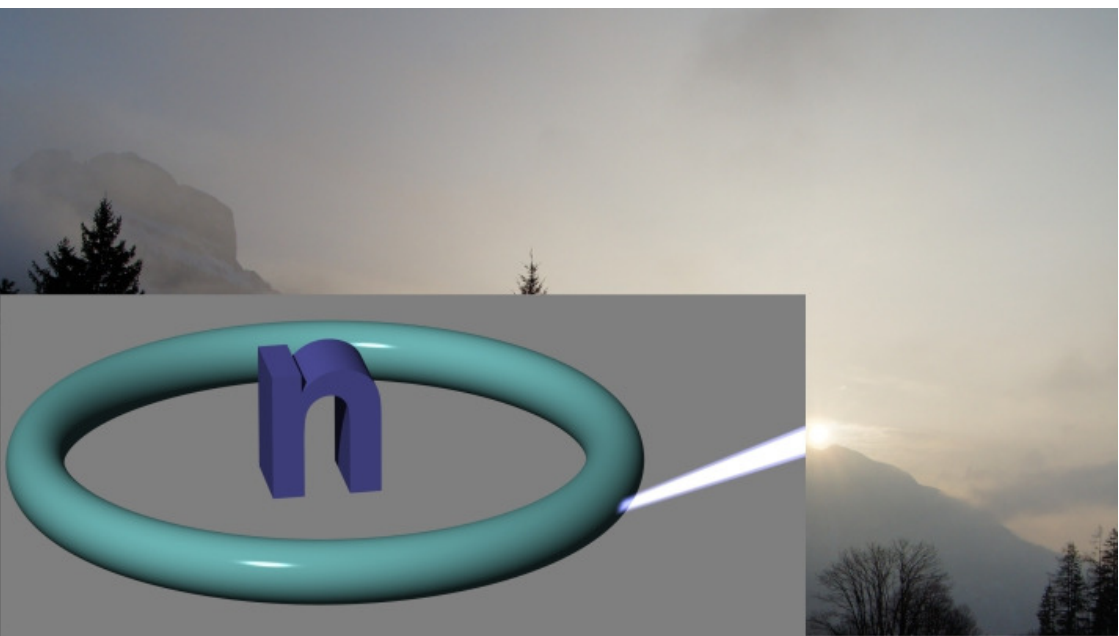


Bad Aussee (Austria), February 25th-March 1st 2024

The 12th European NESY Winterschool & Symposium on Neutron and Synchrotron Radiation

Including topical highlight lectures on Crystallographic Methods &
The 1st Austrian Crystallography Day ACD' 24



General

Preface

The **NESY Winterschool & Symposium** is the traditional forum for Austrian neutron- and synchrotron radiation (NESY) users, with the aim to present and discuss new scientific achievements and to educate young academics in this field. The event was established already in 1999 with the 1st *NESY Winterschool Planneralm* and was since then organised bi-annually until 2019. Due to the Covid pandemic the event was cancelled in 2021, but was replaced by the NESY User Symposium 2022 that took place at the Montanuniversität Leoben. Now we are very happy to be back with the **12th European NESY Winterschool & Symposium 2024 on Neutron and Synchrotron Radiation**.

While in the first couple of years this traditional event was “School only”, it developed into a mixed format of “School and Symposium”. The tutorials in the morning introduce a large variety of NESY techniques employed by Austrian users at Europe’s large scale research facilities. After a “skiing break” in the afternoon, the scientific part with *keynote lectures* and *contributed scientific talks* takes place. Finally, open-end *poster sessions* with drinks and discussions conclude the meeting days.

This year, starting from Sunday to Monday, a complementary satellite event, the **1st Austrian Crystallographer Days (ACD’24)** takes place. The ACD’ 24 fit perfect to this year’s NESY thematic focus on *Crystallographic Methods*. The smooth transition between these two events is illustrated by *two shared keynote lectures* on Monday afternoon. We are very glad to have attracted excellent keynote- and tutorial speakers from Austria, but also international speakers from large scale research centres, like the ESRF, ILL, DESY/FLASH and the FZ Jülich & HC-H2. Besides the focus on crystallographic methods, a broad range of topics from biology, physics, chemistry and materials science up to fundamental quantum-physical topics will be covered as well.

All in all, we have **42 NESY contributions** - 12 Tutorials, 3+2 invited keynote lectures, 13 contributed lectures, and 12 posters - which means that the dominant part of the roughly 65 participants contribute actively to the success of the event.

We are grateful for the financial support from the Forschungszentrum Jülich and the Helmholtz Cluster for sustainable and Infrastructure-Compatible Hydrogen Economy (HC-H2). Many thanks for the sponsoring from the companies Boehringer-Ingelheim, Anton Paar and

Bruker AXS. The sponsoring money will allow us to bestow two young scientist awards: one for the best lecture and one for the best poster. We also thank all tutorial speakers and invited speakers for agreeing to come on their own costs, and to many others who have contributed in one or another way. We are most grateful to Nadine Aichberger and Heike Noll for taking over a considerable part of the organisational issues. Special thanks go to Gerhard Popovski for the layout and assembly of this abstract booklet.

We are looking forward to an inspiring and enjoyable NESY Winterschool and Symposium 2024 in Bad Aussee.

Leoben, February 2024

Rainer T. Lechner & Oskar Paris

General Program		12 th NESY Winterschool & Symposium	
		Program	
Monday	Sunday February 25 th		
	12:00-13:45	ACD'24 Registration	
	13:45-14:00	ACD'24 Opening	
Tuesday	14:00-14:30	B. Stöger Two in one, twice the fun. Crystals composed of different structures.	
	14:30-15:00	K. Dziubek Stunning lessons from extreme condition crystallography at the European synchrotrons	
Wednesday	15:00-15:30	Coffee Break	
	15:30-16:00	M. Unterlass Unlocking novel hybrid materials through hydrothermal synthesis synchrotrons	
Thursday	16:00-16:30	D. Ingele Glancing incidence X-ray analysis for the nondestructive characterization of layered materials synchrotrons	
	16:30-17:00	G. Redhammer Neutron diffraction in applied mineralogy synchrotrons	
Friday	17:00-18:30	Come Together & ACD'24 Poster Session	
	18:30-20:00	Dinner together	
Poster			
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Monday February 26 th	
Morning Session	
9:00-9:30	W. Keller Home source versus synchrotron: do we still need our local X-ray instruments?
9:30-10:00	J. Keckes Intragranular structural properties characterized by dark-field X-ray microscopy
10:00-10:30	Individual Lunch & NESY Registration
10:30-11:00	R.T.Lechner Crystal Structure of Nanocrystals impacts Optical Output
10:00-11:30	D. Haselbach Analysing dynamic protein assemblies with cryo electron microscopy
11:30-12:00	spare time slot
12:00-13:00	Individual Lunch & NESY Registration
Afternoon Session (Chair: O. Paris)	
13:15-13:30	NESY Opening R.T.Lechner (MU Leoben)
13:30-14:30	<i>ACD & NESY keynote: T. Grüne (Univ. Wien)</i> Electron crystallography – the future for chemical structure analysis
14:30-15:30	<i>NESY & ACD keynote: T.C. Hansen (ILL, Grenoble)</i> Neutron diffraction at ILL: focus on in-situ powder diffraction
15:30-16:00	Coffee & Tea with Snacks
16:00-17:00	<i>NESY Tutorial: H. Amenitsch (TU Graz @ ELETTRA)</i> Synchrotron Radiation - Instrumentation & Techniques

Monday

Tuesday

Wednesday

Thursday

Friday

Poster

General Program		12 th NESY Winterschool & Symposium	
Monday	17:00-18:00	<i>NESY Tutorial: M. Fally (Univ. Wien)</i> Holography with light & optics with neutrons	
	18:00-19:00	Dinner together	
	Evening Session (Chair: H. Amenitsch)		
	20:00-21:00	<i>Keynote Lecture: C. Detlefs (ESRF, Grenoble)</i> X-ray diffraction – from ideal single crystals and powders to real materials	
	21:00-	Poster Session	
Tuesday	Tuesday February 27 th		
Wednesday	Morning Session (Chair: M. Fally)		
	8:40-9:40	<i>NESY Tutorial: J. Keckes (ESI @ ÖAW & MU Leoben)</i> X-ray and Neutron Diffraction on Polycrystalline Materials	
	9:40-10:40	<i>NESY Tutorial: V. Holý (Charles Univ., Prague)</i> X-ray scattering from epitaxial layers and multilayers	
	10:40-11:00	Break: Coffee & Tea	
	11:00-12:00	<i>NESY Tutorial: T. Pavkov-Keller (KFU Graz)</i> Diffraction on Protein Crystals	
Thursday	12:00-16:30	Lunch Break	
	16:30-17:00	Coffee & Tea with Snacks	
	Afternoon Session (Chair: J. Keckes)		
Friday	17:00-17:20	<i>Contributed Talk: M. Meindlhumer (MU Leoben)</i> In situ X-ray Nanodiffraction Analysis of Multiaxial Stress-Strain Transfer across an Indenter-Sample Interface during in situ Indentation	
	17:20-17:40	<i>Contributed Talk: L.A. Lumper (MU Leoben)</i> High-Temperature Synchrotron Radiation Characterization of Novel Phases in Bronze: Unraveling Structural Mysteries	
Poster			
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17:40-18:00	<i>Contributed Talk: T. Ziegelwanger (MU Leoben)</i> High Strain-Rate Thermomechanical fatigue of thin Cu films revealed by synchrotron X-ray diffraction
18:00-18:10	Break
18:10-18:30	<i>Contributed Talk: K. Kutleša (MU Leoben)</i> Microstructure and residual stress gradients in Al-CrSiN thin films revealed by X-ray nanodiffraction: Precipitation-induced crack arrest at sublayer interfaces
18:30-18:50	<i>Contributed Talk: B. Seligmann (MU Leoben)</i> High-temperature deformation of a multi-phase γ -TiAl based alloy - Insights from in-situ tensile experiments using synchrotron radiation
19:00-20:00	Dinner together
Evening Session	
20:00-	Poster Session

Monday

Tuesday

Wednesday

Wednesday February 28th

Morning Session (Chair: K. Hradil)

8:40-9:40	<i>NESY Tutorial: S. Kowarik (TU Graz)</i> Surfaces and Interfaces Unveiled: A Primer on GIXD and GISAXS
9:40-10:40	<i>NESY Tutorial: G. Pabst (KFU Graz)</i> Small-Angle X-ray and Neutron Scattering (SAXS/SANS): A Primer with Applications in Life Sciences
10:40-11:00	Break: Coffee & Tea
11:00-12:00	<i>NESY Tutorial: C. Rameshan (MU Leoben)</i> Synchrotron based in-situ NAP-XPS
12:00-16:30	Lunch Break
16:30-17:00	Coffee & Tea with Snacks

Thursday

Friday

Poster

Afternoon Session (Chair: G. Pabst)	
17:00-17:20	<i>Contributed Talk: K. Peter (BOKU Wien)</i> Exploring Spider Silk: X-ray Nanobeam Investigation for Medical Advancements
17:20-17:40	<i>Contributed Talk: P.A. Wieser (TU Graz)</i> Monitoring Micelle-assisted Electrosynthesis of Mesoporous PtNi by in operando GISWAXS
17:40-17:50	Break
17:50-18:10	<i>Contributed Talk: M. Fratschko (TU Graz)</i> Crystallographic Properties of MOF Thin Films Investigated by Rotated Grazing Incidence X-Ray Diffraction
18:10-18:30	<i>Contributed Talk: M. Seyffertitz (MU Leoben)</i> In-situ SAXS investigation of a supercapacitor using conductive metal-organic framework electrodes with ordered cylindrical microporosity and aqueous electrolytes
19:00-20:00	Dinner together
Evening Session (Chair: C. Rameshan)	
20:00-21:00	<i>Keynote Lecture: R. Treusch (FLASH, DESY Hamburg)</i> X-ray Free-Electron Lasers: What it takes for perfect snapshots and movies in the nanocosmos

Thursday February 29 th	
Morning Session (Chair: R. Resel)	
8:40-9:40	<i>NESY Tutorial: C. Prehal (PLU Salzburg)</i> Neutron and Synchrotron Operando Techniques for Energy Materials and Catalysis
9:40-10:10	<i>Research Infrastructures:</i> Reports on Larges Scale Research Activities in Austria

10:10-10:40	<i>Research Infrastructures:</i> R.T. Lechner & H. Abele ESUO & ENSA ... the European User Organisations & their work
10:40-11:00	Break: Coffee & Tea
11:00-12:00	Meeting of the ÖPG-Division NESY
12:00-16:30	Lunch Break
16:30-17:00	Coffee & Tea with Snacks
Afternoon Session (Chair: C. Prehal)	
17:00-17:20	<i>Contributed Talk:</i> E. Skrentny (FZ Jülich) X-ray Absorption Microscopy to Measure Concentration Profiles in Battery Electrolytes
17:20-17:40	<i>Contributed Talk:</i> S. Stock (MU Leoben) Exploring Hydrogen Physisorption in Nanopore Confinement: Insights from In-situ Small-Angle Neutron Scattering
17:40-17:50	Break
17:50-18:10	<i>Contributed Talk:</i> T. Pogrietz (MU Leoben) HE-XRD measurements of H crystal structure interaction in synchrotron
18:10-18:30	<i>Contributed Talk:</i> T. Berger (MU Leoben) Perovskite-type Oxides in Methanol Steam Reforming: Overcoming the Challenges of Conventional Catalytic Systems
19:00-20:00	Dinner together
Evening Session (Chair: S. Kowarik)	
20:00-21:00	<i>Keynote Lecture:</i> H-G. Steinrück (FZ Jülich) Using (coherent) operando X-Ray methods to quantitatively understand electrochemical systems
21:00-	Poster Session

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Poster

General Program		12 th NESY Winterschool & Symposium	
Monday	Friday March 1 st		
	Morning Session (Chair: K. Hradil)		
	8:40-9:40	NESY Tutorial: P. Kregsamer (TU Wien) X-ray Fluorescence Analysis (XRF) - a Tutorial	
	9:40-10:40	NESY Tutorial: H. Michor (TU Wien) Tutorial on inelastic and quasi-elastic neutron scattering	
	10:40-11:00	Break: Coffee & Tea	
Tuesday	11:00-12:00	NESY Tutorial: S. Sponar Quantum Mechanics with Neutron Interferometry	
	12:00-12:30	Prizes & Closing R.T. Lechner (MU Leoben)	
Wednesday			
Thursday			
Friday			
Poster			
10		Bad Aussee, February 25 th -March 1 st 2024	

Monday**Afternoon**

NESY & ACD keynote, 14:30-15:30

**NEUTRON DIFFRACTION AT ILL: FOCUS ON IN-SITU
POWDER DIFFRACTION**Thomas C. Hansen

Institut Laue-Langevin

The neutron facility Institut Laue-Langevin (ILL) provides unique diffractometers to answer crystallographic questions. Certain of those received important upgrades in the frame of the Endurance program. In situ neutron powder diffraction can inspect processes in condensed matter. Only a few high-intensity powder diffractometers at intense neutron sources allow for this. D20 at ILL provides the highest available intensity in constant wavelength neutron powder diffraction. A stationary, curved, linear position sensitive detector allows for in-situ diffraction studies down to a second and encourages the use of complex sample environments with inherently small sample sizes. D20 adapts to various levels of crystallographic complexity and rapidity of an observed phenomenon.

As one example among others, neutron diffraction determines the Li diffusion pathway in solid-state Li-ion conductors. Development of better electrode materials in terms of gravimetric and volumetric energy density, temperature operation range and cycling stability needs understanding of lithium intercalation phenomena. Operando diffraction techniques are well suited here. Electrochemical cells based on a neutron-transparent Ti-Zr-alloy allow to collect neutron diffraction patterns with reasonable statistics and no other Bragg peaks than those of the electrode material, permitting detailed structural determination of electrode materials by Rietveld refinement during operation.

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Poster

NESY Tutorial, 16:00-17:00

SYNCHROTRON RADIATION - INSTRUMENTATION & TECHNIQUES

Heinz Amenitsch

Institute of Inorganic Chemistry, Graz University of Technology,
Stremayergasse 9/V, Graz, Austria & Austrian SAXS beamline @
ELETTRA

This presentation should give an overview from the fundamental aspects of X-ray interaction and their application till the practical issues for the design of an X-ray experiment. The following topics will be covered:

- Short introduction to X-ray interaction with matter
- What can you learn from X-rays?
- How are X-rays produced?
- How does a synchrotron work?
- Beamline components and outline
- FEL's and other new sources
- How to design my own beamline?

NESY Tutorial, 17:00-18:00

HOLOGRAPHY WITH LIGHT & OPTICS WITH NEUTRONS

Martin Fally

University of Vienna

Light optical holography can be used to record artificial structures - for example volume holographic gratings - in suitable materials. These gratings then might serve as diffractive optical elements for cold and very cold neutrons.

In this tutorial three topics are addressed:

- a. the basic concepts of light optical holography and photo-neutron-refractive materials are presented
- b. neutron optics employing such artificial gratings is discussed
- c. an alternative model to the dynamical theory of diffraction is introduced (rigorous coupled wave analysis).

The latter predicts and describes multiwave coupling which occurs when neutrons are coherently diffracted from artificial structures.

Finally, we will show applications for those neutron-diffractive optical elements, e.g., as components of a neutron interferometer.

Evening

Keynote Lecture, 20:00-21:00

X-RAY DIFFRACTION – FROM IDEAL SINGLE CRYSTALS AND POWDERS TO REAL MATERIALS

Carsten Detlefs

ESRF

Many textbooks describe x-ray diffraction rather briefly, discussing only idealized systems such as defect-free single crystals and perfect powders. Industrially relevant materials rarely fall into these categories. Instead, they are full of “defects” that govern their macroscopic properties. Such materials are typically structured over many length scales, from the size of an electronic or structural component that can be several millimetres or more, to defects of the crystal lattice on the atomic scale. Moreover, in order to understand failure modes or to improve manufacturing, it is important to understand the dynamic transformation of the material’s microstructure in-situ or in-operando.

In this presentation, I will present a few selected examples of how the ESRF can be used to study the multi-scale structure of such real materials – with particular emphasis on high-energy x-ray diffraction.

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Evening

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Poster

Tuesday

Morning

NESY Tutorial, 8:40-9:40

X-RAY AND NEUTRON DIFFRACTION ON
POLYCRYSTALLINE MATERIALSJozef Keckes

Montanuniversität Leoben

Structural research stands as an indispensable pillar of scientific progress, offering unparalleled insights into material structures across diverse fields. This contribution aims to underscore the distinctive possibilities and robustness of the two-dimensional diffraction approach. In this contribution, basics of two-dimensional diffraction will be discussed in the first part in order to emphasize unique possibilities and the strength of the approach. Subsequently, the second part presents didactic examples drawn from experiments conducted at prominent European synchrotron and neutron facilities. Specifically, this presentation will showcase results predominantly from ID06 and ID13 at ESRF, P03, P05, and P07 at Petra III, and STRESS-SPEC at FRM II. These outcomes serve as demonstrations of the potential to characterize the structure-property relationship in engineering components within the microelectronic and metal industries. The primary focus will be on elucidating the details of residual stresses and microstructure, leveraging the insights gained from these advanced research facilities.

NESY Tutorial, 9:40-10:40

X-RAY SCATTERING FROM EPITAXIAL LAYERS AND
MULTILAYERSVáclav Holý

Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Praha, Czech Republic

High-resolution x-ray scattering (small-angle scattering, reflection and diffraction) is routinely used for structure investigation of thin epitaxial layers and multilayers. Experimental data are usually represented as a map of the scattered intensity in reciprocal space (reciprocal-space map, RSM). From the position of the diffraction peaks in a RSM it

is possible to determine exactly the lattice parameters of the layer(s) relatively to the substrate, the shape of the diffraction maxima is affected by structure defects (quasi-point defects like small precipitates, stacking faults or dislocation loops, line defects – misfit and threading dislocations). The reciprocal-space distribution of small-angle scattering close to the origin of reciprocal space is influenced by small volume defects (voids, cracks or precipitates with different electron density), while the x-ray reflection data depend mainly on the morphology of free surface and buried interfaces (roughness, surface islands, etc.). The tutorial lecture will present the basics of theoretical description of x-ray scattering (kinematical and semikinematical approximations), including the elements of theory of diffuse scattering from defects. The lecture will be completed by a number of experimental results comprising various types of classical semiconductor heterostructures, oxide epitaxial layers and layers of topological insulators.

NESY Tutorial, 11:00-12:00

DIFFRACTION ON PROTEIN CRYSTALS

Tea Pavkov-Keller

Institute of Molecular Biosciences, University of Graz, Austria

Understanding protein structures has profound implications in various fields, including drug design, enzyme engineering, and the understanding of disease mechanisms. Protein X-ray crystallography plays an important role in unraveling the structures and functionalities of biomolecules, offering insights into the molecular mechanics of life. Central to this technique is the phenomenon where protein crystals diffract X-rays, a critical process that unveils the protein's atomic three-dimensional structure.

The fundamental principles of X-ray crystallography, including protein crystallization, the diffraction of X-rays by protein crystals, data processing, structure determination, refinement and analysis will be presented. Furthermore, the recent advancements in diffraction techniques, such as electron diffraction and free-electron laser X-ray crystallography will be discussed. These cutting-edge technologies have revolutionized our ability to visualize proteins at near-atomic resolutions, opening new frontiers in structural biology.

References:

1. A. Liljas, L. Liljas, M.R. Ash, G. Lindblom, P. Nissenm M.

Kjeldgaard, Textbook of Structural Biology, Series in Structural Biology, 2 Rev ed., 2016, Pp: 612.

2. B. Rupp, Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, New York: Garland Science, Taylor and Francis Group, 2010.

Afternoon

Contributed Talk, 17:00-17:20

IN SITU X-RAY NANODIFFRACTION ANALYSIS OF MULTIAXIAL STRESS-STRAIN TRANSFER ACROSS AN INDENTER-SAMPLE INTERFACE DURING IN SITU INDENTATION

Michael Meindlhumer (1), Manfred Burghammer (2), Aicha Asma
Medjahed (2), Doris Steinmüller-Nethl (3), Juraj Todt (1), Jozef
Keckes (1)

(1) Department of Materials Science, Montanuniversität Leoben, (2)
ESRF - The European Synchrotron, (3) Carbon Competence GmbH

Nanoindentation is routinely used to determine local mechanical properties of materials such as hardness and Young's modulus. Especially for the testing of thin films, nanoindentation is used on materials approaching hardness close to diamond, the indenter tip's material. Yet, the correlation between the deformation of the indenter and the stress-strain evolution within sample remains still unknown.

Contrary, in-situ cross-sectional X-ray nanodiffraction (CSnanoXRD) coupled with indentation has given new insights into the elasto-plastic deformation of thin films during indentation. To test the mechanical response of the indenter tip, a diamond wedge indenter tip with a radius of 2µm was coated with a 3.8µm thick diamond thin film using hot-filament chemical vapour deposition. Focused ion beam milling at the edges of the wedge ensured uniform signal during the CSnanoXRD experiment. In following, the in-situ indentation setup was used to determine experimentally the multi-axial stress distributions across both the diamond-coated indenter and the tested nanocrystalline diamond with a resolution of 80nm. The multi-axial stress results yielded a maximum stress of -13GPa evaluated in direction of contact. Detailed stress analysis revealed accumulation of residual stress gradients both in the diamond indenter tip and sample up to depths of 1µm after the experiment. The results give unprecedented insights into the deformation of both indenter and tested material.

Contributed Talk, 17:20-17:40

HIGH-TEMPERATURE SYNCHROTRON RADIATION CHARACTERIZATION OF NOVEL PHASES IN BRONZE: UNRAVELING STRUCTURAL MYSTERIES

Lea A. Lumper, Verena Maier-Kiener

Montanuniversität Leoben

Monday

Bronze, widely used in electronic components, and musical instruments, presents a fascinating avenue for exploring phase transitions in multi-phase materials. This study, conducted on Cu 20 m.% Sn (bell metal), employs high-temperature high energy X-ray diffraction to investigate four intermetallic phases and their transformations up to 535°C. Notably, our analysis unveils two previously undiscovered metastable phases, termed HEX_β and HEX_γ , characterized by a hexagonal-related structure.

Tuesday
Afternoon

Electrical resistance measurements further hint at an ordered structure in the novel $\text{HEX}_\beta/\text{HEX}_\gamma$ phases, evident from their enhanced conductivity compared to conventional phases. Additionally, high-temperature nanoindentation is employed to meticulously analyze the mechanical properties of these newfound phases, and transmission electron microscopy is applied to gain insight into crystallographic structure. Strikingly, HEX_β and HEX_γ exhibit hexagonal-related structures under ordered conditions, with mechanical deformation behavior akin to the well-known δ phase in bronze.

Wednesday

In conclusion, this study leverages high-temperature synchrotron radiation to unveil the structural nuances of bronze, spotlighting the enigmatic HEX_β and HEX_γ phases. The quest for understanding their crystallographic and mechanical characteristics beckons, marking a crucial step toward unraveling the unknown intricacies of these fascinating bronze phases.

Thursday

Friday

Poster

Contributed Talk, 17:40-18:00

HIGH STRAIN-RATE THERMOMECHANICAL FATIGUE OF THIN CU FILMS REVEALED BY SYNCHROTRON X-RAY DIFFRACTION

Tobias Ziegelwanger, Michael Reisinger (2), Kostya Hlushko(1), Steven van Petegem(3), Michael Meindlhumer(1), Juraj Todt(1), Jozef Keckes(1)

(1) Department of Materials Physics, Montanuniversitaet Leoben, 8700 Leoben, Austria. (2) KAI Kompetenzzentrum Automobil- u. Industrieelektronik GmbH, 9524 Villach, Austria (3) Photons for Engineering and Manufacturing, Paul Scherrer Institute, 5232 Villigen, Switzerland

Smart Power Devices in automotive applications may face short circuit events with strong current pulses, heating the device to 300°C and above. As these pulses are as fast as 200 μ s, characterization methods are limited, and a fundamental understanding of the thermal fatigue at such high strain-rates is still lacking. In this contribution, in-situ synchrotron X-ray diffraction has been performed on dedicated test chips, which can replicate short-circuit events with heating rates of up to 10⁶ K/s. At the MS-Powder beamline located at Paul Scherrer Institute, a custom detector with an acquisition rate of 20 kHz allowed access to the timescales in question. Results showed compressive stresses of -391 MPa at a peak temperature of 525°C, while similar measurements using wafer curvature and a heating rate of 0.1 K/s resulted only in -50 MPa. Furthermore, cycling the sample for 5000 times resulted in a lowered maximum stress of -153 MPa at similar peak temperatures. This weakening can be associated with the formation of microscopic voids and cracks in the Cu metallization. In summary, the results provide novel information on the thermomechanical fatigue of thin Cu films and are an excellent example of modern synchrotron research.

Contributed Talk, 18:10-18:30

MICROSTRUCTURE AND RESIDUAL STRESS GRADIENTS IN ALCrSiN THIN FILMS REVEALED BY X-RAY NANODIFFRACTION: PRECIPITATION-INDUCED CRACK ARREST AT SUBLAYER INTERFACES

Kevin Kutleša (1), Michael Meindlhumer (1), Alice Lassnig (2),
Rostislav Daniel (1), Michael Tkadletz (1), Asma Medjahed (3), Jozef
Keckes (1)

(1) Montanuniversität Leoben, (2) Erich Schmid Institute of Materials
Science, (3) ESRF - The European Synchrotron Radiation Facility

The functional properties of wear-resistant transition metal nitride (TMN) thin films are predetermined by their cross-sectional microstructure and residual stress gradients. Currently, assessing the interplay between annealing treatments and microstructural changes as well as functional properties in these films represents a nontrivial challenge. In this contribution, microstructural design based on correlative nanoscale characterization methods was performed in order to enhance the fracture behaviour of AlCrSiN thin films.

Structural properties and residual stress gradients of the films were characterized by cross-sectional synchrotron X-ray nanodiffraction (CSnanoXRD) at the ID13 beamline of the ESRF in Grenoble. Using multilayer Laue lenses (MLL) the beam size on the sample was $\sim 75 \times 75 \text{ nm}^2$. Cross-sectional scans of $\sim 50 \text{ }\mu\text{m}$ thick lamellae were scanned with a step size of 50 nm, the two-dimensional data collected with an EigerX 4M detector was evaluated with the pyFAI software package. Additional complementary insights into the microstructure were obtained using SEM, TEM and APT. Mechanical properties of the thin films were assessed through in situ bending tests on freestanding microcantilevers prepared by focussed ion beam milling. The experiments revealed a complex microstructure-property correlation that was utilized to design a novel type of microstructure with a crack-arrest mechanism.

Monday

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Poster

Contributed Talk, 18:30-18:50

HIGH-TEMPERATURE DEFORMATION OF A MULTI-PHASE γ -TiAl BASED ALLOY - INSIGHTS FROM IN-SITU TENSILE EXPERIMENTS USING SYNCHROTRON RADIATION

Benjamin Seligmann (1), Michael Musi (1), Petra Spoerk-Erdely (2),
Thomas Antretter (3), Bernd Schwebke (4), Emad Maawad (4),
Helmut Clemens (1)

(1)Department of Materials Science, Montanuniversität Leoben, (2)
Institute of Materials Science, Joining and Forming, Graz University
of Technology, (3) Chair of Mechanics, Montanuniversität Leoben, (4)
Helmholtz-Zentrum Hereon, Institute of Materials Physics, Geesthacht

Titanium aluminide alloys serve as alternatives to nickel-based materials in aerospace applications such as turbojet engines due to their weight-saving potential reducing fuel consumption and CO₂ emissions. As their service temperature reaches up to 750°C, it is crucial to investigate the temperature dependence of their mechanical properties.

This study focuses on the so-called TNM alloy (Ti-43.5Al-4Nb-1Mo-0.1B, in at.%), which comprises the majority γ phase (L1₀ structure) as well as the ordered α_2 (D0₁₉ structure) and β_o (B2 structure) phases. The investigated microstructure consists mainly of lamellar α_2/γ colonies and globular γ , while the β_o phase is situated at grain boundaries.

In-situ high-energy X-ray diffraction tensile experiments were conducted at the beamline P07B at PETRA III, Deutsches Elektronen-Synchrotron, Hamburg, Germany, using synchrotron radiation with a mean photon energy of 87.1 keV. A tensile setup was extended by an inductive heating setup. Experiments were performed under ambient atmosphere ranging from room temperature to 800°C.

This experimental setup enabled the detection of the elastic-plastic transition of individual phases at different load stages. For the first time, these experiments could be conducted on a γ -TiAl based alloy at elevated temperatures in order to study the tensile deformation behavior and load partitioning between the individual phases as a function of temperature.

Wednesday

Morning

NESY Tutorial, 8:40-9:40

SURFACES AND INTERFACES UNVEILED: A PRIMER ON GIXD AND GISAXS

Stefan Kowarik

Institute of Chemistry, NAWI Graz, University of Graz, 8010 Graz, Austria.

This tutorial offers an introduction to Grazing Incidence X-ray Diffraction (GIXD) and Grazing Incidence Small Angle X-ray Scattering (GISAXS) as important techniques for the characterization of thin films and interfaces at the molecular and atomistic level. An overview of the fundamentals of X-ray diffraction for materials with reduced dimensionality for GIXD but also the interplay between structure factor and form factor is given. We will detail the experimental configurations, including X-ray sources, goniometers, and detectors highlight the challenges faced during experiments.

Applications ranging from highly ordered inorganic single crystals to weakly ordered polymer thin films will be discussed, illustrating the broad utility of these techniques. In further case studies we will demonstrate the ability of GIXD and GISAXS to monitor in operando processes, providing real-time insights into the dynamic behaviors of materials under working conditions or during crystal growth.

NESY Tutorial, 9:40-10:40

SMALL-ANGLE X-RAY AND NEUTRON SCATTERING (SAXS/SANS): A PRIMER WITH APPLICATIONS IN LIFE SCIENCES

Georg Pabst

Biophysics, Institute of Molecular Biosciences, NAWI Graz, University of Graz, 8010 Graz, Austria.

Small-angle scattering is a well-established and remarkably versatile non-invasive technique within the realms of physics, chemistry, and life sciences for probing nanostructured materials. This tutorial lecture delves into the intricacies of SAXS and SANS, where the specific interactions of X-rays and neutrons with matter allow for the selective

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enhancement or nullification of contrast, enabling unparalleled insights into the structural details even in the absence of crystalline order.

The focal point of this tutorial lies in the joint analysis of SAXS and SANS data, utilizing compositional modeling and advanced optimization techniques to unleash the full potential of these approaches. Throughout the tutorial, attention will be drawn to the practical application of SAXS/SANS, using selected examples of lipid nanoparticles that mimic biological membranes. The discussion will not only showcase the advantages of the techniques but will also illuminate potential disadvantages and pitfalls that researchers should be mindful of and avoid. By incorporating both experimental and analytical workflows, attendees will gain a comprehensive understanding of the capabilities and limitations of SAXS/SANS, empowering them to navigate the nuances of this powerful tool in their own research endeavors.

NESY Tutorial, 11:00-12:00

SYNCHROTRON BASED IN-SITU NAP-XPS

Christoph Rameshan

Montanuniversität Leoben, Chair of Physical Chemistry

In-situ X-ray photoelectron spectroscopy (XPS) has emerged as a powerful technique for probing the surface chemistry and electronic structure of materials under realistic operating conditions. This advanced analytical method enables the study of dynamic processes occurring at the atomic and molecular levels, offering unparalleled insights into the behaviour of materials in their native environments.

By employing in-situ XPS, researchers can investigate catalysts, electrodes, and other functional materials directly within their operational settings, providing a comprehensive understanding of surface reactions, catalytic transformations, and electrochemical processes. The real-time monitoring capabilities allow for the observation of transient species and reaction intermediates, elucidating reaction pathways and mechanisms that would be elusive using conventional ex-situ methods.

With the synchrotron's key advantage to produce intense, tuneable, and collimated X-rays, in-situ XPS can probe at conditions close to real applications. Furthermore, it facilitates high-resolution spectroscopy, enabling advanced scientific research in materials science, catalysis and electrochemistry, fostering breakthroughs in understanding and manipulating matter at the atomic and molecular levels.

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Contributed Talk, 17:00-17:20

EXPLORING SPIDER SILK: X-RAY NANOBEAM INVESTIGATION FOR MEDICAL ADVANCEMENTS

Karolina Peter (1), Aida Naghilou (2), S. Stadlmayr (2), L. Ploszczanski (1), J. Liu (3), M. Sztucki (3), M. Burghammer (3), C. Riekel (3), S. Kalbfleisch (4), G. Sinn (1), C. Radtke (2), H.C. Lichtenegger (1))

(1) Universität für Bodenkultur Wien, (2) Medizinische Universität Wien, (3) ESRF, (4) MAX IV

Spider silk, developed over 400 million years, holds promise for nerve conduits and regeneration due to its support for Schwann cells (SCs). Our research unveils how subtle silk variations impact SC movement autoclaving impedes while ethanol treatment enhances their motility along *Trichonephila edulis* spider's major-ampullate (MA) silk. Nanobeam X-ray diffraction at ESRF revealed stiffness changes in autoclaved fibers and ultrastructural shifts in ethanol-treated and autoclaved ones. Understanding SCs' mechanosensitivity drove our focus on strain-induced ultrastructural alterations. X-ray experiments at MAX IV, Nanomax, examined Tubuliform (TU) and MA silk from *Trichonephila inaurata* spider's egg protective layer, highlighting differences in nanocrystal arrangements and mechanical properties. In-situ tensile humidity cell tests at ESRF exhibited humidity and stretching rate influence on silk structure. Preliminary data suggest significant variations, warranting further discussion. Our work sheds light on silk's dynamic behavior under strain and humidity, contributing crucial insights into potential biomedical applications.

Contributed Talk, 17:20-17:40

MONITORING MICELLE-ASSISTED ELECTROSYNTHESIS OF MESOPOROUS PTNi BY IN OPERANDO GISWAXS

Philipp Aldo Wieser (1), Heinz Amenitsch (1), Simone Dal Zilio (2)
(1) Graz University of Technology, (2) Consiglio Nazionale delle Ricerche

Micelle-assisted electrosynthesis of mesoporous alloys has attracted a lot of interest recently, as these mesoporous films show promising properties for Fuel Cells, sensors, etc. However, previous studies have shown

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differences in the performance of these films depending on a variety of synthetic parameters, e.g., deposition rates and loading, suggesting changes in the morphology of the deposited films that hinder their successful application.

To understand and mitigate these morphological changes, we have characterized mesoporous PtNi films during electrochemical deposition by in operando Grazing Incidence Small and Wide Angle X-ray Scattering. The electrochemical deposition of PtNi was performed at potentials ranging from -0.6 to -1.0 V vs AgCl, from an aqueous electrolyte containing a triblock copolymer surfactant, Pluronic P-123, as micellar templating agent.

Our custom developed miniaturized electrochemical cell with Kapton entrance windows and an X-ray beam path of 3 mm through the electrolyte in combination with the brilliant Synchrotron Source at the SAXS beamline at Elettra allowed us to monitor the growth of the mesoporous films with a temporal resolution of 1 s. The combination of the structural data from GISAXS, the chemical information from GIWAXS analysis and the chronoamperometry give novel insights into the kinetics of the micelle-assisted electrosynthesis process.

Contributed Talk, 17:50-18:10

CRYSTALLOGRAPHIC PROPERTIES OF MOF THIN FILMS INVESTIGATED BY ROTATED GRAZING INCIDENCE X-RAY DIFFRACTION

Mario Fratschko (1), Narges Taghizade (1), Mercedes Linares-Moreau (1), Jan Fischer (2), Ian Howard (2), Paolo Falcaro (1), Egbert Zojer (1), Roland Resel (1)

(1) Graz University of Technology, (2) Karlsruhe Institute of Technology

Thin films of the pillared metal-organic framework Cu₂(bdc)₂(dabco) are investigated in terms of their crystal structure and the orientation of the internal framework (i.e. the pore structure) relative to the substrate surface. Two thin films were prepared via layer-by-layer and ceramic-to-MOF conversion methods on distinct substrates. These films were analyzed using grazing incidence X-ray diffraction (GIXD), employing a rotated GIXD technique capturing diffraction patterns at various rotation angles with a 2D-detector, enabling comprehensive reciprocal space investigation[1]. The unknown thin film crystal structure of Cu₂(bdc)₂(dabco) was determined via density functional theory modelling and confirmed using rotated-GIXD. Besides phase identification,

various strategies can be used to analyze rotated-GIXD data, e.g., pole figures can be calculated[2]. Two different types of preferred crystal orientation of the Cu₂(bdc)₂(dabco) are found, one type shows epitaxial alignment (axial texture) relative to the crystal surface and the other a defined out- of-plane orientation (uniplanar texture) of the crystals. These alignments imply different pore structures of the MOF relative to the substrate surface. This work shows that rotated GIXD experiments combined with theoretical modelling allows the solving crystal structures from thin films, additionally it is an excellent tool to study the orientational distribution of MOF crystals within thin films.

Contributed Talk, 18:10-18:30

IN-SITU SAXS INVESTIGATION OF A SUPERCAPACITOR
USING CONDUCTIVE METAL-ORGANIC FRAMEWORK
ELECTRODES WITH ORDERED CYLINDRICAL
MICROPOROSITY AND AQUEOUS ELECTROLYTES

Malina Seyffertitz (1), Chloe Balhatchet (2), Sebastian Stock (1), Max Rauscher (1), Alex Forse (2), Heinz Amenitsch (3), Oskar Paris (1)
(1) Montanuniversitaet Leoben, Austria, (2) University of Cambridge, United Kingdom, (3) Graz University of Technology, Austria

Electric double layer capacitors (EDLCs), also known as supercapacitors, emerged as a vital research field addressing the growing demand for efficient electrical energy storage. Owing to their high power density, EDLC devices could be of particular importance for applications in electric vehicles, smart power grids and intermittent energy sources in light of managing the transition from fossil fuels to renewable energy. This poster showcases the applicability of X-ray transmission (XRT), (anomalous) Small Angle X-ray Scattering ((A)SAXS) and Small-Angle Neutron Scattering (SANS) for investigating fundamental processes taking place in the porous activated carbon working electrode of an electric double-layer capacitor with 1 M RbBr aqueous electrolyte at different applied potentials. XRT and incoherent neutron scattering are employed to determine global ion- and water- concentration changes and associated charge-balancing mechanisms. We demonstrate the suitability of SAXS and SANS, respectively, to get complementary information on local ion and solvent rearrangement in nanoconfinement, but also underscore the limitations of simple qualitative models, asking for more quantitative descriptions of water–water and ion–water interactions via detailed atomistic modelling approaches.

Evening

Keynote Lecture, 20:00-21:00

X-RAY FREE-ELECTRON LASERS: WHAT IT TAKES FOR
PERFECT SNAPSHOTS AND MOVIES IN THE NANOCOSMOSRolf Treusch

DESY/FLASH Hamburg

In this lecture, I will familiarize you with the basic ingredients and the working principles of a high repetition rate X-ray Free-Electron Laser (FEL) such as FLASH and the European XFEL at and near the Deutsches Elektronen-Synchrotron DESY in Hamburg. Accelerator-based Free-Electron Lasers combine the best of two worlds: on one hand the easy tunability down to X-rays like for other synchrotron radiation sources and on the other hand the high degree of coherence as well as ultrashort femtosecond pulses like a laser – and all this along with extreme intensities, even in the X-ray range. Hence FELs are the perfect radiation sources to shine light on nanoworld dynamics and, e.g., follow ultrafast chemical reactions, see how materials demagnetize in less than a trillionth of a second, or take snapshots of the geometrical shape and structure of nano-objects in a single flash. This talk presents some basic research examples from FLASH to illustrate the scientific potential of extreme ultraviolet (XUV) and X-ray FELs.

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NESY Tutorial, 8:40-9:40

NEUTRON AND SYNCHROTRON OPERANDO TECHNIQUES FOR ENERGY MATERIALS AND CATALYSIS

Christian Prehal

Paris Lodron University Salzburg, Department of Chemistry and
Physics of Materials, Jakob-Haringer-Straße 2a, 5020 Salzburg

Operando Neutron and Synchrotron techniques have emerged as pivotal in deciphering complex chemical and physical processes in energy storage, catalysis, and beyond. Attendees of this tutorial lecture will gain insights into the working principles, advantages, and limitations of operando absorption spectroscopy, operando microscopy, operando tomography, and operando diffraction.

Focusing on post-lithium-ion batteries, we explore operando small and wide-angle X-ray scattering (SAXS/WAXS) alongside small-angle neutron scattering (SANS) to unveil nanoscale electrochemical phase transitions during battery cycling. Specifically, I will demonstrate how operando SAXS and SANS combined with machine-learning-assisted stochastic modeling allow quantification of the nanoscale phase evolution during the discharge and charge of Lithium-Sulfur batteries [1] and Lithium-air batteries [2]. Both examples demonstrate that often, only the simultaneously recorded device data during an operando measurement allows the development of robust models for time-resolved scattering or spectroscopy data.

References:

- [1] C. Prehal, V. Wood, et al. Nature Communications 13, 6326 (2022)
- [2] C. Prehal, S.A. Freunberger et al. PNAS 118, 14, e2021893118 (2021)

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Research Infrastructure, 10:10-10:40

ESUO & ENSA ... THE EUROPEAN USER ORGANISATIONS & THEIR WORK

Rainer T. Lechner, Hartmut Abele

(1) Chair of Physics, Montanuniversitaet Leoben, Austria, (2) ATI, TU Wien

Here only a short overview will be given of the Synchrotron and Neutron User organisations in Europe (ESUO & ENSA) that are trying to unify the users voice. Especially, we act as partners for the European facilities' organisations for photons (LEAPS) and Neutrons (LENS). The combined work of users and facilities on European level succeeded in the new project NEPHEWS that enables again trans national access (TNA) for experiments at photon and neutron sources. The possibilities within NEPHEWS will be outlined. Additionally a short outlook is given on a new proposal that will be submitted by LEAPS where ESUO will be a direct partner.

Afternoon

Contributed Talk, 17:00-17:20

X-RAY ABSORPTION MICROSCOPY TO MEASURE CONCENTRATION PROFILES IN BATTERY ELECTROLYTES

Emil Skrentny (1)(2), Marten Huck (1)(2), Andreas Kuhlmann (1)(2), Hans-Georg Steinrück (1)(2)

(1) Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy (INW), Am Brainery Park 4, 52428 Jülich, Germany, (2) RWTH Aachen University, Institute of Physical Chemistry, Landoltweg 2, 52074 Aachen, Germany

Toward lifetime and performance predictions of batteries, foundational and quantitative understanding of ion transport is imperative. While this understanding and the quantification of associated transport parameters has historically relied on interpreting electrochemical measurements, imaging and spectroscopic methods to directly probe velocity and concentration profiles upon cell polarization have recently provided new insight. [1]

We are developing novel X-ray microscopy setups to operando and directly measure concentration profiles in polarized electrochemical cells using laboratory and synchrotron X-ray sources and dedicated

electrochemical cells. Our methodology uses the relationship between salt concentration and X-ray absorption. First results will be presented, with focus on the LiTFSI in PEO polymer electrolyte system. While LiTFSI/PEO has been investigated over decades, its transport parameters are still debated. Two recent studies show different concentrations profiles upon polarization of Li—LiTFSI/PEO—Li symmetric cells. [2][3] We hope to shed light on this discrepancy with our new X-ray absorption microscopy data set. We anticipate that the novel methodology can contribute to the efficient determination of electrolyte transport properties and thereby support knowledge-based optimization of electrolytes.

- [1] Mistry et al., Adv. Energy Mater. 13, 2203690 (2023).
 [2] Steinrück et al., EES 13, 4312 (2020).
 [3] Hoffman et al., JES 170, 090517 (2023).

Contributed Talk, 17:20-17:40

EXPLORING HYDROGEN PHYSISORPTION IN NANOPORE CONFINEMENT: INSIGHTS FROM IN-SITU SMALL-ANGLE NEUTRON SCATTERING

Sebastian Stock (1,2), Malina Seyffertitz (1), Nikolaos Kostoglou (1),
 Max Valentin Rauscher (1), Bruno Demé (2), Oskar Paris (1)

(1) Montanuniversität Leoben, (2) Institute Laue Langevin

This study investigates the low-pressure supercritical Hydrogen (H_2) and Deuterium (D_2) adsorption in a nanoporous activated carbon cloth, investigated by small-angle neutron scattering (SANS). The SANS measurements were carried out at the Institute Laue-Langevin (ILL) using the high-resolution diffractometer D16, which allowed us to cover a wide range q-range and thus pore sizes. The physisorption of adsorbate molecules in the pore space leads to changes in the SANS signal, which are described by an analytical pore scattering functions resembling slit-like pores. The pore-size-dependent physical density of the confined adsorbate molecules was calculated by employing a hierarchical contrast model covering three distinct pore classes, roughly resembling meso-, supermicro- and ultramicropores. From these calculations we find the adsorbate density in the smallest pores of ~ 0.7 nm to exceed the bulk solid density of H_2 at 77K. For D_2 adsorption there is strong evidence of similar densification from the analysis of the intermolecular correlation peak. The D_2 density calculated from the hierarchical model is apparently lower, which might be due to an exchange of H with D on surface functional groups of the carbon material.

Contributed Talk, 17:50-18:10

HE-XRD MEASUREMENTS OF H CRYSTAL STRUCTURE INTERACTION IN SYNCHROTRON

Thomas Pogrietz(1,2), Matthias Eichinger(3), Adam Weiser(4), Juraj
Todt(2), Gregor Mori(3), Dominik Brandl(1), Gerald Ressel(1), Jozef
Keckes(2)

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Austria (2) Erich Schmid Institute of Materials Science, Austrian
Academy of Sciences, A-8700 Leoben, Austria (3) Montanuniversität
Leoben, Chair of General and Analytical Chemistry: RG – Corrosion,
A-8700 Leoben, Austria (4) Czech Academy of Sciences, Institute of
Physics of Materials, CZ-61600 Brno, Czech Republic

Amidst the increasing interest in hydrogen as a green energy solution across diverse industries, understanding hydrogen's interaction with crystal structures in materials is paramount. This presentation unveils a novel method of in situ synchrotron cross-sectional micro X ray diffraction on steel with comparable ferrite and austenite phase fractions, coupled with electrolytic hydrogen charging, addressing phase-selective crystal structure swelling and in-plane stress evolution. This method showcases that sustained charging at a constant current density induces significant expansion solely in the austenitic crystal structure, while leaving the lattice parameter of the ferrite unaffected. As the expansion of the austenite near the surface encounters resistance from the underlying material, it triggers a formation of in-plane compressive stresses reaching ~150 MPa. Furthermore, the swelling of austenite induces in plane compressive stresses in the ferrite, peaking at 600 MPa. Notably, the lower stress levels in the austenitic phase align with observed near-surface plastic deformation through scanning electron microscopy. Moreover, this methodology facilitates the estimation of an effective hydrogen diffusion coefficient within the austenite phase under specific assumptions. This presentation sheds light on the nuanced dynamics of hydrogen-material interactions, offering insights critical for ensuring material integrity in hydrogen-rich environments.

Contributed Talk, 18:10-18:30

PEROVSKITE-TYPE OXIDES IN METHANOL STEAM REFORMING: OVERCOMING THE CHALLENGES OF CONVENTIONAL CATALYTIC SYSTEMS

Tobias Berger (1), Hedda Drexler (1), Florian Schrenk (1), Lorenz Lindenthal (1), Raffael Rameshan (1), Christoph Rameshan (1)

(1) Chair of Physical Chemistry, Montanuniversitaet Leoben

This study investigates the release of chemically stored hydrogen via Methanol Steam Reforming (MSR), emphasizing in-situ experiments at DESY (Deutsches Elektronen Synchrotron). Conventional catalysts, e.g. Cu/ZnO/Al₂O₃, suffer activity losses due to occurring sintering processes necessitating the exploration of new kinds of catalytic materials, e.g. in the form of perovskite-type oxides. Specifically, Nd_{0.6}Ca_{0.4}Fe_{1-x}B_xO₃ and Pr_{0.6}Ca_{0.4}Fe_{1-x}B_xO₃, B-site doped with Cu, Ni, or Co, were examined for enhanced MSR catalysis.

In-depth analyses, including catalytic tests and Scanning Electron Microscopy (SEM), were complemented by in-situ X-Ray Diffraction (XRD) measurements at DESY beamline P02.1. These experiments provided valuable insights into structural changes during the conditions of MSR. Notably, all materials exhibited catalytic activity, with Cu-doped catalysts standing out, achieving over 30% conversion and 100% selectivity below 300°C. Furthermore, in-situ XRD confirmed catalyst stability as well as the formation of a stable metallic Cu phase during the reductive pretreatment steps.

The study highlights the controlled modulation of catalytic properties by B-site doping with a focus on the effectiveness of Cu-doped catalysts for MSR, which is further proven by the unique contributions of time-resolved pXRD experiments.

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Keynote Lecture, 20:00-21:00

USING (COHERENT) OPERANDO X-RAY METHODS TO QUANTITATIVELY UNDERSTAND ELECTROCHEMICAL SYSTEMS

Hans-Georg Steinrück

(1) Forschungszentrum Jülich GmbH, Institute for a Sustainable Hydrogen Economy (INW), Am Brainergy Park 4, 52428 Jülich, Germany (2) RWTH Aachen University, Institute of Physical Chemistry, Landoltweg 2, 52074 Aachen, Germany

Quantitative insight into structural (physical and electronic) and morphological properties on an absolute scale and under reactions conditions is imperative towards understanding atomic- to meso-scale mechanisms and processes in electrochemical systems. Interpreted in the context of device performance, this knowledge can be used for rational design of and new concepts for improved materials. Following a brief introduction, two examples will be discussed in detail.

The first topic concerns charge and mass transport in various electrolytes. Here, we used a combination of operando X-ray photon correlation spectroscopy, small angle X-ray scattering, and X-ray absorption microscopy to measure electrolyte velocity and concentration fields upon cell polarization. The results were combined with macroscopic and microscopic theory to quantify and rationalize transport numbers, and to provide length-scale bridging insight into ion transport. The second topic covers desalination batteries. Here, we employed (quasi-high-throughput) operando high-energy X-ray diffraction microscopy to spatially resolve ion intercalation mechanisms in realistic flow-by desalination reactors. We focus on atomic- to electrode-level insight into structural changes and ion selectivity in manganese oxides and iron phosphate electrodes.

The final part of the talk will be devoted to future opportunities to utilize coherent and high-brilliance X-rays to study dynamic processes in energy storage materials.

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NESY Tutorial, 8:40-9:40

X-RAY FLUORESCENCE ANALYSIS (XRF) - A TUTORIAL

Peter Kregsamer

TU Wien - Atominstitut

For the energy range from 1 – 100 keV absorption of X-rays is the dominant effect. The consequent emission of characteristic X-rays (X-ray fluorescence) and their detection is used in X-ray fluorescence spectroscopy (XRF). Elements of the periodic table from Na upwards to the heaviest ones can be detected. Quantitative results for samples containing various elements in the range from 100% down to 1 ppm can be obtained routinely. In principle the technique is non-destructive, the sample can be returned to the customer in the original state. Otherwise a well-selected specimen will be used for the analysis.

Several technological developments can extend the detectable elements' range, the lower limits of detection can be brought down by orders of magnitude, and imaging techniques can be applied as well as chemical speciation.

The fundamentals of XRF and limiting influence factors will be discussed and selected advanced applications presented.

NESY Tutorial, 9:40-10:40

TUTORIAL ON INELASTIC AND QUASI-ELASTIC NEUTRON SCATTERING

Herwig Michor

Institute of Solid State Physics, TU Wien

Inelastic neutron scattering (INS) is a fundamental microscopic technique to study the energy and momentum dependence of excitations related to lattice-, spin-, and orbital degrees of freedom in solids. Quasi-elastic neutron scattering (QENS) is a closely related form of INS applied to study excitations related to random interactions such as diffusive motion in liquids, biomolecular dynamics or paramagnetic spin-fluctuations. We will review the principles of INS and QENS, some basic instrumental setups and methods.

As practical examples we briefly spotlight INS and QENS studies of

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some rare earth intermetallic compounds with respect to magnetic excitations related to crystalline electric field effects as well as paramagnetic fluctuations.

NESY Tutorial, 11:00-12:00

QUANTUM MECHANICS WITH NEUTRON INTERFEROMETRY

Stephan Sponar

Atominstitut - TU Wien

Neutron interferometry, where an interference effects of matter waves passing through a perfect silicon- crystal interferometer is observed, has established a powerful tool for investigation of fundamental quantum mechanical concepts with massive particles. This technique enabled several text-book experiments, such as demonstrations of 4π spinor symmetry of spin-1/2 particles, spin superposition, gravitationally induced phase and topological phase effect, as well as studies of characteristics of intrapartite entanglement, i.e., entanglements between different degrees of freedom [3]. In my lecture I will give a detailed introduction into the dynamical theory of diffraction, which is the basis for the observed interference fringes in neutron interferometry. Furthermore, beside the well-known text book experiment I will give an overview of more recent research activities, covering topics like weak values and weak measurements, which have been used to directly reconstruct the neutron's wave function inside the interferometer, to demonstrate anti-commuting properties of Pauli spin matrices, or determination of a new type of a which-path observable.

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P-1 (ACD'24)	Kirill Kuhlmann	Ancestral reconstruction leads to first crystal structure of tocopherol cyclase involved in vitamin E production
P-2 (ACD'24)	Christoph Grninger	Electron Diffraction on Proteins – Small crystals matter
P-3 (ACD'24)	Nikolina Todorovic	Crystal structure and structure-based IgE epitope prediction of the domestic cat allergen Fel d 4
P-4 (ACD'24)	Tamara Đorđević	Structural characterization of thallium (Tl) hosts in environmental samples
P-5 (ACD'24)	Bernhard Gadermaier	<i>Operando</i> X-ray powder diffraction to monitor the charge and discharge processes in LiCoO ₂ using a laboratory diffractometer
P-6 (ACD'24)	Gerald Giester	Syntheses and crystal structures of K ₂ Zr(SeO ₄) ₃ and K ₂ Zr ₂ O(SeO ₄) ₄ , two novel anhydrous zirconium oxysalts
P-7 (ACD'24)	Herta Effenberger	Ammonium-iron-sulfites from a burning coal-mine dump
P-8 (ACD'24)	Tea Pavkov-Keller	The molecular architecture of Lactobacillus S-Layer: Assembly and attachment to teichoic acids
P-9 (NESY)	Max Valentin Rauscher	Dynamics of Capacitive Water Desalination from In Operando SAXS using Synchrotron Radiation
P-10 (NESY)	Josef Simbrunner	Correlation between 2- and 3-dimensional crystallographic lattices for epitaxial analysis
P-11 (NESY)	Michael Musi	Phase transformation behavior of a γ -TiAl based alloy during spark plasma sintering – An in-situ diffraction study

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P-12 (NESY)	Giulia Tam- burini	Crystallinity of Eu-doped Poly(L-lactic acid) Microspheres by Emulsification
P-13 (NESY)	Fabian Gasser	Intensity Corrections for Grazing Incidence X-ray Diffraction
P-14 (NESY)	David Ober- steiner	Characterization of phase transformation and precipitation behavior in a novel Cu-modified near- α Ti alloy for additive manufacturing
P-15 (NESY)	Thomas Ruh	Characterization of CO ₂ Conversion Catalysts – A Case Study
P-16 (NESY)	Hedda Drexler	Unraveling the mysteries of B-site doped ferrite catalysts
P-17 (NESY)	Georg Urstöger	Advanced X-ray Characterization of Zeolites
P-18 (NESY)	Muhammad Zubair Khan	Layer-Dependent Magnetic Ordering in Natural and Engineered 2D Magnetic insulators
P-19 (NESY)	Malina Seyf- fertitz	Investigating aqueous electrolytes in nanoconfinement at charged interfaces using in-situ small-angle X-ray and neutron scattering
P-20 (NESY)	Rainer T. Lechner	ESUO - The European Synchrotron and FEL User Organisation: A brief introduction

P-1 (ACD'24)

ANCESTRAL RECONSTRUCTION LEADS TO FIRST CRYSTAL STRUCTURE OF TOCOPHEROL CYCLASE INVOLVED IN VITAMIN E PRODUCTION

Kirill Kuhlmann, Christoph Grininger, Tea Pavkov-Keller

Institute for Molecular Biosciences, University of Graz

Tocopherols are a class of organic chemical compounds synthesized exclusively by photosynthetic organisms and oxygenic cyanobacteria. The most popular isomer (RRR)- α -tocopherol (Vitamin E), is frequently used as antioxidant for polyunsaturated fatty acids protection in food industry, cosmetics, and other industrial fields.

Tocopherol cyclases (TCs) are a protein family of membrane associated enzymes which are essential for tocopherol synthesis in photosynthetic organisms. They catalyze the formation of a chromanol headgroup from

hydroquinone precursor such as 2-methyl-6-phytyl-1,4-benzoquinone (MPBQ) and 2,3-dimethyl-6-phytyl-1,4-benzoquinone (DMPBQ) yielding δ - and γ -tocopherol respectively. Due to the hydrophobic nature of the enzyme, standard expression and purification protocols do not yield sufficient amount of soluble protein for subsequent structure determination experiments.

Through a combination of artificial intelligence structure prediction models as well as common ancestor sequence reconstruction (ASR) we identified a novel TC variant derived from *Nostoc* sp. PCC 7120 where we successfully expressed and purified a substantial amount ultimately yielding crystals diffracting up to 4 Å. The structure reveals a fold with four overlapping β -sheets with a putative active site where we suggest a putative enzyme mechanism.

P-2 (ACD'24)

ELECTRON DIFFRACTION ON PROTEINS – SMALL CRYSTALS MATTER

Christoph Grininger (1), Gerhard Hofer (2), Laszlo Schooltink (1),
Moussa Faye (3), Mauro Gemmi(3), Tea Pavkov-Keller (1)

(1) Institute for Molecular Biosciences – Structural Biology,
University of Graz, Graz, Austria (2) Department of Materials and
Environmental Chemistry, Stockholm University, Stockholm, Sweden
(3) Istituto Italiano di tecnologia, Pontedera, Italy

3D electron diffraction (ED) is an uprising method for the structural characterization of nanocrystalline materials. This also includes beam sensitive materials like protein crystals.

A bottleneck in the structural characterization of macromolecules with X-ray diffraction is crystallization. Often the needed crystal size cannot be achieved despite extensive optimization of crystallization conditions. Nevertheless, the yield of needle clusters, microcrystals and almost two-dimensional platelets is a silver lining. Those crystals – too small for X-ray crystallography – could be applied to microcrystal electron diffraction methods. Additionally it is a fast method that could soon outperform X-ray crystallography for cases like ligand screening. So far we were able to establish the basic workflow for data collection with our instrument setup, a Zeiss Libra 120 plus TEM with an OMEGA energy filter and a TVIPS TemCam-XF416(ES) detector. We collected continuous rotation electron diffraction data for the zeolite ZSM-5 and protein nanocrystals (lysozyme, der f 20 like) under cryo conditions.

Optimization of protein crystallization for perfectly suitable ED samples is yet an obstacle to overcome to reach structure resolutions comparable to X-ray diffraction.

With these fundamental achievements we are on track to apply ED to more challenging crystals and also solve novel protein structures in the future.

P-3 (ACD'24)

CRYSTAL STRUCTURE AND STRUCTURE-BASED IGE EPIOTOPE PREDICTION OF THE DOMESTIC CAT ALLERGEN FEL D 4

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Throughout the years pets have been recognized as one of the major sources of indoor allergens posing a great risk for the development of IgE-mediated diseases such as allergenic rhinitis and asthma. To date, the WHO/IUIS database reports eight cat allergens. Among these allergens, the frequency of IgE recognition is found to be the highest for Fel d 1, Fel d 4 and Fel d 7 making them the most important cat allergens. Fel d 4 belongs to the lipocalin protein family with a common 8-stranded beta-barrel fold and a hydrophobic cavity. Fel d 4 shares high sequence identity with the allergens from dog (Can f 6) and horse (Equ c 1) contributing to polysensitization. The structural analysis of these allergens and linear and conformational epitope studies are valuable assets for the development of diagnostic approaches as well as specific immunotherapies. In this study, we cloned the major cat allergen Fel d 4, expressed it in *E. coli* and purified it with nickel affinity chromatography and size-exclusion chromatography. Recombinantly produced allergen showed a typical lipocalin fold upon circular dichroism measurement and a high thermal stability. Furthermore, we determined the crystal structure of the rFel d 4 using X-ray crystallography. Subsequently, we performed in silico epitope prediction analysis, which suggested possible linear and conformational B-cell epitopes that could serve as a starting point for further epitope studies.

P-4 (ACD'24)

STRUCTURAL CHARACTERIZATION OF THALLIUM (Tl)
HOSTS IN ENVIRONMENTAL SAMPLESTamara Đorđević (1,2), Michael Stöger-Pollach (1), Sabine Schwarz
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The discovery of new Tl-bearing occurrences in the last decade suggests that secondary Tl-minerals are more common than previously thought and can play an important role in attenuating the dispersion of Tl from contamination sources. As a result, it is critical to characterize potential secondary Tl-minerals that could form in various environments.

Our current project aims to investigate weathering processes and their nano- and microcrystalline products that result from sulfidic Tl-rich ores, as well as synthetic, mineral-like Tl-bearing oxides and oxy salts. To achieve this goal, we investigate both selected naturally Tl-bearing ore deposits and adjacent mining wastes and technosols for their mineralogical and geochemical properties, as well as synthesised mineral-like Tl-compounds.

We have shown that in Tl-rich environmental samples we encounter minerals that (i) are known but have not previously been reported at the locality of interest, (ii) have not previously been observed and exhibit a wide range of crystallinity, or (iii) are amorphous and have never been described. We were able to structurally characterise several novel or poorly described Tl-phases by combining X-ray diffraction methods with electron microscopy techniques (SEM-EDX, TEM-EBSD, TEM-EELS, TEM-EDX).

T. Đorđević gratefully acknowledges the financial support of the Austrian Science Fund (FWF) [P 36828-N].

P-5 (ACD' 24)

Operando X-RAY POWDER DIFFRACTION TO MONITOR
THE CHARGE AND DISCHARGE PROCESSES IN LiCoO_2
USING A LABORATORY DIFFRACTOMETERBernhard Gadermaier, Ilie Hanzu, Martin Wilkening

Graz University of Technology

The physical properties of any material are closely linked to its structure. Capturing the structural changes of battery active materials dur-

ing operation is a no-trivial task. Laboratory X-ray diffraction, being non-invasive and non-destructive, is perfectly suited for such measurements especially if performed *in situ* or *operando*. Typically, such measurements are performed at highly brilliant beamlines but using the right setup, such measurements can be performed *at home* using a laboratory X-ray powder diffractometer. The cell design is here even more important since the cell must be sufficiently transparent for X-rays while preventing moisture and air from entering the cell.

Using the current collector, a 20 μm thick aluminum foil, and epoxy glue to seal the coin cell, we found a suitable setup to prevent moisture ingress. The cell has been cycled under stable conditions for more than 10 days while being transparent enough to monitor the Bragg peaks in reflection mode during cycling. We used Co and Cu $K\alpha$ radiation to monitor the change of LiCoO_2 during charging and discharging by focusing on the 003 reflection. This showed that LiCoO_2 progresses through a two-phase evolution followed by a continuous lattice expansion as lithium is extracted during charging.

P-6 (ACD' 24)

SYNTHESES AND CRYSTAL STRUCTURES OF $\text{K}_2\text{Zr}(\text{SeO}_4)_3$ AND $\text{K}_2\text{Zr}_2\text{O}(\text{SeO}_4)_4$, TWO NOVEL ANHYDROUS ZIRCONIUM OXYSALTS

Gerald Giester, Manfred Wildner

Universität Wien, Institut für Mineralogie und Kristallographie

The crystal chemistry of zirconium oxysalts with $(\text{XO}_4)^{2-}$ or $(\text{XO}_3)^{2-}$ ($\text{X} = \text{S}, \text{Se}$) anions, synthesized under mild-hydrothermal conditions below 250 $^\circ\text{C}$, has been the subject of our research since several years [1-5]. Recently, four new representatives were obtained, among them two triclinic anhydrous compounds, both incorporating potassium.

The complex structure of $\text{K}_2\text{Zr}(\text{SeO}_4)_3$ is built from ZrO_6 octahedra, SeO_4 tetrahedra and KO_n ($n=7,8,10$) polyhedra. ZrO_6 octahedra are corner-linked to selenate groups, arranged in slabs parallel to (1 0 1) which further include part of the KO_n polyhedra. These building units are separated from each other by layers of further KO_n polyhedra embedded in between.

The structure of $\text{K}_2\text{Zr}_2\text{O}(\text{SeO}_4)_4$ is characterized by dimers of edge-sharing ZrO_7 pentagonal bipyramids, decorated by SeO_4 tetrahedra via shared edges. Along [1 0 0] the dimers are corner-linked via the oxo-oxygen to infinite chains which are interconnected by SeO_4 tetrahedra to two-dimensional units arranged parallel (0 0 1). Distorted

KO₈ polyhedra, sharing common faces and edges to form chains parallel [1 0 0], are situated between these sheets.

Literature:

1. Giester G, Wildner M (2018) *Monatsh Chem* 149: 1321-1325
2. Wildner M, Giester G (2019) *Monatsh Chem* 150: 593-603
3. Giester G, Talla D, Wildner M (2019) *Monatsh Chem* 150: 1877-1892
4. Wildner M, Lengauer C, Effenberger H, Giester G (2022) *Monatsh Chem* 153: 139-151
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P-7 (ACD' 24)

AMMONIUM-IRON-SULFITES FROM A BURNING COAL-MINE DUMP

Herta Effenberger (1), Béla Fehér (2), Sándor Szakáll (3), Martin Ende (1), Judith Mihály (4), István Sajó (5), László Kótai (4), Dávid Szabó (6)

(1) Universität Wien, (2) Herman Ottó Museum Miskolc, (3) University of Miskolc, (4) Research Centre for Natural Sciences Budapest, (5) University of Pécs, (6) University Budapest

Ammonium-iron-sulfites from a burning coal dump in an abandoned open coal pit (Pécs-Vasas, Mecsek Mountains, South Hungary) were investigated.

(NH₄)₉Fe³⁺(SO₃)₆ is metastable and decomposes quickly. The [Fe³⁺(SO₃)₆] clusters are linked by (NH₄) groups.

(NH₄)₂Fe²⁺(SO₃)₂ forms [Fe(SO₃)₂] layers. The crystal structure is topologically equivalent to the buetschliite-type selenites and carbonates. About 8 % of the Fe³⁺ ions are displaced (0.64 Å).

In (NH₄)₂Fe³⁺(OH)(SO₃)₂·H₂O the [FeO₆] octahedra are corner linked to buckled [Fe(OH)(SO₃)₂] chains. They are connected by hydrogen bonds to the H₂O and (NH₄) groups. As the Ow atom has site-symmetry m2m, the H₂O molecule exhibits a site disorder. Neither a reduction of symmetry nor superstructure reflections were observed. Despite the small crystal (6 × 7 × 65 μm³), the half-occupied H atom position was refined without any restrictions (variable atomic coordinates and isotropic displacement parameter). X-ray data were collected at a Stoe-StadiVari diffractometer equipped with a Dectris Pilatus 300 K pixel detector and an Incoatec IμS micro-focus X-ray tube.

For details see Fehér et al. (2023): *Mineralogy and Petrology* 117, 231–245.

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P-8 (ACD' 24)

THE MOLECULAR ARCHITECTURE OF LACTOBACILLUS S-LAYER: ASSEMBLY AND ATTACHMENT TO TEICHOIC ACIDS

Tea Pavkov-Keller (1), Theo Sagmeister(1), Nina Gubensäk(1), Christoph Buhlheller(1), Christoph Grininger(1), Markus Eder(1), Anđela Đorđić(1), Claudia Millán(2), Ana Medina(2), Pedro Alejandro Sánchez Murcia(3), Francesca Berni(4), Ulla Hynönen(5), Djenana Vejzović(1), Elisabeth Damisch(1), Natalia Kulminskaya(1), Lukas Petrowitsch(1), Monika Oberer(1), Airi Palva(5), Nermina Malanović(1), Jeroen Codée(4), Walter Keller(1), Isabel Usón (2,6)

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S-layers are crystalline arrays found on bacterial and archaeal cells. *Lactobacillus* is a diverse family of bacteria known especially for potential gut health benefits. This study focuses on the S-layer proteins from *Lactobacillus acidophilus* and *Lactobacillus amylovorus* common in the mammalian gut. Atomic resolution structures of *Lactobacillus* S-layer proteins SlpA and SlpX exhibit domain swapping and the obtained assembly model of the main S-layer protein SlpA aligns well with prior electron microscopy and mutagenesis data. The S-layer's pore size suggests a protective role, with charged areas aiding adhesion. A highly similar domain organization and interaction networks is observed across the *Lactobacillus* genus. Interaction studies revealed conserved binding areas specific for attachment to teichoic acids. The structure of the SlpA S-layer and the suggested incorporation of SlpX, as well as its interaction with teichoic acids lays the foundation for deciphering its role in immune responses and for developing effective treatments for a variety of infectious and bacteria-mediated inflammation processes, opening new opportunities for targeted engineering of the S-layer or *lactobacilli* bacteria in general.

P-9 (NESY)

DYNAMICS OF CAPACITIVE WATER DESALINATION FROM IN OPERANDO SAXS USING SYNCHROTRON RADIATION

Max Valentin Rauscher (1), Oskar Paris (1), Malina Seyffertitz (1),
Heinz Ammenitsch (2), Sylvio Haas (3)

(1) Montanuniversität Leoben, Chair of Physics, (2) Institute of Inorganic Chemistry, Graz University of Technology, (3) Deutsches Elektronen-Synchrotron DESY

Nanoporous carbon electrodes are used in capacitive deionization (CDI), an increasingly important method for brackish water treatment. The present study uses synchrotron radiation to investigate the intricacies of CD by in-operando Small Angle X-ray Scattering (SAXS). First proof of principle experiments were carried out at the SAXS beamline at ELETTRA and DESY using a customized desalination cell. The experimental setup, designed for small- and wide-angle X-ray scattering enables time-resolved observation of changes of the X-ray transmission- and scattering signals due to ion-electrosorption in the carbon nanopores during desalination. This information is complementary to the simultaneously measured electrochemical information and the conductivity of the electrolyte, providing information on local ion dynamics and its efficacy under diverse conditions. First experiments were done using MSP20-carbon powder and CsCl electrolyte at concentrations of 5 and 25mM with 0, 1 and 5ml/min flow rates. Significant changes of the ion concentration changes between static condition and high flow rate can be observed. Conductivity measurements of the effluent stream indicate little to no salt removal during 1, and 5ml/min flow rate. Ex-situ measurements with NaCl, however, reveal that the cell is operating as expected making the first measurements with CsCl all the more interesting.

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P-10 (NESY)

CORRELATION BETWEEN 2- AND 3-DIMENSIONAL CRYSTALLOGRAPHIC LATTICES FOR EPITAXIAL ANALYSIS

Josef Simbrunner (1), Jari Domke (2), Torsten Fritz (2), Roman Forker (2), Roland Resel (3)

(1) Medical University Graz, (2) Friedrich Schiller University Jena, (3) Graz University of Technology

While the crystalline properties of an epitaxially grown thin film can be studied in three dimensions by X-ray methods like grazing inci-

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dence X-ray diffraction (GIXD), the first monolayer is only accessible by surface sensitive methods that allow the determination of a two-dimensional lattice like low-energy electron diffraction (LEED).

Rotated GIXD measurements on epitaxially grown film are compared with distortion-corrected LEED experiments of molecular monolayers. The theoretical basis has been derived which provides a mathematical relationship between the six lattice parameters of the three-dimensional case with the three parameters obtained for the surface unit cell, together with their orientation to the single crystalline substrate.

The selected examples showed three possible scenarios of crystal growth on top of an ordered monolayer: (1) In PTCDA/Ag(111) and P2O/Ag(111) the growth of a single polymorph was obtained with congruent two-dimensional lattices in the monolayer and multilayer. (2) In DCV4T-Et₂/Ag(111) three different polymorphs with various cell parameters, orientations and azimuthal alignments were observed in the multilayer. Whereas their three-dimensional lattices differ significantly, their surface unit cells converge to a single unit cell in the monolayer. (3) In trans-DBPen/Cu(111) strong lattice distortion and distinct molecular re-alignments from the monolayer to epitaxially grown crystals were observed.

P-11 (NESY)

PHASE TRANSFORMATION BEHAVIOR OF A γ -TiAl BASED ALLOY DURING SPARK PLASMA SINTERING – AN IN-SITU DIFFRACTION STUDY

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Their outstanding property portfolio, including low density and high creep resistance, makes intermetallic γ -TiAl based alloys excellent candidates for structural high-temperature applications in the automotive and aerospace industries. A powder metallurgical processing technique of growing interest is spark plasma sintering (SPS). It offers fast production times and the ability to control the microstructure and, thus, the mechanical properties by adjusting the dwell temperature with respect to the phase diagram. Due to short dwell times, the kinetics of the phase transformations have a particular impact on the final microstructure. Consequently, this work presents an investigation of the phase evolution of a W-containing γ -TiAl based alloy during an SPS

process adapted for high-energy X-ray diffraction (HEXRD). In-situ heating HEXRD experiments utilizing a special powder sample holder grant valuable insights into the non-equilibrium and equilibrium phase transitions, e.g. an $\alpha/\alpha_2 \rightarrow \gamma$ transformation at low temperatures to approach thermodynamic equilibrium and the γ dissolution at higher temperatures. Additionally, the ordering behavior of the individual phases and the dependence of their lattice parameters on temperature and phase composition are investigated. Complementary microstructural characterization by scanning electron microscopy and electron backscatter diffraction shed light on the influence of the occurring phase transformations on the microstructural evolution.

P-12 (NESY)

CRYSTALLINITY OF EU-DOPED POLY(L-LACTIC ACID) MICROSPHERES BY EMULSIFICATION

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This study explores a novel approach to regulate the crystallinity of PLA microspheres by emulsification. Through powder and grazing incidence X-ray diffraction with synchrotron radiation, together with calorimetric and spectroscopic analyses, it has been observed that poly(L-lactic acid) (PLLA) microspheres, whether pure or doped with europium, exhibit an adjustable crystalline fraction achieved through emulsification at temperatures ranging from 20 to 80°C. Specifically, the pure PLLA microspheres show a range from 16% to 35%, while the doped ones from 30% to 50%. Significantly, a comprehensive analysis, comparing macro- and micro-analysis, supports a model in which emulsification temperature influences the ratio of amorphous to α -phase crystalline components within each PLLA microsphere. Additionally, unlike bulk material, the microspheres exhibit no infrared-active changes in the molecular unit after exposure to X-rays. These results pave the way for innovative strategies to produce radiation-resistant microspheres with controlled crystallinity.

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P-13 (NESY)

INTENSITY CORRECTIONS FOR GRAZING INCIDENCE
X-RAY DIFFRACTION

Fabian Gasser (1), Josef Simbrunner (2), Mario Fratschko (1), Marten Huck (3), Hans-Georg Steinrück (3), Roland Resel (1)

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Grazing Incidence X-ray Diffraction (GIXD) is a powerful technique to investigate crystal structures of thin films. The unit cell of a crystal structure can be determined from the position of the different Bragg peaks in a GIXD map. The intensity of the individual peaks is related to the so-called structure factor. To compare measured peak intensities to calculated structure factors a variety of correction factors need to be applied to experimental GIXD data. This work primarily focuses on the Lorentz correction, a geometric correction factor with diverse analytical formulas and mathematical derivations reported in literature. We present a simple yet effective procedure to determine integrated peak intensities, explicitly taking into account Lorentz correction. To verify and benchmark our novel approach, measurements were performed on model systems at beamline XRD1, Elettra Trieste and on laboratory x-ray sources. The procedure is systematically applied to three samples exhibiting distinct textures: 3D powders, 2D powders (i.e., uniplanar textured) and biaxially textured films. We demonstrate how peak integration can be simplified by taking advantage of the different symmetries inherent in these textures. Our study significantly contributes to the fundamental understanding and utilization of GIXD for quantitative texture analysis based on geometrically corrected peak intensities.

P-14 (NESY)

CHARACTERIZATION OF PHASE TRANSFORMATION AND
PRECIPITATION BEHAVIOR IN A NOVEL CU-MODIFIED
NEAR- α Ti ALLOY FOR ADDITIVE MANUFACTURING

David Obersteiner (1), Thomas Klein (2), Sophie Primig (3), Michael Musi (1)

(1) Department of Materials Science, Montanuniversität Leoben (2) LKR Light Metals Technologies, AIT Austrian Institute of Technology (3) School of Materials Science & Engineering, UNSW Sydney

Near α Ti-alloys are widely used for structural components up to service

temperatures of 550 °C. While conventional manufacturing techniques prevail, additive manufacturing (AM) has gained significant interest recently due to its ability to produce complex geometries and efficient material usage. However, AM techniques have proven to be challenging fabrication processes with numerous variables affecting microstructure evolution. Complex thermal conditions and a layer-wise build-up often lead to pronounced textures and, consequently, anisotropic mechanical properties. One fundamental way to address challenges such as microstructure evolution during AM is the development of new alloying concepts. However, this relies on a profound understanding of the influence of the alloying elements on the material's thermodynamics and transformation kinetics.

In this work, in-situ small-angle (SAXS) and wide-angle X-ray scattering (WAXS) experiments were performed to study a novel near α Ti alloy for high-temperature applications. In particular, the effect of Cu on the phase transformation and precipitation behavior was investigated. While WAXS provided insights into present phases under varying heat treatment conditions, the formation of nm sized inter-metallic precipitates could be observed simultaneously by SAXS. The results of this study grant a deeper understanding of the complex phase evolution of a newly developed high temperature Ti alloy optimized for AM.

P-15 (NESY)

CHARACTERIZATION OF CO₂ CONVERSION CATALYSTS – A CASE STUDY

Thomas Ruh, Tobias Berger, Christoph Rameshan

Montanuniversität Leoben, Chair of Physical Chemistry

In our Sparkling Science 2.0 project “CO₂ Conversion” (www.co2-umwandlung.at), we study processes to close the carbon dioxide cycle via CO₂ utilization – e.g. by capturing CO₂ from industrial exhaust gases and using it as feedstock for chemical reactions. As CO₂ is a very stable molecule, catalysts to facilitate those reactions are paramount. A thorough understanding of catalytic materials (e.g. composition and structure – both in bulk and at the surface) is crucial to design catalysts that perform well under industrially relevant conditions. That means a multitude of methods is needed to first characterize the material and – in a second step – assess relevant properties like catalytic activity, resilience against coking, high-temperature stability and so on. In this case study we demonstrate our methods using a commercially

available catalyst as an example (that will be needed as benchmark for further comparisons with materials we synthesize ourselves). Our methods include: Scanning electron microscopy (surface morphology), X-ray diffraction (lab-based to verify phase purity, synchrotron-based for in-situ studies under reaction conditions), X-ray photoelectron spectroscopy (lab-based characterization of surface species, synchrotron-based for high-pressure studies), and tests of various catalytic reactions.

P-16 (NESY)

UNRAVELING THE MYSTERIES OF B-SITE DOPED FERRITE CATALYSTS

Hedda Drexler (1), Tobias Berger (1), Lorenz Lindenthal (1),
Jonathan Rollenitz (1), Raffael Rameshan (1), Florian Schrenk (1),
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Deutsches Elektron-Synchrotron (DESY)

Perovskite-type oxides are an interesting class of materials that is applicable in various fields like SOFCs or catalytic reactions for carbon capture and utilization (CCU). Due to their structure of ABO_3 various elements of the periodic table can be used on the A- and B-site, as long as they still enable a stable structure (e.g according to the Goldschmidt tolerance factor). Furthermore, both sites can be doped with additional elements to enhance a process called exsolution. Hereby, B-site elements are migrating from the host lattice to the surface and are forming stable nanoparticles. Various elements like Co, Cu, Fe, Ni or mixtures thereof can be applied at the B-site, forming very active catalytic species at already low amounts of B-site dopants.

The exsolution process was investigated via pXRD and total scattering (DESY Beamline P02.1) under reductive conditions in the temperature range of 200 – 800 °C. $Nd_{0.6}Ca_{0.4}FeO_{3-\delta}$ (NCF) and $Nd_{0.6}Ca_{0.4}Fe_{0.9}Co_{0.1}O_{3-\delta}$ (NCF-Co10) were compared regarding their exsolution properties. The results of both techniques, with a focus on the evaluation via pair distribution function (PDF) are presented, as information over the bond lengths, coordination number and the occupancies give interesting in-sights into the exsolution process and the nanoparticle formation.

P-17 (NESY)

ADVANCED X-RAY CHARACTERIZATION OF ZEOLITES

Georg Urstöger, Ehmann Heike, Heiner Santner

Anton Paar GmbH

Porous materials such as zeolites are often characterized by scattering methods such as X-ray diffraction (XRD) and small-angle X-ray scattering (SAXS). Anton Paar produces state-of-the-art XRD and SAXS systems for the laboratory that can also be equipped with a wide range of non-ambient attachments (for measurements under e.g. variable temperature, pressure, relative humidity, or gas atmospheres). Using both XRD and SAXS under ambient and non-ambient conditions allows a more in-depth understanding of the sample in question and its properties as they reveal information such as crystal structure, phase content, pore size, specific surface, particle/crystallite size, etc.

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P-18 (NESY)

LAYER-DEPENDENT MAGNETIC ORDERING IN NATURAL AND ENGINEERED 2D MAGNETIC INSULATORS

Muhammad Zubair Khan (1) , Nico Klingner(2), Sergio Valencia(3), Gregor Hlawacek(2), Sebastian Wintz(3), Ulrich Kentsch(2), , Markus Weigand(3), Daniel Knez(4) Florian Kronast(3), Christian Teichert(1), and Aleksandar Matković(1)

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2D materials offer potential performance advantages over current Si-based technologies, and by bringing new functionalities they could also enable novel device concepts. One such example is magneto-resistive random-access memory (MRAM). In case of 2D magnetic insulators in MRAMs, ultra-thin antiferromagnetic barriers in combination with regular (non-magnetic) metals could lead to the development of future memory elements, computing in memory concepts, and self-reconfiguring circuits. Advantages of 2D magnetic insulators are that

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the need for ferromagnetic electrodes is lifted, and that due to their van der Waals nature they both enable atomically sharp interfacing and could be brought closer to the logic elements as magnetic metal ion diffusion is not an issue. The research in magnetic 2D insulators focuses on synthetic iodides, which suffer from a lack of ambient stability. So far, naturally occurring layered magnetic materials have been overlooked. These minerals offer a unique opportunity to explore complex air-stable layered systems with high concentration of magnetic ions. Thus far, only our consortium has reported the presence of weak ferromagnetism in atomically thin naturally occurring Fe-rich phyllosilicates at room temperature. Here, we explore structure to magnetism relation of natural and engineered 2D magnetic insulators using spatially and spectral resolved X-ray data.

P-19 (NESY)

INVESTIGATING AQUEOUS ELECTROLYTES IN
NANOCONFINEMENT AT CHARGED INTERFACES USING
IN-SITU SMALL-ANGLE X-RAY AND NEUTRON SCATTERING

Malina Seyffertitz (1), Sebastian Stock (1,4), Max Valentin Rauscher (1), Christian Prehal (2), Sylvio Haas (3), Lionel Porcar (4), Oskar Paris (1)

Montanuniversität Leoben, Austria, 2 ETH Zürich, Switzerland, now at Paris-Lodron-Universität Salzburg, Austria, 3 Deutsches Elektronen-Synchrotron DESY, Germany, 4 Institut Laue-Langevin ILL, France

Electric double layer capacitors (EDLCs), also known as supercapacitors, emerged as a vital research field addressing the growing demand for efficient electrical energy storage. Owing to their high power density, EDLC devices could be of particular importance for applications in electric vehicles, smart power grids and intermittent energy sources in light of managing the transition from fossil fuels to renewable energy. This poster showcases the applicability of X-ray transmission (XRT), (anomalous) Small Angle X-ray Scattering ((A)SAXS) and Small-Angle Neutron Scattering (SANS) for investigating fundamental processes taking place in the porous activated carbon working electrode of an electric double-layer capacitor with 1 M RbBr aqueous electrolyte at different applied potentials. XRT and incoherent neutron scattering are employed to determine global ion- and water- concentration changes and associated charge-balancing mechanisms. We demonstrate the suitability of SAXS and SANS, respectively, to get complementary

information on local ion and solvent rearrangement in nanoconfinement, but also underscore the limitations of simple qualitative models, asking for more quantitative descriptions of water–water and ion–water interactions via detailed atomistic modelling approaches.

P-20 (NESY)

ESUO - THE EUROPEAN SYNCHROTRON AND FEL USER ORGANISATION: A BRIEF INTRODUCTION

Rainer T. Lechner

Chair of Physics, Montanuniversitaet Leoben, Austria

The European Synchrotron and FEL User Organisation (ESUO) was founded in 2010 to represent all European photon science users. Today, ESUO represents about 30 000 users of the European synchrotron (SR) and Free-Electron Laser (FEL) facilities

Users from around 30 European & Middle East countries are represented by ESUO. The ESUO main goal can be seen in creating a truly European photon science community. ESUO's main objectives can be summarised in the following list:

- **Advocating** open access to European light sources
- **Forming** a pan-European light source user community.
- **Minimizing** administrative obstacles.
- **Increasing** competition to increase competitiveness.
- **Training** scientists hands-on.
- **Assisting** industry in innovation.

More details and current activities can be found on: esu.eu

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Sponsors

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Epilogue

While both scientific large-scale facilities for neutrons and X-rays (NESY) and the mythical monster of Loch Ness (Nessie) capture our imagination with their enigmatic presence, they exist in vastly different realms of reality.

NESY facilities, like neutron and X-ray scattering centers, are sophisticated scientific instruments designed to probe the structure and behavior of matter at the atomic and molecular level. These facilities are essential for research across a multitude of disciplines, including physics, chemistry, materials science, and biology. Scientists utilize them to analyze the properties of materials, investigate the structure of complex molecules, and understand fundamental processes governing various phenomena. NESY facilities are meticulously engineered and operated to provide precise and controlled experimental conditions, facilitating groundbreaking discoveries and advancements in our understanding of the natural world.

On the other hand, Nessie, the legendary creature purported to inhabit the waters of Loch Ness in Scotland, represents a different kind of fascination—one rooted in folklore, mystery, and myth. Despite numerous alleged sightings and fervent speculation over the years, there is no concrete scientific evidence supporting the existence of Nessie. Instead, the legend of Nessie has captured the public’s imagination, inspiring countless stories, expeditions, and debates about the unknown depths of Loch Ness.

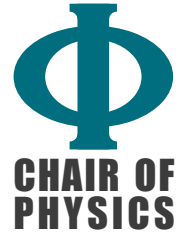
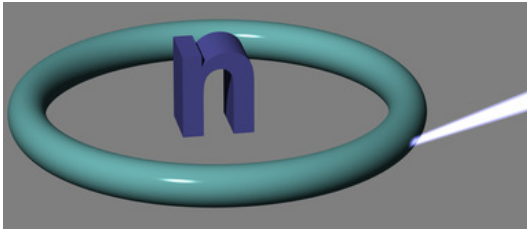
In essence, while NESY facilities represent the pinnacle of human ingenuity and scientific exploration, Nessie symbolizes the enduring allure of the unexplained and the mysteries that continue to captivate our curiosity. Both serve as reminders of humanity’s insatiable thirst for knowledge and our enduring fascination with the unknown, albeit in vastly different contexts.

ChatGPT on “Write something comparing scientific large scale facilities for neutrons and x-rays (NESY) with the monster of Loch Ness (Nessie)”

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	Wednesday					
		Thursday				
			Friday			
				Poster		
54					Bad Aussee, February 25 th -March 1 st 2024	



*Abstract Book assembled by Gerhard Popovski & Rainer T. Lechner,
Chair of Physics, Montanuniversität Leoben, Austria, February 23rd 2024.*



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