SNI2022

GERMAN CONFERENCE FOR RESEARCH WITH SYNCHROTRON RADIATION, NEUTRONS AND ION BEAMS AT LARGE FACILITIES

Freie Universität Berlin, Rostlaube
September 5th – 7th, 2022
Europe/Berlin Time Zone

supported by

Senatsverwaltung für Wirtschaft, Energie und Betriebe | BERLIN

CONFERENCE BOOK

CONFERENCE BOOK: GENERAL INFORMATION, PROGRAMME AND ABSTRACTS

EDITOR:

Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
www.helmholtz-berlin.de

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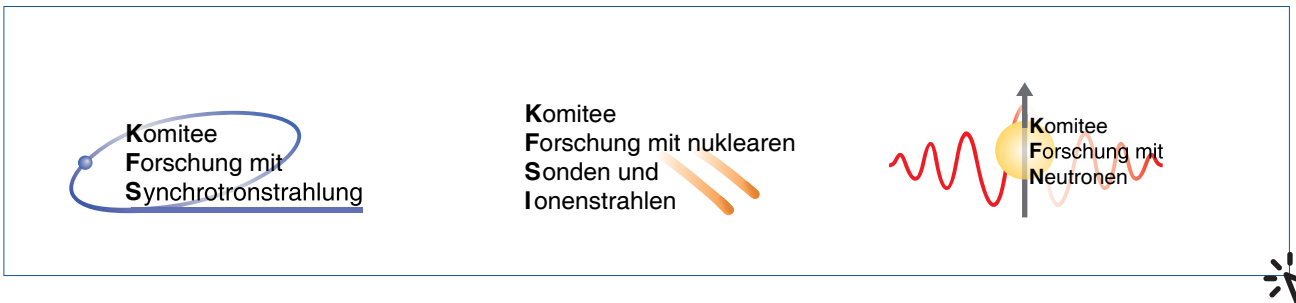
COMMITTEES



SNI2022 is organised on the initiative of the Komitee Forschung mit Synchrotronstrahlung (KFS), the Komitee Forschung mit Neutronen (KFN) and the Komitee Forschung mit Sonden und Ionenstrahlen (KFSI). Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) acts as local organiser.

Programme Committee:
Komitee Forschung mit Synchrotronstrahlung (KFS)
Komitee Forschung mit Neutronen (KFN)
Komitee Forschung mit Sonden und Ionenstrahlen (KFSI)

Local Organisers:
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Olaf Schwarzkopf, HZB
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Zita Hüsges, HZB
Sandra Fischer, HZB

Contact Local Organisers:
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Berlin, 25th August 2022

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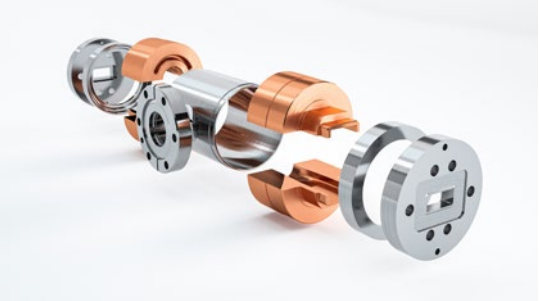

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SPECS Surface Nano Analysis GmbH
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WELCOME

Dear Participants of the SNI2022 Conference,

Since the last conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities, the SNI2018, has taken place in Garching, many of our fundamental believes have severely been shaken up. By the spread of Fake-News, putting in question knowledge as the basis for the decision of our society; by the increase in natural disasters occurring worldwide, bellwether of an accelerating global climate change; by the outbreak of the Covid-19 pandemic, now in its third year of putting at risk the health of humankind; and, this year, on February 24, by the attack of the Russian Federation on the Ukraine, overthrowing security and peace order in Europe and beyond.

In times like this, however, it is most important to proactively promote the progress which has been achieved towards finding, developing and ultimately implementing solutions against such global challenges. The SNI2022 conference offers us, the user community of large-scale Synchrotron Radiation, Neutron and Ion Beam research facilities, an opportunity to do so – to put forward the breadth of scientific and technological areas to which research at these world-wide outstanding facilities contributes to.

Towards this goal, the conference programme committee has put the focus of the meeting on the presentation and discussion of research achievements towards solutions for the global challenges we face. This includes, as non-exhaustive list, research for a carbon-neutral society, a sustainable energy system, energy-efficient information technologies and, last but not least, global health issues. Contributions cover thereby the entire breath of outstanding research from curiosity driven investigations of fundamental principles to application-oriented development of materials and devices.

These solution-oriented sessions will be complemented by methodological sessions, dedicated to the discussion of all current aspects of source, instrument, and technique development. Digitalisation and automation –from the source to the instrument, from the measurement process itself to an online data analysis in real-time– will thereby play a key role, as well as the discussion of novel machine learning algorithms and, more generally, of artificial intelligence-based approaches. Many of these developments rely on the sustainable funding within the ErUM framework of the Federal Ministry of Education and Research (BMBF), a world-wide unique tool to foster collaborations between University research groups and “their” facilities.

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A session dedicated to the interaction between facilities and industry, innovation and transfer completes the programme. Highlighting the societal relevance of research at large scale facilities will also be the topic of the public lecture, organised as part of the program of the SNI2022.

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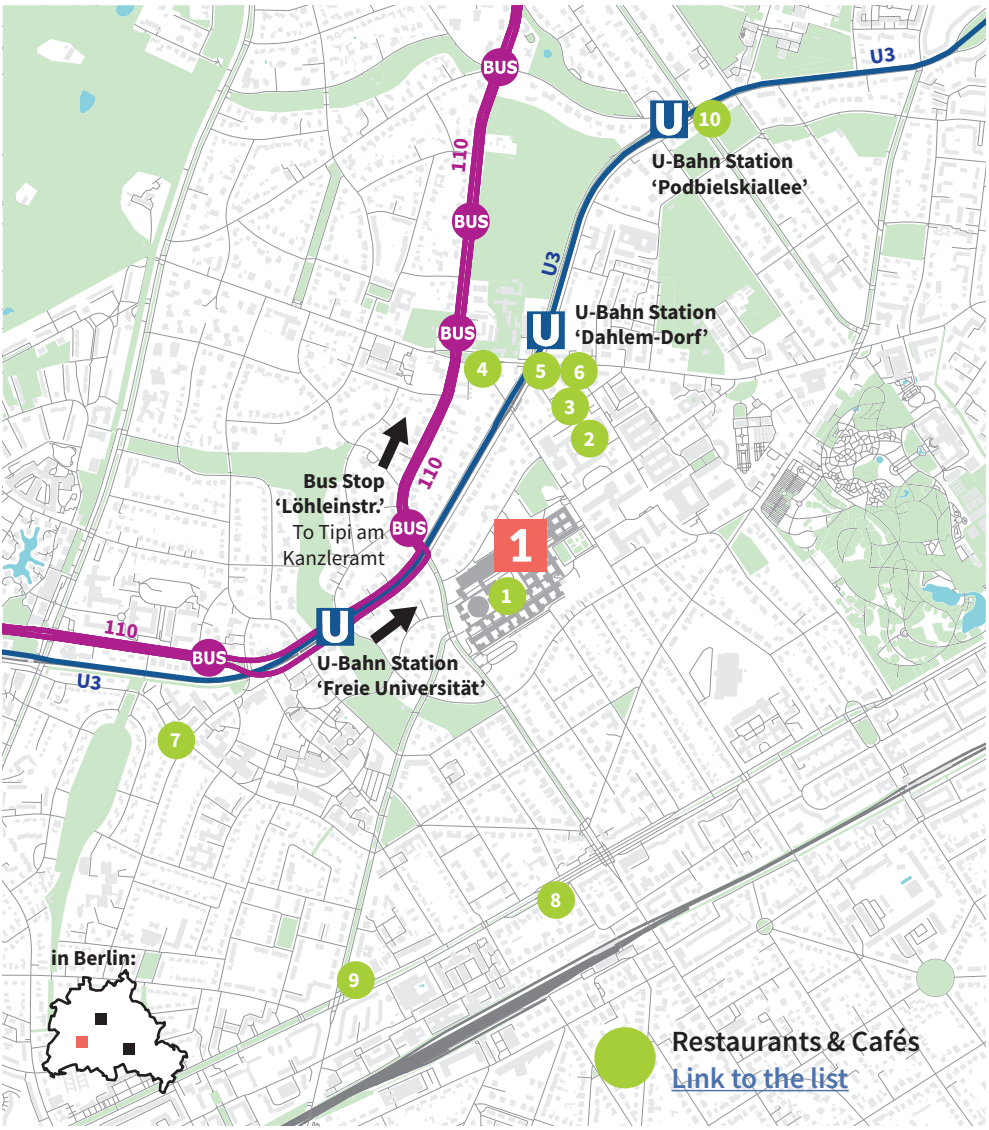
The local organizers, together with the chair persons of the KFS, KFN and KFSI, wish you all a very successful meeting, stimulating discussions, across disciplines and experimental techniques, resulting in many ideas for new ground-breaking research projects.

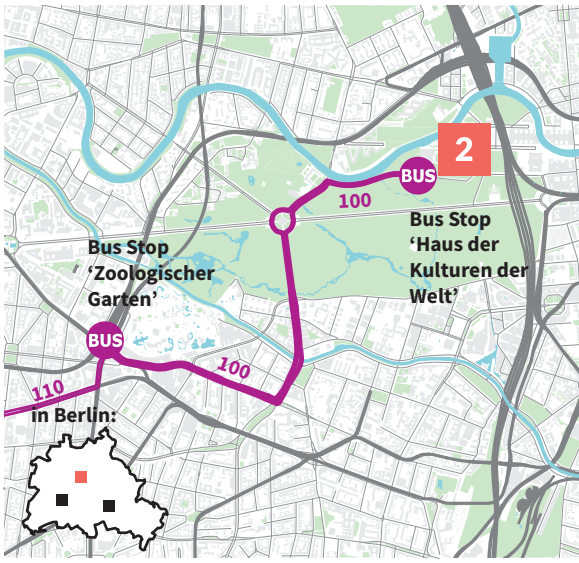
And, last but not least, enjoy your time in Berlin!

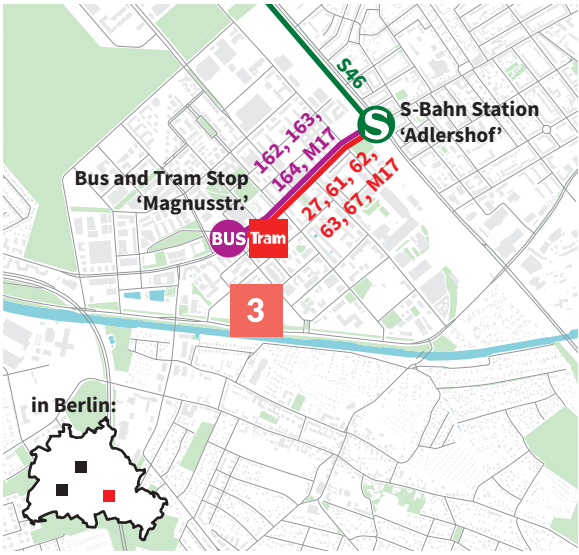
Welcome to SNI2022!

Jan Lüning
Conference Chair

LOCATION







1

SNI 2022, September 5th–7th, 2022
Freie Universität Berlin, Rostlaube
Habelschwerdter Allee 45
(Entrance: Thielplatz),
14195 Berlin-Dahlem

2

Reception, September 6th, 2022
"TIPI AM KANZLERAMT"
Große Querallee
(between "Kanzleramt" and
"Haus der Kulturen der Welt"),
10557 Berlin

3

Visit BESSY II, September 7th, 2022
BESSY II
Albert-Einstein-Straße 15,
12489 Berlin

RESTAURANTS IN THE AREA

	LOCATION	DISTANCE FROM THE CONFERENCE (BY FOOT)	ADDRESS	PRICE	TYPE	OPENING HOURS	LUNCH OFFER	TYPE OF CUISINE
1	**Mensa FU II*** (Payment by Conference bons or MensaCard only!)	0 min.	Otto-von-Simson-Str. 26, 14195 Berlin	€	Cafeteria	Mo. - Fr.: 8:00 a.m.–3:30 p.m. ; Lunch: Mo. – Fr.: from 11:00 a.m. – 2:30 p.m.	✓	Daily changing lunch offers and snacks
2	**“Eßkultur” Restaurant** at the Ethnological Museum	9 min.	Takustr. 38–40, 14195 Berlin	€€	Cafeteria	Mo. - Fr.: 12:00 p.m. – 3:00 p.m.	✓	International cuisine, daily changing lunch offers
3	**“Eßkultur” Cafeteria** at the Museum Dahlem	10 min.	Lansstr. 8, 14195 Berlin	€€	Cafeteria	Tue. - Thu.: 12:00 p.m. – 5:00 p.m.	✗	Pastries, Cake and Coffee
4	**“Alter Krug”**	11 min.	Königin-Luise- Straße 52, 14195 Berlin	€€	Restaurant	10:00 a.m. – 12:00 a.m.	✓	German cuisine
5	**Restaurant “Piaggio”**	11 min.	Königin-Luise-Straße 44, 14195 Berlin	€€	Restaurant	12:00 p.m. – 12:00 a.m.	✓	Italian cuisine
6	**"Luise" Gastronomie**	11 min..	Königin-Luise- Straße 40, 14195 Berlin	€€	Restaurant	10:00 a.m. – 1:00 a.m.	✓	German & Italian cuisine
7	Restaurant Cafe Creperie **“Aux Delices Normands”**	13 min.	Ihnestraße 29, 14195 Berlin	€€	Bistro	9:00 a.m. – 6:00 p.m.	✗	Fresh salads, soup, Crepes, German cuisine
8	**“Marinella”**	13 min.	Unter den Eichen 94, 12205 Berlin	€€	Restaurant	11:30 a.m. – 12:00 a.m.	✓	Italian cuisine: homemade pasta
9	**“Trattoria Romana”**	14 min.	Unter den Eichen 84 D, 12205 Berlin	€€	Restaurant	9:00 a.m. – 2:00 a.m.	✓	Italian cuisine
10	**“Eierschale”** Dahlem	22 min.	Podbielskialle 50, 14195 Berlin	€€	Restaurant	Su. - Thu.: 9:00 a.m. – 9:00 p.m. Fr. - Sa.: 10:00 a.m. – 4.00a.m.	✓	International cuisine: Pizza, Pasta, Burger, Ice Cream

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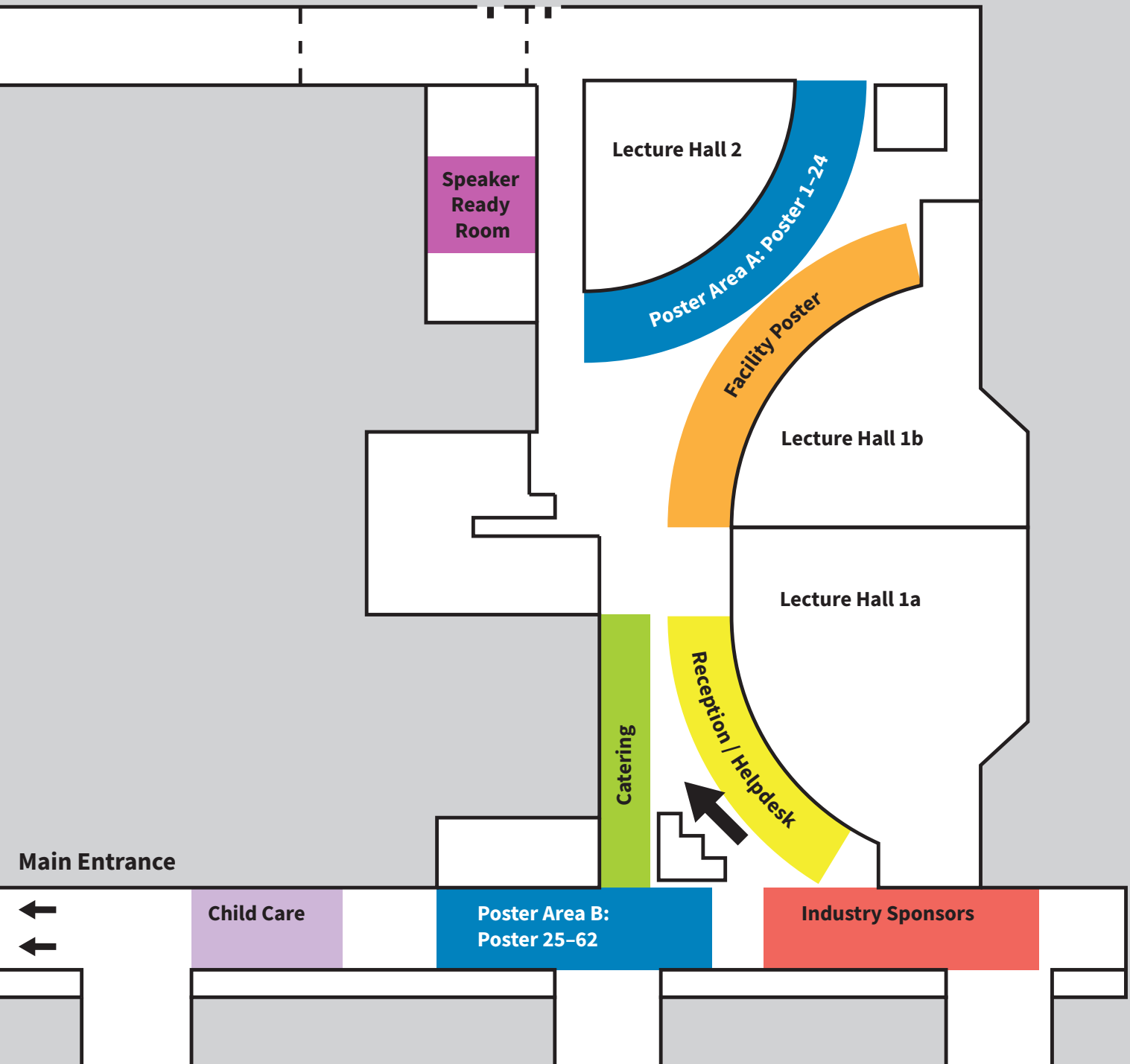
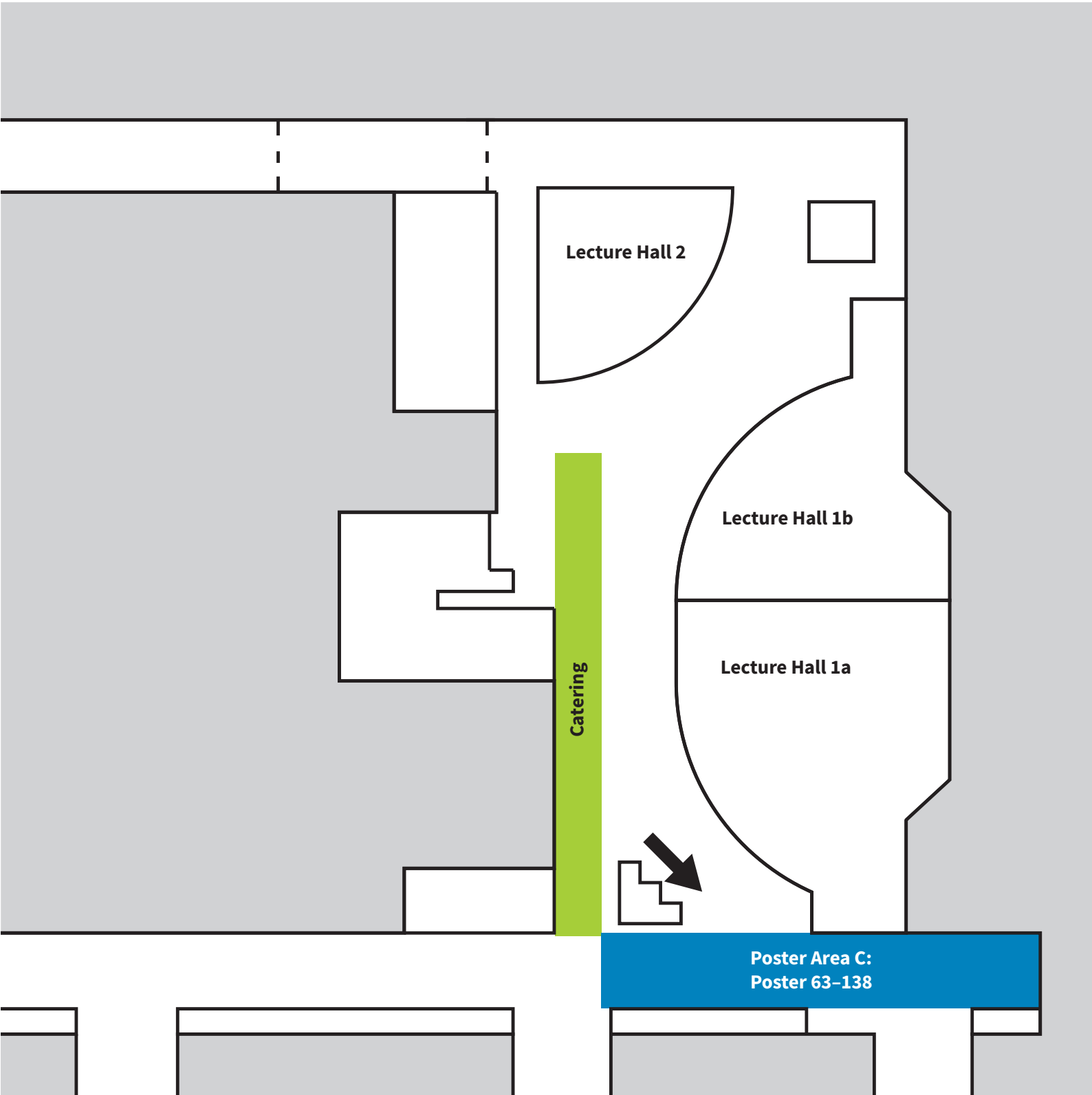
ROSTLAUBE | GROUND FLOOR



ROSTLAUBE | FIRST FLOOR

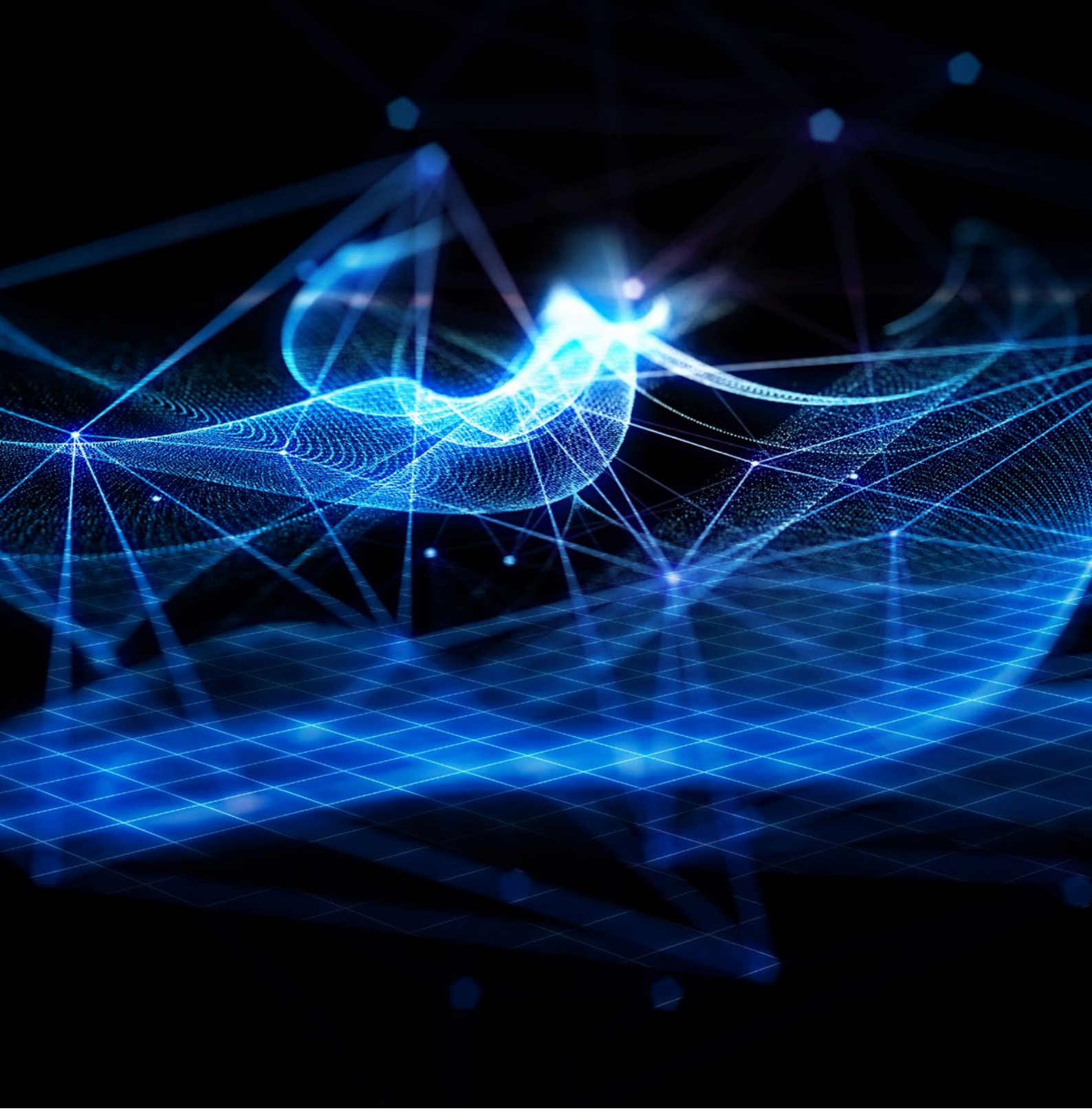


PROGRAMME
5TH – 7TH SEPTEMBER

TO OVERVIEW MONDAY, 5TH SEP.

TO OVERVIEW TUESDAY, 6TH SEP.

TO OVERVIEW WEDNESDAY, 7TH SEP.



MONDAY, 5TH SEPTEMBER

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PROGRAMME

08:00	*Registration*		
09:00	*Welcome*		
09:15	**PLENARY TALK | HS 1A** Structural Disorder in Photovoltaic Absorber Materials – Curse or Blessing for the Solar Cell? – *Susan Schorr (FU Berlin & HZB)*		
10:00	**PLENARY TALK | HS 1A** Ion-Track Nanotechnology: from the filter production to highly sensitive biomimetic sensors and energy materials – *Maria Eugenia Toimil-Morales (GSI)*		
10:45	*Coffee break*		
11:15	**PARALLEL SESSION | HS 1A** Methods & Instruments Development 1	**PARALLEL SESSION | HS 1B** Energy	**MICROSYMPOSIUM | HS 2** Data & Digitalization
12:45	*Lunch break*		
13:45	**KEYNOTE TALK | HS 1A** Unveiling the Dynamic Behavior of Catalysts through *In-Situ* Microscopy and *operando* Spectroscopy – *Beatriz Roldan Cuenya (FHI der MPG)*		
14:15	**MICROSYMPOSIUM | HS 1A** *In-situ* & *operando* Studies in Solid State Research	**MICROSYMPOSIUM | HS 1B** Earth, Environmental & Climate Sciences	**MICROSYMPOSIUM | HS 2** Artificial Intelligence for Large-scale Facilities
15:45	*Coffee break*		
16:15	**POSTER SESSION 1**		
18:15	*Break*		
19:00	**PUBLIC LECTURE | HS 1A** Materie im Licht von Großgeräten: von Nanometern und Femtosekunden – *Frank Schreiber (U Tübingen)*		

Instructions:
Tables of the day are linked to the sessions.
Tables of sessions are linked to the abstracts.

MON 9:15-10:00 | HÖRSAAL 1A | INV-01

PLENARY TALK

STRUCTURAL DISORDER IN PHOTOVOLTAIC ABSORBER MATERIALS – CURSE OR BLESSING FOR THE SOLAR CELL?

Presenter: Susan SCHORR
Author: Susan SCHORR (1,2)

Thin film solar cells, the most promising and cost-efficient PV technology, is based on compound semiconductors with a high absorption coefficient for sun light, such as Cu(In,Ga)Se2, organic metal halide perovskites or kesterites (Cu2ZnSn(S,Se)4). Solar cells based on the first two materials show very high power conversion efficiencies but contain very scarce elements (such as In) or very toxic elements (such as Pb), which would be problematic for their large-scale use. Kesterite-based thin film solar cells are considered as the only critical raw material free PV technology, but their efficiency is comparably lower. Finding alternative semiconductor materials with suitable properties (such as ternary nitrides) remains a task of utmost importance for the widespread use of renewable energies.

To understand the origin of the PV performance and stability it is essential to first understand the crystal structure and structural disorder (static and dynamic) in the absorber material. Kesterites as well the ternary nitride ZnGeN2 contain electronic similar elements which have a very similar atomic scattering factor. We make use of their different neutron scattering lengths enabling us to distinguish these elements in the crystal structure analysis by neutron powder diffraction. The organic part in hybrid halide perovskites makes neutrons particularly useful in such investigations given their sensitivity to hydrogen and ability to distinguish clearly between carbon and nitrogen.

Affillation
1: Helmholtz-Zentrum Berlin für Materialien und Energie, Department Structure and Dynamics of Energy Materials, Germany;
2: Freie Universitaet Berlin, Institute of Geological Sciences, Germany

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MON 10:00-10:45 | HÖRSAAL 1A | INV-02

PLENARY TALK

ION-TRACK NANOTECHNOLOGY: FROM THE FILTER PRODUCTION TO HIGHLY SENSITIVE BIOMIMETIC SENSORS AND ENERGY MATERIALS

Presenter: Maria Eugenia TOIMIL-MOLARES
Author: Maria Eugenia TOIMIL-MOLARES

The existing and future accelerator facilities at GSI and FAIR offer unique opportunities for interdisciplinary research. After a short insight into activities devoted to Materials Research with high-energy ions at GSI, the presentation focuses on current activities on ion track nanotechnology. On their way through matter, swift heavy ions with GeV energy deposit enormous energy densities along their trajectory, causing long nanoscopic damage trails known as ion tracks. Ion-track technology utilizes the small track size (few nm) combined with the extensive track length (up to 100 µm and more) to synthesize and control the properties of unique high aspect ratio nanostructures and, in particular, tailored nanochannels and nanowires. Several examples will illustrate the design and study of biomimetic nanopores and how electrodeposition and ion-track nanotechnology provide an excellent platform for studying the size-dependent properties of nanowires and developing unique 3-D and multi-component nanostructure assemblies. The arrangement of nanowires into stable 3-D architectures enables their implementation, e.g., in thermoelectric, catalytic, or sensing devices.

Affillation
GSI Helmholtzzentrum, Germany

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PARALLEL SESSION
MONDAY, 5TH SEPTEMBER

METHODS & INSTRUMENTS DEVELOPMENT 1			
Time	**Place**	**Presenter**	**Title**
Mon 11:15-11:30	Hörsaal 1a	Sergiu LEVCENKO	A novel XEOL spectroscopy setup at the X-ray absorption spectroscopy beamline P65 of PETRA III
Mon 11:30-11:45	Hörsaal 1a	Simon BODE	Developments in X-Ray Micro-Diffraction Imaging for the 3D Characterization of Crystal Defects
Mon 11:45-12:00	Hörsaal 1a	Sven TOLEIKIS	FLASH2020+: A fully coherent soft X-ray light source at MHz repetition rate
Mon 12:00-12:15	Hörsaal 1a	Michal KAMINSKI	Magnetic X-ray standing waves
Mon 12:15-12:30	Hörsaal 1a	Robert FARLA	New capabilities for high-pressure experiments at the Large Volume Press end-station P61B
Mon 12:30-12:45	Hörsaal 1a	Thales V. A. G. DE OLIVEIRA	Terahertz-driven nonlinear dynamics: New opportunities arising from accelerator-based THz sources

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MON 11:15-11:30 | HÖRSAAL 1A | MET1-01

PARALLEL SESSION

A NOVEL XEOL SPECTROSCOPY SETUP AT THE X-RAY ABSORPTION SPECTROSCOPY BEAMLINE P65 OF PETRA III

Presenter: Sergiu LEVCENKO
Authors: Sergiu LEVCENKO (1), Regina BILLER (2), Timo PFEIFFELMANN (1), Konrad RITTER (1), Hans H. FALK (1), Taowen WANG (3), Susanne SIEBENTRITT (3), Edmund WELTER (2), Claudia S. SCHNOHR (1)

X-ray excited optical luminescence (XEOL) with a synchrotron radiation source is a powerful tool to study the correlation between the radiative properties of a material and its structure and chemistry. By tuning the X-ray energy across an absorption edge of interest, XEOL can often provide an absorption spectrum and new insights into the origin of the luminescence. It is also of advantage to combine XEOL with a conventional X-ray absorption fine structure (XAFS) technique as it opens the possibility to answer the question whether element or site selectivity is observed in the XEOL data. Here, we describe the newly implemented setup to perform steady-state XEOL spectroscopy and simultaneous XEOL and XAFS characterization (2D-XEOL-XAFS) at beamline P65 of PETRA III, Hamburg, which delivers tunable hard X-ray photons in the range of 4 – 44 keV.

A state-of-the-art optical detection system offers a wide wavelength range of 300 – 1700 nm with a high spectral resolution and a customer designed He-flow cryostat allows a controlled sample temperature within the range of 5 – 300 K. The setup performance is illustrated by typical case studies, including the low temperature XEOL on polycrystalline CuInSe2 thin film, single crystalline GaN thin film and single crystalline ZnO bulk semiconductor samples. The presented examples will demonstrate that this setup will provide to the user community the basis for enhanced information from XEOL spectroscopy applied on various material systems.

Affillation
1: Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Germany; 2: Deutsches Elektronen-Synchrotron DESY, A Research Centre of the Helmholtz Association,Germany; 3: Laboratory for Photovoltaics, Department of Physics and Materials Science, University of Luxembourg, Luxembourg

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MON 11:30-11:45 | HÖRSAAL 1A | MET1-02

PARALLEL SESSION

DEVELOPMENTS IN X-RAY MICRO-DIFFRACTION IMAGING FOR THE 3D CHARACTERIZATION OF CRYSTAL DEFECTS

Presenter: Simon BODE
Authors: Simon BODE (1), Daniel HÄNSCHKE (1), Merve KABUKCUOGLU (1,2), Simon HAAGA (3), Elias HAMANN (1), Andreas DANILEWSKY (2), Tilo BAUMBACH (1,3)

The Karlsruhe Institute of Technology (KIT) continuously develops and applies 2D and 3D X-ray diffraction imaging techniques for the characterization of crystalline bulk materials. Combining topographic and tomographic principles, recently developed X-ray diffraction laminography (XDL) facilitates non-destructive 3D imaging of dislocation structures with µm-resolution in laterally extended samples like wafers.

Here, we report on a novel mobile set-up for flexible micro-diffraction imaging, enabling, e.g. XDL and rocking curve imaging. The set-up exhibits high angular and spatial precision and stability for both reciprocal and 3D tomographic real space sampling at the same time. In order to exploit a wide range of synchrotron beam properties, the set-up can be flexibly integrated into different beamline infrastructures and has already proven its capabilities at the KIT synchrotron, the ESRF, and PETRA III. Recent studies facilitated by the instrument allowed comparing experimental results with simulations based on a suitable theoretical approach describing the diffraction-based contrast formation. The obtained deeper understanding allowed enhancing the methodology and extending the capabilities of techniques like XDL, e.g. for accessing additional information about Burgers vectors directly from XDL data.

These recent methodical and instrumental developments will be presented by means of exemplary studies focusing on dislocation nucleation and evolution in semiconductor wafers.

Affillation
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MON 11:45-12:00 | HÖRSAAL 1A | MET1-03

PARALLEL SESSION

FLASH2020+: A FULLY COHERENT SOFT X-RAY LIGHT SOURCE AT MHz REPETITION RATE

Presenter: Sven TOLEIKIS
Author: Sven TOLEIKIS, for the whole FLASH2020+ team

FLASH is the only high-repetition-rate FEL in the XUV/soft X-ray regime worldwide. Based on superconducting accelerator technology developed at DESY, it can provide up to 8000 pulses/s for experiments in such diverse fields as atomic, molecular, and optical physics, chemistry, condensed matter and nanoscience, life science, warm dense matter research, and FEL physics and technology, including development of new methods and instrumentation.

With FLASH2020+, a major upgrade of the FLASH facility has started to meet the new requirements of the growing soft-x ray user community. The design of the FEL beamlines aims at photon properties suitable to the needs of future user experiments with high repetition rate XUV and soft X-ray radiation. By the end of the project, both existing FEL lines at FLASH will be equipped with fully tunable undulators capable of delivering photon pulses with variable polarization. The use of the external seeding at 1 MHz in burst mode is part of the design of the new FLASH1 beamline to provide fully coherent radiation, while FLASH2 will exploit novel lasing concepts based on different undulator configurations. The new FLASH2020+ will rely on an electron beam energy of 1.35 GeV that will extend the accessible wavelength range to the oxygen K-edge with variable polarization. The facility will be completed with new laser sources for pump and probe experiment and new experimental stations.

Affillation
DESY, Germany

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MON 12:00-12:15 | HÖRSAAL 1A | MET1-04

PARALLEL SESSION

MAGNETIC X-RAY STANDING WAVES

Presenter: Michal KAMINSKI
Authors: Michal KAMINSKI, Heiko SCHULZ-RITTER, Martin TOLKIEHN

A new method for studying the magnetic structures of crystalline materials at the atomic level is reported. A completely new perspective appears due to the combination of the site-selectivity of the diffraction-based X-ray standing waves (XSW) technique and sensitivity to magnetic properties of the X-ray magnetic circular dichroism (XMCD) spectroscopy. The XSW method makes use of the standing wave appearing as a result of an interference between the incoming and the Bragg reflected electromagnetic waves. In the magnetic X-ray standing waves (MXSW) technique, a circular polarisation of the incoming beam is used to additionally gain magnetic information via the dichroism in the absorption of the standing wave. Due to the utilisation of the X-ray interference field, the phase information is preserved, so the magnetic structure can be studied directly. When the magnetic atoms are located on some non-equivalent positions, a standing wave with appropriate periodicity, which moves across the lattice as the sample is rocked through the reflection domain, can enhance the contribution of one sublattice and decrease the impact of the other one, thus causing a modulation in the XMCD signal. The shape of modulation is characteristic for a given distribution of the magnetic moments and yields directly a structural information. In the presentation, the MXSW theory based on the dynamical theory of X-ray diffraction, as well as first experimental results, will be presented.

Affillation
DESY Hamburg, Germany

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Back to programme Monday, 5th September

MON 12:15-12:30 | HÖRSAAL 1A | MET1-05

PARALLEL SESSION

NEW CAPABILITIES FOR HIGH-PRESSURE EXPERIMENTS AT THE LARGE VOLUME PRESS END-STATION P61B

Presenter: Robert FARLA

Authors: Robert FARLA (1), Shrikant BHAT (1), Adrien NERI (2), Shuailing MA (1,3), Artem CHANYSHEV (2), Kristina SPEKTOR (1,4), Christian LATHE (1,5), Stefan SONNTAG (1), Tomoo KATSURA (2)

At the end-station P61B of the high-energy wiggler beamline at PETRA III, a Large Volume Press (LVP) 'Aster-15' is installed and operational for user experiments at high pressures and temperatures (HPT: 30 GPa, 2300 K) to solve big questions in Earth / Materials sciences and High-P Chemistry. The standard setup features 2 Ge-detectors for energy-dispersive X-ray diffraction (ED XRD) at 30 – 160 keV, and a white-beam microscope for radiography. Using various anvil-cell assemblies, mm-sized polycrystalline samples can be investigated in the LVP to document phase relations in-situ, as well as physical properties such as viscosity. Recently, two new techniques have been developed for the LVP, ultrasonic interferometry and acoustic emissions (AE) detection. The first method features a piezo-sensor that transmits pulses and receives echoes at specific MHz sine-wave frequencies to measure the two-way travel time in the sample at HPT. Combined with length measurements of the sample by radiography, the wave speeds are calculated and compared to seismic wave propagation in the Earth's interior. The second newly available technique, at HPT and stress conditions, uses specialized AE sensors on all anvils to detect and localize events in samples prone to brittle behavior caused by processes such as dehydration reactions or phase changes. Furthermore, a dedicated glovebox is available to prepare assemblies in a controlled atmosphere for sensitive materials, such as nitrides and hydrides.

Affillation

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MON 12:30-12:45 | HÖRSAAL 1A | MET1-06

PARALLEL SESSION

TERAHERTZ-DRIVEN NONLINEAR DYNAMICS: NEW OPPORTUNITIES ARISING FROM ACCELERATOR-BASED THz SOURCES

Presenter: Thales V. A. G. DE OLIVEIRA
Authors: Thales V. A. G. DE OLIVEIRA, Jan-Christoph DEINERT, Sergey KOVALEV

Strong-field terahertz (THz) radiation offers a direct way to resonantly drive highly relevant low-energy modes in matter, e.g., lattice vibrations, molecular rotations, spin precession and the motion of (quasi-) free electrons. Using these pulses as a pump in ultrafast experiments enables the study of dynamic processes in solid-state, chemical and eventually biological systems. The TELBE THz facility at Helmholtz-Zentrum Dresden-Rossendorf (HZDR) is a strong-field THz-source offering multicycle, CEP stable THz pulses with an exceptionally high spectral density at a repetition rate up to 500 kHz. Therefore, TELBE is ideally suited for the research on THz-driven nonlinear dynamics and resonant control of a number of low-energy degrees of freedom. In this contribution, we present recent scientific results on nonlinear THz frequency conversion, spin dynamics and superconductor spectroscopy. In addition, we present a newly developed synchronization technique used at TELBE, which enabled nanoscale imaging and local spectroscopy with high-field THz excitation.

Affillation
Helmholz-Zentrum Dresden-Rossendorf, Germany

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PARALLEL SESSION
MONDAY, 5TH SEPTEMBER

ENERGY			
Time	**Place**	**Presenter**	**Title**
Mon 11:15-11:30	Hörsaal 1b	Claudia S. SCHNOHR	Elucidating the local structure of V substitutes in In2S3 for intermediate band thin film solar cells
Mon 11:30-11:45	Hörsaal 1b	Juanita HIDALGO	Unraveling low-temperature dependent phase transitions in methylammonium-free lead halide perovskites by in-situ X-ray diffraction
Mon 11:45-12:00	Hörsaal 1b	Tolga Han ULUCAN	Operando Characterization Studies of Ni and Co Based Ammonia Decomposition Catalysts
Mon 12:00-12:15	Hörsaal 1b	Simone MASCOTTO	Mechanistic understanding of metal nanoparticle formation via exsolution
Mon 12:15-12:30	Hörsaal 1b	Tommy HOFMANN	Hybrid Thermoelectric Materials Based on Porous Silicon: Linking Macroscopic Transport Phenomena to Microscopic Structure and Elementary Excitations
Mon 12:30-12:45	Hörsaal 1b	Jan-Dierk GRUNWALDT	New Opportunities of Synchrotron Light for Unraveling Dynamics and Bridging the Complexity Scales in Catalysis

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MON 11:15-11:30 | HÖRSAAL 1B | ENER-01

PARALLEL SESSION

ELUCIDATING THE LOCAL STRUCTURE OF V SUBSTITUTES IN In2S3 FOR INTERMEDIATE BAND THIN FILM SOLAR CELLS

Presenter: Claudia S. SCHNOHR

Authors: Elaheh GHORBANI (1), Martin SCHILLER (2,3), Hans H. FALK (2), Leonard A. WÄGELE (3), Stefanie ECKNER (2), Francesco D'ACAPITO (4), Roland SCHEER (3), Karsten ALBE (1), Claudia S. SCHNOHR (2)

Intermediate band solar cells have been proposed as a promising route to overcome the intrinsic efficiency limit of single junction solar cells. A potential intermediate band absorber material is vanadium doped indium sulfide, In2S3:V. Based on electronic considerations, it is usually assumed that V occupies octahedrally coordinated In sites, although geometrical considerations would favor tetrahedral In sites. In this study, we have therefore combined experimental X-ray diffraction and X-ray absorption spectroscopy with ab initio theoretical calculations to elucidate the incorporation of V in In2S3:V thin films grown with different V content and different growth temperatures. Both, experiment and theory, show that the lattice constant decreases with increasing V content. Furthermore, the crystallinity of the material diminishes upon V incorporation. Most importantly, though, (i) comparing the shape and position of the measured and calculated X-ray absorption edge of V, (ii) comparing experimentally determined and calculated V-S bond lengths, and (iii) evaluating the calculated heat of solution of V on different lattice sites all indicate that V is incorporated on octahedral rather than tetrahedral lattice sites in the In2S3 matrix. For this material system, the electronic benefit of octahedral coordination thus indeed outweighs the mechanical stress induced by the significant local lattice relaxation associated with incorporation of V on octahedral In sites.

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MON 11:30-11:45 | HÖRSAAL 1B | ENER-02

PARALLEL SESSION

UNRAVELING LOW-TEMPERATURE DEPENDENT PHASE TRANSITIONS IN METHYLAMMONIUM-FREE LEAD HALIDE PEROVSKITES BY IN-SITU X-RAY DIFFRACTION

Presenter: Juanita HIDALGO
Authors: Juanita HIDALGO (1,2), Joachim BRETERNITZ (1), Susan SCHORR (1)

Lead halide perovskites have shown to be excellent candidates for solar energy conversion. Methylammonium-free compositions have demonstrated higher thermal stability and an optimal bandgap compared to the prototypical CH3NH3PbI3 (MAPI) [1]. Given that compositional mixing has been a strategy to achieve the optimal optoelectronic properties, it is necessary to unravel the structural phases for the mixed-ion perovskites in a wide range of operating temperatures, such as very low temperatures for space applications. Herein, we explored the structure of methylammonium-free CsyFA1-yPb(BrxI1-x)3 by low-temperature in-situ powder X-ray diffraction at the beamline KMC-2 (BESSY II, at the HZB) for a set of temperatures from 23 K to 300 K. We observed that as the I- anion was substituted by Br-, the transformation into non-perovskite phases was suppressed. In addition, different phase transition temperatures were seen as the Br content increased. In general, the phase transition pathways in methylammonium-free lead halide perovskites were highly dependent on composition. Hence, a phase diagram for the set of studied compositions was elaborated. This fundamental structural understanding provides the basis for the design of more robust and efficient energy materials to function at a broad range of extreme temperature conditions.

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[1] An, Y.; Hidalgo, J.l; et al. Structural Stability of Formamidinium- And Cesium-Based Halide Perovskites. ACS Energy Lett. 2021, 6 (5), 1942–1969

Affillation
1: Helmholtz-Zentrum Berlin für Materialien und Energie; 2: School of Materials Science and Engineering, Georgia Institute of Technology, USA

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MON 11:45-12:00 | HÖRSAAL 1B | ENER-03

PARALLEL SESSION

OPERANDO CHARACTERIZATION STUDIES OF Ni AND Co BASED AMMONIA DECOMPOSITION CATALYSTS

Presenter: Tolga Han ULUCAN
Authors: Tolga Han ULUCAN (1), Jihao WANG (2), Jan TERNIEDEN (1), Malte BEHRENS (2), Claudia WEIDENTHALER (1)

The efficient storage of H2 in a perspective hydrogen economy is still an unsolved problem. Among others, ammonia (NH3) is regarded as a promising H2 carrier molecule that can be used for the on-site generation of H2 for fuel cells or directly in NH3 solid-oxide-fuel cells. Previous studies on NH3 decomposition catalysts showed high complexity of structure-property relationships. Several factors, e.g., catalyst structure, crystallite size, microstructure, or amorphous phases, can significantly influence the catalytic properties. In this study, Ni and Co catalysts on MgO support were synthesized via the conventional co-precipitation method. 10 and 20 at. % metal loaded catalysts with different pre-conditioning treatments were characterized by several ex-situ methods and tested for their performance in the decomposition of NH3 in a conventional plug-flow reactor.

Operando total scattering experiments during temperature-dependent NH3 decomposition were conducted at P02.1 at DESY. A special gas-flow cell connected to a gas dosing system and a mass spectrometer for product gas analysis has been used.

Ex-situ XAFS experiments were performed at P65 (DESY) to investigate the local structures around Co and Ni atoms. The combination of different characterization data enables structure investigations on different length scales. The structure-performance relations give insights into how different catalysts and processing conditions affect the catalytic activity for NH3 decomposition.

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MON 12:00-12:15 | HÖRSAAL 1B | ENER-04

PARALLEL SESSION

MECHANISTIC UNDERSTANDING OF METAL NANOPARTICLE FORMATION VIA EXSOLUTION

Presenter: Simone MASCOTTO
Authors: Simone MASCOTTO, Benedikt EHRHARDT, Benjiamin RUDOLPH, Filippo COLOMBO

The process of metal exsolution attracts since several years the interest of the scientific community because it represents a smart approach to prepare advanced metal-oxide nanocomposites through dopant segregation from a mixed conducting oxide matrix for applications in energy conversion, catalysis, and data storage. However, little is known about the formation mechanism of exsolved metal nanoparticles, and particularly about the interplay between the different steps of the process, i.e. dopant reduction, nucleation and nanoparticle growth. To tackle this, synchrotron methods represent a unique opportunity because they enable comprehensive understanding of the nanoparticle segregation process due to their high statistical significance and real-time operation.

In the present paper, the analysis of the exsolution of mono and bimetallic nanoparticles will be addressed by combining in-situ small-angle X-ray scattering (SAXS), X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS). Due to the high complementary character of these techniques it was possible to understand the correlation between the reduction and growth mechanisms during the exsolution of bimetallic Fe-Ni nanoparticles. Also, the use of SAXS combined with XRD enabled to obtain information about the size, shape and distribution of both surface- and bulk-segregated nanoparticles in powder and thin-film materials, providing insightful morphological information at different scales.

Affillation
University of Hamburg, Germany

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MON 12:15-12:30 | HÖRSAAL 1B | ENER-05

PARALLEL SESSION

HYBRID THERMOELECTRIC MATERIALS BASED ON POROUS SILICON: LINKING MACROSCOPIC TRANSPORT PHENOMENA TO MICROSCOPIC STRUCTURE AND ELEMENTARY EXCITATIONS

Presenter: Tommy HOFMANN

Authors: Tommy HOFMANN (1), Natalia GOSTKOWSKA-LEKNER (1,2), Haider HASEEB (1,2), Manfred MAY (3), Patrick HUBER (3), Klaus HABICHT (1,2)

Organic-inorganic hybrids are a novel class of thermoelectric materials that obtained increasing attention in recent years. It is envisioned to exploit complementary thermal and electronic properties of organic and inorganic materials to excel the thermoelectric performance of the individual constituents. Here, we present macroscopic transport measurements and microscopic scattering studies on structure and dynamics on hybrids that combine mesoporous silicon with 10 nm wide pores and the conducting polymer P3HT. These studies are part of the DFG-funded research project #402553194.

After a brief project description, the first part of the presentation focuses on macroscopic electronic transport measurements that elucidate a thermally activated charge transport in mesoporous silicon. A Meyer-Neldel rule becomes evident and points towards multi-phonon assisted hopping as microscopic transport mechanism. Inelastic neutron scattering studies are at the forefront of the second part of our contribution. They probe the phonon dispersion of porous Si across the Brillouin zone and are an important step towards a comprehensive understanding of thermal transport in porous silicon. The final part of the presentation provides a detailed account on charge transport in the hybrids. In this context, grazing incidence wide-angle X-ray scattering experiments shall reveal the relevance of the P3HT morphology in mesoporous silicon for conductive pathways in the hybrids.

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MON 12:30-12:45 | HÖRSAAL 1B | ENER-06

PARALLEL SESSION

NEW OPPORTUNITIES OF SYNCHROTRON LIGHT FOR UNRAVELING DYNAMICS AND BRIDGING THE COMPLEXITY SCALES IN CATALYSIS

Presenter: Jan-Dierk GRUNWALDT
Authors: Florian MAURER, Jan-Dierk GRUNWALDT

Heterogeneous catalysis is the key for the sustainable production of chemicals, clean air, and energy conversion technologies. This is also closely related to minimizing CO2-emissions and the energy transition. The energy transition to renewable resources is a major challenge, which cannot be achieved by the current catalytic processes. New catalysts need to be discovered and developed in a knowledge-based way. However, the structure of catalysts steadily changes, especially under working conditions. Furthermore, the active site is usually part of a complex environment. Synchrotron light is hereby essential for a rational design and with each generation of new synchrotron light sources a new impetus has been found to catalysis.

Examples both from chemical energy storage (priority program SPP2080, www.spp2080.org) and emission control (collaboration research center CRC1441 “TrackAct”, www.trackact.kit.edu) will be presented demonstrating that synchrotron radiation sources including in-situ and *operando* studies are the key for understanding the dynamics and to further develop catalysts. Synchrotron radiation also allows to cover better and better the various complexity scales in terms of time and length (atomic scale information to mm/cm/m-scale). Hence, both time-resolved, new spectroscopic and new microscopic techniques are required.

Affillation
Karlsruhe Institute of Technology, Germany

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MICROSYMPOSIUM

MONDAY, 5TH SEPTEMBER

DATA & DIGITALIZATION			
Time	**Place**	**Presenter**	**Title**
Mon 11:15-11:45	Hörsaal 2	Bridget MURPHY	DAPHNE4NFDI: DAta from PHoton and Neutron Experiments for NFDI
Mon 11:45-12:00	Hörsaal 2	Astrid SCHNEIDEWIND	ErUM – Data. An initiative on digital transformation in science performed at Large Scale Facilities
Mon 12:00-12:15	Hörsaal 2	Oonagh MANNIX	Making metadata manageable – lessons learned in HMC Hub Matter
Mon 12:15-12:30	Hörsaal 2	Tobias RICHTER	Data Management and Data Analysis Activities for Photon and Neutron Science in Europe
Mon 12:30-12:45	Hörsaal 2	Christoph KOCH	Enabling the digitalization of experimental materials science

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MON 11:15-11:45 | HÖRSAAL 2 | DATA-01

MICROSYMPOSIUM

DAPHNE4NFDI: DATA FROM PHOTON AND NEUTRON EXPERIMENTS FOR NFDI

Presenter: Bridget MURPHY
Authors: Anton BARTY (1), Lisa AMELUNG (1), Christian GUTT (2), Astrid SCHNEIDEWIND (3), Wiebke LOHSTROH (4), Jan-Dierk GRUNWALDT (5), Sebastian BUSCH (6), Tobias UNRUH (7), Frank SCHREIBER (8), Bridget MURPHY (9)

The photon and neutron science community encompasses users from a broad range of scientific disciplines. With the advent of high-speed detectors and increasingly complex instrumentation, the community faces a common need for high-level rapid data analysis and the challenge of implementing research data management for increasingly large and complex datasets. The aim of DAPHNE4NFDI is to create a comprehensive infrastructure to process data from photon and neutron infrastructures according to the FAIR principles (Findable, Accessible, Interoperable, Reusable).

DAPHNE4NFDI brings together users representing key scientific application domains with the large-scale research facilities in photon and neutron science in order to advance the state of data management in the community. Key tasks to be addressed in DAPHNE4NFDI are:

1) Improve metadata capture through consistent workflows supported by user-driven online logbooks that are linked to the data collection;

2) Establishment of community repositories processed data, new reference databases and analysis code for published results, linked, where possible, to raw data sources, to sustainably improve access to research data;

3) Develop, curate and deploy user-developed analysis software on facility computing infrastructure through common data analysis portals.

Financed through the DFG National Research Data Infrastructure programme, DAPHNE4NFDI aims to have impact across the wider European and international photon and neutron community.

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MON 11:45-12:00 | HÖRSAAL 2 | DATA-03

MICROSYMPOSIUM

ErUM – DATA. AN INITIATIVE ON DIGITAL TRANSFORMATION IN SCIENCE PERFORMED AT LARGE SCALE FACILITIES

Presenter: Astrid SCHNEIDEWIND
Authors: Astrid SCHNEIDEWIND (1), Martin ERDMANN (2)

ErUM is a BMBF framework on Universe and Matter oriented research requesting large instruments: Astroparticle Physics, Elementary Particle Physics, Accelerator Physics, Hadron and nuclear Physics, Astronomical Research and Research with Synchrotron Radiation, with Nuclear Probes and Ion Beams and Research with Neutrons.

ErUM-Data sets the stage for successful future research in the named fields on facilities with German contribution. Exploiting and developing digital techniques creates new opportunities for research and recognition, and speeds up the innovation processes. Connecting the relevant communities and structures strengthens the digital competences, boosts the efficiency and speeds up developments. Joint effort multiplies the outcome and increases the impact on the society and on other research areas, but also the awareness on the potential of digital transformation.

In a first step, projects on software and algorithms, AI / ML are under evaluation for funding. The ErUM-Data-Hub, as the central networking and transfer point supporting scientists, was stablished in April 2022. Now, our work focuses on strengthening the synergies between the ErUM-Data and NFDI initiatives; future BMBF calls on research data management and infrastructures will be strategically prepared. In addition, ErUM-Data-Hub offers a series of training workshops on AI/ML for beginners as well training future trainers.

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MON 12:00-12:15 | HÖRSAAL 2 | DATA-04

MICROSYMPOSIUM

MAKING METADATA MANAGEABLE – LESSONS LEARNED IN HMC HUB MATTER

Presenter: Oonagh MANNIX
Authors: Oonagh MANNIX (1,2), Gerrit GÜNTHER (1,2), Markus KUBIN (1,2), Luigia CRISTIANO (1,2), Gabriel PREUSS (1,2), Vivien SERVE (1,2), Pascal WALTER (1,2), Heike GÖRZIG (1), Ants FINKE (1,2)

In the Helmholtz Metadata Collaboration (HMC) Hub Matter we strive to make metadata manageable by improving the capacity of infrastructure to engage with researchers, and by improving the capacity of researchers to engage with infrastructure.

This is achieved through information gathering using both quantitative and qualitative methods to identify gaps in capacity and infrastructure. We construct technical bridges between infrastructure and researchers by working on concrete use cases [1], and bridge the gap between researchers and infrastructure through training and community building.

In our presentation we provide an overview of the hub activities, and the activities of the wider HMC platform. Along the way you will get an idea of how to make your own metadata manageable and how HMC can support you with this.

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[1] https://doi.org/10.18429/JACoW-ICALEPCS2021-WEBL05

Affillation
1: Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; 2: Hub Matter Helmholtz Metadata Collaboration

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MON 12:15-12:30 | HÖRSAAL 2 | DATA-05

MICROSYMPOSIUM

DATA MANAGEMENT AND DATA ANALYSIS ACTIVITIES FOR PHOTON AND NEUTRON SCIENCE IN EUROPE

Presenter: Tobias RICHTER
Author: Tobias RICHTER

FAIR data has been on the agenda by funding agencies for a long time. At the same time datasets from experiments increase in number and volume. Keeping track of data and the compute power required put a strain on many users of large scale facilities. To support scientists the European Open Science Cloud is taking shape in many disciplines. Most of the funding comes in the form of time limited projects and the communities are expected to provide a path to sustain these efforts. This approach comes with some advantages and challenges. With PaNOSC and ExPaNDS two large collaborations in the field of photon and neutron science come to an end soon.

The presentation will provide an overview of ongoing work for services in data cataloguing, curation, sharing/publication, processing and analysis. This will detail some of the ongoing challenges. In addition there will be an outlook of how and where work can hopefully continue.

Affillation
European Spallation Source, Sweden

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MON 12:30-12:45 | HÖRSAAL 2 | DATA-06

MICROSYMPOSIUM

ENABLING THE DIGITALIZATION OF EXPERIMENTAL MATERIALS SCIENCE

Presenter: Christoph KOCH
Authors: Christoph KOCH, Markus KÜHBACH, Sherjeel SHABIH, Sandor BROCKHAUSER, Claudia DRAXL

Experimentally exploring the properties and uses of materials and improving them for particular purposes has been a major driving force for advancing the way people live over the last millennia. Materials characterization techniques have now reached the level of detail that makes them converge with ab-initio computations based on fundamental building blocks: atoms and the electrons they share. During the last decades computers have surpassed the capacity of humans in the extraction of patterns in large amounts of data. It is thus a very natural consequence to involve their strengths also in further accelerating materials development and our capability of gaining knowledge of the fundamental physics and chemistry of materials. However, while it may be a very obvious idea to digitalize materials science, a number of obstacles must be overcome for this to have a chance to realize on a large (global) scale.

In this talk we will introduce the activities of the NFDI-consortium FAIRmat in enabling and promoting the digitalization of experimental materials data by establishing standards and tools for collecting necessary metadata to reproducibly describe the different steps involved in acquiring and processing experimental data. [1] Using illustrative examples, we will also highlight the importance of providing state-of-the-art community-specific online data processing capabilities, in order to encourage laboratories to invest and participate in this process.

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[1] Nature 604 (2022) 635

Affillation
Humboldt-Universität zu Berlin, Germany

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Back to programme Monday, 5th September

MON 13:45-14:15 | HÖRSAAL 1A | INV-03

KEYNOTE TALK

UNVEILING THE DYNAMIC BEHAVIOR OF CATALYSTS THROUGH IN-SITU MICROSCOPY AND OPERANDO SPECTROSCOPY

Presenter: Beatriz ROLDAN CUENYA
Author: Beatriz ROLDAN CUENYA

Climate change concerns have spurred a growing interest in developing environmentally friendly technologies for energy generation (i.e. green H2 from water splitting) and to re-utilize CO2 in thermal catalysis applications where it is reacted with green H2 to produce methanol and high-order hydrocarbons. Moreover, the electrochemical reduction of CO2 into value-added chemicals and fuels offers an additional possibility to store renewable energy. It is of particular interest to develop efficient, selective and durable (electro)-catalysts that can operate under mild reaction conditions. This requires a fundamental understanding of their structure and surface composition under reaction conditions.

This talk will make use of a multi-technique in-situ/*operando* experimental approach to provide new insights into thermal and electrochemical conversion of CO2, as well as the oxygen evolution reaction. Aspects that will be discussed include: (i) the design of size- and shape-controlled catalytically active nanoparticle (NP) pre-catalysts, (ii) the understanding of the active state formation, (iii) the correlation between the dynamically evolving structure and composition of the (electro-)catalysts under *operando* reaction conditions and their catalytic performance, (iv) the role of the support on the activity and selectivity. Our studies are expected to open up new routes for the reutilization of CO2 through its direct conversion into industrially valuable chemicals and fuels.

Affillation
Fritz Haber Institute of the Max Planck Society, Germany

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MICROSYMPOSIUM

MONDAY, 5TH SEPTEMBER

IN-SITU AND OPERANDO STUDIES IN SOLID-STATE RESEARCH			
Time	**Place**	**Presenter**	**Title**
Mon 14:15-14:30	Hörsaal 1a	Mahmoud AL HUMAIDI	Impact of the substrate temperature on the shell growth and bending direction of core-shell nanowires
Mon 14:30-14:45	Hörsaal 1a	Patrick ZELLER	In-situ/operando characterization of solid-liquid electrified interfaces with total electron yield
Mon 14:45-15:00	Hörsaal 1a	Christoph HUGENSCHMIDT	In-situ spectroscopy and imaging of lattice defects using positron annihilation
Mon 15:00-15:15	Hörsaal 1a	Kristina SPEKTOR	In-situ studies of hydrogenation reactions and phase relations of hydrogen-rich hydrides at gigapascal pressures by synchrotron and neutron diffraction
Mon 15:15-15:30	Hörsaal 1a	Anatoliy SENYSHYN	Lithium distribution and transfer in high-power 18650-type Li-ion cell at multiple length scales
Mon 15:30-15:45	Hörsaal 1a	Paolo DOLCET	Tracking Pt single sites on ceria using advanced operando X-ray techniques

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MON 14:15-14:30 | HÖRSAAL 1A | OPER-01

MICROSYMPOSIUM

IMPACT OF THE SUBSTRATE TEMPERATURE ON THE SHELL GROWTH AND BENDING DIRECTION OF CORE-SHELL NANOWIRES

Presenter: Mahmoud AL HUMAIDI
Authors: Mahmoud AL HUMAIDI (1), Jochen KALT (1), Ali ALHASSAN (1), Dmitri NOVIKOV (2), Ullrich PIETSCH (3), Tilo BAUMBACH (1,4)

Nanowire bending can be obtained by performing no rotation of the nanowire core during deposition of a lattice-mismatched shell [1]. This bending offers an approach for strain engineering and fabrication of nanowires with novel geometries. The variation of the axial strain magnitude across the nanowire diameter induces charge carrier drifting toward the tensily strained regions, resulting in an electron-hole separation which can be beneficial for photonic and photoelectric applications [2]. Additionally, the direction of the nanowire bending determines the polarization of the emitted light in an excited core-shell system [3]. Therefore, the understanding and the ability of controlling the shell growth distribution around the nanowire core and the resulting nanowire curvature is essential for engineering of the nanowire bending. In this work we report on the determination of the GaAs-(In,Ga)As core-shell nanowire bending direction with respect to the flux direction of the growth materials in a molecular beam epitaxy (MBE) reactor. Our findings were observed using scanning electron microcopy and in-situ X-ray diffraction measurements and give an insight onto the strain variation in the bent nanowires.

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[1] M. Al-Humaidi, et.al., Nanotechnology 33 015601 (2022)
[2] F. Boxberg , et.al., Nano Letters, 10, 1108–1112 (2010)
[3] R. B. Lewis, et.al., Nano Letters, 18 2343 (2018)

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MON 14:30-14:45 | HÖRSAAL 1A | OPER-02

MICROSYMPOSIUM

IN-SITU/OPERANDO CHARACTERIZATION OF SOLID-LIQUID ELECTRIFIED INTERFACES WITH TOTAL ELECTRON YIELD

Presenter: Patrick ZELLER
Authors: Juan J. VELASCO VÉLEZ, Patrick ZELLER

Most of the electrochemistry processes occur within a thin layer of water or solution at the electrolyte/electrode interfaces, commonly denoted as the electrical double layer (EDL). Surface sensitive techniques based in electron detection are not easily applicable in presence of liquids due to the short inelastic mean free path (IMFP) of the photoelectrons. In spite, the total fluorescence yield (TFY) detection technique is considered as bulk sensitive and is commonly used in-situ X-ray absorption spectroscopy (XAS) characterization due to its simplicity to use. Meanwhile the total electron yield (TEY) is considered surface sensitive but it is not easily applicable in *operando* electrochemical experiments with aqueous electrolyte. In order to understand the process that take part within the EDL, we have developed over the years different in-situ X-ray absorption spectroscopy (XAS) approaches based in TEY mode detection technique to characterize the species present at the liquid/electrode interfaces under relevant electrochemical conditions. Using two different approaches based in the use of thin film graphene membranes and in the synchronous lock-in detection of the TEY we were able to overcome these limitations. In this talk, we will illustrate the operation of these approaches with an example of the electrodeposition of copper onto the working electrode. The right system operation will be validated with complementary in-situ electron spectroscopy measurements.

Affillation
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MON 14:45-15:00 | HÖRSAAL 1A | OPER-03

MICROSYMPOSIUM

IN-SITU SPECTROSCOPY AND IMAGING OF LATTICE DEFECTS USING POSITRON ANNIHILATION

Presenter: Christoph HUGENSCHMIDT
Author: Christoph HUGENSCHMIDT

In materials science, positron annihilation is widely applied for the detection and characterization of lattice defects on an atomic scale. The coincident Doppler-broadening (CDB) spectrometer at the high intensity positron source NEPOMUC provides a powerful non-destructive technique for element-selective defect spectroscopy and defect imaging by using the world's only operational positron microbeam. Example are the 2D-imaging of the oxygen vacancy concentration in thin-film high-temperature superconductors or the formation of open-volume defects in light metal alloys during plastic deformation. In fundamental research, the in-situ measurement of the equilibrium vacancy concentration as function of temperature allows, e.g. the determination of the vacancy formation enthalpy in solids as recently demonstrated for Lanthanum. In addition, future in-*operando* studies on solid samples – i.e. in gaseous atmosphere and/or at applied electric fields – will be enabled by using a new gas pressure cell.

Affillation
FRM II, Technische Universität München, Germany

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MON 15:00-15:15 | HÖRSAAL 1A | OPER-04

MICROSYMPOSIUM

IN-SITU STUDIES OF HYDROGENATION REACTIONS AND PHASE RELATIONS OF HYDROGEN-RICH HYDRIDES AT GIGAPASCAL PRESSURES BY SYNCHROTRON AND NEUTRON DIFFRACTION

Presenter: Kristina SPEKTOR

Authors: Kristina SPEKTOR (1,2), Doreen BEYER (1), Wilson CRICHTON (3), Dmitrii DRUZHBIN (3), Shrikant BHAT (2), Robert FARLA (2), Takanori HATTORI (4), Holger KOHLMANN (1), Ulrich HÄUSSERMANN (5)

We report on the in-situ analysis of hydrogenation reactions at gigapascal pressures aimed at producing new ternary metal hydrides with high H/M ratios and metal atoms attaining unusual oxidation states and H coordinations. The experiments are based on large volume press (LVP) high pressure methodology and employed ammonia borane, BH3NH3, as a hydrogen source. LVP methodology offers excellent opportunities for in-situ diffraction studies at high pressures and temperatures because sample environments can be stably maintained and controlled over extended periods of time. Importantly, it can be applied at both synchrotron and neutron facilities which is especially advantageous for hydride research. We demonstrate that LVP hydrogenations can be routinely performed at pressures beyond 10 GPa and can potentially be pushed to up to 20 GPa. We show that gigapascal hydrogenations open up for new families of main group hydrides, in particular hypervalent Si hydrides. Furthermore, we demonstrate the complementary use of in-situ synchrotron and neutron studies for characterizing the formation and structures of polymorphic Na3NiH5 which features a new and unusual homoleptic hydrido complex NiH5^(3-).

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MON 15:15-15:30 | HÖRSAAL 1A | OPER-05

MICROSYMPOSIUM

LITHIUM DISTRIBUTION AND TRANSFER IN HIGH-POWER 18650-TYPE Li-ION CELL AT MULTIPLE LENGTH SCALES

Presenter: Anatoliy SENYSHYN
Author: Anatoliy SENYSHYN

The operation of state-of-the-art Li-ion batteries is supplemented by the active transport of electrons and lithium ions exchanged between the positive and negative electrode materials during cycling. In the majority of studies reported in literature the lithium distribution was typically probed in the static equilibrium (for example in the fully charged state in the graphite anode), neglecting the evolution of the distribution under real charging conditions, influence of C-rates etc. In the current contribution, the lithiation kinetics of the positive and negative electrode materials in a commercial LFP|C 18650-type lithium-ion battery were investigated using various techniques: spatially-resolved neutron diffraction, X-ray diffraction computed tomography (CT) using high-energy synchrotron radiation and µm-sized beams, X-ray CT and electrochemical characterization. The lithium distribution in the cathode and anode are probed at different SOCs and at different length scales, where it has been found, that heterogeneities of the lithium distribution appear over length, height and thickness of the electrode stripes.

These non-uniform distributions affect cycling stability, aging characteristics, uniformity, safety and lifetime. Methods capable of monitoring the lithium distribution throughout the electrode thickness open up very interesting perspectives for its control and manipulation, such as using an engineered current density profile through adopted electrode morphology.

Affillation
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MON 15:30-15:45 | HÖRSAAL 1A | OPER-06

MICROSYMPOSIUM

TRACKING Pt SINGLE SITES ON CERIA USING ADVANCED OPERANDO X-RAY TECHNIQUES

Presenter: Paolo DOLCET
Authors: Paolo DOLCET (1), Florian MAURER (1), Arik BECK (1,2), Maria CASAPU (1), Jan-Dierk GRUNWALDT (1,3)

Supported noble metal-based catalysts are widely applied in catalysis, one of the most prominent one being emission control. To efficiently use these scarce and costly metals, the noble metal-support interaction in Pt/CeO2 has gained strong attention. This interaction enhances the low-temperature CO oxidation activity and offers the unique possibility to atomically disperse Pt on CeO2 and use it most efficiently.

In the present study, we aim at the identification, generation, and preservation of the active Pt species. In a first step, cationic Pt single sites were anchored in 4-fold coordinated nano-pockets on the CeO2 surface. This species is not active for oxidation reactions, until they agglomerate to form small Pt clusters. We were able to track this process by *operando* high energy resolved fluorescence detected X-ray absorption spectroscopy (HERFD-XAS) at the Pt L3-edge. The agglomeration can be controlled by a careful reduction using reductive pulses. As the formation of such clusters is directly linked to the abundance of noble metal atoms on the surface, we systematically increased the surface noble metal concentration of a well-defined Pt/CeO2 catalyst. In this way, the CO oxidation rate could be improved strongly by increasing the surface noble metal concentration. This behavior underlines that the agglomeration of Pt species in the oxidized state is crucial and its control can improve these catalysts.

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MICROSYMPOSIUM
MONDAY, 5TH SEPTEMBER

EARTH, ENVIRONMENTAL & CLIMATE SCIENCES			
Time	**Place**	**Presenter**	**Title**
Mon 14:15-14:30	Hörsaal 1b	Florian ADOLPHI	Cosmic links between climate archives to improve our understanding of paleoclimate dynamics
Mon 14:30-14:45	Hörsaal 1b	Nicolas WALTE	Current state of the SAPHiR instrument for neutron science under high pressure and high and low temperature conditions at FRM II and recent offline applications
Mon 14:45-15:00	Hörsaal 1b	Christian STERNEMANN	Electronic and structural properties of iron-bearing compounds at pressure and temperature: Applications in Earth sciences
Mon 15:00-15:15	Hörsaal 1b	Thomas HANSEN	Neutron diffraction revealing gas hydrate structure and behaviour
Mon 15:15-15:30	Hörsaal 1b	Messaoud HARFOUCHE	Understanding the Accumulation Mechanism of Pb in Industrial Aerea in Jordan: XAFS Study of the Structural Behavior
Mon 15:30-15:45	Hörsaal 1b	Sara SAVATOVIĆ	X-ray phase-contrast tomography for evaluating the impact of environmental changes on marine life

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MON 14:15-14:30 | HÖRSAAL 1B | EART-01

MICROSYMPOSIUM

COSMIC LINKS BETWEEN CLIMATE ARCHIVES TO IMPROVE OUR UNDERSTANDING OF PALEOCLIMATE DYNAMICS

Presenter: Florian ADOLPHI
Author: Florian ADOLPHI

Past climate changes provide unique insights into the behaviour of the Earth system under different conditions. In order to obtain the full spatiotemporal picture of the underlying dynamics, we must combine different sites and archives from different parts of the system such as ice cores, speleothems, or sediments. Having one consistent and precise chronology is one of the major challenges in this endeavour. Different dating methods vary in precision and accuracy, limiting our ability to infer robust conclusions about the drivers and feedbacks of major climate swings in the past.

Cosmogenic radionuclides such as 10Be and 14C provide a powerful tool to tackle this challenge. Their atmospheric production varies globally in response to changes in the galactic cosmic ray flux. Subsequently, the radionuclides are deposited nearly everywhere and become incorporated in paleoclimate archives such as tree-rings, speleothems, ice-cores, and sediments. Hence, each of these archives stores a record of variations of the cosmic ray flux, a signal that can then be used to date and synchronize them.

I will show how we can use this principle to improve our understanding of rapid climate changes during the last ice age, by combining ice-cores, speleothems and tree-rings, and discuss the implications for paleoclimate dynamics.

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MON 14:30-14:45 | HÖRSAAL 1B | EART-02

MICROSYMPOSIUM

CURRENT STATE OF THE SAPHiR INSTRUMENT FOR NEUTRON SCIENCE UNDER HIGH PRESSURE AND HIGH AND LOW TEMPERATURE CONDITIONS AT FRM II AND RECENT OFFLINE APPLICATIONS

Presenter: Nicolas WALTE
Authors: Nicolas WALTE (1), Christopher HOWARD (2), Hans KEPPLER (2)

SAPHiR, the Six Anvil Press for High Pressure Radiography and Diffraction, belongs to a suite of new instruments at the FRM II neutron source in Garching. The instrument will provide high pressure and temperature environments for in-situ neutron measurements of polycrystalline samples, fluids, and melts. The pressure is generated by a cubic multi-anvil press, currently capable of reaching 15 GPa, with sample volumes of 10-50 mm3 and temperatures up to 2300 K. For neutron diffraction, SAPHiR employs the time-of-flight method, where scattered neutrons are measured with three position sensitive helium-3 detector banks and a wavelength-shifting-fibre scintillator detector system. Applications of SAPHiR include crystallography of light-element-bearing phases, phase transitions, reaction kinetics, high-resolution radiography, and rheological studies. In addition to high-temperature experiments, samples can be investigated at ~80 K using a cryo-system that employs liquid nitrogen cooled jackets that enclose the anvils. The start of in-situ neutron measurements and external user operation is currently projected for 2023; until that time, SAPHiR is being used offline for scientific studies. We present a current application; by simulating olivine-metal textures of pallasite meteorites using high strain-rate deformation of model systems, we reaffirm their formation by cosmic collisions that occurred in the early solar system.

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MON 14:45-15:00 | HÖRSAAL 1B | EART-03

MICROSYMPOSIUM

ELECTRONIC AND STRUCTURAL PROPERTIES OF IRON-BEARING COMPOUNDS AT PRESSURE AND TEMPERATURE: APPLICATIONS IN EARTH SCIENCES

Presenter: Christian STERNEMANN
Author: Christian STERNEMANN

The study of iron in iron-bearing compounds at extreme thermodynamic conditions is highly important to understand the redox-chemistry and physical properties of planetary matter because of iron's abundance, chemical complexity and structural diversity. The electronic and structural properties of such compounds at pressure and temperature can be constrained by a suite of X-ray methods available nowadays of which X-ray emission spectroscopy is capable to determine iron's spin state, electronic properties and local coordination. While these experiments can be conducted at pressure using dedicated diamond anvil cell technology, heating the sample in parallel still poses a challenge, particularly if an extended data collection time for spectroscopic studies is required. Two different approaches are discussed applying emission detection via von Hámos type spectrometers. First, laser heating with a standard Yb-YAG laser is used in combination with synchrotron-radiation-based X-ray emission enabling in-situ spin-state imaging. Second, X-ray heating is applied at the hard X-ray free electron laser. Here, a sequence of X-ray pulses heats and probes the sample with the aim to explore the electronic structure of iron compounds in the solid and the melt.

We acknowledge funding by the BMBF via projects 05K10PEC (laser-heating) and 05K19PE2 (X-ray heating, von Hamos spectrometer) and thank the DFG for financial support via STE1079/4-1 within FOR2125/ CarboPaT (spin-state imaging).

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MON 15:00-15:15 | HÖRSAAL 1B | EART-04

MICROSYMPOSIUM

NEUTRON DIFFRACTION REVEALING GAS HYDRATE STRUCTURE AND BEHAVIOUR

Presenter: Thomas HANSEN
Author: Thomas HANSEN

Neutron diffraction always played a mayor role in the discovery of new phases of ice, most recently in that of the high pressure phase ice XIX, but also in the two negative pressure phases, ice XVI and XVII, both obtained from gas hydrates.

The formation and decomposition of the gas hydrates of sI type (CO2 and methane in particular) has been studied early on extensively by in-situ neutron diffraction at the high intensity powder diffractometer D20 at ILL. The work was driven by the possibility of CO2 storage inside hydrate deposits at continental shelf ocean floors and permafrost sediments and the simultaneous extraction of methane from those deposits. Also the possible seasonal formation and decomposition of CO2 hydrate on the planet Mars was a driving force to these investigations.

As a by-product, the structure of the second ambient pressure phase of ice, ice Ic, has been elucidated, as this phase, long time considered to be cubic, appears frequently in the decomposition of gas hydrates. Also, the origin of the so-called anomalous self-preservation of gas hydrates at “higher” temperatures could be explained in the context of understanding the relation of the ice phases Ih and Ic.

Neutron diffraction further revealed the peculiar thermal expansion behaviour of sI and sII gas hydrates as a function of the guest molecules.

The contribution resumes some of the most prominent results in ice and gas hydrates obtained at D20 in the last two decades.

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MON 15:15-15:30 | HÖRSAAL 1B | EART-05

MICROSYMPOSIUM

UNDERSTANDING THE ACCUMULATION MECHANISM OF Pb IN INDUSTRIAL AREA IN JORDAN: XAFS STUDY OF THE STRUCTURAL BEHAVIOR

Presenter: Messaoud HARFOUCHE
Authors: Messaoud HARFOUCHE (1), Riyad JABER (2), Bashar AL-SMADI (2)

Very high concentrations of lead (Pb) (up to 1.7 wt%) were found in arable soils nearby the Industrial City of Sahab, south east of Amman, Jordan; where many factories are located among them factories for recycling batteries.

The goal of this study was to determine the redox state and the nature of Pb binding in the soil matrix in order to understand the accumulation mechanism. Quantitative and qualitative analyses were done to specify, quantify and determine presence of heavy metals, particularly Pb, in sampling location. A combination of chemical extraction methods and spectroscopy was applied to characterize the redox state and binding environment to Pb in the soil. It was found that Pb concentration decreased with depth, while Pb oxidation state increased inversely proportional to the top surface. More precisely, XAFS (X-ray Absorption Fine Structure) derived structural parameters illustrate the presence of Pb on the surface in a mixture between the metallic and the oxide forms; while it gradually oxidizes with depth presenting a highly disordered PbOS-like structure at short and medium range order.

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MON 15:30-15:45 | HÖRSAAL 1B | EART-06

MICROSYMPOSIUM

X-RAY PHASE-CONTRAST TOMOGRAPHY FOR EVALUATING THE IMPACT OF ENVIRONMENTAL CHANGES ON MARINE LIFE

Presenter: Sara SAVATOVIĆ

Authors: Sara SAVATOVIĆ (1,2), Fabio DE MARCO (1,2), Vittorio DI TRAPANI (1,2), Ginevra LAUTIZI (1,2), Marco MARGINI (1,2), Mirta SMODLAKA TANKOVIĆ (3), Christina WOOD (4), Giuliana TROMBA (2), Adriano CONTILLO (2), Pierre THIBAULT (1,2), Irene ZANETTE (2)

Global climate change, as well as the increase in plastics production and the resulting large volume of litter entering marine ecosystems, have emerged as critical environmental priorities in recent years. Variations in sea temperature and rising microplastic contamination can have adverse consequences on marine organisms.

For example, an undistorted 3D representation of sea star anatomy can reveal how temperature changes affect their development and physiology. Furthermore, such a representation can be used to examine clogging or damage of the filtering channels in sea sponges due to microplastics.

To this end, we used X-ray phase-contrast imaging techniques to visualize and assess possible morphological changes in samples from different environmental conditions.

Data was collected at the SYRMEP beamline at Elettra, using speckle-based (SBI) and propagation-based X-ray imaging (PBI) techniques.

Because of its simplicity, PBI is a widely used phase imaging technique. However, the necessary single-material assumption is not applicable to starfish and sea sponges (containing skeletal and soft tissue). On the other hand, SBI provides quantitative phase-contrast data on heterogeneous samples.

We employed stitching techniques to measure entire specimens at high resolution, which allowed us to inspect the smallest features. Microplastic detection was also facilitated by the high resolution and the quantitative values yielded by SBI.

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MICROSYMPOSIUM

MONDAY, 5TH SEPTEMBER

ARTIFICIAL INTELLIGENCE FOR LARGE-SCALE FACILITIES			
Time	**Place**	**Presenter**	**Title**
Mon 14:15-14:30	Hörsaal 2	Erik THIESSENHUSEN	Reconstruction of SAXS data using Invertible Neural Networks
Mon 14:30-14:45	Hörsaal 2	Shah NAWAZ	Domain Adaptation for Serial Crystallography Data
Mon 14:45-15:00	Hörsaal 2	Vahid RAHMANI	Robust Image Classification with Machine Learning for Data Reduction in Crystallography
Mon 15:00-15:15	Hörsaal 2	Silja FLENNER	Machine learning denoising for nanotomography enabling in-situ experiments
Mon 15:15-15:30	Hörsaal 2	Yaroslav ZHAROV	Deep Learning for Synchrotron-based Tomography
Mon 15:30-15:45	Hörsaal 2	Amir TOSSON	Application of AutoEncoder in denoising correlation function of X-ray photon correlation spectroscopy

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MON 14:15-14:30 | HÖRSAAL 2 | AIFA-01

MICROSYMPOSIUM

RECONSTRUCTION OF SAXS DATA USING INVERTIBLE NEURAL NETWORKS

Presenter: Erik THIESSENHUSEN
Authors: Erik THIESSENHUSEN (1), Thomas KLUGE (1), Nico HOFFMANN (1), Melanie RÖDEL (1), Michael BUSSMANN (2), Thomas COWAN (1)

The understanding of laser-solid interactions is important to the development of future laser-driven particle and photon sources, e.g., for tumor therapy, astrophysics or fusion. Currently, these interactions can only be modeled by simulations which need verification in the real world. Consequently, in 2016, a pump-probe experiment was conducted by Thomas Kluge to examine the laser-plasma interaction that occurs when an ultrahigh-intensity laser hits a solid density target. To handle the nanometer spatial and femtosecond temporal resolution of the laser-plasma interactions, Small-Angle X-Ray Scattering (SAXS) was used as a diagnostic to reconstruct the laser-driven target. However, the reconstruction of the target from the SAXS diffraction pattern is an inverse problem which are often ambiguous and has no closed-form solution. We aim to simplify the process of reconstructing the target from SAXS images by employing Neural Networks due to their speed and generalization capabilities. To be more specific, we use a conditional Invertible Neural Network (cINN) to resolve the ambiguities with a probability density distribution. In consequence, the cINN is trained on simulated diffraction patterns and their respective ground truth parameters. The cINN is able to accurately reconstruct simulated- as well as preshot data. The performance on main-shot data remains unclear due to the fact that the simulation might not be able to explain the governing processes.

Affillation
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MON 14:30-14:45 | HÖRSAAL 2 | AIFA-02

MICROSYMPOSIUM

DOMAIN ADAPTATION FOR SERIAL CRYSTALLOGRAPHY DATA

Presenter: Shah NAWAZ

Authors: Shah NAWAZ (1), Vahid RAHMANI (1), Jaisinh BHOSALE (1,2), Shabarish Pala Ramakantha SETTY (1), David PENNICARD (1), Heinz GRAAFSMA (1,3)

In recent years, serial femtosecond crystallography has made remarkable progress for the measurement of macromolecular structures and dynamics using intense femtosecond duration pulses from X-ray Free Electron Laser. In these experiments, X-ray pulses are fired at a jet of protein crystals, and the resulting diffraction pattern is measured for each pulse. If the pulse hits protein crystals, the resulting diffraction pattern is recorded, known as Bragg peaks. However, most of the time the beam does not hit a crystal. As a result, out of the hundreds of thousands of patterns, only a small fraction is useful, so there is tremendous potential for data reduction. In recent years, machine learning models are leveraged to encode Bragg peaks and background to classify patterns into either hit or miss, resulting in considerable data reduction.

In serial femtosecond crystallography, experimental settings may change in an experiment along with different detector types producing differing patterns. Thus, machine learning models must withstand these variations to effectively deploy them in experiments. However, recent work observed that machine learning models trained on data taken from one experimental setting perform poorly on data extracted from another. It is well understood that drop in performance occurs due to domain gap. In this work, we will develop divergence and adversarial based domain adaptation methods to minimize this drop with an aim to build a robust model.

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MON 14:45-15:00 | HÖRSAAL 2 | AIFA-03

MICROSYMPOSIUM

ROBUST IMAGE CLASSIFICATION WITH MACHINE LEARNING FOR DATA REDUCTION IN CRYSTALLOGRAPHY

Presenter: Vahid RAHMANI

Authors: Vahid RAHMANI (1), Shah NAWAZ (1), Jaisinh BHOSALE (1), David PENNICARD (1), Shabarish PALA RAMAKANTHA SETTY (1), Heinz GRAAFSMA (1,2)

Recent serial crystallography experiments at FELs produce a large amount of data, where typically the proportion of useful images containing crystal diffraction (hit fraction) is about 5-10%. Demands on data storage could be greatly reduced by rejecting bad images before saving them to disk, but this requires reliable methods for detecting these images that do not rely on expert tuning or intervention during the experiment. Traditional machine learning methods successfully classify diffraction patterns, but the major challenge is cross-domain performance, in which a classifier trained on one dataset cannot necessarily be applied to data collected with different samples and experimental settings. In this paper, we propose a real-time, automatic, and parameter-free method based on machine learning which performs well across different experimental settings(cross-domain) to classify diffraction patterns as hit and miss diffraction patterns. Our method describes each diffraction pattern by a vector, consisting of the number of keypoints (Bragg spots) in different areas of the image. Our Modified FAST keypoint detector algorithm is used for Bragg's peak finding. The Modified and parallelized FAST algorithm is designed to work computationally efficient compared to the traditional FAST algorithm. Our initial experimental results show a significant improvement in decreasing the domain gap when a ML classifier is trained by new image descriptor, and tested by another unseen dataset.

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MON 15:00-15:15 | HÖRSAAL 2 | AIFA-04

MICROSYMPOSIUM

MACHINE LEARNING DENOISING FOR NANOTOMOGRAPHY ENABLING IN-SITU EXPERIMENTS

Presenter: Silja FLENNER
Authors: Silja FLENNER (1), Stefan BRUNS (1), Elena LONGO (2), Martin MÜLLER (1), Imke GREVING (1)

The nanotomography setup at the imaging beamline P05 at the PETRA III storage ring at DESY is optimized for full-field hard X-ray microscopy. It offers spatial resolutions down to 50 nm in absorption and phase contrast with scan times down to below one minute and is therefore optimized for in-situ studies. Noise is one of the major limitations for full-field nanotomography, in particular when a high time resolution is required. Here, machine learnig techniques can help to improve the image quality for fast and standard tomography.

Standard scans can be denoised via a new approach without the need of any reference scan: The projections are split into two independent stacks which are reconstructed separately. One of the reconstructed stacks is used as a reference for training while the other one serves as input. Machine learning also enabled a decrease of the total scan time down to 6 s by using a high quality scan as a reference. This approach is especially beneficial for in-situ experiments requiring high temporal resolution, where a high-quality reference scan is performed before and after the actual in-situ experiment.

Due to the high flexibility of the beamline, a wide range of in-situ setups are accessible (e.g. humidification, corrosion). These ML approaches prove to be very powerful tools, outperforming conventional filters by eliminating noise without blurring relevant structural features, thus enabling quantitative analysis in different scientific fields.

Affillation
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MON 15:15-15:30 | HÖRSAAL 2 | AIFA-05

MICROSYMPOSIUM

DEEP LEARNING FOR SYNCHROTRON-BASED TOMOGRAPHY

Presenter: Yaroslav ZHAROV
Authors: Yaroslav ZHAROV, Alexey ERSHOV, Thomas VAN DE KAMP, Mathias HURST, Sabine BREMER, Janes ODAR, Tomas FARAGO, Tilo BAUMBACH

KARA synchrotron facility at Karlsruhe Institute of Technology (KIT) is capable of producing large amount of tomographic data (100TB/week) by implementing high-throughput experiments using robotic sample exchanger and full automation. It is impossible to process and analyze the resulted data using conventional techniques, which usually rely on manual work of experts. Our institution aims to assist scientists in all stages of data analysis, thus we develop and deploy a wide variety of automatized analysis approaches. Recently we turned our efforts to the Deep Learning (DL) — relatively novel techniques which are proven to provide superior accuracy results, flexibility, and robustness while working with large data sets.

We will showcase several approaches for automated data analysis using Neural Networks. These approaches cover various stages of imaging and analysis pipeline — from the data correction to the quantitative analysis of sample's properties.

We will show DL-based sinogram inpainting to reduce tomographic imaging artifacts, unsupervised localization of samples inside large volumetric image, weakly supervised and fully supervised segmentation for annotation and morphological analysis. We also present an example of a large-scale morphometric study of a Medaka fish for the ambitious task of genotype-phenotype association in model organisms.

Affillation
Karlsruhe Institute of Technology, Germany

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MON 15:30-15:45 | HÖRSAAL 2 | AIFA-06

MICROSYMPOSIUM

APPLICATION OF AUTOENCODER IN DENOISING CORRELATION FUNCTION OF X-RAY PHOTON CORRELATION SPECTROSCOPY

Presenter: Amir TOSSON
Authors: Amir TOSSON, Sonja TIMMERMANN, Nimmi Das ANTHUPARAMBIL, Christian GUTT

X-ray photon correlation spectroscopy (XPCS) is a coherent scattering technique that benefits from the new generation of synchrotron sources, such as X-ray free-electron lasers (XFELs). It allows capturing a very broad range of timescales and length scales. Exploiting the multi-speckle techniques, the sample is probed by coherent X-rays and the scattered intensity is recorded as a function of time. Fluctuations in speckle patterns are tracked and defined by the normalized intensity correlation function. This quantitative measuring of these time-dependent fluctuations provides valuable information on the dynamics of the probed sample.

In XPCS experiments, noisy data is still one of the most common challenging problems that keep scientists up at night. The randomness of photon scattering and instrumentation instabilities are the most common kinds of noise that can affect the accuracy of the measurement [5]. We introduce a new denoising approach to enhance the signal-to-noise ratio correlation functions. It is based on 1D convolutional neural network AutoEncoder (1D-CNN-AE) models. The model is trained to capture the most important parts of the input image. The model is to learn to perform the lower-dimensional projection for input data (higher-dimensional). Then, a clean image is reconstructed by a sequence of transposed convolutional layers. We trained our model with 2M 1D images covering different use cases. It can perform noise removal with accuracy up to 85%.

Affillation
Siegen Universität, Germany

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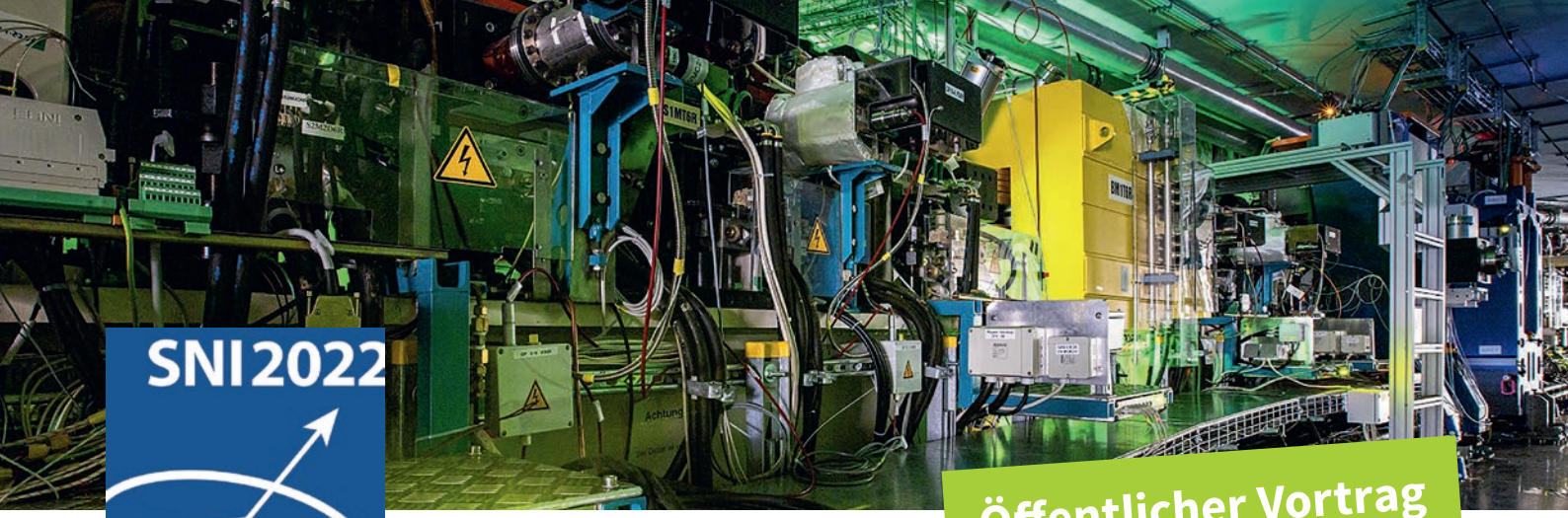

SNI2022

Öffentlicher Vortrag

MATERIE IM LICHT VON GROSSGERÄTEN:

von Nanometern und Femtosekunden

PROF. FRANK SCHREIBER
Universität Tübingen

Mit konkreten Beispielen und Perspektiven für die Zukunft wird Frank Schreiber erläutern, wie die Forschung an Großgeräten dazu beiträgt, nicht nur unsere Welt besser zu verstehen, sondern auch Lösungen für die drängenden gesellschaftlichen Herausforderungen zu entwickeln. Am Anfang steht immer die Neugier – und am Ende oft auch ein Produkt.

Mehr Informationen finden Sie hier:

ORT UND ZEIT:

Freie Universität Berlin, Rostlaube, Hörsaal 1a
Montag, 5. September 2022 um 19:00 Uhr

POSTER SESSION 1
MON, 5TH SEP. 16:15 – 18:15

ENERGY		
Board	**Presenter**	**Title**
1	Ana PALACIOS SAURA	Does the solvent matter? - Influence of the solvent in hybrid halide perovskites precursor solution
2	Daniel M. TÖBBENS	Cation order determination in Kesterite-type quaternary semiconductors by Multiple Edge Anomalous Diffraction (MEAD)
3	Sonja BLASEIO	Investigating transition processes of Cu/Cu-oxide foams during CO2RR by operando Quick-X-ray Absorption Spectroscopy (Quick-XAS)
4	Lukas GROSSMANN	Unveiling the Lithium Depth Profile Upon Lithiation of Extracted Silicon-Based Anodes
5	Galina GURIEVA	Cu/Zn disorder and point defects vs. efficiency and stability in Cu2ZnSn(S,Se)4 monograin solar cells
6	Götz SCHUCK	Parameterization of temperature-dependent atomic displacement parameters in chlorine-substituted MAPbI3
7	Mohan LI	Gold nanowire network fabricated by ion-track nanotechnology and its electrochemical properties
8	Hans H. FALK	Peculiar bond length dependence in (Ag,Cu)GaSe2 thin film alloys revealed by X-ray absorption spectroscopy
9	Konrad RITTER	Local atomic structure of kesterite type materials
10	Simon DIETZMANN	Synthesis of Atomically Dispersed Electrocatalyst by Imprinting with Different Template Ions through Carbonization and Analysis by XAS
11	Raul GARCIA-DIEZ	Studying energy materials under operating conditions by soft X-ray spectroscopy in the new OÆSE endstation: Case study of a Cu-based electrocatalyst
12	David MATZDORFF	Structural disorder in Cu-based quaternary chalcogenides: the role of the divalent cation
13	Joachim BRETERNITZ	In-situ diffraction of halide perovskites reveals light-induced structural changes
14	Steffen CZIOSKA	X-ray absorption spectroscopy of electrochemical catalysts under demanding conditions

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EARTH, ENVIRONMENTAL AND CLIMATE SCIENCES		
17	Christian LATHE	Synchrotron investigations of phase A, Mg7Si2O8(OH)6 dehydration in Large Volume Press (LVP), beamline P61B at PETRA III / DESY
18	Lélia LIBON	The fate of subducted magnesite in the Earth's lower mantle
19	Silke MERCHEL	Accelerator mass spectrometry (AMS) for the determination of long-lived cosmogenic radionuclides in stony meteorites – Now without chemical preparation
20	Marcel DICKMANN	Porosimetry of Metal Organic Frameworks and Polymeric Membranes by means of Positron Annihilation Lifetime Spectroscopy

IN-SITU AND OPERANDO STUDIES IN SOLID-STATE RESEARCH		
25	Anton DAVYDOK	Scanning X-ray nanodiffraction for nanomechanical in-situ tests
26	Itziar SERRANO-MUNOZ	Synchrotron X-Ray Refraction during in-situ heat treatments
27	Canrong QIU	Instrumentation and data analysis software for operando high energy surface X-ray diffraction
28	Anna REIS	Strain relaxation of epitaxially constrained α-(Al,Ga)2O3 thin films investigated by in-situ X-ray diffraction
29	Alberto VIANI	Time-evolution of microstructure during hardening of magnesium phosphate cements from synchrotron X-ray micro-Computed Tomography
30	Alberto VIANI	Nucleation of amorphous precursor in magnesium phosphate cements from in-situ X-ray techniques
31	Holger KOHLMANN	In-situ studies of order-disorder effects in FePd3Hx
32	Laura GUASCO	Kinetics of hydrogen absorption by in-situ neutron/X-ray reflectometry
33	Doreen BEYER	Exploration of formation and polymorphism of K2SiH6 at high pressures and temperatures via in-situ synchrotron diffraction
34	Patrick ROTHWEILER	In-situ ReflEXAFS Investigations on Nb treated in N2 gas atmospheres at elevated Temperatures
35	Konstantin SKUDLER	Operando NEXAFS investigating Lithium Sulfur Batteries
36	Dirk LÜTZENKIRCH-EN-HECHT	In-situ, time-resolved analysis of ZnO nanoparticle formation by simultaneous EXAFS and XRD
37	Lukas VOSS	Investigation of sputter deposited Co- and Cu-nitride thin films using grazing incidence EXAFS
38	Lisa RANDOLPH	Nanoscale subsurface dynamics of solids upon high-intensity femtosecond laser irradiation observed by grazing-incidence X-ray scattering

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IN-SITU AND OPERANDO STUDIES IN SOLID-STATE RESEARCH		
39	Antonia HERZOG	Operando Insights into Bimetallic Cu-based Nanocubes during Static and Pulsed CO2 Electroreduction toward Liquid Products
40	Bärbel KRAUSE	Real-Time Study of Solid-State Reactions at the Pd/a-Ge Interface
41	Armin HOELL	The source of twinning in FCC nanoparticles: high concentration of vacancies
42	Klara SUCHAN	Two step phase-segregation process revealed in mixed halide MHPs by simultaneous in-situ X-ray diffraction and Photoluminescence spectroscopy.
43	Justus JUST	Multimodal combined in-situ / operando XAS/XRD/UV-vis measurements reveal complex transformation processes in energy materials
44	Jochen KLEIN	Operando X-Ray Absorption Spectroscopy (XAS) to probe potential dependant changes of PtCo nanoparticles during oxygen reduction reaction (ORR)
45	Jochen KALT	Reversed bending in GaAs/(In,Ga)As/GaAs nanowire heterostructures
46	Olivia GOUGH	In-situ observations of organic all-small-molecule vacuum-thermally-evaporated bulk heterojunction film growth using ellagic acid as a templating layer
47	Abhijeet GAUR	Investigating the effect of reaction condition parameters on the reversible S-O exchange at the active sites of MoS2 based hydrotreating catalysts by ME-XAS
48	Ali ALHASSAN	Correlating the wetting angle of the Ga droplet with polytypism in as-grown GaAs nanowires using XRD and GISAXS
49	Taseer ANJUM	Lattice thermal expansion of as-grown GaAs nanowires due to optical excitation measured by X-ray pump probe experiment
50	Carolin REHERMANN	Influence of the Anti-Solvent Drop on the Film Formation Processes in Mixed-Halide Perovskites by in-situ multimodal Spectroscopy and X-Ray scattering
51	Anton PLECH	Simultaneous strain detection during in-situ thin film growth analysis
52	Radek SEVCIK	Effect of boron on the reaction of magnesium phosphate ceramics: an in-situ synchrotron SAXS-WAXS study
53	Samuel STRUZEK	Characterization of industrial relevant catalytic materials for emission control using X-ray absorption spectroscopy
54	Shweta SHARMA	Hard X-ray tomography for 3D spatially-resolved multiscale and multimodal characterization of non-model catalysts
55	Fahim KARIMI	Characterisation of LiBH4-MgH2 reactive hydride composite system with scattering and imaging methods using neutron and synchrotron radiation
56	Oliver KORUP	Fixed-bed Reactor for Operando Structure-Activity Profiling
57	Johannes KAA	X-ray emission measurements from X-ray heated matter contained in a DAC: A study of FeS

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METHODS AND INSTRUMENTS DEVELOPMENT 1		
63	Thomas C. ROSSI	Electronic effects in Photoexcited Epitaxial Zinc Oxide Nanorods Investigated by Transient X-ray Absorption Linear Dichroism
64	Sylvio HAAS	The new Small Angle X-ray Scattering beamline for Materials Research at PETRA III (SAXSMAT – P62)
65	Sylvio HAAS	SAXS/WAXS Tomography at the SAXSMAT beamline P62 at PETRA III
66	Daniel CLEMENS	Transfer Program of Neutron Scattering Instrumentation from BER II
67	Christian STERNEMANN	Materials Science and Soft-Matter Research at Beamline BL9 of DELTA
68	Matthias DREIMANN	Enabling time-resolved two-color experiments with the split-and-delay unit at FLASH2
69	J. CORREA	First user experiments of the PERCIVAL soft X-ray imager
70	Jonathan CORREA	Development of Timepix4 readout for experiments at synchrotrons and FELs
71	Arnab MAJUMDAR	Calculation of neutron and X-Ray scattering data from Molecular Dynamics simulations through optimal use of computation resources
72	Christoph HAUF	A new home for three versatile powder diffractometers - the optimized thermal beamport SR8 at the research neutron source Heinz Maier-Leibnitz
73	Michael HOFMANN	High accuracy positioning with an industrial robot system for neutron residual stress analysis
74	Ioanna MANTOUVALOU	SyncLab – combined X-ray imaging and spectroscopy measurements at the synchrotron and in the laboratory
75	Gregor NOWAK	The Material Engineering Diffractometer BEER at the European Spallation Source (ESS)
76	Thomas GUTBERLET	Optimization of a target with microchannel cooling for high-current accelerator-driven neutron sources
77	Michael HAUMANN	KMC-3 at BESSY (Berlin): a versatile beamline for tender-energy, rapid-scan, and operando X-ray absorption spectroscopy at cryogenic or ambient temperatures
78	Weimin GAN	A unique quenching and deformation dilatometer for combined in-situ neutron diffraction at STRESS-SPEC
79	Kai SCHÜLER	Moderate-resolution XES using a full-cylinder von Hamos spectrometer
80	Mathias HURST	Guided hierarchical in-situ X-ray nano-laminography enabling the investigation of damage nucleation in alloy sheets
81	Alessandra HENKEL	CFEL TapeDrive 2.0: Conveyor belt-based sample delivery system for multi-dimensional serial crystallography

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METHODS AND INSTRUMENTS DEVELOPMENT 1		
82	Tilo BAUMBACH	Status and Prospects of 3D Laminographic Imaging at KIT
83	Dmitry GORKOV	KOMPASS – the polarized cold neutron triple-axis spectrometer optimized for polarization analysis.
84	Wolfgang MORGEN-ROTH	NanoExtreme: Nano-focus end-station with double-sided CO2 laser heating for experiments at ID27@ESRF
85	Vladimir KAGANER	X-ray diffraction from strongly bent crystals and resolution of a bent-crystal spectrometer for XFEL pulses
86	Jochen FENSKE	An Engineering Diffractometer for the High Brilliance Neutron Source (HBS)
87	J. Mia LAHEY-RUDOLPH	TapeDrive 2.0 – an efficient sample environment for serial protein crystallography.
88	Michaela ZAMPONI	Applications with the high resolution neutron backscattering spectrometer SPHERES
89	Nils WAUSCHKUHN	Reconstruction of TiO2-HfO2 gratings with scanning-free grazing emission X-ray fluorescence
90	Frank SEIBOTH	Aberration correction for nanofocusing X-ray optics
91	Mikhail LYUBOMIRSKIY	Multi-beam X-ray ptychography using coded probes
92	Henning MARKÖTTER	Tomographic Imaging Capabilities with hard X-Rays at BAMline (BESSY II)
93	Stefan SCHIPPERS	ErUM-FSP T05 - "Aufbau von APPA bei FAIR"
94	Berit MARX-GLOWNA	High sensitive X-ray polarization microscopy
95	Marvin KOWALSKI	Construction of a fast non-linear X-ray shutter system
96	Ivo ZIZAK	A piezo-modulated active grating for selection of X-ray pulses separated by one nanosecond
97	Yutaka YOSHIDA	Mössbauer Spectroscopic Camera for Operando Measurements
98	Mahdi MOHAMMADI BIDHENDI	Single-shot temporal characterization of XUV FEL Pulses
99	Rebecca SPIECKER	Bragg Magnifier Optics for Dose-Efficient X-Ray Imaging with µm-Resolution
100	Angelica CECILIA	The IMAGE Beamline at the KIT Synchrotron Light Source
101	Wolfgang CALIEBE	Advanced X-Ray Absorption Spectroscopy at P64/PETRA III and options for PETRA IV
102	Oliver FORSTNER	Progress report of the LISEL@DREAMS project
103	Maren HOOCK	Nuclear forward scattering of photochemical and catalytically active iridium scomplexes
104	Ankita NEGI	Ptychography for Phase Retrieval in Nuclear Resonance Scattering

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METHODS AND INSTRUMENTS DEVELOPMENT 1		
105	Carlos SATO BARALDI DIAS	HIKa – Hierarchical Imaging Karlsruhe
106	Ioannis TZIFAS	High-pressure irradiation platform at GSI, Helmholtz Center for heavy ion research
107	Anna K. SAMBALE	In-situ X-ray investigations in material research using advanced experimental instruments
108	Mattias ÅSTRAND	Simple proximity effect correction for 50 kV electron-beam lithography on thick resist layers for the fabrication of X-ray optics
109	André WÄHLISCH	Experimental determination of differential scattering coefficients for nickel by means of linearly polarized X-ray radiation
110	Rudolf RÜFFER	A new Nuclear Resonance beamline at the new Extremely Brilliant Source of ESRF
111	Prerana CHAKRABARTI	Micro-Xray diffraction for highly absorbing samples at P06
112	Fabian WESTERMEIER	The Coherence Applications Beamline P10 at PETRA III
113	Mykola SHCHERBININ	Ray tracing simulation for Bragg magnifiers
114	Azat KHADIEV	Particle- and Phase-selective X-ray spectroscopy with Micro- and Macrobeams: The Case of (SmS)1.19TaS2 Nanotubes
115	Jonas SCHLEGEL	Pulsed Neutron Beam at the N4DP Instrument
116	Martin DIEROLF	The Munich Compact Light Source – a laboratory-scale synchrotron facility for bio-medical research and more
117	J. Michael KLOPF	THz Research at FELBE & TELBE – Pushing the Limits of the Ultrafast and Ultrasmall

DATA AND DIGITALIZATION		
120	Angelica CECILIA	Towards Serial Computed Tomography based on Automated Data Acquisition and Analysis Pipelines for Large Scale 3D Morphological Studies
121	Will SMITH	Progress on Measurement Automation and FAIR Data at Energy Materials In-situ Laboratory
122	Jiri VYSKOCIL	Alpaka-SSB: A Case Study of Implementing Performance Portable Ptychography Reconstruction Algorithms in C++
123	Simeon EHRIG	Alpaka-ePIE: Performance Portable Reconstruction of Ptychography Data
124	Klaus KIEFER	SECoP and metadata - the sample environment communication protocol
125	Klaus KIEFER	Sample Environment Communication Protocol (SECoP)

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DATA AND DIGITALIZATION		
126	Abhijeet GAUR	XAS reference database under DAPHNE4NFDI
127	Jiatu LIU	On-the-fly data reduction and analysis for complex multimodal experiments
128	Gudrun LOTZE	NUrF: Streamlining liquid handling and data processing and analysis for SANS beamlines
129	Markus OSTERHOFF	snip – digital users' lab book
130	Lars BOCKLAGE	NEXUS - A new software to evaluate modern nuclear resonant scattering experiments
131	David PAPE	HELIPORT - An Integrated Research Data Lifecycle
132	Philipp JORDT	DAPHNE4NFDI: DAta from PHoton and Neutron Experiments; Electronic Lab Notebooks from a Science Case Perspective
133	Linus PITHAN	SciCat – Implementing a data catalogue for individual research groups and large scale facilities
134	Jonas GRAETZ	First steps towards automated FAIR data collection at university labs
135	Linus PITHAN	Machine learning based data analysis in reflectometry (X-ray and neutron) and grazing incidence X-ray diffraction

ARTIFICIAL INTELLIGENCE FOR LARGE-SCALE FACILITIES		
136	Maksim ZHDANOV	Surrogate modelling for GISAXS reconstruction via gradient descent
137	Christopher KLOSE	Coherent Correlation Imaging: Resolving fluctuating states of matter
138	Martin RADTKE	Getting more efficient - The use of Bayesian optimization and Gaussian processes at the BAMline

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MON 16:15-18:15 | BOARD 1 | P1-ENER-01

POSTER SESSION

DOES THE SOLVENT MATTER? – INFLUENCE OF THE SOLVENT IN HYBRID HALIDE PEROVSKITES PRECURSOR SOLUTION

Presenter: Ana PALACIOS SAURA
Authors: Ana PALACIOS SAURA (1), Joachim BRETERNITZ (1), Armin HOELL (1), Susan SCHORR (1,2)

The efficiency of solar cells based on hybrid halide perovskites (HHPs) as absorber materials has increased from 3.8% in 2009 [1] to 25.8% in 2021 [2]. Commonly, HHPs are synthesized from solution thus it is crucial to understand the underlying mechanism of how the crystallization occurs [3]. Small angle X-ray scattering measurements at the BESSY II synchrotron source were performed at the four-crystal monochromator beamline of the Physikalisch-Technische Bundesanstalt [4] using the HZB ASAXS instrument [5]. We probe the precursor solutions of (FA,MA)Pb(I,Br)3 in various solvents to comprehend the influence of the solvent in the crystallization path. We show that the solvent has a major influence on the agglomerates, much stronger than the effect of anion or cation substitution. Our model explains the atomic arrangements in the agglomerates prior to crystallization.

[1] Kojima, A. et al, J. Am. Chem. Soc., 2009, 131, 6050–6051.
[2] Min, H. et al, Nature, 2021, 598, 444–450.
[3] Flatken, M. A. et al, J. Mater. Chem. A, 2021, 9, 13477–13482.
[4] Krumrey, M. et al, Nucl. Instrum. Methods Phys. Res., Sect. A, 2001, 467, 1175–1178.
[5] Hoell, A. et al, DE102006029449, 2007.

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MON 16:15-18:15 | BOARD 2 | P1-ENER-02

POSTER SESSION

CATION ORDER DETERMINATION IN KESTERITE-TYPE QUATERNARY SEMICONDUCTORS BY MULTIPLE EDGE ANOMALOUS DIFFRACTION (MEAD)

Presenter: Daniel M. TÖBBENS
Authors: Daniel M. TÖBBENS, Susan SCHORR

Quaternary chalcogenide semiconductors Cu2B(II)C(IV)X4 (B(II) = Zn, Fe, Ga; C(IV) = Sn, Ge, Si; X = S, Se) frequently contain isoelectronic cations. Structures are often derived by cation ordering from the cubic sphalerite type or the hexagonal wurtzite type crystal structure. Kesterite or wurtz-kesterite structures are characterized by the presence of Cu(I)-B(II) and Cu(I)-C(IV) layers (perpendicular to the longest crystallographic axis). Stannite or wurtz-stannite structures are formed with cations arranged in B(II)-C(IV) and pure Cu(I) layers. The cation arrangement is crucial for the electronic properties of the compound. Multiple Edge Anomalous Diffraction (MEAD) works particularly well to determine this. MEAD was used to confirm the cation structure type of Cu2FeSnS4, Cu2GaGeS4, Cu2ZnSnSe4, Cu2ZnSiSe4 and Cu2ZnGeSe4. Materials crystallizing in the kesterite structure in particular are prone to cation disorder within the Cu(I)-B(II) layers. Depending on the compound, the degree of cation disorder can change heavily with off-stoichiometry or thermal treatment. In these cases, MEAD spectra supply a robust way of quantification. This works particularly well for compounds where all cations are isoelectric, like Cu2ZnGeSe4. In other cases, joint Rietveld refinement is a better way to determine cation occupation factors. This method, too, profits from prior MEAD analysis firmly establishing the overall distribution, thus limiting the range of potential options.

Affillation
Helmholtz-Zentrum Berlin, Germany, Department Structure and Dynamics of Energy Materials

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MON 16:15-18:15 | BOARD 3 | P1-ENER-03

POSTER SESSION

INVESTIGATING TRANSITION PROCESSES OF Cu/Cu-OXIDE FOAMS DURING CO2RR BY OPERANDO QUICK-X-RAY ABSORPTION SPECTROSCOPY (QUICK-XAS)

Presenter: Sonja BLASEIO

Authors: Sonja BLASEIO (1), Abhijit DUTTA (2), Motiar RAHAMAN (3), Kiran KIRAN (2), Alexandra DWORZAK (1), Björn MAHRT (1), Peter BROEKMANN (2), Mehtap OEZASLAN (1)

Electrochemical CO2 reduction reaction (CO2RR) on copper electrodes is a promising alternative for large-scale production of hydrocarbons. The morphology of the Cu materials i.e. structure and 'chemical state' strongly influence the performance of the CO2RR. In this work, we have investigated the kinetics of both electrochemical oxide-metal reduction and CO2RR on np-Cu foams as catalyst precursor annealed at four different temperatures in air using *operando* Quick-XAS. The XANES data was analyzed by LCF and PCA to monitor the potential dependent changes of the chemical state of Cu. Based on the Cu K-edge XANES and EXAFS data, we show that the annealing temperature strongly influences the population of the Cu(II) species within the as prepared foams. Starting from the different ratios of Cu(0):Cu(I):Cu(II), the oxide-metal transition processes are shifted in the cathodic direction by applying potential steps of 100 mV. However, in all np-Cu foams this transition always occurs before the production of hydrocarbons starts. The potential jump experiments of several hundreds of mV lead to different kinetics of the oxide-metal reduction. These transition processes and the resulting structure of the np-Cu foams have a huge impact on the product distribution for CO2RR. Altogether, our results provide deeper insights into the oxide-metal transition processes to form the catalytically active Cu species for hydrocarbon formation during CO2RR.

Affillation

1: TU Braunschweig, Germany; 2: University Bern, Switzerland; 3: University of Cambridge, United Kingdom

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MON 16:15-18:15 | BOARD 4 | P1-ENER-04

POSTER SESSION

UNVEILING THE LITHIUM DEPTH PROFILE UPON LITHIATION OF EXTRACTED SILICON-BASED ANODES

Presenter: Lukas GROSSMANN
Authors: Lukas GROSSMANN (1), Jiri VACIK (2), Ralph GILLES (1)

A prominent strategy to increase the capacity of Lithium Ion Batteries is the use of silicon as anode material. However, the volumetric increase of silicon upon lithiation regularly results in a low cycling stability of the material. Our strategy is based on a partial lithiation of silicon to ~30%, which leads to a significant gain in cycling stability while maintaining a high capacity. The knowledge of the lithium distribution across such silicon electrodes is crucial to assess their behavior in working cells. In our study, we use Neutron Depth Profiling (NDP) on extracted silicon-based anodes to reveal the lithium depth distribution after different formation and lithiation steps. Thereby, we investigated three states of charge (SOC) and the formation with and without LiNO3 as electrolyte additive, which can significantly increase the cycling stability of silicon. Our results show that lithium is evenly distributed in depth across all studied electrodes. The formation already leads to a lithium concentration of ~9 µmol/cm^2, which is inferred to be a consequence of lithium which is irreversibly bound in the as-formed solid-electrolyte-interface (SEI). With increasing SOC (15 %, 30 %) the lithium concentration consistently increases. Also, we observe a significant swelling of the electrode during the lithiation process. Notably, the LiNO3 electrolyte additive leads to a higher lithium content in the SEI, which is a first indicator of differences in the formation process.

Affillation
1: Heinz Maier-Leibnitz Zentrum (MLZ), Technical University Munich, Germany; 2: Nuclear Physics Institute CAS, Husinec-Rez, Czech Republic

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MON 16:15-18:15 | BOARD 5 | P1-ENER-05

POSTER SESSION

Cu/Zn DISORDER AND POINT DEFECTS VS. EFFICIENCY AND STABILITY IN Cu2ZnSn(S,Se)4 MONOGRAIN SOLAR CELLS

Presenter: Galina GURIEVA

Authors: Galina GURIEVA (1), Kaia ERNITS (2), Nikita SIMINEL (3), Alicia MANJON SANZ (4), Melanie KIRKHAM (4), Dieter MEISSNER (2,5), Susan SCHORR (1,6)

Kesterite-type based thin film solar cell technologies are mainly based on polycrystalline absorber layers. A promising low cost alternative technology uses kesterite-type Cu2ZnSn(S,Se)4 (CZTSSe) monograins which are fixed in a polymer matrix to form a flexible solar cell.

It is agreed in literature that large band tailing observed in Cu-based kesterite-type semiconductors causes voltage losses limiting the efficiency of kesterite-based devices. The Cu/Zn disorder, which is always present in these compounds, is discussed as a possible reason for band tailing. The experimental determination of the order parameter Q which is a quantitative measure of the degree of Cu/Zn disorder requires a differentiation between the isoelectronic cations Cu+ and Zn2+ which is not possible by conventional X-ray diffraction. An in-depth analysis of neutron diffraction data provides information on the cation distribution in the crystal structure allowing the determination of type and concentration of intrinsic point defects. On the other hand, neutron diffraction requires large sample volumes, thus monograins offer the unique possibility to correlate structural disorder in kesterite-type absorbers with device performance parameters.

We present correlative trends between chemical composition, Cu/Zn disorder, intrinsic point defects as well as the optical bandgap energy of CZTSSe monograins and the stability as well as power conversion efficiency of respective Photovoltaic devices.

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MON 16:15-18:15 | BOARD 6 | P1-ENER-06

POSTER SESSION

PARAMETERIZATION OF TEMPERATURE-DEPENDENT ATOMIC DISPLACEMENT PARAMETERS IN CHLORINE-SUBSTITUTED MAPbI3

Presenter: Götz SCHUCK
Authors: Götz SCHUCK (1), Daniel M. TÖBBENS (1), Susan SCHORR (1,2)

In basic research on energy materials, such as hybrid perovskites, the temperature-dependent (TD) investigation of the crystal structure plays a prominent role. However, the atomic displacement parameters (ADP) determined in the TD crystal structure investigations are rarely put into a wider context with physical properties, in contrast to many other features resulting from these investigations. This is despite the fact that the temperature dependence of ADPs can be parameterized relatively easily with the help of an Einstein or Debye model, at least for results from single crystals.[1] For powder diffraction (PD) investigations, this approach is also feasible in principle, but here an analysis is complicated on the one hand by the interfering factors interacting in the background function (diffuse scattering, etc.). On the other hand, the intensity of the Bragg reflexes measured with PD is also influenced, for example, by structural or local disorder, so that these effects can falsify the determination of absolute values of the ADPs. One method of determining the absolute values of ADPs from PD is to use the relative change of ADPs (i.e. the change from one temperature step to the next), which then allows parameterization using an Einstein or Debye model also for PD data. This method is demonstrated by means of investigations on chlorine-substituted MAPbI3.[2]

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[1] Dudka, A.P. et al., J. Appl. Cryst. 2019, 52, 690.
[2] Schuck, G. et al., J. Phys. Chem. C 2022, 126, 5388.

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MON 16:15-18:15 | BOARD 7 | P1-ENER-07

POSTER SESSION

GOLD NANOWIRE NETWORK FABRICATED BY ION-TRACK NANOTECHNOLOGY AND ITS ELECTROCHEMICAL PROPERTIES

Presenter: Mohan LI

Authors: Mohan LI (1,2), Nils ULRICH (1,2), Ina SCHUBERT (1), Christina TRAUTMANN (1,2), Maria Eugenia TOIMIL-MOLARES (1)

The electrochemical characterization of free-standing Au nanowire networks synthesized by ion-track technology and electrodeposition is presented. The fabrication process employs irradiation of polycarbonate foils with heavy ions followed by chemical track etching. In this work, the foils were irradiated sequentially from four directions with 1–2 GeV Au ions at the UNILAC accelerator of GSI. Subsequent chemical etching of the ion tracks results in templates with interconnecting nanochannels which are then filled with gold by potentiostatic electrodeposition. Nanowire growth rate and homogeneity are tuned by varying the deposition potential. The technique provides precise control of the nanowire size, interconnectivity, and composition. By dissolving the polymer template, free-standing nanowire networks are obtained showing remarkable mechanical stability. Because of their large surface area, the networks are of interest for catalytic processes. Their catalytic activity towards methanol oxidation is recorded by cyclic voltammetry (CV) in an alkaline electrolyte and reveals significantly higher current densities than with a planar gold electrode. They also showed very stable long-term performance, with the current density dropping by only 5 % during 200 CV cycles of the oxidation reaction.

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MON 16:15-18:15 | BOARD 8 | P1-ENER-08

POSTER SESSION

PECULIAR BOND LENGTH DEPENDENCE IN (Ag,Cu)GaSe2 THIN FILM ALLOYS REVEALED BY X-RAY ABSORPTION SPECTROSCOPY

Presenter: Hans H. FALK
Authors: Hans H. FALK (1), Stefanie ECKNER (1), Konrad RITTER (1), Sergiu LEVCENKO (1), Timo PFEIFFELMANN (1), Edmund WELTER (2), William N. SHAFARMAN (3), Claudia S. SCHNOHR (1)

Cu(In,Ga)Se2 is a widely used material for solar cell absorbers, reaching efficiencies of more than 22 %. The incorporation of Ag enables a reduced deposition temperature, which benefits the growth of thin film solar cells. Furthermore, Ag alloying leads to a wider optical band gap and thus improves the photovoltaic conversion efficiency. Contrary to other semiconductor alloys, however, the band gap increase occurs even though the crystal lattice expands. Moreover, the Ga-Se bond length of (Ag,Cu)GaSe2 is predicted by theoretical calculations to decrease with increasing Ag content. This prediction is counterintuitive, since in other chalcogenide alloys, for example Cu(In,Ga)Se2, all bond lengths increase as the lattice expands. To unravel this mystery, we studied the element-specific bond lengths of (Ag,Cu)GaSe2 alloys using extended X-ray absorption fine structure spectroscopy (EXAFS). The polycrystalline thin films were grown on Mo-coated soda lime glass by a single stage co-evaporation process at a temperature of 550°C. The average Ag-Se and Cu-Se bond lengths determined by EXAFS clearly increase with increasing Ag content whereas the Ga-Se bond length decreases despite the expansion of the chalcopyrite lattice. Thus, (Ag,Cu)GaSe2 thin film alloys indeed exhibit the predicted counterintuitive bond length dependence. Correlating this peculiar structural behavior with the electronic band structure will contribute to a deeper understanding of (Ag,Cu)GaSe2 alloys.

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MON 16:15-18:15 | BOARD 9 | P1-ENER-09

POSTER SESSION

LOCAL ATOMIC STRUCTURE OF KESTERITE TYPE MATERIALS

Presenter: Konrad RITTER
Authors: Konrad RITTER (1), Galina GURIEVA (2), Silvana BOTTI (3), Susan SCHORR (2,4), Claudia S. SCHNOHR (1)

With the growing need for energy, research of renewable energies such as photovoltaics is focusing on new compounds. Kesterite type materials, usually just referred to as kesterites, are based on typically non toxic, relatively earth abundant elements and the resulting compounds are very stable to environmental conditions. However, thin film solar cells made from kesterite absorbers are far behind their theoretical limit of ~30 % conversion efficiency. In high performing kesterite devices the absorber layer deviates from ideal stoichiometry. Different elements in the structure can be completely or partially replaced, known as alloying, to overcome the performance deficit. Amongst a multitude of methods used to characterize and understand kesterites, synchrotron based Extended X-ray Absorption Fine Structure Spectroscopy (EXAFS) has proven highly useful. It enabled a comparison of the local atomic structure of different off-stoichiometric kesterites and kesterite alloys. Low temperature measurements resolved subtle changes in the element specific bond lengths and enabled a correlation with point defect concentrations obtained from neutron diffraction studies. Temperature-dependent EXAFS unveiled the force constants of the cation anion bonds and the static disorder in selected stoichiometric kesterites. Combining these local structural parameters with ab initio theoretical calculations provided insight into the origins of the band gap bowing observed for kesterite alloys.

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MON 16:15-18:15 | BOARD 10 | P1-ENER-10

POSTER SESSION

SYNTHESIS OF ATOMICALLY DISPERSED ELECTROCATALYST BY IMPRINTING WITH DIFFERENT TEMPLATE IONS THROUGH CARBONIZATION AND ANALYSIS BY XAS

Presenter: Simon DIETZMANN
Authors: Simon DIETZMANN, Asad MEHMOOD, Ana DE OLIVEIRA GUILHERME BUZANICH, Tim-Patrick FELLINGER

Atomically dispersed metal-nitrogen doped carbons (M-N-C) are promising catalyst for small molecule activation such as O2, CO2 and N2. These single atom catalysts are acting on the border between homogenous and heterogenous catalyst. Thus, combining advantages of both worlds such as high atomic efficiency in homogenous catalysis and the ready application for example as electrocatalysts in proton exchange membrane (PEM) fuel cells. Many examples of transition metal nitrogen doped carbons (TM-N-C) are known today but are missing controlled synthesis of the active site. Recently, our group facilitated the synthesis of purely pyrrolic TM-N4 sites using Mg or Zn ions as imprinters.[1] The variety of other potential imprinter ions motivates the exploration of formation of e.g. pyridinic N4 sites, which are considered important in the community. Synthetic control on the selective formation of specific active sites would allow for better understanding of structure-property relations to activity, selectivity, catalyst stability and better insights into the reaction mechanism. These new materials will be characterized at the BAMline (BESSY II) by X-ray absorption spectroscopy (XAS) measurements. Additionally, carefully characterized (such as by single crystal X-ray diffractometry) nitrogen ligated metal complexes will be synthesized as reference materials and measured in the same XAS set-up.

[1] T. P. Fellinger et al, J. Am. Chem. Soc. 2021, 143, 18010-18019.

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MON 16:15-18:15 | BOARD 11 | P1-ENER-11

POSTER SESSION

STUDYING ENERGY MATERIALS UNDER OPERATING CONDITIONS BY SOFT X-RAY SPECTROSCOPY IN THE NEW OÆSE ENDSTATION: CASE STUDY OF A CU-BASED ELECTROCATALYST

Presenter: Raul GARCIA-DIEZ

Authors: Raul GARCIA-DIEZ (1), Regan G. WILKS (1,2), Johannes FRISCH (1), Wolfgang BREMSTELLER (1), Marianne VAN DER MERWE (1), Enggar WIBOWO (1), Mihaela GORGOI (1,2), Elmar KATAEV (1), Catalina JIMENEZ (1), Mauricio ARCE (1), Will SMITH (1), Anna EFIMENKO (1), Dirk WALLACHER (3), Marcus BÄR (1,2,4,5)

In context of the growing need for a more sustainable energy sector, significant efforts have been devoted to the quest for more efficient electrocatalyst materials for energy conversion and storage devices such as water electrolyzers, fuel cells and batteries. Thus, in-situ studies of promising energy materials in conditions close to real operation are of crucial importance for understanding of the performance-limiting mechanisms occurring at the electrochemical interfaces. The combination of soft X-ray absorption (XAS) and emission (XES) spectroscopies is an established method that can probe atom-specifically the (local) chemical and electronic structure of solid, liquid, and gaseous samples, providing insights into their electrochemical activity. For this purpose, in the Energy Materials In-situ Laboratory Berlin (EMIL) at the BESSY II synchrotron facility, we have set up the Operando Absorption and Emission Spectroscopy at EMIL (OÆSE) endstation that allows photon-in/photon-out spectroscopic studies of energy materials under operating conditions.

In this work, we show the first experimental results obtained at OÆSE in the field of electrocatalysis and battery research, showcasing the capabilities of the available sample environments and the 2-color EMIL beamline. As a case study, we present the in-situ growth of copper hydroxide monitored by Cu L-edge XAS, with special focus on the meta-stable intermediate CuIII(OH)3, revealed at hydrolysis-relevant operating conditions.

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MON 16:15-18:15 | BOARD 12 | P1-ENER-12

POSTER SESSION

STRUCTURAL DISORDER IN CU-BASED QUATERNARY CHALCOGENIDES: THE ROLE OF THE DIVALENT CATION

Presenter: David MATZDORFF
Authors: David MATZDORFF (1,2), Galina GURIEVA (1), Denis CHEPTIAKOV (3), Susan SCHORR (1,2)

Thin film photovoltaics enable short energy payback time and minimum use of high purity materials, addressing the urgent need for cost-competitive renewable energy technologies.

Cu-based quaternary chalcogenides are promising semiconductors for PV applications, due to use of non-toxic and earth abundant elements as well as long term stability to environmental conditions. But Cu-Zn disorder in kesterite-type Cu2ZnSn(S,Se)4 absorbers has been blamed for the poor efficiency of related solar cells. Thus an exchange of Zn by Mn may offer a way to avoid this structural disorder. In this context we studied Cu2MnGeS4, Cu2MnGeSe4 as well as Cu2MnSnS4 and Cu2MnSnSe4. Covering a bandgap energy range of 1.1 to 1.7 eV these semiconductors are potential absorber materials for single junction as well as tandem solar cells.

For an in-depth study of the crystal structure and structural disorder, it is essential to distinguish between the electronically similar elements Cu, Mn and Ge. Due to a very similar atomic scattering factor of these elements, conventional X-ray diffraction fails. Therefore, we performed neutron diffraction experiments and took advantage of different neutron scattering lengths of the respective elements to determine the cation distribution in the unit cell, the basis to conclude on the crystal structure and structural disorder. We show that these semiconductors adopt crystal structure types which hinder a structural disorder as observed in the Zn-containing counterparts.

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MON 16:15-18:15 | BOARD 13 | P1-ENER-13

POSTER SESSION

IN-SITU DIFFRACTION OF HALIDE PEROVSKITES REVEALS LIGHT-INDUCED STRUCTURAL CHANGES

Presenter: Joachim BRETERNITZ
Authors: Joachim BRETERNITZ (1), Ivo ZIZAK (1), Susan SCHORR (1,2)

Halide perovskites as materials for solar cells have made a spectacular appearance in the last 10 years. With solar cell efficiencies maxing at 25.7 %, they are close to conventional solar cell materials,[1] while having the advantage of low temperature processing and thin absorber layers. Many different compositions deriving from MAPbI3, the signature material, have been employed to push the solar cell efficiencies higher, spanning a wide variety of perovskite-type crystal structures.[2]

The structural response to external stimuli – such as light – is , however, surprisingly different from conventional semiconductor materials, which can often be thought as highly ordered, very rigid structures. Using in-situ studies conducted at the mySpot beamline at the BESSY II synchrotron light source (HZB),[3] we uncover that light affects the atomic structure of hybrid halide perovskites notably and almost immediately. We show that these changes have a reversible and an irreversible contribution and we elucidate some effects of halide composition on the structural response to light. The understanding of the underlying aspects of these light-induced effects is highly relevant for their use as solar cell materials.

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[1] https://www.nrel.gov/pv/cell-efficiency.html, accessed 27/04/22
[2] J. Breternitz, in Crystallography in Materials Science, Ed. S. Schorr. C. Weidenthaler, de Gruyter, 2020.
[3] I. Zizak, JLSRF, 2016, 2, 101.

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MON 16:15-18:15 | BOARD 14 | P1-ENER-14

POSTER SESSION

X-RAY ABSORPTION SPECTROSCOPY OF ELECTROCHEMICAL CATALYSTS UNDER DEMANDING CONDITIONS

Presenter: Steffen CZIOSKA
Authors: Steffen CZIOSKA, Alexey BOUBNOV, Erisa SARACI, Jan-Dierk GRUNWALDT

The investigation of electrochemical catalysts by *operando* X-ray absorption spectroscopy (XAS) is essential to understand the processes occurring at the material-electrolyte interface under reaction conditions, with the goal to subsequently improve the catalyst. Electrochemical reactions of high interest are, for instance, water splitting (OER, HER) for the production of green hydrogen, and the CO2 reduction reaction for production of high-value chemical products.

However, under industrially relevant conditions with high current densities, dynamic potential changes and elevated temperatures, *operando* XAS measurements become extremely challenging, due to the strong O2 bubble evolution on the catalyst surface during water splitting. We show that by a combined approach of electrochemical flow cells, refined spectroscopic approaches and advanced data analysis, it is possible to unravel the structural changes and the mechanism even under strong bubble evolution at high potentials of up to 1.6 V and temperatures of up to 80 °C.

While at our initial approach we relied at special XAS-infrastructures (especially QuickXAS), we were able to improve and extend our approach to conventional XAS beamlines, appealing to a wide range of users.

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MON 16:15-18:15 | BOARD 17 | P1-EART-01

POSTER SESSION

SYNCHROTRON INVESTIGATIONS OF PHASE A, $Mg_7Si_2O_8(OH)_6$ DEHYDRATION IN LARGE VOLUME PRESS (LVP), BEAMLINE P61B AT PETRA III / DESY

Presenter: Christian LATHE

Authors: Christian LATHE (1,2), Monika KOCH-MÜLLER (1), Bernd WUNDER (1), Oona APPELT (1), Shrikant BHAT (2), Robert FARLA (2)

One of the still open questions with respect to the Deep Water Cycle is, how and to what extent H_2O is brought into the deeper mantle. Experimentally, dense hydrous magnesium silicates (DHMS) have been proven to exist, and hence are considered as the main carriers of H_2O into the mantle via subduction [1]. One of the DHMS, phase A, is viewed as a key carrier of water to the deeper mantle and its dehydration is discussed as cause of earthquakes. The P/T coordinates of the reaction

phase A + clinoenstatite = forsterite + water (1)

are of significant importance and not well constrained. We examined reaction (1) by means of in-situ X ray diffraction (XRD) measurements with the LVP at PETRA III. We used in-situ energy dispersive XRD to study the phase transition (1) between 7 – 10 GPa and 690 – 880 °C. To prevent water escaping form the sample container, the starting materials were encapsulated in Ti capsules with water in exess. Ti is inert, adequately transparent to the diffracted X rays and the capsules can be closed water-tight. Our results confirm the data reported by [1] and it can be concluded that the assemblage phase A + clinoenstatite will only transport H_2O into deeper levels of the mantle in case of cold slabs [2].

[1] Wunder, Contrib. Mineral. Petrol. (1998) 132: pp. 111-120.
[2] Lathe, et al., Eur. J. Mineral. (2022), 34, 201–213, 2022.

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MON 16:15-18:15 | BOARD 18 | P1-EART-02

POSTER SESSION

THE FATE OF SUBDUCTED MAGNESITE IN THE EARTH'S LOWER MANTLE

Presenter: Lélia LIBON

Authors: Lélia LIBON (1), Georg SPIEKERMANN (2), Melanie SIEBER (1,3), Johannes KAA (4), Serena DOMINI-JANNI (5), Mirko ELBERS (1), Ingrid BLANCHARD (1), Christian ALBERS (6), Nicole BIERDERMANN (4), Wolfgang MORGENROTH (1), Karen APPEL (4), Catherine MCCAMMON (5), Anja SCHREIBER (3), Vladimir RODDATIS (3), Konstantin GLAZYRIN (7), Rachel HUSBAND (7,4), Louis HENNET (8), Max WILKE (1)

Subduction of carbon-bearing phases throughout Earth's history may be an important mechanism of sourcing carbon to the Earth's lower mantle. As carbon has very low solubility in mantle silicates, it is primarily present in accessory phases such as carbonates, diamond, or metal carbides. Previous studies indicate that more than half of the carbonate contained in the oceanic crust may reach the lower mantle. Experimental results show that magnesite can be stable up to deep lower mantle conditions and may be considered the most probable carbonate present in the deep Earth. However, our understanding of magnesite's stability in contact with bridgmanite, the most abundant mineral in the lower mantle, remains incomplete.

Hence, to investigate the system MgCO3-(Mg,Fe)SiO3, we conducted a combination of high-pressure experiments using multi-anvil press and laser-heated diamond anvil cells (LH-DAC). Our results suggest a two-step process that starts with melting at temperatures below the mantle geotherm indicated by our multi-anvil press experiments, followed by crystallization of diamond from the melt produced. Therefore, magnesite will not remain stable in the lower mantle and will instead melt at upper-most lower mantle conditions, fostering diamond formation. Consequently, the melting of recycled crust and chemical transfer to the surrounding mantle will hinder the transport of carbon deeper into the lower mantle.

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MON 16:15-18:15 | BOARD 19 | P1-EART-03

POSTER SESSION

ACCELERATOR MASS SPECTROMETRY (AMS) FOR THE DETERMINATION OF LONG-LIVED COSMOGENIC RADIONUCLIDES IN STONY METEORITES – NOW WITHOUT CHEMICAL PREPARATION

Presenter: Silke MERCHEL

Authors: Martin MARTSCHINI, Robin GOLSER, Oscar MARCHHART, Alexander WIESER, Silke MERCHEL

Long-lived radionuclides in meteorites are a result of the interaction with cosmic rays. Therefore, the concentrations of these cosmogenic nuclides (CNs) record the irradiation history of extraterrestrial matter. Reconstruction parameters of interest are:

1) preatmospheric size and shielding depth of the body in space (meteoroid)
2) irradiation time in space (irradiation age)
3) identification of complex exposure, i.e., repeated collisions or inherited CNs from preexposure at the surface of the meteoroid's parent body (asteroid, Moon, Mars)
4) residence time on Earth (terrestrial age) for meteorite finds.

Accelerator mass spectrometry (AMS) is the method-of-choice for the detection of long-lived CNs such ^{10}Be, ^{14}C, ^{26}Al, ^{36}Cl and ^{41}Ca ($t_{1/2}$ = 6 ka-1.4 Ma). However, tedious radiochemical separation to deplete matrices and isobars was a prerequisite for AMS hindering fast and reasonable analysis until recently. Now, the world-wide unique ion-laser interaction mass spectrometry (ILIAMS) system developed at the Vienna Environmental Research Accelerator provides isobar suppression by up to eleven orders of magnitude. Hence, ILIAMS-assisted AMS enables the direct detection of ^{26}Al/^{27}Al (~10^{-10}) and ^{41}Ca/^{40}Ca (~10^{-11}) in crushed stony meteorites containing intrinsic ~1% Al and Ca. Isobars from the natively-abundant elements (15% Mg, 1‰ K) do not cause any analysis problem making radiochemical separation redundant.

Acknow.: We thank D. Heinlein and L. Ferrière for precious samples.

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MON 16:15-18:15 | BOARD 20 | P1-EART-04

POSTER SESSION

POROSIMETRY OF METAL ORGANIC FRAMEWORKS AND POLYMERIC MEMBRANES BY MEANS OF POSITRON ANNIHILATION LIFETIME SPECTROSCOPY

Presenter: Marcel DICKMANN

Authors: Marcel DICKMANN (1), Rhea VERBEKE (2), Timothée STASSIN (2), Werner EGGER (1), Rob AMELOOT (2), Ivo VANKELECOM (2), Ricardo HELM (1), Günther DOLLINGER (1)

Porous materials, such as synthetic membranes or metal organic frameworks (MOFs), have emerged as promising materials due to their high selectivity in absorbing or separating compounds from complex mixtures. Polyamide membranes are currently the state-of-the-art to desalinate sea water and river water or filter waste water, while MOFs can be used for both large-volume applications (adsorption, catalysis, gas storage) and integrated, high-value applications (gas sensors, low-k dielectrics, drug delivery). While the morphology of polymeric membranes and MOFs can be evaluated with widely available techniques, characterizing their intrinsic pore size and pore volume is extremely challenging.

Positron Annihilation Lifetime Spectroscopy (PALS) is a non-destructive and powerful method to obtain pore size information in the nano meter range. The technique can be considerably enhanced using a mono-energetic positron beam of variable energy. Thus, depth profiling in MOFs, MOF thin films, and desalination membranes with layered structures of less than 10 nm is possible.

The use of PALS on porous materials enables the determination of their synthesis-structure-performance relationship which is crucial for their future design and to unravel their application potential. We will present latest results of selected MOF- and membrane materials, characterized by PALS. Additionally, a comparison with complementary techniques will be shown.

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MON 16:15-18:15 | BOARD 25 | P1-OPER-01

POSTER SESSION

SCANNING X-RAY NANODIFFRACTION FOR NANOMECHANICAL IN-SITU TESTS

Presenter: Anton DAVYDOK
Authors: Anton DAVYDOK, Christina KRYWKA

Mechanical properties of modified and novel developed materials are taking an important place the in the further development and mass-product implementation due to direct influence on possible application and life-time of future products. Micro and nanomechanics demonstrate different behavior compared to well-studied macro analogies and require special investigation approaches and instrumentation. In this presentation, we will introduce the applicability of instrumentation for in-situ micromechanical tests developed at the Nanofocus Endstation of the P03 beamline at PETRA III (DESY, Hamburg). The station is operated by Helmholtz-Zentrum Hereon and offers unique conditions for mechanical tests coupled with X-ray nanodiffraction. The highly stabile experimental setup is dedicated to structural analysis with sub-micron precision. The X-ray beam is focused down to a size of only 250 x 250 nm^2 by means of KB-mirrors. The strong focus on materials science at P03 is demonstrated by the wide range of in-situ micromechanical experiments already performed, such as indentation testing of coatings, glasses and metallic glasses with high strain resolution of up to 10^-5. Detailed technical specification of the beamline and the indenters will be shown, as well as results obtained during the experiment.

Affillation
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MON 16:15-18:15 | BOARD 26 | P1-OPER-02

POSTER SESSION

SYNCHROTRON X-RAY REFRACTION DURING IN-SITU HEAT TREATMENTS

Presenter: Itziar SERRANO-MUNOZ
Authors: Itziar SERRANO-MUNOZ (1), Ilaria ROVEDA (1), Andreas KUPSCH (1), Bernd R. MÜLLER (1), Giovanni BRUNO (1,2)

In this work, synchrotron X-ray refraction radiography (SXRR) was combined with in-situ heat treatment to monitor microstructure and porosity evolution as a function of temperature. The investigated material was a laser powder bed fusion (LPBF) manufactured AlSi10Mg, where the initial eutectic Si network is known to break down into larger particles with increasing temperature. Such alloy is also prone to thermally induced porosity (TIP). We show that SXRR allows detecting the changes in the Si-phase morphology upon heating, while this is currently possible only using scanning electron microscopy. SXRR also allows observing the growth of pores, usually studied via X-ray computed tomography, but on much smaller fields-of-view. Our results show the great potential of in-situ SXRR as a tool to gain in-depth knowledge of the susceptibility of any material to thermally induced damage and/or microstructure evolution over statistically relevant volumes.

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MON 16:15-18:15 | BOARD 27 | P1-OPER-03

POSTER SESSION

INSTRUMENTATION AND DATA ANALYSIS SOFTWARE FOR OPERANDO HIGH ENERGY SURFACE X-RAY DIFFRACTION

Presenter: Canrong QIU
Authors: Canrong QIU, Timo FUCHS, Jochim STETTNER, Matthias GREVE, Olaf MAGNUSSEN

Insights into the structure of solid-liquid interfaces under reaction conditions are indispensable in many materials-science fields such as catalysis, corrosion, and thin-film growth. High energy surface X-ray scattering (HESXRD) is a promising technique, which allows one to determine the atomic scale structure of such interfaces with high time resolution. We here describe dedicated instrumentation and software for HESXRD measurements. Specifically, we developed an automatic beamstop placement system that can protect the employed 2D detector from beam damage at the numerous positions of intense Bragg peaks. The system can autonomously place up to 50 beamstops within 2 mins with an accuracy of < 0.1 mm. Furthermore, we also developed a series of Python-based software tools to deal with the demanding data analysis required in the application of HESXRD, including CTR data extraction from large amounts of detector images (typically >2000 frames for a full dataset), structural modeling for resolving atomic scale interfacial structure from the extracted CTR data, and software for fast monitoring of the structural evolution under dynamic conditions. These software packages have been well tested and optimized to make them user-friendly, fault-tolerant, highly performant, and extendible. We demonstrate the use of this instrumentation and software by data obtained for Pt and oxide electrocatalysts under reaction conditions.

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MON 16:15-18:15 | BOARD 28 | P1-OPER-04

POSTER SESSION

STRAIN RELAXATION OF EPITAXIALLY CONSTRAINED α-(Al,Ga)2O3 THIN FILMS INVESTIGATED BY IN-SITU X-RAY DIFFRACTION

Presenter: Anna REIS
Authors: Anna REIS, Michael HANKE, Achim TRAMPERT

Over the past two decades Ga2O3 in its thermodynamically stable β-phase has attracted large scienfic interest due to its ultra-wide bandgap of 4.8 eV enabeling the implementation of high power electronic devices. Lately also the metastable α-phase of Ga2O3 has recieved growing attention. Among the Ga2O3 polymorphs it has the largest bandgap of 5.3 eV and due to being isostructural to Al2O3 ternary (Al,Ga)2O3 can be alloyed across the full compositional range allowing for bandgap engineering between 5.3 eV and 8.8 eV. In order to effectively design heterostructure devices detailed knowledge about strain formation and relief is of fundamental interest.

Thin α-(Al,Ga)2O3 films were epitaxially grown on a-Al2O3 via molecular beam epitaxy and probed in-situ by X-ray diffraction at the PDI's PHARAO facility (U125/2-KMC) at BESSY II. Grazing incidence diffraction patterns of the orthogonal (00.6) and (30.0) lattice planes reveal the in-plane strain dynamics of the interface. In the first monolayers the (Al,Ga)2O3 is found to be completely strained whereas afterwards a partially relaxed layer is formed on top. Within deposition of the first 10-15 nm in-plane compressive strain accumulates preferably along the [100]-direction whilst along [001] strain is relieved exposing the anisotropy of the strain relaxation behaviour.

These findings will lead to a more conclusive understanding of the Al2O3/α-(Al,Ga)2O3 interface enabeling the effective design of high power electronic devices.

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MON 16:15-18:15 | BOARD 29 | P1-OPER-05

POSTER SESSION

TIME-EVOLUTION OF MICROSTRUCTURE DURING HARDENING OF MAGNESIUM PHOSPHATE CEMENTS FROM SYNCHROTRON X-RAY MICRO-COMPUTED TOMOGRAPHY

Presenter: Alberto VIANI
Authors: Alberto VIANI (1), Petra MÁCOVÁ (1), Lucia MANCINI (2)

The reaction in water between MgO and KH2PO4, leading to the formation of a cement at room temperature, has been followed in time with synchrotron X-ray micro-Computed Tomography. The quantitative analysis of the reconstructed volumes allowed to link the development of the microstructure to the reaction mechanisms. The first reaction product is amorphous; the amorphous-to-crystalline conversion, occurring during hardening, has a profound impact on the microstructural development and, therefore, on the properties of the cement body. The results pointed to a coarsening of the pore-matrix microstructure with time, in striking contrast with previous models predicting a decrease in total porosity. During crystallization, the amorphous phase is replaced with a material of higher density, filling the space differently (because of its elongated crystal habit). This process leads to the enlargement of the pores and the formation of new voids. The internal surface of pores and their shape become more irregular. This was confirmed by the increase in the pore surface fractal dimension, the increase in specific surface area of pores, the increase in connectivity density of the pore network and in the increased complexity of the corresponding skeleton. Such mechanism explains why models which did not consider the amorphous-to-crystalline transformation and treated the cement reaction as a through-solution process, failed in predicting the time-evolution of porosity and cement performance.

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MON 16:15-18:15 | BOARD 30 | P1-OPER-06

POSTER SESSION

NUCLEATION OF AMORPHOUS PRECURSOR IN MAGNESIUM PHOSPHATE CEMENTS FROM IN-SITU X-RAY TECHNIQUES

Presenter: Alberto VIANI
Authors: Alberto VIANI (1), Petra MÁCOVA (1), Marta PÉREZ ESTÉBANEZ (2)

In-situ synchrotron X-ray diffraction and small angle X-ray scattering indicated that in its early stages, the reaction pathway of magnesium phosphate cements involves the formation of an amorphous precursor, first detected as nanoparticles which organize themselves into larger domains. Crystallization occurs from this precursor (already containing the structural motives of the crystalline counterpart) by increasing the long-range order through relatively minor structural rearrangements. The process is compatible with multi-steps nucleation involving non-classical mechanisms, as observed in Ca-carbonates and phosphates, therefore, indicating ways to control the transformation to improve cement design.

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MON 16:15-18:15 | BOARD 31 | P1-OPER-07

POSTER SESSION

IN-SITU STUDIES OF ORDER-DISORDER EFFECTS IN FePd3Hx

Presenter: Holger KOHLMANN
Authors: André GÖTZE, Holger KOHLMANN

The intermetallic compound FePd3 attracts interest due to its physical, magnetic, and catalytic properties. Two phases are known in the atomic ratio of 1:3 of iron to palladium atoms. Fe0.25Pd0.75 crystallizes in the cubic close packing and its ordered variant FePd3 in the AuCu3 type. FePd3 with a high degree of crystallographic order shows a higher hydrogen incorporation at high hydrogen pressures compared to less ordering [1]. The hydrogenation at moderate hydrogen pressures as well as possible changes in structure and properties are investigated with in-situ studies like thermal analysis, neutron, and X-ray powder diffraction. At room temperature and deuterium pressure of 8 MPa the hydride FePd3D0.047(9) is formed and deuterium atoms are incorporated at [Pd6] octahedral sites. This formation results in a decrease of long-range order. Further heating experiments up to the Curie temperature of 495(8) K at moderate hydrogen pressures of 8 MPa show a behaviour of a 3D Ising or Heisenberg model. In addition, a decrease in the level of order is observed indicating an influence of the order of FePd3 by hydrogen incorporation and the magnetic orientation.

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[1] Flanagan, T.B.; Majchrzak, S.; Baranowski, B. A chemical reaction strongly dependent upon the degree of order of an alloy: The absorption of hydrogen by Pd3Fe. Philos. Mag. 1972, 25, 257–262, doi:10.1080/14786437208229233.

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MON 16:15-18:15 | BOARD 32 | P1-OPER-08

POSTER SESSION

KINETICS OF HYDROGEN ABSORPTION BY IN-SITU NEUTRON / X-RAY REFLECTOMETRY

Presenter: Laura GUASCO

Authors: Laura GUASCO (1), Yury KHAYDUKOV (1), Sabine PUETTER (2), Luca SILVI (3), Mariano PAULIN (3), Thomas KELLER (1), Bernhard KEIMER (1)

The study of hydrogen diffusion and storage in different materials is crucial for the realization of a hydrogen economy and implementation of sustainable energy sources in the automotive industry. Among the most widely used techniques to study hydrogen absorption in thin films we find neutron (NR) and X-ray reflectometry (XRR). XRR allows to track the thickness changes of the absorbing layer, while NR gives additional direct information about the absorbed hydrogen content. Nonetheless, NR is a relatively time-consuming measurement, with a sensitivity limit that greatly depends on the counting time. Recently we have developed a way to implement conventional reflectometry techniques for fast kinetics studies through resonant neutron reflectometry, or RNR [1]. Thanks to the combined information given by in-situ XRR and RNR performed at NREX, we were able to observe peculiarities in the absorption process of niobium, a well-known H-absorber largely studied in the past, that were never reported before [2]. In this talk we will discuss the current results as well as give a brief overview on possible future perspectives and further insights which can be achieved by combining neutrons simultaneously with different complementary techniques.

[1] L. Guasco, Y. Khaydukov et al., "'Resonant neutron reflectometry for hydrogen", Nat. Commun. 13, 1486 (2022)
[2] L. Guasco, Y. Khaydukov et al., "Kinetics of hydrogen absorption in niobium films with RNR", in preparation

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MON 16:15-18:15 | BOARD 33 | P1-OPER-09

POSTER SESSION

EXPLORATION OF FORMATION AND POLYMORPHISM OF K2SiH6 AT HIGH PRESSURES AND TEMPERATURES VIA IN-SITU SYNCHROTRON DIFFRACTION

Presenter: Doreen BEYER

Authors: Doreen BEYER (1), Kristina SPEKTOR (1,2), Olga VEKILOVA (2), Shrikant BHAT (3), Robert FARLA (3), Sergey SIMAK (4), Holger KOHLMANN (1), Ulrich HÄUSSERMANN (2)

Hydrogenation reactions employing gigapascal pressures (in a range from 4 to 10 GPa) afford unique all-hydrido hypervalent [SiH6]2- complexes in the crystalline hydridosilicate K2SiH6 [1]. Here we report on in-situ diffraction studies of reactions using KSi and KSiH3 as precursors. The experiments are based on large volume press (LVP) high pressure methodology and employed ammonia borane, BH3NH3, as a hydrogen source. We find that K2SiH6 forms at pressures around 8 GPa and comparatively low temperatures, below 300 °C, as a trigonal polymorph which at increased pressures (~13 GPa) is stable up to 750 °C upon melting. Upon pressure release K2SiH6 transforms into a cubic polymorph adopting the K2PtCl6 type structure, which can be recovered at ambient pressure. Theoretical calculations suggest that a third polymorph with a hexagonal structure is stable in the narrow pressure range 3 – 5 GPa. K2SiH6 is a semiconductor with a calculated (indirect) band gap of about 2 eV. In addition, the possible existence of metallic substitution variants K2Si1-xAlxH6 and K2Si1-xPxH6 is suggested by theoretical calculations.

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[1] Puhakainen, K.; Benson, D.; Nylén, J., Konar, S.; Stoyanov, E.; Leinenweber, K.; Häussermann, U. 2012 Angew. Chem. Int. Ed. 51, 3156-3160

Affillation
1: Universität Leipzig, Germany; 2: Stockholm University, Sweden; 3: Deutsches Elektronen-Synchrotron DESY, Germany; 4: Linköping University, Sweden

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MON 16:15-18:15 | BOARD 34 | P1-OPER-10

POSTER SESSION

IN-SITU REFLEXAFS INVESTIGATIONS ON Nb TREATED IN N2 GAS ATMOSPHERES AT ELEVATED TEMPERATURES

Presenter: Patrick ROTHWEILER
Authors: Patrick ROTHWEILER, Franz ECKELT, Moritz WEISS, Lukas VOSS, Frederic BRAUN, Jonas KLÄS, Florian BROCKNER, Dirk LÜTZENKIRCHEN-HECHT

On polished Nb metal bulk samples, time-resolved X-ray absorption spectroscopy investigations in reflection mode (ReflEXAFS) were done in dilute N2 gas atmospheres at elevated temperatures. Such a treatment is frequently used for the processing of Nb RF-cavities used in modern particle accelerators. The samples were investigated at the Nb K-edge to access the structural changes of the bulk material during the processing in N2. The treatments consisted of three phases: (a) the pre-heating at 900 °C under high-vacuum for 1 h, (b) the gas exposure for 1 h at temperatures between 900 °C and 1200 °C at a pressure of 3 mbar, (c) the cool down to room temperature under high-vacuum conditions. All samples were prepared in a high-vacuum cell with a base pressure of 10–6 mbar and accessible temperatures of up to 1200 °C. In addition to the in-situ ReflEXAFS measurements recorded using incidence angles close to the critical angle, ex-situ X-ray reflectivity and ex-situ ReflEXAFS measurements for different angles were performed before and after the treatments. Further, studies on the electron field emission of the Nb samples were carried out in the form of I-V characteristics – the latter provides the maximum electric field that can be potentially applied in particle accelerators. A detailed analysis of the data will be presented at the conference.

We gratefully acknowledge financial support from the German Federal Ministry of Education and Research (BMBF) under project No. 05H18PXRB1.

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MON 16:15-18:15 | BOARD 35 | P1-OPER-11

POSTER SESSION

OPERANDO NEXAFS INVESTIGATING LITHIUM SULFUR BATTERIES

Presenter: Konstantin SKUDLER
Authors: Konstantin SKUDLER (1), Alina KRIVOI (1), Rukiya MATSIDIK (2), Sunel DE KOCK (3), Matthias MÜLLER (1), Claudia ZECH (1)

Lithium sulfur batteries with their high specific capacities are promising alternatives to conventional lithium-ion batteries, yet there are some degradation mechanisms limiting their cycle stability. One of the most investigated effects is the polysulfide shuttle which is thought to continuously decrease the batteries' capacity. In the project of the DFG Priority Programme "Polymer-based Batteries" the goal is to bond the sulfur to the cathode inhibiting the polysulfide shuttle.

Investigating the chemical processes in lithium sulfur batteries to optimize capacity and cycling stability, *operando* NEXAFS measurements are performed to analyze the bond states of sulfur. The typical *operando* sulfur NEXAFS spectra depend on the state of charge and the number of already performed cycles and especially give hints on how the polysulfides act inside the cell.

For a more detailed understanding of the NEXAFS data for polymer cathodes, theoretical modeling of NEXAFS spectra is performed as another part of the project. For paradigmatic sulfide molecules, these spectra have been experimentally verified to further increase the quality of the spectrum deconvolution of working batteries.

Additionally, battery properties regarding various measurement techniques such as Electrochemical Impedance Spectroscopy (EIS) have been modeled and analyzed. We found correlations between electrochemical and NEXAFS data which help to better understand the processes inside the battery from another perspective.

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MON 16:15-18:15 | BOARD 36 | P1-OPER-12

POSTER SESSION

IN-SITU, TIME-RESOLVED ANALYSIS OF ZnO NANOPARTICLE FORMATION BY SIMULTANEOUS EXAFS AND XRD

Presenter: Dirk LÜTZENKIRCHEN-HECHT

Authors: Franz ECKELT (1), Dirk LÜTZENKIRCHEN-HECHT (1), Ankica SARIC (2), Martina VRANKIC (2), Lukas VOSS (1), Patrick ROTHWEILER (1), Frederic BRAUN (1)

Combined, simultaneous EXAFS-XRD are in particular interesting for time-resolved studies of chemical reactions in the liquid phase, which can hardly be investigated by XRD alone. Here the formation of ZnO nanoparticles is studied by a combination of Quick-EXAFS and XRD that provides information about the precursor materials (i.e. molecules) in solution and the nanocrystalline ZnO species formed in the course of the reaction. The synthesis is carried out in a dedicated cell made of carbon-reinforced PTFE. The sealed cell is equipped with a heater for temperatures of up to ca. 300°C, temperature sensors and a magnetic stirrer. Two Kapton windows allow to properly adjust the X-ray beam path within the solution and to measure the growth process of the nanoparticles in the solution with transmission mode EXAFS and XRD. As an example, the formation of ZnO nanoparticles in different solvents was successfully investigated here. For this, EXAFS and XRD measurements were carried out at the Zn K-edge. The measurements clearly show the advantages of the different measurement methods. At the beginning of the synthesis, the smallest proportions of the ZnO nanoparticles can be detected using the EXAFS measurements and the volume proportion of the nanoparticles in the sample can be determined using linear combination fits. XRD only show distinct diffraction peaks for larger particles. On the other hand, the particle size and shape, as well as the growth rate can be deduced from XRD.

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MON 16:15-18:15 | BOARD 37 | P1-OPER-13

POSTER SESSION

INVESTIGATION OF SPUTTER DEPOSITED Co- AND Cu-NITRIDE THIN FILMS USING GRAZING INCIDENCE EXAFS

Presenter: Lukas VOSS

Authors: Lukas VOSS, Frederik BRAUN, Franz ECKELT, Patrick ROTHWEILER, Dirk LÜTZENKIRCHEN-HECHT

Due to their high electrical conductivity and chemical stability, the nitrides of 3d transition metals (M = Cr, Mn, Fe, Co, Cu, Ni) are interesting materials for applications e.g. in catalysis and energy storage. Here, the samples were deposited on float glass substrates by reactive sputtering processes from metal targets in a miniaturized vacuum chamber, that was integrated into the beamline P64 at the PETRA III storage ring at DESY (Hamburg, Germany) for in-situ analysis. The QEXAFS monochromator in combination with gas-filled ionization chambers as detectors and the recently realized reflectometer allow a time resolution of a few seconds per spectrum. Several CoN samples were prepared using different sputtering currents in a pure nitrogen atmosphere under a constant pressure of 0.20 mbar. During deposition in-situ ReflEXAFS at the Co K-edge were carried out at an incident angle of 0.25°.

Additionally ex-situ XRD were taken to calculate the lattice constant and crystallite sizes. All results show the zinc-blende structure for CoN and an increasing surface roughness from which the growth exponent was calculated. Cu-nitride samples were prepared from a Cu-metal target using identical conditions (0.20 mbar, 10 mA), however with different nitrogen/argon gas mixtures. ReflEXAFS were performed for various incident angles around the critical angle for both CoN and CuN samples. A detailed analysis of the measured data will be presented.

Affillation
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MON 16:15-18:15 | BOARD 38 | P1-OPER-14

POSTER SESSION

NANOSCALE SUBSURFACE DYNAMICS OF SOLIDS UPON HIGH-INTENSITY FEMTOSECOND LASER IRRADIATION OBSERVED BY GRAZING-INCIDENCE X-RAY SCATTERING

Presenter: Lisa RANDOLPH

Authors: Lisa RANDOLPH (1), Özgül ÖZTÜRK (1), Mohammadreza BANJAFAR (2,3), Thomas PRESTON (2), Jan-Patrick SCHWINKENDORF (2), Toshinori YABUUCHI (4,5), Mikako MAKITA (2), Nicholas DOVER (6), Christian RÖDEL (7), Sebastian GÖDE (2), Yuichi INUBUSHI (4,5), Gerhard JAKOB (8), Johannes KAA (2), Akira KON (16), James KOGA (16), Dmitriy KSENZOV (1), Takeshi MATSUOKA (9,10), Mamiko NISHIUCHI (16), Michael PAULUS (11), Sripati RAHUL (2), Frederic SCHON (1), Keiichi SUEDA (5), Yasuhiko SENTOKU (12), Tadashi TOGASHI (4,5), Mehran VAFAEE-KHANJANI (8), Michael BUSSMANN (13,14), Thomas COWAN (3,13), Mathias KLÄUI (8), Carsten FORTMANN-GROTE (2), Lingen HUANG (13), Adrian MANCUSO (2,15), Thomas KLUGE (13), Christian GUTT (1), Motoaki NAKATSUTSUMI (2,9)

The interaction of intense laser pulses with solid matter initiates ultrafast surface electron density modulations on the nanometer scale, which provides a basis for technological developments in areas from surface ablation, material micro processing to relativistic plasma optics[1]. Currently, a lack of appropriate surface and subsurface methodology to track density dynamics with sufficient spatial and temporal resolution restricts quantitative understanding, and eventual control, of the laser-solid interaction and the subsequent energy transport into the bulk. We recently proposed a novel method for in-situ visualization of nanometer depth-resolved density dynamics by grazing-incidence X-ray small-angle scattering[2] using an XFEL. Measuring non-specular diffuse X-ray scattering patterns allows us to

cont.

[1] T. Kluge et al, Phys. Rev. X 8, p. 031068 (2018)
[2] S. K. Sinha et al, Phys. Rev. B 38, pp. 2297-2311 (1988)

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1: Universität Siegen, Germany; 2: European XFEL, Germany; 3: Technische Unversiät Dresden, Germany; 4: Japan Synchrotron Radiation Research Institute (JASRI), Japan; 5: RIKEN SPring-8 Center, Japan; 6: Imperial College London, UK; 7: Technische Universität Darmstadt, Germany; 8: Universität Mainz, Germany; 9: Open and Transdisciplinary Research Institute, Osaka University, Japan; 10: Graduate School of Engineering, Osaka University, Japan; 11: Technische Universität Dortmund, Germany; 12: Institute of Laser Engineering, Osaka University, Japan; 13: Helmholtz-Zentrum Dresden-Rossendorf, Germany; 14: Center for Advanced Systems Understanding (CASUS), Germany; 15: Department of Chemistry and Physics, La Trobe Institute for Molecular Science, La Trobe University, Australia; 16: QST-Kansai, KPSI, Kyoto, Japan

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cont.

access ... different depths inside strongly coupled dense plasmas with nm spatial and ps time resolution. Our first proof-of-principle experiments showed how the surface ablation and density perturbation following the fs laser pulse interaction with multilayer samples develop over time [3]. This new methodology will open new possibilities for characterization of (sub)surface dynamics and will allow the benchmarking of physics models and simulations with relevance to laser material processing and high-energy-density science.

[3] L. Randolph et al., arXiv 2012.15076

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MON 16:15-18:15 | BOARD 39 | P1-OPER-15

POSTER SESSION

OPERANDO INSIGHTS INTO BIMETALLIC Cu-BASED NANOCUBES DURING STATIC AND PULSED CO2 ELECTROREDUCTION TOWARD LIQUID PRODUCTS

Presenter: Antonia HERZOG

Authors: Antonia HERZOG, Hyo Sang JEON, Janis TIMOSHENKO, Clara RETTENMAIER, Martina RÜSCHER., Mauricio LOPEZ LUNA, Stefanie KÜHL, Felix T. HAASE, Uta HEJRAL, Arno BERGMANN, Beatriz ROLDAN CUENYA

The electrochemical reduction of CO2 can significantly contribute to mitigate the energy crisis by closing the carbon cycle and storing renewable energy in valuable multicarbon fuels and chemicals. Promising catalysts are Cu2O nanocubes, which can convert undesired CO2 efficiently into multiple C2+ hydrocarbons. However, the broad selectivity remains a major drawback and needs to be tuned toward energy dense liquids. The introduction of a second metal as Ag and Zn already showed improved catalytic performance and selectivity. However, in-situ and *operando* studies are missing to understand the coupling process of the bimetallic and to improve in this way the catalyst further. Here, we investigated the morphology, chemical state, and composition of the Cu-Ag catalyst under static CO2RR and of the Cu-Zn catalyst under pulsed CO2RR conditions by means of ex situ, in-situ and time-resolved synchrotron-based *operando* characterization techniques. By the addition of Ag NPs on Cu2O, we doubled the Faradaic efficiency of alcohols, while observing the formation of Cu-Ag distances in *operando* Ag K-edge EXAFS. The decoration of Cu2O with a ZnOx shell and the application of pulsed CO2RR into the oxidation regime of Zn could significantly enhance the ethanol selectivity. By using time-resolved *operando* characterization techniques we were able to track the evolution of the CuZn alloy and ZnO species in *operando* Zn K-edge and the dynamic lattice evolution of Cu in *operando* XRD.

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MON 16:15-18:15 | BOARD 40 | P1-OPER-16

POSTER SESSION

REAL-TIME STUDY OF SOLID-STATE REACTIONS AT THE Pd/a-Ge INTERFACE

Presenter: Bärbel KRAUSE

Authors: Bärbel KRAUSE (1), Gregory ABADIAS (2), David BABONNEAU (2), Tilo BAUMBACH (1), Alessandro COATI (3), Anny MICHEL (2), Anton PLECH (1), Andrea RESTA (3), Alina VLAD (3), Peter WOCHNER (4)

Controlled solid-state reactions at the metal/semiconductor interface are indispensable for the production of semiconductor devices. Undesired solid-state reactions, however, can reduce their performance and accelerate their degradation. Combining in-situ studies during deposition and annealing of ultrathin Palladium layers (0 – 30 nm) on amorphous Germanium, we have studied the impact of the as-deposited interface on subsequent nucleation and growth processes at the metal/semiconductor interface. The structure formation during sputter deposition was monitored using a unique combination of simultaneous synchrotron XRR, XRD, and optical stress measurements [1,2]. The subsequent annealing process was observed by XRD. The real-time synchrotron experiments were complemented by in-situ XPS and AFM measurements. Interestingly, the XRD analysis requires approaches typically known from epitaxial thin films and nanostructures. Our results provide a detailed picture of the complex interface formation in laterally isotropic metal/semiconductor systems, advancing thus the understanding and control of the interface-mediated phase formation and stress build-up in semiconductor devices.

[1] B. Krause et al., ACS Applied Materials and Interfaces, 2016, 8, 34888-34895
[2] B. Krause et al., ACS Applied Materials and Interfaces, 2019, 11, 39315-39323

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MON 16:15-18:15 | BOARD 41 | P1-OPER-17

POSTER SESSION

THE SOURCE OF TWINNING IN FCC NANOPARTICLES: HIGH CONCENTRATION OF VACANCIES

Presenter: Armin HOELL
Authors: Ilia SMIRNOV (1), Zbigniev KASZKUR (1), Armin HOELL (2)

FCC nanoparticles (NPs) are often observed (e.g. via TEM) in different morphologies: cuboctahedron (CUB), decahedral (DEC), or icosahedral. For a long time, the appearance of one or another morphology was considered from the point of view of the minimum free energy per atom. However, the mechanism of the twinning formation has not yet been described.

Our approach allows us to perform computational simulations of a twinning: high concentration of vacancies in a regular CUB model with subsequent relaxation leads to transformation of CUB into multitwinned NPs (with XRD pattern similar to DEC). Synchrotron radiation helped us to verify this concept. During long lasting exposures of ~2.3 nm Au NPs by X-ray beams with different flux intensities, various types of NP growth were observed and accompanied with:

- Accumulation of vacancies under low-flux synchrotron radiation: WAXS and SAXS analysis reveals growth of the mean particle size and decrease of NPs density;
- Quick accumulation followed by release of vacancies under high flux X-ray beam. WAXS and SAXS analysis shows decrease of the mean NPs diameter and growth of NPs density.

This indirect observation of vacancies is an important step to understand the development and evolution of NPs morphology.

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MON 16:15-18:15 | BOARD 42 | P1-OPER-18

POSTER SESSION

TWO STEP PHASE-SEGREGATION PROCESS REVEALED IN MIXED HALIDE MHPS BY SIMULTANEOUS IN-SITU X-RAY DIFFRACTION AND PHOTOLUMINESCENCE SPECTROSCOPY

Presenter: Klara SUCHAN
Authors: Klara SUCHAN (1), Justus JUST (2), Pascal BECKER (3), Carolin REHERMANN (3), Roland MAINZ (3), Ivan SCHEBLYKIN (1), Eva UNGER (1,3)

The compositional stability of mixed halide perovskite semi-conductors is limited by the light or electrical bias induced phase segregation, restricting the exploitation of the entire bandgap range. To identify the mechanism and cause of light-induced phase-segregation phenomena (photo-segregation), we combine insights from in-situ X-ray diffraction, nano-XRF and photoluminescence spectroscopy during illumination. We quantify the halide redistribution in-situ during segregation as well as its kinetics and further follow the interconnected charge carrier distribution. We apply currently discussed thermodynamic models directly to the experimental data to check their feasibility and to estimate the energy gained by segregation.

We propose a modified gap-model, resulting in a two-step segregation process. The first step corresponds to the nucleation of photo-segregation, which is thermodynamically driven by the energy reduction of charge carriers accumulating in I-rich domains. This is followed by an extended slow segregation phase connected to long lived modifications of the material. Our experimental results highlight the importance of understanding the interplay behind light induced modifications and self-healing capabilities in metal halide perovskites.

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MON 16:15-18:15 | BOARD 43 | P1-OPER-19

POSTER SESSION

MULTIMODAL COMBINED IN-SITU/OPERANDO XAS/XRD/UV-VIS MEASUREMENTS REVEAL COMPLEX TRANSFORMATION PROCESSES IN ENERGY MATERIALS

Presenter: Justus JUST
Author: Justus JUST

Meeting the raising demand for in-situ and in-*operando* studies on material systems especially for energy applications we developed an in-situ investigation platform at the Balder beamline at the MAX IV synchrotron. It consists of specialized sample environments, data analysis tools and multimodal real-time measurements of X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD) as well as optical spectroscopy (PL and UV-vis).

The Balder beamline at the 4th generation MAX IV synchrotron is dedicated to X-ray absorption and emission spectroscopy in the energy range of 2 – 45 keV, with a beamsize down to 50 x 50 µm and a flux of ~1013 ph/s. A recently developed diffraction endstation allows to perform simultaneous measurements of XAS and XRD with time resolutions down to 1s or 10ms, respectively. Here, an FPGA based trigger controller synchronizes all experimental read outs with the monochromator energy motion.

Combining such multimodal real-time measurements with specially developed sample-environments and data evaluation procedures allows us to unravel complex processes during formation and operation of energy related solid state materials. Herein, we will present first results obtained on:

1) the crystallization of perovskite semiconductors for photovoltaic applications

2) the evolution of bimetallic Pt-Pd catalysts during methane oxidation as well as

3) the cation reorganization during charge/ discharge cycling of LNMO based Li-ion batteries.

Affillation
MAX IV Laboratory, Sweden

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MON 16:15-18:15 | BOARD 44 | P1-OPER-20

POSTER SESSION

OPERANDO X-RAY ABSORPTION SPECTROSCOPY (XAS) TO PROBE POTENTIAL DEPENDANT CHANGES OF PtCo NANOPARTICLES DURING OXYGEN REDUCTION REACTION (ORR)

Presenter: Jochen KLEIN
Authors: Jochen KLEIN, Marek JANSSEN, Alexandra DWORZAK, Sonja BLASEIO, Mehtap OEZASLAN

PtCo alloy catalysts are highly active for the oxygen reduction reaction (ORR). The structure and composition of those nanoparticles have a strong influence on the catalytic activity and durability.

In this work, PtCo nanoparticles supported on high surface area carbon (HSAC) were investigated using *operando* XAS. Operando XAS is a powerful tool to gain insights into the identification of the catalytically active sites under ORR conditions. The PtCo alloy NPs show higher specific ORR activities (592±171 µA/cmPt2 at 0.9 V(RHE)) compared to commercial Pt/C catalysts (187±29 µA/cmPt2).

XAS measurements were performed in an in-house electrochemical flow cell with a three electrode arrangement. To monitor the electronic and geometric changes of Pt and Co inside the NPs during the ORR, XAS spectra of the Pt LIII and the Co K edges were measured as a function of the applied potential (0.2, 0.4, 0.7, 0.8, 0.9, 1.0 V(Ag/AgCl)) in oxygen saturated 0.1 M HClO4 electrolyte.

Analysis of the white line intensity from the Pt LIII edge XAS data shows that the oxidation state is highly dependant on the applied potential with reduction taking place below and oxidation above 0.7 V(Ag/AgCl). Very remarkably, the Co K edge shows that Co appears in metallic as well as in an oxidized state throughout the experiment. Furthermore the partial coordination number of Pt and Co (N(Pt-Co)) indicates a potential-dependant change of the intermixture of both metals.

Affillation
TU Braunschweig, Germany

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MON 16:15-18:15 | BOARD 45 | P1-OPER-21

POSTER SESSION

REVERSED BENDING IN GaAs/(In,Ga)As/GaAs NANOWIRE HETEROSTRUCTURES

Presenter: Jochen KALT

Authors: Jochen KALT (1), Ali ALHASSAN (1), Mahmoud HUMAIDI (1), Dmitri V. NOVIKOV (2), Taseer ANJUM (3), Uli PIETSCH (3), Tilo BAUMBACH (1,4)

In this study, we investigate the flexibility and elasticity of bent nanowire heterostructures in a core/shell/shell growth process. An ideal technique to quantify the smallest changes in the orientation of nanowire ensembles, i.e. tilting and bending, and to trace the evolution of axial strain during shell growth is time-resolved X-ray diffraction. The samples were grown in a portable MBE chamber with X-ray transparent Be windows, installed on the heavy load diffractometer of beamline P23 at PETRA III. This allowed to investigate the process in-situ, i.e. during deposition of the shells. First, GaAs nanowires were epitaxially grown on Si(111) substrates, covered by their native oxide. Second, an (In,Ga)As shell was deposited asymmetrically on one side of the nanowires, which forces the nanowires to bend. Subsequently, an outer GaAs shell was grown on the same nanowire side, inducing compressive strain on the (In,Ga)As layer and therefore forcing the nanowire to partially straighten. The evolution of the induced unconventional strain field and nanowire bending were observed by changes of the Ga(111) Bragg peak profile, which was recorded at several stages of the shell growth process. The results will help to quantify the tensile and compressive strains induced by the two different shells and to understand their competing influence on the shape.

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MON 16:15-18:15 | BOARD 46 | P1-OPER-22

POSTER SESSION

IN-SITU OBSERVATIONS OF ORGANIC ALL-SMALL-MOLECULE VACUUM-THERMALLY-EVAPORATED BULK HETEROJUNCTION FILM GROWTH USING ELLAGIC ACID AS A TEMPLATING LAYER

Presenter: Olivia GOUGH
Authors: Olivia GOUGH (1), Andreas EJDRUP LAURITZEN (1), Zhenlong LI (1), Mathias HUSS-HANSEN (2)

The growth mode of organic molecules is important to consider when designing all small-molecule (SM) solar cells, as it can have a large impact on structure. Using a templated layer in such devices gives control over structure; having control over the orientation of molecules deposited leads to enhanced optoelectronic properties, which in turn give better solar cell efficiencies. The real-time growth evolution of vacuum-deposited all SM bulk heterojunction thin films using ellagic acid (EA) as a templating layer on glass are reported, via in-situ grazing incidence wide angle X-ray scattering (GIWAXS). The GIWAXS data were obtained via depositions in a purpose-built chamber, MINERVA, on the I07 beamline at Diamond Light Source. We report that the use of a thin film of EA beneath a bulk heterojunction film leads to a favourable orientation of donor molecules. Furthermore, the changes in morphology are reflected in electronic properties, and mobilities are given for transistors of pure donor films with and without a templating layer. In order to correlate changes in structure with surface morphology, atomic force microscopy (AFM) is used. Finally, full devices including the EA templating layer will be fabricated, in order to demonstrate their improved device efficiency when compared against devices without the EA layer. The use of this molecule is an exciting prospect in terms of the broader renewable energy picture; EA is cheap, readily available and derived from fruits.

Affillation
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MON 16:15-18:15 | BOARD 47 | P1-OPER-23

POSTER SESSION

INVESTIGATING THE EFFECT OF REACTION CONDITION PARAMETERS ON THE REVERSIBLE S-O EXCHANGE AT THE ACTIVE SITES OF MoS2 BASED HYDROTREATING CATALYSTS BY ME-XAS

Presenter: Abhijeet GAUR

Authors: Abhijeet GAUR (1,2), Martin HØJ (3), Matthias STEHLE (1), Marc-André SERRER (1,2), Magnus Zingler STUMMANN (3), Camille LA FONTAINE (4), Valérie BRIOIS (4), Jan-Dierk GRUNWALDT (1,2)

The high sensitivity of modulation excitation spectroscopy (MES) coupled X-ray absorption spectroscopy (XAS) has been exploited in-situ to unravel the minute differences in active site composition of Co-MoS2 and MoS2 hydrotreating catalysts under the influence of H2S and H2O. These MoS2 based catalysts are active for hydrodesulfurization and hydrodeoxygenation in chemical industry and new biomass-related processes. MoS2/Co-MoS2 catalysts (varying metal loadings) were investigated at Co K/Mo K-edges. Experiments were performed at the ROCK beamline, SOLEIL in a quartz microreactor at 400, 450 and 500°C under H2O/H2S or 1-propanol/H2S. Multivariate curve resolution alternating least squares (MCR-ALS) analysis was performed to determine and confirm the different Co species present. Transient XAS at Mo/Co K-edge revealed minute levels of S-O exchange at sulfided Mo/Co sites. ME-XAS analysis showed that increase in metal loading stabilizes the catalyst against the unwanted S-O exchange whereas increase in temperature makes the catalyst more prone to such process. Comparison of cycling experiments using 1-propanol vs. H2S with H2O vs. H2S revealed that H2O was more effective for S-O exchange than 1-propanol. Thus, ME-XAS in addition to changes on catalyst surfaces can also evaluate the comparative degree of changes due to the variation in reaction conditions. In general, combination of these methods can be very useful to resolve the minute phase transitions under dynamic conditions

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MON 16:15-18:15 | BOARD 48 | P1-OPER-24

POSTER SESSION

CORRELATING THE WETTING ANGLE OF THE Ga DROPLET WITH POLYTYPISM IN AS-GROWN GaAs NANOWIRES USING XRD AND GISAXS

Presenter: Ali ALHASSAN

Authors: Ali ALHASSAN (1), Mahmoud AL-HUMAIDI (1,2), Jochen KALT (1,2), Ewen BELLEC (3), Taseer ANJUM (4), Julian JAKOB (1,2), Tobias SCHULLI (3), Ullrich PIETSCH (4), Tilo BAUMBACH (1,2)

In III-V nanowire (NW) based devices, a high control over the crystal quality is required because it dictates the opto-electronic properties. GaAs NWs are often fabricated by molecular beam epitaxy using the self-catalyzed vapour-liquid-solid mode, where a liquid Ga catalyst droplet at the apex of the NW drives the axial crystal growth. The wetting angle of the droplet determines the crystal structure of the NWs which mainly consists of the zinc blende (ZB) and wurtzite (WZ) crystal phases when grown along the [111] crystallographic direction. Regardless of the high degree of control over the crystal phase during latter growth stages, the NW base remains defective as it is challenging to control polytypism at the beginning of the NW growth due to transients in the droplet wetting angle. Moreover, important surface properties i.e. competition between neighboring NWs for the same source materials, and diffusion effects influence the droplet wetting angle.

The aim here is to trace the mean contact angle of Ga droplets on the substrate surface and on as-grown GaAs NW stumps at the early stages of nanowire growth, and correlate the droplet contact angle with the crystal structure of the NW stumps underneath. To do so, grazing incidence small angle X-ray scattering and asymmetric X-ray diffraction are performed on Ga droplets deposited by MBE onto Si 111 substrates and on NW stumps with the Ga droplets on top.

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MON 16:15-18:15 | BOARD 49 | P1-OPER-25

POSTER SESSION

LATTICE THERMAL EXPANSION OF AS-GROWN GaAS NANOWIRES DUE TO OPTICAL EXCITATION MEASURED BY X-RAY PUMP PROBE EXPERIMENT

Presenter: Taseer ANJUM

Authors: Taseer ANJUM (1,2), Francisca LARGO (1), Waheed SALEHI (1), Matthias RÖSSLE (3), Oliver BRANDT (2), Lutz GEELHAAR (2), Ullrich PIETSCH (1)

We investigated the transient structural response in the ensemble of AlxIn1-xAs/GaAs core-shell NWs, grown on Si (111) substrate when irradiated with femtosecond laser pulses via X-ray pump-probe experiment at the KMC3-XPP beamline of BESSY II. The structural variation is introduced via a pulsed laser heating and the transient response is registered via X-ray diffraction by fulfilling the Bragg's condition in the reciprocal space. Femtosecond laser irradiation of solids excites photoelectrons from valance band to conduction and triggers a cascade of fundamental dynamical processes that occur on the picosecond to nanosecond time scales like excitation and thermal equilibration of phonons. Diffracted intensity from the sample is recorded by a two-dimensional Pilatus detector. During the time-resolved hard X-ray diffraction experiment, we measured the lattice thermal strain as a function of laser incident fluence and as a function of NW diameter by examining the transient shift of the 111-peak position of the NW ensemble. Through time-resolved X-ray pump-probe experiments we identified the dynamics of the structural response of two NW samples due to laser excitation. NWs with smaller diameters take longer to release the stored heat in comparison to NWs with bigger diameters where the relaxation is faster.

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MON 16:15-18:15 | BOARD 50 | P1-OPER-26

POSTER SESSION

INFLUENCE OF THE ANTI-SOLVENT DROP ON THE FILM FORMATION PROCESSES IN MIXED-HALIDE PEROVSKITES BY IN-SITU MULTIMODAL SPECTROSCOPY AND X-RAY SCATTERING

Presenter: Carolin REHERMANN

Authors: Carolin REHERMANN (1), Tim KODALLE (2), Jonathan SLACK (3), Nobumichi TAMURA (3), Carolin M. SUTTER-FELLA (2), Eva L. UNGER (1,4,5)

Metal-halide perovskites evolved over the last decade due to their outstanding optical properties [1] as a photoactive material in various optoelectronic devices. All devices require high-quality thin films, mainly morphological but also regarding ionic homogeneity.

While mixed materials of the MAPb(BrxI1-x)3 series can be synthesized, recent studies have highlighted microscopic ionic heterogeneity, originating from the synthesis of the sample. Intrinsic heterogeneous formation processes via competing pathways, rationalize ionic heterogeneities within the MAPb(BrxI1-x)3 series prepared without an anti-solvent drop. Depositing an anti-solvent is an established method to prepare high-quality perovskite films.

We rationalize the formation mechanism by utilizing the three anti-solvents types for the MAPb(BrxI1-x)3 series via structural and optical in-situ characterization. We answer the questions: Does the anti-solvent facilitate more homogeneous samples ionically by “quenching” or worsen the inhomogeneity by inducing the system to crystallize in different phases? The answer strongly depends on how the anti-solvent acts, either as a medium forcing the whole system into oversaturation, including the formation of solvate phases, or by removing the original solvent, possibly preventing the formation of solvate phases. Rationalizing the underlying mechanisms of the anti-solvent drop helps to understand and control their effect on homogeneity and morphology of final thin films.

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MON 16:15-18:15 | BOARD 51 | P1-OPER-27

POSTER SESSION

SIMULTANEOUS STRAIN DETECTION DURING IN-SITU THIN FILM GROWTH ANALYSIS

Presenter: Anton PLECH
Authors: Anton PLECH, Yannis KLÜGL, Tilo BAUMBACH, Bärbel KRAUSE

In-situ analysis of the structure evolution in thin-film growth can be performed with synchrotron-compatible vacuum chambers, such as the magnetron sputtering setup at KIT. In addition to atomic-scale and microscale structure determination by X-ray methods the macroscopic strain can be accessed by an optical setup. A deposited thin film producing an in-plane stress leads to a macroscopic bending of a thin substrate. We have developed a laser-based curvature attachment to the sputter chamber, which is based on a holographic multi-beam imager. A curvature between 2*10^-5 and 1 m^-1 can be resolved with 1 second time resolution.

Affillation
Institute for Photon Science and Synchrotron Radiation, Karlsruhe Institute for Technology, Germany

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MON 16:15-18:15 | BOARD 52 | P1-OPER-28

POSTER SESSION

EFFECT OF BORON ON THE REACTION OF MAGNESIUM PHOSPHATE CERAMICS: AN IN-SITU SYNCHROTRON SAXS-WAXS STUDY

Presenter: Radek SEVCIK
Authors: Radek SEVCIK, Lucie ZARYBNICKA, Petra MACOVA, Alberto VIANI

Boron, introduced as boric acid or borax in the raw mix of magnesium phosphate ceramics, is known to influence the reaction path during ceramic hardening, mostly retarding the crystallization reaction. Despite the numerous studies, a thorough understanding of the mechanism of action of boron is still far to be reached.

In this work the reaction has been followed in-situ in a combined synchrotron SAXS-WAXS time-resolved experiment. The WAXS results indicated that boric acid effectively retarded the crystallization, compared to the neat ceramic formulation. However, during this extended induction time, the SAXS curves exhibited a striking time-evolution, with the formation of scattering objects with a sharp distribution of sizes centered at about 60 nm and rapidly growing up to 200 nm. This marked a difference with the SAXS curves of the neat ceramic, which, in agreement with a recent study, showed the nucleation of a gel-like amorphous precursor of the crystalline magnesium orthophosphate, characterized by large clusters separated by an average distance of the order of 10 – 12 nm with a shorter correlation length (i.e. mesh size).

It is proposed that the structure of the amorphous intermediate precursor is altered thanks to the crosslinking ability of B, forming B-P connectivities, eventually hindering the amorphous-to-crystalline transformation. This is in agreement with recent diffraction and NMR results, and ruled out the crystallization boron magnesium phosphates.

Affillation
Institute of Theoretical and Applied Mechanics of the Czech Academy of Sciences

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MON 16:15-18:15 | BOARD 53 | P1-OPER-29

POSTER SESSION

CHARACTERIZATION OF INDUSTRIAL RELEVANT CATALYTIC MATERIALS FOR EMISSION CONTROL USING X-RAY ABSORPTION SPECTROSCOPY

Presenter: Samuel STRUZEK

Authors: Samuel STRUZEK, Tim DELRIEUX, Anna ZIMINA, Danielle SANTOS GONCALVES, Joachim CZECHOWSKY, Florian MAURER, Jan-Dierk GRUNWALDT

Synchrotron-based characterization of catalytic materials is usually conducted on model powder catalyst systems. X-ray absorption spectroscopy (XAS) is hereby a powerful tool to determine oxidation state and structure of the catalytically active species. However, to bridge the complexity scales to industrial systems, more realistic systems need to be studied as well.

For such systems the investigations of structural gradients are challenging. Therefore, new catalyst and reactor designs are mandatory to enable *operando* and spatially resolved measurements.

In this study which is part of the CRC 1441, we present pilot *operando* XAS studies which were performed on CO oxidation catalysts. The catalysts were used both as model powders and coated layers on monoliths.

To avoid large temperature gradients and deviations between the temperature and its setpoint, a planar chip design with integrated heating was used to simulate monolithic structures.

For both coated systems similar trends were observed between the oxidation state of catalysts and the reaction temperature. Furthermore, the coated planar samples showed a rather high conversion rate for CO oxidation. These findings will be used as basis for simultaneous planar laser induced fluorescence and XAS measurements for non-invasive evolution investigations of the gas phase and the catalyst structure.

Affillation
Karlsruher Institut für Technologie, Germany

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MON 16:15-18:15 | BOARD 54 | P1-OPER-30

POSTER SESSION

HARD X-RAY TOMOGRAPHY FOR 3D SPATIALLY-RESOLVED MULTISCALE AND MULTIMODAL CHARACTERIZATION OF NON-MODEL CATALYSTS

Presenter: Shweta SHARMA
Authors: Shweta SHARMA (1), Srashtasrita DAS (1), Dario FERREIRA SANCHEZ (2), Vasyl MARCHUK (1), Dmitry DORONKIN (1), Tim DELRIEUX (1), Jan-Dierk GRUNWALDT (1), Thomas SHEPPARD (1)

Hard X-ray tomography can be used to investigate the complex hierarchical structure of solid catalysts in 3D space. Moreover, when combined with *operando* methodology, and an additional characterisation method such as X-ray absorption spectroscopy, tomography can be used to establish the link between catalyst structure and activity, producing 3D spatially-resolved volumes of catalysts at work with chemical contrast.[1,2] Here we apply conventional tomography to investigate the physical properties of automative emission control catalysts (2 wt% Pt/Al2O3 washcoated monoliths). Analysing porosity, washcoat thickness and catalytic performance enables to optimise the coating procedure. Furthermore, *operando* hard X-ray spectrotomography was used to observe gradients in oxidation state and local chemical composition as a function of washcoat thickness in Cu-SSZ-13 washcoated monoliths for NH3-SCR process. This method has now been extended to structured composite catalysts consisting of dual layers or mixed monolayer of Pt/Al2O3 (NH3 oxidation function) and Cu-SSZ-13 zeolite (NOx reduction function) to examine the distribution of ammonia and oxidation states of Cu species in the washcoat of the working technical catalyst in 3D space. This can be used to achieve an in-depth understanding of catalyst performance, promoting targeted design of structured catalysts in emission control.

[1] J. Becher et al., Nat. Catal. 4, 1 (2021).
[2] D. Sanchez et al., Angew. Chem. Int. Ed. 60, 18 (2021).

Affillation
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MON 16:15-18:15 | BOARD 55 | P1-OPER-31

POSTER SESSION

CHARACTERISATION OF LiBH4-MgH2 REACTIVE HYDRIDE COMPOSITE SYSTEM WITH SCATTERING AND IMAGING METHODS USING NEUTRON AND SYNCHROTRON RADIATION

Presenter: Fahim KARIMI
Author: Fahim KARIMI

Reversible solid-state hydrogen storage is a key technology for pollutant-free energy conversion. The so-called “reactive hydride composite” (RHC) systems are a special class of solid-state hydrogen storage materials that are promising for mobile applications, owing to their high gravimetric capacity and low reaction enthalpy. In this work, the composite system LiBH2–MgH2 is investigated using synchrotron- and neutron radiation based probing methods that can be applied to characterize such systems from nanoscopic levels up to macroscopic scales.

Affillation
Helmholtz Zentrum Hereon, German

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MON 16:15-18:15 | BOARD 56 | P1-OPER-32

POSTER SESSION

FIXED-BED REACTOR FOR OPERANDO STRUCTURE-ACTIVITY PROFILING

Presenter: Oliver KORUP
Authors: Birte WOLLAK (1), Thomas SHEPPARD (2), Diego ESPINOZA (1), Dmitry DORONKIN (2), Marina STURM (3), Ann-Christin DIPPEL (3), Olof GUTOWSKI (3), Oliver KORUP (1,4), Michael SCHMIDT (4), Raimund HORN (1,4)

A major goal in catalysis research is to optimize catalytic processes based on knowledge. A crucial step towards this goal is to holistically understand catalysts and their complex structure-activity relationships through appropriate experiments, such as operando studies. Currently, most operando catalysis studies at synchrotron radiation facilities are performed with very small sample geometries, typically <1.5 mm diameter reactors, which often restricts catalytic activity measurements to the reactor in- and outlet. Here we introduce a fixed-bed profile reactor capable of simultaneously measuring spatially-resolved operando concentration-, temperature-, and XAS or XRD profiles through a catalyst bed. This approach can be used to probe chemical and structural gradients within working catalytic reactors.

The oxidative dehydrogenation of C2H6 to C2H4 over a MoO3/gamma-Al2O3 catalyst was used as a test system to develop the combined methodology.

The introduced reactor pushes operando catalysis research to a new level, due to the acquisition of spatially-resolved chemical and structural information which is directly correlated based on the position within the reactor. This combined methodology will generate interest from scientists, engineers and researchers in heterogeneous catalysis and reaction engineering in academia and industry alike, because it is a meaningful, versatile and accessible approach to understand and optimize a broad range of catalytic processes.

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MON 16:15-18:15 | BOARD 57 | P1-OPER-33

POSTER SESSION

X-RAY EMISSION MEASUREMENTS FROM X-RAY HEATED MATTER CONTAINED IN A DAC: A STUDY OF FES

Presenter: Johannes KAA

Authors: Johannes KAA (1,2), Christian STERNEMANN (2), Karen APPEL (1), Christian ALBERS (2), Khachiwan BUAKOR (1), Valerio CERANTOLA (1), Anand DWIVEDI (1), Mirko ELBERS (3), Lélia LIBON (3), Mikako MAKITA (1), Motoaki NAKATSUTSUMI (1), Alex PELKA (1), Sylvain PETITGIRARD (4), Christian PLÜCKTHUN (5), Thomas PRESTON (1), Christoph SAHLE (6), Robin SAKROWSKI (2), Georg SPIEKERMANN (4), Nicola THIERING (2), Metin TOLAN (2,7), Max WILKE (2), Ulf ZASTRAU (1), Zuzana KONOPKOVA (1)

The novel approach of combining a diamond anvil cell sample environment with X-ray heating and MHz resolved X-ray diffraction measurements has been recently introduced to the High-Energy-Density (HED) instrument of the European XFEL (EuXFEL) [1]. It enables measurements of the samples' structure at static high pressures (p) and extreme temperatures (T) and, in future, also at unique thermodynamic conditions induced by e.g. laser shock compression with a nanosecond time resolution [2].

We implemented a von-Hámos spectrometer in the vacuum chamber Interaction chamber 1 (IC1) of HED dedicated for X-ray emission spectroscopy (XES) measurements at extreme p/T conditions and exploited the X-ray heating after a successful proof-of-principle experiment [3]. We successfully applied the final setup for spin sensitive Fe Kβ and Kα fluorescence measurements from the FeS system at conditions close to the Mars' cores' p/T including melting. The temperatures and changes in the samples' structure were monitored with simultaneously measured X-ray diffraction (XRD). The spin state of iron changed during heating from an initial low or medium to higher average spin states.

In addition to that we explored the capabilities of the new setup to measure X-ray pulse-resolved Fe Kβ and Kα emission spectra, which would allow for spin measurements on a microsecond time scale.

[1] [Liermann et al.
[2] Cerantola et al. (2021)
[3] Kaa et al. (2022)

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1: European XFEL, Schenefeld, Germany; 2: Technische Universität Dortmund, Dortmund, Germany; 3: Universität Potsdam, Potsdam, Germany; 4: ETH Zürich, Zürich, Switzerland; 5: Deutsches Elektronen-Synchrotron, Hamburg, Germany; 6: European Synchrotron Radiation Facility ESRF, Grenoble, France; 7: Universität Göttingen, Göttingen, Germany

MON 16:15-18:15 | BOARD 63 | P1-MET1-01

POSTER SESSION

ELECTRONIC EFFECTS IN PHOTOEXCITED EPITAXIAL ZINC OXIDE NANORODS INVESTIGATED BY TRANSIENT X-RAY ABSORPTION LINEAR DICHROISM

Presenter: Thomas C. ROSSI

Authors: Thomas C. ROSSI (1,2), Conner P. DYKSTRA (2), Tyler N. HADDOCK (2), Rachel WALLICK (2), John H. BURKE (2), Cecilia M. GENTLE (2), Gilles DOUMY (3), Anne Marie MARCH (3), Renske M. VAN DER VEEN (1,2)

Understanding the electronic structure and dynamics of semiconducting materials at the atomic level is crucial for the realization and optimization of devices in solar energy and photocatalysis. Unidimensional carrier transport in oriented nanorod arrays is a promising development for enhanced performances in solid-state solar cells. Epitaxial ZnO nanorods in particular have emerged as promising candidates due to the piezophototronic tunability of electronic conduction. Here, we report on the picosecond dynamics of atoms and charge carriers in photoexcited epitaxial ZnO nanorods by time-resolved X-ray absorption linear dichroism. The transient signal is composed of incoherent atomic thermal motion and non-local screening of the core-hole potential by photogenerated electron-hole pairs. In addition, we observe transient phase-space filling in the pre-edge. Our results open new perspectives for the study of charge carriers in photoexcited semiconductor materials from an atomic perspective, which should prove useful in materials and devices composed of multiple chemical elements.

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MON 16:15-18:15 | BOARD 64 | P1-MET1-02

POSTER SESSION

THE NEW SMALL ANGLE X-RAY SCATTERING BEAMLINE FOR MATERIALS RESEARCH AT PETRA III (SAXSMAT – P62)

Presenter: Sylvio HAAS
Authors: Sylvio HAAS, Xiao SUN, André CONCEICAO, Saskia PFEFFER

The new SAXSMAT beamline P62 at PETRA III (DESY) is dedicated to perform combined small- and wide-angle X-ray scattering. The SAXSMAT beamline is focusing on anomalous SAXS, SAXS tomography (invariant rotation or tensor), and single or combined SAXS and WAXS. The beamline aims at in-situ and *operando* characterization of structural and functional materials, and catalytic and electrochemical processes by a combination of SAXS/WAXS, and multi-probe imaging techniques.

The SAXS-instrument consists of a 13m long and 1m diameter evacuated tube system in which the SAXS detector can be continuously moved along the beam direction. In front of the SAXS-tube, a specially designed cone allows the installation of a WAXS detector for simultaneous SAXS/WAXS measurements. A vacuum compatible Eiger2 X 9M detector and a customized Eiger2 X 4M-DESY detector are used as SAXS and WAXS detector, respectively. The sample area is an open space that allows the installation of different kinds of sample environments setups either from P62 or from the users.

Within this contribution the following topics will be presented:

- Current status and performance of the SAXSMAT beamline
- Showcase for anomalous SAXS/WAXS to determine an organic surfactant layer on top of metallic nanoparticles
- Showcase for SAXS tensor tomography to obtain a 3D representative model in real space describing the nanostructure
- Showcase for in-situ synthesis study of the formation of ZnO particles

Affillation
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MON 16:15-18:15 | BOARD 65 | P1-MET1-03

POSTER SESSION

SAXS / WAXS TOMOGRAPHY AT THE SAXSMAT BEAMLINE P62 AT PETRA III

Presenter: Sylvio HAAS
Authors: Sylvio HAAS, Xiao SUN, André CONCEICAO, Saskia PFEFFER

For many scientific questions gaining three-dimensional insight, coupled with the ability to probe structures across multiple length scales of a specimen can provide precious information. The SAXSMAT beamline provide dedicated instrumentation for the spatially-resolved mapping of the orientation and degree of organization of hierarchical nanostructures and, then deciphering the intricate interplay of mechanisms acting at different scales – from the atomic to the macroscopic, which is crucial for the development of new functionalities and new materials, since multifunctionality is a matter of design strategy.

The dedicated SAXS/WAXS-CT approach at the SAXSMAT beamline is composed of a sample environment, two detectors and a pipeline for data acquisition, treatment, and online reconstruction. The sample environment consists of a stack of high-resolution nano-positioners allowing translation horizontally and vertically as well as a rotary stage on top where the sample is positioned. An additional rotary stage is used to tilt the rotation axis, as required for the tensor tomography technique. Moreover, a pico-scale feedback system for online correction of potential misalignment of the sample during the measurement is also utilized. The acquired images are submitted to an in-house workflow accelerated by graphics processing units (GPUs) for the data processing and tomographic reconstruction.

Here we present the setup installed at SAXSMAT beamline P62 as well as the first results.

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MON 16:15-18:15 | BOARD 66 | P1-MET1-04

POSTER SESSION

TRANSFER PROGRAM OF NEUTRON SCATTERING INSTRUMENTATION FROM BER II

Presenter: Daniel CLEMENS

Authors: Daniel CLEMENS, Thomas WILPERT, Peter SMEIBIDL, Sebastian GERISCHER, Klaus KIEFER, Dirk WALLACHER, Axel RUPP, Roland STEITZ

Beginning in 2013 when the shut-down of the Berlin Experimental Reactor (BER II) in December 2019 was announced, the management of Helmholtz-Zentrum Berlin (HZB) was offering HZB's highly competitive, in part unique neutron scattering instrumentation and sample environment to neutron scattering facilities all over the world. A large number of collaborating institutions concluded contracts with HZB or are in the preparation of such, so that there is confidence that all 24 (incl. SPAN 25) BER II instruments, a substantial part of the neutron guides and shielding will have found new homes at collaborating neutron science centers in Germany, in Europe and overseas. Until now 12 instruments have been delivered out of which 4 instruments have already taken up user service again at their new destinations. A team of scientists, units of the administration and the technicians that once guaranteed for the continuous successful operation of the instruments at BER II reoriented to the necessary processes that ensure successful transfer of the experimental stations to their new locations. We describe these processes and the status of the transfer project which is an enormously important activity for keeping the valuable BER II experimental facilities available to the international user community.

Affillation

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MON 16:15-18:15 | BOARD 67 | P1-MET1-05

POSTER SESSION

MATERIALS SCIENCE AND SOFT-MATTER RESEARCH AT BEAMLINE BL9 OF DELTA

Presenter: Christian STERNEMANN

Authors: Michael PAULUS (1), Christian ALBERS (1), Steffen BIEDER (1), Jennifer BOLLE (1), Steffen CORNELIUS (2), Susanne DOGAN (1), Kevin LEHNINGER (1), Marc MORON (1), Mike MORON (1), Julia NASE (1), Robin SAKROWSKI (1), Patrick SCHLENZ (2), Eric SCHNEIDER (1), Göran SURMEIER (1), Nicola THIERING (1), Bridget MURPHY (1,3,4), Metin TOLAN (1,5), Christian STERNEMANN (1)

Beamline BL9 of the DELTA synchrotron radiation facility (Dortmund, Germany) is dedicated to grazing-incidence X-ray diffraction and X-ray reflectivity studies with focus on materials science and soft matter research. Since the end of 2020, a new 7-Tesla superconducting wiggler serves as radiation source providing X-rays in the energy range between 6 keV and 27 keV. The beamline is equipped with a MAR345 image plate scanner and a Pilatus-100k detector. Various sample environments support temperature conditions between 10 K and 1350 K and pressures up to 5 kbar for in-situ studies. We present the beamline characteristics along with selected examples of typical X-ray reflectivity and wide angle X-ray scattering experiments performed recently in order to demonstrate its capabilities for user experiments.

We acknowledge funding of the superconducting wiggler by the DFG via project INST 212/330-1 AOBJ: 619186. The experiments were supported by the BMBF via 05K19PEA, by Germany's Excellence Strategy – EXC 2033 – Project-ID 390677874, by the DAAD via project 57560563 and by the project NanoQI which receives funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 862055.

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MON 16:15-18:15 | BOARD 68 | P1-MET1-06

POSTER SESSION

ENABLING TIME-RESOLVED TWO-COLOR EXPERIMENTS WITH THE SPLIT-AND-DELAY UNIT AT FLASH2

Presenter: Matthias DREIMANN

Authors: Matthias DREIMANN (1), Dennis ECKERMANN (1), Sebastian ROLING (2), Marion KUHLMANN (3), Sven TOLEIKIS (3), Frank WAHLERT (2), Rolf TREUSCH (3), Elke PLÖNJES-PALM (3), Helmut ZACHARIAS (1)

A split-and-delay unit (SDU) for the extreme ultraviolet (XUV) and soft X-ray region has been built that enables time-resolved experiments for users at the beamlines FL23 and FL24 at the free-electon laser in Hamburg (FLASH2). Geometric wavefront splitting at a sharp edge of a beamsplitting mirror is applied to split the incoming X-ray into two beams. Ni and Pt coatings at grazing incidence angles can be chosen in order to cover the whole spectral range of FLASH2 up to hν = 1800 eV. In the variable beam path with a grazing incidence angle of ϑ = 1.8° the total transmission ranges in the order of T > 0.50 for 100 eV < hν < 650 eV with the Ni coating and T > 0.06 for hν < 1800 eV for the Pt coating. For the fixed beam path with a grazing incidence angle of ϑ = 1.3° a transmission of T > 0.61 with the Ni coating and T = 0.23 with a Pt coating is achieved. XUV pump/XUV probe experiments are possible within a delay range from -5 ps < Δt < +19ps with a nominal time resolution of t = 65.8 as. Latest work is presented which shows the current capability of the SDU and future techniques to perform time-resolved experiments with two distinct photon energies. A FEL beam with both photon energies is provided by FLASH and the desired energy band in each beam path is separated by the means of gratings or filters within the SDU.

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MON 16:15-18:15 | BOARD 69 | P1-MET1-07

POSTER SESSION

FIRST USER EXPERIMENTS OF THE PERCIVAL SOFT X-RAY IMAGER

Presenter: J. CORREA

Authors: J. CORREA (1,2), A. MARRAS (1,2), C.B. WUNDERER (1,2), S. LANGE (1,2), V. VARDANYAN (1,2), F. KRIVAN (1), V. FELK (1), I. SHEVYAKOV (1), N. GUERRINI (3), B. MARSCH (3), I. SEDGWICK (3), T. NICHOLLS (3), G. CAUTERO (4), D. GIURESSI (4), R.H. MENK (4,5), L. STEBEL (4), D. ANGELIS (4), W. NICHOLLS (6), P. SHIKHALIEV (6), U. PEDERSEN (6), A. GREER (6), N. TARTONI (6), H.J. HYUN (7), S.Y. RAH (7), F. ORSINI (8), A. DAWIEC (8), B. PFAU (9), F. BUETTNER (10), R. BATTISTELLI (10), M. HOESCH (1), K. BAGSCHIK (1), E. PLOENJES (1), M. MEHRJOO (1), K. KHARITONOV (1), M. RUIZ-LOPEZ (1), B. KEITEL (1), H. GRAAFSMA (1,2,11)

The PERCIVAL detector is a CMOS imager specifically designed for the soft X-ray regime. In 2020, although still in a development phase, it served its two first user experiments, at a Storage Ring (SR) and also at a Free Electron Laser (FEL). We will report some preliminary results and sketch future plans.

With its 2 Megapixels, 27 um pixel size, and 4 x 4 cm^2 active area, PERCIVAL can provide images with high spatial resolution. Moreover, its fast readout was designed to reach speeds up to 300 frames per second. In fully optimised mode, the sensor dynamic range its expected to cover a range from 16e- to 3.5 Me-. The development, jointly carried by 5 light sources will enable increased science yield from today's FEL and SR sources in the soft X-ray regime.

In collaboration with groups at the Helmhotz Zentrum Berlin (HZB) and Max-Born Institute (MBI), we used the P04 XUV beamline at PETRA-III to perform holographic imaging of topological materials (in particular skyrmions) at an energy of 780eV. Together with colleagues from FLASH, we used the beamline FL24 at the FLASH2 FEL to perform ptychographic imaging of plasma treated surfaces at an energy range between 92 and 462eV. Both experiments benefited from the very large dynamic range provided by the PERCIVAL detector.

The development will go on in order to reach the nominal specification parameters. In the meantime, new user experiments with a high impact factor will be scheduled and will help us to speed up the process.

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MON 16:15-18:15 | BOARD 70 | P1-MET1-08

POSTER SESSION

DEVELOPMENT OF TIMEPIX4 READOUT FOR EXPERIMENTS AT SYNCHROTRONS AND FELS

Presenter: Jonathan CORREA

Authors: Jonathan CORREA (1), Alexandr IGNATENKO (1), David PENNICARD (1), Sabine LANGE (1), Sergei FRIDMAN (1), Sergej SMOLJANIN (1), Heinz GRAAFSMA (1,2)

Timepix4 is a versatile readout chip, developed by CERN on behalf of the Medipix4 collaboration. The DESY detector group develops readout systems for the chip, to be used at modern synchrotrons and FELs. Timepix4 has two operating modes. The photon counting mode will be able to replace Medipix3-based readout systems like LAMBDA in their existing applications: SAXS/WAXS. Other, like power diffraction, can benefit from a 10 times higher count rate. The timestamping mode will replace its predecessor Timepix3. Techniques using correlation analysis, e.g. XPCS and XCCA, will benefit the most of the ns time resolution. Also, it will be useful for pump-probe experiments as well as enable time-resolved experiments with single-bunch time resolution at PETRA IV.

A carrier board for a single chip has been designed, produced and tested. The layout of the board allows for 2-chip tiled systems. For this first iteration, a commercially available readout board hosting a powerful SoC has been chosen. Data (up to 160 Gbps per chip) is transferred to a control PC over Firefly optical links. Chip testing, as well as firmware and software developments are currently in progress. The next step is development of multi-chip modules. Custom readout boards carrying 3 chips are currently under design. In the long term, multi-megapixel systems composed of multi-chip modules will be developed enabled by TSV technology. Such systems would be in high demand for large continuous detectors in photon science.

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MON 16:15-18:15 | BOARD 71 | P1-MET1-09

POSTER SESSION

CALCULATION OF NEUTRON AND X-RAY SCATTERING DATA FROM MOLECULAR DYNAMICS SIMULATIONS THROUGH OPTIMAL USE OF COMPUTATION RESOURCES

Presenter: Arnab MAJUMDAR
Authors: Arnab MAJUMDAR (1), Sebastian BUSCH (1), Muller MARTIN (2,3)

We address the computation of X-Ray and neutron scattering data from molecular dynamics simulations. Optimization of computation time is particularly crucial for large or long simulations. There are multiple software solutions available; we have chosen sassena for our work. Sassena inherits distributed memory parallelization (MPI) from its previous version. This work further augments vectorization and shared-memory parallelization (OpenMP) into it and bolsters the computing speed of sassena by up to an order of magnitude. Furthermore, the introduction of shared memory parallelization introduces the possibility of doing hybrid parallelization. As a long-term goal, we aim to use the benefit of this optimization to validate the simulation of hydrogen storage materials with neutron scattering data.

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MON 16:15-18:15 | BOARD 72 | P1-MET1-10

POSTER SESSION

A NEW HOME FOR THREE VERSATILE POWDER DIFFRACTOMETERS – THE OPTIMIZED THERMAL BEAMPORT SR8 AT THE RESEARCH NEUTRON SOURCE HEINZ MAIER-LEIBNITZ

Presenter: Christoph HAUF
Authors: Christoph HAUF (1), Milan GRUJOVIC (1), Michael HEERE (1,2), Anatoliy SENYSHYN (1)

The neutron powder diffractometer SPODI is one of the most active instruments at the research neutron source Heinz Maier-Leibnitz. However, the demands of the user community far exceed the available beam time. Therefore, the thermal beamport SR8 will be optimized to allow the simultaneous operation of the three powder diffractometers SPODI, FIREPOD and ERWIN. Due to the unique characteristics of the three instruments, which will be presented in detail, they will be able to cater for a wide range of experimental demands.

SPODI is going to remain the high-resolution option in this suite of instruments. Due to neutron guides with optimized geometries, SPODI will feature a 20% increase of the neutron flux, while retaining its flat resolution curve with typical small FWHMs of below 0.35°. Careful Monte-Carlo simulations show that the neutrons transmitted through the SPODI monochromator can be efficiently re-utilized by the powder diffractometer FIREPOD in simultaneous operation.

With a planned neutron flux of 2*10^7 n/s cm^2 – one order of magnitude more than SPODI – and its eight large area detectors, FIREPOD will be a dedicated high throughput instrument, ideally suited for a broad range of fast parametric studies. Finally, ERWIN will complement the current single crystal option RESI. It is characterized by a large curved 2D detector with a virtually seamless coverage of ~135° and a choice of three different monochromators allowing for a broad range of usable wavelengths.

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MON 16:15-18:15 | BOARD 73 | P1-MET1-11

POSTER SESSION

HIGH ACCURACY POSITIONING WITH AN INDUSTRIAL ROBOT SYSTEM FOR NEUTRON RESIDUAL STRESS ANALYSIS

Presenter: Michael HOFMANN
Authors: Martin LANDESBERGER (1), Oguz KEDILIOGLU (2), Lijiu WANG (1), Michael HOFMANN (1), Weimin GAN (3), Heinz-Günter BROKMEIER (4)

The Heinz Maier-Leibnitz Zentrum (MLZ) operates at FRM II the neutron strain scanner STRESS-SPEC, which was one of the first neutron diffractometers at which large industrial robots for sample handling and positioning were used. However, industrial robots are still limited in their use due to insufficient absolute positioning accuracies of up to ± 0.5 mm in some cases. Usually, an absolute positioning accuracy of 10 % of the smallest gauge volume size – which in case of modern neutron diffractometers is in the order of 1x1x1 mm^3 – is necessary to allow accurate strain tensor determination and correct centering of local texture measurements. The original robot setup at the neutron diffractometer STRESS-SPEC has therefore been upgraded to a high accuracy positioning/metrology system. We will give a short introduction on the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50 µm or better during measurement of the full strain tensor, the sample position is tracked by an optical metrology system and actively corrected, which we will show in detail.

In addition, a newly designed laser furnace can be mounted at the robot flange to conduct, for example, texture measurements at elevated temperatures of up to 1300 °C. A brief overview of the STRESS-SPEC instrument and its capabilities using the new robot setup will be given.

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MON 16:15-18:15 | BOARD 74 | P1-MET1-12

POSTER SESSION

SyncLAB – COMBINED X-RAY IMAGING AND SPECTROSCOPY MEASUREMENTS AT THE SYNCHROTRON AND IN THE LABORATORY

Presenter: Ioanna MANTOUVALOU
Authors: Ioanna MANTOUVALOU (1), Leona BAUER (1), Richard GNEWKOW (1), Adrian JONAS (2), Frank FÖRSTE (2), Birgit KANNGIESSER (2)

Due to new hardware and methodological developments, the performance of laboratory spectrometers has improved significantly. This allows conducting experiments in the laboratory which were up until recently restricted to synchrotron radiation facilities. By combining measurements in the laboratory with more specialized investigations at large scale facilities, both the users as well as the beamline scientists benefit, as beamtime can be utilized more efficiently, knowledge and technology transfer is initiated and new application fields can be accessed.

In the framework of the joint research group SyncLab between the HZB and the TU Berlin, various experiments at the BLiX (Berlin laboratory for innovative X-ray technologies) are possible for users. For XAFS measurements on heterogeneous samples, fast XRF mapping can be performed with laboratory spectrometers before beamtime, rendering the localization of regions of interest feasible. For transmission XAFS in the soft X-ray range a laboratory setup offers the possibility for static and transient measurements before or after beamtime. Therewith, e.g. sample preparation can be checked concerning thickness and absorption edge jumps at the respective edges. Additional reference spectra can be collected and sample degradation tests at wavelength are feasible.

We present showcases of the synergy effects offered by the combination of synchrotron and laboratory experiments leading to optimized use of measurement time and resources.

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MON 16:15-18:15 | BOARD 75 | P1-MET1-13

POSTER SESSION

THE MATERIAL ENGINEERING DIFFRACTOMETER BEER AT THE EUROPEAN SPALLATION SOURCE (ESS)

Presenter: Gregor NOWAK

Authors: Gregor NOWAK (1), Přemysl BERAN (2,3), Jan ŠAROUN (2), Peter LUKÁŠ (2), Jochen FENSKE (1), Mustapha ROUIJAA (1), Dirk-Jan SIEMERS (1), Rüdiger KIEHN (1), Jörg BURMESTER (1), Martin MÜLLER (1), Robin WORACEK (3)

The upcoming ToF-diffractometer BEER (Beamline for European Materials Engineering Research) [1] as a joint project of NPI (CZ) and Hereon (GER) at the ESS, is focused on in–situ studies of microstructures, textures, residual stresses and material phases in material processing.

The long, high brilliance pulse of the ESS allows BEER a flexible shaping of the incident neutron spectrum by a new unique modulation technique [2]. The time encoded extraction of several short pulses from one long ESS pulse, raises substantial the counting statistics up to an order of magnitude in the detector read-out without compromising the resolution compared to conventional single pulse extraction methods for diffraction on low crystal symmetries. For complex crystal symmetries or multi-phase materials, pulse shaping methods are in place. The pulse extraction techniques [3] are enabled by a sophisticated chopper cascade, which offers a broad intensity/resolution range needed for example for in-situ experiments on a quenching and deformation dilatometer.

We present the current status of BEER, its expected performance, the sample environment planed for day one and future upgrades.

[1] K.H. Andersen, et al., NIM A, 957, 163402, (2020)
[2] M. Rouijaa, R. Kampmann, J. Šaroun, J. Fenske, P. Beran, M. Müller, P. Lukáš, A. Schreyer, NIM A, 889, 7-15, (2018)
[3] J. Šaroun, J. Fenske, M. Rouijaa, P. Beran, J. Navrátil, P. Lukáš, A. Schreyer, M. Strobl, J. Phys.: Conf. Ser., 746, 012011, (2016)

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MON 16:15-18:15 | BOARD 76 | P1-MET1-14

POSTER SESSION

OPTIMIZATION OF A TARGET WITH MICROCHANNEL COOLING FOR HIGH-CURRENT ACCELERATOR-DRIVEN NEUTRON SOURCES

Presenter: Thomas GUTBERLET

Authors: Qi DING (1,2), Jörg WOLTERS (3), Johannes BAGGEMANN (1), Ulrich RÜCKER (1), Paul ZAKALEK (1), Jingjing LI (1), Yannick BESSLER (3), Thomas GUTBERLET (1), Thomas BRÜCKEL (1), Ghaleb NATOUR (2,3)

With the decommissioning of older fission-based neutron sources in Europe in recent years, the available capacity on neutrons for science and access is becoming critical for neutron users. To provide an alternative approach to the realization of neutron facilities, the High Brilliance Neutron Source (HBS) project has been initiated at the Jülich Centre for Neutron Science (JCNS) of the Forschungszentrum Jülich GmbH. It aims at developing a high-current accelerator-driven neutron source (Hi-CANS) to deliver high-brilliant neutron beams for neutron scattering. One of the key components is the neutron producing target that generates free neutrons by proton induced nuclear reactions with an energy well below the spallation threshold. For HBS, a solid tantalum target with a sophisticated internal microchannel water-cooling structure was developed for a 70 MeV pulsed proton beam with a peak current of 100 mA and an average power of 100 kW. The high-current requires a design minimizing proton accumulation within the tantalum target to avoid blistering problems. The high-power density requires an optimization of the microchannel cooling structure to reduce temperatures and to minimize thermo-mechanical stresses. Proton implantation was optimized with Monte-Carlo code FLUKA. Steady state and transient analysis on cooling effect of the target in operation were performed with ANSYS. The details of these investigations and the resulting microchannel target design will be presented.

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MON 16:15-18:15 | BOARD 77 | P1-MET1-15

POSTER SESSION

KMC-3 AT BESSY (BERLIN): A VERSATILE BEAMLINE FOR TENDER-ENERGY, RAPID-SCAN, AND OPERANDO X-RAY ABSORPTION SPECTROSCOPY AT CRYOGENIC OR AMBIENT TEMPERATURES

Presenter: Michael HAUMANN
Authors: Michael HAUMANN, Paul BEYER, Stefan MEBS, Holger DAU

The beamline KMC-3 at BESSY II (Berlin) is a bending magnet source with a double-crystal monochromator. In two BMBF/PT-DESY funded projects and a pending ErUM-Pro application we pursue instrumentation and scientific research at KMC-3 in a broad collaborative framework (UniSysCat Excellence Cluster Berlin, Helmholtz-Center Berlin). KMC-3 offers an extended energy range (ca. 2 – 15 keV), including EXAFS and XANES at the phosphorus and sulfur K-edges and at various L-edges in the tender-energy regime. Rapid data acquisition capabilities enable EXAFS scans within seconds and time-resolved single-energy experiments with 100 µs per data point, using an energy-resolving 13-element silicon-drift detector for fluorescence monitoring at count rates up to 4 Mcps per channel. Permanent facilities for cryo-XAS (closed-cycle liquid-He cryostat, 5 – 320 K) and *operando*-XAS at room temperature using electrochemistry (potentiostats) or light-excitation (pulsed diodes, 5 ns tunable OPO-laser) are available. These facilities are accessible via the BESSY beamtime application system. Next steps are installation of extended sample environments (flow-through cells, gas and media supplies) and further improved efficient data acquisition. Experiments using our XAS facilities have resulted in numerous high-ranking publications in recent years. KMC-3 is a partly unique station for studying wide-ranged topics and yields high-quality XAS data due to fast energy-resolving fluorescence detection.

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MON 16:15-18:15 | BOARD 78 | P1-MET1-16

POSTER SESSION

A UNIQUE QUENCHING AND DEFORMATION DILATOMETER FOR COMBINED IN-SITU NEUTRON DIFFRACTION AT STRESS-SPEC

Presenter: Weimin GAN
Authors: Li XIAOHU (1,2), Solis CECILIA (1), Weimin GAN (1), Hofmann MICHAEL (2)

A modified quenching and deformation dilatometer (TA instruments DIL 805A/D/T) is now in operation at MLZ. It is customized for running neutron scattering measurements during the temperature/deformation treatment of the sample, in particular neutron diffraction at STRESS-SPEC (phase, texture, and lattice strain) and neutron small angle scattering at SANS-1. The bulk length change of dilatometer specimens is successfully combined with in-situ neutron diffraction patterns for analyzing dynamic processes in metallic materials.

In this contribution a detailed introduction to the unique dilatometer is given and examples of user experiments for studying engineering materials highlight the application of the added insight provided by combining diffraction at STRESS-SPEC and dilatometry.[1]

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[1] X.H. Li et al., Adv. Eng. Mater. 2021, 2100163
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MON 16:15-18:15 | BOARD 79 | P1-MET1-17

POSTER SESSION

MODERATE-RESOLUTION XES USING A FULL-CYLINDER VON HAMOS SPECTROMETER

Presenter: Kai SCHÜLER
Authors: Kai SCHÜLER, Yves KAYSER, Christian STADELHOFF, Burkhard BECKHOFF

Spectrometers realized in the von Hamos geometry are characterized by moderate- to high-energy resolution and very efficient in terms of reflectivity times the solid angle of detection when equipped with a full-cylinder highly annealed pyrolytic graphite. The von Hamos spectrometer employed at PTB allows to discriminate sensitively between energy shifts of emission lines ($E/\Delta E = 1000$ to 2700). Thus, it represents a good instrument to conduct X-Ray Emission Spectroscopy (XES) measurements.

The alignment of the von Hamos spectrometer of the PTB is critical to optimize the response function and the detection efficiency. Parametric optimization routines for enhanced alignment reliability and reproducibility were developed, which also consider the position of the optic and the sample position and base on geometrical reflection computations. By means of the routines, the alignment of the von Hamos spectrometer is to be no longer empirical, but rather subject to a reproducible parametric optimization procedure.

The alignment routines have been applied to measure energetical shifts of the Kβ emission lines of different nickel-manganese-cobalt electrodes. It could be shown that different electrode materials can be discriminated by means of XES based on their electronic configuration.

Affillation
Physikalisch-Technische Bundesanstalt, Germany

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MON 16:15-18:15 | BOARD 80 | P1-MET1-18

POSTER SESSION

GUIDED HIERARCHICAL IN-SITU X-RAY NANO-LAMINOGRAPHY ENABLING THE INVESTIGATION OF DAMAGE NUCLEATION IN ALLOY SHEETS

Presenter: Mathias HURST
Authors: Mathias HURST (1,2), Lukas HELFEN (1,3), Thilo MORGENEYER (4), Heikki SUHONEN (5), Jussi-Petteri SUURONEN (6), Ante BULJAC (4,7), Francois HILD (7), Tilo BAUMBACH (1,2), Daniel HÄNSCHKE (1)

Non-destructively, X-ray nano-tomography enables in-situ studies with 3D spatial resolutions below 100nm. With a generalised geometry nano-laminography allows for flat, laterally extended samples. However, for high-resolution in-situ studies the intrinsically limited FOV hinders identification and tracking of ROIs within evolving bulk samples.

Here we introduce guided hierarchical in-situ 3D X-ray nano-imaging, enabling us to search for, identify and track ROIs. The approach makes use of zoomable projection microscopy, acquiring alternating high- and low-resolution volumes with on-the-fly phase and 3D reconstruction. This allows anticipating sample changes and displacements of high-resolution ROIs. While on-the-fly 3D reconstruction is achieved by GPU-based pipelines, suitable on-the-fly phase retrieval remains challenging. Thus, the suitability of the quasi-particle approach for the required fast measurement and fast phase retrieval of holographic projection microscopy data is demonstrated, non-iteratively, with a single propagation distance and suited beyond the restrictions of contrast-transfer-function based methods.

Finally, we employ guided hierarchical in-situ nano-laminography to investigate damage initiation in alloy sheets. During gradually induced macroscopic deformation, we follow nanoscale clusters of voids and intermetallic particles over many loading steps and identify the cracking of intermetallic particles as main damage initiation process inside the bulk.

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MON 16:15-18:15 | BOARD 81 | P1-MET1-19

POSTER SESSION

CFEL TAPEDRIVE 2.0: CONVEYOR BELT-BASED SAMPLE DELIVERY SYSTEM FOR MULTI-DIMENSIONAL SERIAL CRYSTALLOGRAPHY

Presenter: Alessandra HENKEL

Authors: Alessandra HENKEL (1), Julia MARACKE (1), Anna MUNKE (1), Aida RAHMANI MASHHOUR (1), Patrick REINKE (1), Martin DOMARACKY (1), Holger FLECKENSTEIN (1), Johanna HAKANPÄÄ (2), Jan MEYER (2), Alexandra TOLSTIKOVA (2), Jerome CARNIS (1), Philipp MIDDENDORF (1), Luca GELISIO (1), Oleksandr YEFANOV (1), Henry N. CHAPMAN (1,3,4), Dominik OBERTHÜR (1)

Serial crystallography (SX) at both X-ray Free-electron Lasers (XFELs) and synchrotrons offers the possibility to collect data at non-cryogenic temperature almost radiation damage free and enables time-resolved crystallography of irreversible reactions. To ensure the necessary steady delivery of new micron-sized crystals, many new means of sample delivery have been developed. Described here is a novel conveyor belt-based sample delivery system, the completely re-designed and re-engineered second generation of the CFEL TapeDrive. It is optimized for fast installation at beamlines, ease of use, low sample consumption and precise adjustment of several sample delivery parameters like ligand concentration, pH and sample temperature. Through combination of these parameters and the additional possibility for time-resolved experiments, CFEL TapeDrive 2.0 enables multi-dimensional serial crystallography experiments. It can now be used as standard instrumentation at beamline P11 at PETRA III (DESY, Germany) and is suitable for serial Laue crystallography with polychromatic X-rays. In the future, parts of the system will be automated to achieve rapid ligand screening with micron-sized crystals in various sample environments.

By introducing the CFEL TapeDrive 2.0, a platform for user-friendly multi-dimensional serial crystallography, we provide a novel approach for structural biology to further reveal details about how macromolecules keep our biological world turning.

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MON 16:15-18:15 | BOARD 82 | P1-MET1-20

POSTER SESSION

STATUS AND PROSPECTS OF 3D LAMINOGRAPHIC IMAGING AT KIT

Presenter: Tilo BAUMBACH

Authors: Daniel HÄNSCHKE (1), Lukas HELFEN (1,2,3), Elias HAMANN (1), Marcus ZUBER (1,4), Simon BODE (1,4), Mathias HURST (1,4), Thilo MORGENEYER (5), Merve KABUKCUOGLU (1), Tilo BAUMBACH (1,4)

The Karlsruhe Institute of Technology (KIT) is continuously progressing in the design and construction of methodology and instrumentation for 3D X ray computed laminography (CL), including the implementation of suitable algorithms for data processing and analysis.

CL has unique capabilities for 3D imaging of flat and laterally extended objects exceeding the detector view field, in particular enabling screening large sample areas in combination with zooming in on selected regions of interest for high-resolution 3D imaging without need for sample dissection. Thus, CL allows truly non-destructive hierarchical imaging particularly suited for in-situ and *operando* studies under real-world conditions.

In collaboration with the ESRF and DESY, we have established a pool of complementary instrumentation for 3D CL, taking advantage of the unique X-ray beam properties of beamlines at the KIT synchrotron, ESRF, PETRA III, as well as in the lab. With absorption, propagation-based phase contrast, grating interferometry, fluorescence, and Bragg diffraction, complementary contrast modes are available and we cover a wide range of length scales, e.g., achieving highest spatial resolution by X-ray microscopy modalities.

Here, we will overview the status and the future prospects of our laminography portfolio and we will present some of our current applications, e.g., the 3D in-situ investigation of metal sheets during tensile testing and the study of crystal defect dynamics in semiconductor wafers.

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MON 16:15-18:15 | BOARD 83 | P1-MET1-21

POSTER SESSION

KOMPASS – THE POLARIZED COLD NEUTRON TRIPLE-AXIS SPECTROMETER OPTIMIZED FOR POLARIZATION ANALYSIS.

Presenter: Dmitry GORKOV
Authors: Dmitry GORKOV (1,2), Manuel MÜLLER (1,2), Georg WALDHERR (2), Alexander GRÜNWALD (1,2), Jonas STEIN (1), Stephan GIEMSA (3), Peter BÖNI (3), Markus BRADEN (1)

KOMPASS is a polarized cold-neutron three axes spectrometer (TAS) currently undergoing its final construction phase at the MLZ in Garching. The instrument is designed to exclusively work with polarized neutrons and optimized for zero-field spherical neutron polarization analysis for measuring all elements of the polarization matrix.

In contrast to other TASs, KOMPASS is equipped with a unique polarizing guide system. The static part of the guide system hosts a series of three polarizing V-cavities providing a highly polarized beam with expected polarization above 98 %. The exchangeable straight and parabolic front-end guide sections allow adapting the instrument resolution for any particular experiment and provide superior energy- and Q-resolution values when compared with the existing conventional guide and instrument concepts [1, 2].

In combination with the end position of the cold neutron guide NL-1, the large doubly focusing monochromator and analyzer, the secondary V-cavity for analysis of polarization of scattering beam, the KOMPASS TAS will be very well suited to study various types of weak magnetic order and excitations in variety of complex magnetic structures. Special emphasis was put on a compact design of the instrument in order to maximize intensity.

[1] M. Janoschek et al., Nucl. Instr. and Meth. A 613 (2010) 119.
[2] A. C. Komarek et al., Nucl. Instr. and Meth. A 647 (2011) 63.

The construction of KOMPASS is funded by the BMBF through the Verbundforschungsprojekt 05K19PK1.

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MON 16:15-18:15 | BOARD 84 | P1-MET1-22

POSTER SESSION

NanoExtrem: NANO-FOCUS END-STATION WITH DOUBLE-SIDED CO2 LASER HEATING FOR EXPERIMENTS AT ID27@ESRF

Presenter: Wolfgang MORGENROTH
Authors: Wolfgang MORGENROTH (1,2), Mohamed MEZOUAR (2), Gastón GARBARINO (2), Markus HERRMANN (3), Sandro JAHN (3), Lélia LIBON (1), Max WILKE (1)

The ESRF has built a new high pressure beamline for nano-focused X-ray diffraction, fluorescence and imaging at the extremely brilliant source EBS. The upgraded beamline is in operation since end of 2021.

In the framework of the joint BMBF-funded project 'NanoExtrem', research groups from the Universities of Potsdam and Cologne have been contributing to the construction of this end-station by providing personnel and instrumentation:

- 15 – 60 keV in monochromatic mode, additional 'pink' beam mode
- beam focus of down to ~250 nm at 17 keV to achieve pressures >500 GPa
- XRD detection using EIGER2 X CdTe 9M detector
- sample goniometers for nano-focusing, YAG and CO2 laser heating or heavy duty experiments like Paris-Edinburgh cell or a 4 K cryostat
- in preparation: new experiments exploiting coherence of the beam and providing X-ray imaging capabilities.

This 'high-flux nano-XRD' beamline is optimized for the needs of the geo- and materials-science community for in-situ XRD and XRF studies at extreme conditions. It will be possible to study materials relevant to processes of the deep Earth or other planetary bodies in an unprecedented manner. We will present the overall design and provide first insights to performance parameters commissioned and used in first user experiments.

We acknowledge many divisions within the ESRF for construction and the German BMBF for financial support. BMBF project 'NanoExtrem' 05K2019: 05K19IP2 (Potsdam) and 05K19PK2 (Köln).

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1: Institut für Geowissenschaften, Universität Potsdam, Germany; 2: ESRF – The European Synchrotron, Grenoble, France; 3: Institut für Geologie und Mineralogie, Universität zu Köln, Germany

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MON 16:15-18:15 | BOARD 85 | P1-MET1-23

POSTER SESSION

X-RAY DIFFRACTION FROM STRONGLY BENT CRYSTALS AND RESOLUTION OF A BENT-CRYSTAL SPECTROMETER FOR XFEL PULSES

Presenter: Vladimir KAGANER
Authors: Vladimir KAGANER (1), Ilia PETROV (2), Liubov SAMOYLOVA (2)

The resolution function of a spectrometer based on a strongly bent single crystal is evaluated. It is shown that the resolution is controlled by two parameters: (i) the ratio of the lattice spacing of the chosen reflection to the crystal thickness and (ii) a single parameter comprising crystal thickness, its bending radius, distance to a detector, and anisotropic elastic constants of the crystal. X-ray diffraction from a bent single crystal can be treated kinematically when the bending radius is small compared with the critical radius given by the ratio of the Bragg-case extinction length for the actual reflection to the Darwin width of this reflection. The critical radius varies, depending on the X-ray energy, the crystal and the reflection, from centimeters to meters. In a cylindrically bent diamond plate, the Poisson effect on bending is compensated by the elastic anisotropy, and the displacement field does not vary over the depth. In this case, the spectral resolution is limited by the crystal thickness, rather than the extinction length, and can be better than the resolution of a planar dynamically diffracting crystal. It amounts to the ratio of the lattice spacing for the actual reflection to the crystal thickness. As an example, for the (220) reflection from diamond crystal of a thickness of 40 µm, the energy resolution of 3 x 10^(-6) can be reached. These results allow one to optimize the parameters of the bent-crystal spectrometers for the XFEL radiation pulses.

Affillation
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MON 16:15-18:15 | BOARD 86 | P1-MET1-24

POSTER SESSION

AN ENGINEERING DIFFRACTOMETER FOR THE HIGH BRILLIANCE NEUTRON SOURCE (HBS)

Presenter: Jochen FENSKE
Authors: Jochen FENSKE, Igor KRASNOV

The HBS is a high brilliance accelerator driven neutron source currently in the design process. It provides different target stations that follow the same duty cycle but offer different frequencies and pulse length. Further cold and thermal moderators are used to adjust the neutron spectrum. The target stations with their moderators thus allow choosing the parameters best fitting to an instrument or instrument class. We here present the design and expected performance of an engineering diffractometer for one of the target stations at the HBS. While optimized for straining scanning measurements the design of the instrument will allow further the analysis of textures and the investigations of phase transitions.

Affillation
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MON 16:15-18:15 | BOARD 87 | P1-MET1-25

POSTER SESSION

TAPEDRIVE 2.0 – AN EFFICIENT SAMPLE ENVIRONMENT FOR SERIAL PROTEIN CRYSTALLOGRAPHY.

Presenter: J. Mia LAHEY-RUDOLPH
Authors: J. Mia LAHEY-RUDOLPH, Leif HOLTHUSEN, Manfred RÖSSLE

Serial crystallography experiments require a continuous delivery of microcrystals to the X-ray beam. There are several features an ideal sample delivery should show: First, owing to the small crystal size, a high signal to noise ratio (SNR) is vital for successful experiments. Second, high hit-rates are desirable to minimize both necessary beamtime and sample consumption. Last but not least, the setup should be robust and easy to use, but flexibly adaptable to different experimental designs.

In cooperation with Suna Precision, we have developed a tape drive that transports a slurry of microcrystals onto an ultrathin porous polymer foil, and into the X-ray beam.

In this new tapedrive version, liquid scattering is reduced and SNR optimized by blotting away excess mother liquor and if applicable ligand buffer before the quasi-naked crystals are illuminated. The tapedrive setup, which will be installed at the new ID29 beamline at the ESRF in Grenoble, allows time-resolved observation of conformational changes in crystallized proteins using different triggers like light-activation, pH jump or chemical mixing via diffusion. This contribution will offer solutions and advice against the frequent problem of crystal settling and highlight ongoing experiments investigating preferential crystal orientation.

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MON 16:15-18:15 | BOARD 88 | P1-MET1-26

POSTER SESSION

APPLICATIONS WITH THE HIGH RESOLUTION NEUTRON BACKSCATTERING SPECTROMETER SPHERES

Presenter: Michaela ZAMPONI
Authors: Marcella Carbrera BERG, Michaela ZAMPONI

The neutron backscattering spectrometer SPHERES (SPectrometer for High Energy RESolution) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It covers a dynamic range of ± 31μeV with a high resolution of about 0.66μeV and a good signal-to-noise ratio. The instrument performance has been improved over the recent years by different measures. The intensity has been more than doubled by the upgrade of the PST chopper and the focusing guide. The signal-to-noise ratio can be significantly improved by employing the new background chopper.

SPHERES enables investigations on a broad range of scientific topics, accessing dynamic processes up to a timescale of a few ns. Since it is sensitive to the incoherent scattering from hydrogen, SPHERES is particular well suited to study dynamic processes in soft matter and biological systems such as, polymer and protein motions or water motion on the surface of proteins. Other typical applications include energy research, such as polymer electrolyte fuel cells and ionic liquids. The high resolution of the spectrometer also enables the observation of hyperfine splitting in magnetic materials.

Affillation
Forschungszentrum Jülich GmbH , Jülich Centre for Neutron Science, Germany

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MON 16:15-18:15 | BOARD 89 | P1-MET1-27

POSTER SESSION

RECONSTRUCTION OF TiO2-HfO2 GRATINGS WITH SCANNING-FREE GRAZING EMISSION X-RAY FLUORESCENCE

Presenter: Nils WAUSCHKUHN

Authors: Nils WAUSCHKUHN (1), Yves KAYSER (1), Victor SOLTWISCH (1), Jonas BAUMANN (2), Burkhard BECKHOFF (1), Philipp HÖNICKE (1)

The complexity of today's nanostructures, especially for semiconductor-related applications, necessitates new metrology techniques. Here, the capability of scanning-free grazing emission X-ray fluorescence (GEXRF) will be demonstrated on two-dimensional nanostructures. TiO2 gratings with variable etching depth, coated with HfO2, are being characterized with respect to their dimensional and analytical properties [1].

Using HfO2-TiO2 grating lines as an example, it is shown that grazing emission X-ray fluorescence provides sub-nm discrimination capabilities for crucial dimensional parameters such as the line height, the line width, the etching depth, and the thickness of HfO2. Furthermore, no sample preparation is needed and GEXRF is a destruction-free method. This enables a subsequent characterization of the same sample with other techniques such as transmission electron microscopy or atomic force microscopy to validate the GEXRF-results.

Due to the illumination from the sample normal, in contrast to grazing incidence techniques, the probed sample volume is only defined by the beam size and therefore compatible with typically sized test fields from semiconductor studies. Furthermore, buried parts of the nanostructure are accessible due to the high penetration characteristics of X-rays.

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[1] P. Hönicke et al., Small 2105776, 2021

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MON 16:15-18:15 | BOARD 90 | P1-MET1-28

POSTER SESSION

ABERRATION CORRECTION FOR NANOFOCUSING X-RAY OPTICS

Presenter: Frank SEIBOTH

Authors: Frank SEIBOTH (1), Adam KUBEC (2), Andreas SCHROPP (1,8), Sven NIESE (4), Peter GAWLITZA (5), Jan GARREVOET (7), Vanessa GALBIERZ (7), Silvio ACHILLES (1), Svenja PATJENS (1), Michael E. STUCKELBERGER (1), Andreas JAHN (6), Satishkumar KULKARNI (1), Wenxin WANG (1), Ayush SHARMA (1), Mikhail LYUBOMIRSKIY (1), Thomas KELLER (1,9), Christian DAVID (3), Christian G. SCHROER (1,8,9)

Nanofocusing X-ray optics such as multilayer Laue lenses (MLL) have reached beam sizes below 10 nm and in principle their manufacturing process has the potential to break the 1 nm barrier. However, minuscule fluctuations during fabrication can lead to imperfect shapes and introduce aberration. Even with suitable at-wavelength metrology a direct improvement on the manufacturing process of X-ray optics can be extremely challenging. On the other hand, this metrology data can be used to fabricate tailor-made refractive phase plates. These additional optical elements pose a solution to correct aberration subsequently[1], similar to visiting an optician to improve eye-sight. I will present recent developments in this area and show applications on X-ray optics like CRLs, NFLs, and MLLs, highlighting diverse fabrication techniques such as laser ablation, additive manufacturing, and FIB milling.

[1] Seiboth et al., Nat. Commun. 8, 14623 (2017)

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MON 16:15-18:15 | BOARD 91 | P1-MET1-29

POSTER SESSION

MULTI-BEAM X-RAY PTYCHOGRAPHY USING CODED PROBES

Presenter: Mikhail LYUBOMIRSKIY

Authors: Mikhail LYUBOMIRSKIY (1), Felix WITTWER (2), Maik KAHNT (3), Frieder KOCH (4), Adam KUBEC (5), Ken Vidar FALCH (1), Jan GARREVOET (1), Martin SEYRICH (1), Christian DAVID (6), Christian G. SCHROER (1,7)

Ptychography is a high-resolution imaging technique known for being capable of reaching sub-10 nm resolution. A coherent beam is required to reach this resolution. Currently, the coherent fraction of the beam for third-generation synchrotron sources is only 10 %. Thus, ptychography needs to isolate the coherent flux. Consequently, more than 90 % of the incoming X-rays are wasted. This reduces the total flux on the sample, which leads to an increased scan time or reduced spatial resolution due to a lower signal-to-noise ratio. The need to choose between high resolution and a large field of view is a show stopper for many experiments. The latest advances in ptychographic algorithms provide the possibility of introducing mutually incoherent modes. This was adapted in recent developments for visible light microscopy with multiple independent beams. The sample is scanned simultaneously, not by one beam but by many, which can be mutually incoherent from each other. Each mode in the algorithm is used to reconstruct one beam and a corresponding region of the sample, expanding the scan area by the number of beams. We have successfully implemented this technique in the X-ray regime using up to 6 beams in parallel. Each beam was uniquely coded, which provided robust disentangling of the diffracted signal from different sample areas and thus artifact-free reconstructed object.

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MON 16:15-18:15 | BOARD 92 | P1-MET1-30

POSTER SESSION

TOMOGRAPHIC IMAGING CAPABILITIES WITH HARD X-RAYS AT BAMLINE (BESSYII)

Presenter: Henning MARKÖTTER

Authors: Henning MARKÖTTER (1), Michael SINTSCHUK (1), Shahabeddin DAYANI (1), Itziar SERRANO MUNOZ (1), Tatiana MISHUROVA (1), Ralf BRITZKE (1), Bernd MÜLLER (1), Andreas KUPSCH (1), Giovanni BRUNO (1,2)

The BAMline at the synchrotron X-ray source BESSYII (Berlin, Germany) is supporting researchers in a wide range of research areas for more than 20 years. These fields include biology, cultural heritage, medicine, and also materials science. As a non-destructive characterization method, synchrotron X-ray imaging, especially tomography with hard X-rays, plays an important role in structural 3D characterization.
A recent upgrade of key equipment at the BAMline expands the imaging capabilities towards shorter acquisition times. Therefore, in-situ and *operando* experiments can now be routinely conducted. Also, different energy resolutions can be set up to optimize flux and energy resolution as desired. This requires an adaptation of the used reconstruction methods in order to perform necessary analyses also during the experiment. In this presentation the equipment, data handling pipeline as well as various examples from material science are presented.

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MON 16:15-18:15 | BOARD 93 | P1-MET1-31

POSTER SESSION

ERUM-FSP T05 – "AUFBAU VON APPA BEI FAIR"

Presenter: Stefan SCHIPPERS
Authors: Stefan SCHIPPERS (1,2), Thomas STÖHLKER (3,4,5)

APPA (Atomic and Plasma Physics and Applications) next to CBM, NUSTAR and PANDA is one of the four research pillars of FAIR. The following research collaborations are acting under the umbrella of APPA:

BIOMAT (biophysics and materials science), FLAIR (physics with low-energy antiprotons), HED@FAIR (plasma physics), SPARC (atomic physics). The common research topic is the exploration of the building blocks and of the phenomena of matter under extreme conditions (high fields, densities, pressures and temperatures).

The BMBF funded collaborative research center ErUM-FSP APPA of German university groups pursues coordinated research projects in the area of accelerator based experiments with heavy ions at the future FAIR installation. Central issues are: Further development of the experimental infrastructure, in particular, research and development for enhancing the scientific capabilities of the existing installations and of the future accelerator and detector systems including the respective base technologies, set-up of the APPA experiments of the modules 0–3 of the modularized start version of FAIR, and realization of the APPA research program during the current FAIR Phase-0.

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1: Justus-Liebig-Universität Gießen, I. Physikalisches Institut; 2: Hemholtz Forschungsakademie Hessen für Fair, Campus Gießen; 3: GSI Helmholtzzentrum für Schwerionenforschung GmbH; 4: Helmholtz-Institut Jena; 5: Friedrich-Schiller-Universität Jena, Institut für Optik und Quantenelektronik

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MON 16:15-18:15 | BOARD 94 | P1-MET1-32

POSTER SESSION

HIGH SENSITIVE X-RAY POLARIZATION MICROSCOPY

Presenter: Berit MARX-GLOWNA

Authors: Berit MARX-GLOWNA (1,2), Benjamin GRABIGER (3), Robert LÖTZSCH (3), Ingo USCHMANN (1,2,3), Annika T. SCHMITT (3), Kai Sven SCHULZE (1,2), Arndt LAST (4), Thomas ROTH (5), Sergey ANTIPOV (6), Hans-Peter SCHLENVOIGT (7), Ilya SERGUEEV (8), Olaf LEUPOLD (8), Ralf RÖHLSBERGER (1,2,8), G.G. PAULUS (1,2,3)

Polarimetry is one of the most versatile and sensitive methods in optics. Since 11 years, we have improved the polarization purity of X-ray polarimeters to the world record of <10^(-10). The new generation of polarimeters has made it possible to measure quantum optical phenomena via nuclear resonant scattering and smallest rotations of the polarization plane up to 0.9 arcsec.

Recently we could discover a polarization-preserving lens material which allows for the first time the combination of precision polarimetry with micro-focused beams without compromising its polarization purity. This breakthrough opens many new fields of application at synchrotrons and XFEL's, because the new technique allows for the first time to investigate small samples, or tiny regions of interest.

Present fields of application of the new technique are the investigation of charge, orbital and spin anisotropies of correlated materials. A key to understand the properties of such materials and compounds can be obtained by investigating these anisotropies on the relevant micro- and nanoscopic length scales. Another actual application of the high-sensitive polarization microscope is the discovery of the vacuum birefringence with high-power lasers. For this experiment a high-precision X-ray polarization microscope is the key-technology, because the effect, as well as the interaction region is very small.

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MON 16:15-18:15 | BOARD 95 | P1-MET1-33

POSTER SESSION

CONSTRUCTION OF A FAST NON-LINEAR X-RAY SHUTTER SYSTEM

Presenter: Marvin KOWALSKI
Authors: Marvin KOWALSKI (1), Michael SPRUNG (2), Michael PAULUS (3), Daniel WESCHKE (2), Michael ZIOLKOWSKI (1), Sonja TIMMERMANN (1), Christian GUTT (1)

A major obstacle of measuring protein samples with X-ray scattering experiments is radiation damage. Especially at facilities with a high photon flux radiation sensitive protein samples can be irreversibly destroyed in fraction of a second of beam exposure. Therefore, to perform X-ray photon correlation spectroscopy (XPCS) measurements of these samples, a fast X-ray shutter system was developed allowing for switching of the X-ray beam in defined time patterns (e.g. logarithmic time scales for building multiple tau correlation functions). This project represents the initial phase of constructing a fast non-linear X-ray shutter system for the Coherence Beamline P10 of PETRA III (DESY, Hamburg). This system consists of 20 amplified piezo actuators (APA200M, CEDRAT TECHNOLOGIES) forming 10 'piezo-shutters', which are connected in series. Each 'piezo-shutter' is capable of running with 10 Hz allowing the system to reach frequencies of up to 100 Hz. Those shutters are operated by an electronic control device designed und produced by the Electronics Development Lab of the University of Siegen and housed in a vacuum vessel produced by the mechanical workshop also located at the University of Siegen. To position the system in the X-ray beam a rotation and translation stage (HUBER Diffraktionstechnik GmbH and Co. KG) is used. First measurements to test the mechanical properties of the system will be conducted at the 'Dortmunder Elektronenspeichering-Anlage' (DELTA) this summer.

Affillation
1: Universität Siegen; 2: DESY; 3: Technische Universität Dortmund

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MON 16:15-18:15 | BOARD 96 | P1-MET1-34

POSTER SESSION

A PIEZO-MODULATED ACTIVE GRATING FOR SELECTION OF X-RAY PULSES SEPARATED BY ONE NANOSECOND

Presenter: Ivo ZIZAK
Authors: Simone VADILONGA, Ivo ZIZAK, Matthias RÖSSLE

A useful property of synchrotron radiation is, beside the stability, brilliance and coherence, that it is made of pulses of radiation. The repetition rate of the pulses is in the MHz frequency range, which is often too fast for many experiments. Thus, the repetition rate of the X-ray pulses has to be adapted to the experiment, different technical implementations exist or have been proposed. We present a novel method of temporal modulation of synchrotron radiation for time-resolved experiments, designed and tested at BESSY II [1]. This method allows to select precisely which X-ray pulse from the synchrotron bunch filling pattern is used for the experiment.

The Bragg reflection on a LiNbO3 piezoelectric crystal is modified using comb shaped electrodes with alternating polarity deposited on the surface of the crystal. When a voltage is applied to the electrodes a periodic deformation of the crystal is induced, acting as a diffraction grating for hard X-rays. Diffraction on such a grating alters the direction of the X-rays and it can be used to modulate the intensity of the X-ray beam. It is possible to modulate the grating amplitude, and to obtain different scattering conditions for different X-ray pulses.

The pulse picker reaches an efficiency up to 34 % of the incoming beam intensity, and we demonstrate a time-resolution of 1 ns, which is independent of the accepted beam size and limited only by the driving electronics.

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[1] https://doi.org/10.1364/OE.438570

Affillation
Helmholtz Zentrum Berlin, Germany

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MON 16:15-18:15 | BOARD 97 | P1-MET1-35

POSTER SESSION

MÖßBAUER SPECTROSCOPIC CAMERA FOR OPERANDO MEASUREMENTS

Presenter: Yutaka YOSHIDA
Authors: Masashi KOBAYASHI (1), Yuka ISHIDA (1), Kazuo HAYAKAWA (1), Yutaka YOSHIDA (1,2), Ralf RÖHLSBERGER (2)

A “57Fe Mößbauer spectroscopic camera [1]” is becoming attractive because of recent advances in detector technology, in particular, due to the development CMOS cameras for X-rays, providing us with an extremely low readout noise. Such Mössbauer imaging techniques would allow us to take “photographs” every minute separately for different hyperfine spectral components with a spatial resolution of several micrometres or even sub-micrometres. So, we could achieve “Non-destructive Operando measurements” of the system studied, following the dynamical atomic motions and the chemical reactions in the vital industrial materials such as iron steel and functional materials. So far, we have reported mainly a mapping technique by focusing the ɣ-rays down to several 10 micrometres. Subsequently, we measured both the transmitted ɣ-rays and the reemitted conversion and Auger electrons and the 6 keV-X-rays via scanning a focused 14.4 keV ɣ-ray across the sample. We applied this mapping technique for imaging Fe impurities in Si solar cells to understand the origin of conversion efficiency degradation in photovoltaics. In addition, we have further developed a direct imaging technique for 14.4keV ɣ-rays which are converted to visible light by a Scintillator (HAMAMATSU), producing images with a qCMOS camera.

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[1] “Mößbauer spectroscopic camera for *operando* measurement of pattern formation processes”, M. Kobayashi, K. Hayakawa, Y. Yoshida, R. Röhlsberger, Hyperfine Interactions, 243, (2022).

Affillation
1: Shizuoka Institute of Science and Technology, Japan; 2: Helmholtz Institut Jena, Germany

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MON 16:15-18:15 | BOARD 98 | P1-MET1-36

POSTER SESSION

SINGLE-SHOT TEMPORAL CHARACTERIZATION OF XUV FEL PULSES

Presenter: Mahdi MOHAMMADI BIDHENDI
Authors: Mahdi MOHAMMADI BIDHENDI (1), Rosen IVANOV (2), Ivette Jazmin BERMUDEZ MACIAS (2), Juliane ROENSCH-SCHULENBURG (1), Mathias VOGT (1), Mikhail YURKOV (1), Stefan DUESTERER (1)

The free-electron laser of Hamburg operates in the self-amplified spontaneous emission regime, meaning that every pulse has a unique combination of energy, spectrum, arrival time and pulse duration. So it is critical to be able to determine the pulse duration and temporal profile of each pulse. THz field-driven streaking technique has the potential to deliver single-shot pulse duration information basically wavelength-independent and over a large dynamic range (in pulse duration and FEL energy) [1, 2].

Firstly, the XUV pulse arrival time was determined by the streaking and compared to the electron arrival time. Here we find a very good agreement. Using THz streaking, the single-shot pulse duration has been measured over a wide range from 10 fs to 350 fs (FWHM) [2] and correlations with other photon beam parameters have been investigated [3]. In addition, a study of the impact of the number of undulators contributing to the lasing on the pulse duration was performed and compared to the results of 1D and 3D FEL simulations. A comparison of the pulse duration determined by THz streaking with another pulse duration diagnostic, a transverse deflecting structure measuring the modulation of the electron bunch [4] is shown and the advantages, as well as limitations of both techniques, are discussed.

[1] Grguraš et al., Nature Photonics 6 (2012)
[2] R. Ivanov et al., J. Phys. B 53 (2020)
[3] I. Bermúdez et al., Opt. Express 29 (2021)
[4] C. Behrens et al., Nat. Commun. 5 (2014)

Affillation
1: Deutsches Elektronen-Synchrotron, Notkestrasse 85, D-22603 Hamburg, Germany; 2: European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany

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MON 16:15-18:15 | BOARD 99 | P1-MET1-37

POSTER SESSION

BRAGG MAGNIFIER OPTICS FOR DOSE-EFFICIENT X-RAY IMAGING WITH MM-RESOLUTION

Presenter: Rebecca SPIECKER

Authors: Rebecca SPIECKER (1), Holger HESSDORFER (2), Adyasha BISWAL (3), Pauline PFEIFFER (4), Mathias HURST (1), Valerio BELLUCCI (1,5), Angelica CECILIA (2), Tomas FARAGO (2), Annette HERZ (6), Daniel HÄNSCHKE (2), Thomas VAN DE KAMP (2), Yaroslav ZHAROV (1), Marcus ZUBER (2), Mykola SHCHERBININ (1), Elias HAMANN (2), Tilo BAUMBACH (1,2)

Synchrotron-based X-ray imaging of biological samples is often hindered by the radiation dose deployed in the sample, in particular for in vivo imaging and at µm-resolution. Single-distance phase contrast imaging with parallel beam at ~30 keV has the potential for a superior contrast-to-dose ratio, but the limited detection efficiency (~10–20%) of typical scintillator-based high-resolution detectors precludes high overall dose efficiency.

To overcome this bottleneck, we developed a so-called Bragg Magnifier (BM) system optimized for 29–31 keV. By Bragg diffraction from asymmetrically cut silicon single crystals, a 2D magnification of the X-ray beam profile up to a factor 150 is possible, with a sample placed upstream or downstream of the system realizing a microscope (BMM) or beam conditioner (BMC), respectively. In BMM mode and combined with a highly efficient large-area detector, e.g. a high-Z single photon counting detector, an overall detection efficiency of over 90 % can be achieved at ~1 µm effective spatial resolution. In BMC mode, a large beam and thus a cm-sized field of view is achievable even at short beamlines and with the intrinsically small beams of 3rd and 4th generation synchrotrons.

Here, we introduce our BM system and present first experimental results, demonstrating the theoretically predicted high detection efficiency at ~1 µm spatial resolution, as well as an exemplary application of the system to dose-efficient in vivo X-ray imaging of parasitoid wasps.

Affillation

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MON 16:15-18:15 | BOARD 100 | P1-MET1-38

POSTER SESSION

THE IMAGE BEAMLINE AT THE KIT SYNCHROTRON LIGHT SOURCE

Presenter: Angelica CECILIA
Authors: Angelica CECILIA, Elias HAMANN, Rolf SIMON, Tilo BAUMBACH

Here, we will present the status and future perspectives of the recently commissioned IMAGE beamline at the KIT synchrotron. Equipped with two main experimental end-stations for computed laminography and tomography, IMAGE is dedicated to full-field 2D/3D/4D hard X-ray imaging applications in Materials and Life Sciences, with a focus on systematic in-situ and *operando* studies as well as on high sample throughput.

A superconducting wiggler provides a cm-sized beam at the sample location ~40m from the source. In white beam mode, the flux density and energy spectrum is adjustable by tuning the magnetic field of the wiggler in a wide range (1–2.9 T), enabling, e.g., optimizations for fast data acquisition schemes. To protect the beamline components from the high heat load and to adjust the photon flux and it spectral density, sets of pyrolytic graphite and silicon carbide filters can be placed upstream of the beamline optics. In monochromatic mode, either a double multilayer monochromator with an energy bandwidth of ~10E-2 or a Si 111 double crystal monochromator with a bandwidth of ~10E-4 provide X-rays in the energy range from 8 keV to 40 keV, well-suited for absorption or phase contrast imaging with a spatial resolution down to ~1 µm.

After the presentation of the beamline layout, its optics, the related instrumentation as well as the experimental infrastructure, we will report on first application examples and we will provide an outlook on future research activities at IMAGE.

Affillation
Karlsruhe Institute of Technology, Germany

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MON 16:15-18:15 | BOARD 101 | P1-MET1-39

POSTER SESSION

ADVANCED X-RAY ABSORPTION SPECTROSCOPY AT P64 / PETRA III AND OPTIONS FOR PETRA IV

Presenter: Wolfgang CALIEBE
Authors: Wolfgang CALIEBE (1), Aleksandr KALINKO (1), Akhil TAYAL (1), Maria NAUMOVA (1), Claudia SCHWAN (1), Aleksandr KATAEV (2), Marcel GÖRLITZ (1)

X-ray Absorption Spectroscopy (XAS) is a standard analytical method in the application of synchrotron radiation in science. XAS itself provides various important element-specific information on the sample like the oxidation state of the investigated element, its local symmetry and distance to its neighbours. The low absorption by X-rays allow measurements in various sample environments under different conditions, like reactors for homogeneous or heterogeneous catalysis.

Several advanced methods in XAS have been implemented at beamline P64 at PETRA III: A fast-oscillating monochromator reduces the time for one absorption scan from a few minutes to the sub-s time regime, which allows to follow chemical reactions in more detail. The combination of a high-resolution emission spectrometer with XAS reduces the life-time broadening of the absorption edge, which provides more precise information on the local symmetry, and high resolution emission spectroscopy of valence electrons gives additional information on the ligands, which are difficult to get with other methods. Fast, high-resolution cameras can be used for spatially resolved spectra on the micron-length scale with sub-minute time resolution. Photo-excitation of the sample with a high-power laser-pulse is used to study the excited state in light-harvesting metal-organic complexes. All these methods profit from the high flux which is available at PETRA III.

We envision to continue and extend this program at PETRA IV.

Affillation
1: DESY, Germany; 2: Universität Paderborn, Germany

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MON 16:15-18:15 | BOARD 102 | P1-MET1-40

POSTER SESSION

PROGRESS REPORT OF THE LISEL@DREAMS PROJECT

Presenter: Oliver FORSTNER
Authors: Oliver FORSTNER (1,2), Vadim GADELSHIN (3), Kurt STIEBING (4), Klaus WENDT (3)

LISEL (Low energy Isobar SEparation by Lasers) is a project at the DREAMS (DREsden Accelerator Mass Spectrometry) facility at HZDR to widen the applications of AMS by extending the range of measurable (radio-) nuclides. It is a collaboration between the University of Jena and the University of Mainz together with the HZDR. LISEL will use the element selective laser photodetachment of negative ions to suppress unwanted isobars at the low energy side of an AMS system. To achieve this the ions will be thermalized in a radio frequency ion beam cooler where they will be overlapped with a strong laser beam. The laser radiation is produced by a tunable Ti:Sapphire laser pumped by a frequency-doubled, high repetition Nd:YAG laser. The laser system was developed at the University of Mainz and is currently installed at the Frankfurt low-energy storage ring FLSR to acquire spectroscopic data of atomic and molecular negative ions. The LISEL cooler is constructed at the University of Jena and will be commissioned in a test setup. A summary of the full setup and the updated instrumental design as well as results from the storage ring measurements will be presented.

Affillation
1: Friedrich-Schiller-Universität Jena; 2: Helmholtz-Institut Jena; 3: Johannes Gutenberg-Universität Mainz; 4: Goethe Universität Frankfurt

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MON 16:15-18:15 | BOARD 103 | P1-MET1-41

POSTER SESSION

NUCLEAR FORWARD SCATTERING OF PHOTOCHEMICAL AND CATALYTICALLY ACTIVE IRIDIUM COMPLEXES

Presenter: Maren HOOCK

Authors: Maren HOOCK (1), Olaf LEUPOLD (2), Alexander HAAG (3), Yanik BECKER (3), Andreas OMLOR (1), Jonathan OLTMANNS (1), Lukas KNAUER (1), Tim HOCHDÖRFFER (1), René STEINBRÜGGE (2), Atefeh JAFARI (2), Ilya SERGEEV (2), Ralf RÖHLSBERGER (2,4), Werner R. THIEL (3), Hans-Jörg KRÜGER (3), Peter J. SADLER (5), Volker SCHÜNEMANN (1)

Iridium complexes have highly interesting photochemical, photophysical and catalytic properties. They are used for example in Iridium-containing organic light-emitting diodes (OLEDs), organic solar cells and automotive exhaust catalysts. Recently, iridium complexes have also been used to initiate “water oxidation reactions“. They could also be used for directed photoredox catalysis for photodynamic cancer therapy of hypoxic tumors. Recently nuclear forward scattering (NFS) on 193Ir at 73 keV has been established at beamline P01, PETRA III, DESY, Hamburg [1]. We have applied 193Ir-NFS in order to yield information about the electronic properties of selected catalytically active Iridium complexes via the determination of the quadrupole splitting. First results show that even chemical modifications of distant ligand bonds not in the direct vicinity of the iridium atom already leads to different electronic properties, which are manifested in different quadrupole splittings.

[1] P. Alexejev, O. Leupold, I. Sergueev, M. Herlitschke, D. F. McMorrow, R. S. Perry, E. C. Hunter, R. Röhlsberger, H.- C. Wille, Scientific Reports 9, 5097 (2019)

Affillation

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MON 16:15-18:15 | BOARD 104 | P1-MET1-42

POSTER SESSION

PTYCHOGRAPHY FOR PHASE RETRIEVAL IN NUCLEAR RESONANCE SCATTERING

Presenter: Ankita NEGI
Authors: Ankita NEGI (1,2), Lars BOCKLAGE (1), Leon Merten LOHSE (1,3), Sven VELTEN (1,4), Dimitrios BESSAS (8), Christina BRANDT (2), Guido MEIER (5), Ralf RÖHLSBERGER (1,6,7)

Nuclear Resonance Scattering of Synchrotron Radiation (NRS) probes the hyperfine interaction of Mössbauer nuclei by measuring their radiative decay as temporal beat patterns. At present, these time spectra are interpreted with established models and fitted with software tools like CONUSS.

In our experiment at ESRF, we investigated the resonant interaction of X-rays from the synchrotron Mössbauer source (SMS) at beamline ID-18 with a standard 2.5 µm enriched Fe-foil containing (57) Fe Mössbauer nuclei. Our aim is to develop a “Ptychography-like” phase retrieval technique for NRS so that we can computationally retrieve the energy spectra and phase response of samples from their measured temporal beat patterns in a model independent way. Keeping the crystal at rest, we moved our sample with respect to the illuminating beam from the Synchrotron passing through a “mask” ((57) FeBO(3) crystal from the SMS in this case) by mounting it on a Mössbauer drive. This is the equivalent of energetically moving the probe beam across the object in conventional ptychography. Using a multiple-event time digitizer (Fastcom MCS6A) based data acquisition system, we collected 2-D spectra for the (57) Fe-foil in different magnetization directions with respect to the incoming X-ray beam polarization.

The 2-D spectra are used as inputs for our ptychographic phase retrieval engine which operates iteratively by projecting to the Fourier and the overlap constraint in the forward model of the experiment.

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MON 16:15-18:15 | BOARD 105 | P1-MET1-43

POSTER SESSION

HIKA – HIERARCHICAL IMAGING KARLSRUHE

Presenter: Carlos SATO BARALDI DIAS
Authors: Carlos SATO BARALDI DIAS (1), Mateusz CZYZYCKI (1), Dmitri NOVIKOV (2), Tilo BAUMBACH (1)

The HIKa (Hierarchical Imaging Karlsruhe) is the new experimental station being constructed in Hamburg from a collaboration between KIT and DESY. This station is being designed as a versatile imaging platform for various purposes including hierarchical imaging and high throughput 3D imaging for both life and material science, as well as in vivo imaging. Initially, an instrument, named MiQA (Microscope and Quality Assurance), will serve as a multipurpose X-ray optical table for both fundamental experiments aiming at the development of X-ray imaging, and also as a reliable platform for routine X-ray imaging measurements mentioned above. The HIKa station is located at the Ada Yonath Hall on the P23 beamline and has a permanent KIT staff dedicated to the project. The current construction phase is planned to be completed by the end of 2022, followed by MiQA scientific commissioning in 2023.

In the meantime, experiments conducted at P23 current experimental station already demonstrated the technical viability of the project by combining the beamline infrastructure at DESY with the expertise from KIT and also produced original and new results in the field of X-ray imaging.

With the construction of the HIKa station, DESY will add yet another imaging beamline to its portfolio but with the technical expertise of KIT. Future imaging instruments will follow MiQA, increasing the beamline portfolio and leading to interesting scenarios for future research with synchrotron radiation at DESY.

Affillation
1: Karlsruher Institut für Technologie, Germany; 2: Deutsches Elektronen-Synchrotron, Germany

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MON 16:15-18:15 | BOARD 106 | P1-MET1-44

POSTER SESSION

HIGH-PRESSURE IRRADIATION PLATFORM AT GSI, HELMHOLTZ CENTER FOR HEAVY ION RESEARCH

Presenter: Ioannis TZIFAS

Authors: Ioannis TZIFAS (1), Kay-Obbe VOSS (1), Eugenia-Maria TOIMIL-MOLARES (1), Maik LANG (2), Christopher SCHROECK (1,3), Christina TRAUTMANN (1,4)

The growing demand for new engineering applications (i.e. energy, catalysis, space technology) requires materials capable of operating under extreme conditions. Replication of extreme environments provides also valuable information in many areas of geosciences by giving new insights into new thermodynamic pathways and their phase diagrams. The pressure extreme itself can trigger the formation of novel phases, however previous and very recent experiments demonstrate that materials simultaneously exposed to swift heavy ion irradiation and static pressure develop new structures with unique properties. In this contribution, we present the high-pressure irradiation platform at GSI, where materials under high static pressure are exposed to high-energy heavy-ion irradiation and in-situ analyzed by Raman spectroscopy. The compression is achieved by placing a miniaturized sample (thickness 20-30 µm, diameter ~100 µm) into a hole of a metallic gasket and squeezing it between two opposite diamonds. The irradiation is conducted with a collimated beam through the gasket to avoid ion-beam-induced activation and coloration of the diamonds. Monitoring beam-induced structural changes in the pressurized sample are provided by on-line Raman spectroscopy through the diamond anvils. The complete characterization of the materials under pressure also includes the use of synchrotron X-ray spectroscopy at the extreme condition's beamline at DESY prior and after the ion irradiation at GSI.

Affillation

1: GSI Helmholtzzentrum für Schwerionenforschung, Germany; 2: University of Tennessee, Knoxville, Tennessee 37996; 3: Goethe Universität Frankfurt, 60438 Frankfurt,Germany; 4: Technische Universität Darmstadt, 64289 Darmstadt, Germany

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MON 16:15-18:15 | BOARD 107 | P1-MET1-45

POSTER SESSION

IN-SITU X-RAY INVESTIGATIONS IN MATERIAL RESEARCH USING ADVANCED EXPERIMENTAL INSTRUMENTS

Presenter: Anna K. SAMBALE

Authors: Eric EUCHLER (1), Anna K. SAMBALE (1), Konrad SCHNEIDER (1), Constantin HARDER (2), Stephan V. ROTH (2,3), Markus STOMMEL (1,4)

Two recently developed experimental devices for investigating deformation-induced structural evolution in soft matter are now available. The devices exploit the capabilities of a modern synchrotron beamline to enable advanced and highly precise materials-science experiments, in which X-ray scattering is registered for various deformation scenarios, e.g. quasi-static and impact loading. The devices can be operated in monotonic as well as cyclic mode and are implemented into a beamline at DESY (Germany). Hence, relevant experimental parameters, such as displacement, force and temperature, are recorded synchronously with the individual X-ray scattering patterns. Results of recent studies shed new light on the deformation and failure behavior of polymer materials. The focus was on an improved understanding of the kinetics of strain-induced crystallization in natural rubbers and the orientation of such crystallites under inhomogeneous strain fields. Furthermore, molecular and nanoscale mechanisms behind the deformation-induced defect nucleation and growth at crack tips were studied in-situ. Measurements of the deformation-induced nanostructure evolution of thin layers on flexible substrates were realized by performing in-situ grazing-incidence (GI) experiments using a special GI tower for the stretching devices. Besides this, electrical resistance measurements can be performed to correlate nanostructural changes with the conductivity of (semi-)conducting composites.

Affillation

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MON 16:15-18:15 | BOARD 108 | P1-MET1-46

POSTER SESSION

SIMPLE PROXIMITY EFFECT CORRECTION FOR 50 KV ELECTRON-BEAM LITHOGRAPHY ON THICK RESIST LAYERS FOR THE FABRICATION OF X-RAY OPTICS

Presenter: Mattias ÅSTRAND
Authors: Mattias ÅSTRAND, Thomas FRISK, Hanna OHLIN, Ulrich VOGT

Electron-beam lithography (EBL) is relevant to the synchrotron community as it enables the production of high resolution nanodevices that are typically used at beamlines, such as Fresnel zone plates (FZPs) for focusing X-ray beams. We investigate a direct-write process for efficient FZP fabrication that is based on writing features in a thick resist layer. Dose insufficiency may be observed for narrow features if the dose itself is not adjusted. We present a dose study, a theory for understanding the proximity effect in our samples, and a method for correction. This knowledge is translated to high-quality FZPs, produced by 50 kV EBL (fast writing) on AR-P 6200 resist (CSAR 62, compatible with further nanoprocessing), implemented successfully at NanoMAX (MAX IV) and P06 (PETRA III).

Affillation
KTH Royal Institute of Technology, Sweden

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MON 16:15-18:15 | BOARD 109 | P1-MET1-47

POSTER SESSION

EXPERIMENTAL DETERMINATION OF DIFFERENTIAL SCATTERING COEFFICIENTS FOR NICKEL BY MEANS OF LINEARLY POLARIZED X-RAY RADIATION

Presenter: André WÄHLISCH
Authors: André WÄHLISCH (1), Malte WANSLEBEN (1,2), Jan WESER (1), Ina HOLFELDER (1), Yves KAYSER (1), Burkhard BECKHOFF (1)

The incorporation of scattered X-ray radiation (i.e., Rayleigh and Compton scattering) can provide additional information compared to conventional X-ray fluorescence (XRF) analysis, which is commonly used for element-sensitive investigations. In particular, matrix effects due to light elements can be investigated under ambient conditions using scattered X-rays, even when their XRF radiation can not be detected due to absorption in air. To this end, accurate and reliable descriptions of the X-ray scattering fundamental parameters are required for a quantitative interpretation of the X-ray scattering process. These scattering coefficients are highly anisotropic. Thus, differential scattering coefficients have to be determined in dependence of the scattering angle. Furthermore, utilizing polarized X-ray radiation adds another directional dependency. We present a metrological study on the determination of differential scattering coefficients, utilizing highly polarized synchrotron radiation. The utilized setup consists of a sample manipulator and a silicon drift detector mounted on a detector arm. They allow for rotational selection of angle of incidence, exit angle, polar and azimuthal scattering angles, resulting in a flexible experimental approach. We present a description of the instrument and the measurement methodology, an analysis of the involved uncertainty budget, and compare our experimental results to available databases based on calculations.

Affillation
1: Physikalisch-Technische Bundesanstalt, Germany; 2: Helmut Fischer GmbH

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MON 16:15-18:15 | BOARD 110 | P1-MET1-48

POSTER SESSION

A NEW NUCLEAR RESONANCE BEAMLINE AT THE NEW EXTREMELY BRILLIANT SOURCE OF ESRF

Presenter: Rudolf RÜFFER
Authors: Aleksandr CHUMAKOV, Rudolf RÜFFER

In 2024, the pioneering Nuclear Resonance beamline (ID18) at the ESRF will get a successor: a brand-new Nuclear Resonance beamline (ID14) at the new Extremely Brilliant Source (EBS) of ESRF. Cornerstones of the new beamline are pursuing (i) spectroscopies with extreme spatial resolution, (ii) studies of atomic dynamics with extreme energy resolution, and eventually (iii) exploiting all advantages of the ESRF-EBS.

Studies with extreme spatial (~150 nm) and extreme energy (~50 mueV) resolution will profit by two new instruments, Nanoscope and Spectrograph, respectively. In both cases, the improvement in resolution goes without essential losses of flux, i.e., keeping nearly the same count rate.

In order to assure stable operation with extreme spatial and energy resolution, the second optics hutch (containing optics of high-resolution monochromators, synchrotron Mössbauer source, and Spectrograph) and the new fourth experimental hutch (hosting Nanoscope) will be equipped with thermal isolation and with a high-quality air conditioning system providing temperature stability of about 0.1°C. Eventually, advanced instrumentation, beamline control systems, and evaluation software complete the new beamline.

The Nanoscope and Spectrograph instruments should already be available to users by end of 2022, still at ID18, and shall move to ID14 in 2023. ID18 is planned to be operational until second half of 2023 and user service at ID14 is expected to start from the beginning of 2024.

Affillation
ESRF, France

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MON 16:15-18:15 | BOARD 111 | P1-MET1-49

POSTER SESSION

MICRO-XRAY DIFFRACTION FOR HIGHLY ABSORBING SAMPLES AT P06

Presenter: Prerana CHAKRABARTI
Authors: Prerana CHAKRABARTI (1,2), Anna WILDEIS (3), Markus HARTMANN (3), Robert BRANDT (3), Ralph DOEHRMANN (2), Giovanni FEVOLA (2), Christina OSSIG (2,4), Michael ELIAS STUCKELBERGER (2), Jan GARREVOET (5), Ken VIDAR FALCH (5), Vanessa GALBIERZ (5), Gerald FALKENBERG (5), Peter MODREGGER (1,2)

Micro and nano-scale characterization of (poly)-crystalline materials like measuring micro strains, crystallite sizes or local texture requires X-ray diffraction (XRD) with high spatial resolution. This can be achieved by combining XRD with focusing optics such as compound refractive lenses for small spot sizes and lateral scanning of the sample. Further, the utilization of high photon energies is beneficial for investigating highly absorbing samples. Recently, we have demonstrated that a novel goniometer-based setup at the P06 beamline of PETRA III provides XRD data with a spot size of approximately 2 micrometer at a photon energy of 35 keV. This goniometer provides up to 5D scans for the complete characterization of reciprocal space as a function of sample position. The combination of high spatial resolution and high photon energy allowed us to examine martensitic steels, which constitute the material of choice for suspension springs in vehicles due to their excellent resiliency in the high cycle fatigue regime.
We demonstrate that the local strain in martensitic steel samples can be measured with approximately 4 micrometer spatial resolution and sensitivities better than 0.001. This setup will enable the study of the impact of microscopic residual stress on short crack propagation in spring steels, still an open and topical question in materials science, for the first time.

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MON 16:15-18:15 | BOARD 112 | P1-MET1-50

POSTER SESSION

THE COHERENCE APPLICATIONS BEAMLINE P10 AT PETRA III

Presenter: Fabian WESTERMEIER
Authors: Fabian WESTERMEIER (1), Nimmi Das ANTHUPARAMBIL (1,2), Vijay KARTIK (1), Zhe REN (1), Rustam RYSOV (1), Daniel WESCHKE (1), Han XU (1), Michael SPRUNG (1)

The Coherence Beamline P10 at PETRA III, DESY, is dedicated to coherent X-ray scattering experiments using X-ray Photon Correlation Spectroscopy (XPCS) and Coherent Diffraction Imaging (CDI) techniques as well as holographic imaging. Mostly, the beamline operates in the energy range of 5-17 keV. It consists of two 12m long experimental hutches which house various experimental setups.

Here we want to present the three setups which are commonly used for XPCS and Bragg-CDI experiments. 1) A SAXS/WAXS instrument, where the detector can be translated between 0 and 30 degrees at a sample to detector distance of 5 m. By reducing the sample to detector distance to 2 m, the accessible angular range can be extended to 45 degrees. This setup is thus ideally suited to probe an extended q-range up to atomic length-scales. 2) An ultra-small angle X-ray scattering setup, where the detector is positioned at a sample to detector distance of around 21 m. This long pathway allows it to use a large fraction of the coherent flux in an unfocused X-ray beam, while providing a fairly strong speckle visibility. This setup is therefore ideally suited for radiation sensitive samples. 3) A six-circle diffractometer setup which allows to satisfy different diffraction conditions to mainly perform Bragg-CDI experiments. Here, a beam spot of around 1 micrometer^2 is routinely used, and several microscopes allow to monitor and position the sample.

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MON 16:15-18:15 | BOARD 113 | P1-MET1-51

POSTER SESSION

RAY TRACING SIMULATION FOR BRAGG MAGNIFIERS

Presenter: Mykola SHCHERBININ
Authors: Mykola SHCHERBININ (1), Adyasha BISWAL (2), Rebecca SPIECKER (1), Elias HAMANN (3), Tilo BAUMBACH (3)

The target system for presented simulations is a Bragg magnifier (BM). It consists of up to four asymmetrically cut single crystals for magnifying the small synchrotron beam cross section. The system can be used either as microscope or for large field-of-view imaging.

Polychromatic light beam reflection from several perpendicularly oriented crystal surfaces leads to an inhomogeneous light intensity distribution on a detector plane. Due to dispersion of the monochromator the light beam obtains a certain transversal spatial chromatic distribution. The light reflection from the crystals of the BM which follow downstream is determined by their Bragg reflection curve that is sensitive to wavelength. It means that the initially rectangular beam will lose almost all its intensity in those parts where the Bragg condition is not fulfilled. This phenomenon is observed experimentally by a photodetector as a distinctive 'diagonal' intensity distribution. The described pattern strongly depends on the size and angular divergence of the source, characteristics of crystal lattice and overall geometry of the system.

As this phenomenon significantly restricts an actual field of view of a setup, the foremost task is to find the setup parameters for which the illuminated area will fill the whole field of view of the detector. Monte Carlo polychromatic light source simulation and a mathematical apparatus for crystal dynamical diffraction are applied to trace the light path through the system.

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MON 16:15-18:15 | BOARD 114 | P1-MET1-52

POSTER SESSION

PARTICLE- AND PHASE-SELECTIVE X-RAY SPECTROSCOPY WITH MICRO- AND MACROBEAMS: THE CASE OF (SmS)1.19TaS2 NANOTUBES

Presenter: Azat KHADIEV

Authors: Azat KHADIEV (1), Madhenahalli Bhyrappa SREEDHARA (2), Dmitri NOVIKOV (1), Reshef TENNE (2)

The purpose of this study is to show the advantages of the DAFS (Diffraction Anomalous Fine Structure) spectroscopy and microbeam XANES techniques in the analysis of nanotube (NT) powders containing a sufficient number of different phases. Contrary to conventional XAFS, DAFS allows measuring the XAFS-like signal from a certain phase separately by choosing the proper diffraction peak, thus providing phase-selectivity. Microbeam spectroscopy allows one to focus the beam on a certain particle and perform XANES.

In order to understand the growth and stability of SmS-TaS2 NT a set of powders was synthesized at different temperatures. XRD and TEM have shown that the NT abundancy falls down with temperature. The shape of the DAFS spectra also changes: the intensity of Ta L3 ‘white’ line decreases with temperature. The microbeam XANES measured on single SmS-TaS2 NTs also shows higher Ta L3 ‘white’ line intensity in comparison to the powder. Such dependence of ‘white’ line intensity on NT abundancy can be explained by the difference in the interaction of SmS and TaS2 in bulk SmS-TaS2 crystals and NT. In the bulk SmS-TaS2 crystals it was found that SmS layer act as a donor of electrons for the TaS2 part. In the NT due to the curvature of the layer, the number of the SmS units is smaller than in the crystals, thus SmS part donates fewer electrons. Therefore, in NT there should be more Ta 5d band vacancies in comparison to bulk, thus providing a more intense Ta L3 ‘white’ line in XANES.

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MON 16:15-18:15 | BOARD 115 | P1-MET1-53

POSTER SESSION

PULSED NEUTRON BEAM AT THE N4DP INSTRUMENT

Presenter: Jonas SCHLEGEL
Authors: Jonas SCHLEGEL (1), Robert NEAGU (1), Markus TRUNK (2), Roman GERNHÄUSER (1), Ralph GILLES (2), Zsolt REVAY (2), Bastian MÄRKISCH (1)

Neutron Depth Profiling (NDP) is a non-destructive, isotope-specific, high-resolution nuclear analytical technique, which is often used to probe concentration profiles of lithium, boron, nitrogen, helium and several other light elements in different host materials. The N4DP instrument is located at the Prompt Gamma Activation Analysis (PGAA) beam line of Heinz Maier-Leibnitz Zentrum (MLZ), which provides a cold neutron flux up to 5×10^{10} $s^{-1}cm^{-2}$. When a neutron is captured by a specific nucleus, charged particles with well-defined energies are emitted back-to-back, and one of them is detected by a double sided silicon strip detector (DSSSD). The energy loss of the charged particles traveling through the host material is related to the depth of origin at a resolution level down to tens of nanometers.

The delayed part of the background from the neutron activation is time-dependent and increases, depending on the sample, in the course of the measurement until saturation is reached. Although the N4DP instrument achieves good signal to background ratio, one can still improve this ratio by determining the time-dependent background from activation. This is possible by using a pulsed neutron beam, which can be generated by a newly developed chopper.

This project is supported by the BMBF, Contract Nos. 05K16WO1, 05K19WO8.

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MON 16:15-18:15 | BOARD 116 | P1-MET1-54

POSTER SESSION

THE MUNICH COMPACT LIGHT SOURCE – A LABORATORY-SCALE SYNCHROTRON FACILITY FOR BIOMEDICAL RESEARCH AND MORE

Presenter: Martin DIEROLF
Authors: Martin DIEROLF (1,2), Benedikt GÜNTHER (1,2), Johannes BRANTL (1,2), Johannes MELCHER (1,2), Bernhard GLEICH (2), Klaus ACHTERHOLD (1,2), Julia HERZEN (1,2), Franz PFEIFFER (1,2,3,4)

Synchrotron X-ray sources have allowed scientists to push the frontiers of X-ray imaging towards nanometer-scale resolutions and extremely high sensitivities. However, for many of the developed techniques, the transfer from the synchrotron back to preclinical or even clinical imaging is not straightforward. This is mainly due to the rather different characteristics of the X-ray tube sources typically employed in the latter cases. The Munich Compact Light Source (MuCLS) at the Technical University of Munich bridges this performance gap and aims at providing an X-ray facility that allows to apply modern synchrotron techniques in a university research laboratory setting. It consists of a commercial inverse Compton X-ray source (Lyncean Technologies Inc., Fremont, USA) and a beamline with two endstations designed and constructed by TUM scientists [1, 2].

The various applications utilize the – for a laboratory source – unique properties of the MuCLS beam [2]: The narrow tunable spectrum allows to perform quantitative computed tomography (CT) without beam-hardening, K-edge imaging or absorption spectroscopy. The relatively high flux density enables radiation therapy studies, high-resolution micro-CT and fast dynamical imaging. Finally, the partial coherence of the source enables grating-based phase-contrast and dark-field imaging, as well as propagation-based imaging.

[1] E. Eggl et al., J. Sync. Rad. 23, 1137 (2016)
[2] B. Günther et al., J. Sync. Rad. 27, 1395 (2020)

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MON 16:15-18:15 | BOARD 117 | P1-MET1-55

POSTER SESSION

THZ RESEARCH AT FELBE & TELBE – PUSHING THE LIMITS OF THE ULTRAFAST AND ULTRASMALL

Presenter: J. Michael KLOPF
Authors: J. Michael KLOPF (1), Sergey KOVALEV (1), Jan DEINERT (1), Alexej PASHKIN (2), Stephan WINNERL (2), Peter MICHEL (1), Manfred HELM (2)

The THz sources of FELBE and TELBE are powerful and versatile tools for the study of many types of materials. The low energy dynamics in materials can be related to the motion of charges or resonant motion of the lattice. The interaction between charges and the lattice gives rise to correlated processes in certain materials as well as other exotic phenomena in low dimensional systems and quantum structures. The THz-driven structural dynamics of soft materials (e.g. water, proteins, etc.) also occur at THz energies and are another important new field of exploration. In all of these types of studies, the ultrashort high-field coherent THz pulses of FELBE and TELBE sources are ideally suited for driving and probing the dynamics of these systems to bring forth a greater understanding.

Furthermore, by coupling the FELBE and TELBE sources with scattering-Scanning Nearfield Optical Microscope (s-SNOM) instrumentation, it is possible to probe the resonant coupling of the THz field with the charge distribution (plasmons) or the lattice (phonon polaritons). The s-SNOM technique provides optical information with spatial resolution far below the diffraction limit.

The critical tools needed to continue to develop and enhance the research at FELBE and TELBE are made possible by the BMBF ERUM projects presented below.

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MON 16:15-18:15 | BOARD 120 | P1-DATA-01

POSTER SESSION

TOWARDS SERIAL COMPUTED TOMOGRAPHY BASED ON AUTOMATED DATA ACQUISITION AND ANALYSIS PIPELINES FOR LARGE SCALE 3D MORPHOLOGICAL STUDIES

Presenter: Angelica CECILIA
Authors: Tomas FARAGO, Angelica CECILIA, Alexey ERSHOV, Evelina AMETOVA, Yaroslav ZHAROV, Tilo BAUMBACH

We aim to extend the synchrotron based tomography towards Serial Computed Tomography with AI-assistance from data acquisition to analysis of 3D volumes, which has the potential to enable systematic large-scale comparative 3D morphological studies on the µm scale. Here, we report on the developments towards smart and automated data acquisition and analysis pipelines for such studies.

We employ a highly automated CT acquisition set-up developed at KARA synchrotron for time-resolved and high-throughput CT experiments. It contains a robotized sample changer and substantial automation of the complete workflow from data acquisition to analysis. The system contains a 3D data-driven feedback loop: during the scan, image data are fed into GPUs of a computing server and immediately after the data acquisition the complete 3D reconstructed volume is available for further analysis, quality assurance and control of the experiment. We have developed unsupervised deep learning methods to automatically localize samples in large tomographic volumes, useful for in-situ measurements and for data reduction in large series.

After acquisition, the data is re-reconstructed with various fine-tuned pre- and post-processing steps (e.g. ring removal). We then employ robust state-of-the-art deep learning techniques to process the series of 3D volumes. We will demonstrate the potential of our developments to enhance 3D X-ray imaging by various case studies.

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MON 16:15-18:15 | BOARD 121 | P1-DATA-02

POSTER SESSION

PROGRESS ON MEASUREMENT AUTOMATION AND FAIR DATA AT ENERGY MATERIALS IN-SITU LABORATORY

Presenter: Will SMITH

Authors: Will SMITH (1), Andreas BALZER (1), Anna EFIMENKO (1), Raul GARCIA-DIEZ (1), Michael GOETTE (1), Mihaela GORGOI (1), Gerrit GUENTHER (1), Michael HÄVECKER (1,2), Huiling HE (1), Sebastian KAZARSKI (1), Sebastian SACHSE (1), Simone VADILONGA (1), Markus WEIGAND (1), Regan WILKS (1)

The Energy Materials In-Situ Laboratory Berlin (EMIL) at BESSY II, with its unique analytical instrumentation in direct combination with scientifically- and industrially-relevant deposition tools, is now in user operation. The project comprises a complex 2-color undulator-based beamline delivering X-rays with photon energies between 80 and 10000 eV and 5 end stations dedicated to diverse techniques like scanning transmission X-ray microscopy, *operando* fluorescence spectroscopy or energy-dependent photoelectron spectroscopy. These experiments are striving to make the data they produce Findable Accessible Interoperable and Reproducible (FAIR), as well as providing easy to use tools to control experiments for the range of techniques performed. Devices from the beamline and the end stations are integrated with EPICS. The experiments are orchestrated by Bluesky, a python library for experiment control and collection of scientific data and metadata. Bluesky can be operated by different means, either by a GUI, Jupyter Notebooks or IPython. Additionally, an electronic logbook is implemented that is automatically written by the machine and can be freely modified by the users. Finally, data are automatically exported into NeXus format and uploaded to the ICAT repository. This work presents the progress of the project, looks at the problems that have been overcome and discusses what is still to be done.

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MON 16:15-18:15 | BOARD 122 | P1-DATA-03

POSTER SESSION

ALPAKA-SSB: A CASE STUDY OF IMPLEMENTING PERFORMANCE PORTABLE PTYCHOGRAPHY RECONSTRUCTION ALGORITHMS IN C++

Presenter: Jiri VYSKOCIL
Authors: Jiri VYSKOCIL (1,2), Simeon EHRIG (2), Nico HOFFMANN (2), Michael BUSSMANN (1,2)

Ptychography is a method of reconstructing images of nanometer-scale from a set of diffraction patterns obtained by illuminating said object without the need for putting lenses between it and the illumination source. The Single Side Band ptychographic reconstruction method (SSB) analyzes 4D data obtained from a scanning electron microscope utilizing the largest possible volume of Fourier space to create high efficiency phase contrast images. Such a reconstruction, notably when it is to be done on the edge devices at a beamline in real-time, requires a well performing implementation. Support for different computing architecture can be achieved by introducing a performance portability layer such as Alpaka - an open-source header-only C++ abstraction library for accelerator development which provides performance portability across processor types through the abstraction of the underlying levels of parallelism. Alpaka code compiles to binaries supporting multi-threaded CPUs, GPUs from multiple vendors, and FPGAs. When the vendors release new hardware, the user does not need to be aware of the implementation specifics, as this will be handled by the Alpaka library. In our case study, we have chosen SSB to show how to use Alpaka's facilities to write C++ reconstruction codes which can be executed on most contemporary parallel architectures without the need to be aware of their specific differences on the level of algorithm implementation.

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MON 16:15-18:15 | BOARD 123 | P1-DATA-04

POSTER SESSION

ALPAKA-ePIE: PERFORMANCE PORTABLE RECONSTRUCTION OF PTYCHOGRAPHY DATA

Presenter: Simeon EHRIG

Authors: Simeon EHRIG (1), Silvio ACHILLES (2), Andreas SCHROPP (2), Dieter WEBER (4), Alexander CLAUSEN (4), Jiri VYSKOCIL (3), Christian SCHROER (2), Oleh MELNYK (5), Knut MÜLLER-CASPARY (4), Nico HOFFMANN (1), Michael BUSSMANN (2)

Ptychography is a computational imaging method required to numerically retrieve the projection of an object from a set of measured diffraction patterns. Each individual diffraction pattern represents a partially overlapping area of the object. The corresponding inverse problem, i.e. the image reconstruction, can be solved by projection-based or gradient-based algorithms. There are several implementations that have been developed and optimized for a specific system and are difficult to port to a new system. In contrast, we will be introducing the alpaka library along with a generic C++ implementation of the ePIE algorithm and Python bindings. The alpaka library follows the write once, run everywhere principle, which means that a single C++ implementation can run on GPUs from different vendors, but also on CPU and FPGA. Additionally, alpaka also simplifies the development workflow: we will be demonstrating how a tomography extension of the alpaka-ePIE code benefits from the ability to debug GPU code with CPU tools. Finally, the Python bindings improve compatibility with existing software workflows and allow easy parallelization across many GPUs by LiberTEM. The updates of the object function and illumination function are concurrently retrieved, merged, and redistributed. This cycle is run until convergence of the reconstruction. The reconstruction code is then evaluated using experimental data from various experimental setups for X-ray and electron microscopy.

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MON 16:15-18:15 | BOARD 124 | P1-DATA-05

POSTER SESSION

SECoP AND METADATA – THE SAMPLE ENVIRONMENT COMMUNICATION PROTOCOL

Presenter: Klaus KIEFER

Authors: Klaus KIEFER (1), Georg BRANDL (7), Niklas EKSTRÖM (4), Enrico FAULHABER (3), Thomas HERRMANNSDÖRFER (6), Bastian KLEMKE (1), Thorsten KRACHT (5), Anders PETTERSSON (4), Lutz ROSSA (1), Markus ZOLLIKER (2)

The integration of sample environment (SE) equipment in a beam line experiment is a complex problem both in the physical world and in the digital world. Different experiment control software offers different interfaces for the connection of SE equipment. Therefore, it is time-consuming to integrate new SE or to share SE equipment between facilities.

To tackle this problem, the International Society for Sample Environment (ISSE) developed the Sample Environment Communication Protocol (SECoP) to standardize the communication between instrument control software and SE equipment (see [1] and references therein). SECoP offers, on the one hand, a generalized way to control SE equipment. On the other hand, SECoP holds the possibility to transport SE metadata in a well-defined way.

Using SECoP as a common standard for controlling SE equipment and generating SE metadata will save resources and intrinsically give the opportunity to supply standardized and FAIR data compliant SE metadata. It will also supply a well-defined interface for user-provided SE equipment, for equipment shared by different research facilities and for industry.

In this contribution we will give an overview of the present status of SECoP and the developments within the SECoP@HMC project supported by the Helmholtz Metadata Collaboration.

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[1] K. Kiefer, et al. (2020). An introduction to SECoP – the sample environment communication protocol. Journal of Neutron Research, 21(3-4), pp.181–195

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MON 16:15-18:15 | BOARD 125 | P1-DATA-06

POSTER SESSION

SAMPLE ENVIRONMENT COMMUNICATION PROTOCOL (SECoP)

Presenter: Klaus KIEFER

Authors: Thomas HERRMANNSDÖRFER (1), Klaus KIEFER (2), Georg BRANDL (3), Niklas EKSTRÖM (4), Enrico FAULHABER (5), Bastian KLEMKE (2), Thorsten KRACHT (6), Anders PETTERSON (4), Lutz ROSSA (2), Markus ZOLLIKER (7)

We would like to introduce a software and initiative that takes care of the standardization of communication between instrument control software, sample environment (SE) equipment, and acquisition of metadata as well, the Sample Environment Communication Protocol (SECoP). To tackle these challenges of data acquisition in daily laboratory routine, the International Society for Sample Environment (ISSE) developed the Sample Environment Communication Protocol (SECoP) to standardize the communication between instrument control software and SE equipment (see [1] and references therein). SECoP offers, on the one hand, a generalized way to control SE equipment. On the other hand, SECoP holds the possibility to transport SE metadata in a well-defined way. Using SECoP as a common standard for controlling SE equipment and generating SE metadata will save resources and intrinsically give the opportunity to supply standardized and FAIR data compliant SE metadata. It will also supply a well-defined interface for user-provided SE equipment, for equipment shared by different research facilities and for industry. In this Poster Session presentation we will give an overview of the present status of SECoP and the developments within the SECoP@HMC project supported by the Helmholtz Metadata Collaboration.

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[1] K. Kiefer, et al. (2020). An introduction to SECoP – the sample environment communication protocol. Journal of Neutron Research, 21(3-4), pp.181–195

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MON 16:15-18:15 | BOARD 126 | P1-DATA-07

POSTER SESSION

XAS REFERENCE DATABASE UNDER DAPHNE4NFDI

Presenter: Abhijeet GAUR
Authors: Abhijeet GAUR (1,2), Dmitry DORONKIN (1,2), Sebastian PARIPSA (3), Wolfgang MALZER (4), Christopher SCHLESIGER (4), Jan-Dierk GRUNWALDT (1,2), Birgit KANNGIESSER (4), Dirk LÜTZENKIRCHEN-HECHT (3)

Photon and neutron science communities encompass users from a broad range of disciplines facing the common need for high-level, rapid data analysis and the challenge of implementing research data management. Within the DAPHNE4NFDI consortium, an important pilot project is to develop a reference database in the field of X-ray absorption as well as X-ray emission spectroscopy and related techniques. In this field, data are often evaluated by comparing them to previously measured or calculated spectra. Automatic, also on the fly, data processing requires a repository with high quality reference data, including metadata, from reliable sources. This sets high requirements concerning both spectral quality and documentation of the measurements. The initial focus is to setup an XANES/EXAFS database of raw and processed data with the aim of an interface for the user for data submission as well as an API for data analysis software. An automated assessment of data quality including a manual peer review possibility will be established with the results saved in the metadata. Users could judge the quality and the usability of each data set by looking at these quality criteria. The purpose of the present contribution is to intensify the discussion in the XAS community regarding the importance of metadata/data fields and quality assurance criteria as well as interface and API functionality to be included in the planned reference database. This will optimize the reusability of the data.

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MON 16:15-18:15 | BOARD 127 | P1-DATA-08

POSTER SESSION

ON-THE-FLY DATA REDUCTION AND ANALYSIS FOR COMPLEX MULTIMODAL EXPERIMENTS

Presenter: Jiatu LIU
Authors: Jiatu LIU (1), Mahesh RAMAKRISHNAN (1), Matteo CIAMBEZI (1), Eva UNGER (2), Jinzhao LI (2), Justus JUST (1)

As the acquisition of large experimental data sets has become a routine in the in-situ characterization of chemical processes at synchrotron/neutron facilities, a quick display and reduction of the data during one experiment session is extremely helpful as researchers can make good use of the beamtime according to the physiochemical information offered on the fly. A python-based multimodal data reduction software (MDRS) is developed to visualize data collected from multiple collection modules and reduce them to human-readable form.

MDRS, with dockable tabs and adjustable parameters as the user-interface, is able to generate time-series plots or load from previously generated plots, memorize data for comparison, and show data acquired according to the time stamps. It is a growing project that can encompass data reading modes/pipelines written by users with minimal modification of the code.

The current version of MDRS can handle four modules of data, i.e. X-ray absorption spectroscopy (XAS), diffraction (XRD), visible light reflection and photo-luminescence spectroscopy. The reduction of XAS in the extended region borrowed the already developed Larch functions. The XRD pipelines go as far as peak identification and phase index based on time-series data. The software will be demonstrated with an in-situ study of hybrid perovskite material formation processes applying in-situ a slot-die coating.

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MON 16:15-18:15 | BOARD 128 | P1-DATA-09

POSTER SESSION

NUrF: STREAMLINING LIQUID HANDLING AND DATA PROCESSING AND ANALYSIS FOR SANS BEAMLINES

Presenter: Gudrun LOTZE
Authors: Gudrun LOTZE (1), Cedric DICKO (2), Judith HOUSTON (3), Simon HEYBROCK (3), Adrian RENNIE (1)

Automated liquid handling systems perform various liquid handling tasks, e.g., pipetting, sample preparation, and cuvette washing. Those devices are now standard at bioSAXS beamlines [1]. They save on labour and free up resources to focus on analysis instead of repetitive tasks.

However, the application of such systems at SANS beamlines is in its infancy. The most recent systems involve (i) an in-line liquid chromatography system to separate and subsequently measure biomacromolecules and their complexes [2]; and (ii) microfluidics cells [3]. The significant difficulty is the optimization of sample volume, concentration and deuteration state.

We recently developed a simultaneous measurement platform combining SANS, UV-vis, fluorescence, and densitometry: the NUrF [4].

On the software side, we propose a new outline for hdf5 files for all neutron sources using the NUrF experimental configuration. The new file format follows the NeXus data format [5] and integrates smoothly with the scipp Python library [6] facilitating data processing and future analysis.

Overall, this contribution illustrates how automatic liquid handling needs to go hand in hand with automatic data processing, visualization, and analysis to make efficient use of neutron beamtime and to reveal unexpected events in the sample.

[1] doi:10.1107/S1399004714026959
[2] doi:10.1107/S1600576716016514
[3] doi:10.1039/C7LC00179G
[4] doi:10.1063/5.0011325
[5] https://scipp.github.io/scippnexus/
[6] doi:10.3233/JNR-190131

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MON 16:15-18:15 | BOARD 129 | P1-DATA-10

POSTER SESSION

SNIP – DIGITAL USERS' LAB BOOK

Presenter: Markus OSTERHOFF
Authors: Markus OSTERHOFF (1,2,3), Sebastian MOHR (1,2), Sarah KÖSTER (1,3)

Conducting and steering experiments (including alignment, sample treatment and conditions, actual measurements, and preliminary analysis) is a highly creative process. In the realm of hand-crafted log books, a lot of freedom was used to combine printouts with annotations and sketches. This process mirrored the progress and decisions of the experiment.

In recent years, lots of electronic log books have been built. We find that the creative process of free note-keeping has been disregarded, while formalities are overemphasized and take increasing amounts of time. Also, important machine parameters (e.g. motor positions, detector and microscope images) cannot be easily accessed/referenced, even with facility-developed log books.

We propose "snip", a digital users' lab book combining hand-crafted entries with computer-generated contents. External software (e.g. control software, detector and microscope computers etc.) create and send standardised "snippets" representing the experiment; the users then curate these snippets and add annotations. The "analogue mode of operation" is maintained to a large degree, but instead of printouts now "true digital copies" are used and "glued into the book". The snippets carry certain pieces information as meta-data, e.g. motor positions or images. Before "gluing in", users can adapt the actual "view" (size, ROI etc.), and then annotate with pen entry.

The web-based software allows for collaborative (real-time and distributed) read/write.

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MON 16:15-18:15 | BOARD 130 | P1-DATA-11

POSTER SESSION

NEXUS – A NEW SOFTWARE TO EVALUATE MODERN NUCLEAR RESONANT SCATTERING EXPERIMENTS

Presenter: Lars BOCKLAGE
Author: Lars BOCKLAGE

Applications of nuclear resonant scattering with synchrotron radiation range from biology and chemistry over material science to hard-X-ray quantum optics. The method relies on measuring quantum beats during the de-excitation of Mössbauer resonances. Interpretation of those data is not straight forward and dedicated software tools are needed. Especially, a prior design of an experiment is of great importance in quantum optical studies. Existing evaluation software written in FORTRAN (CONUSS, REFTIM, MOTIF) focus on fitting a single sample or measurement, which is often not sufficient to properly describe full data sets or modern experimental setups with many objects in the beam path.

NEXUS is a Python extension written in C++ with a highly object-oriented approach and special emphasis on simulating and fitting any kind of experimental condition. Modern optimization routines offer not only to fit multiple data sets in parallel but also to design experiments beforehand to specific target parameters.

We present the basic structure of NEXUS and a few showcases where it has been applied to material science and quantum optical experiments with Mössbauer nuclei. Those experiments include experiments with synchrotron Mössbauer sources, magnetic multilayers, nuclear polarimetry, interferometry for nuclear ptychography, nuclear waveguides, and the creation of a nuclear quantum memory.

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MON 16:15-18:15 | BOARD 131 | P1-DATA-12

POSTER SESSION

HELIPORT – AN INTEGRATED RESEARCH DATA LIFECYCLE

Presenter: David PAPE
Authors: Oliver KNODEL, David PAPE, Martin VOIGT, Thomas GRUBER, Jeffrey KELLING, Mani LOKAMANI, Stefan MÜLLER, Guido JUCKELAND

HELIPORT is a data management solution that aims at making the components and steps of the entire research experiment's life cycle discoverable, accessible, interoperable and reusable according to the FAIR principles.

Among other information, HELIPORT integrates documentation, scientific workflows, and the final publication of the research results - all via already established solutions for proposal management, electronic lab notebooks, software development and devops tools, and other additional data sources. The integration is accomplished by presenting the researchers with a high-level overview to keep all aspects of the experiment in mind, and automatically exchanging relevant metadata between the experiment's life cycle steps.

Computational agents can interact with HELIPORT via a REST API that allows access to all components, and landing pages that allow for export of digital objects in various standardized formats and schemas. An overall digital object graph combining the metadata harvested from all sources provides scientists with a visual representation of interactions and relations between their digital objects, as well as their existence in the first place. Through the integrated computational workflow systems, HELIPORT can automate calculations using the collected metadata.

By visualizing all aspects of large-scale research experiments, HELIPORT enables deeper insights into a comprehensible data provenance with the chance of raising awareness for data management.

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MON 16:15-18:15 | BOARD 132 | P1-DATA-13

POSTER SESSION

DAPHNE4NFDI: DATA FROM PHOTON AND NEUTRON EXPERIMENTS; ELECTRONIC LAB NOTEBOOKS FROM A SCIENCE CASE PERSPECTIVE

Presenters: Philipp JORDT
Authors: Philipp JORDT (1), Alexander HELDMANN (2), Wiebke LOHSTROH (2), Bridget MURPHY (1)

The photon and neutron science community encompasses users from a broad range of scientific disciplines answering to increasingly complex questions and requiring more and more interdisciplinary work across different scientific fields producing more and larger datasets. The more elaborate instrumentation and data evaluation requires more know-how to successfully publish the scientific findings.

The aim of DAPHNE4NFDI is to create a comprehensive infrastructure to process research data from large scale photon and neutron infrastructures according to the FAIR principles (Findable, Accessible, Interoperable, Repeatable). A key to successfully provide well documented and searchable research data is the addition of fully-fledged electronic lab notebooks (ELN).

Here we present our latest findings on the requirements and evaluations on existing ELN worked out in an joint collaboration in the neutron and X-ray community. A comparison between different ELN concepts is given. The implementation of the TUM workbench ELN at the FRM II is presented, together with a first evaluation of the resulting experience. Furthermore, the advantages and hurdles to implement a workflow to auto ingest scientific data into an ELN will be presented.

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MON 16:15-18:15 | BOARD 133 | P1-DATA-14

POSTER SESSION

SciCat – IMPLEMENTING A DATA CATALOGUE FOR INDIVIDUAL RESEARCH GROUPS AND LARGE SCALE FACILITIES

Presenters: Linus PITHAN
Authors: Linus PITHAN (1), Philipp JORDT (2), Tobias RICHTER (3), Frank SCHREIBER (1), Bridget MURPHY (2)

SciCat is a modern and flexible data catalogue that suites the needs of both, large scale research facilities as well as individual research groups e.g. at universities. Within DAPHNE4NFDI we find these two use-cases and currently evaluate the use of SciCat for different scenarios.

Since SciCat was initially build to serve Photon- and Neutron sources (the development started at PSI and ESS), it provides community specific features like the homogenized search API that has been developed within PANOSC & EXPANDS. To serve individual research groups as a tool for research data management some use-case specific extensions are needed e.g. to manually ingest data into the catalogue through a web frontend.

On this Poster Session we aim to give an overview on specific use-cases of SciCat within DAPHNE, present DAPHNE-contributions to SciCat and show first evaluation results related to SciCat used on university group level.

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MON 16:15-18:15 | BOARD 134 | P1-DATA-15

POSTER SESSION

FIRST STEPS TOWARDS AUTOMATED FAIR DATA COLLECTION AT UNIVERSITY LABS

Presenter: Jonas GRAETZ
Authors: Jonas GRAETZ (1,2), Santanu MAITI (1,2), Christian BÄR (1,2), Wolfgang GRUBER (1,2), Tobias ZECH (1,2), Klaus GÖTZ (1,2), Tobias UNRUH (1,2)

FAIR (Findable, Accessible, Interoperable, Reusable) research data management is an essential building block towards distributed interdisciplinary collaborations and the long-term sustainability of project-driven research. The DAPHNE4NFDI project aims to establish federated data and software catalogs for Photon and Neutron (PaN) experiments with particular focus on integrating German university labs specialized in PaN-based research in close collaboration with the large scale facilities [1]. Making research data FAIR especially requires digitized lab workflows consistently capturing all data, metadata and lab notes that are used for subsequent scientific analyses.

We present initial results and progress in establishing such an integrated workflow combining user-provided lab-notes with rich instrumental metadata in a common catalog at our custom-built VAXSTER SAXS/GISAXS instrument and its sample-environments. The strong resemblances with respective instruments at large scale facilities allow to adapt typical approaches used at beamlines: automated collection of metadata from the instrument control software and integration with detector images into NeXus/HDF5 files, automated application of basic data reduction tools, and use of SciCat [2] to keep systematic records of all machine- and user-provided information.

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[1] https://gepris.dfg.de/gepris/projekt/460248799
[2] https://scicatproject.github.io/

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MON 16:15-18:15 | BOARD 135 | P1-DATA-16

POSTER SESSION

MACHINE LEARNING BASED DATA ANALYSIS IN REFLECTOMETRY (X-RAY AND NEUTRON) AND GRAZING INCIDENCE X-RAY DIFFRACTION

Presenter: Linus PITHAN
Authors: Linus PITHAN, Vladimir STAROSTIN, Alessandro GRECO, Valentin MUNTEANU, Alexander GERLACH, Alexander HINDERHOFER, Frank SCHREIBER

Machine learning (ML) based approaches are a relatively new option to determine physical sample properties from scattering data. After training, ML models can yield results several orders of magnitudes faster than conventional methods. Here we present two of our current research lines in the context of ML applied to scattering data.

Reflectometry is an established technique to extract thin film parameters such as thickness, roughness and scattering length density. However, these physical properties are generally not be extracted directly from reflectivity data, but are instead refined during an iterative fitting process (inverse problem). Once trained, artificial neural networks are very efficient in addressing these problems [1] . We present our ML-based approach to extract parameters of organic thin films on Si.

Grazing incidence wide-angle X-ray scattering (GIWAXS) is used to record reciprocal space. We use ML-based approaches to analyse GIWAXS data and study the complex crystallization process of organic-inorganic perovskites. We adopted the Faster Region-based CNN architecture to the specific needs of scattering data and perform automated phase identification, unit-cell determination and online tracking of the perovskite crystallisation process [2]).

For both techniques we provide python packages (mlreflect and mlgixd, GIXI) for online data analysis on facility infrastructure.

[1] Greco et al, J.Appl.Cryst. 2019 52 1342 & 2022 55 362
[2] Starostin et al, npj Comp.Mat. 2022 8 101

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MON 16:15-18:15 | BOARD 136 | P1-AIFA-01

POSTER SESSION

SURROGATE MODELLING FOR GISAXS RECONSTRUCTION VIA GRADIENT DESCENT

Presenter: Maksim ZHDANOV
Authors: Maksim ZHDANOV (1), Lisa RANDOLPH (2), Marina GANEVA (3), Thomas KLUGE (1), Christian GUTT (2), Nico HOFFMANN (1)

Small-angle X-ray scattering at grazing incidence (GISAXS) is a modern 2D X-ray imaging modality employed in material research to study nanoscale materials. The reconstruction of material properties based on experimentally acquired GISAXS images can be seen as ill-posed inverse imaging problems due to the involved image formation processes in the Fourier domain. Currently, analysis of GISAXS data is a highly time-consuming process as it relies on iterative reconstruction using numerical simulation code such as BornAgain. It motivates the application of machine learning techniques to efficiently solve the reconstruction property and hence reduce the computational cost of the analysis. We propose a novel approach based on a differentiable surrogate model of GISAXS simulation software. The differentiability of the model allows one to calculate gradients with respect to the model parameters. Therefore, it is possible to perform gradient descent to calculate optimal material properties for a given scattering pattern. The proposed framework significantly reduces the time of data analysis while achieving high accuracy of reconstruction.

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MON 16:15-18:15 | BOARD 137 | P1-AIFA-02

POSTER SESSION

COHERENT CORRELATION IMAGING: RESOLVING FLUCTUATING STATES OF MATTER

Presenter: Christopher KLOSE

Authors: Christopher KLOSE (1), Felix BÜTTNER (2,3,4), Wen HU (3), Claudio MAZZOLI (3), Kai LITZIUS (2), Riccardo BATTISTELLI (4), Ivan LEMESH (2), Jason BARTELL (2), Mantao HUANG (2), Christian GÜNTHER (5), Michael SCHNEIDER (1), Andi BARBOUR (3), Stuart WILKINS (3), Geoffrey BEACH (2), Stefan EISEBITT (1,6), Bastian PFAU (1)

Fluctuations are ubiquitous in magnetically and charge ordered systems, spanning orders of magnitude in space and time. Real-space access to fluctuating states is impeded by a dilemma between spatial and temporal resolution. Averaging over an extended period of time (or repetitions) is key for the majority of high-resolution imaging experiments, especially in weak contrast systems. If, by lack of better knowledge, averaging is indiscriminate, it leads to a loss of temporal resolution and to motion-blurred images.

We present coherent correlation imaging (CCI) – a high-resolution, full-field imaging technique that realizes multi-shot, time-resolved imaging of stochastic processes. The key of CCI is the classification of camera frames that correspond to the same physical state by combining a correlation-based similarity metric with powerful classification algorithm developed for genome research.

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MON 16:15-18:15 | BOARD 138 | P1-AIFA-03

POSTER SESSION

GETTING MORE EFFICIENT – THE USE OF BAYESIAN OPTIMIZATION AND GAUSSIAN PROCESSES AT THE BAMline

Presenter: Martin RADTKE
Authors: Martin RADTKE, Ana BUZANICH, Cafer Tufan CAKIR

For more than 20 years, BAM is operating the BAMline at the synchrotron BESSY II in Berlin Adlershof. During this time, the complexity of the setup and the amount of data generated have multiplied. To increase the effectiveness and in preparation for BESSY III, algorithms from the field of machine learning are increasingly used.

In this paper, several examples in the areas of beamline alignment and measurement time optimization based on Bayesian optimization (BO) with Gaussian processes (GP) are presented. BO is a method for finding the global optimum of a function using a probabilistic model represented by a GP. The advantage of this method is that it can handle high-dimensional problems, does not depend on the initial estimate, and also provides uncertainty estimates.

The first example is the automatic alignment of our double multilayer monochromator (DMM).

The second example is the optimization of measurement time in XRF scanning. Here we will show the advantage of the BO GP approach over point-by-point scanning.

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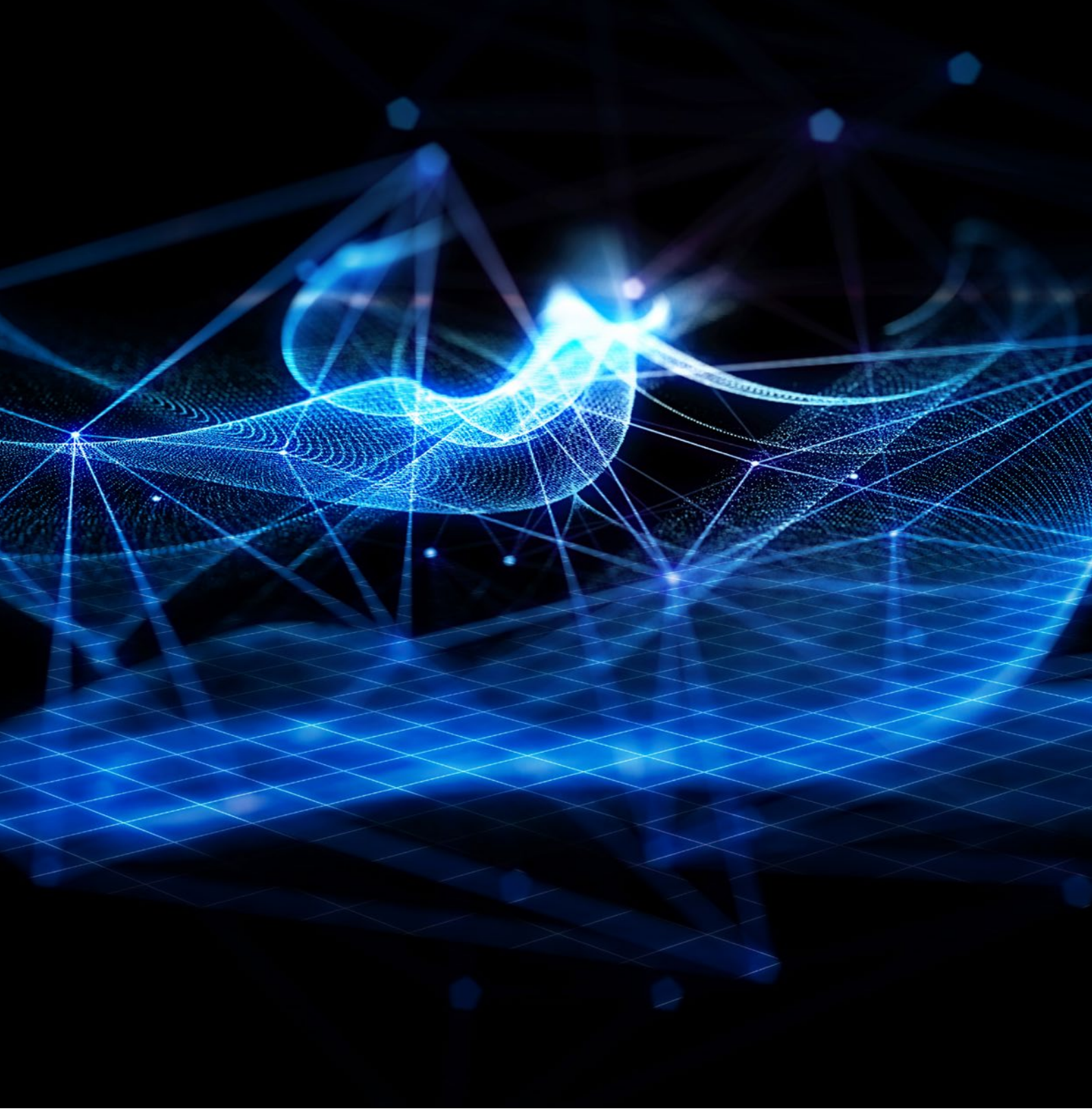

TUESDAY, 6TH SEPTEMBER

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TUESDAY, 6TH SEP.

PROGRAMME

09:00	News from KFS, KFN and KFSI		
09:15	Keynote Talk | HS 1a COVID19: The pandemic Response in Structural Biology – *Andrea Thorn (U Hamburg)*		
09:45	*Keynote Talk | HS 1a* From µm to mm scale – the Application of Ions in Radiobiology and Radiation Medicine – *Judith Reindl (UdBW München)*		
10:15	*Coffee break*		
10:45	MICROSYMPOSIUM | HS 1A Magnetism in 4d and 5d Transition Metal Compounds (65 years Mößbauerspectroscopy)	MICROSYMPOSIUM | HS 1B Multi-scale Protein Dynamics	MICROSYMPOSIUM | HS 2 Industry, Innovation & Transfer
12:15	*Lunch break*		
13:15	KEYNOTE TALK | HS 1A Probing interfacial Structure and Dynamics around Nanoparticles with X-rays and Neutrons – *Mirijam Zobel (RWTH Aachen)*		
13:45	PARALLEL SESSION | HS 1A Methods & Instruments Development 2	PARALLEL SESSION | HS 1B Health, Life & Biology	PARALLEL SESSION | HS 2 Materials Engineering
15:15	*Coffee break*		
15:45	POSTER SESSION 2		
17:45	*Break*		
18:15	*Reception / **Tipi am Kanzleramt***		

Instructions:
Tables of the day are linked to the sessions.
Tables of sessions are linked to the abstracts.

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TUE 9:15-9:45 | HÖRSAAL 1A | INV-05

KEYNOTE TALK

COVID19: THE PANDEMIC RESPONSE IN STRUCTURAL BIOLOGY

Presenter: Andrea THORN
Author: Andrea THORN

During the COVID-19 pandemic, structural biologists rushed to solve the structures encoded by the SARS-CoV-2 genome in order to understand the viral infection cycle and to enable drug design. Over 2000 structures of SARS-CoV-2 proteins were released in a short time span, which immediately were used to understand how the virus hijacks human cells, drug and vaccine design. However, errors often occur in even the most careful structure determination - and may be even more common among these structures. The Coronavirus Structural Task Force [1] has responded to this challenge by rapidly evaluating and reviewing all of these structures. In addition, we provided improved models for key structures online, set up a website (www.insidecorona.net) and data base. We also engaged in outreach activities, writing blog posts for scientists and the public alike, refining structures live on Twitch and offering a 3D printable virus model. We were an ad hoc collaboration of 26 researchers across nine time zones, brought together by the desire to fight the pandemic. Still, we were able to rapidly establish a host of COVID-19 related research, forge friendships and collaborations across national boundaries, spread knowledge about the virus and provide improved models for drug discovery projects.

Now, after more than two years, we have consolidated our collective knowledge about the virus, and can leverage this insight for the question:

What is next?

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[1] https://doi.org/10.1038/s41594-021-00593-7

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TUE 9:45-10:15 | HÖRSAAL 1A | INV-06

KEYNOTE TALK

FROM MICROMETER TO MILIMETER SCALE – THE APPLICATION OF IONS IN RADIOBIOLOGY AND RADIATION MEDICINE

Presenter: Judith REINDL
Author: Judith REINDL

Human cells are constantly exposed to ionizing radiation of different quality, which can cause severe damage in the genome. These damages can lead to cell death or cancer formation. Especially new types of radiotherapy using ions, such as carbon ions or protons, and the planning of manned missions into deep space create the need to understand the effects of particle radiation to eucaryotic cells and organisms. It is well known that particle radiation with a high linear energy transfer (LET) (>10keV/µm) shows an enhanced biological effect compared to low-LET radiation, such as photons. To investigate the basic mechanisms of the radiation damage of ions accelerator based research using ion microbeams, with beam sizes in the order or below 1µm are necessary.

Furthermore, using accelerator based facilities it is possible to investigate new therapy approaches such as proton minibeam radiotherapy (pMBT), which exploits the small angle scattering of particles in tissue to spare the healthy tissue but treat the tumor with conventional dose distribution.

This talk focuses on the techniques and studies in radiobiological and medical research to be performed on accelerators. Main focus lies on the mechanistic studies to explain the enhanced biological effectiveness of particles, explorative studies to perform biological dosimetry on high-LET particle tracks and preclinical studies on pMBT.

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MICROSYMPOSIUM

TUESDAY, 6TH SEPTEMBER

MAGNETISM IN 4D AND 5D TRANSITION METAL COMPOUNDS (65 YEARS MÖßBAUER SPECTROSCOPY)			
Time	**Place**	**Presenter**	**Title**
Tue 10:45-11:15	Hörsaal 1a	Ilya SERGEEV	Nuclear Resonance Scattering on 193Ir Mossbauer transition at P01, PETRA III.
Tue 11:15-11:45	Hörsaal 1a	Hans-Henning KLAUSS	µSR study of Sr2RuO4: superconductivity with broken time reversal symmetry under various perturbations
Tue 11:45-12:00	Hörsaal 1a	Alexandre BERTIN	K2ReCl6: an unconventional Jahn-Teller system?
Tue 12:00-12:15	Hörsaal 1a	Volker SCHÜNEMANN	Magnetic hyperfine interaction and molecular modes in Dy containing single molecule magnets

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TUE 10:45-11:15 | HÖRSAAL 1A | MÖSS-01

MICROSYMPOSIUM

NUCLEAR RESONANCE SCATTERING ON 193Ir MOSSBAUER TRANSITION AT P01, PETRA III.

Presenter: Ilya SERGEEV
Authors: Ilya SERGEEV, Olaf LEUPOLD

The recent interest in understanding the physical properties of systems containing 5d transition metals makes attractive the method of Mössbauer spectroscopy (in energy or time domain) on Ir nuclear transitions. Most Mössbauer spectroscopy studies were performed using the 73 keV nuclear transition on 193Ir. This transition shows an untypical high E2/M1 multipolarity mixing ratio.

In this presentation, an overview of the recently established nuclear resonance scattering of synchrotron radiation on 193Ir (time-domain Mössbauer spectroscopy) will be presented [1]. As compared to conventional Mössbauer spectroscopy, the method does not require the preparation of the radioactive source which is difficult for this transition. The setup which includes the medium-resolution monochromators and the efficient fast detector will be described.

The method was applied to measure magnetic and other hyperfine parameters on several Ir-containing compounds, including elemental Ir, magnetic Ir-Fe alloys, iridium-chlorine bioinorganic materials, and iridate perovskite Sr2IrO4 [1]. For the last compound, we also studied the orientation of the spin alignment versus the applied external magnetic field. Here, the E2 / M1 multipolarity of the transition provides valuable additional information which is not available for pure M1 transition as will be shown in the presentation.

[1] P.Alexeev et al., Sci. Rep., 9, 5097 (2019)

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TUE 11:15-11:45 | HÖRSAAL 1A | MÖSS-03

MICROSYMPOSIUM

µSR STUDY OF Sr2RuO4: SUPERCONDUCTIVITY WITH BROKEN TIME REVERSAL SYMMETRY UNDER VARIOUS PERTURBATIONS

Presenter: Hans-Henning KLAUSS
Authors: Vadim GRINENKO (1,2,3), Shreenanda GHOSH (2), Rajib SARKAR (2), Debarchan DAS (4), Zurab GUGUCHIA (4), Naoki KIKUGAWA (5), Fabian JERZEMBECK (6), Ilya SHIPULIN (3), Andrew MACKENZIE (6,7), Hubertus LUETKENS (4), Bastian ZINKL (8), Manfred SIGRIST (8), Yoshiteru MAENO (9), Rustem KHASANOV (4), Clifford HICKS (10), Hans-Henning KLAUSS (2)

In this talk, I will present the results of our muon spin rotation (µSR) experiments targeted to test various scenarios for multicomponent superconductivity that breaks time reversal symmetry (BTRS) in Sr2RuO4. Our motivation is based on the mean-field theory predictions that depending on the structure of the multicomponent superconducting order parameter, the superconducting (T_c) and T_BTRS split for some perturbations and do not split for others. Our systematic µSR study demonstrates that the transitions split under uniaxial pressure for both <100> and <110> stresses [1]. In contrast, no splitting of the transitions is observed under hydrostatic pressure and in the samples with suppressed T_c by disorder or chemical doping [2]. These results, combined with theoretical analysis, point to a chiral dxz ± idyz superconductivity in Sr2RuO4. However, our recent study shows a very strong sensitivity of BTRS superconductivity to orthorhombic distortions. This observation is consistent with missing specific heat anomaly at T_BTRS indicating finely-tuned superconductivity in Sr2RuO4, in which the gain in condensation energy associated with the onset of time reversal symmetry breaking transition is very small. In this talk, I will also discuss the relationship of our µSR data with ultrasound experiments.

[1] V. Grinenko, et al., Nat. Phys. 17, 748–754 (2021).
[2] V. Grinenko, et al., Nat Commun 12, 3920 (2021).

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TUE 11:45-12:00 | HÖRSAAL 1A | MÖSS-05

MICROSYMPOSIUM

K2ReCl6: AN UNCONVENTIONAL JAHN-TELLER SYSTEM?

Presenter: Alexandre BERTIN
Authors: Alexandre BERTIN (1), Tusharkanti DEY (1), Daniel BRÜNING (1), Dmitry GORKOV (1,2), Kevin JENNI (1), Astin KRAUSE (1), Petra BECKER (3), Ladislav BOHATÝ (3), Daniel KHOMSKII (1), Thomas LORENZ (1), Markus BRADEN (1)

Antifluorite compounds of chemical formula K2MX6 (where M is a 4d/5d transition metal and X=Cl,Br) can exhibit various crystallographic phase transitions, often understood by the softening of rotary phonon modes of the ligand octahedra surrounding the central transition metal. Among this family, K2ReCl6 exhibits on cooling four distinct structural phases and may constitute a playground to investigate the interplay between spin-orbit coupling (SOC) and Jahn-Teller (JT) effect. Indeed, the 5d3 electronic ground state in the weak SOC limit (Russel-Saunders scheme) does not show any orbital degeneracy. On the other hand, in the strong SOC limit (jj-coupling scheme), the j=3/2 ground state is JT active. The question whether one of the crystallographic phase transitions is JT driven will be tackled by presenting a detailed temperature dependent structural study of K2ReCl6 and of its non magnetic counterpart K2SnCl6 by means of powder and single crystal X-ray diffraction. With high resolution single crystal neutron diffraction experiments and considering the monoclinic symmetry of the low temperature phase the magnetic structure was solved. Frustration is only partially lifted by the structural distortions and the magnetic order causes further symmetry reduction. Finally, the strong magneto-elastic effect observed by thermal expansion measurements will be discussed with the key ingredients (domain re-orientation and weak ferromagnetism) provided by these structural studies.

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TUE 12:00-12:15 | HÖRSAAL 1A | MÖSS-06

MICROSYMPOSIUM

MAGNETIC HYPERFINE INTERACTION AND MOLECULAR MODES IN Dy CONTAINING SINGLE MOLECULE MAGNETS

Presenter: Volker SCHÜNEMANN
Author: Volker SCHÜNEMANN

With the contemporary evolution of spintronics, molecular electronics and quantum computing, single-molecule magnets (SMMs) arouse an immense amount of interest. Lanthanide-based compounds and especially Dy-containing ones are among the best high-performance SMMs, characterized by long relaxation times of the magnetization reversal and high blocking temperatures. As a novel method for the characterization and understanding of these molecular materials, synchrotron-based 161Dy Nuclear Forward Scattering (NFS), delivers complementary information to conventionally applied magnetization measurement techniques [1]. In this contribution we will also present investigations of the vibrational properties of Dy containing SMMs obtained via 161Dy Nuclear Inelastic Scattering (NIS) [2]. NIS allows to determine the partial phonon density of states (pDOS) which includes all vibrational modes involving displacement of the Dy. Simulations using density functional theory (DFT) have made it possible to assign observed bands to specific molecular modes.

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[1] L. Scherthan, S. F. M. Schmidt, H. Auerbach, T. Hochdörffer, J. A. Wolny, W. Bi, J. Zhao, M. Y. Hu, T. Toellner, E. E. Alp, D. E. Brown, C. E. Anson, A. K. Powell, V. Schünemann, Angew. Chemie Int. Ed. 58, 3444 (2019)
[2] L. Scherthan, R.F. Pfleger, H. Auerbach, T. Hochdörffer, J. A. Wolny, W. Bi, J. Zhao, M. Y. Hu, E. E. Alp, C. E. Anson, R. Diller, A. K. Powell, V. Schünemann, Angew. Chem. Int. Ed., 59, 8818 (2020)

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TU Kaiserslautern, Germany

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MICROSYMPOSIUM

TUESDAY, 6TH SEPTEMBER

MULTI-SCALE PROTEIN DYNAMICS – INSIGHTS FROM NEUTRONS, X-RAYS AND SIMULATION			
Time	**Place**	**Presenter**	**Title**
Tue 10:45-11:15	Hörsaal 1b	Martin WEIK	Dynamics of amyloid fibers and their hydration water as studied by neutron scattering and molecular dynamics simulations
Tue 11:15-11:45	Hörsaal 1b	Anita GIRELLI	Diffusion of antibodies in solution: from individual proteins to phase separation domains
Tue 11:45-12:00	Hörsaal 1b	David VON STETTEN	Serial time-resolved crystallography at the T-REXX endstation at PETRA III
Tue 12:00- 12:15	Hörsaal 1b		Discussion

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TUE 10:45-11:15 | HÖRSAAL 1B | PROT-01

MICROSYMPOSIUM

DYNAMICS OF AMYLOID FIBERS AND THEIR HYDRATION WATER AS STUDIED BY NEUTRON SCATTERING AND MOLECULAR DYNAMICS SIMULATIONS

Presenter: Martin WEIK

Authors: Kevin POUNOT (1,2), Giorgio SCHIRO (3), Yann FICHOU (4), Martine MOULIN (2), Michaela ZAMPONI (5), Michael HAERTLEIN (2), Tilo SEYDEL (2), Annette LANGKILDE (6), Douglas J. TOBIAS (7), Frank SCHREIBER (1), Martin WEIK (3)

Protein amyloid fiber formation is the pathological hallmark in various neurodegenerative diseases such as Parkinson's and Alzheimer's. The physico-chemical origin of protein fibrilation, as well as the role that hydration-water might play remain elusive. We combine elastic and quasi-elastic neutron spectroscopy and molecular dynamics simulations on the intrinsically disordered proteins α-synuclein (involved in Parkinson disease) and tau (involved in Alzheimer disease) to investigate both structural and dynamical properties of the protein-hydration water system. One of our findings is an increased water translational diffusion on fiber surfaces, suggesting that hydration-water entropy might be one of the driving forces for amyloid fiber formation.

Affillation

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TUE 11:15-11:45 | HÖRSAAL 1B | PROT-03

MICROSYMPOSIUM

DIFFUSION OF ANTIBODIES IN SOLUTION: FROM INDIVIDUAL PROTEINS TO PHASE SEPARATION DOMAINS

Presenter: Anita GIRELLI
Author: Anita GIRELLI

We investigated the diffusion of a model system for liquid-liquid phase separation (LLPS), which is a biological mechanism for the formation of intracellular organelles. The solution of ɣ-globulin and PEG spontaneously separates and reaches a gel state due to the high concentration of the more concentrated of the two phases.

The hierarchy of motions requires probing the sample from nanometers to micrometers and time scales from ps to hundreds of seconds. This is achieved by a combination of light, neutron, and X-ray scattering. At LLPS domains length scale X-ray photon correlation spectroscopy (XPCS) reveals correlation functions that show typical characteristics of ballistic motion as seen for colloidal gels. The experimental results are compared with simulated data based on the Cahn-Hilliard equation.

Qualitative comparability is obtained by adding a strong dependence of the protein mobility on protein concentration. The validity of this assumption is confirmed by probing the diffusion on the protein length scale and below with neutron quasi-elastic scattering and XPCS [1,2].

The combination of Neutron Spin Echo and XPCS allows to access the diffusion at protein length scale over 10 orders of magnitude.

We acknowledge contributions by the groups of Frank Schreiber, Christian Gutt, Tilo Seydel and Foivos Perakis, the allocation of beamtime from DESY, ILL, XFEL, FRM II, and funding from BMBF.

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[1] Girelli et al., Mol. Pharm. 18 (11), 2021
[2] Reiser et al., Nat. Comm., subm.

Affillation
University of Tübingen, Germany

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TUE 11:45-12:00 | HÖRSAAL 1B | PROT-05

MICROSYMPOSIUM

SERIAL TIME-RESOLVED CRYSTALLOGRAPHY AT THE T-REXX ENDSTATION AT PETRA III

Presenter: David VON STETTEN

Authors: David VON STETTEN (1), Michael AGTHE (1), Gleb BOURENKOV (1), Briony A. YORKE (2), Godfrey S. BEDDARD (3), Marina NIKOLOVA (1), Ivars KARPICS (4), Thomas GEHRMANN (1), Jochen MEYER (1), Uwe RISTAU (1), Stefan FIEDLER (1), Pedram MEHRABI (5), Eike-Christian SCHULZ (5), Friedjof TELLKAMP (6), Nils HUSE (5), Arwen R. PEARSON (5), Thomas R. SCHNEIDER (1)

The T-REXX endstation on the EMBL beamline P14 at PETRA III is in user operation since 2018 and is dedicated to time-resolved serial synchrotron crystallography. The collimated P14 X-ray beam is refocussed for T-REXX with a compound refractive lens (CRL) transfocator to provide a 10x10 µm2 beam with a flux of about 2x1012 photons/s at 12.7 keV. The space around the sample position is designed to be open and flexible to accommodate diverse crystal presentation devices and is equipped with a beam shaping device providing an on-axis viewer, beam shaping apertures, a motorized beamstop, and a scintillator for visualising the X-ray beam. For standard operation, an Eiger 4M detector is used, and other area detector systems have been evaluated.

For pump/probe experiments, a laser system (355 nm) for light-based triggering and a droplet injector for mixing with ligands are available. First experiments have yielded promising results using microfluidic flow cells as well as patterned silicon chips with temperature and humidity control. The Eiger 4M offers a time-resolution of 1.35 ms, and the typical data collection time for one time-point is on the order of one hour. In the future, the Hadamard technique will be employed to reach sub-millisecond timescales by detector gating or X-ray beam modulation.

Access to T-REXX is provided via the EMBL user program (smis.embl-hamburg.de). Funding from the BMBF via the Verbundforschung-Programm (05K16GU1, 05K19GU1) is gratefully acknowledged.

Affillation

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MICROSYMPOSIUM

TUESDAY, 6TH SEPTEMBER

INDUSTRY, INNOVATION AND TRANSFER			
Time	**Place**	**Presenter**	**Title**
Tue 10:45-11:00	Hörsaal 2	Thomas SHEPPARD	New Horizons for Catalyst Characterisation using Hard X-ray Tomography
Tue 11:00-11:15	Hörsaal 2	Arnold MÜLLER	The Ionplus AG – An example of commercializing new innovations in ion beam technologies
Tue 11:15-11:30	Hörsaal 2	Sophie BOUAT	What do large-scale facilities bring to industry?
Tue 11:30-11:45	Hörsaal 2	Simon JACQUES	Lubricating Industrial Science
Tue 11:45-12:00	Hörsaal 2	Alberto DEGIOVANNI	High frequency linacs for proton therapy: the journey from conception to industrialization
Tue 12:00-12:15	Hörsaal 2	Ralph GILLES	Neutrons are a perfect tool to study in-situ and/or operando industrially relevant topics for innovation and transfer, e.g. electromobility and gas turbines

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TUE 10:45-11:00 | HÖRSAAL 2 | INDU-01

MICROSYMPOSIUM

NEW HORIZONS FOR CATALYST CHARACTERISATION USING HARD X-RAY TOMOGRAPHY

Presenter: Thomas SHEPPARD
Authors: Sebastian WEBER, Srashtasrita DAS, Shweta SHARMA, Thomas SHEPPARD

Recent developments in synchrotron hard X-ray tomography have opened a flexible toolbox for characterisation of catalysts and functional materials. Here we highlight applications in two focal areas:

(i) hard X-ray ptychographic tomography (PXCT) for quantitative 3D imaging of catalysts at the nanoscale;

(ii) *operando* hard X-ray spectrotomography for chemical imaging of catalysts at work.

The first case outlines a strategy for studying pore networks in solid catalysts, including hierarchically-structured materials with at least two distinct pore size distributions. The role of PXCT is compared with complementary X-ray and electron imaging methods to visualise pore networks in 3D space from micro- to nanoscale. Further applications include the study of carbon deposition (coking) and other common deactivation mechanisms in solid catalysts, along with the potential for quantitative structural analysis at <50 nm 3D spatial resolution. The second case focuses on *operando* tomography combined with XANES to study technical catalyst materials under realistic reaction conditions. This includes observation of 3D structural and chemical gradients within washcoated Cu/zeolite and Pt/alumina monoliths for emissions control reactions such as NOx reduction and NH3 oxidation. By focusing on two possible examples which may assist our understanding of catalysts from model to technical scale, we aim to improve awareness of hard X-ray tomography in the catalysis community and chemical industry.

Affillation
Karlsruhe Institute of Technology, Germany

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TUE 11:00-11:15 | HÖRSAAL 2 | INDU-02

MICROSYMPOSIUM

THE IONPLUS AG – AN EXAMPLE OF COMMERCIALIZING NEW INNOVATIONS IN ION BEAM TECHNOLOGIES

Presenter: Arnold MÜLLER

Authors: Arnold MÜLLER (1), Hans-Arno SYNAL (1), Joël BOURQUIN (2), Lukas WACKER (1), Martin SUTER (1), Andreas HERRMANN (2), Rudolf PFENNINGER (1)

The laboratory of ion beam physics (LIP) at ETH Zurich has a long tradition in developing new instrumentations in the field of ion beam physics. Especially in accelerator mass spectrometry (AMS) major breakthroughs were achieved in terms of measurement stability, efficiency and costs. Prominent examples of developments are the most compact radiocarbon AMS system MICADAS (Mini Carbon Dating System) or the fully automized graphitization equipment (AGE). In order to make these innovations available to the scientific community, seven members of LIP decided in 2013 to found the Ionplus AG as a spin-off company. Since then, the Ionplus AG was steadily growing with nowadays more than 25 full time employees and a production site located in Dietikon ZH with more than 1200 m^2 manufacturing space. In this contribution an overview will be given, how the Ionplus AG successfully commercialized new innovations in ion beam technologies.

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TUE 11:15-11:30 | HÖRSAAL 2 | INDU-03

MICROSYMPOSIUM

WHAT DO LARGE-SCALE FACILITIES BRING TO INDUSTRY?

Presenter: Sophie BOUAT

Authors: Sophie BOUAT (1), Eric MOSSANG (2), Paul TAFFOREAU (3), Elodie BOLLER (3), Ludovic PINIER (4), Xavier SEBASTIAN (4), Adrian LOSKO (5), Rudolf SCHÜTZ (5), Michael SCHULZ (5), Zsolt REVAY (5), Zeljko ILIC (5,6,8), Eric MAUERHOFER (7), Thomas BRÜCKEL (7,8), Ralph GILLES (5)

Industry is often facing scientific questions to improve its products or to bring solutions to unresolved topics. Most of the time, conventional techniques provide satisfactory answers, but some issues can still remain unaddressed. How to follow material evolution history during product lifetime in energy harvesting devices? How to detect clog formation in sub-marine pipelines under deep seas? Conventional characterization methods only give access to a part of the solution: only a few numbers of devices can be observed with classical methods; exploring deeply inside a sub-marine pipeline is out of reach of all commonly used techniques in oil and gas industry. Large-scale facilities can bring answers thanks to their powerful beams both in terms of intensity and flux and their ability to accommodate large samples. A synchrotron such as the ESRF can observe hundreds of devices at a time, thanks to the micro-tomography beamline dedicated to industry, thus following material evolution during product lifetime in one go. The MLZ-FRM II neutron reactor provides a high-energy, high-flux neutron beam that can get through the thick pipeline walls, showing that detecting clog inside a sub-marine pipeline in deep seas is feasible.

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TUE 11:30-11:45 | HÖRSAAL 2 | INDU-04

MICROSYMPOSIUM

LUBRICATING INDUSTRIAL SCIENCE

Presenter: Simon JACQUES
Authors: Simon JACQUES, Stephen PRICE

Finden Ltd provides state-of-the-art measurement and analysis services to industrial clients across sectors. In this presentation, an industrial case study will be presented where advanced methods are used to study deposits on engine components.

Coking of engine components reduces efficiency and lifetime of engines (automotive, marine, aviation) through increased wear. Lubricants not only act to reduce friction of such components, key for wear and fuel economy but they also play a key role in engine thermal management and cleanliness. Where and how deposit forms varies based on the engine, its application, but can be limited by additives in the lubricating oil.

The engine component temperature and lubricant residence time unsurprisingly correlate to coke formation. Coked components have poorer thermal conductivity and act to insulate the engine components, this can lead to localised increases in temperature, which in extreme cases can lead to physical failure. Coke material, if shed, can travel around the engine, blocking filters and narrow regions away from their point of formation.

Both neutron and X-ray conventional and chemical imaging are used to locate, identify and understand the nature of coking deposits on engine components, allowing for the better design of lubricants to extend engine lifetime and improve fuel efficiency.

Affillation
Finden, United Kingdom

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TUE 11:45-12:00 | HÖRSAAL 2 | INDU-05

MICROSYMPOSIUM

HIGH FREQUENCY LINACS FOR PROTON THERAPY: THE JOURNEY FROM CONCEPTION TO INDUSTRIALIZATION

Presenter: Alberto DEGIOVANNI
Author: Alberto DEGIOVANNI

The company AVO (Advanced Oncotherapy), with its subsidiary A.D.A.M. (Application of Detectors and Accelerators to Medicine), a CERN spin-off, has been working to the realization and construction of the first high frequency linear accelerator for proton therapy applications: LIGHT (Linac for Image Guided Hadron Therapy). The modular and compact solution is based on innovation and technologies used in the world of particle accelerators for research and have been transferred and adapted to the needs of therapy with charged ions.

The Design, Development and Industrialization process is presented, starting with the conception, the first prototyping and the steps towards the industrial certification.

Affillation
AVO-ADAM, Switzerland

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TUE 12:00-12:15 | HÖRSAAL 2 | INDU-06

MICROSYMPOSIUM

NEUTRONS ARE A PERFECT TOOL TO STUDY IN-SITU AND/OR OPERANDO INDUSTRIALLY RELEVANT TOPICS FOR INNOVATION AND TRANSFER, E.G. ELECTROMOBILITY AND GAS TURBINES

Presenter: Ralph GILLES
Author: Ralph GILLES

Neutrons are a unique tool with their properties as high depth of penetration in materials, weak interaction with matter, high sensitivity to distinguish adjacent elements of the periodic table (e.g. important in battery cathode materials consisting of element combinations of Mn, Ni, Co or Fe) and high sensitivity of light ones elements (Li, H, O, N) to characterize industrial related problems on different length scales.

For example, the electrochemical processes in batteries can be tracked during operation or the in-situ filling of electrolytes in cells can be visualized. Fully functional batteries or individual components can be measured from the atomic level up to the cm range using various dedicated neutron methods.

In the field of gas turbines, which work under strong forces and high temperatures, so-called high-temperature alloys (superalloys) are characterized with neutrons. Real working conditions are realized with sophisticated test machines. The detailed description of the microstructure (including precipitation kinetics and phase transformations) of these alloys leads to an optimization of alloy development on an industrial scale.

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[1] R. Gilles, How neutrons facilitate research into gas turbines and batteries from development to engineering applications, Journal of Surface Investigations: X-Ray, Synchrotron and Neutron Techniques, (2020), 14, Suppl. 1, S69.

Affillation
TU München, Germany

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TUE 13:15-13:45 | HÖRSAAL 1A | INV-07

KEYNOTE TALK

PROBING INTERFACIAL STRUCTURE AND DYNAMICS AROUND NANOPARTICLES WITH X-RAYS AND NEUTRONS

Presenter: Mirijam ZOBEL
Author: Mirijam ZOBEL

Nanostructured solid-liquid and solid-gas interfaces play a key role not only during nanoparticle formation, but in a plethora of surroundings spanning from geochemical processes to heterogenous catalysis. Despite much progress in fine-tuning nanoparticle properties themselves, our understanding of the very interface of nanoparticles interacting with their surroundings is still limited.

By joining insights form pair distribution function (PDF) and quasielastic neutron scattering (QENS), we aim to achieve an advanced understanding of the structure and dynamics of nanoscale interfaces. In contrast to classical crystallographic approaches, the PDF is utmost suited to characterize short-range order, allowing us to investigate solvent structures around colloidal, 3 – 15 nm sized metal oxide nanoparticles. We can access solvation shells and their extension into the bulk liquid via double-difference PDFs (dd-PDF), when subtracting contributions from bulk solvents and nanoparticles from the dispersion signal. Hereby, we can tackle solvation structures ranging from non-polar and polar organic ones to water, and down to nanoparticle concentrations of merely 0.3 wt%. This dd-PDF approach can further be readily transferred to gain detailed insight into nanoparticle-support interactions in heterogeneous catalysis. Since structural reorganization at interfaces often affects dynamical properties concurrently, we tackle the interfacial dynamics of water at nanoparticle surfaces with QENS.

Affillation
RWTH Aachen, Germany

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PARALLEL SESSION
TUESDAY, 6TH SEPTEMBER

METHODS AND INSTRUMENTS DEVELOPMENT 2			
Time	**Place**	**Presenter**	**Title**
Tue 13:45-14:00	Hörsaal 1a	Thomas GUTBERLET	The HBS Project for a Next Generation Accelerator Based Neutron Source
Tue 14:00-14:15	Hörsaal 1a	Robert NEAGU	Time and Spatial Resolved Neutron Depth Profiling with the N4DP Instrument
Tue 14:15-14:30	Hörsaal 1a	Sakshath SADASHIVAIAH	Time-resolved studies of photoexcited spin and phonon dynamics using optical pump - nuclear resonant scattering probe experiments
Tue 14:30-14:45	Hörsaal 1a	Rajendra Prasad GIRI	Time-resolved measurements from liquid-vapor interfaces using synchrotron-based optical pump - X-ray probe technique
Tue 14:45-15:00	Hörsaal 1a	Justine SCHLAPPA	Time-resolved Resonant Inelastic X-ray Scattering at SCS instrument, European XFEL – design and commissioning of the Heisenberg RIXS spectrometer
Tue 15:00-15:15	Hörsaal 1a	Brian Richard PAUW	X-ray Scattering for Nanostructure Quantification, and the Quest for the Perfect Experiment

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TUE 13:45-14:00 | HÖRSAAL 1A | MET2-01

PARALLEL SESSION

THE HBS PROJECT FOR A NEXT GENERATION ACCELERATOR BASED NEUTRON SOURCE

Presenter: Thomas GUTBERLET

Authors: Thomas GUTBERLET (1), Ulrich RÜCKER (1), Eric MAUERHOFER (1), Paul ZAKALEK (1), Johannes BAGGEMANN (1), Jingjing LI (1), Alexander SCHWAB (1), Qi DING (1), Zhanwen MA (1), Sebastian EISENHUT (2), Jörg VOIGT (1), Klaus LIEUTENANT (1), Andreas LEHRACH (3), Olaf FELDEN (3), Ralf GEBEL (3), Romuald HANSLIK (4), Yannick BESSLER (4), Oliver MEUSEL (5), Holger PODLECH (5), Winfried BARTH (6), Thomas BRÜCKEL (1)

High current accelerator driven neutron sources (HiCANS) with high brilliance neutron provision present an attractive alternative to classical neutron sources of fission reactors and spallation sources to provide scientist with neutrons to probe and analyze the structure and dynamics of matter. The Jülich Centre for Neutron Science (JCNS) is leading a project to develop, design and demonstrate such an accelerator driven high-brilliance neutron sources (HBS) as an efficient and cost-effective alternative to reactor and spallation sources as next generation of neutron sources. Basic features of HBS are a high current proton accelerator, a compact neutron production and moderator unit, an optimized neutron transport system to provide thermal and cold neutrons with high brilliance and a full suite of high performing epithermal, thermal and cold neutron instruments.

The project aims at construction of a scalable neutron source for a user facility with open access and service for the various and changing demands. Embedded within an international collaboration with partners from Germany, Europe and Japan the Jülich HBS project offers best flexible solutions to scientific and industrial users. The overall conceptual design of HBS was published in a report recently. The current status of the project, progress and next steps regarding accelerator, target, moderators and beam delivery development, milestones and the vision for the future neutron landscape will be presented.

Affillation

1: Forschungszentrum Jülich GmbH, JCNS, Germany; 2: Technische Universität Dresden, Germany; 3: Forschungszentrum Jülich GmbH, IKP-4, Germany; 4: Forschungszentrum Jülich GmbH, ZEA-1, Germany; 5: Goethe Universität Frankfurt, Helmholtz Research Academy Hesse for FAIR (HFHF), Germany; 6: GSI Darmstadt, HI Mainz/JGU Mainz, Germany

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TUE 14:00-14:15 | HÖRSAAL 1A | MET2-02

PARALLEL SESSION

TIME AND SPATIAL RESOLVED NEUTRON DEPTH PROFILING WITH THE N4DP INSTRUMENT

Presenter: Robert NEAGU

Authors: Robert NEAGU (1), Markus TRUNK (2), Lukas WERNER (1), Roman GERNHÄUSER (1), Ralph GILLES (2), Zsolt REVAY (2), Bastian MÄRKISCH (1)

Neutron Depth Profiling is a non-destructive, isotope-specific, high-resolution nuclear analytical technique, which is often used to probe concentration profiles of lithium, boron, nitrogen, helium and several other light elements in different host materials. The N4DP instrument is located at the Prompt Gamma Activation Analysis beam line of Heinz Maier-Leibnitz Zentrum , which provides a cold neutron flux up to 5×10^{10} $s^{-1}cm^{-2}$. When a neutron is captured by a specific nuclide, charged particles with well-defined energies are emitted. The energy loss of the charged particles traveling through the host material is related to the depth of origin at a resolution level up to tens of nanometers.

We applied NDP to study the lithium-ion concentration gradient in energy storage systems, e.g. Li-ion batteries. Here, NDP reveals the evolution of immobilized lithium, which is one of the main causes of battery lifetime limitation. Furthermore, the status of the ongoing development towards 4D profiling is presented, where not only the concentration gradient, but also the lateral position of probes as well as its time evolution will be measured. For this, a highly segmented Si-based detector with 32×266 stripes, including integrated electronics, were tested. Using a camera-obscura geometry setup, we aim for lateral resolutions down to 100 µm × 100 µm and highest time resolutions using a newly developed elliptical focussing neutron guide. This project is supported by the BMBF, Contract No. 05K16WO1, 05K19WO8.

Affillation

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TUE 14:15-14:30 | HÖRSAAL 1A | MET2-03

PARALLEL SESSION

TIME-RESOLVED STUDIES OF PHOTOEXCITED SPIN AND PHONON DYNAMICS USING OPTICAL PUMP – NUCLEAR RESONANT SCATTERING PROBE EXPERIMENTS

Presenter: Sakshath SADASHIVAIAH

Authors: Sakshath SADASHIVAIAH (1,2), Ilya SERGUEEV (3), Benedikt EGGERT (4), Olaf LEUPOLD (3), Tim HOCHDÖRFFER (5), Christina MÜLLER (5), Andreas OMLOR (5), Joachim LANDERS (4), Soma SALAMON (4), Richard A BRAND (4), Katharina OLLEFS (4), Hans-Christian WILLE (3), Juliusz Adam WOLNY (5), Heiko WENDE (4), Ralf RÖHLSBERGER (1,2,3,6)

Simultaneous access to spin and lattice dynamics is vital to solve fundamental questions of phase transitions in materials with strong spin-phonon coupling. Nuclear resonance scattering (NRS), which is not limited by optical selection rules, is an ideal candidate that provides full access to spin dynamics and the instantaneous phonon density of states (pDOS) of Mössbauer-active nuclei [1,2]. We developed an optical laser pump – NRS probe experimental setup at the beamline P01, PETRA III, DESY, Hamburg. By investigating the time-resolved dynamics immediately after laser excitation, we identified the exact phonon modes that assist the co-operative propagation of laser induced spin transition in a spin-crossover complex [2]. In 3 micrometer thick Fe foils excited by 250 fs laser pulses, we obtained the time-evolution of thermodynamic parameters such as the vibrational entropy and the mean force constant by evaluation of the time dependent pDOS. The time resolution is limited to 100 ps due to the pulse width of synchrotron radiation at PETRA III. In FeRh thin films excited by the ultrashort laser pulses, we observe a slow relaxation of the spin coherence over 10 ns although the Lamb-Mössbauer factor (and temperature) indicates that the transition from antiferromagnetic (ground) to the ferromagnetic (excited) state occurs on a timescale of 300 ps.

[1] S. Sakshath et al, Hyperfine Interact. 238, 1 (2017).
[2] S. Sadashivaiah et al, J. Phys. Chem. Lett. 12, 3240 (2021).

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TUE 14:30-14:45 | HÖRSAAL 1A | MET2-04

PARALLEL SESSION

TIME-RESOLVED MEASUREMENTS FROM LIQUID-VAPOR INTERFACES USING SYNCHROTRON-BASED OPTICAL PUMP – X-RAY PROBE TECHNIQUE

Presenter: Rajendra Prasad GIRI
Authors: Rajendra Prasad GIRI (1), Svenja HÖVELMANN (1,2), Lukas PETERSDORF (1), Jonas WARIAS (1), Andrea SARTORI (1), Matthias GREVE (1), Florian BERTRAM (2), Olaf MAGNUSSEN (1,3), Bridget MURPHY (1,3)

Optical pulses have been routinely used in the last two decades to study the structural and dynamic changes in solids [1]. Currently, there is a growing interest on investigating those phenomena in liquids, such as liquid metals, aqueous solutions and room temperature ionic liquids, close to their surfaces and interfaces.

Here, we investigate the thermally induced capillary wave dynamics at liquid mercury-vapor and water-vapor interfaces at Liquid Interfaces Scattering Apparatus (LISA) at P08 beamline [2], PETRA III (DESY) in Hamburg. Optically induced electron solvation dynamics at water and water-based salt solutions-vapor interfaces has also been investigated. First measurements from a crystalline Bi (111) sample have confirmed a time resolution of 85 ± 2 ps from the setup. Capillary wave dynamics at water-vapor and mercury-vapor interfaces were investigated with IR (1030 nm) laser excitation by following the electron density and interface roughness using X-ray reflectivity (XRR) and time response (TR) pump-probe studies. In addition, UV (258 nm) laser excitation at the vapor interface of halide-based salt solutions indicates interesting dynamics close the surface. Our recent developments at the diffractometer to cover the time range between sub ns and s will also be discussed.

[1] P. Reckenthaeler et al., Phys. Rev. Lett. 102, 213001 (2009)
[5] B. M. Murphy et al., J. Synchrotron Rad. 21, 45 (2014)

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TUE 14:45-15:00 | HÖRSAAL 1A | MET2-05

PARALLEL SESSION

TIME-RESOLVED RESONANT INELASTIC X-RAY SCATTERING AT SCS INSTRUMENT, EUROPEAN XFEL – DESIGN AND COMMISSIONING OF THE HEISENBERG RIXS SPECTROMETER

Presenter: Justine SCHLAPPA

Authors: Justine SCHLAPPA (1), Benjamin VAN KUIKEN (1), Zhong YIN (1), Sergii PARCHENKO (1), Martin TEICHMANN (1), Natalia GERASIMOVA (1), Piter MIEDEMA (1), Giuseppe MERCURIO (1), Robert CARLEY (1), Carsten BROERS (1), Jan Torben DELITZ (1), Luigi ADRIANO (1), Manuel IZQUIERDO (1), Serguei MOLODTSOV (1), Andreas SCHERZ (1), Yingying PENG (2), Giacomo C. GHIRINGHELLI (2), Stefan NEPPL (3,4), Friedmar SENF (3,4), Frank SIEWERT (3), Christian WENIGER (3), Annette PIETZSCH (3), Alexander FOEHLISCH (3,4), Simo J. HUOTARI (5), Torben REUSS (6), Simone TECHERT (6), Tim LAARMANN (6)

The User Consortium Heisenberg RIXS (hRIXS) spectrometer was built in order to enable time-resolved resonant inelastic X-ray scattering (tr-RIXS) studies at the soft X-ray SCS instrument, European XFEL. The motivation was providing instrumentation for dynamic inelastic X-ray scattering studies for the two user communities, one with focus on complex and quantum materials, e.g. high-temperature superconductors and the other one with focus on chemical systems, e.g. photoactive catalysts. The design goal was on one hand a high energy resolution, potentially allowing the exploration of the Heisenberg limit for tr-RIXS studies and on the other hand a possibly effortless operation.

The hRIXS spectrometer was installed in 2020/2021 and commissioned in May 2021. Very recently, first tr-RIXS experiments took place, in close collaboration with the user communities. The results look very promising and indicate that hRIXS, in combination with the unique features of the European XFEL and the SCS beamline [1], provides currently the best performance for soft X-ray RIXS studies at a FEL.

In the presentation I will explain the design of the hRIXS spectrometer and give an overview of the available parameters. Further, I will show some of the commissioning results and discuss the currently obtained performance. I will conclude with an outlook for tr-RIXS studies.

[1] Tschentscher, T. et al., Photon beam transport and scientific instruments at the European XFEL, Appl. Sci. 7, 592 (2017).

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1: European XFEL, Germany; 2: Politecnico di Milano, Italy; 3: HZB, Germany; 4: University of Potsdam, Germany; 5: University of Helsinki, Finland; 6: DESY, Germany

TUE 15:00-15:15 | HÖRSAAL 1A | MET2-06

PARALLEL SESSION

X-RAY SCATTERING FOR NANOSTRUCTURE QUANTIFICATION, AND THE QUEST FOR THE PERFECT EXPERIMENT

Presenter: Brian Richard PAUW
Authors: Brian Richard PAUW, Glen SMALES

Measuring an X-ray scattering pattern is relatively easy, but measuring a steady stream of high-quality, useful patterns requires significant effort and good laboratory organization.

Such laboratory organization can help address the reproducibility crisis in science, and easily multiply the scientific output of a laboratory, while greatly elevating the quality of the measurements. We have demonstrated this for small- and wide-angle X-ray scattering in the MOUSE project (Methodology Optimization for Ultrafine Structure Exploration).

With the MOUSE, we have combined a comprehensive and highly automated laboratory workflow with a heavily modified X-ray scattering instrument. This combination allows us to collect fully traceable scattering data, within a well-documented, FAIR-compliant data flow (akin to what is found at the more automated synchrotron beamlines). With two full-time researchers, our lab collects and interprets thousands of datasets, on hundreds of samples, for dozens of projects per year, supporting many users along the entire process from sample selection and preparation, to the analysis of the resulting data.

This talk will briefly introduce the foundations of X-ray scattering, present the MOUSE project, and will highlight the proven utility of the methodology for materials science. Upgrades to the methodology will also be discussed, as well as possible avenues for transferring this holistic methodology to other instruments.

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PARALLEL SESSION
TUESDAY, 6TH SEPTEMBER

HEALTH, LIFE AND BIOLOGY			
Time	**Place**	**Presenter**	**Title**
Tue 13:45-14:00	Hörsaal 1b	Niccolò PERUZZI	Bimodal X-ray and neutron µCT provides new insights on the corrosion of Mg-based biodegradable implants in bone
Tue 14:00-14:15	Hörsaal 1b	Nicole MATEJKA	Migration behavior of U87 glioblastoma cells after irradiation with varying LET
Tue 14:15-14:30	Hörsaal 1b	Felix ROOSEN-RUNGE	Towards a comprehensive picture of temperature-responsive elastin-like peptides
Tue 14:30-14:45	Hörsaal 1b	Svenja C. HÖVELMANN	Influence of saccharides on photo-induced structural changes in lipid membranes studied with X-ray diffraction
Tue 14:45-15:00	Hörsaal 1b	Heinrich HAAS	Investigation of Molecular Organization Inside RNA Nanomedicines by Small Angle Scattering
Tue 15:00–15:15	Hörsaal 1b	Viviane KREMLING	Small Compound Crystal Screening of SARS-CoV-2 Methyltransferases

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TUE 13:45-14:00 | HÖRSAAL 1B | LIFE-01

PARALLEL SESSION

BIMODAL X-RAY AND NEUTRON µCT PROVIDES NEW INSIGHTS ON THE CORROSION OF Mg-BASED BIODEGRADABLE IMPLANTS IN BONE

Presenter: Niccolò PERUZZI

Authors: Niccolò PERUZZI (1), Silvia GALLI (2), Heike HELMHOLZ (3), Alessandro TENGATTINI (4,5), Florian WIELAND (3), Regine WILLUMEIT-RÖMER (3), Robin WORACEK (6), Ann WENNERBERG (7), Martin BECH (1)

Magnesium (Mg) is an attractive resorbable material for orthopedic and dental applications, but needs to be alloyed with other metals to tune its corrosion rate and its mechanical properties. Substantial knowledge is still lacking on how corrosion really occurs, which hinders tailoring the corrosion rate in a controlled fashion.

Recently, we have explored combined X-ray and neutron micro-computed tomography (µCT) for the study of Mg-implants alloyed with gadolinium.[1] We have now extended our analysis to other types of Mg-based alloys as well (paper in preparation).

Mini-screws (2 mm in size) of 3 different Mg-based alloys were implanted in the legs of rabbits for 9 months. After euthanasia, small blocks of bone centered around the implants were extracted and critical point dried. The samples were scanned with bimodal µCT at the NeXT-Grenoble beamline of ILL, with effective voxel size around 7 µm. After digital volume registration, segmentation was performed by applying clustering methods to the bivariate histogram.

The multimodal analysis revealed phases within the screws that would not be visible with X-ray µCT alone. Those parts are presumably a remainder of still non-corroded alloy, while the rest of the implant has instead transitioned to a composition more similar to that of bone, rich in hydrogen, calcium, phosphorus and oxygen. A comparison with 2D X-ray elemental mapping of similar samples confirmed our hypothesis.

[1] Peruzzi et al., DOI: 10.1016/j.actbio.2021.09.047

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TUE 14:00-14:15 | HÖRSAAL 1B | LIFE-02

PARALLEL SESSION

MIGRATION BEHAVIOR OF U87 GLIOBLASTOMA CELLS AFTER IRRADIATION WITH VARYING LET

Presenter: Nicole MATEJKA
Authors: Nicole MATEJKA, Sarah RUDIGKEIT, Matthias SAMMER, Judith REINDL

Glioblastoma multiforme is the most common malignant brain tumor with a very poor prognosis. Despite multimodal treatment, the tumor often recurs in the vicinity of 1–2 cm to the primary tumor.

In this study, the migration behavior of U87 glioblastoma after low- and high-LET irradiation is analyzed to figure out whether the migration is influenced by radiation exposure.

For the migration assay, the cells were seeded in Ibidi Culture-Inserts to generate a cell-free gap of about 500 µm between two cell populations. Irradiation was performed with 55 MeV carbon ions and 20 MeV protons at SNAKE located at the 14 MV tandem accelerator in Garching (GER). The closure of the gap after irradiation was observed by phase-contrast microscopy under live-cell conditions.

There are differences in the migration behavior of cells regarding their velocity and directness visible. Cells irradiated with high-LET carbons tend to be faster, but have lost all orientation. Low-LET proton irradiation cause also a loss of orientation but has nearly no effect on the cell speed. When only one cell population on one side of the gap was irradiated, the cells are better oriented regardless of the radiation type. However, the one-sided proton irradiation leads to a slowdown of the cells.

Our results show that with different irradiation conditions the migration behavior changes and indicate that the close presence of non-irradiated cells has a strong effect on the migration behavior of the whole population.

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TUE 14:15-14:30 | HÖRSAAL 1B | LIFE-03

PARALLEL SESSION

TOWARDS A COMPREHENSIVE PICTURE OF TEMPERATURE-RESPONSIVE ELASTIN-LIKE PEPTIDES

Presenter: Felix ROOSEN-RUNGE

Authors: Tatiana MOROZOVA (1), Olga MATSARSKAIA (1), Zeina WEHBE (1), Sarah WALDIE (2), Nicolas A. GARCIA (3), Michael M. KOZA (1), Martine MOULIN (1), Valerie LAUX (1), Michael HAERTLEIN (1), Trevor FORSYTH (1), Jean-Louis BARRAT (1), Felix ROOSEN-RUNGE (2)

Elastin-like peptides (ELPs) are biomolecules mimicking the hydrophobic repeat units of elastin, a protein providing elasticity to biological tissues such as lung, ligaments and blood vessels. ELPs undergo a hydrophobic collapse upon crossing a lower critical solution temperature (LCST). Due to their stimulus-responsive properties, ELPs are of interest for a broad range of applications including advanced biomaterials, protein purification and drug delivery. While the hydrophobic collapse is believed to be key for the elastic properties of elastin, a comprehensive mechanistic characterisation of the static and dynamic aspects of the collapse has not yet been obtained. In particular, the dynamical state within the collapsed hydrophobic domains of elastin is debated (fluid-like structure vs. a more specific stacking). By combining SANS, QENS, molecular dynamics simulations and selective deuteration, we investigate the temperature response of short and long ELPs. Neutron data indicate differences in the behaviour of short and long ELPs, and, in agreement with simulations, a shift towards more compact ELP structures with increasing temperature is observed. Using our results, we aim at establishing a framework for the investigation of stimulus-responsive molecules and materials.

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TUE 14:30-14:45 | HÖRSAAL 1B | LIFE-04

PARALLEL SESSION

INFLUENCE OF SACCHARIDES ON PHOTO-INDUCED STRUCTURAL CHANGES IN LIPID MEMBRANES STUDIED WITH X-RAY DIFFRACTION

Presenter: Svenja C. HÖVELMANN

Authors: Svenja C. HÖVELMANN (1,2), Jonas E. WARIAS (1), Rajendra P. GIRI (1), Karin HANSEN (1), Jule KUHN (1), Andrea SARTORI (1), Philipp JORDT (1), Chen SHEN (2), Franziska REISE (4), Olaf M. MAGNUSSEN (1), Thisbe LINDHORST (4), Bridget M. MURPHY (1,3)

Understanding the dynamics of structure and interfacial tension in phospholipid membranes containing photoswitchable glycolipids is of fundamental interest for cell-cell interactions and for potential health science applications such as drug delivery. Therefore, we investigate photoswitchable azobenzene-glycolipid molecules embedded in a 1,2-dipalmitoyl-phosphatidylcholine (DPPC) Langmuir film and vesicles as a model system. We use multiple measurement technics to characterise the structural changes, their evolution and time scales with absorption spectroscopy, Langmuir isotherms, X-ray reflectivity, grazing incident X-ray diffraction, X-ray and Neutron small angle scattering. The azobenzene-glycolipids switch reversibly between their trans- and cis-conformation by illumination with UV and blue light and induce a reversible structural change in the membrane they are embedded. These studies were performed on multiple mixed monolayers and vesicles with varying number of sugar groups in the head group to investigate the relevance of the saccharides. Differences in terms of their switching behaviour and membrane conformations will be discussed.

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TUE 14:45-15:00 | HÖRSAAL 1B | LIFE-05

PARALLEL SESSION

INVESTIGATION OF MOLECULAR ORGANIZATION INSIDE RNA NANOMEDICINES BY SMALL ANGLE SCATTERING

Presenter: Heinrich HAAS

Authors: Heinrich HAAS (1), Olga MATSARSKAIA (2), Thomas NAWROTH (3), Christoph WILHELMY (3), Lukas UEBBING (3), Jorge MORENO (1), Sahadat SHEIKH (1), Martin SCHROER (4), Clement BLANCHET (5), Dmitri SVERGUN (5), Peter LANGGUTH (3)

With the recent breakthroughs in the development of mRNA-based COVID-19 vaccines, messenger RNA (mRNA) nanomedicines have been gaining great public attention. Therapeutic application of mRNA requires delivery systems, in order to protect the mRNA from rapid degradation, facilitate cellular uptake and convey translation into protein by the ribosomes. Typically, nanoparticle formulations, as obtained by self-assembly processes between RNA and positively charged lipids or polymers are used for mRNA delivery. The biological activity of these products my depend in a complex manner from the molecular composition and conditions during manufacturing. Here, the internal organization within such nanoparticle systems was investigated to detail, in order to provide a basis for the correlation of structural and functional coherencies.

Small angle X-ray scattering (SAXS) and small angle neutron scattering (SANS) measurements were used to investigate the internal structure of the mRNA nanoparticles. For the lipoplex systems, repeating lipid bilayers were found to be the dominating structural feature inside the particles. The degree of internal organization depended on the lipid composition and preparation protocol. These structural characteristics were correlated with the biological behavior of the systems. Such insight can serve as a basis for better justifying or refining specification limits and critical quality attributes for such nanoparticulate pharmaceutical products.

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TUE 15:00–15:15 | HÖRSAAL 1B | LIFE-06

PARALLEL SESSION

SMALL COMPOUND CRYSTAL SCREENING OF SARS-CoV-2 METHYLTRANSFERASES

Presenter: Viviane KREMLING

Authors: Viviane KREMLING (1), Janina SPRENGER (1), Dominik OBERTHÜR (1), Oleksandr YEFANOV (1), Marina GALCHENKOVA (1), Philipp MIDDENDORF (1), Luca GELISIO (1), Jerome CARNIS (1), Christiane EHRT (2), Sven FALKE (1), Antonia KIENE (1), Bjarne KLOPPROGGE (1), Henry CHAPMAN (1)

Non-structural protein 10 (nsp10), nsp14, and nsp16 are part of the RNA synthesis complex which is crucial for viral replication in SARS-CoV-2. Nsp14 and nsp16 exhibit methyltransferase activity needed for mRNA capping and are active in heterodimeric complexes with the enzymatic inert nsp10. It has been shown that inactivation of any of these proteins interferes severely with viral replication, making them promising drug targets against COVID-19. As only limited information on ligands binding to nsp10–nsp16 is available, we use X-ray crystallography to test small compound libraries (~ 200 compounds) containing potential methyltransferase-binders that were soaked into protein crystals prior to diffraction. We obtained ~30 data sets of the nsp10-16 complex with purine derivatives bound to different positions of the active site. Promising compounds are being tested in binding and activity assays. In parallel, we are testing small peptides by small-angle-X-ray scattering (SAXS) that potentially disrupt the complex formation with nsp10. Nsp14 will be screened in the same way since the enzymatic activity is similar to nsp16. Our results may contain inhibitors that can serve as novel drugs against COVID-19.

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PARALLEL SESSION
TUESDAY, 6TH SEPTEMBER

MATERIALS ENGINEERING			
Time	**Place**	**Presenter**	**Title**
Tue 13:45-14:00	Hörsaal 2	Cem ÖRNEK	In-situ Corrosion Studies at Electron Synchrotrons – Pushing the Limits of Experimental Resolution
Tue 14:00-14:15	Hörsaal 2	Christopher GARVEY	Millisecond Timescale Diffraction During a Piezo-Electric Cycle
Tue 14:15-14:30	Hörsaal 2	Srashtasrita DAS	Multimodal hard X-ray tomography to study degradation and composition of Pt/Rh gauze catalysts during NH3 oxidation
Tue 14:30-14:45	Hörsaal 2	Joana REBELO KORNMEIER	Onset of yielding – macro and micro evidence
Tue 14:45-15:00	Hörsaal 2	Axel GRIESCHE	The Debye-Waller Factor for Temperature Distribution Determination in NBEI Experiments: A Case Study for GTAW
Tue 15:00.15:15	Hörsaal 2	Massimo FRITTON	Microstructural evolution during hot deformation and cooling in VDM© Alloy 780 studied via in-situ high energy X-ray diffraction

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TUE 13:45-14:00 | HÖRSAAL 2 | MAEN-01

PARALLEL SESSION

IN-SITU CORROSION STUDIES AT ELECTRON SYNCHROTRONS – PUSHING THE LIMITS OF EXPERIMENTAL RESOLUTION

Presenter: Cem ÖRNEK

Authors: Cem ÖRNEK (1), Jinshan PAN (2), Dirk ENGELBERG (3), Alfred LARSSON (4), Ulrich LIENERT (5), Francesco CARLÀ (6), Gary HARLOW (7), Ammar AKSOY (1), Bilgehan ŞEŞEN (1), Fan ZHANG (8), Edvin LUNDGREN (4), Hadeel HUSSAIN (6), Ulf KIVISÄKK (9), Steve OOI (10)

This talk will summarise undertaken in-situ corrosion experiments at electron synchrotrons to understand the complex nature of corrosion and hydrogen embrittlement of high-strength steel and duplex stainless steel. Grazing-incidence X-ray measurements (diffraction, reflectivity, fluorescence) coupled with electrochemical methods (current, potential, impedance) were performed during corrosion exposure. As a result, it has been understood that the dissolution of Fe precedes the oxidation of Mo and Ni, followed by rapid dissolution of Cr, leading to intense anodic current transients.

The talk will also summarise recent in-situ time- and space-resolved hydrogen-induced lattice strain measurements using high-energy X-ray diffraction (83–96 keV). Miniature-sized tensile specimens (50 x 3 x 1 mm^3 gauge volume) were subjected to constant electrochemical hydrogen charging at constant tensile loading over time. Hydrogen absorption resulted in lattice strains across the specimen thickness, showing tensile and compressively strained regions. Moreover, austenite grains at the near-surface gradually transformed into quasi nickel hydrides. However, the hydrides reverted instantaneously upon the termination of hydrogen charging, indicating a metastable nature. The research has shown that it is essential to capture these degradation processes in real-time with high spatial and temporal resolution and high sensitivity to reveal momentary events that can only be seen when measured in-situ.

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TUE 14:00-14:15 | HÖRSAAL 2 | MAEN-02

PARALLEL SESSION

MILLISECOND TIMESCALE DIFFRACTION DURING A PIEZO-ELECTRIC CYCLE

Presenter: Christopher GARVEY
Authors: Christopher GARVEY (1), Stephen MUDIE (2), Vitor SENCADAS (3)

The structural changes in a fibre mat of electrospun fibroin during the piezo-electric cycle were investigated with X-ray scattering. The poor signal to noise ratio of a single shot X-ray measurement is overcome by a triggered mode of data acquisition. This data acquisition mode, where acquisitions are synchronized with the piezo cycle, consisting of multiple shots added together for an extended time binning, overcomes the limitations of X-ray flux both in the low and high flux regimes. These limitations are imposed by the intensity of the X-ray source which should be sufficient to provide sufficient signal to noise in the duration of the X-ray exposure (e.g. lab source), and the potential for sample damage by the X-ray source during a single shot experiment at high fluxes (e.g. synchrotron X-ray source). The isotropic scattering X-ray data spans a range of scattering vectors, q, 0.1 < q < 3.5 Å-1 a regime where scattering presents as a number of very poorly defined and size broadened Bragg peaks. With compression the peaks incrementally shift and increase in intensity while the small angle scattering signal increases. We suggest that this change is due to an increase in the ordering of the material with an increase in the grain boundaries of these ordered domains responsible for the small angle scattering signal.

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TUE 14:15-14:30 | HÖRSAAL 2 | MAEN-03

PARALLEL SESSION

MULTIMODAL HARD X-RAY TOMOGRAPHY TO STUDY DEGRADATION AND COMPOSITION OF Pt/Rh GAUZE CATALYSTS DURING NH3 OXIDATION

Presenter: Srashtasrita DAS

Authors: Srashtasrita DAS (1), Michael STUECKELBERGER (2), Jan POTTBACKER (3), Sven JAKOBTORWEIHEN (3), Raimund HORN (3), Thomas SHEPPARD (1)

Catalytic etching of Pt/Rh gauze catalysts during oxidation of NH3 to NO (in Ostwald process) leads to surface reconstruction of smooth wire gauzes into cauliflower-like structures, resulting in decreased catalytic activity and selectivity. To examine this structural degradation, we investigated the distribution of Pt and Rh in the catalyst using complementary hard X-ray tomography techniques – scanning transmission X-ray tomography (STXM-CT), ptychographic X-ray computed tomography (PXCT) and X-ray fluorescence tomography (XRF-CT) at the P06 beamline of PETRA III (DESY, Hamburg), at energies above and below the Rh K-edge (23.300 keV and 23.208 keV respectively). Single wires of 60-76 µm diameter were extracted from catalyst gauzes aged for 24h, 50h, 100h, and 50 days. STXM-CT performed with a 3D spatial resolution of ~2.5 µm allowed to study the distribution of Rh within the catalyst as a function of reaction time. Additionally, PXCT enabled the study of composition of an individual cauliflower with a 3D spatial resolution of 100-150 nm. This study provides new insights into bulk-material chemical gradients accompanying the structural degradation of Pt/Rh catalyst, important for improving reactor design and catalyst performance. Advanced material characterization using tomography with chemical contrast is shown as an ideal method to probe the structure of challenging samples, generally not feasible using conventional methods.

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TUE 14:30-14:45 | HÖRSAAL 2 | MAEN-04

PARALLEL SESSION

ONSET OF YIELDING – MACRO AND MICRO EVIDENCE

Presenter: Joana REBELO KORNMEIER
Authors: Joana REBELO KORNMEIER (1), Simon VITZTHUM (2), Michael HOFMANN (1), Maximilian GRUBER (2), Emad MAAWAD (3), António C. BATISTA (4), Wolfram VOLK (2)

Numerical prediction of springback in sheet metals is still a challenge nowadays. Especially for high strength steels, precise modelling of the elastic behaviour is crucial, because of the non-linearity and decrease of Young's modulus during forming processes. In this study, a temperature-dependent evaluation method [1] is investigated and further improved. Matching the thermoelastic effect with the microscopic material behaviour shows that the temperature minimum can be considered for the evaluation of the onset of yielding, i.e. the maximum yield stress at zero plastic strain (YS0). The basic assumption for this is that the point in time of the temperature minimum is the equilibrium between elastic cooling and plastic heating induced by deformation. To verify this hypothesis, in-situ synchrotron diffraction experiments are performed with an interstitial free low carbon steel, while monitoring the temperature changes in the respective samples. The suitability and validity of the thermoelastic effect for material characterization and the determination of the onset of yielding has been analysed using lattice strains evaluated based on the peak shift of several lattice planes and dislocation density estimated by micro strains due to peak broadening. The results prove existing assumptions and clearly qualifies the thermoelastic effect for material characterization on a microstructural basis.

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[1] S.Vitzthum et al., Procedia Manufacturing 29 (2019) 490-497.

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TUE 14:45-15:00 | HÖRSAAL 2 | MAEN-05

PARALLEL SESSION

THE DEBYE-WALLER FACTOR FOR TEMPERATURE DISTRIBUTION DETERMINATION IN NBEI EXPERIMENTS: A CASE STUDY FOR GTAW

Presenter: Axel GRIESCHE

Authors: Axel GRIESCHE (1), Tobias MENTE (1), Thomas KANNENGIESSER (1), Nikolay KARDJILOV (2)

In Neutron-Bragg-Edge Imaging (NBEI) in-situ experiments, we studied the phase transitions in martensitic steel sheets during butt-welding [1]. Gas tungsten arc welding was used with a motorized torch allowing automated weldments. The austenitization in the heat affected zone underneath the welding head could be clearly visualized. Also, the retransformation into the martensitic phase upon cooling. However, we observed an unexpected additional change in transmission at $\lambda = 0.44$ nm that is at a wavelength larger than the wavelength of the Bragg edges of both the martensitic and austenitic phases. We attribute this change to the Deybe-Waller-Factor that describes the temperature dependence of coherent scattering at a crystal lattice [2]. With help of temperature field simulations that were calibrated by the reading of an attached thermo couple during welding, we could show that the Debye-Waller factor can produce an additional image contrast.

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[1] Griesche, A.; Pfretzschner, B.; Taparli, U. A.; Kardjilov, N.: Time-Resolved Neutron Bragg-Edge Imaging: A Case Study by Observing Martensitic Phase Formation in Low Temperature Transformation (LTT) Steel during GTAW. Appl. Sci. 2021, 11, 10886.

[2] Ramadhan, R.S.; Kockelmann, W.; Minniti, T.; Chen, B.; Parfitt, D.; Fitzpatrick, M.E.; Tremsin, A.S.: Characterization and application of Bragg-edge transmission imaging for strain measurement and crystallographic analysis on the IMAT beamline. J. Appl. Crystallogr. 2019, 52, 351–368.

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TUE 15:00.15:15 | HÖRSAAL 2 | MAEN-06

PARALLEL SESSION

MICROSTRUCTURAL EVOLUTION DURING HOT DEFORMATION AND COOLING IN VDM© ALLOY 780 STUDIED VIA IN-SITU HIGH ENERGY X-RAY DIFFRACTION

Presenter: Massimo FRITTON

Authors: Massimo FRITTON (1), Frank KÜMMEL (1), Andreas KIRCHMAYER (2), Andreas STARK (3), Masood Hafez HAGHIGHAT (4), Bodo GEHRMANN (4), Steffen NEUMEIER (2), Ralph GILLES (1)

Ni-based polycrystalline superalloys are developed for use in demanding conditions, e.g. for the hot sections of modern gas turbines or jet engines. In such environments, the material is typically challenged by a combination of high tensile loads, high temperatures, and oxidizing atmospheres. In this study, the polycrystalline Ni-based superalloy VDM© Alloy 780 was investigated, which consists of ɣ-matrix, ɣ'-hardening phase, δ- and η-high-temperature phases, and traces of NbC, and was developed for higher operating temperatures than the widely used alloy 718. High-energy X-ray diffraction experiments were performed in-situ during hot compression with synchrotron radiation to mimic the forging process. In the first part of the experiments, i.e the hot forming, the formation, and development of the crystallographic texture were investigated. During plastic deformation, subgrain formation, recrystallization, and rotation of the grains into preferred orientations were observed. In the second part, directly after the hot forming, the microstructural evolution at cooling rates of 10 °C/min, 100 °C/min, and 1000 °C/min were studied. The recrystallized fraction is highest at the slowest cooling rate and vice versa. The experiments helped to elucidate the material behaviour throughout the manufacturing process to further optimize the precipitation behaviour and thus the mechanical properties of the alloy.

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POSTER SESSION 2
TUE, 6TH SEP. 16:15 – 18:15

MAGNETISM AND FUNCTIONAL MATERIALS		
Board	**Presenter**	**Title**
1	Alevtina SMEKHOVA	Synchrotron X-rays for structural and magnetic studies of high-entropy alloys
2	Jorge TORRES	Room-temperature presence of high-spin state in spin-crossover molecule thin layers on graphite measured by X-ray absorption spectroscopy
3	Frank WEBER	YNi2B2C – a model superconductor to investigate electron-phonon coupling
4	Xiao SUN	Tuning the structural and magnetic properties of iron oxide nanoparticles
5	Dmitriy KSENZOV	Faster chiral versus collinear magnetic order recovery after optical excitation revealed by femtosecond XUV scattering
6	Klaus HABICHT	Heat Transport in Quantum Materials - The Intriguing Phonon Physics in Ever Surprising SrTiO3
7	Franziska ZAHN	Atomic-scale structure and vibrations in RESbS rare-earth pnictide chalcogenides
8	Artem FEOKTYSTOV	On the magnetization reduction in iron oxide nanoparticles
9	Xingchen SHEN	Full phonon softening above the charge-density-wave phase transition in 2H-TaSe2
10	Eugen WESCHKE	Soft X-Ray XMCD at 30 Tesla: A New Pulsed Magnetic Field Setup at BESSY II
11	Leila NOOHINEJAD	Capturing proton dynamics in the phase transitions of incommensurate organic ferroelectrics using synchrotron X-ray diffraction.
12	Yunxia ZHOU	Phase transtion in La0.6Sr0.4CoO3-δ thin films by ion irradiation
13	Nazim MAMEDOV (MAMMADOV)	Magnetic Topological Insulators MnBi2Te4·n(Bi2Te3) (n = 0, 1, …, 6): is there a 3D-2D crossover and transition to 2D ferromagnetism?
14	Doru C. LUPASCU	A study of the local fields in bismuth ferrite using different radioactive tracer ions
15	Fouad KERAMSI	Novel theoretical prediction of physical properties of phases Max
16	Carolin SCHMITZ-ANTONIAK	XMCD of a molecular diamagnet: The peculiar case of Pd(II)

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OTHER		
Board	**Presenter**	**Title**
17	Michael STUCKELBERGER	X-rays meet Neutrons meet Ions meet Electrons meet Lasers meet Magnets: Combined Access to Multiple Facilities through EU Project "ReMade@ARI"
18	Antje VOLLMER	LEAPS IDEA – Inclusion, Diversity, Equity, and Anti-discrimination
19	Antje VOLLMER	Science Diplomacy – overcoming social and economic imbalances by research, development and higher education

HEALTH, LIFE AND BIOLOGY		
Board	**Presenter**	**Title**
25	Nimmi Das ANTHUPARAMBIL	Kinetics of aggregation of low density lipoproteins and evolution of protein gelation dynamics of an egg yolk gel
26	Nils SCHUTH	Tryptophan regulates Drosophila zinc stores
27	Christopher GARVEY	Swelling behaviour of mucin particles by extended q-range small angle neutron scattering
28	Sonja TIMMERMANN	Non-linear radiation effects on the dynamics of cooked egg white investigated by X-ray photon correlation spectroscopy
29	Janes ODAR	A pipeline for a three-dimensional X-ray phase contrast Xenopus laevis atlas
30	Manfred WEISS	Facilities for Macromolecular Crystallography at the HZB
31	Manfred S. WEISS	Fragment screening by macromolecular crystallography – efficient workflow for users at BESSY II
32	Mohammad Sayed AKHUNDZADEH	Dose rate dependent X-ray induced dynamics in dense antibody-protein solutions (Ig-PEG and BSA)
33	Katja FRENZEL	Quantitative analysis of trace elements in pancreatic carcinoma and pancreas sections by reference-free X-ray Fluorescence analysis
34	Christian BECK	Short-time transport properties of bidisperse suspensions of immunoglobulins and serum albumins consistent with a colloid physics picture
35	Thomas VAN DE KAMP	Serial tomography and semi-automatic analysis of insects
36	Clement E. BLANCHET	Biological SAXS in Corona time: automation, remote operation and scientific projects
37	Sarah RUDIGKEIT	CeCILE – intelligent detection, tracking and cell cycle evaluation of eukaryotic cells on phase-contrast live-cell videos
38	Jessica NEUBAUER	Design of a preclinical proton minibeam radiotherapy facility
39	Ilaria MOSCA	Dynamic cluster formation, viscosity and diffusion in monoclonal antibody solutions

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HEALTH, LIFE AND BIOLOGY		
40	Selina L. STORM	EMBL@PETRA4 – an Integrated Facility for Structural Biology and Imaging
41	Gleb BOURENKOV	Biological crystallography and X-ray imaging on EMBL@PETRA III beamlines
42	Pauline PFEIFFER	Small wasps, big data: Revealing the morphology, development and behavior of parasitoid wasps using synchrotron X-ray imaging
43	Stefan FIEDLER	Implementation of a robotic system for crystal transfer and storage after remotely controlled harvesting as part of the MX pipeline at EMBL Hamburg
44	Jonas ALBERS	High Throughput Tomography (HiTT) of biological samples on EMBL Beamline P14 on PETRA III
45	Thomas NAWROTH	Specific Structure Resolution of Pharmaceutical Carriers by Contrast Variation: D-SANS and (A)SAXS
46	Gudrun LOTZE	What makes chalky teeth crumble? A multimodal high-resolution XRF and WAXS study on MIH-teeth
47	Lukas KNAUER	The pH value influences vibrational modes of the iron-sulfur protein Apd1
48	Helena TABERMAN	The High-Throughput Macromolecular Crystallography Beamline P11 at PETRA III
49	Rajni RAJNI	X-ray Fluorescence Imaging of Human Atherosclerotic Plaques

MULTI-SCALE PROTEIN DYNAMICS		
50	Sharmistha DUTTA	Origins of enhanced aurophilicity in stimuli-responsive dimer complexes and the role of “host-guest” interactions

SOFT MATTER AND LIQUIDS		
Board	**Presenter**	**Title**
51	Max WILKE	Ion association in hydrothermal aqueous NaCl solutions: Implications for the microscopic structure of supercritical water
52	Lukas PETERSDORF	X-ray pump-probe studies of aqueous salt solution interfaces
53	Florian TRINTER	Photoemission studies on a liquid jet at the PETRA III beamline P04

INDUSTRY, INNOVATION AND TRANSFER		
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59	Philipp HÖNICKE	Accurate determination of X-ray fundamental parameters at PTB
60	Marc THIRY	EASI-STRESS - European Activity for Standardisation of Industrial residual STRESS characterisation

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62	Josephine GUTEKUNST	Polymer compound refractive X-ray lenses for easy customization

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63	Ezzeldin METWALLI	Simultaneous SAXS/SANS method: A novel nanoanalytical tool
64	Stefan SCHIPPERS	A Free-Electron Target for the Heavy-Ion Storage Rings at FAIR
65	Andreas OSTERMANN	The Macromolecular Neutron Single Crystal Diffractometer BIODIFF for Proteins at the Heinz Maier-Leibnitz Zentrum
66	Thomas HANSEN	Accurate determination of bound coherent neutron scattering lengths by Bragg diffraction
67	Anna ZIMINA	Catalysis at the CAT-ACT X-ray spectroscopy beamline at KIT Light Source
68	Olaf HOLDERER	High-resolution neutron spin echo spectroscopy with the J-NSE “PHOENIX” at MLZ
69	Martin MEVEN	High Pressure Options for Single Crystal Diffraction at MLZ
70	Klaus LIEUTENANT	Latest developments of the program VITESS for the simulation of neutron scattering instruments and virtual neutron experiments
71	Andreas SCHROPP	PtyNAMi: Ptychographic Nano-Analytical Microscope
72	Peter FEUER-FORSON	RAY-X: a modern software architectural basis for RAY, RAY-UI and REFLEC
73	Edmund WELTER	Perspectives for analytical XAFS spectroscopy at PETRA IV
74	Ivo ZIZAK	mySpot Station at BESSY II: Diffraction Tomography and Time Resolution
75	Frieder KOCH	Swift Heavy Ion Irradiation and in-situ analysis capabilities of the M-branch at the GSI UNILAC
76	Markus APPEL	Recent Achievements and Future Perspectives of Neutron Backscattering at IN16B
77	Leon JACOBSE	Advanced HE-SXRD Studies for Electrocatalysis
78	Mahesh RAMAKRISHNAN	A novel fast synchronized setup for combined in-situ X-ray Diffraction and X-ray absorption spectroscopy at MAX IV
79	Armin HOELL	Structure and Composition of Size-Tunable Ni–Cu Core–Shell Nanoparticles as analyzed by ASAXS
80	O'Neill GEORGE	Simulations using NCrystal and Geant4 for innovative solid-state neutron detectors
81	Imke GREVING	In-situ nanotomography at the imaging beamline P05

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83	Chen SHEN	The high-resolution diffraction beamline P08 at PETRA III
84	Ricardo HELM	The Pulsed Low-Energy Positron System PLEPS
85	Johannes MITTENEDER	Micrometer positron beam at the Scanning Positron Microscope
86	Volodymyr BARAN	The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY
87	Abdel AL-FALOU	A compact high-temperature furnace for SANS magnets.
88	Anton TREMSIN	Applications of high resolution event counting MCP/Timepix detectors at soft X-ray and energy-resolved neutron imaging beamlines
89	Analía FERNÁNDEZ HERRERO	Feasibility research for the production of next generation X-ray optics
90	Anico KULOW	Illustration of resonant ptychographic X-ray computed tomography
91	Dirk WALLACHER	Sample Environment at BESSY-II
92	Azat KHADIEV	In-Situ X-ray Diffraction and Imaging P23 Beamline at PETRA III: status and prospects
93	Nele THIELEMANN-KÜHN	4f electronic excitations and their role for magnetization dynamics
94	Nele THIELE-MANN-KÜHN	DynaMaX: Endstation for ultra-fast dynamics at BESSY II
95	Jan RUBECK	PETRA III: P03/MiNaXS - current status and future plans
96	Thomas KELLER	Fast kinetics in thin films by intensity modulated neutron refectometry
97	Andrey SOKOLOV	At-Wavelength Metrology facility for EUV, XUV and tender X-ray diffrac-tive optics at BESSY-II
98	Ronan SMITH	Directional Dark-Field X-ray Imaging: A Comparison of a 2D Talbot Array Illuminator and Sandpaper as Optical Elements
99	Christian GOLLWITZER	Small-angle X-Ray scattering: characterization of arbitrarily shaped nanoparticles using Debye's equation
100	Thomas KRIST	Polarizing Neutron Optics from NOB Nano Optics Berlin
101	Robin SCHÜRMANN	Traceable concentration measurements of nanoparticle suspensions using SAXS and photocentrifugation
102	Wilko MIDDENTS	Angular distribution in Rayleigh scattering of linearly polarized hard X-rays

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METHODS AND INSTRUMENTS DEVELOPMENT 2		
103	Lars BREUER	Electronic vs. Nuclear sputtering of Coronene
104	Thomas GUTBERLET	Time of flight measurements using a compact solid methane moderator
105	Thiago R. F. PEIXOTO	The hard X-ray momentum microscopy end station at PETRA III
106	Christoph SCHLUETER	HAXPES at PETRA III: electronic structure, operando devices and in-situ catalysis
107	Markus OSTERHOFF	GINIX – Göttingen Instrument for Nano-Imaging with X-rays
108	Adam KUBEC	XRnanotech - Achromatic X-ray Lens and recent developments in nanostructured X-ray optics
109	Konstantin GLAZYRIN	Sub-micrometer focusing setup for high-pressure crystallography at the Extreme Conditions beamline at PETRA III
110	Deniz WONG	PEAXIS - A High Resolution RIXS Endstation for Solid-State Energy and Quantum Materials
111	Jörg EVERS	Nuclear quantum optics - from pulse shaping to coherent control at synchrotron radiation sources
112	Peter MODREGGER	Ptychographic Reconstruction With Object Initialization
113	Leon Merten LOHSE	Light-matter coupling of quantum emitters in hard X-ray waveguides
114	Adyasha BISWAL	2D Bragg beam conditioner for large field-of-view X-ray imaging

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118	Stephanos KARAFILUDIS	Evolution of mesoporous structures in Mg-,Ni- and Co-phosphate compounds
119	Benjamin NEDING	Three-dimensional X-ray diffraction for microstructure mapping on the grain level
120	Susanne HENNINGER	Precipitation kinetics in Al-alloy 7050 studied by SAXS, WAXS and numerical modeling
121	Simon BODE	Quasi in-situ Investigation of Dislocation Dynamics in Semiconductor Materials by X-ray Diffraction Imaging
122	Jan ROSIGKEIT	Phase Transformations in TiAl during Selective Laser Melting (SLM) studied by X-ray Diffraction
123	Moritz HOESCH	Active Sites of Te in Hyperdoped Si by Hard X-ray Photoelectron Kikuchi-Diffraction
124	Yue YU	Optical constants of MgF2 thin film in the VUV and EUV energy range with improved accuracy
125	Peter STARON	P61A: The new materials science high energy white beam beamline at PETRA III

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MATERIALS ENGINEERING		
126	Anastasiia KUZNETSOVA	The methods of neutron diffraction calculation
127	Mohd Saif SHAIKH	Phase evolution of Te-hyperdoped Si upon furnace annealing
128	Yi LI	Chlorine doping of MoSe2 flakes by ion implantation
129	Florian WIELAND	In-situ X-ray diffraction experiments of Magnesium alloys at physiological salt concentrations
130	Chaitali SOW	Unraveling the Spatial Distribution of Catalytic Non-Cubic Au Phases in a Bipyramidal Microcrystallite by X-ray Diffraction Microscopy
131	Marc-André NIELSEN	Residual stresses in additively manufactured aluminum alloys and 316L steel
132	Kai SCHLAGE	Innovative Sputter Deposition for Flexible Thin Film Engineering
133	Christopher SCHRÖCK	Swift heavy ion irradiation of bismuth nanowires pressurized in diamond anvil cells
134	Malte BLANKENBURG	Multi-modal characterisation of engineering materials at the inline branch P21.2 of the Swedish Materials Science beamline (SMS) at PETRA III

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TUE 15:45-17:45 | BOARD 1 | P2-MAGN-01

POSTER SESSION

SYNCHROTRON X-RAYS FOR STRUCTURAL AND MAGNETIC STUDIES OF HIGH-ENTROPY ALLOYS

Presenter: Alevtina SMEKHOVA

Authors: Alevtina SMEKHOVA (1), Alexei KUZMIN (2), Konrad SIEMENSMEYER (1), Chen LUO (1), James TAYLOR (1), Sangeeta THAKUR (3), Florin RADU (1), Eugen WESCHKE (1), Ana GUILHERME BUZANICH (4), Götz SCHUCK (1), Ivo ZIZAK (1), Kirill YUSENKO (4)

The advantages of synchrotron radiation as high brilliance, energy tunability and a variable polarisation of X-ray photons offer unique opportunities to study novel multifunctional materials and multicomponent systems in element-specific ways unattainable by laboratory methods. Together with the possibility to perform the experiments under different sample environment conditions, it allows unravelling the precise role of individual components in certain macroscopic properties of complex compounds. Such knowledge, in turn, is crucial to design new materials with exceptional performance properties demanded by modern technologies.

Herein, the single-phase fcc Al0.3CrFeCoNi high-entropy alloy has been chosen as an appropriate model system for element-specific structural and magnetic studies with X-rays from the BESSY II synchrotron radiation facility (HZB, Berlin). Multi-edge X-ray absorption spectroscopy (EXAFS) combined with reverse Monte Carlo (RMC) simulations was used to probe the details of local coordination and the internal structure relaxations at the atomic scale in the most unbiased manner. The surface oxidation was probed by XANES while the net magnetic moments of surface atoms were probed by XMCD after in-situ cleaning with different methods. The outcomes of the synchrotron studies on a local scale and their connection to the macroscopic magnetic properties are discussed.

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TUE 15:45-17:45 | BOARD 2 | P2-MAGN-02

POSTER SESSION

ROOM-TEMPERATURE PRESENCE OF HIGH-SPIN STATE IN SPIN-CROSSOVER MOLECULE THIN LAYERS ON GRAPHITE MEASURED BY X-RAY ABSORPTION SPECTROSCOPY

Presenter: Jorge TORRES

Authors: Jorge TORRES (1), Lalminthang KIPGEN (1), Sascha OSSINGER (2), Sangeeta THAKUR (1), Clara W.A. TROMMER (2), Ivar KUMBERG (1), Rahil HOSSEINIFAR (1), Evangelos GOLIAS (1), Sebastien HADJADJ (1), Jendrik GÖRDES (1), Chen LUO (3), Kai CHEN (3), Florin RADU (3), Felix TUCZEK (2), Wolfgang KUCH (1)

The bistability of spin-crossover molecules (SCMs) in the high-spin (HS) and low-spin (LS) states, which can be induced by external stimuli such as light, temperature, pressure, magnetic or electric fields, puts them amongst the most promising candidates for realizing molecular spintronics. However, contacting SCMs with solid surfaces often results in the loss of spin-crossover behavior. Herein, we report on the combined light- and temperature-induced spin switching of sub-, mono- and multilayer coverages of the SCM [Fe{H2B(pz)(pypz)}2] sublimed on a highly oriented pyrolytic graphite (HOPG) surface. The switching kinetics and cooperativity between the SCMs is studied by X-ray absorption spectroscopy (XAS) at the VEKMAG end station at BESSY II. Analysis of the XAS spectra shows that the light-induced excited spin-state trapping (LIESST) at a temperature of 10 K resulted in twice the HS fraction than the thermally induced spin-state transition. On the other hand, the largest number of LS-state molecules is reached at 60 K, while the transition temperature T1/2 (50 % HS and 50 % LS) is located at 300 K.

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TUE 15:45-17:45 | BOARD 3 | P2-MAGN-03

POSTER SESSION

YNi2B2C – A MODEL SUPERCONDUCTOR TO INVESTIGATE ELECTRON-PHONON COUPLING

Presenter: Frank WEBER
Authors: Frank WEBER (1), Philipp KURZHALS (1), Rolf HEID (1), Claude MONNEY (2), Alexandre IVANOV (3), Vladimir STROCOV (4), Dmitry REZNIK (5)

Electron-phonon coupling (EPC), i.e., the scattering of lattice vibrations by electrons and vice versa, is ubiquitous in solids and can lead to emergent ground states such as superconductivity and charge-density wave order. The strength of EPC in emergent superconducting materials is routinely assessed by ab-initio calculations. However, the accuracy of such calculations is difficult to check.

Here, we report on a comprehensive study of the lattice dynamics in the strong-coupling superconductor YNi2B2C. Employing thermal neutron spectroscopy, we report phonon properties over the full dispersion range, E ≤ 160 meV. At many points we could deduce the intrinsic phonon linewidth and compare it to prediction based on density-functional perturbation theory. Overall, we find excellent agreement. Studies including angle-resolved photoemission spectroscopy revealed that the most prominent phonon anomalies can only be explained by taking into account the dependence of the EPC on both, the electron-momentum k and the phonon-momentum q [1]. We show that strong phonon broadening can occur in the absence of both Fermi surface nesting and lattice anharmonicity, if EPC is strongly enhanced for specific values of electron-momentum, k. This new scenario likely applies to a wide range of compounds.

[1] Kurzhals et al., Nature Communications 13, 228, doi:10.1038/s41467-021-27843-y (2022).

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TUE 15:45-17:45 | BOARD 4 | P2-MAGN-04

POSTER SESSION

TUNING THE STRUCTURAL AND MAGNETIC PROPERTIES OF IRON OXIDE NANOPARTICLES

Presenter: Xiao SUN
Authors: Xiao SUN (1), Akhil TAYAL (1), Oleg PETRACIC (2), Sylvio HAAS (1)

Due to their biocompatibility and magnetic properties, iron oxide nanoparticles (NPs) are especially interesting for applications such as targeted drug delivery and hyperthermia therapy. According to its oxidation states, iron may form various crystal structures and thus show different magnetic properties. FeO is a bulk antiferromagnet with a rock salt crystal structure at room temperature. Bulk magnetite and maghemite are ferrimagnet with TC = 858K and 948K, respectively. However, they show different magnetic properties in nanoscale due to the finite size effect.

We observe a shift in the hysteresis loops of various sizes of iron oxide NPs (5 – 20nm). This is due to an exchange interaction between the magnetite core and a shell with disordered surface spins. In order to understand the origin of the exchange bias effect, we studied their crystallographic structure using X-ray total scattering experiments with pair distribution function analysis. The ratio of different phases of iron oxide was obtained using X-ray absorption spectroscopy. The morphology of the particles was characterized using scanning electron microscopy and small angle scattering. The relationship between the composition of the NPs and the exchange bias effect is studied. Furthermore, the magnetic properties of the samples can be tuned by oxidation or reduction via different annealing procedures. These results provide important information for the manipulation of the exchange bias in oxide NPs.

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TUE 15:45-17:45 | BOARD 5 | P2-MAGN-05

POSTER SESSION

FASTER CHIRAL VERSUS COLLINEAR MAGNETIC ORDER RECOVERY AFTER OPTICAL EXCITATION REVEALED BY FEMTOSECOND XUV SCATTERING

Presenter: Dmitriy KSENZOV

Authors: Nico KERBER (1,2), Dmitriy KSENZOV (3), Frank FREIMUTH (1,4), Flavio CAPOTONDI (5), Emanuele PEDERSOLI (5), Ignacio LOPEZ-QUINTAS (6), Boris SENG (1,2,7), Joel CRAMER (1,2), Kai LITZIUS (1,2), Daniel LACOUR (7), Hartmut ZABEL (1,2,8), Yuriy MOKROUSOV (1,2,4), Mathias KLÄUI (1,2), Christian GUTT (3)

Magnetization configurations with a fixed chirality are currently investigated intensively due to their fascinating properties such as enhanced stability and efficient manipulation by the current. The chiral wall spin structure is of key importance as it governs the dynamical properties of DWs and skyrmions. While the investigation of static structures and slow dynamics of chiral magnetic structures has been intensified recently, experimental studies addressing the ultimate fs-ns dynamics of the chirality have been elusive so far. In our work, we employ circularly polarized light pulses of the FERMI FEL and investigate the X-ray magnetic scattering evolution of the chiral order of DWs in magnetic thin film samples. Using samples with interfacial DMI and perpendicular magnetic anisotropy exhibiting labyrinth-like domain patterns, we measure in the same experiment both the contribution of ferromagnetic order and the average chirality at the DW. A key step of this experimental work is the comparison of the collinear ferromagnetic order dynamics and the chiral order dynamics. We subsequently investigated the origin of the faster recovery of the chiral signal by performing numerical simulations of the scattering signal, which reproduce the experimental findings. Our study paves the way for future investigations of fundamental aspects such as, e.g., the dependence of the timescales of the chiral order build-up on the absolute strength of the DMI by varying the heavy metal layers.

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TUE 15:45-17:45 | BOARD 6 | P2-MAGN-06

POSTER SESSION

HEAT TRANSPORT IN QUANTUM MATERIALS – THE INTRIGUING PHONON PHYSICS IN EVER SURPRISING SrTiO3

Presenter: Klaus HABICHT
Authors: Klaus HABICHT (1,2), Danny KOJDA (1), Katharina FRITSCH (1), Tommy HOFMANN (1), Thomas KELLER (3,4)

The model perovskite SrTiO3 is well-known for its strongly anharmonic phonon properties underlying the intriguing physics of soft phonon modes. A plethora of unusual thermal transport properties derive from the interplay of ferroelectricity, phonon softening, quantum fluctuations and topological properties, including Poiseuille flow of phonons and the elusive coupling of phonons in SrTiO3 to magnetic fields. We gain new insights by establishing a link between the macroscopic specific heat cp of SrTiO3 signalizing the displacive structural phase transition, and the soft-phonon behavior in the R-corner of the Brillouin zone. We devise a cp model which is situated intermediate between the oversimplified Debye model and computationally expensive first-principles calculations. Our model replicates the temperature evolution of the specific-heat anomaly close to the cubic-to-tetragonal structural phase transition. We demonstrate that the entropy-derived critical exponents are compatible with the Heisenberg universality class in the tetragonal phase and also mean-field Landau behavior in the cubic phase. Our analysis identifies the R-point soft phonons to be responsible for both, the specific-heat anomaly close to TC and a sizeable amount of specific heat in the temperature range below ~10 K. Consequently, the correlation between changes in the phase transition and the Debye temperature can be traced back to be microscopically rooted in the soft phonon physics.

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TUE 15:45-17:45 | BOARD 7 | P2-MAGN-07

POSTER SESSION

ATOMIC-SCALE STRUCTURE AND VIBRATIONS IN RESbS RARE-EARTH PNICTIDE CHALCOGENIDES

Presenter: Franziska ZAHN
Authors: Franziska ZAHN (1), Christopher BENNDORF (2), Hans H. FALK (1), Konrad RITTER (1), Eva ZOLLNER (1), Sergiu LEVCENKO (1), Edmund WELTER (3), Oliver OECKLER (2), Claudia S. SCHNOHR (1)

Rare-earth pnictide chalcogenides, REPnCh, represent an intriguing class of materials, showing special physical properties in terms of electronic and magnetic characteristics, topological effects and charge density waves. The crystal structure of these materials consists of different atomic layers. Pn monolayers alternate with RE-Ch double-layers and there is no Pn-Ch bonding. The presence of charge density waves marks the phase transition from semiconductor to metal with increasing temperature. Furthermore, the RE species has a major influence on the formation of charge density waves. Therefore, RESbS compounds with RE = La, Ce, Pr and Nd were investigated to gather further knowledge on this matter. Extended X-ray absorption fine structure spectroscopy (EXAFS) was performed at ten different temperatures ranging from 20 K to 295 K at the Sb K-edge in transmission mode. The analysis of the temperature-dependent EXAFS data yields structural parameters such as static disorder, thermal vibrations and bond lengths of the Sb atoms in the Pn monolayers. Sb, Sb2O3 and LaSb samples serve as reference materials and were also measured as a function of temperature. The spectra of the Sb sample closely resemble those of the RESbS compounds and provide a particularly important reference for a detailed analysis. This systematic investigation of different RESbS compounds adds to the fundamental understanding of the physical properties of this still mostly unstudied class of materials.

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TUE 15:45-17:45 | BOARD 8 | P2-MAGN-08

POSTER SESSION

ON THE MAGNETIZATION REDUCTION IN IRON OXIDE NANOPARTICLES

Presenter: Artem FEOKTYSTOV

Authors: Artem FEOKTYSTOV (1), Tobias KÖHLER (1,2,3), Oleg PETRACIC (2), Emmanuel KENTZINGER (2), Tanvi BHATNAGAR-SCHÖFFMANN (2,3,4), Mikhail FEYGENSON (5,6), Nileena NANDAKUMARAN (2,3), Joachim LANDERS (7), Heiko WENDE (7), Antonio CERVELLINO (8), Ulrich RÜCKER (2), András KOVÁCS (4), Rafal E. DUNIN-BORKOWSKI (4), Thomas BRÜCKEL (2,3)

Iron oxide nanoparticles are presently considered as promising objects for various medical applications including targeted drug delivery and magnetic hyperthermia. The nanoparticle solution in water has to possess large enough saturation magnetization to react on external magnetic field. However, there remains several unsolved questions regarding the effect of size onto nanoparticle overall magnetic behavior. One aspect is the reduction of magnetization as compared to bulk samples. A detailed understanding of the underlying mechanisms of this reduction will improve the particle performance in the applications.

There are several proposed models for the spatial distribution of the magnetization, which include the presence of a magnetic core-shell structure, spin disorder around defects and a reduced magnetization in the core due to reversed moments and frustration. In this work we combine neutron and synchrotron X-ray scattering techniques with magnetometry, transmission electron microscopy (TEM), elemental analysis and Mössbauer spectroscopy to study nanoparticles of various sizes and to obtain as complete as possible picture of their properties. We find that the nanoparticles possess a macroscopically reduced saturation magnetization, mostly due to the presence of antiphase boundaries as observed with high-resolution TEM and X-ray scattering and to a lesser extent due to a small magnetically depleted surface layer and cation vacancies.

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TUE 15:45-17:45 | BOARD 9 | P2-MAGN-09

POSTER SESSION

FULL PHONON SOFTENING ABOVE THE CHARGE-DENSITY-WAVE PHASE TRANSITION IN 2H-TaSe2

Presenter: Xingchen SHEN
Authors: Xingchen SHEN, Frank WEBER

Research on charge-density-wave (CDW) ordered transition-metal dichalcogenides continues to unravel new states of quantum matter correlated to the intertwined lattice and electronic degrees of freedom. Here, we report an inelastic X-ray scattering investigation of the lattice dynamics of the canonical CDW compound 2H-TaSe2 complemented by angle-resolved photoemission spectroscopy. Our results provide evidence for a previously unknown precursor phase above the CDW transition temperature TCDW. The phase at temperatures between T* (= 128.7 K) and TCDW (= 121.3) is characterized by a fully softened phonon mode, an increasing static CDW superlattice peak and no detectable change in the electronic band structure on cooling below T*. Thus, 2H-TaSe2 exhibits increasing structural before electronic order emphasizing the important lattice contribution to CDW transitions. Furthermore, our results rule out the central-peak scenario for the CDW transition in 2H-TaSe2.

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TUE 15:45-17:45 | BOARD 10 | P2-MAGN-10

POSTER SESSION

SOFT X-RAY XMCD AT 30 TESLA: A NEW PULSED MAGNETIC FIELD SETUP AT BESSY II

Presenter: Eugen WESCHKE
Authors: Oleksandr PROKHNENKO (1), Shingo YAMAMOTO (2), Benedikt EGGERT (3), Hiroyuki NOJIRI (4), Eugen WESCHKE (1)

The UE-46 PGM1 soft X-ray beamline at BESSY II, Helmholtz-Zentrum Berlin, has a successful history of studying magnetic materials and transition metal oxides in magnetic fields up to 7 Tesla. This capability was recently expanded by a new pulsed magnetic field setup that comprises a lN2-cooled magnet driven by a capacitor bank. It provides magnetic field pulses of 4 ms duration with a peak magnetic field of up to 30 Tesla. Equipped with a He flow cryostat, experiments can be carried out in a range between 8 K and room temperature. The setup has so far been commissioned for XMCD measurements by sample drain current.

30 Tesla pulses require waiting times of 5 minutes, allowing for about 100 pulses in a typical shift of 12 hours. With a rather low noise level achieved, changes in the XMCD of the order of one percent can be monitored. Selected examples will be presented, including magnetic transitions in 3d-4f intermetallics as well as XMCD in transition metal oxides. Using a reduced peak field of 12 Tesla allows for a higher repetition rate. While this is still a rather high field in soft X-ray applications, a set of element-selective hysteresis curves can be obtained within a few hours. A full set of field-dependent XMCD spectra would require one user shift.

The instrument is now open for proposals in a friendly user mode. Further, it is being developed towards the use for resonant soft X-ray scattering with applications to magnetic and correlated electron materials.

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TUE 15:45-17:45 | BOARD 11 | P2-MAGN-11

POSTER SESSION

CAPTURING PROTON DYNAMICS IN THE PHASE TRANSITIONS OF INCOMMENSURATE ORGANIC FERROELECTRICS USING SYNCHROTRON X-RAY DIFFRACTION

Presenter: Leila NOOHINEJAD
Authors: Leila NOOHINEJAD (1), Sander VAN SMAALEN (2), Carsten PAULMANN (3), Martin TOLKIEHN (1)

We will present the recent advances in the field of modulated molecular crystals with an emphasis on the links between incommensurability, intermolecular interactions, and ferroelectric properties of the materials [1]. The importance of detailed knowledge of the modulated structure for understanding the crystal chemistry and the functional properties will be presented using selected examples of incommensurate modulations in organic ferroelectrics .

Supramolecular compounds are of interest as ferroelectric materials because they have a low density and are cheap to produce, furthermore it is easy to design based on the acidity and base strength of their building blocks. The co-crystals of 5,5´-dimethyl-2,2´-bipyridine or Phenazine (as bases), with haloanilic acids are among several recently discovered hydrogen-bonded organic ferroelectrics where the acid and base blocks are connected through O—H…N bonds. The co-crystals undergo modulated paraelectric-ferroelectric phase transitions upon cooling and heating [2]. The temperature-dependent structural phase transitions of these co-crystals have been studied using synchrotron X-ray diffraction at the P24 beamline, DESY. The (3+1)-D precise atomic models were obtained using the superspace approach. We found the origin of phase transitions are in a result of the proton dynamics in intermolecular, O—H…N bond.

[1] L. Noohinejad, Aperiodic Molecular Ferroelectric Crystals, University of Bayreuth, 2016.
[2] S. Horiuchi,et.al , RSC. Adv., 2019, 9.

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TUE 15:45-17:45 | BOARD 12 | P2-MAGN-12

POSTER SESSION

PHASE TRANSTION IN La0.6Sr0.4CoO3-δ THIN FILMS BY ION IRRADIATION

Presenter: Yunxia ZHOU

Authors: Yunxia ZHOU (1,2), Lei CAO (1,3), Andreas HERKLOTZ (4), Diana RATA (4), René HÜBNER (1), Suqin HE (5), Felix GUNKEL (5), Tomas DUCHON (6), Ulrich KENTSCH (1), Manfred HELM (1), Shengqiang ZHOU (1)

Perovskite oxides exhibit rich physics related to ionic defects. In particular, the defect concentration and distribution alter the lattice parameters and affect the competitive interplay between strongly correlated electrons, enabling numerous applications as sensors, catalysts, and memristive devices. In this work, helium-ion irradiation is demonstrated as an effective, low-temperature tool to modulate the vacancy profiles in epitaxial La0.6Sr0.4CoO3-δ thin films. A significant lattice expansion solely along the out-of-plane direction is observed. By proper tuning of the irradiation parameters, the resistivity is increased up to several orders of magnitude. It indicates a phase transition from perovskite to Brownmillerite. These results offer a new playground for optimizing oxide-based spintronic and electronic devices.

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TUE 15:45-17:45 | BOARD 13 | P2-MAGN-13

POSTER SESSION

MAGNETIC TOPOLOGICAL INSULATORS MnBi2Te4·n(Bi2Te3) (n = 0, 1, …, 6): IS THERE A 3D-2D CROSSOVER AND TRANSITION TO 2D FERROMAGNETISM?

Presenter: Nazim MAMEDOV (MAMMADOV)
Authors: Nazim MAMEDOV (MAMMADOV) (1,2), Ziya ALIEV (2,1), Imamaddin AMIRASLANOV (1,2), Yegana ALIYEVA (2,1)

Magnetic topological insulators, belonging to the homologous series MnBi2Te4·n(Bi2Te3) with integer n varying from zero to infinity are derivatives of the first magnetic topological insulator MnBi2Te4 and represent systems with tunable magnetic and surface properties. They are currently in the focus of numerous studies going worldwide. However, until now these studies including ours [1] have been limited to the systems with index n smaller than 4.

We have successfully prepared the systems with higher n values and expect that systems with n=5 and 6 are very likely to have magnetically decoupled MnBi2Te4 layers, because of the increased number n of the non-magnetic Bi2Te3 layers between every two neighboring magnetic MnBi2Te4 layers. Temperature dependent neutron scattering studies of the system with n=3 [2] have disclosed still 3D character of magnetism. It is expected that system with n=4 will be bordering the 3D and 2D ferromagnetic cases while higher n systems will host purely 2D magnetism and bring about qualitatively new conditions for the realization of quantum anomalous Hall state. Facilitation of low temperature neutron studies of MnBi2Te4·n(Bi2Te3) with n=4, 5 and 6 will be discussed with interested research groups.

[1] Z. S. Aliev et al. / Journal of Alloys and Compounds 789 (2019) 443
[2] Ding et. al./ Phys. D: Appl. Phys., 54 (2021) 174003

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TUE 15:45-17:45 | BOARD 14 | P2-MAGN-14

POSTER SESSION

A STUDY OF THE LOCAL FIELDS IN BISMUTH FERRITE USING DIFFERENT RADIOACTIVE TRACER IONS

Presenter: Doru C. LUPASCU
Authors: Doru C. LUPASCU, Thien Thanh DANG, Juliana SCHELL, Marianela ESCOBAR-CASTILLO, Daniil LEWIN, Astita DUBEY

This work presents the study of the local electric and magnetic fields in multiferroic bismuth ferrite (BiFeO3: BFO) using Time Differential Perturbed Angular Correlation (TDPAC) spectroscopy. The measurements were carried out in a wide range of temperatures up to 850°C, after the implantation of various radioactive tracer ions: 181Hf, 111In and 111mCd. The experimental results reflect the obedience to the Landau theory and the Brillouin-Weiss equation of local electric polarization and magnetization, respectively. Particularly, a huge coupling between local electric and magnetic fields has been found in anti-ferromagnetic order. With the support of ab-initio DFT simulations, we are able to discuss the site-assignment for the probe nucleus, and conclude that under our experimental conditions, the 111mCd is replacing the Bi-atom at the A-site, 181Hf and 111In probes substitute the Fe-atom at the B-site of the general perovskite structure ABO3.

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TUE 15:45-17:45 | BOARD 15 | P2-MAGN-15

POSTER SESSION

NOVEL THEORETICAL PREDICTION OF PHYSICAL PROPERTIES OF PHASES MAX

Presenter: Fouad KERAMSI
Authors: Fouad KERAMSI (1), Moued MEBREK (2)

In this work, we have studied the magnetic stability, structural, electronic, elastic, magnetic, and thermodynamic properties of the Fen+1CdCn and Mnn+1SiCn. To realize this study, we used the linearly augmented plane wave method (FP-LAPW) based on density functional theory implanted in Wien2k code. The exchange–correlation potential is treated with the local density approximation LSDA.

The formation energies were calculated for the three compounds and showed that these compounds are thermodynamically stable in a ferromagnetic spin configuration. Further analysis was done to check the mechanical and dynamical stability based on Born criteria and phonon spectra. The result shows that the increase in the stacked layer increases the rigid layer mode and the metallicity of the compounds. To understand such behavior, both analysis based on electron density and topological analysis of electron density was done. Additionally, we show that the total magnetic moment increases while the number of layers increases. The study also used the quasi-harmonic method to predict some relevant thermal properties of the three stable compounds.

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TUE 15:45-17:45 | BOARD 16 | P2-MAGN-16

POSTER SESSION

XMCD OF A MOLECULAR DIAMAGNET: THE PECULIAR CASE OF Pd(II)

Presenter: Carolin SCHMITZ-ANTONIAK
Authors: Carolin SCHMITZ-ANTONIAK (1), Alevtina SMEKHOVA (2), Detlef SCHMITZ (2), Natalya V. IZAROVA (3), Maria STUCKART (4), S. Fatemeh SHAMS (3), Konrad SIEMENSMEYER (2), Frank M.F. DE GROOT (5), Paul KÖGERLER (3,4)

Soft X-ray magnetic circular dichroism (XMCD) was used to investigate the magnetism of Pd(II) ions in polyoxopalladate (POP) molecules composed of a central Pd(II) ion surrounded by a distorted cubic shell of eight oxygen ions, which is in turn encapsulated in a cuboctahedral cavity of 12 Pd(II) ions in square-planar oxygen coordination environments stabilised by capping groups [1]. XMCD at the Pd M3,2 edges accompanied by simulations based on charge transfer multiplet calculations and density functional theory unravel three different states of Pd(II) ions [2]:

(i) Conventional diamagnetism in a square-planar O4 coordination environment,

(ii) paramagnetism of central Pd(II) ions caused by four additional out-of-plane oxygen anions, and

(iii) an unusual diamagnetic state in the diamagnetic/paramagnetic crossover region modified by significant mixing of states and facilitated by the substantial 4d spin-orbit coupling.

The two diamagnetic states can be distinguished by characteristic XMCD fine structures, thereby overcoming the common limitation of XMCD to ferro-/ferrimagnetic and paramagnetic materials in external magnetic fields.

We thank HZB for allocation of synchrotron radiation beamtime and access to the CoreLab Quantum Materials. For kind support we thank the HZB staff, particularly E. Weschke and E. Schierle. Partly funded by the Helmholtz Association (VH-NG-1031).

[1] Chubarova et al., Angew. Chem. Int. Ed. 47, 9542 (2008)
[2] Smekhova et al., Comm. Chem. 3, 96 (2020)

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TUE 15:45-17:45 | BOARD 17 | P2-OTH-01

POSTER SESSION

X-RAYS MEET NEUTRONS MEET IONS MEET ELECTRONS MEET LASERS MEET MAGNETS: COMBINED ACCESS TO MULTIPLE FACILITIES THROUGH EU PROJECT “REMADE@ARI”

Presenter: Michael STUCKELBERGER
Author: Michael STUCKELBERGER

Traditional access to large-scale analytical research infrastructures (ARI) such as X-ray, neutron, or ion-beam facilities relies on facility-specific proposal systems. While this mono-modal concept is well established and satisfies a broad user community, it has several shortcomings. For example, time-sensitive experiments that require subsequent access to several ARI are hardly manageable due to a lack of coordination, and similar proposals tend to be submitted to multiple ARI by experienced users, which leads to unbalanced distribution of access.

With the EU project ReMade@ARI, we propose a different approach. For research in the field of Circular Economy that is of utmost societal relevance, ReMade@ARI offers coordinated access to more than 50 European analytical research infrastructures, comprising the leading sources for X-ray, neutron, and ion beams, with joint proposal evaluation. Beyond access, ReMade@ARI offers comprehensive services with senior scientists, facility experts, and trained young researchers realizing a user service of unprecedented quality. Particular attention is attributed to the implementation of attractive formats to support Circular Industry.

In ReMade@ARI, the most significant large-scale analytical research infrastructures join forces to pioneer a support hub for materials research facilitating a step change to the Circular Economy, which may serve as model for joint facility access in other fields of research.

Affillation
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TUE 15:45-17:45 | BOARD 18 | P2-OTH-02

POSTER SESSION

LEAPS IDEA – INCLUSION, DIVERSITY, EQUITY, AND ANTI-DISCRIMINATION

Presenter: Antje VOLLMER
Author: Antje VOLLMER (1,2)

LEAPS, the league of the accelerator-based photon sources in Europe, casts an eye on all dimensions of diversity. Fighting any kind of discrimination and going into bat for equal opportunities and inclusion is a matter of course and an uncompromising commitment of all LEAPS facilities.

Although science is ruled by objectivity and rationality, thus expected to be impervious to discrimination, the reality is, that researchers still face systemic unequality or limited opportunities.

Discrimination, imbedded socially and culturally in all our interactions with others, mostly occurs unmindfully, unintentionally, and non-deliberately. Openly displayed acts of discrimination, racism, anti-Semitism, xenophobia or homophobia, to name a few, are rarely seen in science; unconscious bias, however, happens day-to-day.

It is necessary and urgent to unlearn unconscious discriminatory behavioral habits and set up safeguards in our scientific institutions to make them more inclusive, fairer, and as a result more creative and successful.

LEAPS IDEA wants to discuss Inclusion, Diversity, Equity, and Anti-discrimination, gives an impressive number of best practice examples from the LEAPS facilities and provides a tool box to tackle the IDEA-ideas.

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TUE 15:45-17:45 | BOARD 19 | P2-OTH-03

POSTER SESSION

SCIENCE DIPLOMACY – OVERCOMING SOCIAL AND ECONOMIC IMBALANCES BY RESEARCH, DEVELOPMENT AND HIGHER EDUCATION

Presenter: Antje VOLLMER
Author: Antje VOLLMER (1,2)

Globalization brings us all closer together, the internet allows a free flow of information around the world, global challenges can be addressed jointly. At the same time, we also face a lack of equal opportunities around the globe, disintegration, national self-interest, and in parts a breaking apart of international cooperation.

Here we will try to illustrate how networks of research facilities bring together a very diverse international scientific community where the mission of the advancement in science is finely intermixed with a firm societal commitment. The importance of international collaboration as a peace-keeping and societal way-paving vehicle is illustrated taking Europe and the Middle East as examples and is extended to initiatives like “Synchrotron for Africa”.

Large scale facilities have always been multi-disciplinary, multi-national melting pots and are therefore the perfect crucible for this task. They are often the crystal nucleus for political and societal cooperations and the source point for international activities, for interdisciplinary work and for global teamwork.

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TUE 15:45-17:45 | BOARD 25 | P2-LIFE-01

POSTER SESSION

KINETICS OF AGGREGATION OF LOW DENSITY LIPOPROTEINS AND EVOLUTION OF PROTEIN GELATION DYNAMICS OF AN EGG YOLK GEL

Presenter: Nimmi Das ANTHUPARAMBIL

Authors: Nimmi Das ANTHUPARAMBIL (1,4), Anita GIRELLI (2), Sonja TIMMERMANN (1), Anastasia RAGULSKAYA (2), Mohammad Sayed AKHUNDZADEH (1), Marvin KOWALSKI (1), Fabian WESTERMEIER (4), Michael PAULUS (3), Nafisa BEGAM (2), Fajun ZHANG (2), Frank SCHREIBER (2), Michael SPRUNG (4), Christian GUTT (1)

The kinetics of heat-induced aggregation and microscopic dynamics of protein gelation of a fresh hen egg yolk are studied using in-situ X-ray photon correlation spectroscopy along with ultra-small-angle X-ray scattering. Two non-equilibrium processes occur in the egg yolk when the temperature is increased to above 65 ˚C, viz, aggregation of low-density lipoproteins (LDLs) and gelation of egg yolk proteins. The size of LDL aggregate is positively correlated to the amount of heat provided and the waiting time, thus a certain size of aggregate is achieved for a specific pair of temperature and waiting time. The microscopic dynamics reveal a sudden decrease in relaxation rate at the onset of gelation and a subsequent steady-state ballistic dynamics when the elastic protein gel is formed. The non-equilibrium dynamics of protein gelation are found to be temperature independent above 75 ˚C. These findings will be valuable not only in understanding the process of protein gelation but also in estimating the extent of temperature stability of LDLs when utilized as a drug delivery carrier.

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TUE 15:45-17:45 | BOARD 26 | P2-LIFE-02

POSTER SESSION

TRYPTOPHAN REGULATES DROSOPHILA ZINC STORES

Presenter: Nils SCHUTH

Authors: Nils SCHUTH (1), Erika GARAY (2), Alessandra BARBANENTE (3), Carlos TEJEDA-GUZMÁN (2), Daniele VITONE (3), Beatriz OSORIO (2), Adam H. CLARK (4), Maarten NACHTEGAAL (4), Michael HAUMANN (5), Holger DAU (5), Alberto VELA (1), Fabio ARNESANO (3), Liliana QUINTANAR (1), Fanis MISSIRLIS (2)

Zinc deficiency is a mayor public health concern as it is estimated to affect up to a third of the global population. Zinc deficiency is commonly attributed to inadequate absorption of the metal. Instead, we show that body zinc stores in Drosophila melanogaster depend on tryptophan consumption. Hence, a dietary amino acid regulates zinc status of the whole insect – a finding consistent with the widespread requirement of zinc as a protein cofactor. Specifically, the tryptophan metabolite kynurenine is released from insect fat bodies and induces the formation of zinc storage granules in Malpighian tubules, where 3-hydroxykynurenine and xanthurenic acid act as endogenous zinc chelators. Kynurenine functions as a peripheral zinc-regulating hormone and is converted into a 3-hydroxykynurenine-zinc-chloride complex, precipitating within the storage granules. Thus, zinc and the kynurenine pathway – well-known modulators of immunity, blood pressure, aging and neurodegeneration – are physiologically connected.

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TUE 15:45-17:45 | BOARD 27 | P2-LIFE-03

POSTER SESSION

SWELLING BEHAVIOUR OF MUCIN PARTICLES BY EXTENDED Q-RANGE SMALL ANGLE NEUTRON SCATTERING

Presenter: Christopher GARVEY
Authors: Christopher GARVEY (1), Cheng CAO (2), Liliana DE CAMPO (3), Jitendra MATA (3)

Mucins and mucin-like molecules are an important group of biomacromolecules characterized by a charged and highly glycosylated linked peptide backbone. The fundamental structural unit is a bottle-brush-like structure which may be organized into higher level aggregates or networks. The electrostatic interactions between polymer chains are of interest to understand the transport properties of these gels since gel forming attractive interactions are opposed by the electrostatic chain repulsion. In this study we have examined dilute solutions of the particles formed by pig gastric mucin (PGM) in increasing ionic strength by small angle neutron scattering (SANS) over an extended range of scattering vectors to encompass the hierarchical nature of the PGM particles. Ultra small angle neutron scattering measurements made on the Bonse-Hart type diffractometer KOOKABURRA are sensitive to the radius of gyration of the particles and the electrostatic interactions between particles. Conventional pin-hole SANS measurements were made on the two SANS instruments BILBY and QUOKKA . These measurements were sensitive to the electrostatically mediated intra-particle mucin chain correlations and thus the degree of compaction within the particle. The dependence of the scattered intensity over the extended range of scattering vectors in this study reveals the interrelationships between chain and particle electrostatic interactions.

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TUE 15:45-17:45 | BOARD 28 | P2-LIFE-04

POSTER SESSION

NON-LINEAR RADIATION EFFECTS ON THE DYNAMICS OF COOKED EGG WHITE INVESTIGATED BY X-RAY PHOTON CORRELATION SPECTROSCOPY

Presenter: Sonja TIMMERMANN

Authors: Sonja TIMMERMANN (1), Nimmi Das ANTHUPARAMBIL (1,2), Nafisa BEGAM (3), Anita GIRELLI (3), Mario REISER (4), Marc MORON (5), Marvin KOWALSKI (1), Mohammad AKHUNDZADEH (1), Hanna-Friederike POGGEMANN (6), Maximilian SENFT (3), Dennis GUTMÜLLER (3), Sebastian RETZBACH (3), Michael PAULUS (5), Fabian WESTERMEIER (2), Michael SPRUNG (2), Fajun ZHANG (3), Frank SCHREIBER (3), Christian GUTT (1)

Hen egg white is known to form a three-dimensional gel network during heating, which plays an important role in many food-manufacturing sections. The state-of-the-art method for investigating dynamics on length and time scales of the protein network is X-ray photon correlation spectroscopy (XPCS), but radiation damage is the limiting factor. We have performed XPCS measurements at ultra-small angles (USAXS) on hen egg samples with six different fluxes to investigate dose and dose rate dependencies. The samples were prepared with two concentrations of sodium chloride and have been cooked to temperatures in the range of 70 – 80°C resulting in a variety of gel network structures responding to radiation damage in different ways.

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TUE 15:45-17:45 | BOARD 29 | P2-LIFE-05

POSTER SESSION

A PIPELINE FOR A THREE-DIMENSIONAL X-RAY PHASE CONTRAST XENOPUS LAEVIS ATLAS

Presenter: Janes ODAR

Authors: Janes ODAR (1), Rebecca SPIECKER (1,2), Yaroslav ZHAROV (1), Fee WIELATH (3), Marcus ZUBER (2), Thomas VAN DE KAMP (2), Alexey ERSHOV (1), Tomas FARAGO (2), Elias HAMANN (2), Philipp VICK (3), Kerstin FEISTEL (3), Tilo BAUMBACH (1,2)

The African clawed frog (Xenopus laevis) is an important model organism to study development and disease. Its embryos are routinely utilized to investigate early developmental processes like gastrulation, neurulation and organogenesis. The first anatomical 2D atlas based on light microscopy images of cut samples was presented in 1991 to serve as a compendium of different developmental stages. Up to today this work is the most important reference for the development of X. laevis.

The opaqueness of the embryos prevents a 3D investigation of embryogenesis by traditional methods. While the low absorbing soft tissues impede X-ray absorption tomography in laboratories, synchrotron X-ray phase-contrast micro-tomography enables the analysis of whole embryos in 3D with cellular resolution. To further enhance the contrast of the tissues for AI post-processing an additional staining approach may be employed.

Here we present a pipeline of sample fixation, staining, high-throughput X-ray microtomography and optimized post-processing in order to create a 3D atlas of X. laevis early developmental stages that will substantially complement the existing 2D atlas. Moreover, this pipeline provides the large X. laevis community with a guideline to create their own X-ray phase-contrast data in the future while facilitating data comparability. Finally these data will broaden our understanding of gene functions, mutations and the influence of external factors to environmental factors.

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TUE 15:45-17:45 | BOARD 30 | P2-LIFE-06

POSTER SESSION

FACILITIES FOR MACROMOLECULAR CRYSTALLOGRAPHY AT THE HZB

Presenter: Manfred WEISS
Authors: Tatjana BARTHEL, Laila BENZ, Thomas CROSSKEY, Ronald FOERSTER, Paula FROELING, Christine GLESS, Thomas HAUSS, Michael HELLMIG, Frank LENNARTZ, Uwe MUELLER, Gert WEBER, Jan WOLLENHAUPT, Markus WAHL, Manfred WEISS

The Macromolecular Crystallography (MX) group at the Helmholtz-Zentrum Berlin (HZB) has been in operation since 2003. Since then, three state-of-the-art synchrotron beam lines (BL14.1-3) for MX have been built up on a 7T-wavelength shifter X-ray source. Currently, the three beam lines represent the most productive MX-stations in Germany, with nearly 4000 PDB depositions (Status 04/2022). BLs14.1 and 14.2 are energy tunable in the range 5.5-15.5 keV, while beam line 14.3 is a fixed-energy side station operated at 13.8 keV. All three beam lines are equipped with state-of-the-art detectors: BL14.1 with a PILATUS3S 6M detector, BL14.2 with a PILATUS3S 2M and BL14.3 with a PILATUS 6M detector. BL14.1 and BL14.2 are in regular user operation providing close to 200 beam days per year and about 600 user shifts to approximately 100 research groups across Europe. Recently remote beamline operation has been established successfully at BL14.1 and BL14.2. BL14.3 is been equipped with a MD2 micro-diffractometer, a HC1 crystal dehydration device and a REX nozzle changer making it suitable for room temperature experiments. Additional user facilities include office space adjacent to the beam lines, a sample preparation laboratory, a biology laboratory (safety level 1) and high-end computing resources. On the Poster Session a summary on the experimental possibilities of the beam lines and the ancillary equipment provided to the user community will be given.

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TUE 15:45-17:45 | BOARD 31 | P2-LIFE-07

POSTER SESSION

FRAGMENT SCREENING BY MACROMOLECULAR CRYSTALLOGRAPHY – EFFICIENT WORKFLOW FOR USERS AT BESSY II

Presenter: Manfred S. WEISS
Authors: Jan WOLLENHAUPT (1), Tatjana BARTHEL (1), Elmir JAGUDIN (2), Dirk WALLACHER (1), Thomas HAUSS (1), Frank LENNARTZ (1), Thomas CROSSKEY (1), Uwe MÜLLER (1), Andreas HEINE (3), Tobias KROJER (2), Manfred S. WEISS (1)

To develop biochemical tool compounds or lead structures in drug discovery, screening for small organic molecules called fragments became a predominant technique in the last decade. Carried out as a crystallographic screening it reveals not only the identity of the bound fragments, but also their 3D-positioning inside the binding site of the protein under study. At the macromolecular crystallography (MX) beamlines at BESSY II, a dedicated workflow was established for the user community to foster efficient and convenient screening.[1] It is based on several unique developments, one being the very diverse F2X fragment libraries that deliver high hit rates, mostly in the range of 20–25%.[2] Using the EasyAccess Frame, fast and comfortable crystal soaking and harvesting is ensured.[3] After data collection at the state-of-the-art MX beamlines at BESSY II, data analysis is highly automated and conveniently interfaced via the FragMAXapp setup at HZB.[4] Beyond efficient screening and identification of fragment hits, HZB also offers methods of hit evolution to higher potency using a growing by catalog approach via Frag4Lead.[5]

[1] Wollenhaupt, J. et al. J. Vis. Exp. 2021, 62208 (2021).
[2] Wollenhaupt, J. et al. Structure 28, 694-706.e5 (2020).
[3] Barthel, T. et al. J. Appl. Crystallogr. 54, 376–382 (2021).
[4] Lima, G. M. A. et al. Acta Crystallogr. Sect. D Struct. Biol. 77, 799–808 (2021).
[5] Metz, A. et al. Acta Crystallogr. Sect. D Struct. Biol. 77, 1168–1182 (2021).

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TUE 15:45-17:45 | BOARD 32 | P2-LIFE-08

POSTER SESSION

DOSE RATE DEPENDENT X-RAY INDUCED DYNAMICS IN DENSE ANTIBODY-PROTEIN SOLUTIONS (IG-PEG AND BSA)

Presenter: Mohammad Sayed AKHUNDZADEH

Authors: Mohammad Sayed AKHUNDZADEH (1), Anita GIRELLI (2), Sonja TIMMERMANN (1), Nimmi Das ANTHUPARAMBIL (1), Marvin KOWALSKI (1), Anastasia VLADIMIROVNA RAGULSKAYA (2), Hanna-Friederike POGGEMANN (2), Nafisa BEGAM (2), Maximilian SENFT (2), Mario REISER (3), Fabian WESTERMEIER (4), Michael SPRUNG (4), Fajun ZHANG (2), Frank SCHREIBER (2), Christian GUTT (1)

There is a general interest in studying protein dynamics in crowded solutions with aspects of phase separation, protein crystallization, gelation, and the protein glass transition. The dynamics of protein systems are often heterogeneous in nature and need to be measured on length scales ranging from micrometers to nanometers and corresponding time scales ranging from second to micro-seconds. This time-space window can be accessed via X-ray Photon Correlation Spectroscopy (XPCS) utilizing the coherent X-ray beam from third-generation synchrotron facilities. By measuring fluctuations in X-ray speckle patterns we can investigate the spatial and temporal properties of the sample simultaneously, and the heterogeneous processes can be studied using a multi-speckle two-time correlation function. However, proteins are very susceptible to radiation damage, especially in water environments, which requires to study the effects of dose and dose rate on the measured dynamic properties.

Here, we investigate the radiation-induced dynamics in dense antibody-protein (immunoglobulin G (IgG) and the Bovine serum albumin (BSA). By applying different X-ray doses and dose rates we observe a pronounced dose rate dependence on the shape and relaxation rate of the intermediate scattering functions of the protein systems.

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TUE 15:45-17:45 | BOARD 33 | P2-LIFE-09

POSTER SESSION

QUANTITATIVE ANALYSIS OF TRACE ELEMENTS IN PANCREATIC CARCINOMA AND PANCREAS SECTIONS BY REFERENCE-FREE X-RAY FLUORESCENCE ANALYSIS

Presenter: Katja FRENZEL

Authors: Katja FRENZEL (1), Yves KAYSER (1), Andrea HORNEMANN (1), Arne HOEHL (1), Petros MOURATIDIS (2), Ian RIVENS (2), Chelsea NIKULA (3), Alex DEXTER (3), Burkhard BECKHOFF (1), Gail TER HAAR (2)

To assess innovative medical therapeutic approaches the physical and chemical analysis of organic tissues with reliable and preferably traceable methods is essential. Reference-free X-ray Fluorescence (XRF) allows to monitor treatment effects via the spatial distribution of the absolute elemental mass depositions of trace elements within samples using radiometrically calibrated instrumentation and reliable knowledge of atomic fundamental parameters.

Within the RaCHy project malignant and benign pancreatic tissue sections of mice were analysed to assess radiotherapy treatment induced changes. Pancreas of healthy mice, mice with pancreatic cancer treated with radiotherapy or with untreated pancreatic cancer were extracted and sectioned. The dried tissue sections were fixated on glass or quartz slides and analysed by reference-free XRF to investigate differences and changes of the spatial absolute elemental mass depositions distribution of Na, Mg, P, S, Cl, K and Ca between samples.

As it is important to be aware of changes inflicted on biological samples during probing, repetitive measurements allowing for the investigation of X-ray irradiation-induced changes in binding states of carbon and nitrogen compounds were conducted. In addition, over-time binding state degradation of carbon and nitrogen compounds of the tissue samples were observed.

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TUE 15:45-17:45 | BOARD 34 | P2-LIFE-10

POSTER SESSION

SHORT-TIME TRANSPORT PROPERTIES OF BIDISPERSE SUSPENSIONS OF IMMUNOGLOBULINS AND SERUM ALBUMINS CONSISTENT WITH A COLLOID PHYSICS PICTURE

Presenter: Christian BECK

Authors: Christian BECK (1,2), Marco GRIMALDO (2), Hender LOPEZ (3), Stefano DA VELA (1,4), Benedikt SOHMEN (5), Fajun ZHANG (1), Martin OETTEL (1), Jean-Louis BARRAT (6), Felix ROOSEN-RUNGE (7), Frank SCHREIBER (1), Tilo SEYDEL (2)

The crowded environment of biological systems such as the interior of living cells is occupied by macromolecules with a broad size distribution. This polydispersity changes the dependence of the diffusive dynamics of given tracer macromolecules on the volume fraction from the known dependence in a monodisperse solution. The resulting size-dependence of diffusive transport crucially influences the function of a living cell. Here, we investigate a simplified model system consisting of two constituents in aqueous solution, namely of the proteins bovine serum albumin (BSA) and bovine polyclonal gamma-globulin (Ig), systematically controlling the total volume fraction and ratio of these constituents. From high-resolution quasi-elastic neutron spectroscopy, the short-time diffusion coefficients for BSA and Ig, respectively, in the mixture are individually extracted and show substantial deviations from the diffusion coefficients measured in monodisperse solutions. These deviations are modeled quantitatively using computational results for the short-time rotational and translational diffusion in a two-component hard sphere system with two distinct, effective hydrodynamic radii. We find that a simple colloid picture describes short-time diffusion in binary mixtures well. Notably, the self-diffusion of the smaller protein BSA in the mixture is faster than the diffusion in a pure BSA solution, whereas the self-diffusion of Ig in the mixture is slower than in the pure Ig solution.

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TUE 15:45-17:45 | BOARD 35 | P2-LIFE-11

POSTER SESSION

SERIAL TOMOGRAPHY AND SEMI-AUTOMATIC ANALYSIS OF INSECTS

Presenter: Thomas VAN DE KAMP
Authors: Thomas VAN DE KAMP (1), Philipp D. LÖSEL (2), Vincent HEUVELINE (2), Lars KROGMANN (3), Tilo BAUMBACH (1)

Insects fulfill key functions in our ecosystems and form the basis for complex food webs. Although the global insect decline has been apparent for decades, its true extent and the associated consequences of decreasing biodiversity are still unclear. Investigations of insect biology, evolution and morphology are therefore highly relevant not only for scientific questions but to a large extent also for society. However, the relative wealth of genetic data collected in recent years is hardly matched by comparative 3D morphological information.

Serial X-ray microtomography experiments at the KIT Light Source demonstrated the value of the method for the digitization and 3D analysis of large scientific collections of extant and fossil specimens. In this presentation we highlight recent results, including fossil parasites, peculiar mandibles in minute wasps and a comprehensive repository for ant morphology.

Despite the ongoing advances in X-ray imaging, analyzing insect micro-CT data is still often tedious and time-consuming. Especially the manual segmentation of large and complex datasets remains a major bottleneck for large comparative studies. We developed Biomedisa ("Biomedical Image Segmentation App") as an open-source online platform for semi-automatic segmentation of large volumetric datasets. Here, we demonstrate how to employ this software for the semi-automatic segmentation of insect micro-CT data.

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TUE 15:45-17:45 | BOARD 36 | P2-LIFE-12

POSTER SESSION

BIOLOGICAL SAXS IN CORONA TIME: AUTOMATION, REMOTE OPERATION AND SCIENTIFIC PROJECTS

Presenter: Clement E. BLANCHET
Authors: Clement E. BLANCHET, Melissa GRAEWERT, Cy JEFFRIES, Daniel FRANKE, Dmitri SVERGUN

The last years of pandemic with lasting lockdowns and travel restrictions have been challenging for the mobile user community of large-scale scientific facilities. Synchrotron beamlines were urged to develop new ways to work under these conditions, in particular for experiments aiming at better describing the virus and developing therapeutics or vaccines against Covid-19.

Biological solution Small Angle X-ray Scattering (BioSAXS) is a key method in biophysics and structural biology. It provides information on the size and shape of biological macromolecules and assembly in solution. It is one of the synchrotron techniques helping in the fight against the SARS-CoV-2 virus.

The P12 beamline of EMBL Hamburg (on PETRA III), is dedicated to BioSAXS. We shall present here the response of the P12 team to the current pandemic and describe the beamline automation that allowed a smooth transition from on-site visits to a full remote/mail-in mode.

We shall also specifically highlight Covid-related projects carried out at P12. For example, the receptor-binding domain of the spike protein was measured in presence of nanobodies that could neutralize the virus. The stoichiometry and topology of the nsp7+8 complexes of the virus replication transcription complex were determined using SAXS and mass spec. SAXS has also been particularly useful to study and characterize the lipid nanoparticles employed to package nucleic acids in mRNA vaccine used against Covid.

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TUE 15:45-17:45 | BOARD 37 | P2-LIFE-13

POSTER SESSION

CeCILE – INTELLIGENT DETECTION, TRACKING AND CELL CYCLE EVALUATION OF EUKARYOTIC CELLS ON PHASE-CONTRAST LIVE-CELL VIDEOS

Presenter: Sarah RUDIGKEIT
Authors: Sarah RUDIGKEIT (1), Hai HUANG (2), Julian REINDL (1), Helmut MAYER (2), Judith REINDL (1)

The reaction of tissue to irradiation is based on the radiation effects on single cells. The most notable reactions of cells to irradiation are cell cycle arrest, proliferation, and cell death. We present a new approach to investigate these biological endpoints in one experiment: The use of long-term live-cell phase-contrast videos analyzed by a deep-learning-based algorithm called CeCILE (Cell Classification and In-vitro Lifecycle Evaluation).

After irradiation, the cells were imaged for up to 5 days. The created videos were then analyzed by CeCILE, which is based on a faster RCNN algorithm for object detection and is trained on a hand-labelled dataset of microscopic videos. In these videos, all cells were assigned to one of four classes, which defines the cells' state in the cell cycle. Then, a tracking algorithm assigns an individual ID to every cell in the video. The tracking is conducted employing hidden Markov models to simulate the cell movements and states and an embedded recursive Bayesian filter to predict their behaviors via inference.

In conclusion, we are able to investigate the behavior of irradiated cells in one simple experiment on a single cell basis. The first version of CeCILE was able to achieve similar results compared to state-of-the-art assays. The upgrade with the Markov-model-based tracking allows to go further by inspecting the behavior of every single cell by evaluating the cell-cycle, the lineages, and the circumstances of cell death.

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TUE 15:45-17:45 | BOARD 38 | P2-LIFE-14

POSTER SESSION

DESIGN OF A PRECLINICAL PROTON MINIBEAM RADIOTHERAPY FACILITY

Presenter: Jessica NEUBAUER
Authors: Jessica NEUBAUER, Tarik GENCASLAN, Aikaterini ROUSSETI, Gerd DATZMANN, Michael MAYERHOFER, Günther DOLLINGER, Judith REINDL

Spatial fractionated radiotherapy using protons, so-called proton minibeam radiotherapy (pMBRT), was developed for better sparing of normal tissue in the entrance channel of radiation. Preclinical in-vivo experiments, conducted with pMBRT in animal models, support the prospects. Progressing towards clinical usage, pMBRT research should overcome technical and biomedical limitations of the current irradiation test stages and animal models.

This work discusses the design of a preclinical pMBRT facility. Two major parts, which have to be designed and constructed, are the dose monitor and the range shifter. To monitor high local dose rates, a parallel plate ionization chamber was constructed. As electrodes aluminum coated mylar foils were used. Here, we present the final prototype construction and first reference measurements. We show beam spreading simulations of different materials, which can be used as range shifter. Also we present the possibility of using a hybrid range shifter split in two parts, one in vacuum and one in air. This supports keeping beam size small and offers maximum flexibility. Additionally we introduce a possible quality assurance procedure, which has to be conducted to be able to apply the pMBRT in small animals with sufficient small beam size, positioning accuracy as well as lateral and axial dose profiles. For this purpose we show first pilot studies of a cancer model which will be used as a preliminary stage of the animal model.

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TUE 15:45-17:45 | BOARD 39 | P2-LIFE-15

POSTER SESSION

DYNAMIC CLUSTER FORMATION, VISCOSITY AND DIFFUSION IN MONOCLONAL ANTIBODY SOLUTIONS

Presenter: Ilaria MOSCA
Authors: Ilaria MOSCA (1,2), Kevin POUNOT (2), Christian BECK (2), Olga MATSARSKAIA (1), Christoph GRAPENTIN (3), Tilo SEYDEL (1), Frank SCHREIBER (2)

Antibodies play an essential role in the immune response of mammals. Monoclonal antibodies (mAbs) are particularly relevant for therapeutic approaches due to their high target specificity. The pharmaceutical challenge is to formulate highly concentrated antibody solutions to achieve a significant therapeutic effect and to simultaneously minimize their viscosity for subcutaneous injection [1]. Since the understanding of macroscopic viscosity requires a deep knowledge on protein diffusion and dynamic cluster formation [2,3], we study the self-diffusion of mAbs in aqueous solution as a function of the type of antibody and of their concentration, by quasi-elastic neutron spectroscopy (QENS). QENS allows to unambiguously determine the hydrodynamic cluster size [4] and gain information on the internal dynamics, which can be compared to results obtained by MD simulations. As a reference, we use polyclonal IgG solutions [5], thus obtaining a comprehensive picture of mAb diffusion.

[1] V. I. Razinkov, et al.: J. Biomol. Screen. 2015 Apr, 20 (4);
[2] S. von Bülow, et al.: PNAS May 14, 2019, 116 (20);
[3] M. Heinen, et al.: Soft Matter 2012, 8, 1404;
[4] M. Grimaldo, et al.: Quarterly Reviews of Biophysics 2019, 52, e7.

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TUE 15:45-17:45 | BOARD 40 | P2-LIFE-16

POSTER SESSION

EMBL@PETRA4 – AN INTEGRATED FACILITY FOR STRUCTURAL BIOLOGY AND IMAGING

Presenter: Selina L. STORM
Authors: Selina L. STORM, Gleb BOURENKOV, Elizabeth DUKE, Clement BLANCHET, Michael AGTHE, David VON STETTEN, Stefan FIEDLER, Dmitri SVERGUN, Matthias WILMANNS, Thomas R. SCHNEIDER

As a partner of DESY in the planning PETRA IV, EMBL is proposing an Integrated Facility for Structural Biology and Imaging. The facility will offer both easy-to use, robust, and remotely accessible measurement services and cutting-edge capabilities for tackling the most challenging experiments. Services supporting the preparation of samples and for the of experimental data will be offered in an integrated fashion.

The core of the facility is proposed to consist of endstations for static and time-resolved small-angle X-ray scattering (BioSAXS) and macromolecular crystallography (MX), and medium-resolution high-throughput phase-contrast X-ray imaging (HiTT).

BioSAXS will benefit from PETRA IV beam by shorter data collection times, lower sample consumption and unprecedented time resolution. Novel SAXS experiments will become possible to bridge the gap between the synchrotron-based and XFEL studies.

For MX, the increased brilliance of PETRA IV will increase throughput and enable the collection of diffraction data to higher spatial resolution from small and/or less-ordered crystals, time-resolved crystallography will have access to shorter time-scales.

The increased coherence of PETRA IV will revolutionize X-ray based imaging imaging. We will provide X-ray imaging in an operational mode facilitating its use by a wide user community for answering biological questions. Scale-bridging and correlative imaging will be offered in cooperation with other providers of imaging technologies.

Affillation
EMBL Hamburg, Germany

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TUE 15:45-17:45 | BOARD 41 | P2-LIFE-17

POSTER SESSION

BIOLOGICAL CRYSTALLOGRAPHY AND X-RAY IMAGING ON EMBL@PETRA III BEAMLINES

Presenter: Gleb BOURENKOV

Authors: Gleb BOURENKOV, Isabel BENTO, Saravanan PANNEERSELVAM, David VON STETTEN, Michael AGTHE, Selina STORM, Kirill KOVALEV, Marina NIKOLOVA, Stefan FIEDLER, Jonas ALBERS, Elizabeth DUKE, Thomas R. SCHNEIDER

P13 is a high-flux high-throughput MX beamline (10^13 ph/s, 4-16 keV, >= 15 µm beam diameter). An upgrade of the X-ray optics towards providing a top-hat beam profile is in preparation.

P14 is tunable (6-30 keV) and can be operated in two modes: 'collimated' and 'micro-focusing', between which the user can toggle within 20 seconds. In collimated mode, a top-hat beam, that can be shaped to any size between 20 and 300 µm is provided for optimized conditions for high-resolution crystallography and large macromolecular complexes. Using high energy photons up to 26.7 keV in combination with an recently installed EIGER2 16M CdTe detector, extraordinary data quality is obtained in such experiments. In micro-focusing mode, the recently upgraded KB system enables data acquisition by serial methods as well as fast time resolved experiments with sub-ms time resolution.

At both P13 and P14 a high throughput-mode configuration (>30 samples per hour) is available and has been recently used in a screening campaign by an industrial customer.

Building on the beam quality and versatility of P14, we recently established a high-throughput pipeline for phase contrast X-ray imaging at sub cellular resolution (0.2–0.7 µm voxel, 1 mm FOV, <5 min data collection). The method has found important applications as a targeting or scale-bridging tool in multi-modal imaging applications.

For access: smis.embl-hamburg.de. Funding from the BMBF via the Verbundforschung-Programm is gratefully acknowledged.

Affillation
EMBL Hamburg Unit c/o DESY, Germany

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TUE 15:45-17:45 | BOARD 42 | P2-LIFE-18

POSTER SESSION

SMALL WASPS, BIG DATA: REVEALING THE MORPHOLOGY, DEVELOPMENT AND BEHAVIOR OF PARASITOID WASPS USING SYNCHROTRON X-RAY IMAGING

Presenter: Pauline PFEIFFER
Authors: Pauline PFEIFFER (1), Rebecca SPIECKER (2), Thomas VAN DE KAMP (3), Lars KROGMANN (1)

Within parasitoid wasps, Chalcidoidea is one of the most speciose superfamilies with estimated 500.000 predominantly parasitoid species. They parasitize a variety of host stages and insect orders. Since they kill their host at the end of their development, they fulfill a key role as antagonists in natural and managed ecosystems and are therefore of great economic value as biological pest control. The evolution of the parasitoid lifestyle led to a great diversification, a wide range of life history strategies and miniaturization. Due to their small size and high diversity, little is known about the larval and pupal morphology. To study morphology, development and behavior, we examined numerous species within Chalcidoidea at different life stages exhibiting different life history strategies using synchrotron-micro-computed tomography (SR-µ-CT). This non-invasive imaging technique allowed high-throughput image acquisition of the external and internal morphology in a high resolution and a subsequent detailed virtual reconstruction, interactive manipulation and analysis of this data. We created an open-access and interactive 3D reconstruction of the internal and external morphology of the model organism Nasonia vitripennis (Pteromalidae) as an atlas for other scientists and students, identify and describe the immature stages of Ooencyrtus telenomicida (Encyrtidae) and show the emergence of Trichogramma cacoeciae (Trichogrammatidae) using dose-efficient in-vivo imaging.

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TUE 15:45-17:45 | BOARD 43 | P2-LIFE-19

POSTER SESSION

IMPLEMENTATION OF A ROBOTIC SYSTEM FOR CRYSTAL TRANSFER AND STORAGE AFTER REMOTELY CONTROLLED HARVESTING AS PART OF THE MX PIPELINE AT EMBL HAMBURG

Presenter: Stefan FIEDLER

Authors: Stefan FIEDLER (1), Moises BUENO (2), Vamsee PALNATI (1), Thomas GEHRMANN (1), Doris JAHN (1), Elias BOEHME (1), Liliana KOLWICZ-CHODAK (1), Jochen MEYER (1), Uwe RISTAU (1), Jeremy SINOIR (3), Maria GARCIA ALAI (1), Thomas SCHNEIDER (1)

The Integrated Facility for Structural Biology located at the European Molecular Biology Laboratory (EMBL) at PETRA III in Hamburg provides a highly integrated environment for the automated and remotely controlled preparation, measurement and structure analysis of protein crystals. A key element of this pipeline is a Crystal Direct Harvester (EMBL Grenoble, ARINAX (Moirans, France)) for the automated harvesting of crystals that is located in the Sample Preparation and Characterisation Laboratory (https://www.embl.org/groups/sample-preparation-characterisation/) adjacent to the beamlines. The Crystal Harvester can harvest protein crystals onto sample pins (SPINE standard) and has been interfaced with a robotic transfer system. This system is based on the MARVIN (Multi-Axis Robotic Versatile INstaller) robotic sample changer used at the beamlines. It transfers the cryo-cooled and mounted crystals into standardized SPINE baskets kept in a large storage dewar. Once filled, the baskets can be transported to one of the synchrotron beamlines for structure determination. This new robotic sample transfer system is removing one of the last manual steps in the automation pipeline for protein crystallography. It allows a more efficient use of CDHarvester and provides the option to operate the system remotely which becomes particularly important during times when in-situ operation is not always possible.

Affillation

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TUE 15:45-17:45 | BOARD 44 | P2-LIFE-20

POSTER SESSION

HIGH THROUGHPUT TOMOGRAPHY (HiTT) OF BIOLOGICAL SAMPLES ON EMBL BEAMLINE P14 ON PETRA III

Presenter: Jonas ALBERS
Authors: Jonas ALBERS, Gleb BOURENKOV, Marina NIKOLOVA, Ivars KARPICS, Thomas R. SCHNEIDER, Elizabeth DUKE

The state of the art MX EMBL beamline P14 on PETRA III has been adapted to perform high-resolution phase contrast tomography. We take advantage of the coherent top hat beam to acquire X-ray tomograms with submicron voxel sizes in a few minutes. Each acquisition is automatically performed at four different propagation distances; phase contrast information is then extracted using the contrast transfer function algorithm. The complete imaging interface is integrated in the MXCuBE graphical user interface and data processing, such as phase-retrieval and tomographic reconstruction can be triggered automatically following successful data acquisition. By utilizing the computational resources of the EMBL Hamburg beamline compute cluster the data processing was reduced to a few minutes ensuring a high throughput data collection pipeline.

We have used the beamline to image a wide variety of biological samples both stained and unstained ranging from resin embedded cell organoids with a diameter of ~100µm, to small organisms such as platynereis. In addition both resin and paraffin embedded tissue samples such as brain, kidney or lung have been imaged.

Therefore, due to its flexibility, high-resolution and high-throughput P14's imaging setup is a promising development to study large cohorts of biological samples as a standalone application or in a correlative approach with other imaging modalities such as electron microscopy.

Access is provided via the EMBL Hamburg User Program.

Affillation
EMBL Hamburg Unit c/o DESY, Germany

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TUE 15:45-17:45 | BOARD 45 | P2-LIFE-21

POSTER SESSION

SPECIFIC STRUCTURE RESOLUTION OF PHARMACEUTICAL CARRIERS BY CONTRAST VARIATION: D-SANS AND (A)SAXS

Presenter: Thomas NAWROTH

Authors: Thomas NAWROTH (1), Christoph WILHELMY (1), Lukas UEBBING (1), Peter LANGGUTH (1), Raphael JOHNSON (2), Markus SAENGER (3), Heinz SCHMIDBERGER (3), Jorge Moreno HERRERO (4), Sahadat SHEIKH (4), Heinrich HAAS (4), Urgur SAHIN (4), Guenther GOERIGK (5), Peter BOESECKE (6), Alberto BRAVIN (6), Martin SCHROER (7), Clement BLANCHET (8), Melissa GRAEWERT (8), Dmitri SVERGUN (8), Aurel RADULESCU (9), Ralf SCHWEINS (10), Olga MATSARSKAIA (10)

Pharmaceutical nanocarriers are complexes composed of frame materials, e.g. lipids or polymers, and medically active materials, such as bio-chemical drugs or biological agents, e.g. proteins or mRNA. The structure is the key to the medical application and safety. The formulation depends on the application pathway, which may be oral (tablets, capsules), pulmonary (inhalation), intramuscular (tissue injection), parenteral (blood injection), or intracranial (brain injection). Success, patient security and structure issues increase in this sequence.

The structure determination by solution scattering and imaging of neutrons and synchrotron X-rays is enforced by specific component labeling by deuteration in SANS, magnetic material scattering, or heavy metal scattering, absorption and fluorescence (ASAXS, imaging), in combination with DLS as µm size range extension.

We have investigated the structure and development of pharmaceutical nanocarriers in original form (static) and upon simulated application (dynamic, space-time resolved) by contrast labeling via selective deuteration and lanthanide complexes. The studies were done by SANS, SAXS and ASAXS with lipid and polymer frame carriers and surface modification by an artificial protein shell for specific bio-targeting, e.g. in cancer therapy. The application of the complementary neutron and X-ray methods combines the detection of deuterated lipids and mRNA without radiation damage with high resolution scattering, focussing and flux.

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TUE 15:45-17:45 | BOARD 46 | P2-LIFE-22

POSTER SESSION

WHAT MAKES CHALKY TEETH CRUMBLE? A MULTIMODAL HIGH-RESOLUTION XRF AND WAXS STUDY ON MIH-TEETH

Presenter: Gudrun LOTZE

Authors: Gudrun LOTZE (1), Sebastian KALBFLEISCH (2), Carina KAMPLEITNER (3,4,5), Clemens WENIGER (2), Zdenek MATEJ (2), Satishkumar KULKARNI (6), Thomas F. KELLER (6), Surya Snata ROUT (7), Imke GREVING (7), Stefan TANGL (3,4), Katrin BEKES (8)

Molar incisor hypomineralization (MIH) is a worldwide growing developmental dental condition in paediatric dentistry with a prevalence of up to 44 % [1].

MIH-teeth are highly prone to fracture and caries as hardness, elasticity, and acidic resistance of the enamel barrier are deteriorated. It is unclear why the mechanical properties with respect to the mineral phases are so significantly compromised. Sound enamel exhibits high stiffness and hardness. The drastic difference indicates structural changes in MIH. However, the MIH-enamel microstructure, its orientations, and chemical composition are unknown over multiple length scales.

To characterize these differences and to close this gap in the structure-property relationship in MIH, we have studied MIH-enamel and sound enamel with high-resolution scanning WAXS and XRF recently at a synchrotron. We will present the experimental design, its challenges, and the first results of correlated data of simultaneous WAXS and XRF measurements.

This contribution will be the first one showing enamel with sub-500nm and sub-100nm beam size spatial resolution.

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[1] Bekes, K., Molar Incisor Hypomineralization - A Clinical Guide to Diagnosis and Treatment, Springer, 2020. https://doi.org/10.1007/978-3-030-31601-3

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TUE 15:45-17:45 | BOARD 47 | P2-LIFE-23

POSTER SESSION

THE pH VALUE INFLUENCES VIBRATIONAL MODES OF THE IRON-SULFUR PROTEIN Apd1

Presenter: Lukas KNAUER

Authors: Hendrik AUERBACH (1), Lukas KNAUER (1,2), Kathrin STEGMAIER (2), Aleksandr CHUMAKOV (3), Antonio PIERIK (2), Volker SCHÜNEMANN (1)

The iron sulfur protein Apd1 has a [2Fe-2S] cluster coordinated by two cysteines and two histidines. In bacteria, plants, fungi, and unicellular pathogenic eukaryotes Apd1 is found, but not in Metazoe, while its in-vivo function is still unclear [1]. In order to investigate the influence of the protonation state of the histidine on the electronic properties of the histidine coordinated iron-ion three samples with different pH values were prepared. The samples were measured on the Nuclear Resonance Beamline ID18 at European Synchrotron Radiation Facility (ESRF) in Grenoble by nuclear forward scattering (NFS) and nuclear inelastic scattering (NIS) on 57Fe at 14.4 keV [1]. The NFS measurements showed that with increasing pH, the isomer shift decreases. This can be attributed to the anionic character of the histidine in the deprotonated state, which leads to a shortening of the bond length between the iron ion and the Nδ of the histidine. NIS experiments allow to identify individual vibrational cluster modes with a possible functional relevance with regard to electron transfer.

[1] Stegmaier, K., Blinn, C. M., Bechtel, D. F., Greth, C., Auerbach, H., Müller, C. S., Jakob, V., Reijerse, E. J., Netz, D. J. A., Schünemann, V., and Pierik, A. J. (2019) Apd1 and Aim32 Are Prototypes of Bishistidinyl-Coordinated Non-Rieske 2Fe-2S Proteins. Journal of the American Chemical Society 141, 5753–5765 10.1021/jacs.8b13274 PMID 30879301

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TUE 15:45-17:45 | BOARD 48 | P2-LIFE-24

POSTER SESSION

THE HIGH-THROUGHPUT MACROMOLECULAR CRYSTALLOGRAPHY BEAMLINE P11 AT PETRA III

Presenter: Helena TABERMAN

Authors: Helena TABERMAN (1), Clemente BORGES (1), Spyros CHATZIEFTHYMIOU (1), Eva CROSAS (2), Andrey GRUZINOV (1), Bernhard KISTNER (1), Guillaume POMPIDOR (1), Jialing SONG (1), Johanna HAKANPÄÄ (1)

P11 is a diverse instrument for macromolecular crystallography[1] with energy range of 5.5-28 keV having Eiger2 X 16M as a stationary detector and the possibility of using a CdTe-detector for higher energies. Beam size from 200x200 µm to 4x9 µm can be used with a maximum photon flux of 1.3x10^13 ph/s at 12 keV. The automatic sample changer is based on unipucks with a capacity of 23 pucks (368 samples) having a mount-unmount cycle of ~36 s, bringing the beamtime/sample to ca. 2 min.

P11 allows the adjustment to non-standard experiments e.g. serial synchrotron crystallography with sample delivery on solid supports or tape-drive setup[2]. After establishing the remote connection using FastX-access via dedicated remote machine in 2020, the mode of operation has changed almost exclusively to remote.

This year MXCuBE will be employed as the default control software with the integration to ISPyB. Furthermore, development of parallel autoprocessing pipelines in addition to the currently used XDSAPP-based [3], and the implementation of strategy calculations are carried out. These imrovements are synchronising P11 with the EMBL beamlines for the future uniform structural biology village at PETRA IV.

[1] Burkhardt A., et al., Status of the crystallography beamlines at PETRA III. Eur. Phys. J. Plus 131, 56 (2016)
[2] Beyerlein K. R., et al., Mix-and-diffuse serial synchrotron crystallography. IUCrJ 4, 769-777 (2017)
[3] Sparta KM, et al., XDSAPP2.0. J. Appl. Cryst. 49, 1085-1092 (2016)

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TUE 15:45-17:45 | BOARD 49 | P2-LIFE-25

POSTER SESSION

X-RAY FLUORESCENCE IMAGING OF HUMAN ATHEROSCLEROTIC PLAQUES

Presenter: Rajni RAJNI

Authors: Rajni RAJNI (1,2), Peter MODREGGER (1,2), Mallika KHOSLA (1,2), Prerana CHAKRABARTI (1,2), Kathryn M. SPIERS (3), Bükem TANÖREN (4), Özgül ÖZTÜRK (1), Mehmet BURCIN UNLU (4,5)

According to the World Health Organization cardiovascular diseases (CVD) are the most common cause of death globally. Associated atherosclerotic plaques develop in roughly two stages. At first, a plaque is composed of a lipid-rich core covered by a fibrous cap, which is prone to rupture, leading to strokes. Then the plaque is stabilized by progressive calcification. Scanning acoustic microscopy (SAM) constitutes a method that potentially can differentiate between stable and unstable plaques by determining the Ca concentration. However, SAM only reveals relative and not absolute Ca concentrations. We have used synchrotron radiation-induced X-ray fluorescence in order to quantify Ca concentrations in atherosclerotic plaque samples (N=5), which serves as a gold standard for SAM. We found a robust correlation (0.96) between the median Ca concentrations retrieved by X-ray fluorescence and acoustic impedance values determined by SAM. This preliminary result is a first step toward establishing SAM as a potential new modality for the medical diagnosis of atherosclerotic plaques.

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TUE 15:45-17:45 | BOARD 50 | P2-PROT-01

POSTER SESSION

ORIGINS OF ENHANCED AUROPHILICITY IN STIMULI-RESPONSIVE DIMER COMPLEXES AND THE ROLE OF "HOST-GUEST" INTERACTIONS

Presenter: Sharmistha DUTTA
Authors: Sharmistha DUTTA, Dmitry KHAKHULIN, Chris MILNE

Luminescent stimuli-responsive compounds based on ligand-supported Au(I) molecular systems offer unique photophysical properties making them promising candidates for a large variety of technological applications including chemical sensing, medical diagnostics, bioimaging, and OLED devices. The special properties of such complexes are typically related to pronounced noncovalent interactions and particularly aurophilicity, which involves the formation of a weak bond between gold atoms in an electronically excited state. Both in solid and solution phases the weak aurophilic interaction is strongly affected by the nearest environment of the complex such as counter ions and solvent molecules, which can coordinate the gold centers enhancing the effect of aurophilicity.

We are investigating the formation of aurophilic bonds in solvated dinuclear Au(I) complexes upon electronic transition to the emissive excited state. Optical studies suggest that the effect strongly depends on the solvent environment and on the presence of counter ions while the exact electronic and structural origins of enhanced aurophilicity remain unclear. Combining pump-probe X-ray absorption spectroscopy with high energy resolution (HERFD-XAS) and wide-angle X-ray scattering (WAXS) in the solution we aim to visualize the local redistribution of electron density as well as the drastic changes in molecular structure when a weak aurophilic bond is formed in the triplet excited state.

Affillation
European XFEL GmbH, Germany

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TUE 15:45-17:45 | BOARD 51 | P2-SOFT-01

POSTER SESSION

ION ASSOCIATION IN HYDROTHERMAL AQUEOUS NaCl SOLUTIONS: IMPLICATIONS FOR THE MICROSCOPIC STRUCTURE OF SUPERCRITICAL WATER

Presenter: Max WILKE
Authors: Mirko ELBERS (1), Christian SCHMIDT (2), Christian STERNEMANN (3), Christoph J. SAHLE (4), Sandro JAHN (5), Christian ALBERS (3), Robin SAKROWSKI (3), Hlynur GRETARSSON (6), Martin SUNDERMANN (6), Metin TOLAN (3), Max WILKE (1)

We present a combined in-situ X-ray Raman scattering (XRS) and ab initio molecular dynamics (AiMD) simulations study of aqueous NaCl solutions at high pressure and temperature to reveal the microscopic structure and to investigate the influence of the alkali halide on the hydrogen-bond network up to supercritical conditions. Hydrothermal fluids are of high importance for various industrial applications and for material and heat transport in Earth's crust. By probing the oxygen K-edge of the salt solution, unique information is obtained about the oxygen's local coordination. The measured XRS spectra exhibit systematic temperature dependence, the relative course of which is nicely reproduced by spectral calculations based on AiMD simulations structures. This combined analysis reveals a net destabilizing effect of the dissolved ions, which is reduced with rising temperature. An increased formation of contact ion pairs and larger polyatomic clusters at higher temperatures can be identified as a driving force behind the increasing similarities of the NaCl solution and pure water in terms of spectral and structural differences. These findings are of significant importance for geochemical processes involved in the formation of ore deposits and comprehend the understanding of ion-solvent interaction.

We thank: BMBF (05KP16PE1), DFG: STE1079/2-1, STE1079/4-1 (FOR2125, CarboPaT), STE1079/6-1, WI 2000/22-1, EXC 2033 - 390677874 RESOLV and PETRA III (P01, 20180388), ESRF (ID20, ES-863).

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TUE 15:45-17:45 | BOARD 52 | P2-SOFT-02

POSTER SESSION

X-RAY PUMP-PROBE STUDIES OF AQUEOUS SALT SOLUTION INTERFACES

Presenter: Lukas PETERSDORF

Authors: Lukas PETERSDORF (1), Svenja HÖVELMANN (1), Rajendra GIRI (1), Nicolas HAYEN (1), Karin HANSEN (1), Andrea SARTORI (1), Matthias GREVE (1), Florian BERTRAM (3), Olaf MAGNUSSEN (1), Bridget MURPHY (1,2)

Aqueous salt solution interfaces have an importance not only in biological transport processes but also in atmospheric chemistry. Processes of electrons at the liquid-vapor-interface can have timescales from seconds up to femtoseconds, which are excellent for time-resolved pump-probe studies. Our pump-probe studies on various liquid samples, such as SrCl2, ErCl3, RbBr, with different characteristics (pH and concentration) or layering behavior could extend the understanding for temporal processes on the liquid-vapor-interface.

The probed electron solvation dynamics and ion rearrangements at the interface are induced by a UVC laser pulse. For the characterization of these excitation and solvation dynamics surface sensitive measurement techniques are included in our studies, for instance X-ray reflectivity, X-ray fluorescence spectroscopy, and time response pump-probe studies in the time range of ps and s at the LISA liquid scattering facility at P08 (DESY).

Operando investigations of the aqueous solutions under a sensor monitored sample environment allow us to distinguish between laser induced and pH, temperature and humidity dependent dynamics. Analyzed pump-probe results show a change in the intensity of the specular reflectivity in a timescale of s. Noticeable SLD and roughness changes in XRR curves indicate a rearrangement of the ion concentration near the surface. The surface sensitive X-ray fluorescence spectroscopy data can affirm interface changes in the electronic structure.

Affillation

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TUE 15:45-17:45 | BOARD 53 | P2-SOFT-03

POSTER SESSION

PHOTOEMISSION STUDIES ON A LIQUID JET AT THE PETRA III BEAMLINE P04

Presenter: Florian TRINTER
Authors: Florian TRINTER (1), Sebastian MALERZ (1), Karen MUDRYK (1), Dominik STEMER (1), Michele PUGINI (1), Tillmann BUTTERSACK (1), Marvin N. POHL (1,2), Iain WILKINSON (3), Uwe HERGENHAHN (1), Stephan THÜRMER (4), Bernd WINTER (1)

We present results obtained with a new experimental station for photoemission studies from liquid samples, introduced in the form of a microjet. This setup, termed EASI (Electronic structure from Aqueous Solutions and Interfaces), has been constructed with an emphasis on the detection of low-kinetic-energy electrons, a field only sparsely explored so far. It can be transported and has been used at various synchrotron-radiation facilities and in the laboratory, then using a He discharge lamp. In this contribution we focus on experiments performed at the P04 beamline of synchrotron PETRA III. Recent results from our work that will be discussed are

1) the demonstration of photoelectron circular dichroism (PECD) from a liquid with chiral constituents (fenchone). PECD is a helicity-dependent intensity asymmetry in photoelectron spectra of chiral molecules, which has widely been explored in the gas phase, but has not been shown in liquids so far.

2) We have developed a protocol to determine binding energies of the electronic states in a liquid on an absolute scale, by referring measured photoelectron energies to the zero-energy cut-off. This procedure is well known from condensed-matter photoemission, but has not been applied to the liquid phase so far. We show examples for concentration-dependent binding-energy changes of solute and solvent states in aqueous solutions, which could not be reliably determined earlier.

Affillation
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TUE 15:45-17:45 | BOARD 59 | P2-INDU-01

POSTER SESSION

ACCURATE DETERMINATION OF X-RAY FUNDAMENTAL PARAMETERS AT PTB

Presenter: Philipp HÖNICKE
Authors: Philipp HÖNICKE, Rainer UNTERUMSBERGER, Katja FRENZEL, Michael KOLBE, Andre WÄHLISCH, Nils WAUSCHKUHN, Burkhard BECKHOFF

The determination of atomic fundamental parameters (FP) is important for reliable quantitative X-ray fluorescence (XRF) analysis. In view of the lack of adequate reference materials and calibration samples quantitative XRF and related methods call for a high accuracy of the X-ray FPs. However, the respective uncertainties of available tabulated data are usually rather large, especially for low-Z elements or L- and M-shell fluorescence lines in the soft X-ray range. To address this issue, different methods for experimental FP determinations have been developed, validated and applied at the Physikalisch-Technische Bundesanstalt (PTB).

In this work, we will present recent results of our activities on the experimental determination of X-ray FP, covering examples for the determination of low-Z K-shell fluorescence yields, L-subshell fluorescence yields, subshell photoionization cross sections and Coster-Kronig transition probabilities.

Affillation
Physikalisch-Technische Bundesanstalt, Germany

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TUE 15:45-17:45 | BOARD 60 | P2-INDU-02

POSTER SESSION

EASI-STRESS – EUROPEAN ACTIVITY FOR STANDARDISATION OF INDUSTRIAL RESIDUAL STRESS CHARACTERISATION

Presenter: Marc THIRY
Authors: Marc THIRY (1), Nikolaj ZANGENBERG (2)

Neutrons and synchrotron X-rays enable non-destructive penetration of metals and alloys and therefore the direct determination of bulk stresses. EASI-STRESS aims at removing the barriers for industry to adopt these techniques into their quality control systems and to validate materials simulation models.

Residual stresses are of key importance across all industrial sectors where metals are used e.g. within the transportation and energy sectors. This includes various industrial segments with widest applicability in advanced materials and advanced manufacturing and processing where the new techniques can be used to qualify new materials or processes to reduce the time-to-market.

The goals of EASI-STRESS are:

- improving synchrotron X-ray and neutron diffraction-based residual stress characterisation tools for the needs of industrial use
- developing European-wide characterisation standards, protocols and data exchange procedures to facilitate the industrial use of the characterisation tools, e.g. through traceability and comparability
- strengthening European industrial uptake of the characterisation tools through open access to data and protocols, development of a test bed service and collaboration/synergy/ standardization activities
- to secure a competitive advantage across European industrial sectors through optimised component design, reduced material use through reduced safety factors (material savings of around 15%) and respective cost reductions.

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TUE 15:45-17:45 | BOARD 61 | P2-INDU-03

POSTER SESSION

NEW SINGLE POINT OF CONTACT FOR INDUSTRY AT BESSYII

Presenter: Paul HARTEN
Author: Paul HARTEN

Representatives of industry continue to demand simple and easy access to large research facilities, both – in terms of processes, and in terms of rules of engagement. AT HZB, we decided to set up a new Single Point of Contact (SPOC) for industrial partners in order to meet those demands.

Our SPOC is located at the top of the first page of the INDUSTRY menu on the homepage of HZB. It is accessed by just one click. A second click opens up an email channel for starting a dialog with the technology transfer and innovation (TTI) department at HZB. TTI interactively clarifies first of all the scope and goals of the desired activity, and subsequently checks the suitability and availability of resources at HZB required to achieve those goals.

From the perspective of an external industrial partner the advantages of our new SPOC comprise

- the ability to cut to the chase with just two clicks,
- a typical response time of two working days for a first offer, and
- TTI acting as large facility guide removes the complexity of entry requirements.

Affillation
HZB, Germany

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TUE 15:45-17:46 | BOARD 62 | P2-INDU-04

POSTER SESSION

POLYMER COMPOUND REFRACTIVE X-RAY LENSES FOR EASY CUSTOMIZATION

Presenter: Josephine GUTEKUNST
Authors: Josephine GUTEKUNST (1), Arndt LAST (2), Joachim SCHULZ (1)

Focused X-rays are used in many analysis applications [1,2] to increase the resolution of an imaging system or reduce experiment time through higher photon flux. For each application the parameters of the optical system need to be chosen carefully. To facilitate this, we have developed sets of X-ray lenses which can be easily adapted to the most common parameters such as focal length and aperture for a given X-ray energy.

Our approach is based on X-ray lenses made with the LIGA technique for focusing in one dimension or (by crossing two lens elements) in two dimensions. The technique offers highest precision, small radii, excellent compactness and it has the advantage that all lens elements are perfectly aligned to each other [3].

In this Poster Session presentation, we will describe the range of parameter of our compound refractive X-ray lenses, give some examples of their use in running beamlines and describe approaches to adapt the parameters.

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[1] B. Kaulich, P. Thibault, A. Gianoncelli and M. Kiskinova, “Transmission and emission X-ray microscopy: operation modes, contrast mechanisms and applications”, J. Phys: Cond. Matter, 23(8): 083002 (2011)
[2] R. Falcone, C. Jacobsen, J. Kirz, S. Marchesini, D. Shapiro and J. Spence, “New directions in X-ray microscopy”, Contemp Phys., 52: 293-318, 2011.
[3] V. Nazmov, E. Reznikova, A. Last, J. Mohr, V. Saile, R. Simon, and M. DiMichiel. X-ray lenses fabricated by liga technology. AIP Conference Proceedings, 879(1): 770-773, 2007.

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TUE 15:45-17:45 | BOARD 63 | P2-MET2-01

POSTER SESSION

SIMULTANEOUS SAXS/SANS METHOD: A NOVEL NANOANALYTICAL TOOL

Presenter: Ezzeldin METWALLI

Authors: Ezzeldin METWALLI (1), Klaus GÖTZ (1), Tobias ZECH (1), Christian BÄR (1), Lionel PORCAR (2), Tobias UNRUH (1)

Exploiting X-ray and neutron beams at the same sample volume enables unprecedented investigations of nanomaterials using small angle scattering (SAS) techniques. A portable small angle X-ray scattering (SAXS) instrument with a proper geometrical dimension was successfully designed, constructed and implemented at D22 zone of Institut Laue Langevin (ILL) in France for simultaneous SAXS/SANS experiments. The newly established nano-analytical method at ILL will open the way for real time investigations of a wide range of innovative nanomaterials and will allow comprehensive in-situ studies on biological systems. Compared with an independent experimental approach, the simultaneous SAXS/SANS experimental approach ensures the exactness of the probed samples, especially for time-resolved studies. For instance, a temporal structural cross-correlation between organic stabilizing agent (cetyltrimethylammonium bromide; CTAB micelles) and gold seeds, which cooperate in the formation of different size/shape of large stabilized gold nanorods during the synthesis process was simultaneously probed [1]. Thus, the new SAXS/SANS experimental setup will indispensably permit to instantaneously analyse and understand the complicated correlated nanostructures of two different types of nanoscale components in the same sample volume.

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[1] T. Zech, E. Metwalli, K. Gotz, I. Schuldes, L. Porcar, T. Unruh, Particle and Particle Systems Characterization, 2022, 39, 2100172.

Affillation

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TUE 15:45-17:45 | BOARD 64 | P2-MET2-02

POSTER SESSION

A FREE-ELECTRON TARGET FOR THE HEAVY-ION STORAGE RINGS AT FAIR

Presenter: Stefan SCHIPPERS
Authors: Carsten BRANDAU (1,2), Alexander BOROVIK JR. (1), Michel DÖHRING (1), Alfred MÜLLER (1), Michael LESTINSKY (2), Stefan SCHIPPERS (1)

As part of the activities of the ErUM-FSP T05 – “Aufbau von APPA bei FAIR”, a free-electron target is presently being built that has a ribbon-shaped electron beam and operates in transverse collision geometry. The target is optimized for applications in the heavy-ion storage rings of the FAIR facility and will initially be installed at the low-energy ion-storage ring CRYRING@ESR. The electron target is one of the major new experimental installations of the international SPARC collaboration at FAIR [1]. The concept of a transverse free-electron target for heavy-ion storage rings for atomic crossed-beams collision experiments opens up many new physics opportunities [1] but has not been realized, yet. The electron target is designed such that it can be fully retracted from the storage ring to behind a gate valve. It will operate with electron energies of up to 12.5 keV and electron densities of up to 10^9 cm^–3. The interaction volume is accessible for photon spectroscopy within a large solid angle. A modularized design allows for easy adaption to the different storage rings of FAIR. In our contribution we will summarize the concept, physics opportunities and the present status of the work which has been financially supported by BMBF (grant numbers 05P15RGFAA, 05P19RGFA1, and 05P21RGFA1).

[1] M. Lestinsky et al., Eur. Phys. Spec. Top., 225 (2016) 797.

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TUE 15:45-17:45 | BOARD 65 | P2-MET2-03

POSTER SESSION

THE MACROMOLECULAR NEUTRON SINGLE CRYSTAL DIFFRACTOMETER BIODIFF FOR PROTEINS AT THE HEINZ MAIER-LEIBNITZ ZENTRUM

Presenter: Andreas OSTERMANN
Authors: Andreas OSTERMANN (1), Tobias SCHRADER (2)

Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules, thus providing important complementary information to that gained by X-ray crystallography. At the FRM II neutron source in Garching near Munich the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is dedicated to the structure determination of proteins. Typical scientific questions address the determination of protonation states of amino acid side chains, the orientation of individual water molecules and the characterization of the hydrogen bonding network between the protein active center and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behavior of an enzyme. BIODIFF is designed as a monochromatic diffractometer and is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. This allows to adapt the wavelength to the size of the unit cell of the sample crystal. Data collection at cryogenic temperatures is possible, allowing studies of cryo-trapped enzymatic intermediates. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography.

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TUE 15:45-17:45 | BOARD 66 | P2-MET2-04

POSTER SESSION

ACCURATE DETERMINATION OF BOUND COHERENT NEUTRON SCATTERING LENGTHS BY BRAGG DIFFRACTION

Presenter: Thomas HANSEN
Authors: Florian GEHLHAAR (1,2), Holger KOHLMANN (2), Henry FISCHER (1), Thomas HANSEN (1)

Bound coherent scattering lengths b(coh) are one of the basic properties of any isotope, and many experimental neutron techniques in condensed matter as well as in nuclear physics rely on these values, determined by many different scientists over decades and collected in various tables. But many of the values listed in these respectable references have large experimental uncertainties, including possible systematic errors, due largely to having been measured decades ago with neutron instrumentation that has since greatly improved.

Therefore, we use the advantages of modern neutron powder diffraction (NPD), like very good counting statistics even on sub-gram samples, for a redetermination of bcoh of important isotopes.

The measurement of integrated Bragg peak intensities I(hkl) using NPD has the huge advantage that the relative peak intensities are affected by a change in one of the sample's b(coh), such that there is no need to normalize the data to an absolute intensity scale, being therefore much less prone to systematic errors than are other techniques used for b(coh) determination. Rietveld refinement then provides the structure factor F(hkl), and in the case of fixed atomic positions, F(hkl) depend only on b(coh) which thus can be determined directly. The strategy for an accurate determination of b(coh) is therefore to use binary or ternary compounds with well-known crystal structures and ideally with a small number of free positional parameters.

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TUE 15:45-17:45 | BOARD 67 | P2-MET2-05

POSTER SESSION

CATALYSIS AT THE CAT-ACT X-RAY SPECTROSCOPY BEAMLINE AT KIT LIGHT SOURCE

Presenter: Anna ZIMINA
Authors: Anna ZIMINA, Danielle SANTOS GONCALVES, Serrer MARC-ANDRE, Lakshmi PANDIT, Daniel EGGART, Jan-Dierk GRUNWALDT

The CAT station at the CATalysis-ACTinide wiggler beamline at KIT focuses on characterization of catalytically active materials under realistic reaction conditions, e.g. in energy related applications, power-to-chemicals and fuels, selective oxidation, sustainable fine chemical processes and emission control for clean air. A special infrastructure including stationary reactive gas supply, gas dosing units and on-line product analysis as well as in-situ and *operando* cells for sample environments close to industrial reactors are essential aspects of CAT. The XAS setup at the CAT station can be combined with advanced setups for complementary characterization techniques like X-ray diffraction and infrared spectroscopy. Recent examples are the long term (over 310 h) *operando* experiments on commercial Co Fischer-Tropsch synthesis catalysts and methanol synthesis on Cu-based catalysts using the elevated pressure setup (up to 50 bar and 450 °C), the direct methane conversion using the high temperature equipment (up to 1050 °C and 20 bar) on Pt/CeO2 based catalysts. The study helped to clarify the deactivation process of FTS catalyst, the structure-activity ratio on CuZn-catalysts during the methanol synthesis and the role of Al promoter and confirmed the strong metal–support interaction in Pt-CeO2 system under reaction conditions.

We gratefully acknowledge the DFG SPP 2080 program, BMBF project “Kopernikus-P2X” and Sino-German DFG-grant for support.

Affillation
KIT, Germany

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TUE 15:45-17:45 | BOARD 68 | P2-MET2-06

POSTER SESSION

HIGH-RESOLUTION NEUTRON SPIN ECHO SPECTROSCOPY WITH THE J-NSE "PHOENIX" AT MLZ

Presenter: Olaf HOLDERER
Authors: Margarita FOMINA, Olaf HOLDERER, Stefano PASINI , Tadeusz KOZIELEWSKI, Michael MONKENBUSCH

Neutron spin echo (NSE) spectroscopy provides the ultimate energy resolution in quasi-elastic thermal and cold neutron scattering spectroscopy. In terms of Fourier-time (τ) – or, equivalently, in terms of the accessible energy (E) – a high resolution means the extension of τ (respectively E) into the regime of μs (neV). Recently, Jülich's neutron spin echo spectrometer (J-NSE) "PHOENIX" at MLZ has been upgraded with superconducting, fringe-field compensated main precession coils, and optimized field shape. Now, the spectrometer offers a broader range of Fourier times relevant for thermally driven fluctuations in biology and soft matter [1]. "PHOENIX" allows to detect the microscopic dynamics of various soft- and biological materials. We present the results of the spectrometer performance after refurbishment and some scientific examples from soft matter dynamics and biology. Latest experiments at the J-NSE investigated protein domain fluctuations under physiological conditions [2], membrane dynamics in lipase-containing microemulsions [3], and internal dynamics of microgel particles [4] which can be used as functional coatings or drug delivery systems.

[1] S. Pasini, et al., Rev. Sci. Instrum. 90, 043107 (2019)
[2] L. Balacescu, et al., Scientific Reports 10, 1570 (2020)
[3] S. Engelskirchen et al., Frontiers in Chemistry, 8, 613388 (2021)
[4] T. Kyrey, et al., Soft Matter, 15, 6536 (2019)

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TUE 15:45-17:45 | BOARD 69 | P2-MET2-07

POSTER SESSION

HIGH PRESSURE OPTIONS FOR SINGLE CRYSTAL DIFFRACTION AT MLZ

Presenter: Martin MEVEN
Authors: Andreas EICH (1,4), Muni POLI (1,2), Martin MEVEN (1,2), Vladimir HUTANU (3), Robert GEORGII (3), Yixi SU (2), Karen FRIESE (4), Andrzej GRZECHNIK (1)

Numerous scientific topics profit from single crystal neutron diffraction. Aside from temperature-dependent studies, high pressure (HP) experiments in particular give important insights into structural and related physical properties. Instruments with high flux at short wavelengths are advantageous for these. Therefore, a BMBF funded project was launched in 2016 to establish HP diffraction studies at MLZ on HEiDi (and its polarized counterpart POLI) focusing on new diamond anvil pressure cells (DAC). Combining optimized neutron optics and short wavelengths (< 1 Å), the new cell designs allow HP studies on tiny samples (<< 0.1 mm^3) up to several GPa and down to low temperatures or simultaneous studies of the same sample in the same cell using neutron and synchrotron/X-ray sources, e.g. on magnetocaloric compounds like MnFe4Si3.

A subsequent BMBF project has been complementing these efforts by clamp cell developments for other single crystal instruments (POLI, DNS and MIRA), better suited for large sample volumes and studies in magnetic fields. Based on detailed simulations, various cells using different alloys and designs with low paramagnetic moments and pressures up to above 1 GPa have been manufactured. Initial tests show promising results[1] with further tests under different conditions (T, P, H) pending. This work is accompanied by 2D detector developments on HEiDi and POLI to increase their efficient use for this kind of studies.

[1] A. Eich et al.; High Press. Res. 41, 88

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TUE 15:45-17:45 | BOARD 70 | P2-MET2-08

POSTER SESSION

LATEST DEVELOPMENTS OF THE PROGRAM VITESS FOR THE SIMULATION OF NEUTRON SCATTERING INSTRUMENTS AND VIRTUAL NEUTRON EXPERIMENTS

Presenter: Klaus LIEUTENANT
Authors: Klaus LIEUTENANT, Lydia FLEISCHHAUER-FUSS, Fabian BEULE, Jörg VOIGT

The VITESS software package has been used since 1999 to simulate neutron scattering instruments and virtual experiments at several neutron sources around the world, e.g. at BER-II, FRM-II, JEEP-II and ESS.

While it had been developed at Helmholtz-Zentrum Berlin during the first two decades of the century, it is now hosted by Forschungszentrum Juelich. Here it is mainly used for simulation of instruments foreseen for the planned new neutron source HBS (Jülich High Brilliance neutron Source) and intruments installed at MLZ (Maier-Leibnitz-Zentrum) close to Munich.

The new version 3.5 has gone through a code redesign and contains some new features that are needed for the simulation of the HBS instrument suite, e.g. a rotating monochromator and improved reading and writing option for MCNP data. At the same time, version 4.0 was completed. It offers a new GUI using Qt and further options for virtual experiments, facilitated by storing the instruments as yaml files and monitor updates during the run. It will be used to offer virtual experiments at MLZ. The upcoming version 3.6 will enable a smooth transition from version 3 to version 4 and show improved visualization features. Finally, version 4.1 will contain all VITESS modules, thus combining the improvement of the versions 3.6 and 4.1.

As an example, a virtual experiment of a diffractometer planned for the HBS will be presented.

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TUE 15:45-17:45 | BOARD 71 | P2-MET2-09

POSTER SESSION

PTyNAMi: PTYCHOGRAPHIC NANO-ANALYTICAL MICROSCOPE

Presenter: Andreas SCHROPP

Authors: Andreas SCHROPP (1), Ralph DÖHRMANN (1), Stephan BOTTA (1), Dennis BRÜCKNER (1), Maik KAHNT (3), Mikhail LYUBOMIRSKIY (1), Christina OSSIG (1), Maria SCHOLZ (1), Martin SEYRICH (1), Michael STÜCKELBERGER (1), Patrik WILJES (1), Felix WITTWER (1), Jan GARREVOET (1), Gerald FALKENBERG (1), Yakub FAM (4), Thomas SHEPPARD (4), Jan-Dierk GRUNWALDT (4), Christian SCHROER (1,2)

Scanning coherent X-ray microscopy (ptychography) with high spatial resolution requires an optimal experimental environment, providing a high coherent flux, excellent mechanical stability and a low background in the measured diffraction data. This requires, for example, a stable performance of all optical components along the entire beam path, high temperature stability, a robust sample and optics tracking system, and a scatter-free environment. The Ptychographic Nano-Analytical Microscope (PtyNAMi), which is installed in the nanohutch of beamline P06 at PETRA III, has been developed within the group 'X-ray Nanosicence and X-ray Optics' at DESY and is optimized in view of these enhanced experimental requirements. It is designed to create nanofocused X-ray beams with sizes of 50 nm (FWHM) and even smaller, which allows one to image objects with high spatial resolution yielding simultaneously local elemental, chemical and structural information of a specimen. Ptychography can be combined with tomographic methods potentially yielding structural information in 3D with a spatial resolution of 10 nm and even below. In this contribution recent results obtained at PtyNAMi will be summarized.

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TUE 15:45-17:45 | BOARD 72 | P2-MET2-10

POSTER SESSION

RAY-X: A MODERN SOFTWARE ARCHITECTURAL BASIS FOR RAY, RAY-UI AND REFLEC

Presenter: Peter FEUER-FORSON

Authors: Peter FEUER-FORSON (1), Peter BAUMGÄRTEL (1), Jannis MAIER (1), Oussama SAYARI (1), Rudi SCHNEIDER (1), Enrico AHLERS (1), Theresa FOLLATH (1), David MEIER (1), Gregor HARTMANN (1), Hartmut SCHIRMACHER (2), Simone VADILONGA (1), Jens VIEFHAUS (1)

RAY-X is an open-source software project with the goal of developing state-of-the-art physics-based ray tracing algorithms, optimised for modern GPUs. Additionally, RAY-X aims to fundamentally modularise and restructure the architecture of the well-known RAY, RAY-UI and REFLEC software.

We have implemented the tracer (the core of RAY) using the Vulkan framework with GLSL shaders, which is an industry leading graphics and computing API providing high efficiency, cross-platform access to modern GPUs. The core code previously implemented in Fortran is being ported to C++ and the design of the software has been updated to a Model-view-presenter pattern. This separation of the interface from the underlying code improves not only software maintenance, but also allows for the use of multiple interfaces. With the higher demand for machine learning assistance in all aspects of beamline research an important application of RAY-UI is the efficient generation of large datasets. As such, two new interfaces are foreseen using the Electron framework: a fully-supported command line interface is already in development, a web-based graphical user interface will follow.

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TUE 15:45-17:45 | BOARD 73 | P2-MET2-11

POSTER SESSION

PERSPECTIVES FOR ANALYTICAL XAFS SPECTROSCOPY AT PETRA IV

Presenter: Edmund WELTER
Author: Edmund WELTER

Over the past 30 years X-ray absorption fine structure spectroscopy (XAFS) developed into an established analytical method used routinely by a large user community working in various fields of science. Today the undulator beamline P65 at the PETRA III storage ring at DESY is available for a broad user community to perform high quality analytical XAFS measurements.

Starting in 2026 PETRA III will be converted into a 4th generation storage ring to provide improved brilliance and a high degree of coherence of the photon beam. While the extremely high brilliance and degree of coherence at 4th generation storage ring sources offer unique possibilities for hitherto impossible experiments they pose some challenges for analytical XAFS spectroscopy. The design of a analytical XAFS and quick scanning XAFS beamline at PETRA IV which will employ the radiation from a short wiggler is currently under investigation. A continuous source like a wiggler can significantly improve the conditions especially for quick scanning XAFS compared to the current undulator beamlines. The aim of this presentation will be to present the design and instrumentation of this new beamline for analytical XAFS at PETRA IV and to discuss the experimental possibilities and possible problems for classical XAFS spectroscopy in comparison to the existing beamline P65 at PETRA III.

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TUE 15:45-17:45 | BOARD 74 | P2-MET2-12

POSTER SESSION

mySPOT STATION AT BESSY II: DIFFRACTION TOMOGRAPHY AND TIME RESOLUTION

Presenter: Ivo ZIZAK
Author: Ivo ZIZAK

New developments at the microfocusing X-ray beamline at BESSY II synchrotron light source [1] are presented. Increased mechanical stability of the beamline allows for the focused beam to be stable over several days, making it possible to develop demanding experimental techniques, e.g. diffraction computer tomography. Wide or small angle scattering can be used to reconstruct the spatial (3-dimensional) distribution of the scattering sources in the studied sample, and combined with the absorption and fluorescence tomography it provides more insight into the functionality of hierarchically structured samples compared to information delivered from each method if they would be performed independently.

To achieve this goal, the triggering scheme of a multi-method experiment was modified, resulting in faster and more accurate timing. As a side-effect, fast time series of diffraction images with the resolution in the range of milliseconds are possible at the mySpot experimental station. Possible applications are the study of transient crystalline changes after triggering a chemical reaction (even irreversibly), or after exposing a sample to the light, electric or magnetic field pulse.

[1] I. Zizak, JLSRF, 2016, 2, 101.

Affillation
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TUE 15:45-17:45 | BOARD 75 | P2-MET2-13

POSTER SESSION

SWIFT HEAVY ION IRRADIATION AND IN-SITU ANALYSIS CAPABILITIES OF THE M-BRANCH AT THE GSI UNILAC

Presenter: Frieder KOCH

Authors: Frieder KOCH (1), Ina SCHUBERT (1), Bruno MERK (1), Daniel SEVERIN (1), Markus BENDER (1,2), Christina TRAUTMANN (1,3)

The M-branch at the universal linear ion accelerator UNILAC of the GSI/FAIR facility in Darmstadt provides three end stations dedicated to international users from materials science and other cross-disciplinary research fields. Ion beams up to uranium of kinetic energy between 3.6 – 11.4 MeV per nucleon are available. In this energy regime, heavy ions induce complex structural modifications within a highly localized nanoscale damage zone. The unique feature of the M-branch is the availability of a variety of in-situ and on-line characterization methods, which can be tailored to the system under investigation.

This contribution aims to give an overview of established (and planned) techniques including SEM, FTIR, UV-vis, XRD, SIMS/SNMS, Raman spectroscopy and a cryo- and high temperature stage. The presentation will also illustrate how swift heavy ions manipulate material properties and simulate cosmic rays to better understand astrochemical processes.

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TUE 15:45-17:45 | BOARD 76 | P2-MET2-14

POSTER SESSION

RECENT ACHIEVEMENTS AND FUTURE PERSPECTIVES OF NEUTRON BACKSCATTERING AT IN16B

Presenter: Markus APPEL
Authors: Markus APPEL (1), Bernhard FRICK (1), Tilo SEYDEL (1), Andreas MAGERL (2), Frank SCHREIBER (3)

Neutron spectroscopy gives unique insight into microscopic dynamics of soft and hard condensed matter and simple or complex liquids. Crystal spectrometers such as IN16B at the Institut Laue-Langevin in Grenoble (France) operating in backscattering provide high energy resolution down to sub-micro-eV. While IN16B serves its international user community for nearly a decade by now, we continuously strive to improve and extend its capabilities with new developments. In this presentation, we will review past, ongoing, and future projects.

A first upgrade phase has been successfully completed and brought into routine user operation with the so-called BATS option (Backscattering And ToF Spectrometer) which offers an energy transfer range increased by more than one order of magnitude. In parallel, the feasibility for a future construction of an ultra-high energy resolution spectrometer based on GaAs 200 could be demonstrated.

The second key enhancement currently ongoing concerns the installation of a 10m long variable focusing/defocusing neutron guide system for the BATS chopper system. This innovative and unique upgrade will bring BATS to its full potential in terms of neutron flux.

As a future step, we propose to extend the instrument's capabilities at low scattering angles, which entails re-designing the low angle analyser section and improvements of the detector arrangement. This will give an advantage in both 'classical' high-resolution backscattering as well as in BATS mode.

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TUE 15:45-17:45 | BOARD 77 | P2-MET2-15

POSTER SESSION

ADVANCED HE-SXRD STUDIES FOR ELECTROCATALYSIS

Presenter: Leon JACOBSE
Authors: Leon JACOBSE (1), Xin DENG (1,2), Herbert OVER (3), Olaf BRUMMEL (2), Vedran VONK (1), Joerg LIBUDA (2), Andreas STIERLE (1)

Efficient electrocatalytic processes are essential for developing technologies based on renewable sources. Detailed characterization of electrocatalysts under operating conditions is required to develop electrocatalytic systems exhibiting optimal reactivity and stability. Such experiments should allow to correlate the surface structure, surface chemistry, and reactivity at the electrode interface. Here, we present two setups developed for high energy surface X-ray diffraction (HE-SXRD) experiments under electrochemical conditions. First, we combine HE-SXRD with the rotating disk electrode (RDE) technique. This allows for characterization of the surface structure, while maintaining well-defined steady-state mass transport conditions. With this setup, we study the changes in the surface structure of Pt(111) under *operando* oxygen reduction and evolution (ORR/OER) conditions. In a second experiment, HE-SXRD is combined with electrochemical in-situ infrared reflection absorption spectroscopy (EC-IRRAS). This provides, simultaneously, information on the surface structure and the interfacial chemistry, enabling a direct correlation between the two. Using this setup, we were able to monitor in a single experiment the behavior of adsorbed CO at a Pt(111) electrode, the electrocatalytic oxidation of adsorbed CO to CO2, and the surface oxidation at higher potentials.

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TUE 15:45-17:45 | BOARD 78 | P2-MET2-16

POSTER SESSION

A NOVEL FAST SYNCHRONIZED SETUP FOR COMBINED IN-SITU X-RAY DIFFRACTION AND X-RAY ABSORPTION SPECTROSCOPY AT MAX IV

Presenter: Mahesh RAMAKRISHNAN
Authors: Mahesh RAMAKRISHNAN (1), Matteo CIAMBEZI (1), Per-Anders CARLSSON (2), Justus JUST (1)

Observation of changes in crystalline structures of materials during chemical reactions and phase transformations remains a challenge in materials science [1-3]. We have developed a setup to perform in-situ X-ray diffraction (XRD) in parallel with X-ray absorption spectroscopy (XAS) at the Balder beamline at MAX IV [4]. This enables us to obtain multi-dimensional information of materials such as long-range crystalline order via XRD, the electronic properties via XAS and short-range correlations via extended X-ray absorption fine structure. The high photon flux (10^12 ph/s) over a wide range of energies (3 – 40 keV) makes it possible to investigate processes with a sub-second resolution with real-time visualization and data analysis capabilities.

The setup consists of ion-chambers and multi-element detectors for XAS measurements in transmission and fluorescence modes, respectively and a hybrid-pixel area detector for XRD measurement. It can also be extended to study in-situ diffraction anomalous fine structure [5] to obtain comprehensive structure-property relationships of materials. We will present the specifics of our experimental setup, the modalities of data acquisition and treatment, and a few examples of measurements carried out with the setup.

[1] Physical Sciences Reviews 5, 20170181 (2020)
[2] Crystals 6, 87 (2016)
[3] Johns. Matthey Technol. Rev. 62, 316–331 (2018)
[4] J. Phys.: Conf. Ser. 712, 012023 (2016)
[5] J. Phys.: Condens. Matter 29, 113002 (2017)

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TUE 15:45-17:45 | BOARD 79 | P2-MET2-17

POSTER SESSION

STRUCTURE AND COMPOSITION OF SIZE-TUNABLE Ni–Cu CORE–SHELL NANOPARTICLES AS ANALYZED BY ASAXS

Presenter: Armin HOELL

Authors: Armin HOELL (1), Maria HEILMANN (2,3), Robert WENDT (1), Carsten PRINZ (2), Ralf BIENERT (2), Jörg RADNIK (2), Ana Guilherme BUZANICH (2), Franziska EMMERLING (2,3)

A facile and efficient methodology is developed for the solvothermal synthesis of size-tunable, stable, and uniform NiCu core–shell nanoparticles (NPs) for various application in catalysis [1]. Their diameter can be tuned in a range from 6 nm to 30 nm and the Ni:Cu ratio is adjustable in a wide range from 1:1 to 30:1. The NPs are structurally characterized by a method combination of transmission electron microscopy, anomalous small-angle X-ray scattering (ASAXS), X-ray absorption fine structure, and X-ray photoelectron spectroscopy. Here, we focus on the ASAXS method and its ability to analyses nanostructure parts and their compositions at ones.

The X-ray absorption edges of Ni and Cu are nearby. Consequently, the strong variation of the anomalous scattering behavior in the energy range from 8 keV to 9 keV is used for this special ASAXS investigation.

ASAXS excluded the hypothesis of a bimetallic core-shell structure and evidenced a core-shell-shell nanostructure. The outer shell is NiO while the inner core is Cu and Ni alloyed. That was proved to be valid for all particle sizes and Ni:Cu ratios. The inner shell is pure Ni dominated.

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[1] Heilmann, M. et al, Adv. Eng. Mater. 2022, 2101308 (1-13).

Affillation

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TUE 15:45-17:45 | BOARD 80 | P2-MET2-18

POSTER SESSION

SIMULATIONS USING NCrystal AND Geant4 FOR INNOVATIVE SOLID-STATE NEUTRON DETECTORS

Presenter: O'Neill GEORGE

Authors: O'Neill GEORGE (1), Povoli MARCO (2), Birch JENS (3), Choolakkal ARUN (3), Getz MICHAEL (2), Kok ANGELA (2), Koybasi OZHAN (2), Moutoussamy EMMANUEL (4), Pedersen HENRIK (3), Rohrich DIETER (1), Slavicek TOMAS (5)

Due to their lack of charge, low-energy neutrons are not detectable in semi-conductors, and instead detectors use expensive or dangerous gases in bulky, immobile devices. The INDet (Improved Neutron DETection) project aims to fix these issues using pulse plasma etching to generate a 3-D silicon diode consisting of a series of sub-structures each with an enriched boron carbide (BxC) coating. By making use of the 10B(n, 11B*) reaction, the fission of the excited nucleus into two charged decay products (α and 7-Li) can be used as a signature for neutrons.

Using 3-D sensors allows for an increase in the apparent thickness of the deposited BxC layer, and thus an increase in conversion efficiency. However, the optimal coverage of boron does not necessarily correspond to the best detection geometry, nor what is manufacturable reliably. Monte Carlo methods are required in order to determine the performance of the detector; to this end, a series of simulations were created using the NCrystal library, developed by the detector group at ESS, which allows for more accurate simulation of sub-keV neutrons within Geant4. These simulations have been compared to existing work and geometries, and will be improved via comparison to 'real-world' scenarios and have shown a detection efficiency of up to 30%.

This presentation will discuss the capabilities of NCrystal, the setup and technique used to simulate many small sub-structures, and the comparison with existing physical devices.

Affillation

1: University of Bergen, Department of Physics and Technology, Bergen, Norway; 2: SINTEF AS, Smart Sensors and Microsystems, MiNaLab, Oslo, Norway; 3: Linköping University, Department of Physics, Chemistry and Biology, Linköping, Sweden; 4: University of Oslo, Centre for Materials Science and Nanotechnology, Oslo, Norway; 5: Czech Technical University, Institute for Experimental and applied Physics, Prague, Czech Republic

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TUE 15:45-17:45 | BOARD 81 | P2-MET2-19

POSTER SESSION

IN-SITU NANOTOMOGRAPHY AT THE IMAGING BEAMLINE P05

Presenter: Imke GREVING
Authors: Imke GREVING (1), Silja FLENNER (1), Elena LONGO (3), Johannes HAGEMANN (2)

The nanotomography setup at the imaging beamline P05 at the PETRA III storage ring at DESY (Hamburg, Germany) operated by the Helmholtz-Zentrum Hereon is optimized for full field imaging in the hard X-ray regime. The transmission X-ray microscope (TXM) offers spatial resolutions down to 40 nm and allows for scan times of below one minute in the fast scan mode, optimized for in-situ studies. Thanks to the very versatile set-up not only X-ray microscopy (XRM) can be performed, but also Zernike phase contrast and cone beam (holotomography) experiments. Thus this instrument is serving as an ideal probe for a wide range of applications from engineering over medicine to biology. The development of innovative nano-materials for example, profits massively from an in-depth knowledge of their three-dimensional inner structures but also requires knowledge about their functional performance. Therefore in-situ applications like nanoindentation, allow a detailed analysis of the 3D inner structure as well as the mechanical response at reasonably short timescales offering an ideal combination for studying materials at the nano scale.

Affillation
1: Helmholtz Zentrum Hereon, Germany; 2: Desy, Germany; 3: Elettra, Italy

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TUE 15:45-17:45 | BOARD 82 | P2-MET2-20

POSTER SESSION

IN-SITU ROLL-TO-ROLL SLOT-DIE COATING SETUP FOR MULTIMODAL XAS/XRD/UV-VIS MEASUREMENTS AT THE BALDER BEAMLINE

Presenter: Matteo CIAMBEZI
Authors: Matteo CIAMBEZI (1), Mahesh RAMAKRISHNAN (1), Jiatu LIU (1), Eva UNGER (2), Jinzhao LI (2), Justus JUST (1)

Solution processable functional materials for photovoltaics, batteries, sensors and photo-electronic devices are increasing their relevance because of their high performances, production flexibility and low cost. A deep understanding of the formation mechanisms of these materials during deposition is key to achieve high performance materials and enable up-scaling towards industrial production.

To this end we developed an endstation for in-situ analysis of solution processed materials by multimodal XAS, XRD and optical spectroscopy. It consists of a small footprint roll-to-roll slot-die coater with annealing and a gas-quenching stages, enabling for simultaneous multimodal measurements. The coating system is fully remotely operated and permits to perform automated high-throughput experiments under varying experimental conditions. Moreover, the platform is very modular for high versatility to the different possible experiments and future upgrades.

Employing combined XAS, XRD and optical spectroscopy this setup permits a complementary investigation of the local structure, crystalline phases, chemical composition, oxidation states and optoelectronic properties in real-time during the deposition and annealing stages. Besides technical developments, we will present first results obtained during in-situ processing of metal halide perovskites for photovoltaic applications.

Affillation
1: MAX IV Laboratory, Sweden; 2: Helmholtz-Zentrum Berlin

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TUE 15:45-17:45 | BOARD 83 | P2-MET2-21

POSTER SESSION

THE HIGH-RESOLUTION DIFFRACTION BEAMLINE P08 AT PETRA III

Presenter: Chen SHEN
Authors: Chen SHEN, Arka DEY, Rene KIRCHHOF, Florian BERTRAM

The high-resolution diffraction beamline P08 at PETRA III provides X-ray diffraction and scattering methods for solid and liquid surfaces and interfaces, with highly monochromatic, low divergent hard X-ray beam (5 ~ 30keV). The beamline hosts a 6-circle diffractometer for experiments at solid surfaces, a double-crystal-beam-tilter for general purpose liquid interfaces diffraction experiments, and a Langmuir GID setup dedicated for Langmuir trough experiments at vapour-water interfaces. In particular, the newly upgraded Langmuir GID setup is optimized for low background grazing incidence X-ray diffraction and small angle scattering experiments, combined with total reflection X-ray fluorescence spectroscopy. Its highly standardized and automated operation ensures easy access for non-X-ray-expert users to conduct studies ranging from biophysics, pharmaceutical sciences to nanotechnology applications.

Affillation
Deutsches Elektronen-Synchrotron DESY, Germany

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TUE 15:45-17:45 | BOARD 84 | P2-MET2-22

POSTER SESSION

THE PULSED LOW-ENERGY POSITRON SYSTEM PLEPS

Presenter: Ricardo HELM
Authors: Ricardo HELM, Marcel DICKMANN, Werner EGGER, Johannes MITTENEDER, Gottfried KÖGEL, Peter SPERR, Günther DOLLINGER

The Pulsed Low-Energy Positron System PLEPS is a user facility for defect depth-profiling by means of positron lifetime measurements using a monochromatic pulsed positron beam of variable implantation energy in the range between 0.5 keV and 20 keV. It is operated at the intense positron source NEPOMUC at the MLZ in Garching, Germany.

PLEPS enables a quantitative and non-destructive characterization of open volume defects, e.g. vacancies, grain boundaries, precipitates or vacancies clusters close to surfaces and in thin films (< 30 nm) and layered structures. Varying the positron beam energy allows defect depth-profiling from 5 nm to 5 µm. A spectrum can be measured within less than 10 minutes for a single implantation energy.

In-situ manipulation of the sample during lifetime measurements is possible: The sample temperature can be varied between 80 K and 600 K. With a new broad band illumination system optically active defects can be detected and identified by manipulating their charged states. Positron drift experiments to explore interfaces and internal surfaces can be performed by applying bias voltages to the samples.

Typical applications comprise the defect identification in semiconductors and insulators, the investigation of irradiation induced defects in materials for fusion and fission, as well as the characterization of nano-voids in glasses, polymers and polymeric membrane layers.

Affillation
Universität der Bundeswehr München

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TUE 15:45-17:45 | BOARD 85 | P2-MET2-23

POSTER SESSION

MICROMETER POSITRON BEAM AT THE SCANNING POSITRON MICROSCOPE

Presenter: Johannes MITTENEDER
Authors: Johannes MITTENEDER, Marcel DICKMANN, Ricardo HELM, Werner EGGER, Günther DOLLINGER

Positron annihilation lifetime spectroscopy is a powerful tool in a wide range of material science. To investigate inhomogeneous defect distributions, e.g. close to fatigue cracks or dispersive alloy, with PALS a monochromatic pulsed positron beam of variable energy with a diameter in the range of 1 µm and a pulse width of 150 ps FWHM is needed.

To this aim the Scanning Positron Microscope (SPM) was developed and built at the Universität der Bundeswehr. To overcome the limit of low count-rates the SPM is currently transferred to the intense positron source NEPOMUC at the MLZ in Garching.

A sophisticated beam preparation, including multiple remoderation steps, is needed to reach a lateral resolution in the micro-meter range. An essential component of the interface is the positron elevator which compensates for the energy loss caused by the remoderation process without altering other important beam properties like time structure and brightness. In this contribution we will give an overview of the current status of SPM, which has become a complete makeover during the reactor shutdown. In addition the latest developments of the positron elevator and the newly developed frequency stabilization system are reported. To ensure proper operation of SPM at NEPOMUC, stable amplitude, stable frequency and stable phase of the RF-signal are crucial.

Affillation
Universität der Bundeswehr München, Germany

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TUE 15:45-17:45 | BOARD 86 | P2-MET2-24

POSTER SESSION

THE POWDER DIFFRACTION AND TOTAL SCATTERING BEAMLINE P02.1 AT PETRA III, DESY

Presenter: Volodymyr BARAN
Authors: Volodymyr BARAN, Henrik JEPPESEN, Alba San José MÉNDEZ, Alexander SCHÖKEL, Tim SCHOOF, Mario WENDT, Sergej WENZ, Martin ETTER

The Powder Diffraction and Total Scattering Beamline P02.1 at the PETRA III synchrotron at the DESY facility in Hamburg, Germany, is a specialized station where researchers from science and industry have the possibility to collect Powder Diffraction (PD) and Total Scattering (TS) data simultaneously with a fixed energy of 60 keV. With a custom-made tandem detector setup consisting of two large area detectors, users can, among others, perform in-situ crystal growth experiments from the amorphous and nanocrystalline state up to the microcrystalline state, collecting simultaneously high-resolution PD data and TS / Pair Distribution Function data on the same sample. The P02.1 beamline offers a variety of sample environments for high-temperature and low-temperature studies, as well as for mechanical treatments. While the aforementioned sample environments are available at the beamline, others are provided on a collaborative basis with DESY users. Besides regular on-site synchrotron experiments, users can also apply for mail-in / rapid access services for PD and/or TS / Pair Distribution Function measurements of samples packed in capillaries. These measurements can then be automatically performed using a robotic system either at room temperature or temperatures in the range between 100 K and 1200 K.

In this presentation, we will inform the scientific community as well as industrial customers about the latest developments at beamline P02.1.

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TUE 15:45-17:45 | BOARD 87 | P2-MET2-25

POSTER SESSION

A COMPACT HIGH-TEMPERATURE FURNACE FOR SANS MAGNETS

Presenter: Abdel AL-FALOU
Authors: Abdel AL-FALOU (1,2), Milan ANTIC (2), Andreas WILHELM (2), Sebastian MÜHLBAUER (2)

Many modern high performance alloys feature ferromagnetic elements like, e.g. Co or Ni. With SANS being a major technique to investigate the nanostructure of these compounds in in-situ conditions, the ever present magnetic scattering can be of similar size as the nuclear signal. Magnetic fields combined with high temperatures can hence be a key ingredient for studies of Co or Ni based superalloys or Steel samples.

We present a prototypical furnace that has been designed to fit the small-scale dimensions (80mm bore) of the available 2.5T magnet at SANS-1, MLZ. The innovations lie in a compact design, with water-cooling based on a 3-D printed Copper structure that is press-fitted to the aluminum dewar. The heating mechanism builds upon often-applied Joule heating of Nb-foils, although the implemented elements differ considerably in size from existing ones. The internal scaffold is exclusively made of ceramics, which displays ideal thermal stability, electric and magnetic irresponsiveness. A sample size of 10mm and a sample temperature of 1500K is foreseen.

The oven, by its small size and application to metallurgic samples, makes excellent use of the SANS-1MAX upgrade that is planned for the upcoming years.

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TUE 15:45-17:45 | BOARD 88 | P2-MET2-26

POSTER SESSION

APPLICATIONS OF HIGH RESOLUTION EVENT COUNTING MCP / STIMEPIX DETECTORS AT SOFT X-RAY AND ENERGY-RESOLVED NEUTRON IMAGING BEAMLINES

Presenter: Anton TREMSIN
Authors: Anton TREMSIN (1), Beamline SCIENTISTS (2)

Recent development of high resolution photon and neutron counting detectors with Microchannel Plates combined with a Timepix readout enables a number of novel experimental studies at soft X-ray synchrotron beamlines as well as neutron imaging/scattering facilities. With these detectors implemented at spallation neutron sources it is now possible to measure simultaneously more than 250,000 neutron transmission spectra, each within a 55 µm pixel. The same technology has been successfully implemented for soft X-ray photon counting applications where time and position of each registered photon is registered with virtually no readout noise and at a large dynamic range with capability to register many simultaneous particles. This paper describes the current status of this detection technology and presents the results of recent studies conducted at neutron and soft X-ray beamlines. Spatially resolved investigation of microstructure and elemental composition within various polycrystalline and single crystal materials, mapping of residual strain, uniformity of texture and location of various crystalline defects, all non-destructively, is enabled by this detection technology implemented at pulsed neutron beamlines. Application of the same detectors for resonant inelastic soft X-ray scattering experiments and the near future capabilities of these detection technology will also be discussed.

Affillation
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TUE 15:45-17:45 | BOARD 89 | P2-MET2-27

POSTER SESSION

FEASIBILITY RESEARCH FOR THE PRODUCTION OF NEXT GENERATION X-RAY OPTICS

Presenter: Analía FERNÁNDEZ HERRERO
Authors: Analía FERNÁNDEZ HERRERO (1), Anke TEICHERT (2), Grzegorz GWALT (1), Stefan REHBEIN (1), Thomas KRIST (1), Alexei ERKO (3), Frank SIEWERT (1)

Next generation of X-ray gratings are essential for the development of avant-garde synchrotron radiation sources and X-ray applications. Nowadays the production of such gratings is based on conventional ruling techniques which limits their design possibilities as well as their availability. To overcome such problems a feasibility research using electron-beam lithography (EBL) for the production of blazed gratings is proposed. Here, we present preliminary results of blazed gratings produced using different numbers of steps for the approximation of the blazed facet and different etch depths. Blaze angle, facet roughness and roughness correlations are systematically analysed for a better control of the production.

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TUE 15:45-17:45 | BOARD 90 | P2-MET2-28

POSTER SESSION

ILLUSTRATION OF RESONANT PTYCHOGRAPHIC X-RAY COMPUTED TOMOGRAPHY

Presenter: Anico KULOW

Authors: Anico KULOW (1), Redhouane BOUDJEHEM (1), Jean-Louis HAZEMANN (1), Samy OULD-CHIKH (2), Javier PÉREZ (3), Julio César DA SILVA (1)

Ptychography is a scanning coherent diffraction imaging technique that has gained much attention over the past decade. Ptychography allows the investigation of microstructures of extended samples with a resolution down to ten nanometers. A coherent probe is used to scan the sample at overlapping positions. For each position, a diffraction pattern is recorded. From these diffraction patterns, the probe and the complex-valued sample transmission function, which corresponds to a map of the complex refractive index, is reconstructed. Ptychographic reconstructions from the sample measured under different angles can be used to reconstruct a 3D volume, like in classical computed tomography. Furthermore, spectral information can be added by repeating a ptychographic experiment at different energies.

With the progress of method and instrumentation, ptychography becomes a standard technique, and is available on various beamlines worldwide. The upcoming of 4th generation synchrotrons with superior coherence properties will increase this trend even more. One of these beamlines is Swing at SOLEIL, which allows for 2D ptychography and 3D ptychographic CT.

We will present mesurements on a Ni wire conducted at Swing to illustrate the method of spectral 2D- and resonant 3D-ptychography. We can extract spectra of the real and imaginary part of the refractive index from the measured ptychographic projections, and determine the electron and atomic density from the reconstructed tomogram.

Affillation

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TUE 15:45-17:45 | BOARD 91 | P2-MET2-29

POSTER SESSION

SAMPLE ENVIRONMENT AT BESSY II

Presenter: Dirk WALLACHER
Authors: Dirk WALLACHER, Bastian KLEMKE, Nico GRIMM, Matthias NEEB, René GRÜNEBERGER, Hermann THIEL, Sebastian GERISCHER, Robert WAHLE, Martin PETSCHE, Jörg DATHE, Klaus KIEFER

The sample environment group supports all beam line experiments at BESSY II as well as the HZB inhouse labs. We provide our experience and a repertoire of sample environment equipment and tools to the beamlines and users groups. We help with the development and construction of novel sample environment components, which can be firmly integrated in the experimental stations or operated as modular and variable sample environment in combination with direct user service.

This presentation focusses on highlights of recent in-situ and in *operando* sample environment developments dedicated to different photon studies in gas absorption properties, catalytic processes, and electro-chemical reactions.

Affillation
Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

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TUE 15:45-17:45 | BOARD 92 | P2-MET2-30

POSTER SESSION

IN-SITU X-RAY DIFFRACTION AND IMAGING P23 BEAMLINE AT PETRA III: STATUS AND PROSPECTS

Presenter: Azat KHADIEV
Authors: Dmitri NOVIKOV, Azat KHADIEV, Yury MATVEEV, Jana RAABE, Atula PODUVAL

The In-situ X-ray diffraction and imaging beamline P23 at the PETRA III (DESY, Hamburg) operates currently with one experimental hutch. A second hutch operated by a joint KIT / DESY cooperation and dedicated to novel hard X-ray microscopy techniques will go into operation at the beginning of 2023. The scientific case of the beamline is concentrating on the physics and chemistry of systems dominated by low dimensional and confinement effects, with an emphasis on in-situ and *operando* techniques.

The undulator source and X-ray optics provide up to 1013 photons/sec into variable spot sizes down to one micrometer in the energy range 5-35 keV. Optionally, the energy can go higher up to 50 keV. The optical layout comprises an LN2-cooled Si(111)/Si(311) double-crystal monochromator, horizontally deflecting plane and collimating mirrors, and adjustable sets of Be CRLs in the optical and as well as experimental hutches. The experimental hutch is equipped with a heavy-load 5+2 circle diffractometer (HUBER), which can carry sample cells with up to 150 kg in horizontal scattering mode and up to 15 kg on the Eulerian cradle in the vertical mode. The experiment instrumentation pool is designed for multiscale analysis of bulk and nanostructured materials and devices: heating chambers, flow LHe-cryostat, piezo-based position stages, and an Andor optical spectrometer are available for the users. An in-situ pulsed deposition chamber becomes available for user projects starting September 2022.

Affillation
Deutsches Elektronen-Synchrotron DESY, Germany

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TUE 15:45-17:45 | BOARD 93 | P2-MET2-31

POSTER SESSION

4f ELECTRONIC EXCITATIONS AND THEIR ROLE FOR MAGNETIZATION DYNAMICS

Presenter: Nele THIELEMANN-KÜHN

Authors: Nele THIELEMANN-KÜHN (1), Tim AMRHEIN (1), Wibke BRONSCH (1), Gina HANDZAR (2), Somnath JANA (2), Niko PONTIUS (2), Robin Y. ENGEL (3), Piter S. MIEDEMA (3), Dominik LEGUT (4), Karel CARVA (5), Unai ATXITIA (2), Benjamin E. VAN KUIKEN (6), Martin TEICHMANN (6), Robert E. CARLEY (6), Laurent MERCADIER (6), Alexander YAROSLAVTSEV (6), Giuseppe MERCURIO (6), Loic LE GUYADER (6), Naman AGARWAL (6), Rafael GORT (6), Andreas SCHERZ (6), Siarhei DZIARZHYTSKI (3), Günter BRENNER (3), Federico PRESSACCO (3), Ru-Pan WANG (3), Jan SCHUNCK (3), Mangalika SINHA (3), Martin BEYE (3), Gheorghe Sorin CHIUZBAIAN (7), Peter OPPENEER (8), Anton TREMSIN (9), Martin WEINELT (1), Christian SCHÜSSLER-LANGEHEINE (2)

Ultrafast magnetic response to optical excitation has been studied for many years. Only recently it has been appreciated that early electronic excitations may play a more important role than just being a transient step in the deposition of energy in the electron system. As f-f electronic excitations in 4f metals are dipole forbidden, a variation of the 4f electronic structure was generally not considered to effect optically driven 4f spin dynamics. From a RIXS experiment at FLASH1 we learned that after exciting the 5d6s valence electrons in Tb with optical laser pulses, the 4f electronic state actually can be affected on ultrashort time scales. The derived spin and orbital momenta define the coupling of the magnetic system to the environment. According to X-ray absorption data obtained from a study at the EuXFEL, we find about 20 % of the Tb atoms to be orbitally excited. The altered state changes the magneto crystalline anisotropy. Our study gives a new dimension to the discussion about optically control of 4f magnetic dynamics, as it provides a femtosecond handle on the 4f spin coupling.

To explore electronic excitations and their role for magnetization dynamics in more detail at the FemtoSpeX slicing facility of BESSY II in the 2nd funding period of the TRR227 – Ultrafast Spin Dynamics, we plan to implement 2D-detection and improve energy resolution within a new experimental setup, based on the recently developed Timepix3 chip for soft-X-ray detection (BMBF financed).

Affillation

1: Freie Universität Berlin, Germany; 2: Helmholtz-Zentrum Berlin, Germany; 3: Deutsches Elektronen-Synchrotron DESY, Germany; 4: IT4Innovations-Czech National Supercomputing Centre, Czech Republic; 5: Charles University, Czech Republic; 6: European XFEL, Germany; 7: Sorbonne Université, France; 8: Uppsala University, Sweden; 9: University of California at Berkeley, USA

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TUE 15:45-17:45 | BOARD 94 | P2-MET2-32

POSTER SESSION

DynaMaX: ENDSTATION FOR ULTRA-FAST DYNAMICS AT BESSY II

Presenter: Nele THIELEMANN-KÜHN

Authors: Nele THIELEMANN-KÜHN (1), Tim AMRHEIN (1), Markus GLEICH (1), Kamil BOBOWSKI (1), Christoph TRABANT (1), Martin HENNECKE (2), Tino NOLL (2), Dieter ENGEL (2), Ilie RADU (2), Bertram FRIEDRICH (2), Stefan EISEBIT (2), Niko POTIUS (3), Christian SCHÜSSLER-LANGEHEINE (3), Martin WEINELT (1)

Central questions in material research, like how fast we can control materials properties and how this can be explained fundamentally are directly addressed by femtosecond (fs) time-resolved spectroscopy. Soft X-ray pulses with fs duration are well suited for such experiments because they allow for highly sensitive, element-specific investigations of transient electronic and magnetic properties. To keep up with the ever growing demand the BMBF financed project DynaMaX was created for optimizing the experimental capabilities at the fs X-ray source FemtoSpeX at BESSY II.

We built a new endstation, including a 3D vector magnet. The magnet allows applying magnet fields up to 1.5 T in all space directions with a sweep-rate up to 1 T/s. Together with the variable X-ray polarization this enables X-ray absorption, reflectivity and diffraction studies with variable geometries.

We developed an environment for in-situ sample preparation with different deposition techniques. We setup a combined system of two UHV chambers, one unit for molecular beam epitaxy and the other for magnetron sputter deposition. For sample characterization with X-rays, the growth unit is connected to the neighbouring PM3 scattering chamber.

The DynaMaX project has successfully increased the experimental capabilities and improved the infrastructure for researches at the FemtoSpex beamline, rendering the setup a world-wide unique fs X-ray source.

Affillation

1: Freie Universität Berlin, Germany; 2: Max-Born Institut, Germany; 3: Helmholtz-Zentrum Berlin, Germany

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TUE 15:45-17:45 | BOARD 95 | P2-MET2-33

POSTER SESSION

PETRA III: P03/MiNaXS – CURRENT STATUS AND FUTURE PLANS

Presenter: Jan RUBECK

Authors: Jan RUBECK (1), Andrei CHUMAKOV (1), Qing CHEN (1), Marc GENSCH (1,2), Benedikt SOCHOR (1), Marie BETKER (1,3), Constantin HARDER (1,2), Anton DAVYDOK (4), Matthias SCHWARTZKOPF (1), Christina KRYWKA (4), Stephan ROTH (1,3)

The P03 beamline at PETRA III, DESY, Hamburg, consist of a micro- (EH1) and a nanofocus (EH2) endstation, both being capable of experiments in transmission, wide- and small-angle X-ray scattering as well as grazing incidence geometries. The microfocus operates in the range of 42 x 20 µm^2, 22 x 13 µm^2 down to 7 x 4 µm2 (using Be-CRLs and intermediate focusing). The nanofocus endstation, operated by Hereon, features routinely a beam size of 350 x 250 nm2 and 1.5 x 1.5 µm2 focussed by a KB-mirrors system. A common, unique feature of all endstations is the exceptionally long and flexible focal distances, 3-8 m in the case of microfocus and 10 cm in the case of the nanofocus. Therefore, a large variety of in-situ sample environments can be implemented at MiNaXS. At the microfocus endstation, we operate a flexible heavy-load 5-axes goniometer (up to 180 kg) optional equipped with a linear translation stage and/or a hexapod (up to 30 kg) for precise alignment. We also offer additional auxiliary equipment for in-situ measurements to our user community, e.g. RF sputter deposition chamber, roll-to-roll spray coating. An adaptive flight-tube enables changes of the SAXS detector distance (from 1.5–9.8 m) addressing the relevant length scales ranging from Angstroms to microns. We also operate a novel, customized ɣ-shaped LAMBDA 9M (X-Spectrum) with a small pixel size (55µm) and a 2 kHz frame rate enabling simultaneous SAXS/WAXS measurements even with sub-millisecond time resolution.

Affillation

1: DESY, Notkestr. 85, D-22607 Hamburg, Germany; 2: TU München, James-Franck-Str. 1, D-85748 Garching, Germany; 3: KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden; 4: Helmholtz Zentrum Hereon, Max-Planck-Straße 1, 21502 Geesthacht, Germany

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TUE 15:45-17:45 | BOARD 96 | P2-MET2-34

POSTER SESSION

FAST KINETICS IN THIN FILMS BY INTENSITY MODULATED NEUTRON REFECTOMETRY

Presenter: Thomas KELLER
Authors: Thomas KELLER, Khaydukov YURY, Guasco LAURA, Keimer BERNHARD

We introduce a method for kinetic neutron reflectometry with a time resolution of a few microseconds. The method is based on periodic excitation of the sample and phase locked modulation of the beam intensity by one radio frequency spin flipper, and requires a neutron detector with time resolution also in the order of 1 microsecond. The output are time resolved reflectivity curves locked to the phase of the sample excitation parameter. The method is compatible with polarization analysis, and also allows to collect phase selective intensity of secondary radiation emitted by the sample, such as Gamma radiation or incoherently scattered neutrons.

Affillation
MPI für Festkörperforschung, Germany

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TUE 15:45-17:45 | BOARD 97 | P2-MET2-35

POSTER SESSION

AT-WAVELENGTH METROLOGY FACILITY FOR EUV, XUV AND TENDER X-RAY DIFFRACTIVE OPTICS AT BESSY II

Presenter: Andrey SOKOLOV
Authors: Andrey SOKOLOV, Frank EGGENSTEIN, Peter BISCHOFF, Yue YU, Peter BAUMGÄRTEL, Matthias MAST, Marcel MERTIN, Ingo PACKE, Franz SCHÄFERS, Jens VIEFHAUS

The At-Wavelength Metrology facility for sophisticated XUV optics such as diffraction gratings is operating since many years at the BESSY II storage ring. As the main instrument a versatile 11-axis UHV-reflectometer is permanently connected to dedicated Optics beamline is available. The setup covers energy ranges of the EUV and XUV. High spectral purity of the incident beam is achieved by a set of 12 absorption filters and a High-Order Suppressor System. It was experimentally tested that it gives a nearly high-order free beam between 13.5 eV and 1800 eV. A flexible sample support system based on an UHV-tripod gives 6 degrees of freedom for a precise alignment and mapping of optical elements under test. Optical elements with sizes up to 360 x 60 x 60 mm^3 have been tested, for samples smaller than 60 x 40 x 10 mm^3 a fast in-vacuum transfer load-lock system is available.

In additional to that a small Reflectometer as a portable end station is used to get access to UV-EUV or X-ray energy ranges. We had tested possibility to operate in lower energy range from 4 eV up to 30 eV at U125-2_NIM beamline. As well accurate measurements in energy range from 2000 eV to 10000 eV were carried out with small Reflectometer attached to KMC-1 beamline. The present status of the metrology facility, their upgrade projects and challenging recent results will be presented at the conference.

Affillation
Helmholtz-Zentrum Berlin für Materialien und Energie (BESSY II), Albert-Einstein-Str. 15, D-12489 Berlin

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TUE 15:45-17:45 | BOARD 98 | P2-MET2-36

POSTER SESSION

DIRECTIONAL DARK-FIELD X-RAY IMAGING: A COMPARISON OF A 2D TALBOT ARRAY ILLUMINATOR AND SANDPAPER AS OPTICAL ELEMENTS

Presenter: Ronan SMITH
Authors: Ronan SMITH (1), Mirko RIEDEL (2,3), Fabio DE MARCO (4,5), Sara SAVATOVIĆ (4,5), Julia HERZEN (2), Richard BOARDMAN (1), Pierre THIBAULT (4,5)

As X-rays pass through a sample, they undergo attenuation, refraction, and scattering. Traditionally, X-ray imaging systems only measured the first effect. Speckle-based imaging is a technique capable of mapping all 3 effects using a standard X-ray Micro-CT setup, with the addition of a 'diffuser' in the beam. This diffuser creates a fluctuating intensity pattern on the detector, and when a sample is placed into the beam the pattern is modified. Attenuation reduces the intensity, while refraction in the sample causes local translations of the pattern on the detector which can be measured, giving the phase-contrast image. Scattering in the sample blurs the pattern, giving the dark-field image. Here, we will be focusing on a special case of this – the directional dark-field image. This is where orientated structures (such as fibers within a carbon fiber reinforced composite) cause an anisotropic scattering. Measuring the direction of this scattering allows the orientation of these structures to be measured without being able to resolve them.

Sandpaper is a popular choice for the diffuser which creates the pattern, however 2D Talbot Array Illuminators have recently been custom made for this application. They have been shown to be effective for phase-contrast imaging, and here we demonstrate their potential for directional darkfield imaging. We compare images produced using sandpaper and a 2D Talbot Array Illuminator at the P05 Beamline of PETRA III.

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TUE 15:45-17:45 | BOARD 99 | P2-MET2-37

POSTER SESSION

SMALL-ANGLE X-RAY SCATTERING: CHARACTERIZATION OF ARBITRARILY SHAPED NANOPARTICLES USING DEBYE'S EQUATION

Presenter: Christian GOLLWITZER
Authors: Jérôme DEUMER (1), Brian PAUW (2), Sylvie MARGUET (3), Dieter SKROBLIN (1), Olivier TACHÉ (3), Michael KRUMREY (1), Christian GOLLWITZER (1)

We propose a versatile software package in the form of a Python extension, named CDEF (Computing Debye's scattering formula for Extraordinary Formfactors), to approximately calculate scattering profiles of arbitrarily shaped nanoparticles for small-angle X-ray scattering (SAXS). CDEF generates a quasi-randomly distributed point cloud in the desired particle shape and then applies the open source software DEBYER [1] for efficient evaluation of Debye's scattering formula to calculate the SAXS pattern.

The usage of the software is demonstrated for the evaluation of scattering data of Au nanocubes with rounded edges, which were measured at the four-crystal monochromator beamline of PTB at the synchrotron radiation facility BESSY II in Berlin. Our implementation is fast enough to run on a single desktop computer and perform model fits within minutes. The accuracy of the method was analyzed by comparison with analytically known form factors.

CDEF is freey available under the terms of the GPL open source license and can be installed directly from PyPI [2]

---

[1] https://github.com/wojdyr/debyer
[2] https://pypi.org/project/CDEF/
[3] https://arxiv.org/abs/2109.06570

Affillation
1: Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany; 2: Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany; 3: Université Paris-Saclay, CEA, CNRS, NIMBE, 91191 Gif-sur-Yvette, France

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TUE 15:45-17:45 | BOARD 100 | P2-MET2-38

POSTER SESSION

POLARIZING NEUTRON OPTICS FROM NOB NANO OPTICS BERLIN

Presenter: Thomas KRIST
Author: Thomas KRIST

In the last decades a variety of polarizing neutron optical devices has been developed in cooperation of NOB and the Helmholtz-Zentrum Berlin, mainly solid state elements where the neutrons are transported in thin silicon wafers with coated walls, but also devices where the neutrons transmit silicon wafers with polarizing coatings.

We show results of solid state polarising benders, solid state collimators with polarizing walls and a solid state radial bender for polarisation analysis over an angular range of 3.8 deg.

Two-dimensional polarisation analysers for an angular range of 5 degrees in both directions are presented.

A polarizing cavity in a guide with a cross section of 60mm x 100mm was built which polarizes neutrons with wavelengths above 2.5 Å.

In all these polarizing devices polarisations of 95 % were realised.

In the last years several polarizing S-benders were build and tested. They had cross sections from 30 mm x 50 mm up to 60mm x 125mm. They were designed for different wavelength ranges, some as low as 2 Å to 6.5 Å.

Typical values for the maximum transmission for the spin up component at a wavelength of 4.4Å are above 65 % with a polarization above 98 % [1].

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[1] Th. Krist, F. Rucker, G. Brandl, R. Georgii: High performance, large cross section S-bender for neutron polarization, Nuclear Inst. and Methods in Physics Research A 698 (2013) 94-97.

Affillation
NOB Nano Optics Berlin GmbH, Germany

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TUE 15:45-17:45 | BOARD 101 | P2-MET2-39

POSTER SESSION

TRACEABLE CONCENTRATION MEASUREMENTS OF NANOPARTICLE SUSPENSIONS USING SAXS AND PHOTOCENTRIFUGATION

Presenter: Robin SCHÜRMANN
Authors: Robin SCHÜRMANN, Jerome DEUMER, Christian GOLLWITZER

The industrial production of high-quality nanoparticles (NPs), as well as biomedical analytical applications, require precise methods to quantify the absolute number concentration of NPs in suspension. In this context, small angle X-ray scattering (SAXS) is a powerful tool to determine the NP size, shape and concentration. In order to calculate the concentration, absolute measurements of the scattering intensity in terms of SI-units are necessary, which require precise knowledge of all experimental parameters. Moreover, the scattering intensity depends significantly on the electron density difference of solvent and NPs, which is often unknown, due to possible differences in the densities of bulk material and NPs [1]. Methods have been established to directly measure the electron density of the NPs by contrast matching with a solvent density gradient [2]. However, these methods are typically limited to a certain density regime and therefore complementary techniques are required to determine the density of the particles. Here a combined approach is presented using SAXS and analytical photocentrifugation to traceably determine the size distribution, density and absolute number concentration of silica NPs. Furthermore, challenges like beam size effects will be discussed, which must be considered in the data treatment to avoid systematic errors by artificial backgrounds.

[1] A. Schavkan et al., Nanomaterials (2019), 9(4), 502
[2] Garcia et al., J. Appl. Cryst. (2015). 48, 20–28

Affillation
Physikalisch-Technische Bundesanstalt (PTB), Germany

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TUE 15:45-17:45 | BOARD 102 | P2-MET2-40

POSTER SESSION

ANGULAR DISTRIBUTION IN RAYLEIGH SCATTERING OF LINEARLY POLARIZED HARD X-RAYS

Presenter: Wilko MIDDENTS

Authors: Wilko MIDDENTS (1,2), Günter WEBER (2,3), Uwe SPILLMANN (3), Philip PFÄFFLEIN (2,3), Alexandre GUMBERIDZE (3), Nikolaus KURZ (3), Thomas KRINGS (4), Sophia STRNAT (5,6), Andrey SURZHYKOV (5,6), Norbert SCHELL (7), Thomas STÖHLKER (1,2,3)

Rayleigh scattering is the dominant contribution to the elastic scattering of hard X-rays on atoms for photon energies below 1 MeV. It is the scattering of a photon on atomic electrons without gain or loss of energy. The angular distribution of Rayleigh scattering strongly depends on the polarization of the incident photon beam [1]. Thus, determining the angular distribution of Rayleigh scattering of a highly linearly polarized photon beam allows for a sensitive test of the underlying theoretical calculations. Vice versa, relying on the calculations, this process allows for a precise determination of the linear polarization of the incident photon beam.

In an experiment at the synchrotron PETRA III at DESY we analyzed the angular distribution of Rayleigh scattering for a linearly polarized X-ray beam with a photon energy of 175 keV on a thin gold target. The scattered radiation was analyzed inside and out of the polarization plane with a Ge(i) detector and a 2D sensitive Compton polarimeter. By leveraging on the theoretical calculations of the scattering process, we were able to determine the polarization characteristics of the incident synchrotron beam with high accuracy. In contrast to the common assumption of a fully linearly polarized synchrotron beam, we can show a slight depolarization of the incident beam as seen already in a previous experiment [2].

[1] A. Surzhykov et al., Phys. Rev. A98, 053403 (2018)
[2] K. H. Blumenhagen et al., New J. Phys.18, 103034 (2016)

Affillation
1: Friedrich-Schiller-Universität Jena, Germany; 2: Helmholtz-Institut Jena, Germany; 3: GSI Helmholtzzentrum für Schwerionenforschung Darmstadt, Germany; 4: Forschungszentrum Jülich, Germany; 5: Physikalisch-Technische Bundesanstalt Braunschweig, Germany; 6: Technische Universität Braunschweig, Germany; 7: Helmholtz-Zentrum Hereon, Geesthacht, Germany

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TUE 15:45-17:45 | BOARD 103 | P2-MET2-41

POSTER SESSION

ELECTRONIC VS. NUCLEAR SPUTTERING OF CORONENE

Presenter: Lars BREUER
Authors: Lars BREUER (1), Tobias HECKHOFF (1), Matthias HERDER (1), Hua TIAN (2), Nicholas WINOGRAD (2), Andreas WUCHER (2)

Electronic sputtering induced by swift heavy ion (SHI) irradiation of solids has been suggested as a relatively soft desorption mechanism for intact molecules in Secondary Ion Mass Spectrometry (SIMS). In order to evaluate the prospects of this “MeV-SIMS” technique as compared to the standard SIMS methodology utilizing nuclear sputtering with projectile energies in the keV range, we have performed a case study using time-of-flight (ToF) mass spectrometry to detect both ionized and neutral particles sputtered from a coronene film. In particular, secondary ion and neutral mass spectra obtained under 4.8 MeV/u Ca, Bi and Au ion impact were compared with those measured under irradiation with keV Ar, C60 and Ar1500 ions. While secondary ions were directly detected using a reflectron ToF spectrometer, sputtered neutral particles were post-ionized using two different laser photoionization schemes, namely vacuum ultraviolet single photon ionization at 157 nm and infrared strong field ionization at wavelengths between 800 and 1300 nm, respectively. In order to assess the photo-induced fragmentation of emitted molecular species, the results measured under ion bombardment were compared in-situ with those induced by thermal evaporation via heating the sample. The measured spectra are interpreted in terms of partial sputter yields, fragmentation patterns, emission velocity distributions and ionization probabilities with emphasis on the emission and/or formation of intact molecular ions.

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TUE 15:45-17:45 | BOARD 104 | P2-MET2-42

POSTER SESSION

TIME OF FLIGHT MEASUREMENTS USING A COMPACT SOLID METHANE MODERATOR

Presenter: Thomas GUTBERLET

Authors: Alexander SCHWAB (1,4), Paul ZAKALEK (1), Ulrich RÜCKER (1), Yannick BESSLER (2), Olaf FELDEN (3), Thomas GUTBERLET (1), Thomas BRÜCKEL (1), Ghaleb NATOUR (2,4)

Long-wavelength neutrons for the investigation of nano-scale materials are an indispensable tool in neutron research. To slow down the free neutrons produced in a large-scale source to energies of a few meV and below, hydrogen-rich materials at cryogenic temperatures are applied.

At the High Brilliance Neutron Source (HBS) project, multiple cold moderators will be positioned inside the same Target-Moderator-Reflector unit (TMR), each providing its own instrument with cold or even very cold neutrons. All of these moderators can therefore be optimized in terms of material, operating temperature and geometry, depending on the requirements of the instrument.

To experimentally investigate the effect of lowering the operating temperature of a compact solid methane moderator to approximately 10 K, a cryogenic system was designed and manufactured at Forschungszentrum Jülich. Time of flight measurements were conducted for various temperatures of the solid methane, using a 45 MeV proton beam provided by the cyclotron JULIC at Forschungszentrum Jülich to produce free neutrons mainly by (p,n) reactions inside a tantalum target. The neutrons were subsequently moderated and guided to a detector cradle equipped with He-3 detectors.

The results will allow a more precise validation of scattering kernels used in Monte Carlo simulations and lead to a more efficient optimization of existing and future cold neutron sources.

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TUE 15:45-17:45 | BOARD 105 | P2-MET2-43

POSTER SESSION

THE HARD X-RAY MOMENTUM MICROSCOPY END STATION AT PETRA III

Presenter: Thiago R. F. PEIXOTO
Authors: Thiago R. F. PEIXOTO (1), Christoph SCHLUETER (1), Gerd SCHÖNHENSE (2), Hans-Joachim ELMERS (2)

The demand for a bulk-sensitive photoemission (PE) imaging probe in momentum space, with high energy and momentum resolution, has been pushing forward the development of new approaches to hard X-ray PE spectroscopy (HAXPES). The use of a time-of-flight (ToF) spectrometer combined with synchrotron radiation has been proving very successful in this regard. The parallel data acquisition scheme of the ToF spectrometer combined with a state-of-the-art delay-line detector and a high flux / high energy resolution hard X-ray beamline allows the fast imaging of PE spectra directly in the k-space and element-selective photoelectron diffraction (HXPD) patterns. Also for valence band (VB) mapping, this ToF momentum microscopy (MoM) approach has overcome fundamental bottlenecks faced by standard hemispherical analysers. Here we present the new HAX-ToF-MoM end station available at the beamline P22, at PETRA III. Our instrument allows high-resolution k-space imaging of core levels and bulk VB of various materials, with field-of-views of 20 Brillouin zones, at photon energies in the range 2.4–8 keV. Recent results obtained at this end station demonstrate the instrument's energy and momentum resolutions comparable to standard hemispherical analysers in the soft X-ray range. This instrument establishes HAX-ToF-MoM as bulk-sensitive spectromicroscopic tool in solid state research available at PETRA III for the investigation of electronic and atomic structures of novel materials.

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TUE 15:45-17:45 | BOARD 106 | P2-MET2-44

POSTER SESSION

HAXPES AT PETRA III: ELECTRONIC STRUCTURE, OPERANDO DEVICES AND IN-SITU CATALYSIS

Presenter: Christoph SCHLUETER
Author: Christoph SCHLUETER

The X-ray undulator beamline (P22) at PETRA III facilitates research in electronic structure, *operando* devices and in-situ catalysis by use of hard X-ray photoelectron spectroscopy (HAXPES) techniques. For this purpose P22 hosts four specialised experimental end stations for high-resolution studies of the electronic and chemical structure of complex materials, realistic device-like structures and catalytic interfaces. The main instrument for conventional HAXPES techniques offers sample cooling and in-situ electrical characterisation for *operando* studies. A separate instrument provides full-field, sub-µm electron spectro-microscopy (HAXPEEM). Additionally, a specialized setup for high-pressure HAXPES applications (POLARIS) recently demonstrated its capabilities at pressures >2.0 bar. Finally, a full-field k-microscope with time-of-flight energy discrimination delivered first fully k-resolved valence band structures in the HAXPES energy range (up to 7 keV). All instruments are implemented and operated in close collaboration with external user groups and as such reflect the wide range of scientific fields currently covered by our community.

Affillation
Deutsches Elektronen Synchrotron DESY, Hamburg, Germany

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TUE 15:45-17:45 | BOARD 107 | P2-MET2-45

POSTER SESSION

GINIX – GÖTTINGEN INSTRUMENT FOR NANO-IMAGING WITH X-RAYS

Presenter: Markus OSTERHOFF
Authors: Markus OSTERHOFF (1,2), Michael SPRUNG (4), Tim SALDITT (1,2,3)

Over more than eleven years, the GINIX endstation situated at PETRA III's coherence beamline P10 has brought light to more than 100 experiments and lots of data to scientists of different fields. Here, we highlight scientific outcomes of selected experiments, and present instrumental challenges and key upgrades that were necessary to achieve these results.

Recent developments in holo-tomo reconstruction and segmentation are also summarised. This includes new phase-retrieval methods like reporter based super-resolution imaging or a combined reconstruction making use of several holographic orders and scattering signals. In AI assisted segmentation, techniques like Optimal Transport address the classification problem.

Finally, we present a Scientific Instrument Proposal for a potential GINIX II at PETRA IV. Combining the benefits of hybrid pixelated detectors, waveguide filtered clean beams, and single-shot high-resolution holographic imaging techniques, imaging resolutions of below 10 nm have just been demonstrated. With GINIX II, a dedicated high-throughput holo-tomo setup is envisaged for virtual histology, pre-clinical research, and diagnostic findings.

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TUE 15:45-17:45 | BOARD 108 | P2-MET2-46

POSTER SESSION

XRnanotech – ACHROMATIC X-RAY LENS AND RECENT DEVELOPMENTS IN NANOSTRUCTURED X-RAY OPTICS

Presenter: Adam KUBEC
Authors: Adam KUBEC (1), Christian DAVID (2), Florian DÖRING (1)

At XRnanotech, a spin-off from the Paul Scherrer Institut (PSI) in Switzerland, we develop X-ray optics to enable experiments at many large-scale research facilities. Our goal is to push the limits of diffractive and refractive X-ray optics by continuously improving the resolution and efficiency enabling new applications in microscopy to make the invisible visible. In X-ray microscopy, Fresnel zone plates (FZPs) are used as high-resolution lenses. Their resolution depends mainly on the size of their smallest outermost zones and many years of development were required in order to push this value into ever-smaller regimes.

New procedures have recently also allowed using 3D-printing methods also in the field of X-ray optical applications. For X-ray energies of several keV, a good transmission and refractive properties are achieved along with low surface roughness. Through its versatility, 3D-printing allows manufacturing various types of geometries, X-ray optics, and (resolution) samples alike. The flexibility of this approach allows for achieving previously inaccessible X-ray optical properties.

It has allowed us to achieve achromatic focusing with X-rays using a combination of diffractive and refractive optical elements, which we demonstrated for the first time.

We will also show some of the recent developments in high efficiency, high resolution, structured beam, and reflection optics.

Affillation
1: XRnanotech, Switzerland; 2: Paul Scherrer Institute, Switzerland

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TUE 15:45-17:45 | BOARD 109 | P2-MET2-47

POSTER SESSION

SUB-MICROMETER FOCUSING SETUP FOR HIGH-PRESSURE CRYSTALLOGRAPHY AT THE EXTREME CONDITIONS BEAMLINE AT PETRA III

Presenter: Konstantin GLAZYRIN

Authors: Konstantin GLAZYRIN (1), Saiana KHANDARKHAEVA (2,3), Timofey FEDOTENKO (1,3), Weiwei DONG (1), Dominique LANIEL (3), Frank SEIBOTH (4), Andreas SCHROPP (4,5), Jan GARREVOET (1), Dennis BRÜCKNER (1,6,7), Gerald FALKENBERG (1), Adam KUBEC (8), Christian DAVID (8), Mario WENDT (1), Sergej WENZ (1), Leonid DUBROVINSKY (2), Natalia DUBROVINSKAIA (3,9), Hanns-Peter LIERMANN (1)

Scientific tasks aimed at decoding and characterizing complex systems and processes at high pressures set new challenges for modern X-ray diffractioninstrumentation in terms of X-ray flux, focal spot size and sample positioning. Presented here are new developments at the Extreme Conditions beamline (P02.2, PETRA III, DESY, Germany) that enable considerable improvementsin data collection at very high pressures and small scattering volumes. Inparticular, the focusing of the X-ray beam to the sub-micrometer level is described, and control of the aberrations of the focusing compound refractivelenses is made possible with the implementation of a correcting phase plate. This device provides a significant enhancement of the signal-to-noise ratio by conditioning the beam shape profile at the focal spot. A new sample alignment system with a small sphere of confusion enables single-crystal data collection from grains of micrometer to sub-micrometer dimensions subjected to pressures as high as 200 GPa. The combination of the technical development of the optical path and the sample alignment system contributes to research and gives benefit son various levels, including rapid and accurate diffraction mapping of samples with sub-micrometer resolution at multimegabar pressures.

Affillation

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TUE 15:45-17:45 | BOARD 110 | P2-MET2-48

POSTER SESSION

PEAXIS – A HIGH RESOLUTION RIXS ENDSTATION FOR SOLID-STATE ENERGY AND QUANTUM MATERIALS

Presenter: Deniz WONG
Authors: Deniz WONG, Christian SCHULZ, Maciej BARTKOWIAK, Klaus HABICHT

PEAXIS (Photo Electron Analysis and resonant X-ray Inelastic Spectroscopy) is a dedicated endstation installed at the beamline U41-PEAXIS at BESSY II that offers high resolution soft X-ray spectroscopy measurements. The endstation combines two X-ray spectroscopic techniques: X-ray photoelectron spectroscopy (XPS) and resonant inelastic spectroscopy (RIXS), which are important in probing electronic structure and excited electronic states in solid-state materials. Here, we highlight scientific insights recently obtained at PEAXIS by RIXS spectroscopy.

Material systems for energy and quantum applications strongly build upon complex and, in part, unique electronic structures. High resolution RIXS explores the coupling of the material's lattice system to its electronic structure and provides insights towards the dynamics and transport properties of tomorrow's functional materials. As a prominent example, the detection of distinct chemical states of oxygen that contributes to the redox reaction inherent to new generation cathodes in Li-ion batteries is discussed. This leads to a better understanding of the mechanism involved in capacity fading and contributes to the development of materials for enhanced battery performance. In addition, selected highlights illustrating unique features of PEAXIS that cater the needs of studying modern material systems in a wide temperature range, exploiting applied voltage devices and employing continuous motion for sensitive samples are shown.

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TUE 15:45-17:45 | BOARD 111 | P2-MET2-49

POSTER SESSION

NUCLEAR QUANTUM OPTICS – FROM PULSE SHAPING TO COHERENT CONTROL AT SYNCHROTRON RADIATION SOURCES

Presenter: Jörg EVERS

Authors: Kilian P. HEEG (1), Andreas KALDUN (1), Cornelius STROHM (2), Christian OTT (1), Rajagopalan SUBRAMANIAN (1), Dominik LENTRODT (1), Johann HABER (2), Hans-Christian WILLE (2), Stephan GOERTTLER (1), Rudolf RÜFFER (3), Christoph H. KEITEL (1), Ralf RÖHLSBERGER (2,4,5,6,7), Thomas PFEIFER (1), Jörg EVERS (1)

Ideas from quantum optics play an important role in studying, controlling, and utilizing light-matter interactions in many regions of the electromagnetic spectrum. This raises the question, whether such concepts could also be utilized to improve or develop applications at hard X-ray energies. Prime candidates for this purpose are Mössbauer nuclei, since they offer exceptionally narrow nuclear resonances, and thereby correspondingly long coherence times. This Poster Session introduces basic concepts of nuclear quantum optics. The focus will be on the temporal- and spectral shaping of X-ray pulses delivered by synchrotron sources, by means of mechanical motions of a resonant target. As a first application, I will show how this can be used to increase the resonant flux, by shifting off-resonant parts of the pulse spectrum onto resonance [1]. Next, I will demonstrate how such shaped pulses can be used to coherently control the dynamics of Mössbauer nuclei [2].

[1] K. P. Heeg et al., Science 357, 375 (2017).
[2] K. P. Heeg et al., Nature 590, 401 (2021).

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TUE 15:45-17:45 | BOARD 112 | P2-MET2-50

POSTER SESSION

PTYCHOGRAPHIC RECONSTRUCTION WITH OBJECT INITIALIZATION

Presenter: Peter MODREGGER
Authors: Felix WITTWER (1,2), Dennis BRÜCKNER (3), Peter MODREGGER (1,2)

In X-ray ptychography, phase retrieval, i.e., the recovery of a complex valued signal from intensity-only measurements, is enabled by exploiting a redundancy of information contained in diffraction patterns measured with overlapping illuminations. Ptychographic reconstruction is generally performed by an iterative minimization procedure of an appropriate cost function. During iteration the bulk phase information has to propagate from the sample edges to the center for bulky samples, which is an inherent limitation of reconstruction speed, if a flat object initialization is used. Here, we experimentally demonstrate that by using a low resolution representation for the object as a starting guess, computational speed and stability can be improved considerably. This approach is computationally fast and compatible with a wide range of ptychographic reconstruction algorithms, which impies a widespread use.

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TUE 15:45-17:45 | BOARD 113 | P2-MET2-51

POSTER SESSION

LIGHT-MATTER COUPLING OF QUANTUM EMITTERS IN HARD X-RAY WAVEGUIDES

Presenter: Leon Merten LOHSE
Authors: Leon Merten LOHSE (1,2), Tim SALDITT (1), Ralf RÖHLSBERGER (2,3)

Enabled by the brilliance of third generation synchrotron radiation sources and advances in instrumentation, the last two decades bore major successes in the emerging field of X-ray quantum optics. A particularly fruitful experimental platform are the sharp nuclear resonances of Mössbauer nuclei, accompanied by their extreme coherence properties [1]. The resonant nuclei can be deposited as thin films in a multilayer structure, which alters the light-emitter coupling efficiency and can be designed to the experimental needs. At the same time, the understanding of hard X-ray waveguides has been advanced to the point where they are routinely employed for nanoscopic imaging experiments and even allow spliting and deflecting beams on a chip [2].

Here we present first experiments of resonant atoms embedded in thin-film X-ray waveguides and coherently probed by synchrotron radiation. Unlike previous experiments, we have coherently coupled the focussed beam into the front end of the waveguide and recorded the forward-transmitted intensity. For the first time, we were able to measure the transmitted photons after propagating through 20-nm-thin waveguides of up to 2 mm length while interacting with the ensemble of quantum emitters. We have observed temporal beatings characteristic for multiple absorption and reemission of the photons.

[1] R. Röhlsberger and J. Evers, “Quantum Optical Phenomena in Nuclear Resonant Scattering,” (2021)
[2] T. Salditt et al., PRL 115, 203902 (2015).

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TUE 15:45-17:45 | BOARD 114 | P2-MET2-52

POSTER SESSION

2D BRAGG BEAM CONDITIONER FOR LARGE FIELD-OF-VIEW X-RAY IMAGING

Presenter: Adyasha BISWAL
Authors: Adyasha BISWAL (1), Rebecca SPIECKER (2), Holger HESSDORFER (3), Elias HAMANN (3), Mykola SCHERBININ (2), Tilo BAUMBACH (2,3)

For X-ray imaging and tomography, the evolution of synchrotron radiation sources has opened new dimensions, especially in terms of flux and coherence. However, the decreasing cross-section of the X-ray source is an impediment, especially for high-throughput imaging of large, cm-sized samples. Large fields of view (FOV) can be reached by scanning the sample, which, conversely, increases scan times and necessitates stitching of 3D volumes in post-processing.

The beam cross section can be expanded by asymmetric Bragg diffraction using large single crystals. We have developed a Bragg magnifier system adapted for energies of 29–31 keV to allow for synchrotron imaging of cm-sized samples even at beamlines with a beam cross section of 2 mm or less. The system is based on up to four silicon crystals to keep the outgoing beam parallel to the incoming beam. Depending on the source parameters, energy and crystal dimensions, the outgoing FOV can reach values of over 5 cm x 5 cm while the high reflectivity (over 90 %) of the Bragg crystals ensures low loss of total photon flux.

The Poster Session presents first experimental results with our 30 keV beam conditioner system. Besides, it discusses parameters that need to be considered for the design of an equivalent system at different energies as well as intrinsic and practical challenges.

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TUE 15:45-17:45 | BOARD 118 | P2-MAEN-01

POSTER SESSION

EVOLUTION OF MESOPOROUS STRUCTURES IN Mg-,Ni- AND Co-PHOSPHATE COMPOUNDS

Presenter: Stephanos KARAFILUDIS
Authors: Stephanos KARAFILUDIS (1,2), Tomasz M. STAWSKI (1), Ana Guilherme BUZANICH (1), Franziska EMMERLING (1,2)

In the last decade mesoporous transition metal phosphates (TMP) captured major interest due to their high electrocatalytic activity useful for H2 generation, supercapacitors or batteries. A mesoporous material (2-50 nm, IUPAC) is highly reactive due to a high surface area and large number of active metal sites while it simultaneously offers significant mass transfer through the molecule, highly suitable for catalytical properties. Typically, the synthesis of mesoporous materials employs a template-based route, which is inefficient in the case of TMPs due to difficulties such as the removal of the used surfactants or the sensitivity of the mesoporous framework. We present a new template-free method including the formation of a precursor phase called M-struvite (NH4MPO4•6H2O, M = Mg2+, Ni2+, Co2+, Cu2+, Zn2+, Fe2+ ...) to synthesize mesoporous and amorphous transition metal phosphates (2–5 nm wide pore channels, specific surface area of 100 m2 g–1 and a pore volume of 0.13 cm3 g–1). This method relies on thermal decomposition of a crystalline M-struvite precursors, i.e. M - NH4PO4.6H2O (M = Mn, Co, Ni etc.) with the coincident degassing of volatile components like H2O or NH3. In addition to this low cost, environmentally friendly and simple one pot synthesis, M-struvites could grow as a recycle product from industrial waste waters and would contribute in such a way to a circular economy of sought-after commodities like phosphorus or transition metals.

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TUE 15:45-17:45 | BOARD 119 | P2-MAEN-02

POSTER SESSION

THREE-DIMENSIONAL X-RAY DIFFRACTION FOR MICROSTRUCTURE MAPPING ON THE GRAIN LEVEL

Presenter: Benjamin NEDING
Authors: Benjamin NEDING (1), Johan HEKTOR (2), Sangbong YI (1)

A fundamental understanding of the relationship between the microstructure and the macroscopic properties of a material is crucial in order to improve existing materials and develop new alloys to meet increasingly challenging demands on engineering materials. In recent years, modelling the mechanical behavior of polycrystalline materials has become a powerful tool in order to bridge the material's microstructure and its resulting macroscopic properties.

Naturally, these models need experimental verification and input parameters in order to reflect reality accurately and, moreover, to further improve. Three-dimensional X-ray diffraction (3DXRD) is one of the most powerful experimental technique for quantifying the microstructure and elastic strain state of a material on the grain level. The material can be quantified and mapped in three dimensions, and individual grains embedded in polycrystalline materials can be studied non-destructively. It also allows tracking changes and studying the response of materials during mechanical loading, heat treatments or other applied fields.

A dedicated instrument for grain mapping was installed at the high-energy materials science beamline P07 at the PETRA III synchrotron radiation source. We will present the status of the instrument along with plans for upgrades and we will present recent results giving an insight in the possibilities of this technique.

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TUE 15:45-17:45 | BOARD 120 | P2-MAEN-03

POSTER SESSION

PRECIPITATION KINETICS IN Al-ALLOY 7050 STUDIED BY SAXS, WAXS AND NUMERICAL MODELING

Presenter: Susanne HENNINGER
Authors: Susanne HENNINGER (1), Jan HERRNRING (2), Peter STARON (1), Benjamin KLUSEMANN (2,3), Martin MÜLLER (1)

Al-alloys are favored as lightweight material in industry due to their high strength-to-weight ratio. Especially alloys of the 7xxx series, which are age-hardenable, are often used in structural components in aerospace and automotive industry. The strengthening precipitates, which lead to their outstanding mechanical properties, are formed by thermal aging processes. The main strengthening phases in these alloys are the metastable η'-phase and the stable η-phase. However, microstructural evolution of these phases is complex as two major alloying elements (Mg, Zn) and two phases are involved.

Numerical modeling is a powerful tool for the description of precipitation kinetics; therefore, a numerical model has been developed that can handle alloys of the 7xxx series. Experimental data is required for evaluation of the model, which can be gained by in-situ SAXS/WAXS experiments. The refined precipitation model can then be used for studying precipitation behavior under non-equilibrium conditions like e.g. in friction stir processing.

In this work simultaneous in-situ SAXS / WAXS measurements using high-energy X-rays were conducted using the alloy AA7050 in T7451. Reversion experiments at four different temperatures (200 – 290 °C) with high temporal resolution were carried out as well as an isothermal experiment and heating ramps. Volume fractions, mean radius and number of precipitates during these time-temperature cycles are compared with predictions of the developed numerical model.

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TUE 15:45-17:45 | BOARD 121 | P2-MAEN-04

POSTER SESSION

QUASI IN-SITU INVESTIGATION OF DISLOCATION DYNAMICS IN SEMICONDUCTOR MATERIALS BY X-RAY DIFFRACTION IMAGING

Presenter: Simon BODE
Authors: Merve KABUKCUOGLU (1,2), Simon BODE (1), Elias HAMANN (1), Simon HAAGA (1,2), Andreas DANILEWSKY (2), Tilo BAUMBACH (1,3), Daniel HÄNSCHKE (1)

Semiconductor materials are key for modern micro- and optoelectronics but plastic deformation by dislocation slip during wafer processing (induced e.g. by handling and annealing) still reduces the fabrication yield and degrades device performance. Moreover, due to the ongoing miniaturization of electronics, the understanding, prediction, and avoidance of processing-induced dislocations and their dynamics becomes more and more relevant, thus motivating both scientific and industrial interest in their systematic investigation.

For the presented study, 2D and 3D X-ray diffraction imaging techniques, namely conventional X-ray white-beam topography and the recently developed X-ray diffraction laminography, were employed. Non-destructively, the methods allow investigating dislocations in large crystals with a 3D resolution of a few µm. Our recent instrumental and methodical progress, including well-defined and monitored sample annealing, now enables so-called quasi in-situ 2D and 3D studies of dislocation dynamics in semiconductor wafers under industrially relevant conditions.

Here, we will show a quasi in-situ study of the evolution of dislocation arrangements in silicon and gallium arsenide wafers, under conditions similar to industrial processing. Our results provide new insight into features of individual dislocations and the mechanisms involved in dense arrangements, as well as the relation of the observed dynamics, the driving thermal forces, and crystallographic properties.

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TUE 15:45-17:45 | BOARD 122 | P2-MAEN-05

POSTER SESSION

PHASE TRANSFORMATIONS IN TiAl DURING SELECTIVE LASER MELTING (SLM) STUDIED BY X-RAY DIFFRACTION

Presenter: Jan ROSIGKEIT
Authors: Jan ROSIGKEIT (1), Peter STARON (1), Emad MAAWAD (1), Erwin KROHMER (2), Martin MÜLLER (1)

Interest in SLM has dramatically expanded in the last several years, owing to the advantages of additive manufacturing (AM) compared to conventional manufacturing. AM attracts strong attention in the area of high performance materials like intermetallic Titanium Aluminide (TiAl) alloys. They represent innovative materials for high-temperature applications in aviation or energy generation, e.g. turbines blades. However, the cyclic heating and cooling during SLM leads to heat treatments of the previous solidified layers changing the phase content and inducing large residual stresses. Therefore, TiAl has so far only been additively manufactured using electron beam melting, which easily facilitates substrate heating to the required temperatures. Nevertheless, SLM of TiAl can also be achieved with sufficient substrate heating. This study focuses on the phase transformations and residual stress build-up as a function of process parameters in order to understand cracking in these alloys. For this, diffraction measurements with high-energy X-rays were performed in-situ during the build process. An SLM chamber was used that had been developed for use at a synchrotron beamline. The influence of process parameters on phase transformations and strain development will be discussed.

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TUE 15:45-17:45 | BOARD 123 | P2-MAEN-06

POSTER SESSION

ACTIVE SITES OF Te IN HYPERDOPED Si BY HARD X-RAY PHOTOELECTRON KIKUCHI-DIFFRACTION

Presenter: Moritz HOESCH

Authors: Moritz HOESCH (1), Mao WANG (2), Shengqiang ZHOU (2), Olena FEDCHENKO (3), Christoph SCHLÜTER (1), Dmitrii POTOROCHIN (1,4), Katerina MEDJANIK (3), Sergey BABENKO (3), Anca CIOBANU (1), Aimo WINKELMANN (5), Hans-Joachim ELMERS (3), Gerd SCHÖNHENSE (3)

n-type doping of Si by the deep chalcogen donor Te in excess of the solubility limit was recently demonstrated to lead to hyperdoped material [1]. Our investigation by hard X-ray photoelectron spectroscopy (hXPS) reveals at least two different Te species with different binding energy and systematically varying concentrations with increasing ion implantation dose. At the highest doping we study the photoelectron scattering patterns using hard X-ray photoelectron diffraction (hXPD) [2]. Substitutional site occupation of both Te monomers as well as dimers is identified with increasing binding energy leading to the main features in the XPS spectra. The sharp hXPD patterns allow the detailed analysis of the local surrounding of the dopant atoms [3]. At the lowest binding energy, an additional species is found and the distinct, rather diffuse hXPD pattern at this binding energy suggests the assignment of this component to a small fraction of Te in clusters.

[1] M. Wang et al. Phys. Rev. Appl. 11 054039 (2019) and references therein.
[2] O. Fedchenko et al NJP 21, 113031 (2019);
[3] O. Fedchenko et al NJP 22, 103002 (2020).

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TUE 15:45-17:45 | BOARD 124 | P2-MAEN-07

POSTER SESSION

OPTICAL CONSTANTS OF MgF2 THIN FILM IN THE VUV AND EUV ENERGY RANGE WITH IMPROVED ACCURACY

Presenter: Yue YU
Authors: Yue YU (1), Andrey SOKOLOV (2), Analía FERNÁNDEZ HERRERO (2), Jens VIEFHAUS (2)

Magnesium fluoride is regarded as an extremely attractive material choice for preparing single layer or multilayer coatings on various optics that are as well demanded for synchrotron radiation beamlines and spectrometers. Even though a considerable number of publications have been devoted to the optical constants of MgF2, the samples under study were mostly deposited by evaporation, ion beam sputtering or mix of these two technologies. Optical constants determination for the magnetron sputtered MgF2 samples have not been found in publications so far. Besides, in the existing publications, the optical constants of MgF2 have rather limited detailization in energy scale. However, one need to note that in the vicinity of the absorption-edges, optical constants vary dramatically, which brings significant difference in calculated reflectivity curve.

In our work, the optical properties of a magnetron sputtered MgF2 single layer film were characterized at the Optics Beamline of BESSY II. Reflection spectra were measured in 12–1800 eV energy range with energy step small enough to obtain every small feature in vicinity of absorption edges. Kramers-Kronig analysis was applied to calculate n and k (refractive index and extinction coefficient). The calculated optical constants were verified by comparing calculated reflectivity at different angular conditions with the measured ones. The detailed process of measurements and analysis will be presented.

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TUE 15:45-17:45 | BOARD 125 | P2-MAEN-08

POSTER SESSION

P61A: THE NEW MATERIALS SCIENCE HIGH ENERGY WHITE BEAM BEAMLINE AT PETRA III

Presenter: Peter STARON
Authors: Guilherme ABREU FARIA, Peter STARON, Martin MUELLER

The study of materials science and engineering topics with synchrotron radiation has incredible potential to shed light on fundamental questions about materials behavior and to investigate and optimize manufacturing processes. However, many experiments on such topics require specific sample geometries or spatially constrained sample environments which limit the scope of possible experiments done with traditional high energy angle-dispersive (AD) techniques.

In complement to AD diffraction, energy-dispersive (ED) diffraction can broaden this scope, as this technique has by default a limited gauge volume in the beam direction with transmission geometry, and can also be used to obtain near surface property gradients in reflection geometry.

P61A is a new PETRA III beamline, operated by Helmholtz-Zentrum Hereon, which was designed and constructed to use these advantageous characteristics for the study of materials science and engineering. The beamline has 10 4 m long damping wigglers as a source, delivering outstanding flux on the range from 20 to 200 keV. Sample and detector positioning were designed for versatile stress and texture measurements, and the beamline is also equipped with a 1 ton load capacity heavy load diffractometer for large sample environments. P61A is in operation since April 2021.

This contribution will discuss the beamline characteristics, how these are being used for materials investigations, and some of the experiments executed since start of operation.

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TUE 15:45-17:45 | BOARD 126 | P2-MAEN-09

POSTER SESSION

THE METHODS OF NEUTRON DIFFRACTION CALCULATION

Presenter: Anastasiia KUZNETSOVA
Authors: Anastasiia KUZNETSOVA (1), Jie LUO (2), Arnab MAJUMDAR (1), Hareesh SHAVANA (3), Veronika REICH (1), Sebastian BUSCH (1), Martin MÜLLER (4)

There are various methods for diffraction pattern calculation of powders, differing in Q-averaging procedures. Three of these were studied in detail:

1) The structure factor formula sums up all the hkl planes for a Q-vectors despite their respective orientations. Only peak intensities are calculated and the peak shape is arbitrary.

2) A Monte Carlo method of averaging used i.a. by the program SASSENA involves a number of random Q-points over which the computed intensity is averaged.

3) The Debye Formula considers only interatomic distances and the integration is taken with respect to scattering angle and the scattering is weighted as the fraction of the Ewald sphere surface area.

The structure factor intensity has to be normalized on the Ewald sphere surface area in order to yield the same result as the Debye formula – with the drawback that the peak shapes are arbitrary. Only a sample of one million Q-points was enough to reproduce the Debye formula for monoatomic powders by the MC method, but still insufficient for biatomic crystals. The time for the monoatomic compound there exceeded an hour (C++) while the Debye calculation is finished on the minutes time scale (python).

Summing up, the Debye formula appears to be the best and the most time-efficient way for crystalline powder diffraction modeling.

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TUE 15:45-17:45 | BOARD 127 | P2-MAEN-10

POSTER SESSION

PHASE EVOLUTION OF Te-HYPERDOPED Si UPON FURNACE ANNEALING

Presenter: Mohd Saif SHAIKH

Authors: Mohd Saif SHAIKH (1,4), Mao WANG (1), Rene HUEBNER (1), Maciej Oskar LIEDKE (2), Maik BUTTERLING (2), Dmytro SOLONENKO (3), Teresa Isabel MADEIRA (3), Zichao LI (1,4), Yufang XIE (1,4), Eric HIRSCHMANN (2), Andreas WAGNER (2), D. R. T. ZAHN (3), Manfred HELM (1,4), Shengqiang ZHOU (1)

Silicon doped with Tellurium (Te), a deep level impurity, at concentrations higher than the solid solubility limit (hyperdoping), was prepared by ion implantation and nanosecond pulsed laser melting. The resulting material exhibits strong sub-bandgap optical absorption showing potential for room-temperature broadband infrared photodetectors. As a thermodynamically metastable system, an impairment of the optoelectronic properties in hyperdoped Si materials occurs upon subsequent high-temperature thermal treatment. The substitutional Te atoms that cause the sub-bandgap absorption are removed from the substitutional sites to form Te-related complexes. In this work, we explore the phase evolution and the electrical deactivation of Te-hyperdoped Si layers upon furnace annealing through the analysis of optical and microstructural properties as well as positron annihilation lifetime spectroscopy. Particularly, Te-rich clusters are observed in samples annealed at temperatures reaching 950 °C and above. Combining the analysis of polarized Raman spectra and transmission electron microscopy, the observed crystalline clusters are suggested to consist of Si2Te3. The defect characterization using positron lifetime spectroscopy suggests the generation of vacancy complexes as a function of temperature, leading to a decrease of sheet carrier concentration.

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TUE 15:45-17:45 | BOARD 128 | P2-MAEN-11

POSTER SESSION

CHLORINE DOPING OF MoSe2 FLAKES BY ION IMPLANTATION

Presenter: Yi LI
Slawomir PRUCNAL (1), Yi LI (1), Mahdi GHORBANI-ASL (1), René HÜBNER (1), René ZIEGENRÜCKER (1), Ulrich KENTSCH (1), Arkady KRASHENINNIKOV (1), Manfred HELM (1), Dietrich R. T. ZAHN (2), Shengqiang ZHOU (1)

The efficient integration of transition metal dichalcogenides (TMDs) into the current electronic device technology requires mastering the techniques of effective tuning of their optoelectronic properties. Specifically, controllable doping is essential. For conventional bulk semiconductors, ion implantation is the most developed method offering stable and tunable doping. In this work, we demonstrate n-type doping in MoSe2 flakes realized by low-energy ion implantation of Cl+ ions followed by millisecond-range flash lamp annealing (FLA). We further show that FLA for 3 ms with a peak temperature of about 1000 °C is enough to recrystallize implanted MoSe2. The Cl distribution in few-layer-thick MoSe2 is measured by secondary ion mass spectrometry. An increase in the electron concentration with increasing Cl fluence is determined from the softening and red shift of the Raman-active A1g phonon mode due to the Fano effect. The electrical measurements confirm the n-type doping of Cl-implanted MoSe2. A comparison of the results of our density functional theory calculations and experimental temperature-dependent micro-Raman spectroscopy data indicates that Cl atoms are incorporated into the atomic network of MoSe2 as substitutional donor impurities.

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TUE 15:45-17:45 | BOARD 129 | P2-MAEN-12

POSTER SESSION

IN-SITU X-RAY DIFFRACTION EXPERIMENTS OF MAGNESIUM ALLOYS AT PHYSIOLOGICAL SALT CONCENTRATIONS

Presenter: Florian WIELAND
Authors: Florian WIELAND (1), Petra MAIER (2), Benjamin CLAUSIUS (2), Regine WILLUMEIT-RÖMER (1)

Biodegradable magnesium (Mg) implants have become a promising material for bone fracture treatment due to their high biocompatibility and good mechanical properties similar to the bone itself. One possibility to control the degradation speed and implant material properties is the usage of alloying elements like Zinc, Zirconium or Dysprosium. In order to understand the degradation behaviour of such magnesium alloys under near-physiological conditions in-situ experiments are needed. In-situ X-ray diffraction experiments with highly focused X-ray beams in the range of 1µm can yield valuable insight into forming precipitates and degradation products. By this, the layer formation at the solid-aqueous interface under aqueous conditions can be studied as a function of time.

We have investigated different magnesium alloys in Ringers solution, which mimics the ion composition in the body. The experiment was performed at the nano focused endstation of the P03, PETRA III, DESY, Hamburg. The alloys were Mg, Mg-Dy, Mg-Zr and Mg-Zn-Zr. We could observe thin layers of calcium carbonate and brucite forming on top of the Magnesium interface. In contrast, Mg-Zn-Zr showed extended layer formation of calcium carbonate and its metastable form Aragonite. The most prominent precipitation formation was observed for this alloy, which increased during the observation time.

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TUE 15:45-17:45 | BOARD 130 | P2-MAEN-13

POSTER SESSION

UNRAVELING THE SPATIAL DISTRIBUTION OF CATALYTIC NON-CUBIC Au PHASES IN A BIPYRAMIDAL MICROCRYSTALLITE BY X-RAY DIFFRACTION MICROSCOPY

Presenter: Chaitali SOW

Authors: Chaitali SOW (1,2), Abhisakh SARMA (1,3), Andreas SCHROPP (1), Dmitry DZHIGAEV (1,4), Thomas F. KELLER (1,5), Christian G. SCHROER (1,5), Milan K. SANYAL (6), Giridhar U. KULKARNI (2)

Tuning of crystal structures and shapes of submicrometer-sized noble metals have revealed fascinating catalytic, optical, electrical, and magnetic properties that enable developments of environmentally friendly and durable nanotechnological applications. Several attempts have been made to stabilize Au, knowing its extraordinary stability in its conventional face-centered cubic (fcc) lattice, into different lattices, particularly to develop Au-based catalysis for industry. Here, we report the results from scanning X-ray diffraction microscopy (SXDM) measurements on an ambient-stable penta-twinned bipyramidal Au microcrystallite (about 1.36 μm in length and 230 nm in diameter) stabilized in noncubic lattice, exhibiting catalytic properties. With more than 82 % of the crystal volume, the majority crystallite structure is identified as body-centered orthorhombic (bco), while the remainder is the standard fcc. A careful analysis of the diffraction maps reveals that the tips are made up of fcc, while the body contains mainly bco with very high strain. The reported structural imaging technique of representative single crystallite will be useful to investigate the growth mechanism of similar multiphase nano- and micrometer-sized crystals.

ACS Nano 2020, 14, 9456_9465.

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Back to programme Tuesday, 6th September

TUE 15:45-17:45 | BOARD 131 | P2-MAEN-14

POSTER SESSION

RESIDUAL STRESSES IN ADDITIVELY MANUFACTURED ALUMINUM ALLOYS AND 316L STEEL

Presenter: Marc-André NIELSEN
Authors: Marc-André NIELSEN (1), Sabine BODNER (2), Emad MAADWAD (1), Jozef KECKES (2), Peter STARON (1), Martin MÜLLER (1)

Additive manufacturing opens up new ways to produce parts with high geometric complexity, e.g., involving internal structures, which led to an increased interest of science and industry in the recent years. The mechanical behavior and load-bearing capacity of additively manufactured components, however, are still not really understood and subject of intensive research efforts. In particular, residual stresses (RS) play an important role, e.g., for the strength and fatigue properties. Therefore, RS distributions were investigated in various parts, fabricated from aluminium alloy powder (AlSi10Mg) and 316L steel using the Laser Powder Bed Fusion (LPBF) technique. The samples consist of simple walls with a wall thickness of about 3 mm and are made in different geometries involving, e.g., different edge curvatures. Residual stress fields were determined using high-energy X-ray diffraction. The diffraction study was carried out in transmission geometry using a photon energy of 87.1 keV that allows to penetrate thicker samples. The influence of specimen geometry and production parameters on the RS state will be discussed. Also, the RS state will be compared with microstructure studies.

Affillation
1: Helmholtz-Zentrum hereon, Germany; 2: Erich Schmid Institute, Montanuniversität Leoben, Austria

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TUE 15:45-17:45 | BOARD 132 | P2-MAEN-15

POSTER SESSION

INNOVATIVE SPUTTER DEPOSITION FOR FLEXIBLE THIN FILM ENGINEERING

Presenter: Kai SCHLAGE
Authors: Kai SCHLAGE (1), Mehdi RAMIN MOAYED (1), Andrey SIEMENS (1), Lars BOCKLAGE (1), Anjali PANCHWANEE (1), Christian ADOLFF (1), Janne LÜTJENS (1), Ralf RÖHLSBERGER (1,2,3)

Highly specialized thin film structures play a crucial role for SNI-related basic research and technological developments. The realization of such films can be arbitrarily challenging due to several different stack materials, 3D shaped substrates, an atomic precision to guarantee their functionality, desired ultra-smooth interfaces, or, if a mass production of identical thin film systems is required. Furthermore, innovative deposition techniques are needed allowing to manipulate or customize thin film properties in an elegant manner.

To address this issue, we have developed two sputter-deposition systems with special mechanics and home-made control software, which enable unique and extreme coating possibilities. The first chamber provides depositions in the lab scale, on substrates up to 30 mm large. The second one is suitable for industrial scale applications and allows homogenous depositions on 200 mm wafers, planar substrates with the length of up to 1000 mm and weight of up to 50 kg, or 3D objects up to a few hundred mm large. The special feature of both devices is the possibility of oblique incidence deposition (OID). With this advanced and at the same time very simple method, magnetic, optical or crystalline properties of thin films can be adjusted according to the final application simply by changing the deposition angles. In this contribution we will introduce the capability of the 2D/3D/OID coating devices and introduce unique several thin film demonstrators.

Affillation
1: Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; 2: Friedrich-Schiller-Universität Jena, Germany; 3: Helmholtz-Institut Jena, Germany

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TUE 15:45-17:45 | BOARD 133 | P2-MAEN-16

POSTER SESSION

SWIFT HEAVY ION IRRADIATION OF BISMUTH NANOWIRES PRESSURIZED IN DIAMOND ANVIL CELLS

Presenter: Christopher SCHRÖCK

Authors: Christopher SCHRÖCK (1,2), Ioannis TZIFAS (1), Kay-Obbe VOSS (1), Lkhamsuren BAYARJARGAL (2), Wilfried SIGLE (3), Ina SCHUBERT (1), Maria Eugenia TOIMIL-MOLARES (1), Björn WINKLER (2), Christina TRAUTMANN (1,4)

The simultaneous exposure of materials to multiple extreme conditions is a field of increasing interest in modern high pressure research. A worldwide unique approach, applying concomitantly high-pressure using diamond anvil cells (DACs) and irradiation with swift heavy ions (SHI) of GeV energies has been pioneered at GSI Helmholtz Center Darmstadt and revealed new effects such as the generation of new phases far from thermodynamic equilibrium or the stabilization of high pressure phases at ambient conditions.

In this report, our activities to exploit intrinsic properties of nanomaterials beneficial for the manipulation of high pressure phase diagrams are presented. As material of interest bismuth was selected, due to its complex and well-characterized high-pressure phase diagram and its sensitivity to SHI irradiation. The experiments require the fabrication of bismuth nanowires by electrodeposition in etched ion-track membranes, compression of miniaturized samples in DACs and subsequent irradiation using relativistic heavy ions of typically several tens of GeV kinetic energy, including in-situ Raman spectroscopy and high pressure X-ray diffraction studies. The aim of this project is to investigate to what extent size effects can be utilized in order to promote SHI-induced high p-T phase transitions and to provide insight into the underlying mechanisms of the combined pressure and irradiation effects.

Affillation

1: GSI Helmholtzzentrum für Schwerionenforschung GmbH, Germany; 2: Institute of Geosciences, Goethe University Frankfurt, Germany; 3: Max-Planck Institute for Solid State Research, Stuttgart, Germany; 4: Department of Materials- and Geosciences, Technical University of Darmstadt, Germany

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TUE 15:45-17:45 | BOARD 134 | P2-MAEN-17

POSTER SESSION

MULTI-MODAL CHARACTERISATION OF ENGINEERING MATERIALS AT THE INLINE BRANCH P21.2 OF THE SWEDISH MATERIALS SCIENCE BEAMLINE (SMS) AT PETRA III

Presenter: Malte BLANKENBURG
Authors: Ulrich LIENERT, Zoltán HEGEDÜS, Malte BLANKENBURG, Sven GUTSCHMIDT, Thomas BÄCKER, Anatoly SHABALIN

It has been demonstrated that high-energy synchrotron radiation is a powerful tool for the structural characterization of polycrystalline bulk materials during thermo-mechanical processing. Pertinent features are high penetration power, large reciprocal space coverage, and high spatial and temporal resolution.

The Swedish Materials Science beamline (SMS) at PETRA III is a recently commissioned high-energy beamline (40 – 150 keV) and user mode has started in August 2019. Here, the in-line branch, P21.2, will be presented which is optimized for multi-modal (WAXS/SAXS/Imaging) *in-situ* and *operando* characterization of bulk materials and surfaces. Characterisations of engineering materials, in particular metals, constitute the largest group of applications. The main features of the beamline design will be described together with the available diffraction, scattering and imaging capabilities. The complementary modalities will be illustrated by case studies characterizing engineering materials.

Affillation
Deutsches Elektronen-Synchrotron (DESY), Germany

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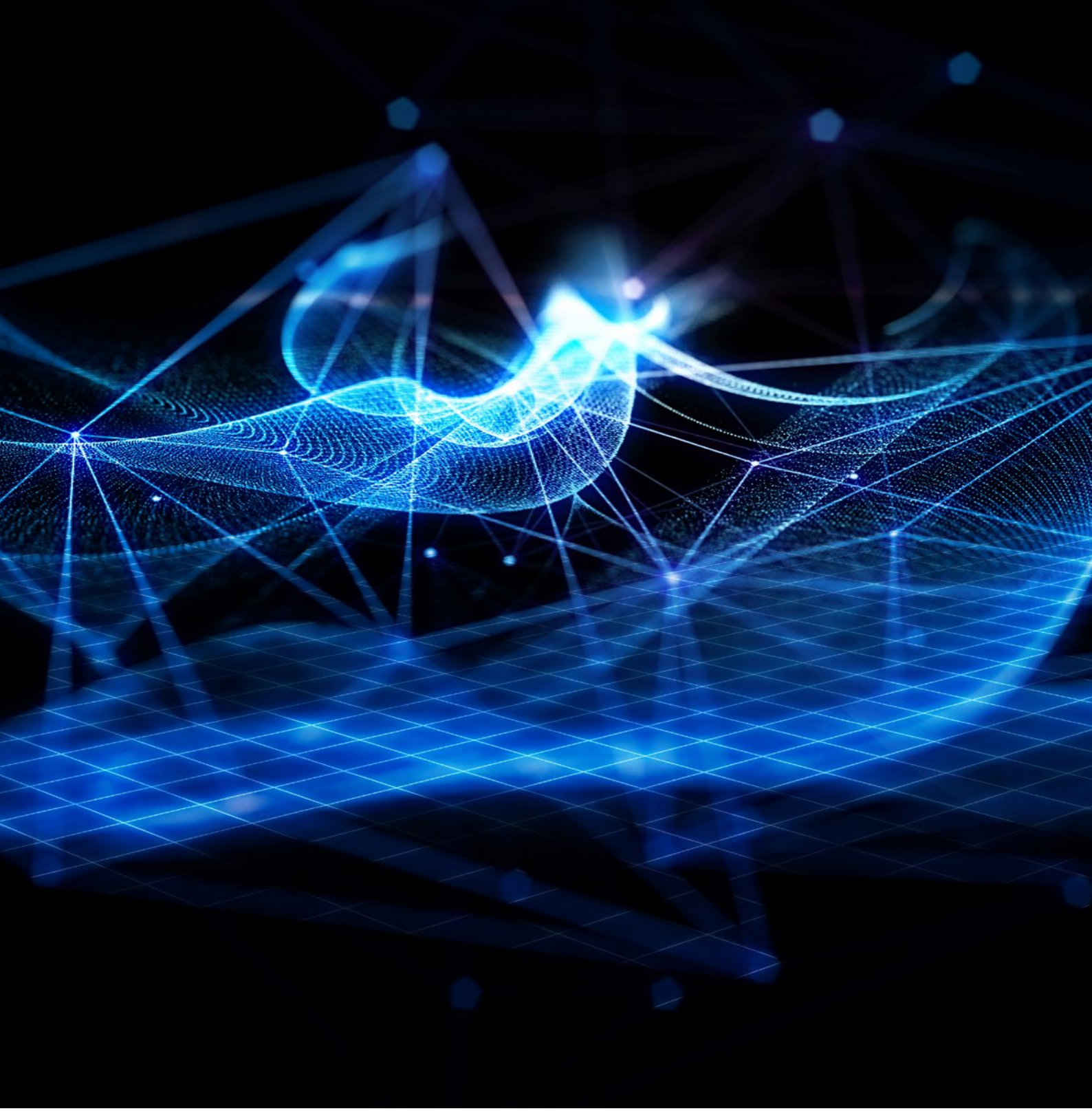

WEDNESDAY, 7TH SEPTEMBER

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WEDNESDAY, 7TH SEP

PROGRAMME

09:00	**PLENARY TALK | HS 1A** When X-rays go Quantum: From Cavity QED to Quantum Imaging – *Ralf Röhlsberger (U Jena & HI Jena)*		
09:45	**KEYNOTE TALK | HS 1A** X-ray Nanofocus for spatially resolved Studies of Mesocrystals – *Ivan Zaluzhnyy (U Tübingen)*		
10:15	*Coffee break*		
10:45	**PARALLEL SESSION | HS 1A** Methods & Instruments Development 3 / In-Situ and Operando Studies	**PARALLEL SESSION | HS 1B** Soft Matter & Liquids	**PARALLEL SESSION | HS 2** Magnetism & Functional Materials
12:15	Awards & Talks by the Awardees		
13:15	Scientific Resumee & Closing		
13:30	*Departure Visit BESSY II*		
14:00–17:00	Visit BESSY II		

Instructions:
Tables of the day are linked to the sessions.
Tables of sessions are linked to the abstracts.

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WED 9:00-9:45 | HÖRSAAL 1A | INV-08

PLENARY TALK

WHEN X-RAYS GO QUANTUM: FROM CAVITY QED TO QUANTUM IMAGING

Presenter: Ralf RÖHLSBERGER
Author: Ralf RÖHLSBERGER (1,2)

The remarkable development of accelerator-driven light sources with their highly brilliant X-rays has brought quantum and nonlinear phenomena at X-ray energies within reach. In this contribution I will describe recent developments in this field and identify future research areas that will be stimulated by this evolution.

Nowadays, X-ray photonic structures like cavities and superlattices are employed as new laboratory to realize quantum optical concepts at X-ray energies. The prime candidates to be chosen as atomic emitters in this field are Mössbauer isotopes. Their extremely small resonance bandwidth facilitates to probe fundamental phenomena of the light-matter interaction like the observation of X-ray superradiance and the collective Lamb, electromagnetically induced transparency with nuclei and Rabi oscillations between nuclear ensembles, which could open new avenues towards nonlinear interactions between X-rays and matter. Ultranarrow nuclear resonances like those of 229Th and 45Sc could facilitate the realization of nuclear clocks with unprecedented accuracy.

Employing higher-order coherences of X-ray fields in the spirit of Glauber could even lead to novel concepts for quantum imaging at X-ray energies with outstanding spatial resolution. The future development of high-brilliance X-ray sources holds great promise for further breakthroughs in this exciting field.

Affillation
1: Helmholtz Institut Jena, Germany; 2: Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

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WED 9:45-10:15 | HÖRSAAL 1A | INV-09

KEYNOTE TALK

X-RAY NANOFOCUS FOR SPATIALLY RESOLVED STUDIES OF MESOCRYSTALS

Presenter: Ivan ZALUZHNYY
Authors: Ivan ZALUZHNYY (1), Frank SCHREIBER (1), Ivan VARTANYANTS (2), Michael SPRUNG (2), Marcus SCHEELE (3)

X-ray diffraction has been used to study the structure of well-ordered crystalline materials since its discovery about a century ago. Nowadays, the excellent parameters of the new synchrotron sources allow us to focus the X-ray flux to a nanometer-scale spots. Apart from the obvious advantages of studying nanoscale objects with a focused X-ray beam, it is also possible to perform a raster scan of a larger sample to obtain spatially-resolved information of its structure. This is especially advantageous to characterize the fabricated nanodevices or study the structure of novel non-crystalline materials. Depending on the typical length scale of the non-uniformity of the sample, different size of the X-ray beam should be chosen. This talk will be focused on spatially resolved studies of mesocrystal superlattices performed at the Coherence beamline P10 of PETRA III. These superlattices are formed from crystal nanoparticles coated with organic ligands. By utilizing the raster scan with an X-ray beam focused to approximately 400 nm, and measuring simultaneously SAXS and WAXS signal with a 2D detector, it is possible to determine the structure of the superlattice and characterize the orientation of individual nanoparticles in the superlattice.

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[1] I. Zaluzhnyy, et al., Nano Lett. 2017, 17(6), 3511-3517.
[2] N. Mukharamova, et al., Small 15, 1904954 (2019).
[3] A. Maier, et al., Adv. Mater. 32, 2002254 (2020).
[4] D. Lapkin, et al., Nat. Commun. 13, 892 (2022).

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PARALLEL SESSION
WEDNESDAY, 7TH SEPTEMBER

METHODS & INSTRUMENTS DEVELOPMENT 3 / IN-SITU AND OPERANDO STUDIES			
Time	**Place**	**Presenter**	**Title**
Wed 10:45-11:00	Hörsaal 1a	Stefan SCHIPPERS	Inner-shell photoionization of silicon and iron ions of astrophysical interest
Wed 11:00-11:15	Hörsaal 1a	Gabriel SPARTACUS	A sample environment for in-situ synchrotron X-ray studies of metal additive manufacturing using electron beam powder bed fusion (E-PBF)
Wed 11:15-11:30	Hörsaal 1a	Daniel SCHICK	Time-resolved resonant magnetic scattering and spectroscopy – Synergy of laser-driven- and synchrotron-soft-X-ray source
Wed 11:30-11:45	Hörsaal 1a	Johannes HAGEMANN	Phase retrieval framework for direct reconstruction of the projected refractive index applied to ptychography and holography
Wed 11:45-12:00	Hörsaal 1a	Olaf MAGNUSSEN	High-energy surface X-ray scattering for electrocatalysis and energy science
Wed 12:00-12:15	Hörsaal 1a	Michael STUCKELBERGER	Correlative X-ray nanoscopy of solar cells: Towards in-situ and operando experiments at diffraction-limited storage rings

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WED 10:45-11:00 | HÖRSAAL 1A | MET3-01

PARALLEL SESSION

INNER-SHELL PHOTOIONIZATION OF SILICON AND IRON IONS OF ASTROPHYSICAL INTEREST

Presenter: Stefan SCHIPPERS
Authors: Stefan SCHIPPERS (1), Ticia BUHR (1), Alexander PERRY-SASSMANNSHAUSEN (1), Alexander BOROVIK JR. (1), Alfred MÜLLER (1), Simon REINWARDT (2), Michael MARTINS (2), Stephan FRITZSCHE (3,4)

We report on recent experimental work on the photoabsorption of atomic and molecular ions that has been carried out at the photon-ion merged-beams setup PIPE [1,2], a permanently installed end station at the XUV beamline P04 of the PETRA III synchrotron radiation source operated by DESY in Hamburg, Germany. Selected results on, e.g., single and multiple L-shell photoionization of low-charged iron ions [3–5] and on single and multiple K-shell photoionization of silicon ions [6,7] will be discussed in an astrophysical context. The results are particularly relevant for the determination of the elemental abundances in the interstellar medium. Moreover, their quality bears witness of the fact that the implementation of the photon-ion merged-beams method at one of the world's brightest synchrotron light sources has led to a breakthrough for the experimental study of inner-shell photoabsorption processes with ions.

Funding by BMBF (grant numbers 05K16RG1, 05K16GUC, and 05K16SJA) is gratefully acknowledged.
[1] S. Schippers et al., X-Ray Spectrometry 49 (2020) 11.
[2] A. Müller et al. , Astrophys. J 836 (2017) 166.
[3] S. Schippers et al., Astrophys. J 849 (2017) 5.
[4] R. Beerwerth et al., Astrophys. J 887 (2019) 189.
[5] S. Schippers et al., Astrophys. J 908 (2021) 52.
[6] A. Perry-Sassmannshausen et al., Phys. Rev. A 104 (2021) 053107.
[7] S. Schippers et al., Astrophys. J (in print) arXiv:2204.08750.

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WED 11:00-11:15 | HÖRSAAL 1A | MET3-02

PARALLEL SESSION

A SAMPLE ENVIRONMENT FOR IN-SITU SYNCHROTRON X-RAY STUDIES OF METAL ADDITIVE MANUFACTURING USING ELECTRON BEAM POWDER BED FUSION (E-PBF)

Presenter: Gabriel SPARTACUS
Authors: Chrysoula IOANNIDOU (1), Hans-Henrik KÖNIG (1), Nick SEMJATOV (2), Gabriel SPARTACUS (1), Martin WILDHEIM (3), Anton LINDAHL (3), Ulf ACKELID (3), Christopher ZENK (2), Carolin KÖRNER (2), Peter HEDSTRÖM (1), Greta LINDWALL (1)

Powder bed fusion (PBF) technologies are successfully implemented processes in additive manufacturing (AM) of metal components. While Laser-PBF (L-PBF) has a larger share of production capacities, Electron beam-PBF (E-PBF) is particularly promising for manufacturing of high-performance alloys that need to be processed at high temperatures and under vacuum.

Synchrotron X-ray characterization techniques (imaging, diffraction and small-angle X-ray scattering) offer real-time and in-situ observations with high spatial and temporal resolution, and have led to profound insights on solidification and microstructure evolution, as well as melt pool and powder dynamics during the L-PBF process.

E-PBF has not yet been studied in such experiments, probably due to the high equipment demands compared to L-PBF. Although L-PBF and E-PBF are conceptually similar, there are significant differences between those, mainly related to the nature of the energy sources, the process steps and the different processing environment, thus, knowledge by synchrotron studies on L-PBF are not transferable to E-PBF. In this work, we present the development of an environment that facilitates in-situ synchrotron X-ray measurements during E-PBF and thus enables studies of electron beam-matter interactions under realistic E-PBF processing conditions. We address the design considerations, the setup details, its implementation at PETRA III, DESY, and the measurement possibilities this sample environment provides.

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WED 11:15-11:30 | HÖRSAAL 1A | MET3-03

PARALLEL SESSION

TIME-RESOLVED RESONANT MAGNETIC SCATTERING AND SPECTROSCOPY – SYNERGY OF LASER-DRIVEN- AND SYNCHROTRON-SOFT-X-RAY SOURCE

Presenter: Daniel SCHICK
Authors: Daniel SCHICK (1), Martin BORCHERT (1), Martin HENNECKE (1), Themistoklis SIDIROPOULOS (1), Julia BRAENZEL (1), Dieter ENGEL (1), Holger STIEL (1), Matthias SCHNUERER (1), Clemens VON KORFF SCHMISING (1), Bastian PFAU (1), Stefan EISEBITT (1,2)

Magnetic heterostructures are the backbone of current and future devices for data storage and processing applications. Their functionalities rely on magnetic interactions within nanolayers and across interfaces between them. The resulting complex spin structures can be resolved with resonant scattering techniques in the soft-X-ray regime (RSXS), even with element-selectivity. RSXS combines significant spectroscopic and magnetic contrast with access to reciprocal space in addition to depth- and lateral spatial resolution. In functionalized magnetic heterostructures, the underlying physical processes can also be disentangled from their intrinsic time scales by utilizing ultrashort soft-X-ray pulses in a pump-probe manner.

Due to the limited access to suitable beamlines and the ~100ps pulse durations of current and future synchrotrons, a great demand for short-pulse and high-brightness soft-X-ray sources is apparent. We present an overview of experiments that have been recently enabled by laser-driven sources in the photon energy range from 150-1500eV with ~10fs-10ps temporal resolution, e.g., RSXS from antiferromagnets, small-angle scattering (SAXS) from magnetic domains, and X-ray magnetic circular dichroism (XMCD) from ferromagnets. We will compare the capabilities of both laser-driven and synchrotron sources also in terms of sample environments and excitation parameters and discuss synergies from combining both approaches.

Affillation
1: Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Germany; 2: Technische Universität Berlin, Institut für Optik und Atomare Physik, Germany

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WED 11:30-11:45 | HÖRSAAL 1A | MET3-04

PARALLEL SESSION

PHASE RETRIEVAL FRAMEWORK FOR DIRECT RECONSTRUCTION OF THE PROJECTED REFRACTIVE INDEX APPLIED TO PTYCHOGRAPHY AND HOLOGRAPHY

Presenter: Johannes HAGEMANN
Authors: Johannes HAGEMANN (1,3,4), Felix WITTWER (1,2), Christian G. SCHROER (1,3,4)

The interaction of an object with a coherent probe often encodes its properties in a complex-valued function, which is then detected in an intensity-only measurement. Phase retrieval methods commonly infer this complex-valued function from the intensity. However, the decoding of the object from the complex-valued function often involves some ambiguity in the phase, e.g., when the phase shift in the object exceeds 2π . Here, we present a phase retrieval framework to directly recover the amplitude and phase of the object. This refractive framework is straightforward to integrate into existing algorithms. As examples, we introduce refractive algorithms for ptychography and near-field holography and demonstrate this method using measured data.

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WED 11:45-12:00 | HÖRSAAL 1A | MET3-05

PARALLEL SESSION

HIGH-ENERGY SURFACE X-RAY SCATTERING FOR ELECTROCATALYSIS AND ENERGY SCIENCE

Presenter: Olaf MAGNUSSEN
Authors: Timo FUCHS (1), Canrong QIU (1), Jan Ole FEHRS (1), Jonas BUNGE (1), Jochim STETTNER (1), Jakub DRNEC (2), Olaf MAGNUSSEN (1)

The need for sustainable energy, reduction of pollutants, and the environmental benign processing of chemicals has spurred worldwide scientific activities in electrochemical energy science and electrocatalysis. These processes occur at the interfaces of solid catalyst materials in contact with complex liquid environments and under conditions involving high reaction rates, pronounced mass transport, and vigorous gas evolution. Because conventional surface analytic techniques cannot directly access these interfaces, the atomic scale surface structure and composition of the catalysts controlling the reactions are notoriously difficult to determine. For a better understanding of structure-property relationships and catalyst degradation mechanisms, experimental approaches are required that provide insight into the atomic and nanoscale interface structure in *operando* under reaction conditions.

We have developed high-energy (40-100 keV) X-ray scattering methods for in-situ and in *operando* studies of the complex interfaces between electrocatalysts and liquid electrolytes under reaction conditions. Here, we will describe our developments in these techniques and dedicated instrumentation and present results of proof-of-principle studies of platinum-based and transition metal oxide electrocatalysts at beamline P21.2 of PETRA III at DESY and ID31 of the ESRF.

Affillation
1: Institute of Experimental and Applied Physics, Kiel University, Germany; 2: European Synchrotron Radiation Facility, Grenoble, France

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WED 12:00-12:15 | HÖRSAAL 1A | MET3-06

PARALLEL SESSION

CORRELATIVE X-RAY NANOSCOPY OF SOLAR CELLS: TOWARDS IN-SITU AND OPERANDO EXPERIMENTS AT DIFFRACTION-LIMITED STORAGE RINGS

Presenter: Michael STUCKELBERGER
Authors: Michael STUCKELBERGER

Today, we exploit scanning X-ray nanoscopy to answer questions about photovoltaic materials: How do interfaces look like in solar cell stacks? How can perovskite semiconductors be manufactured without sacrificing the efficiency due to lateral inhomogeneity? Which defects limit the device performance, and how can they be engineered to be less detrimental? How can solar cells be cost-effectively fabricated using abundant and non-toxic materials?

Based on in-situ and *operando* experiments at DESY, APS, ESRF, and NSLS II, we will showcase examples of multi-modal scanning X-ray nanoscopy measurements during growth and operation of solar cells, involving X-ray beam induced current (XBIC), X-ray fluorescence (XRF), X-ray diffraction (XRD), ptychography, and X-ray excited optical luminescence (XEOL), for which we have developed dedicated instruments. We have found correlations between the optical / electrical performance, composition, and strain, and will highlight the relevance of X-ray nanoscopy for the solar-cell development.

Tomorrow, the questions will be different, and we will be able to use X-ray nanoscopes at novel diffraction-limited storage rings to answer them. Where will be the frontiers of X-ray nanoscopy for in-situ and *operando* energy research? Which challenges arise with the new opportunities, and how can we tackle them? We will present ideas of 'dream experiments' and discuss the challenges related to multi-modal in-situ and *operando* scanning X-ray nanoscopy.

Affillation
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PARALLEL SESSION
WEDNESDAY, 7TH SEPTEMBER

SOFT MATTER AND LIQUIDS			
Time	**Place**	**Presenter**	**Title**
Wed 10:45-11:00	Hörsaal 1b	Henrich FRIELINGHAUS	Ionic liquids with water in porous glasses
Wed 11:00-11:15	Hörsaal 1b	Susanne DOGAN	Influence of perfluorocarbons on model membranes and membrane-protein interactions
Wed 11:15-11:30	Hörsaal 1b	Matthias KÜHNHAMMER	Modelling neutron scattering from foams
Wed 11:30-11:45	Hörsaal 1b	Olaf HOLDERER	Dynamics of a lamellar microemulsion exploited with high Q-resolution with a time-of-flight NSE
Wed 11:45-12:00	Hörsaal 1b	Alevtina SMEKHOVA	Resonant soft X-ray scattering for studies spiral ordering in liquid crystals
Wed 12:00-12:15	Hörsaal 1b	Jörg RADNIK	Energy-resolved X-ray photoelectron spectroscopy measurements on the concentration profile of thin blended poly(vinyl methyl ether)/polystyrene films

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WED 10:45-11:00 | HÖRSAAL 1B | SOFT-01

PARALLEL SESSION

IONIC LIQUIDS WITH WATER IN POROUS GLASSES

Presenter: Henrich FRIELINGHAUS
Authors: Henrich FRIELINGHAUS, Margarita FOMINA, Olaf HOLDERER

The structure and dynamics of the ionic liquid 1-ethyl-3-methylimidazolium acetate (EMIMAc) with certain amounts of water in porous glass with pores of the size 40 and 100 Å is determined in comparison to the bulk liquid. We employed X-ray diffraction to measure the domain structure, and neutron spin echo spectroscopy / neutron backscattering for the dynamics. In confinement, the liquid displays onion-like domain structuring while in bulk the liquid is largely forming a bicontinuous structure similar to microemulsions. This also has an effect on the dynamics of the liquid at high temperatures (373K): The ions in the bulk can diffuse along the domain boundaries while they need to cross the domains in the ordered state in confinement. At low temperatures, the attractive forces of all ions are such strong – we have a highly viscous fluid – such that the diffusion in any direction is similarly slow, and the exact domain structure plays a minor role. The 0.5 mol/mol of water do not change the structure, but reveal changed dynamics in terms of an activation energy. We selectively deuterated the EMIM and either the acetate or water to highlight the mobility of the small molecules. While in larger pores the motion of the hydrogenous portions is facilitated, it indicated stronger hydrogen bonding for the smallest pores. We address this to the distortion of the domains that leaves more room for water in the smaller pores.

Affillation
Forschungszentrum Jülich, Germany

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WED 11:00-11:15 | HÖRSAAL 1B | SOFT-02

PARALLEL SESSION

INFLUENCE OF PERFLUOROCARBONS ON MODEL MEMBRANES AND MEMBRANE-PROTEIN INTERACTIONS

Presenter: Susanne DOGAN
Authors: Susanne DOGAN, Michael PAULUS, Göran SURMEIER, Dominik BIRKWALD, Katharina BRÄGELMANN, Metin TOLAN

We present a surface-sensitive X-ray scattering study on the influence of gaseous and aerolized perfluorocarbons on zwitterionic and anionic phospholipid model membranes and on protein-interface interactions. Lung surfactant is a complex mixture of proteins and lipids which are present at the alveolar-air interface to maintain the respiration cycle. We observed that small molecules of fluorinated gases, such as F-propane and F-butane, can penetrate and accumulate in phospholipid membranes and form islands within alkyl chains. At low initial surface pressures this clustering process trigger the formation of crystallites. The large linear aerolized F-octyl bromide with its polar bromide moiety leads to a dissolution and thus fluidizes the membrane. The globular bicyclic F-decalin molecules penetrate DPPC alkyl chains but cannot accumulate between DPPA molecules due to its size. Since the functionality of the pulmonary surfactant depends sensitively on the proteins it contains, we also investigated the influence of the substances on the protein-membrane interaction using initially simple model proteins. Results show that the adsorption of BSA, regardless of the adsorbate age, is not affected and the interaction with F-decalin is reversible at the buffer-air interface. This study implies that the highly biocompartible and non-toxic FCs might be beneficial in the treatment of lung diseases with injured non-functional lung surfactant in a novel approach for ventilation.

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WED 11:15-11:30 | HÖRSAAL 1B | SOFT-03

PARALLEL SESSION

MODELLING NEUTRON SCATTERING FROM FOAMS

Presenter: Matthias KÜHNHAMMER
Authors: Matthias KÜHNHAMMER, Regine VON KLITZING

Foams are a complex material with different structural motifs. Aqueous foams in particular change their structure over time due to processes like gravitational drainage, Ostwald ripening and coalescence. Because of this complex structure, modelling of small angle neutron scattering (SANS) curves obtained from foams is challenging. Up to now the interpretation of such curves was mostly done on a phenomenological basis, only taking into account isolated features like peak positions. Here, a newly developed model, describing (SANS) data of foams, is presented. The model takes into account the geometry of the foam bubbles and is based on an incoherent superposition of reflectivity curves, arising from the foam films, and a small-angle scattering (SAS) contribution from the Plateau borders. The model is capable of describing the complete scattering curves of a foam stabilized by the standard cationic surfactant (C14TAB) with different water contents, i.e. drainage states, and provides information about the thickness distribution of liquid films inside the foam.

Affillation
TU Darmstadt, Germany

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WED 11:30-11:45 | HÖRSAAL 1B | SOFT-04

PARALLEL SESSION

DYNAMICS OF A LAMELLAR MICROEMULSION EXPLOITED WITH HIGH Q-RESOLUTION WITH A TIME-OF-FLIGHT NSE

Presenter: Olaf HOLDERER

Authors: Olaf HOLDERER (1), Piotr ZOLNIERCZUK (2), Henrich FRIELINGHAUS (1), Michael OHL (3), Michael MONKENBUSCH (3)

Neutron spin echo (NSE) spectroscopy provides the ultimate energy resolution in quasi-elastic thermal and cold neutron scattering spectroscopy. A peculiarity of the SNS-NSE [1], the only NSE spectrometer at a pulsed beam port at the moment, is that the q-resolution can be adjusted in certain limits a Poster Sessioniori by choosing the appropriate detector binning and time channel binning. This can be exploited for samples with a strongly varying scattered intensity I(q), e.g. due to Bragg peaks in a crystal or lamellar ordering in microemulsions. The data reduction software DrSpine [2] allows for appropriate slicing and masking for this task.

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WED 11:45-12:00 | HÖRSAAL 1B | SOFT-05

PARALLEL SESSION

RESONANT SOFT X-RAY SCATTERING FOR STUDIES SPIRAL ORDERING IN LIQUID CRYSTALS

Presenter: Alevtina SMEKHOVA

Authors: Alevtina SMEKHOVA (1), Vladimira NOVOTNA (2), Ladislav FEKETE (2), Radu ABRUDAN (1), Mattis FONDELL (1), Vera HAMPLOVA (2)

Resonant Soft X-ray Scattering (RSoXS) is a unique technique for studies various liquid crystal phases and compounds, and significantly complements different laboratory methods. Herein, it is applied to reveal the shortest up-to-now reported value of the helix pitch and the size of coherently scattering domains of newly synthesized room temperature (RT) cholesteric liquid crystal EZL10/10 with a single lactate unit in a molecular chain. The angular position and the broadening of a strong element-specific scattering peak detected only at RT point out the ultra-short pitch of approx. 104 ± 1 nm and the domain size of about five pitches, respectively. The periodicity found agrees well with the surface stripe texture observed by atomic force microscopy at the liquid crystal/air interface.

RSoXS experiment was performed in transmission geometry near the carbon K-edge resonance (within 270 – 290 eV) with linearly polarized X-rays from BESSY II synchrotron radiation facility (HZB, Berlin). Besides, X-ray absorption spectroscopy within the same energy range was used to prove the stability of EZL10/10 molecules under the incident beam. The possibility to directly probe the helix pitch of different sizes, the reversibility of the phase transitions, the peculiarities of space filling and the stability of liquid crystal molecules underline a great promise of soft X-rays in soft matter studies.

We acknowledge Prof. B. Ostrovskii for leading this work and his contribution to the experiment.

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WED 12:00-12:15 | HÖRSAAL 1B | SOFT-06

PARALLEL SESSION

ENERGY-RESOLVED X-RAY PHOTOELECTRON SPECTROSCOPY MEASUREMENTS ON THE CONCENTRATION PROFILE OF THIN BLENDED POLY(VINYL METHYL ETHER)/ POLYSTYRENE FILMS

Presenter: Jörg RADNIK
Authors: Jörg RADNIK, Marcel GAWEK, Sherif MADKOUR, Paulina SZYMONIAK, Hassan OMAR, sAndreas SCHÖNHALS

In this contribution the correlation function of microemulsions, thermodynamically stable mixtures of oil, water and surfactant, is studied with NSE on length scales where structural correlations are important. The typical ”de Gennes narrowing” or structural narrowing is observed with a relaxation time proportional to I(q). The chances and pitfalls related to the q-resolution in neutron spin echo spectroscopy are discussed.

Affillation
Federal Insitute for Material Research and Testing BAM, Germany

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PARALLEL SESSION
WEDNESDAY, 7TH SEPTEMBER

MAGNETISM AND FUNCTIONAL MATERIALS			
Time	**Place**	**Presenter**	**Title**
Wed 10:45-11:00	Hörsaal 2	Victor UKLEEV	Exchange anisotropy in cubic chiral magnets probed by resonant small-angle X-ray scattering
Wed 11:00-11:15	Hörsaal 2	Anjali PANCHWANEE	Magnetic spiral structure engineering in thin films via oblique incidence deposition
Wed 11:15-11:30	Hörsaal 2	Michał DEMBSKI-VILALTA	Potential new vortex phase in antiferromagnetic incommensurate magnet $Ba_2CuGe_2O_7$
Wed 11:30-11:45	Hörsaal 2	Sabrina DISCH	Probing the Disorder Distribution in Ferrite Nanoparticles using Magnetic SANS
Wed 11:45-12:00	Hörsaal 2	Steffen WITTROCK	Small angle elastic X-ray scattering at sub-100nm wavelength exchange magnons
Wed 12:00-12:15	Hörsaal 2	Gyanendra PANCHAL	Study of interfacial magnetism in epitaxial $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ heterostructure via soft X-ray resonant magnetic reflectometry

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WED 10:45-11:00 | HÖRSAAL 2 | MAGN-01

PARALLEL SESSION

EXCHANGE ANISOTROPY IN CUBIC CHIRAL MAGNETS PROBED BY RESONANT SMALL-ANGLE X-RAY SCATTERING

Presenter: Victor UKLEEV

Authors: Victor UKLEEV (1,2), Priya BARAL (3), Chen LUO (1), Florin RADU (1), Pierluigi GARGIANI (4), Manuel VALVIDARES (4), Arnaud MAGREZ (3), Jonathan WHITE (2)

The ground-state helical magnetic structures of cubic chiral systems are well explained by the Bak-Jensen model that considers the interplay between exchange, antisymmetric Dzyaloshinskii-Moriya interaction (DMI), anisotropic exchange interaction (AEI), and cubic anisotropy. The weak cubic anisotropy determines the spin-wave gap and some additional peculiarities of the helix axis orientation under a magnetic field, while the exchange, DMI and AEI are responsible for the helical spiral and its orientation relative to crystal axes. The latter interaction is often neglected due to its weak impact on experimental observations. However, the cubic and exchange anisotropies are important for defining the propagation direction of the helix, and ultimately the orientation of any field-induced skyrmion lattice (SkL) in these materials. Moreover, their role which has been neglected for decades, has been recently found to be manifested in exotic low-temperature states of Cu2OSeO3: tilted conical spiral and disordered SkL. In the present work we use a simple and reliable method based on resonant X-ray scattering (REXS) in vector magnetic fields to quantify the AEI in chiral cubic magnets FeGe [1] and Cu2OSeO3. We find that in the latter material, the AEI is very pronounced at low temperatures < 35 K resulting in the conical spiral pitch variation of 10 % for particular magnetic field orientations relative to crystal axes.

[1] V. Ukleev, et. al., Phys. Rev. Res. 3, 013094 (2021).

Affillation

1: Helmholtz-Zentrum Berlin, Germany; 2: Paul Scherrer Institute, Switzerland; 3: École Polytechnique Fédérale de Lausanne, Switzerland; 4: ALBA Synchrotron Light Source, Spain

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WED 11:00-11:15 | HÖRSAAL 2 | MAGN-02

PARALLEL SESSION

MAGNETIC SPIRAL STRUCTURE ENGINEERING IN THIN FILMS VIA OBLIQUE INCIDENCE DEPOSITION

Presenter: Anjali PANCHWANEE

Authors: Anjali PANCHWANEE (1), Kai SCHLAGE (1), Mehdi RAMIN MOAYED (1), Lars BOCKLAGE (1), Sven VELTEN (1), Sakshath SADASHIVAIAH (2), Aleksandr I. CHUMAKOV (3), Ilya SERGEEV (1), Ralf RÖHLSBERGER (1,2,4,5)

Manipulating the magnetic spin configuration in thin films retains the basis for future development of spintronic-based devices. Here we introduce an application of the oblique incidence deposition (OID) technique [1] to fabricate thin magnetic films with customized magnetic spiral structures. The realization of two arbitrarily crossed OID uniaxial surface anisotropy contributions offer a unique way to precisely shape its depth dependent magnetic spin profile for the specific need of application.

To image the spiral spin profiles in 10 nm thick iron films, we apply the nuclear resonant scattering (NRS) technique [2] along with the X-ray standing wave generator (XSWG) approach. With the XSWG approach a depth resolution of the NRS technique in the nm-regime can be achieved.

For this purpose, we have prepared high quality Ta / SiC superlattices as substrate. The integration of intermediate spacer layers with linear thickness gradient in between the XSWG and OID iron film allows us to selectively illuminate different depths and to determine the spatial orientation of the spins by simply collecting nuclear resonant time spectra at various lateral positions of the sample.

In the present work, we thus introduce a new pathway to design and probe spiral spin configurations in single magnetic films.

[1.] K. Schlage et al., Adv. Funct. Mater. 26, 7423 (2016).
[2]. R. Röhlsberger, Tracts in Modern Physics, Vol. 208 (Springer, Heidelberg, 2004)

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1: Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany; 2: Helmholtz-Institut Jena, 07743 Jena, Germany; 3: ESRF-The European Synchrotron, F-38043 Grenoble, France; 4: Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany; 5: Helmholtz Centre for Heavy Ion Research (GSI), 64291 Darmstadt, Germany

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WED 11:15-11:30 | HÖRSAAL 2 | MAGN-03

PARALLEL SESSION

POTENTIAL NEW VORTEX PHASE IN ANTIFERROMAGNETIC INCOMMENSURATE MAGNET $Ba_2CuGe_2O_7$

Presenter: Michał DEMBSKI-VILLALTA

Authors: Michał DEMBSKI-VILLALTA (1), Sebastian MÜHLBAUER (1), Markus GARST (2), Benjamin WOLBA (2), Eric RESSOUCHE (3), Alexandra A. TURRINI (4), Alexander ENGELHARDT (5)

$Ba_2CuGe_2O_7$ is a quasi-2D insulator characterised by a tetragonal, noncentrosymmetric space group (P-421m) with Dzyaloshinskii–Moriya interactions (DMI). Because of the DMI, at ground state below TN = 3.05 K, it exhibits an almost AF cycloidal spin structure with a pitch of 220 Å. The magnetic structures of $Ba_2CuGe_2O_7$for different temperature and magnetic field values have been the topic of numerous experiments [1] indicating a rich phase diagram with a multitude of incommensurate (IC) phases. Following a recent theoretical prediction, the existence of a vortex phase [2] with non-trivial topological properties in $Ba_2CuGe_2O_7$ has been verified, by means of neutron scattering and bulk measurements of specific heat and AC susceptibility. Despite lacking evidence of any signature of a phase transition in the bulk magnetisation and specific heat measurements, hints towards the presence of a vortex phase were found in the neutron scattering data. There significant measured intensity is seen in the region of interest, noticeably higher than in the paramagnetic phase. This intensity is evenly distributed among four IC satellites on a square plane in reciprocal space, even in the presence of a small in-plane magnetic field component. However, it remains unclear whether the observed phase is due to static long range order or is a fluctuating dynamic texture that is on the verge of ordering.

[1] S. Mühlbauer et al., Phys. Rev. B 86 024417 (2012)
[2] B. Wolba, PhD Thesis, KIT (2021)

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1: Heinz Maier-Leibnitz Zentrum (TUM/FRM II), Germany; 2: Karlsruhe Institute of Technology, Germany; 3: Université Grenoble Alpes, France; 4: Paul-Scherrer Institut, Switzerland; 5: Technical University of Munich, Germany

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WED 11:30-11:45 | HÖRSAAL 2 | MAGN-04

PARALLEL SESSION

PROBING THE DISORDER DISTRIBUTION IN FERRITE NANOPARTICLES USING MAGNETIC SANS

Presenter: Sabrina DISCH

Authors: Dominika ZÁKUTNÁ (1,2), Nahal ROUZBEH (1), Dirk HONECKER (3), Sabrina DISCH (1)

Being intrinsic to nanomaterials, disorder effects crucially determine functional properties such as the magnetic heating performance of magnetic nanoparticles (MNPs), relevant for hyperthermia [1] and thermocatalysis applications [2]. A quantitative interpretation of the nanoscale distribution of structural and spin disorder within MNPs, however, remains a key challenge. Magnetic SANS is a versatile technique to investigate the chemical morphology and magnetization with nanoscale spatial resolution [3].

The classical picture considers single-phase MNPs as a collinearly magnetized core with a structurally and magnetically disordered surface region. We have recently shown that this static idea needs revision as inside MNPs the magnetization is more complex with a significant field-induced growth of the integral moment by a magnetic ordering transition at the structurally disordered surface [4]. On this basis, we derive the intraparticle distribution of the spin disorder energy, giving indirect insight into the structural defect profile in MNPs.

Here, we will present our recent results on the disorder profile in ferrite nanoparticles as affected by synthesis conditions and annealing history of the particles.

[1] A. Lak, S. Disch, P. Bender., Adv. Science 8, 2002682 (2021).
[2] C. Niether et al., Nature Energy 3, 476 (2018).
[3] S. Mühlbauer et al., Rev. Mod. Phys. 91, 015004 (2019).
[4] D. Zákutná, D. Honecker, S. Disch et al., Phys. Rev. X 10, 031019 (2020).

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WED 11:45-12:00 | HÖRSAAL 2 | MAGN-05

PARALLEL SESSION

SMALL ANGLE ELASTIC X-RAY SCATTERING AT SUB-100nm WAVELENGTH EXCHANGE MAGNONS

Presenter: Steffen WITTROCK

Authors: Steffen WITTROCK (1), Christopher KLOSE (1), Korbinian BAUMGAERTL (3), Michael SCHNEIDER (1), Tamer KARAMAN (2), Victor DEINHART (1), Lisa-Marie KERN (1), Kathinka GERLINGER (1), Riccardo BATTISTELLI (2), Daniel SCHICK (1), Bastian PFAU (1), Dirk GRUNDLER (3), Stefan EISEBITT (1)

Spin waves are a promising approach to overcome the limitations of CMOS technology in low power computing and processing. A major challenge is the miniaturization of the required magnon-based devices exhibiting exchange magnons with wavelength on the nanometer scale. Here, we tackle the ~100nm magnon wavelength regime by magnonic grating couplers (GCs), which allow a direct electrical rf excitation of the spin waves. We recently demonstrated the approach to efficiently allow for the generation of propagating sub-100nm magnons at the BESSY MAXYMUS scanning transmission microscope (STXM). However, in a real space microscope, such as STXM, essential characteristics of the magnon dynamics, such as its dispersion, cannot be accessed easily. Common other techniques providing such information are either diffraction limited to their optical sources (e.g. BLS spectroscopy) and usually reach their limit when resolving spin waves far below 1µm, or rather cover the elementary magnetic excitations in the Angstrom to nm range (e.g. inelastic scattering techniques with neutrons, electrons, or X-rays).

Here, we demonstrate to close the relevant wavelength detection gap in the 100nm regime by performing elastic magnetic SAXS. We show that the technique reveals a vast amount of information about the excited magnons. Establishing this method will leverage the study of exchange spin waves and related phenomena and, hence, has the potential of becoming a game changer in the field of magnonics.

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WED 12:00-12:15 | HÖRSAAL 2 | MAGN-06

PARALLEL SESSION

STUDY OF INTERFACIAL MAGNETISM IN EPITAXIAL $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ HETEROSTRUCTURE VIA SOFT X-RAY RESONANT MAGNETIC REFLECTOMETRY

Presenter: Gyanendra PANCHAL

Authors: Gyanendra PANCHAL (1), Enrico SCHIERLE (2), Katharina FRITSCH (1), Klaus HABICHT (1,3)

$La_{0.7}Sr_{0.3}MnO_3$ (LSMO) is a material with interesting magnetic properties such as a high Curie temperature of ~378 K and nearly perfect spin polarization, used for the realization of magnetic tunnel junctions, magneto-electric devices, and next generation spintronic devices [1].

In such oxide heterostructures and multilayers, the interface induced magnetic properties are usually discussed in terms of charge transfer, symmetry breaking and interlayer exchange coupling.

Recent studies reported intralayer exchange coupling induced inverse hysteresis in monolithic $La_{2/3}Sr_{1/3}MnO_3/SrTiO_3$ heterostructure by STEM-EELS studies [2]. However, any quantitative determination of the interfacial magnetization regarding such intralayer exchange coupling in the monolithic thin films have not been studied yet.

In the present work, we have prepared epitaxial 20 nm LSMO thin films on single crystalline $SrTiO_3$ substrate and have studied the inverse hysteresis of this heterostructure by detailed DC magnetization measurements. We will further present our study on the microscopic origin of the unique intralayer exchange coupling at the interface and depth-dependent magnetic profiles that we investigated using soft X-ray resonant magnetic reflectivity and XMCD measurements at the Mn and Ti L-edges performed at the undulator beamline UE46-PGM1, BESSY II, Germany.

1. S. Bader et al. Annual Review of Condensed Matter Physics 1, 71 (2010)
2. M. Saghayezhian et al. PNAS, 116 (21), 10309-10316 (2019)

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