristic of theCoarse Condition. The Kneedle algorithm identified 0.0241 mm² as the threshold separating these two α spots. Spots larger than this threshold were extracted from theRefine Conditiondata and scaled to the full sample volume under a truncated-octahedral grain-shape assumption. The estimated 368 ± 5 prior-β grains agreed with an independent estimate of 365 ± 68 from electron backscatter diffraction and Voronoi tessellation.

Conclusion

The proposed method uses logarithmic background extraction from rotating-stage synchrotron XRD images and characterizes continuously observed spots by theirA_max. Geometric pair in-

tegration and Kneedle-based threshold detection on theA_max histogram separate grain boundaryαsignals from prior-βgrain signals. Volume scaling under a truncated-octahedral grain-shape assumption yields the prior-βgrain number without full 3D reconstruction.

Probing Ferroelectric Switching in BaMgF via Quasi In-Situ Dark-Field X-ray Microscopy

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Presentation type: Poster

Barium magnesium fluoride (BaMgF) is a radiation-resistant, uniaxial ferroelectric material with significant potential for nonlinear optical applications, such as frequency conversion, owing to its ultra-broad transparency range.[1] Using this potential for quasi-phase matching requires the fabrication of periodic domain structures through the whole wafer thickness. Although periodic poling is facilitated by a relatively low coercive field and stable domain walls,[2] writing domains smaller than 5 µm remains a persistent challenge, which is potentially due to the pinning of domain walls at crystal defects.

To investigate the fundamental mechanisms limiting domain size, we employed quasi-time-resolved dark-field X-ray microscopy (DFXM) at the ESRF synchrotron beamline ID03. Using resonant Friedel pair contrast, we successfully performed three-dimensional (3D) imaging of ferroelectric domain evolution in BaMgF bulk crystals under applied voltage pulses. Our time-resolved data reveal that domain growth occurs through domain wall motion. We identified a pronounced anisotropy in this process, with domain walls exhibiting both a preferred orientation and direction-dependent velocities. Using periodically patterned metal electrodes, we could write stables domain structures with 15 µm, while smaller structures led to a coalescence of neighboring domains. Notably, no spontaneous back-switching events were observed on the time scales available in our experiment. The data provides unprecedented 3D insights into the ferroelectric switching dynamics of BaMgF and demonstrate the utility of DFXM for visualizing these processes. This approach may proof particularly valuable for the non-destructive, imaging of ferroelectric domain structures in capacitor structures on functional materials.

References

[1] Víllora et al. Opt. Express, 17(15):12362–12378, 2009.
[2] Herr et al. Opt. Mater. Express, 13(8):2158–2164, 2023.

From pixels to bases: Integrating synchrotron X-ray imaging and DNA sequencing of insects

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Presentation type: Poster

The integration of morphological and molecular data is central to modern biodiversity and evolutionary research. However, current workflows often compromise one data source in favor of the other: standard DNA extraction protocols dissolve internal soft tissues, precluding post-extraction imaging and digital preservation, while the impact of high-dose radiation micro-computed tomography (µCT) scanning on DNA integrity remains insufficiently understood. This study systematically evaluates the reciprocal effects of µCT scanning and DNA extraction on insect specimens to develop an optimized workflow that maximizes both phenotypic and genotypic data recovery.

We assessed multiple DNA extraction methods to quantify their effects on internal tissue preservation and examined the influence of varying µCT irradiation doses and durations on DNA quality, quantity, and DNA fragmentation. Our results show that while all DNA extraction methods inherently damage soft tissues to some degree, µCT scanning allows for non-destructive visualization of internal morphology prior to digestion. DNA yield and integrity decrease with increased irradiation time, yet both DNA barcoding and ultraconserved element (UCE) sequencing remain viable when µCT data acquisition parameters are optimized.

These findings demonstrate that careful calibration of scanning and extraction protocols enables the creation of high-quality digital vouchers alongside usable genomic material. The proposed workflow provides a framework for integrating morphological and molecular datasets in natural history collections, preserving both phenotypic and genotypic information from even the most delicate or rare specimens for future research.

A standardized workflow for cross-beamline data harmonization and analysis of cement hydration in X-ray tomography

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Presentation type: Poster

Cement hydration is a complex multiscale set of processes. The early-age mechanisms controlling cement hydration, especially particle dissolution and the transition fromacceleration to deceleration, are still not fully understood. Time-resolved synchrotron X-ray tomography enables 3D imaging of cement hydration and provides access to particle-scale microstructural evolution.

Quantifying particle dissolution during cement hydration using X-ray computed tomography requires consistent analysis of time-resolved 3D datasets. However, datasets acquired from different beamlines often differ in data format, voxel size, field of view and image quality, complicating data handling, spatial alignment and the reproducible application of downstream particle-based analysis methods.

The X-ray imaging studies are carried out for pastes loaded in cylindrical capillaries of diameters dictated by the field of view (FOV) and spatial resolution requirements. The volume reconstructions are carried out with the software available at the beamlines.

In this work, we present a two-stage standardized workflow for synchrotron X-ray tomography studies of cement hydration. The first stage focuses on cross-beamline reconstructed data harmonization and preprocessing, including data format conversion, volume cropping and standardized multi-step 3D precise volume registration, to obtain spatially consistent time-resolved volumes. It is noted that the accurate determination of the evolution of microparticles, after mounting and dismounting the specimens at the beamline, is only possible if volume registration is very good and it is carried out in a robust way. The second stage performs downstream image analysis, including segmentation, particle separation, labeling, particle tracking and dissolution-rate quantification.

The approach is applied to multiscale XCT datasets ofdifferent cementitious materials, ranging from single-phase tricalcium silicate (C3S) and ordinary Portland cement (PC) to low-carbon cements such as limestone calcined clay cement (LC3), acquired across multiple beamlines, including FaXToR-ALBA (voxel size: 0.65µm, FOV: 1.3 mm), Anatomix-SOLEIL (voxel size: 220 nm, FOV: 0.45 mm), ID16B-ESRF (voxel size: 100 nm, FOV: 0.2 mm). The workflow enables reproducible application of particle-based dissolution analysis without the need for dataset-specific adjustments. The proposed framework provides a foundation for integrating multiscale datasets acquired from different beamlines, enabling consistent analysis and facilitating future comparative and systematic studies of cement hydration processes.

Artificial laminar oxide multiferroic magnetoelectric thin film structures - elaboration and characterization

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Presentation type: Poster

Nanometric laminar two-dimensional artificial multiferroic oxide thin films can be elaborated using spinel ferrites and perovskite ferroelectrics like CoFe2O4 and BaTiO3. Such materials can retain their individual ferromagnetic or ferroelectric properties. In the thin epitaxial film regime, a cross coupling and cross-correlation of these properties is possible thanks to strain engineering.

The concepts supporting artificial multiferroic laminar structures, the growth of strained BaTiO3 thin films and the growth of subsequent Co-ferrites will be introduced. With respect to the relative film thickness, a detailed characterization of the elastic behavior of these films will be shown, using several synchrotron radiation techniques including x-ray specular and off-specular diffraction, x-ray absorption spectroscopy, as well as x-ray magnetic circular dichroism.

In-situ Synchrotron X-ray Micro-Tomography and Machine-Learning-Assisted Segmentation of Low-Density Hydrocarbon Phases in Powdered Catalysts

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Presentation type: Poster

A fundamental barrier in understanding catalytic systems under realistic operating conditions is the lack of access to their evolving internal structure. During operation, complex multiphase environments emerge within porous materials due to the formation and accumulation of heavy hydrocarbon species. These processes lead to heterogeneous spatial distributions of solids, liquids, and gases that strongly influence transport phenomena, reaction pathways, and catalyst performance. However, capturing such dynamic structural changes in a non-destructive and spatially resolved manner remains a major challenge due to the limited contrast between coexisting phases.

In this work, synchrotron-based X-ray microtomography was combined with Raman spectroscopy and machine-learning-assisted image segmentation to investigate the formation, redistribution, and removal of hydrocarbon waxes within porous catalyst beds under in-situ thermal treatment conditions. Cobalt-based Fischer–Tropsch catalysts containing accumulated waxes were used as a model multiphase porous system. The multimodal approach enabled visualization and quantitative analysis of low-density hydrocarbon phases and their structural evolution during catalyst regeneration.

A key challenge in characterizing such systems lies in the intrinsically weak contrast between wax-filled and empty pore regions. Even advanced synchrotron-based X-ray microtomography with phase-sensitive imaging struggles to resolve subtle variations due to the minimal absorption contrast between coexisting phases. As a result, conventional threshold-based segmentation approaches fail to reliably capture the internal structure. To overcome this limitation, machine-learning-assisted segmentation was employed, enabling robust phase discrimination and quantitative analysis of wax redistribution during in-situ thermal treatment.

The investigated catalyst consisted of amorphous silica support grains (<100 µm) loaded with cobalt nanoparticles. Spent catalysts containing accumulated wax species were subjected to controlled dewaxing treatments under nitrogen and hydrogen atmospheres at elevated temperatures. In-situ synchrotron X-ray microtomography experiments were performed at the P05 beamline at DESY using sequential tomographic acquisitions during stepwise heating. The study revealed pronounced differences between inert and reductive atmospheres during dewaxing. Under hydrogen flow, wax melting became visible at approximately 100 °C, followed by progressive redistribution and substantial removal above approximately 220 °C. At 330 °C, a significant reduction of intergranular wax was observed together with compaction of the catalyst bed. In contrast, treatment under nitrogen resulted mainly in wax melting and redistribution with limited removal at elevated temperature. Correlative Raman spectroscopy confirmed the gradual reduction of hydrocarbon species after dewaxing.

The integration of in-situ imaging with machine-learning-assisted analysis demonstrates the potential of synchrotron X-ray microtomography for quantitative investigation of weakly contrasted multiphase materials and dynamic low-density phases in porous reactive systems.

Crystal defect dynamics at the solid-liquid interface in silicon – Investigation by X-ray topography and rocking curve imaging.

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Presentation type: Poster

Controlling defect formation during silicon solidification is essential for improving its crystalline quality for photovoltaic solar-cell applications. In particular, understanding how defects are transmitted from the seed crystal into the regrown region, and how they reorganize at the solid–liquid interface, remains a key challenge. In this work, in-situ X-ray radiography and topography are combined to directly visualize the evolution of the solid–liquid interface and follow defect dynamics in real time. In addition, rocking curve imaging (RCI) is used ex-situ to quantify local lattice distortions, misorientation, and possible sub-grain formation during the early stages of silicon regrowth. This approach is applied to different seed materials, including float-zone, Czochralski, and cast-mono silicon, in order to assess the influence of the initial seed quality on defect propagation and reorganization during regrowth.

The observations reveal a characteristic two-stage evolution of defects revealed by their contrast on the X-ray topographs recorded during regrowth. At the initial stage, diagonal contrast features are observed above the first solid–liquid interface. These features are attributed to dislocation glide along {111} characterized only in the first stages. As growth proceeds and the interface becomes more stable, the linear contrasts progressively reorient and become nearly perpendicular to the solid–liquid interface moving upward. This latter contrast type is interpreted as grown-in dislocations expanding along the growth direction, intersecting with the solid-liquid interface to minimize their line tension.

Interestingly, the quasi-perpendicular contrast does not appear in the same form in all samples. In some cases, it appears as sharp, intense, and well-defined individual lines, whereas in others it appears weaker, broader, and more diffuse. Comparison with the RCI peak-position maps suggests that regions showing broadened topographic contrast are often associated to local lattice misorientation and thus to sub-grain formation. This indicates that, in these regions, dislocations may rearrange collectively ultimately polygonising and creating dislocation networks or low-angle boundaries, leading to broadened contrast and measurable local lattice tilt. In contrast, when sharp individual perpendicular contrast is observed, no significant lattice tilt or misorientation is detected in the corresponding RCI maps indicating that the linear contrasts are due to the strain field created by independent propagating dislocations.

These results suggest that the solid–liquid interface plays an active role not only in the transmission of seed defects into the regrown crystal, but also in their reorganization during the transition from the transient stage to the stationary growth regime.

I13-1 Coherence: The multiscale, Multimodel, Ptycho-tomographic End Station at DLS.

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Presentation type: Poster

I13-1 is the longest beamline at Diamond light source (DLS), with 235m source to detector. The beamline optics is defined to preserve the coherence of the source and transported to the sample 220m downstream, allowing to exploit several coherent diffraction imaging modalities both in 2D and 3D samples, such as Ptychography-tomography, Bragg-ptychography, Bragg-CDI, Spectral ptychography. That can be combined with XRF for retrieving elemental composition.

The ptychography-tomography data collection at I13-1 can ramp up to high speeds in the order of 100's kHz, collecting full tomograms in few minutes. In this contribution, we would like to present the new technical features that make the beamline capable to of performing scan at such high repetition rates and present results from the commissioning and initial experiments perform at the beamline.

Also, we would like to present other upgrades happening in the other experimental configurations. That will benefit from the upgrade of the DLS ring to a 4th generation synchrotron in the next 3 years.

Contrast Engineering in NanoCT of Porous Silica through Tailored Intrusion Media

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Presentation type: Poster

Nano X-ray computed tomography (nanoCT) enables non-destructive, three-dimensional characterization of porous microstructures with local visualization and quantification of pore size, shape, and connectivity at spatial resolutions down to ~50 nm. The accuracy of pore metrics depends critically on projection contrast and signal-to-noise. In nanoCT, contrast arises from spatial variations in the complex refractive index, $n = 1 - \delta + i\beta$. Absorption contrast (β), governed by the Beer-Lambert law, provides mass-thickness sensitivity but is often weak for low-Z phases or materials with small attenuation differences. Zernike phase contrast (δ) converts phase shifts into intensity variations, enhancing visibility in weakly absorbing or highly porous materials, but introduces halo and shade-off artifacts that impair segmentation accuracy. To efficiently exploit both modes and broaden applicability across material systems, tailored media intrusion offers a powerful strategy for contrast engineering.

To enhance absorption contrast, gallium is introduced as an intrusion medium into porous silica, increasing X-ray attenuation differences and improving the robustness of reconstructions. Using a modified mercury intrusion porosimetry protocol, previously shown to enhance contrast in electron tomography [1], liquid Ga is pressure-driven into the pore network. In contrast to mercury, Ga remains in the pores after pressure release due to the formation of an interfacial oxide layer [2]. Compared to the unfilled state, Ga infiltration yields a 3.7x increase in absorption contrast and a 29% improvement in apparent interface sharpness. As an addition benefit, the higher electrical conductivity of the Ga-filled sample facilitates focused ion beam milling by reducing charging and sample drift.

For Zernike phase contrast, an intrusion strategy is employed that reduces the refractive-index difference between pore space and silica matrix while maintaining sufficient contrast. Epoxy-based infiltration provides an effective compromise: Pressure-driven infiltration of an epoxy-carbon black mixture decreases halo intensity by 35% and improves shade-off contrast by a factor of 2.7, while still providing sufficient overall contrast for segmentation.

Together, these intrusion strategies enable more reliable segmentation and more robust pore-size statistics. They expand the applicability of nanoCT to materials composed of light elements and with low electrical conductivity, and support a more detailed understanding of structure-property relationships in complex porous systems.

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References

[1] A. Kichigin et al., JTMS 2025, 8, 100068.
[2] A. Schuss et al., 2026, under review.

Improving spatial resolution for Dark-Field X-ray microscopy

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Presentation type: Poster

Dark-field X-ray microscopy (DFXM) is a diffraction-based imaging technique used to image crystalline materials such as metals, ceramics and semiconductors [1]. An objective lens, typically a compound refractive lens (CRL), placed in the diffracted beam path, magnifies a selected diffracting volume and enables spatial mapping of strain and orientation within embedded crystalline elements. However, aberrations and imperfections of the objective and condenser lenses limit the achievable spatial resolution. In this work, we present improvements to both the objective and condenser optics of the DFXM setup at the ID03 beamline at the European Synchrotron Radiation Facility [2].

A Multilayer Laue Lens (MLL) [3] has been integrated into the ID03 beamline to enhance the spatial resolution of the objective optics. Owing to its high numerical aperture (NA), the MLL provides substantially higher spatial resolution than the commonly used compound refractive lenses. Recent measurements achieved a spatial resolution of 50 nm at a photon energy of 19 keV, compared to the 150 nm resolution obtained with the current CRL-based setup. The large angular acceptance of the high-NA objective may also reduce measurement times for highly misoriented samples.

In DFXM, the vertical resolution of layer scans is set by the beam height at the sample, analogous to the section thickness in section topography. To push this limit, new Fresnel zone plate condensers were tested [4], improving the vertical resolution by a factor of two to around 300 nm.

These developments improve the achievable spatial resolution of DFXM and extend its accessible application range toward higher-resolution and higher-magnification measurements. Combined with the existing optics, this work contributes to a multiscale DFXM approach with different resolution and magnification levels tailored to specific applications.

References

[1] Poulsen et al., J. Appl. Crystallogr. (2017)
[2] Isern et al., arXiv (2025)
[3] Gellert et al., Optics Express (2025)
[4] Lebugle et al., Appl. Opt.(2018)

X-ray strain and stress tensor tomography

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Presentation type: Poster

Currently, two major categories of non-destructive, x-ray based methods exist for measuring depth-resolved stress in poly-crystalline materials. But both involve rather complex setups and suffer from anisotropic gauge volumes with aspect ratios of 1:10 or worse. An alternative approach utilizes a pencil beam and x-ray powder diffraction for tomographic reconstruction of local strain and stress tensor components, achieving a more favorable aspect ratio of 1:1. In 2015, it was mathematically demonstrated that using diffraction data from six points on a single diffraction ring, combined with corresponding sample rotations, allows the tomographic reconstruction of the six strain tensor components. However, it was noted that this idea is experimentally challenging and left open the possibility of using fewer rotation axes.

In our presentation, we will demonstrate that employing a single rotation axis and eight segments on two diffraction rings provides sufficient constrains for the tomographic reconstruction of the six strain and stress tensor components. We have used iterative gradient descent to minimize an appropriate cost function, which includes x-ray elastic constants. We tested this innovative approach using control and shot-peened martensite samples at the ID11 beamline of the ESRF Synchrotron Radiation Facility in Grenoble, France. The results showcase the validity of this approach with achieved stress sensitivities of 20 MPa. The influence of photon shot noise and parallax at the detector will be discussed.

Stress tensor tomography utilizes a comparatively simple setup that is compatible with many existing beamlines, which demonstrates its high potential for applications in materials science.

Protein denaturation in heated egg yolk studied with in-situ X-ray holotomography

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Presentation type: Poster

Raw egg yolk is a highly nutritious liquid with many interesting properties. As a stable mixture of water, protein and lipids, it is an excellent emulsifier and widely used in food preparation. When heated, the yolk transforms from a liquid to a grainy gel due to a combination of lipid aggregation, protein denaturation, aggregation and gelation and other processes. This heat-induced solidification of egg yolk makes it a useful model system to study protein denaturation and gelation in biological systems with potential implications also for biopolymers and protein misfolding diseases.

Because water, proteins and lipids have a similar elemental composition and electron density, the contrast in conventional X-ray absorption imaging is too weak to distinguish the different phases. To study the heat-induced transformation of egg yolk, we therefore used in-situ X-ray holotomography at the P05 beamline of PETRA III (DESY, Hamburg). Holotomography is particularly suited for weakly absorbing samples. By using a newly developed in-situ heating chamber, we could follow with sub-micrometer resolution how the liquid yolk changes, how structures desolve and new structures grow as the proteins denature. Our results show the expected coagulation of denatured proteins into large networks. However, we also observed an unexpected rapid aggregation of lipid components into large, spherical globules with diameters around 40 µm.

Reference-free nano-XRF analysis of TaOx memristive devices

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Presentation type: Poster

Tantalum oxide (TaOx) thin films are widely used in resistive switching devices (memristors), where reversible changes in electrical resistance are controlled by nanoscale redistribution of oxygen and the associated modification of local tantalum valence states. These devices operate by the formation and dissolution of localized conductive pathways within the oxide, so called filaments. Although macroscopic electrical measurements show highly reproducible switching behaviour, the underlying nanoscale chemical and structural modifications remain poorly quantified. Conventional electrical and electron microscopy-based techniques primarily provide indirect or surface sensitive information and lack the ability to non-destructively resolve buried elemental distributions in a quantitative manner.

In this work, we applied reference-free nano-X-ray fluorescence analysis (nano-XRF) [1] based on a scanning X-ray microscope with X-ray fluorescence detection. Monochromatic synchrotron radiation in the soft X-ray regime is used to spatially resolve elemental distributions for germanium-based benchmark objects [2], as well as in TaOx-based memristive devices [3]. The method allows absolute quantification without reference materials or calibration samples and provides lateral analytical mapping at the nanoscale, including access to buried functional layers and localization of individual nanoobjects. Distinct, isolated regions of compositional variation were identified in the TaOx devices, indicating spatially heterogeneous oxygen redistribution and changes in tantalum stoichiometry.

The presented nano-XRF approach establishes a non-destructive, element-specific methodology to quantitatively probe nanoscale compositional gradients and buried layer chemistry in complex systems. Memristive devices, which undergo electrically induced redox processes, can be studied nondestructively and quantitatively.

References

[1] B. Beckhoff, Nanomaterials 12, 2255 (2022)
[2] A. Wählisch, R. Unterumsberger, P. Hönicke, J. Lubeck, Y. Kayser, J. Weser, G. Dai, K. Hahm, T. Weimann, C. Seim, S. Rehbein, B. Beckhoff, Small 19, 2204943 (2023).
[3] A. Wählisch, X. Zheng, A. Haidl, J. Weser, C. Stadelhoff, M. Dummin, L. J. Bauer, R. Unterumsberger, I. Valov, B. Beckhoff, Adv. Electron. Mater., accepted (2026).

Computational methods applied in materials studies

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Presentation type: Poster

Contemporary materials science relies on the discovery and optimization of novel crystalline phases using a synergistic combination of predictive computational simulations and subsequent experimental validation. Herein, we present a case study workflow showcasing both the theoretical investigation of chromium hydride [1] and experimental studies of the microstructural properties and defects in chromium thin films.

Firstly, a rigorous ab initio prediction of stable and metastable crystal structures was performed using the CALYPSO code (Crystal Structure Analysis by Particle Swarm Optimization), which only requires the chemical composition of the compound as the initial input parameter. The prediction algorithm was specifically applied to explore the complex phase space of the chromium-hydrogen system, focusing on the structural determination of the Cr2H3 stoichiometry under various energy constraints.

Following the successful identification of the structural candidates with the lowest energy, density functional theory (DFT) calculations were executed within the Quantum ESPRESSO (QE) code, utilized here in evaluating the critical electron-phonon coupling mechanisms that govern the electronic properties and potential superconducting behavior of the predicted hydrides. Through computing the phonon linewidths, Eliashberg spectral functions, and the total coupling strength, the superconducting transition temperature (Tc) could be estimated for the Cr2H3 compound using the McMillan formula.

Alongside these theoretical predictions, epitaxial chromium Cr thin films were grown via radio-frequency (RF) sputtering on KTaO3 (001) substrates. Advanced dislocation density studies were applied to investigate the film growth. These microstructural defect analyses were tailored specifically for cubic crystal systems, focusing on quantifying the density and distribution of threading dislocations. X-ray diffraction spectra were measured to extract these structural parameters using a detailed theoretical framework [2].

By describing the interplay between the CALYPSO structure predictions, Quantum ESPRESSO electron-phonon evaluations, and the X-ray diffraction studies, we provide a comprehensive overview of how computational methods can complement experimental techniques in modern materials science research.