School of XFEL and Synchrotron Radiation Users – SFEL 2024

Book of Abstracts

October 14-18, 2024, Liptovský Ján, Slovakia

Jozef Bednarčík (Ed.)

Pavol Jozef Šafárik University in Košice
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About the SFEL 2024

Pavol Jozef Šafárik University in Košice under the auspices of Ministry of Education, Research, Development and Youth of the Slovak Republic, Ministry of Economy of the Slovak Republic and European X-Ray Free-Electron Laser Facility GmbH in Hamburg organizes School of XFEL and Synchrotron Radiation Users 2024. The school is continuation of the Winter Schools of Synchrotron radiation held in 2011, 2013, 2014 and SFEL 2017, 2018, 2019 and 2022.

The aim of the SFEL2024 school is to facilitate the growth of new Slovak research community of high expertise in high-efficiency RTG laser and synchrotron and neutron sources. The SFEL school is designed for efficient transfer of the rapidly developing know-how in these areas to young generation - researchers and university students. The next aim of the SFEL2024 is strengthening of personal connections between the local Slovak research community and forming scientific teams of XFEL users. Slovak research community thus can take advantage of the fact that Slovakia is a shareholder of European XFEL GmbH Company in Hamburg, but also makes more efficient use of other closely related scientific facilities, including ILL and ESRF in Grenoble and DESY in Hamburg.

The SFEL2024 agenda focuses on a more thorough acquaintance with the selected experimental techniques that make use of the XFEL, synchrotron and neutron radiation. Particular attention is devoted to imaging methods for biological and material applications. The School is implemented in the form of invited tutorial lectures (20 − 45 minutes). Young scientists and PhD students are able to present their experiences with FEL, synchrotron and neutron sources via short oral presentations (10 − 15 min) and/or posters. The target group mainly consists of a wider Slovak and international scientific community with an emphasis on young researchers, PhD and undergraduate students. The contents of the School is focused on the interdisciplinary research with emphasis on physics, material science, chemistry, biology, pharmacy, medical science, and IT technology. Organizers allocate time for both oral and poster presentations for students and young researchers (up to age of 35).

Organizers

School of XFEL and Synchrotron Radiation Users 2024 – SFEL 2024 is jointly organized by following partner institutions:

- European X-Ray Free-Electron Laser Facility GmbH
- Pavol Jozef Šafárik University in Košice
- Technical University in Košice, Faculty of Materials, Metallurgy and Recycling
- Ministry of Education, Research, Development and Youth of the Slovak Republic
- Ministry of Economy of the Slovak Republic
- Commission for coordination of ESFRI activities in Slovak Republic
- Slovak National Center for Popularization of Science and Technology at CVTI

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Norbert Kučerka	Comenius University Bratislava, Slovakia, JINR Dubna, Russia
Juraj Krempaský	Paul Scherrer Institute PSI, Switzerland

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Andrea Putalová	National Centre for Popularisation of Science and Technology in Society, Slovak Centre of Scientific and Technical Information in Bratislava, Slovakia

Location & Venue

Liptov is a historical and geographical region in northern Slovakia with around 140,000 inhabitants. Liptov is one of the most visited regions in Slovakia. There are three public caves: Demänovská Cave of Liberty, Demänovská Ice Cave and Važecká Cave, the biggest ski resort in Slovakia, Jasná, ski park Malinô Brdo, thermal parks of Tatralandia and Bešeňová as well as a UNESCO World Heritage Site of Vlkolínec. Liptovský Ján is the gateway to the world of history, architecture, thermal waters, tourism, flora and fauna, hunting, fishing and sun untouched charm of underground caves.

The hotel SOREA MÁJ is situated in the beautiful scenery of the Low Tatras National Park, at the entrance to the Jánska valley. It is situated at the end of the historic village of Liptovský Ján. Interior and exterior is suitable for family recreation, but also for relaxation and recovery stays, sports camps, congresses, seminars or social events. The hotel area includes the well-known summer swimming pool - TERMAL Paradise with a thermal spring. Lovers of cultural heritage or cycling will definitely have a great time.

Accommodation in single and double rooms, family rooms, suites and rooms for disabled clients. Rooms are equipped with a bathroom, toilet, satellite TV, telephone, safe and balcony. Rooms for disabled clients are situated on the ground floor (without a balcony). WiFi connection. Parking next to the hotel. A varied offer of dishes are served in the hotel restaurant with spectacular views of the West Tatras. Breakfast and dinner are served in a buffet style manner with hot and cold dishes, lunches are served as chosen from the offer. A wide range of cocktails can be enjoyed in the BISTRO café or in the cocktail bar.

Preface

Dear participants

Welcome to Liptovský Ján, small village in beautiful region of Slovak Republic, Low Tatras. On behalf of the Organizing Committee, it is a great honour for me to welcome you here as participants of traditional scientific event - School of XFEL and Synchrotron Radiation Users 2024 „SFEL 2024“. This year it starts on October 14th and ends on October 18th, 2024. Pavol Jozef Šafárik University in Košice jointly with Technical University in Košice, Faculty of Materials, Metallurgy and Recycling under the auspices of Ministry of Education, Research, Development and Youth of the Slovak Republic, Ministry of Economy of the Slovak Republic and European X-Ray Free-Electron Laser Facility GmbH in Hamburg prepared SFEL 2024 as an important event to propagate importance of international cooperation. There are 100 participants from 14 countries registered for the SFEL 2024, majority of them are students, PhD students and young scientists. Together with excellent experts from well-known large scale facilities we will do our best to foster creative community during the SFEL 2024.

The SFEL school is continuation of the Winter Schools of Synchrotron radiation held in 2011, 2013, 2014 and SFEL 2017, 2018, 2019 and 2022. All schools of the series were held here, in Liptovský Ján, where our conference venue offers conditions for friendly and creative atmosphere. The aim of the SFEL 2024 school is to facilitate the growth of a new Slovak research community with high expertise in the area of high-efficiency RTG laser, synchrotron and neutron sources. The SFEL school is designed for efficient transfer of the rapidly developing know-how in these areas to young generation – researchers and university students. The next aim of the SFEL2024 is strengthening of personal connections between the local Slovak research community and actually forming scientific teams of XFEL users, scientific teams of synchrotron or neutron sources users, respectively. Slovak research community thus can take advantage of the fact that Slovakia is a shareholder of the European XFEL GmbH company in Hamburg, but also makes more efficient use of other closely related scientific facilities, including ILL and ESRF in Grenoble and DESY in Hamburg.

Dear colleagues,

I wish you a pleasant stay in Liptovský Ján and I hope very much that the SFEL 2024 accomplishes all your expectations. I would like to express my thanks to all speakers and to all posters contributors for their active participation. They help us to keep scientific level of the SFEL. Last, but not least, I would like to thank to all members of my team from both programme and local committee, respectively.

Liptovský Ján, October 14, 2024 *Pavol Sovák (chairman)*

Contents

EMSA 2024 Program

The table below shows explanation of colors in respective timetables

time	ID	**Name**	Title
			Opening / Closing
			Laboratory X-rays
			Free Electron Lasers
			Synchrotron sources
			Neutron sources
			Poster session
		Session	
		Coffee Break	
		Brakfast / Lunch / Dinner	

Information for presenters

Oral presentations

Present yourself to the session chair at least 15 minutes before the beginning of the session to upload your presentation to the conference room PC using a USB Key. The beamer and screen are set to a 16:9 aspect ratio. Please prepare your slides accordingly. Presentations will be run from the PC which is having Window OS installed together with the Office 2021 suite. Presentation can be prepared in Power Point format or in Adobe PDF format.

Poster presentations

Posters must be 120 cm (height) $\times$ 80 cm (width) (A0 format, portrait). Presenters must provide their own printout of the poster, including title and authors. Session codes will be displayed on the session boards. Material for hanging posters will be available. Please hang your poster during the morning sessions and remove it at the end of the poster session.

October 14, 2024, Monday

11:00–22:00		**Registration**	
12:30–13:30		**Lunch**	
13:45–14:00		**A. Zeleňáková,** **J. Bednarčík** Košice, SK	*Welcoming of participants, introduction to X-ray laboratory session*
		SESSION 1 – LABORATORY X-RAYS – chairman: J. Bednarčík	
14:00–14:45	X-01	**F. Laufek** Prague, CZ	*Introduction to crystallography and X-ray diffraction*
14:45–15:30	X-02	**R. Kužel** Prague, CZ	*Introduction to powder diffraction*
15:30–16:00		**Coffee Break**	
		SESSION 2 – LABORATORY X-RAYS – chairman: R. Kužel	
16:00–16:30	X-03	**M. Dopita** Prague, CZ	*X-ray based techniques applied in materials research*
16:30–17:00	X-04	**T. Roch** Bratislava, SK	*Analysis of thin films by laboratory X-ray sources*
17:00–17:30	X-05	**M. Kusý** Trnava, SK	*Structure determination from a single or series of x-ray diffraction patterns*
17:30–18:00		**Break**	
		OPENING SFEL 2024	
18:00–18:15		**P. Sovák,** **K. Saksl,** **S. Molodtsov**	*Opening SFEL 2024*
18:15–18:30	F-01	**T. Michalek** Bratislava, SK	*Research Infrastructures at the Ministry of Education, Research, Development and Youth*
19:30–22:00		**WELCOME DINNER**	

October 15, 2024, Tuesday

7:30–8:30		**Breakfast**	
		Session 3 – Free Electron Lasers – chairman: P. Sovák	
8:30–9:15	F-02	**S. Molodtsov** XFEL, DE	*Recent Scientific Highlights at European XFEL*
9:15–10:00	F-03	**N. Elleuche** XFEL, DE	*Research Infrastructures in a Changing Global, Environmental and Socio-economical Context: the example of European XFEL*
10:00–10:30	F-04	**C. Milne** XFEL, DE	*Probing dynamics in energy materials using hard X-rays*
10:30–11:00		**Coffee Break**	
		Session 4 – Free Electron Lasers – chairman: J. Krempaský	
11:00–11:30	F-05	**U. Zastrau** XFEL, DE	*High Energy Density science – Research at extreme conditions*
11:30–12:00	F-06	**F. Roth** Freiberg, DE	*Tracking charge transfer dynamics in light harvesting systems by femtosecond time-resolved XPS*
12:00–12:30	F-07	**H. Dürr** Uppsala, SE	*Ultrafast Nanomagnetism*
12:30		**Conference Photo**	
12:30–14:00		**Lunch**	
		Session 5 – Free Electron Lasers – chairman: K. Saksl	
14:00–14:30	F-08	**J. Krempaský** PSI Villigen, CH	*Altermagnetism: the new taxonomy in the century old theory of magnetism?*
14:30–15:00	F-09	**J. Vonka** PSI Villigen, CH	*Hard X-ray scattering in the milli Kelvin domain at SwissFEL*
15:00–15:30	F-10	**L. Juha** CAS Prague, CZ	*Beyond EUV lithography: nanostructuring with XUV/x-ray lasers*
15:30–16:00		**Coffee Break**	
		Session 6 – Free Electron Lasers – chairman: L. Juha	
16:00–16:30	F-11	**I. Barák** SAS Bratislava, SK	*Spore coat protein 2D crystals as a continuing challenge for studies at XFEL*
16:30–17:00	F-12	**J. Uličný** **P. Vagovič** UPJŠ Košice XFEL DE	*2D and 3D MHz X-ray imaging at EuXFEL*

17:00–17:30	F-13	**G. Vankó** Budapest, HU	*Hard X-ray Spectroscopy as an Ultrafast Probe*
17:30–18:00		**Break**	
		SESSION 7 – FREE ELECTRON LASERS – chairman: C. Milne	
18:00–18:30	F-14	**R. Nietubyć** NCNR, PL	*The PolFEL status*
18:30–18:50	F-15	**J. Bulička** CAS Prague, CZ	*Laboratory and Computer Simulations of Radiation Damage to First Wall Materials of Prospective IFE Reactors: Damage Thresholds of Boron Nitride and Tungsten*
18:50–19:10	F-16	**J. Pivoňková** XFEL, DE	*Opportunities for Early Stage Researchers (ESRs) to access research infrastructures via international networks*
19:30–21:00		**DINNER + FOLK PERFORMANCE**	

October 16, 2024, Wednesday

7:30–8:30		**Breakfast**	
		Session 8 – Synchrotron sources – chairman: P. Šiffalovič	
8:30–9:00	S-01	**M. Cesnek** ČVUT Prague, CZ	*Introduction to the charged particle accelerators and their applications*
9:00–10:00	S-02	**V. Hollý** CU Prague, CZ	*Introduction to synchrotron radiation*
10:00–10:30	S-03	**K. Sedlačková** STU Bratislava, SK	*Basic principles of X-ray detectors*
10:30–11:00		**Coffee Break**	
		Session 9 – Synchrotron sources – chairman: V. Holý	
11:00–11:45	S-04	**P. Šiffalovič** IP SAS, SK	*Time-resolved grazing incidence X-ray scattering applied to energy-related materials*
11:45–12:30	S-05	**K. Kosiba** IFW Dresden, DE	*Synchrotron methods applied in materials science*
12:30–14:00		**Lunch**	
		Session 10 – Synchrotron sources – chairman: J. Bednarčík	
14:00–14:30	S-06	**M. Sikora** Solaris, PL	*Research opportunities at SOLARIS synchrotron in the area of materials for future*
14:30–15:00	S-07	**Š. Michalik** Diamond, UK	*Complementarity of the high-energy X-ray scattering and imaging techniques in material science research (but not only) on I12-JEEP beamline at Diamond Light Source*
15:00–15:30	S-08	**R. Mokso** TU Denmark, DK	*The finest details we can visualize with X-ray tomography*
15:30–16:00		**Coffee Break**	
		Session 11 – Synchrotron sources – chairman: M. Dopita	
16:00–16:30	S-09	**Y. Chushkin** ESRF, FR	*Application of Coherent Scattering at the ESRF EBS – progress and challenges*
16:30–17:00	S-10	**Z. Matěj** Max IV, SE	*Azimuthal Integration for Powder Diffraction and Rietveld Refinement*
17:00–17:30	S-11	**J. Kulda** ILL, FR	*From Molecular Dynamics Simulations to Diffuse Scattering Maps*
17:30–18:00		**Break**	

		Session 12 – Synchrotron sources – chairman: A. Zeleňáková	
18:00–18:20	S-12	**G. Gazdowicz** SOLARIS, PL	*ASTRA beamline at SOLARIS: XAS in the tender and hard X-ray range*
18:20–18:40	S-13	**M. Holub** Soleil, FR	*The revealing of Ni2Fe-OH layered double hydroxide magnetic characterization using powerful XAS/XMCD methods*
18:40–19:00	S-14	**V. Girman** UPJŠ Košice, SK	*TEM and synchrotron study of precipitates in Al-based alloys*
19:30–20:30		**Dinner**	
		Session 13 – Free Electron Lasers – chairman: Š. Michalik	
20:30–20:50	F-17	**T. Burian** CAS Prague, CZ	*Focus characterization I: How to measure transverse fluence distributions in focused x-ray FEL beams by ablation imprints*
20:50–21:10	F-18	**V. Vozda** CAS Prague, CZ	*Focus characterization II: AI aided and automated image segmentation for focused beam analyses*
21:10–21:30	F-19	**Š. Jelínek** CAS Prague, CZ	*Focus characterization III: Tightly focused x-ray FEL beams: simulations and experiment*

October 17, 2024, Thursday

7:30–8:30		**Breakfast**	
		SESSION 14 – NEUTRON SOURCES – chairman: D. Uhríková	
8:30–9:15	N-01	**M. Johnson** ILL Grenoble, FR	*The Institut Laue Langevin: a world-leading neutron facility for the next decade of science and innovation*
9:15–9:45	N-02	**L. Gajdoš** ILL Grenoble, FR	*Neutrons for structural biology at ILL*
9:45–10:30	N-03	**N. Kučerka** JINR, RU	*Applications of pulsed reactor neutrons*
10:30–11:00		**Coffee Break**	
		SESSION 15 – NEUTRON SOURCES – chairman: N. Kučerka	
11:00–11:30	N-04	**D. Uhríková** CU Bratislava, SK	*Exogenous lung surfactant for drug delivery: a view through scattering techniques*
11:30–12:00	N-05	**L. Almasy** HUN-REN, HU	*Budapest Neutron Center – science at a medium size reactor with examples on structural studies of ionic liquids*
12:30–14:00		**Lunch**	
14:00–18:00		**Leisure Time**	
		SESSION 16 – POSTER PRESENTATIONS – chairman: P. Sovák	
18:00–19:00	P-01 ... P-14		*POSTER presentations*
19:00–22:00		**FAREVEL DINNER**	

October 18, 2024, Friday

7:30–8:30		**Breakfast**	
		Session 17 – Neutron sources – chairman: N. Kučerka	
8:30–9:15	N-06	**M. Klicpera** CU Prague, CZ	*Neutron scattering in Czech Republic from intermetallics to oxides*
9:15–10:00	N-07	**M. Koza** ILL Grenoble, FR	*Vibrational properties and mass transport in thermoelectric materials studied by neutron spectroscopy*
10:00–10:30	N-08	**A. Martinelli** CNR-SPIN, IT	*Representation Analysis of Magnetic Structure: Theory and Praxis*
10:30–11:00		**Coffee Break**	
		Session 18 – Neutron sources – chairman: A. Martinelli	
11:00–11:20	N-09	**D. Zákutná** CU Prague, CZ	*Disentangling Anisotropy Contributions in Mn-mixed Ferrite Nanoparticles*
11:20–11:40	N-10	**P. Hrubovčák** UPJŠ Košice, SK	*Interaction of magnetic nanocarriers with cell membranes*
11:40–12:00	N-11	**M. Falkowska** Manchester, UK	*Structural investigations of disordered systems using total neutron scattering*
12:00–12:20	N-12	**P. Kopčanský** SAS Košice, SK	*Small-angle scattering and neutron reflectometry methods in the study of magnetic nanoparticles in magnetic fluids and their composites*
		Closing SFEL 2024	
12:20–12:30		**P. Sovák,** **K. Saksl** Košice, SK	*Closing SFEL 2024*
12:30–14:00		**Lunch**	

Part I

Laboratory X-rays

X-01

Introduction to Crystallography and X-Ray Diffraction

František Laufek [1,*]

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14.10.2024, Monday
14:00 – 14:45

Topic 1
Laboratory X-rays

THE TERM CRYSTAL was introduced by the Ancient Greeks and means ice. Greeks used this term for rock-crystals since they thought that the rock-crystals were produced by congelation of water.

Crystallography is a peculiar science, at the same time interdisciplinary – it overlaps with the principal natural sciences of physics, chemistry, mineralogy and biology – and yet rather hermetic. The "basic language of crystallography" is not really difficult, but it is very exact and must be learned. In the lecture, several basic individual terms used in crystallography as e.g. crystal system, symmetry operations, point groups, lattices and space groups, equivalent positions, asymmetric unit will be briefly explained. Crystallography information file (CIF) and related Inorganic Crystal Structure Database – will be discussed. A brief introduction to International Tables for Crystallography, Volume A, will be presented. In a second part of the lecture, a concise historical development of crystallography will be mentioned.

The modern crystallography is based on three fundamentals findings. W.C. Röntgen made the discovery of X-rays in 1895. Soon later, in 1912, M. Laue, F. Knipping and W. Friedrich performed the first X-ray diffraction experiment. The same year, W.H. Bragg and W.L. Bragg wrote their famous equation for the first time. The powder X-ray diffraction method was developed independently by Peter Debye, Paul Scherrer (1916) and by Alfred Hull (1917). A major advance of the powder diffraction method began in the early 1950´s with the introduction of the first commercial high-resolution diffractometers which greatly expand the use of the method. In 1967, a next huge step was taken as Hugo Rietveld published his first whole profile pattern fitting analysis of WO_3. In this work, Hugo Rietveld showed that he could refine a crystal structure having powder diffraction pattern with overlapping reflections.

Subsequent development in the field of powder X-ray diffraction has included usage of synchrotron and neutron sources, in situ investigation of powders and solid materials, solving crystal structures by direct and dual space methods, fundamental parameter approach, quantitative phase analysis, just to name a few.

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X-02

Introduction to Powder Diffraction

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14.10.2024, Monday
14:45 – 15:30

Topic 1
Laboratory X-rays

POWDER DIFFRACTION (PD) is an old technique for the structural and microstructural characterization of materials that is experimentally relatively simple (regardless of the price of a modern powder diffractometer). PD includes not only the analysis of powder samples but also studies of all kinds of polycrystalline materials – bulk materials, and thin films. There are several monographies available devoted to this technique. Much has already been described for example in [1] and more recently in [2]. In addition to original Debye-Scherrer method, nowadays mainly standard – conventional arrangement of the experiment is used. This is the so-called Bragg-Brentano parafocusing geometry with symmetrical $2\theta - \theta$ or $\theta - \theta$ scan when the information contained in each diffraction peak hkl is related only to the corresponding (hkl) planes parallel to the surface, so different peaks are related to different crystallite families.

The information contained in the powder diffraction pattern analysis is quite rich. Each crystalline phase has its typical PD pattern as a fingerprint. Therefore, by using databases like PDF-5+ we can perform *qualitative* and *quantitative* phase analysis (e.g. [1-3]). PD peak positions are also related to the unit cell size, i.e. *lattice parameters* that can be connected to possible non-stoichiometry, lattice defects and residual stresses. Integrated intensities are given by several factors. Mainly by the structure factor – i.e. the *crystal structure* that can be refined or even sometimes solved from the PDXRD pattern (e.g. [4, 5]). They are also determined by the irradiated volume of suitably oriented crystallites, and if their distribution is not random, their *preferred orientation - texture*, can be estimated. Finally, broadening of diffraction peaks can be influenced by *small crystallite sizes* and/or *microstrains* (e.g. due to dislocations) that can also be determined for each phase [e.g. 6, 7]. For detailed analysis of thin films, textures and stresses, asymmetric geometries and often parallel beam techniques are also used.

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X-03

X-ray based Techniques applied in Materials Research

14.10.2024, Monday
16:00 – 16:30

Topic 1
Laboratory X-rays

Milan Dopita [1,*]

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THE X-RAY BASED techniques play a fundamental role in materials research by providing integral insights into the phase composition, morphological, structural, microstructural and real structure properties of materials at various scales. Modern X-ray laboratory equipment, which underwent significant improvements within past years, covering the use of X-ray sources with high flux of photons and various wavelengths, optical elements as monochromators, and X-ray mirrors, and fast, noise-free multidimensional detectors, extends the use of laboratory equipment into the fields which were the dominant domain of synchrotron sources, in past.

In the lecture the experimental possibilities accessible in our X-ray laboratory together with examples of individual applications, with the focus to a special, challenging, or non-commonly used techniques, in materials research, will be shown and discussed in details. It involves unique combination of X-ray diffractometers offering measurements covering a wide range of reciprocal space between q of 0.003 to 21 1/Å (q is a magnitude of reciprocal space vector), which allows the fundamental studies of materials properties in ranges from 0.03 up to 200 nm, in real space. This unique collection of instruments allows nearly any type of laboratory accessible X-ray scattering experiment - measurements of single crystals, polycrystalline bulk and powder materials, nanocrystalline and amorphous samples, thin films, multilayers and epitaxial layers. The instruments can operate with various X-ray wavelengths (Co, Cu, Mo and Ag), and in different geometries: Bragg-Brentano parafocusing geometry, medium resolution parallel beam setting, high resolution geometry, with monochromatic $K\alpha_1$ radiation and in coplanar and non-coplanar (in-plane) mode. Various sample environments, low and high temperature chambers, deformation (tensile and compression) stage, reaction chamber are available for individual diffractometers. Methodologically the instrumentation offers the structure solution and refinement, qualitative and quantitative phase analysis, the real structure of material studies: preferred orientation of crystallites - texture measurements, residual stress measurements, reflectivity measurements, rocking curve measurements, reciprocal space mapping, pair distribution function - total scattering measurements, small angle X-ray scattering and grazing-incidence small angle X-ray scattering.

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X-04

Analysis of Thin Films by Laboratory X-ray Sources

Tomáš Roch [1,*], B. Grančič [1], R. Vrablec [1]

14.10.2024, Monday
16:30 – 17:00

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Topic 1
Laboratory X-rays

Material research of thin films is today very interdisciplinary and important for applications. Beside their chemical composition, electrical, optical or mechanical properties understanding of structure and morphology is crucial in utilizing their potential and mastering production procedures. In this short contribution the typical peculiarities in X-ray structural analysis of thin films are introduced. Low thickness of the studied material in orders of nanometers to few micrometers influences measured diffraction intensity patterns via μt, product of attenuation coefficient μ and the thickness t. Due to penetration depth orders of magnitude larger than thin film thickness, there are special grazing incidence X-ray scattering methods for restricting the probed volume within the sample thickness.

Thin films are typically prepared on suitable substrates, mostly of monocrystalline nature. Beside substrate artefacts the X-ray structural analysis often reveals strong influence of substrate surface symmetry on the thin film morphology and preferential orientation of crystallites. Few presented examples of X-ray structural analysis of transition metal boride thin films prepared by various physical deposition techniques illustrate the development of strong biaxial texture. Deposition parameters and thermal treatment of thin films also strongly influence phase composition and transformations. Although the texture measurement or grazing incidence techniques are routinely realized at synchrotron facilities, to some extend the basic characterization can be performed using laboratory equipment.

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X-05

Structure Determination from a Single or Series of X-ray Diffraction patterns

Martin Kusý [1,*]

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14.10.2024, Monday
17:00 – 17:30

Topic 1
Laboratory X-rays

X-RAY DIFFRACTION methods provide important information about the state of the material structure. Knowledge acquired in this way can be reflected not only in the development of new materials, but also in areas of application and optimization of the service life of tools or machine parts. Many structural parameters can be determined with sufficient precision using a single diffraction measurement, specifically in cases where the sample is a polycrystalline bulk material or a powder with a random arrangement of crystallites. The identification of the phases present, their quantity, the determination of the lattice parameter, the size of the crystallites and micro deformations of the lattice allows, for example, to characterize the efficiency of homogenization annealing, which is a necessary prerequisite for the corrosion resistance of stainless steels or precedes the process of precipitation hardening of precipitation-hardenable alloys.

Samples originating from various stages of laboratory preparation of new materials, industrial production of materials carry with them traces of technological production processes in the form of various structural features. In the case of operated components, the effects of operation in the given environment are superimposed on top of production ones. In many cases, it is therefore necessary to analyse samples that combine, for example, micro-layered textured layers as well as the substrate, increased residual stresses with significant anisotropy, and the like. One of the possibilities to characterize these materials is to reveal and quantify each of these structural characteristics individually, using specific measurements. Another possibility is the simultaneous combined analysis of diffraction records obtained using different experimental conditions, which are subsequently analysed using specialized programs based on the Rietveld method.

As part of the lecture, the results of mostly applied research in the field of metallurgy and production technologies will be presented. Using the evaluation of the size of the lattice parameter of V_4C_3 carbide of high-alloy tool steels for cold work, the effect of rapid solidification during the production of powder particles as a precursor for the production of tools using powder metallurgy will be indirectly demonstrated. Individual measurements of the residual stresses introduced into the surface of the material, as will be shown, have a significant impact on the initiation of corrosion damage to the operating machine components. The combined method of analysing the diffraction records of plasma-nitrided components will demonstrate the presence of a layer of nitrides with the required thickness by a non-destructive method, while at the same time the residual stresses in this layer will be determined.

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Part II

Free Electron Lasers

F-01

Research Infrastructures Governance System in Slovakia

14.10.2024, Monday
18:15 – 18:30

Topic 2
Free Electron Lasers

Tomáš Michalek [1,*]

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In this talk, we will try to shed more light on how the system of research infrastructures governance in Slovakia works and who the relevant actors are. In February 2024, the Government of the Slovak Republic adopted an updated version of the Research Infrastructures Action Plan, which outlines the exact implementation steps on the way to improve the Slovak research infrastructures governance in line with the Research Infrastructures Roadmap adopted in 2021. Among other things, in 2024, the Research Infrastructures Unit was created at the Ministry of Education, Research, Development and Youth. The Unit is, together with the Research Infrastructures Working Group of the Council of the Government, responsible for implementation of the Action Plan. In a joint effort, they will shortly introduce an evaluation procedure for emerging and existing research infrastructures in Slovakia, which will be part of a mechanism to receive a competitive funding from the planned funding scheme. Moreover, the Unit and the Working Group are also going to define a procedure for so called national research infrastructures platforms, which should help them again to receive necessary funding either from Slovak or European funding schemes. Finally, the Unit and the Working Group coordinate the activities of the Slovak research infrastructures in the European Strategy Forum on Research Infrastructures (ESFRI).

F-02

Recent Scientific Highlights at European XFEL

Serguei Molodtsov [1,*]

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15.10.2024, Tuesday
8:30 – 9:15

Topic 2
Free Electron Lasers

The European X-ray Free Electron Laser (XFEL) is a new international research installation that is under operation in the Hamburg area in Germany. The facility generates new knowledge in almost all the technical and scientific disciplines that are shaping our daily life - including nanotechnology, medicine, pharmaceutics, chemistry, materials science, power engineering and electronics. The ultra-high brilliance femtosecond X-ray flashes of coherent radiation are produced in a 3.4-kilometre long European XFEL facility. Most of it is housed in tunnels deep below ground. In its present configuration, the European XFEL comprises 3 self-amplified spontaneous emission (SASE) light sources - undulators operating in energy ranges 3 - 25 keV (SASE 1 and SASE 2) and 0.2 - 3 keV (SASE 3), respectively. The world-unique feature of this XFEL is the possibility to provide up to 27.000 ultra-short flashes (1 - 100 fs) that makes the facility particular suitable for time-resolved X-ray absorption, photoemission, (resonance) inelastic X-ray scattering as well as diffraction and imaging studies in the range of moderate and hard X-ray photons. In this talk an overview of the European XFEL project will be provided and a review of applications as well as directions of further developments will be given.

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F-03

Research Infrastructures in a Changing Global, Environmental and Socio-economical Context: the Example of European XFEL

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15.10.2024, Tuesday
9:15 – 10:00

Topic 2
Free Electron Lasers

DOI: https://doi.org/10.33542/SRU-0350-0

F-04

Probing Dynamics in Energy Materials using Hard X-rays

Christopher Milne [1,*]

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15.10.2024, Tuesday
10:00 – 10:30

Topic 2
Free Electron Lasers

X-RAY spectroscopy and scattering allow a unique combination of electronic and structural information to be obtained from a variety of different types of samples in many different forms (solid, liquid, gas). The extension of these methods into the time domain has allowed measurement of dynamic processes, for example the tracking the photoinduced charge carriers in a functional material [1] or following the photocycle in a light activated protein [2]. In recent years X-rays have started to become routinely used to measure light-activated processes using a pump-probe scheme, where the sample is photoexcited with light and then probed after a variable time delay using an X-ray pulse. These methods can measure dynamics over a broad range of timescales, allowing them to probe everything from protein dynamics to ultrafast electronic spin-state changes in molecular systems. With the recent development of X-ray free electron lasers (XFELs), time-resolved X-ray techniques have moved into the ultrafast regime, where the timescales of electron and nuclear motion can be accessed using the femtosecond X-ray pulses available from these facilities.

This talk will present an overview of how X-ray techniques are being used at XFELs to address energy materials and the type of information the measurements can provide. The talk will introduce the European XFEL, a high-repetition rate XFEL facility located in northern Germany, and its' Femtosecond X-ray Experiments (FXE) instrument [3] which is focussed on measuring ultrafast dynamics in the condensed phase. Finally the presentation will show some examples of the types of measurements XFELs can perform and the scientific questions that can be answered using ultrafast X-ray techniques.

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F-05

High Energy Density Science - Research at Extreme Conditions

Ulf Zastrau [1,*]

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15.10.2024, Tuesday
11:00 – 11:30

Topic 2
Free Electron Lasers

This lecture will introduce the students and audience into the field of the science at high energy density (HED) - that is, above a pressure of 1 Mbar or 100 GPa. Since pressure is energy per volume, or an "energy density", this HED condition is equivalent to any large amount of energy stored in dense matter (solids) at high temperatures and densities, or EM-field strength, accordingly.

First, I will provide an overview where such extreme states of matter can be found - in the universe, in (exo-)planets, inside our planet Earth, and in technical and scientific applications involving powerful lasers. Then I will explain how these states can be produced in the laboratory - usually only for a very short time - and what the methods are to create and characterize them. Finally, I will show how HED science benefits strongly from a precision tools such as a X-ray Free Electron Laser: It provides single-shot short bright x-rays, which can "snapshot" the often rapidly evolving states of matter.

References

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F-06

Tracking Charge Transfer Dynamics in Light Harvesting Systems by Femtosecond Time-resolved XPS

15.10.2024, Tuesday
11:30 – 12:00

Topic 2
Free Electron Lasers

Friedrich Roth [1,*], M. Borgwardt [2], L. Wenthaus [3], D. Kutnyakhov [3], J. Mahl [1], F. Pressacco [3], G. Brenner [3], S. Molodtsov [1,4], O. Gessner [2], W. Eberhardt [3]

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THE STUDY OF EXCITATIONS and their dynamics is of great significance in nature and applied technologies. Many fundamental aspects of our world, such as chemical processes and transport phenomena rely on dynamic reaction chains. At the heart of many emerging sunlight-to-fuel and sunlight-to-electricity concepts are interfacial processes that require an optimized, concerted flow of charge and energy on the molecular level. In order to gain a comprehensive understanding of the fundamental dynamics and scaling laws that enable molecular, interfacial, and macroscopic charge and energy transport, it is necessary to connect processes that evolve on spatial and temporal scales spanning orders of magnitude. As the interface properties change during operation, e. g., under applied electrochemical stimulus or external photoexcitation, and because multiple bulk and interface processes coexist and compete, detailed in operando characterization is urgently needed. Concurrently, interfaces present a challenge in technologies that rely on charge transfer processes. These require advanced experimental probes to shed new light on the underlying physical and chemical processes. Soft X-ray spectroscopy techniques are particularly well suited to monitor electronic and chemical states of matter with the elemental site-specificity and chemical sensitivity that is required to test and improve our fundamental understanding of interfacial chemistry and photophysics in complex systems. This lecture offers an overview of the diverse experiments conducted in recent years using synchrotron radiation sources and free-electron lasers. These have demonstrated that time-resolved XPS provides a distinctive opportunity to investigate the photo-induced interfacial charge transfer dynamics with exceptional site-specificity and a temporal resolution in the picosecond to femtosecond regime across a range of sample systems. Access to the element and chemically specific core-levels provides a unique perspective of the dynamic charge evolution in direct vicinity of the atom from which the core electron is emitted. This unique capability will enable previously unachievable insights into underlying microscopic mechanisms and thus aims to pave the way for a better understanding of emerging photovoltaic and photocatalytic frameworks.

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F-07

Ultrafast Nanomagnetism

15.10.2024, *Tuesday*
12:00 – 12:30

Topic 2
Free Electron Lasers

Hermann Dürr [1,*]

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ONE OF THE KEY DRIVERS for information technology is the quest for "smaller and faster" information processing and storage. The ultimate speed limit is the speed of light. The idea to change and control properties of materials with the help of femtosecond laser pulses, the shortest stimuli in contemporary experimental physics, has, therefore, long intrigued researchers. In this lecture I will focus on how transient femtosecond electric fields can be used to change magnetic properties of materials, in particular how nanoscale spin textures emerge from the laser-induced demagnetized state [1,2].

References

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F-08

Altermagnetism: a New Taxonomy in the Century Old Theory of Magnetism?

Juraj Krempaský [1,*]

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15.10.2024, Tuesday
14:00 – 14:30

Topic 2
Free Electron Lasers

MANGANESE-TELLURIDE (MnTe) is a near room temperature antiferromagnet, which we recently addressed in the context of altermagnetism – as a central topic of condensed-matter physics demonstrating a new type of lifted Kramers spin degeneracy. Is the altermagnetism proving its place on the magnetic family tree as a 3rd distinct magnetic phase without net magnetization, yet with spin polarization which combines merits of ferromagnets and antiferromagnets thought to be fundamentally incompatible? The experimental results from spin- and angle-resolved photoemission spectroscopy carried out at the Swiss Light Source provide us direct evidence: in contrast to ferromagnets or antiferromagnets, altermagnets have a special arrangement of spins with broken parity time reversal symmetry, which are absent in magnetic systems known so far [1]. Detailed imaging of the local altermagnetic ordering vector shows a variety of spin configurations that can be imposed using microstructure patterning combined with thermal cycling in magnetic fields [2]. Finally, with such a field-cooling procedure our recent experimental results indicate evidence of the MnTe altermagnetic d wave spin texture, which motivates exploration of the altermagnetism in the context of superconductors.

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F-09

Hard X-ray Scattering in the milli Kelvin Domain at Swiss-FEL

Jakub Vonka [1,*] M. Clemence [1], B. Pedrini [1], A. Steppke [1,2], D. Kazazis [1], Y. Ekinci [1], M. Bartkowiak [3], G. Aeppli [1,4,5], S. Gerber [1]

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15.10.2024, Tuesday
14:30 – 15:00

Topic 2
Free Electron Lasers

Quantum fluctuations dominate over thermal fluctuations at low temperatures, as manifested by the emergence of quantum many-body ground states and new phases of matter. One of the goals of the new Cristallina-Quantum endstation at SwissFEL is to image these states with hard X-ray pulses, outrunning the beam heating thanks to femtosecond pulse duration. In this talk I will review our commissioning progress on a new dilution refrigerator instrument that has recently entered early pilot user program. I will describe some of the results demonstrating resonant X-ray scattering from magnetic orders down to sub-100mK temperatures, and elaborate on the path towards full scientific exploitation of this unique experimental environment.

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F-10

Beyond EUV Lithography: Nanostructuring with XUV/X-ray Lasers

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15.10.2024, Tuesday
15:00 – 15:30

Topic 2
Free Electron Lasers

NOWADAYS, the mass production of nanostructures for highly integrated electronic circuits (microchips) is dominated by extreme ultraviolet lithography (EUVL). The EUVL technology consists of several processing steps. The key step is represented by a transfer and demagnification of structural motif from either reflective or transmission masks with electromagnetic radiation having a typical wavelength of 13.5 nm delivered most frequently from optimized laser-produced plasma sources. A latent nanostructure is created in a suitable resist in this way. The exposed resist should be etched to evolve the above mentioned demagnified structural motif at the resist-semiconductor interface. Then, further processing steps should be applied to create a wanted 3D structure in semiconducting functional material below the resist layer. We clearly see that many manufacturing steps are needed to manufacture an electronic element exhibiting a very high degree of integration using the conventional EUVL technology. Could new sources of intense XUV/X-ray radiation, i.e., short-wavelength lasers providing the photon flux high enough to erode functional materials in vacuum directly, make possible a remarkable reduction of processing complexity required for the fabrication of highly integrated electronic elements? This talk should give an answer to this question with respect to the progress in radiation sources development and understanding the nature of radiation-induced processes occurring at high dose rates of XUV/X-ray radiation.

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F-11

Spore Coat Protein 2D Crystals as a Continuing Challenge for Studies at XFEL

Imrich Barák[1,*], D. Krajčiková[1], E. Round[2], F. Koua[2], A. Vetráková[1]

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15.10.2024, Tuesday
16:00 – 16:30

Topic 2
Free Electron Lasers

Bacillus subtilis spore coat is an outermost proteinaceous layer which protects the spores in a variety of incidents as in the presence of different toxic chemicals and lytic enzymes or against predation by unicellular and multicellular eukaryotes. The coat, organized in two major morphologically distinct layers known as an outer coat and an inner coat, is composed of at least 70 proteins. The process of the coat assembly represents a central objective of our research. In order to gain structural insights into the spore coat of B. subtilis we have attempted to purify a number of recombinant coat proteins including CotY, and CotZ. We have discovered a number of self-assembled structures including two-dimensional crystals and helical fibres. X-ray free-electron lasers are opening up unique opportunities to image biological materials at high resolution. The European XFEL brings a unique capability of over a 200 increase in pulse repetition rate compared with the LCLS, which vastly increase the efficiency of the method, reducing the time required to carry out a measurement and reducing the quantity of protein required to obtain a structure. Taken together, X-ray FELs have the potential to profoundly impact the field of structural biology. Slovak involvement in User consortium of SFX at XFEL experimental station in Hamburg will be discussed. We will present our first data from XFEL-related to determination of structure of CotY 2D crystals. We aim to develop, in a longer-term perspective, a robust technique for the structural determination of the 2D crystals by studying the model samples (CotY and CotZ coat proteins) to overcome the difficulties of obtaining 3D structures of proteins forming 2D crystals, which are likely the nature of these proteins. To use these 2D lattices of Cot proteins for suitable fusion with proteins of interest for various applications, the determination of their structures is essential. The output of suggested experiments will be manyfold. Firstly, it will provide a basis for understanding the underlying mechanism behind the formation of highly complex cellular structures such as spore coat. Secondly, the determination of the 3D structure of CotY and CotZ will allow us to fit them into already known low-resolution cryo-TEM ternary structures of both proteins. Thirdly, these 3D structures should reveal the attachment sites of single protein molecules in the hexameric forms as well as the attachment of hexamers together, and the formation of the observed 2D lattices. Lastly, the spatial organization of each amino acid in the lattice will allow us to select a suitable site for the attachment of different enzymes, antibodies, etc. to use such structures in nano-biotechnology processes and biomedicine.

F-12

2D and 3D MHz X-ray Imaging at European XFEL

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15.10.2024, Tuesday
16:30 – 17:00

Topic 2
Free Electron Lasers

FIRST MHz rate fourth generation hard X-ray XFEL source European XFEL [1] provide unique opportunity for characterisation of stochastic dynamics occurring in various systems either naturally or response is stimulated by an external force. High repetition rate of pulses (up to 4.5 MHz) together with high flux per pulse allow to record projected X-ray radiograms of dynamic samples and image more then million frames per second with high spatio-temporal resolution. Each such frame is illuminated using ultrashort exposure (fs scale) given by the X-ray pulse duration providing "frozen in time" snapshots of stochastic phenomena. This enable to film fast stochastic processes individual realisations in slow smooth motion. Moreover, EuXFEL SASE1 undulator generate X-ray pulses with three orders higher number of photons per pulse (10^{12} photons) as compared to synchrotrons reaching hard X-ray range up to 24 keV with $\sim$ 20 eV bandwidth. This unique performance allows for implementation of X-ray beam splitting schemes of multiprotection microscopy to obtain 3D snapshots per single pulse of dynamic objects sampled at MHz rate. We will present applications of recently developed MHz XFEL projection X-ray microscopy [2] applied for study of industrially relevant fluidic system behaving stochastically and we will present experimental results from recent characterisation of multi projection MHz X-ray which is being developed under EIC-Pathfinder MHz-Tomoscopy project at SPB/SFX instrument [3].

References

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F-13

Hard X-ray Spectroscopy as an Ultrafast Probe

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15.10.2024, Tuesday
17:00 – 17:30

Topic 2
Free Electron Lasers

ULTRAFAST photo-induced transformations of molecular systems are ubiquitous in various branches of chemistry, physics, molecular biology, and materials science. These processes are essential in photosynthesis and photocatalysis, and have high potential for applications in molecular storage or switching devices, and light-harvesting systems. Understanding the elementary steps and the formation of transient species in related molecular reactions, phase transitions or biochemical function is inevitable. However, the traditional toolset of pump-probe experiments has several limitations, preventing us from capturing many relevant aspects needed to fully understand the underlying ultrafast dynamics. X-ray free electron lasers (XFELs) offer a very rich toolset, particularly when we can work in vacuum, but hard X rays are often the choice when we need to study dynamics in the condensed phase. Exploiting hard X-ray techniques to probe the ultrafast dynamics in pump-probe experiments can provide us with novel element sensitive insights. The intense femtosecond X-ray pulses of XFELs permit us to exploit the X-ray spectroscopy tools with the appropriate time resolution, offering direct access to the changes in the charge, spin and nuclear degrees of freedom during the elementary physical processes of a chemical reaction, photophysical transformation, or biological function. Combining spectroscopy with X-ray solution scattering allows us to simultaneously address both the electronic and structural dynamics of the molecule in the solvent cage, as well as the relaxation of the product molecule and the energy transfer to the solvent. The development in time resolution made it possible to separate the details of these processes, and with the help of quantum chemistry and quantum dynamics the mechanisms are becoming fully understood. Results obtained on light-excited transition-metal-based model systems for photoswitchable or light-harvesting functional molecules, as well as ligand exchange reactions will be shown as examples. We will discuss the applicability of hard X-ray spectroscopy, highlighting successes, challenges, and common misconceptions.

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F-14

The PolFEL Status

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15.10.2024, Tuesday
18:00 – 18:30

Topic 2
Free Electron Lasers

After the transformation of the PolFEL project from an ensemble of FELs covering THz - VUV range of electromagnetic radiation, to a hybrid of accelerator-, plasma harmonics- and solid state lasers-based sources maintaining that range and supplemented with an EUV plasma jet HH generator, the ultimate arrangement of constituting elements has been frozen. The superconducting linac based on two Rossendorf-like accelerating cryomodules and including all superconducting electron gun, has been designed in order to deliver 20 pC – 250 pC electron bunches to superradiant THz undulator. IR-VUV range will be covered by a set of Nd:YLF and Ti sapphire generators and OPAs enabling the flexible choice of wavelength, pulse duration and repetition rate as well as pulse shaping. The light source facility combined in this way will be complemented with a continuous wave, MeV ranged UED beamline dedicated for solid and gasous samples. Currently the major components procurement is being completed, the installation will begin in the half of 2025 aiming at the commissioning and first light in 2026. The efforts to provide a wide range tuneable and coherent electromagnetic radiation source dedicated for fundamental and applied sciences are, on the other hand, intended as an introductory step in FEL science and engineering development in Poland.

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F-15

Laboratory and Computer Simulations of Radiation Damage to First Wall Materials of Prospective IFE Reactors: Damage Thresholds of Boron Nitride and Tungsten

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15.10.2024, Tuesday
18:30 – 18:50

Topic 2
Free Electron Lasers

Elemental tungsten, tungsten alloys, and boron nitride ceramics have been extensively studied as potential materials for the first walls of prospective fusion reactors and other high-energy applications. A crucial factor for these materials is their damage threshold under short-wavelength electromagnetic radiation, which constitutes a significant component of fusion plasma emission. Conventional, well-established methods of determining damage thresholds through surface morphology changes are often hindered by the complex and irregular surfaces of real samples. These materials frequently exhibit complex, poor defined structures, such as foams or sintered nano-powders, making it difficult to detect the subtle initial damage indicative of the threshold. To address this challenge, we propose using ion emissions induced by focused XUV laser radiation as an alternative method for estimating damage thresholds [1]. Radiation damage investigations were conducted on selected first-wall materials using a capillary-discharge XUV laser with ion emissions detected by TOF mass spectrometry [2]. Our findings reveal that hexagonal boron nitride (h-BN) ceramics demonstrate superior resistance to XUV/x-ray radiation damage in a comparison to tungsten-based materials [1]. These results are in close agreement with threshold fluences provided by computer simulations performed with the hybrid simulation code XTANT-3 [3].

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F-16

Opportunities for Early Stage Researchers (ESRs) to Access Research Infrastructures via International Networks

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15.10.2024, Tuesday
18:50 – 19:10

Topic 2
Free Electron Lasers

THIS TALK will outline opportunities for Early Stage Researchers (ESRs), novice applicants, students and entrepreneurial spirits to access research infrastructures at any stage of their career. Spanning from twinning, virtual training, or fast-track access to traineeships, internships, PhD programmes or national networks, newcomers of all ages and experience levels have options to exploit research infrastructures of Europe. A myriad of international, intergovernmental groups support networking and further education, alongside travel funding, especially for users from widening countries like Slovakia, Poland, Hungary or Czech Republic. These projects and networks will be shared. The speaker will also highlight the importance of matchmaking, how to make the first contact with the research infrastructures, or how to be visible in the relevant networks for sustainable career advancement. The session is intended not only for students, but for any scientist looking to start working with Big Science research infrastructures.

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F-17

Focus Characterization I: How to measure Transverse Fluence Distributions in focused X-ray FEL Beams by Ablation Imprints

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16.10.2024, Wednesday
20:30 – 20:50

Topic 2
Free Electron Lasers

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An ccurate and reliable characterization of the fluence distribution [J/cm^2] in the focus of ultra-high intensity laser beam is of great importance in experiments investigating laser-matter interactions, especially with respect to non-linear phenomena. Over the years we have developed a method of ablation imprints that reliably characterizes the fluence distribution in the X-ray laser beam focus. The method is based on laser ablation of a suitable target material at increasing pulse energies ranging from the vicinity of a damage threshold to the maximum achievable pulse energy. Then, beam profile in focus can be reconstructed from the dependence of the ablation imprint size on laser pulse energy. We summarize the instructions on how to perform the measurement and data processing. We also show how the beamline and beam monitors should be made ready for this measurement. In conclusion, we demonstrate advantages and drawbacks of the ablation imprints method on selected results of previous focus characterization experiments.

F-18

Focus Characterization II: AI aided and automated Image Segmentation for focused Beam Analyses

Vojtěch Vozda [1,*], J. Hering [4], J. Kybic [4], T. Burian [1], S. Dziarzhytski [5], V. Hájková [1], J. Chalupský [1], K. Juráňová [1], Š. Jelínek [1,2,3], B. Keitel [5], Z. Kuglerová [1,2], M. Kuhlmann [5], E. Plönjes-Palm [5], B. Petryshak [4], M. Ruiz-Lopez [5], L. Vyšín [1], T. Wodzinski [6], L. Juha [1]

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16.10.2024, Wednesday
20:50 – 21:10

Topic 2
Free Electron Lasers

THE METHOD OF ablation imprints for focused laser beam characterization often requires creating and analyzing many damage patterns. Although the laser beam imprinting can be carried out in tens of minutes, an analysis of imprints usually takes tens of hours to produce final results. Up to several thousands of optical microscope images of ablation imprints must be segmented into parts of imprint and no imprint. This can be done manually, semi-automatically with thresholding and fully automatically with convolutional neural network. We compare the different approaches to image segmentation and show conditions when the analysis can be accelerated. In addition to that, an idea of an AbloCAM project - a universal device for automatic focus characterization – is presented in this talk.

F-19

Focus Characterization III: Tightly focused X-ray FEL Beams: Simulations and Experiment

16.10.2024, Wednesday
21:10 – 21:30

Topic 2
Free Electron Lasers

Šimon Jelínek [1,2,3,*], T. Burian [1], T. Cowan [5], V. Hájková [1], J. Chalupský [1], B. Keitel [4], E. Plönjes-Palm [4], M. Ruiz-Lopez [4], M. Šmíd [5], V. Vozda [1], L. Juha [1]

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PEAK FLUENCE and fluence distribution in a beam focus play a crucial role in interaction experiments observing non-linear phenomena. Full information on the fluence distribution must be known even during the planning phase of the experiment. We can estimate the fluence distribution by using light propagation simulations with Fresnel approximation. This can be done with an ideal beam or with input of beam aberrations revealed by a wavefront sensor which enables us to observe the focus in real time. It is beneficial to check the simulated results with the method of ablation imprints because of its superb resolution and possibility to measure very small foci. The smallest measurable feature in PbI_2 coated CVD diamond target has a typical dimension of 80 nm. A tight focus of 600 nm FWHM was characterized in such experiments. We show how to simulate tightly focused laser beams. We compare these results to those obtained using the ablation imprint method.

DOI: https://doi.org/10.33542/SRU-0350-0

Part III

Synchrotron sources

S-01

Introduction to the Charged Particle Accelerators and their Applications

16.10.2024, Wednesday
8:30 – 9:00

Topic 3
Synchrotron sources

Martin Cesnek [1,*]

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Particle accelerators are indispensable tools in both scientific research and various practical applications, designed to increase the kinetic energy of charged particles such as electrons, protons, and ions. Since the development of early systems like the Van de Graaff generator, these machines have evolved into highly sophisticated devices used across a wide range of fields, from fundamental research to industry.

This lecture delves into the fundamental principles of particle acceleration and provides an overview of the basic types of accelerators, including linear and circular models, classified by their trajectory and underlying acceleration mechanisms. Additionally, it traces the evolution of these accelerators over the years, underscoring their profound contributions to modern science, particularly in areas such as materials science, biology, chemistry, and medicine.

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S-02

Introduction to Synchrotron Radiation

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16.10.2024, Tuesday
09:00 – 10:00

Topic 3
Synchrotron sources

The talk presents the basics of generation of synchrotron radiation as well as its properties (energy spectrum, polarization, time structure, cohererence). The second part of the talk deals with insertion devices (wigglers, undulators), as well as X-ray optics elements (monochromators, lenses, zone plates, etc). In the third part several examples are presented using unique properties of synchrotron radiation, like its coherence (coherent imaging, phase retrieval), energy tunability (absorption spectroscopy methods, anomalous scattering, DAFS, resonant scattering) and unique time structure (pump-probe experiments). If time permits, the talk will be completed by a few examples of our recent results measured at several synchrotron sources

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S-03

Basic Principles of X-ray Detectors

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16.10.2024, Wednesday
10:00 – 10:30

Topic 3
Synchrotron sources

THIS CONTRIBUTION covers the fundamental concepts of X-ray detectors used especially in synchrotron radiation environments. Synchrotron radiation (SR), characterized by its broad energy range and high photon flux, imposes specific requirements on X-ray detectors driving the development of advanced detector technology. A classification of the main families of X-ray detectors will be presented, providing information on their suitability for various SR applications. The core focus will be on semiconductor detectors, which have become essential in SR due to their high energy resolution, high efficiency, compact size, fast response time and versatility. The underlying physical principles governing X-ray detection in semiconductors, including charge carrier generation, charge transport mechanism and signal processing, will be covered. Comparison of different semiconductors and the impact of material properties on detection performance will be discussed with a focus on high-Z materials like GaAs and CdTe particularly suited for high-energy X-ray detection. Spectroscopic characteristics of semiconductor detectors, such as energy resolution, charge collection efficiency, detection efficiency, along with the challenges posed by polarization effects, will be compared across different detector types. Recent advancements in detector technologies (e.g. pixel and hybrid detectors), and the use of novel materials, will be highlighted as key innovations enhancing detector performance. Finally, the issue of radiation damage, which presents a significant challenge in synchrotron environments, will also be addressed, with a focus on how modern detectors are designed to mitigate this problem.

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S-04

Time-resolved Grazing Incidence X-ray Scattering Applied to Energy-related Materials

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16.10.2024, Wednesday
11:00 – 11:45

Topic 3
Synchrotron sources

METAL-HALIDE PEROVSKITES, a promising material for next-generation solar cells, are hindered by challenges such as non-radiative recombination and environmental instability. Real-time insights into the nucleation and growth of these thin perovskite films are crucial for addressing these issues. In-situ grazing-incidence wide-angle X-ray scattering (GIWAXS), combined with in-situ photoluminescence (PL), offers a powerful approach to simultaneously study structural and optoelectronic properties during the growth process. This presentation will review recent advancements in spin-coated, vacuum-deposited, and chemical-vapor-deposited perovskite films, highlighting the valuable insights gained from in-situ GIWAXS-PL studies.

ACKNOWLEDGEMENT This work was supported by the APVV-20-0111 grant.

S-05

Exploring the Microstructure of Additively Manufactured Metals via High Energy X-ray Diffraction

16.10.2024, Wednesday
11:45 – 12:30

Topic 3
Synchrotron sources

Konrad Kosiba [1,*], S. Scudino [1], J. Hufenbach [1], J. Bednarčík [2,3]

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Owing to the layer-by-layer processing, additive manufacturing (AM) of metals is known for the fabrication of near-net shaped components with virtually infinite geometry. This manufacturing principle is reflected in the layer-like microstructure of additively manufactured materials with each layer consisting of solidified melt pools. Extremely, high cooling rates are effective during the solidification, because very small volume units of about 100 µm solidify and this can lead to the formation of metastable phase(s). By depositing subsequent layers, the underlying material, moreover, experiences a short and repetitive heat-treatment. Thereby, alternately tensile and compressive stresses are induced into the deposited material resulting in the formation of macroscopic compressive residual stresses along the building direction. By contrast, residual stresses on a microscale are scarcely explored, especially not via experiments. High-energy diffraction (HE XRD) using a micro-beam exactly allows for such an investigation and is the topic of this talk. Additively manufactured bulk metallic glasses (BMGs) are utilized to explore the microscale residual stresses, because of their lacking long-range order and hence absence of crystals which could eventually distrurb the determination of the microscopoic residual stresses. At first, the formation of bulk metallic glasses and then laser powder bed fusion, which is a widely employed metal AM technology, are introduced. Next, the HE XRD setup used at Deutsches Elektronensynchrotron P21.2 and the extraction of the 2D strain tensor from the recorded 2D patterns are briefly outlined before finally results of strain field maps of LPBF-fabricated BMGs are presented and discussed.

References

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S-06

Research Opportunities at SOLARIS Synchrotron in the Area of Materials for Future

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16.10.2024, Wednesday
14:00 – 14:30

Topic 3
Synchrotron sources

The SOLARIS synchrotron in Krakow is a third-generation light source operating in the medium electron energy range. The first synchrotron light in SOLARIS was observed in 2016, while the first user experiments were performed in 2018. SOLARIS is expanding its activities, developing new beamlines and experimental end-stations as well as providing complementary infrastructure such as cryo-electron microscopes. Research opportunities offered by SOLARIS, the only synchrotron in Central-Eastern Europe, allow for conducting unique scientific projects in fundamental research and applied sciences [1]. It should be emphasized that access to the research infrastructure in SOLARIS is free of charge and provided based on the assessment of the beamtime applications by the international review panel. Financial support to user visits is provided through several schemes, e.g. Horizon Europe projects NEPHEWS and RIANA as well as CERIC-ERIC consortium. We will present the SOLARIS synchrotron project and available infrastructure, provide practical information on access to the infrastructure, and show examples of the research results obtained at the Centre by the Users. A special emphasis will be given to research on quantum materials and materials for sustainable technologies.

Acknowledgement We acknowledge the entire team of SOLARIS Centre and the supporting groups as well as Polish Ministry and Higher Education project: “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” under contract nr 1/SOL/2021/2.

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S-07

Complementarity of the High-Energy X-ray Scattering and Imaging Techniques in Material Science Research (but not only) on I12-JEEP Beamline at Diamond Light Source

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16.10.2024, Wednesday
14:30 – 15:00

Topic 3
Synchrotron sources

IN THIS TALK, I will firstly introduce the high-energy (53 – 145 keV) X-ray experimental station I12-JEEP [1], which is part of the large national synchrotron facility Diamond Light Source (DLS) in Didcot (near Oxford) in the United Kingdom. The I12-JEEP station represents a versatile instrument combining X-ray scattering and imaging techniques used in the structural characterization of metallic and non-metallic materials, chemical products, geological, biological, archaeological, and paleontological samples. The extremely high intensity of synchrotron radiation compared to laboratory X-ray sources allows the realization of in-situ and operando measurements and observations of processes easily with sub-second and millisecond resolution. Secondly, I will describe several selected in situ diffraction, imaging and tomography experiments dedicated to the study of structural changes of different materials (e.g. Ti-, Al-, Ni-based alloys) under loading, heat treatment, mechanical treatment, magnetic field or in-operando during (laser) additive manufacturing processing conditions. In addition, a couple of non-material science related examples will be present to stress the versatility of research achievable on I12-JEEP. Finally, I will make a few remarks about applying for a beamtime at DLS.

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S-08

What is the Finest Details We Can Visualize with X-ray Tomography?

16.10.2024, Wednesday
15:00 – 15:30

Topic 3
Synchrotron sources

Rajmund Mokso [1,*]

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X-RAY MICROSCOPY is a versatile tool to capture the 3D microstructure of a very broad spectrum of materials. Modern X-ray sources with sufficient coherence allow to exploit phase contrast imaging to reconstruct fine details of the microstructure down to several nanometers 3D resolution. In my talk I will reveal the current state-of-the art of phase contrast nano-tomography at the new generation of synchrotron sources and discuss which break-throughs we may expect in the upcoming years.

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S-09

Application of Coherent Scattering at the ESRF EBS - Progress and Challenges

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16.10.2024, Wednesday
16:00 – 16:30

Topic 3
Synchrotron sources

THE FIRST COHERENT SCATTERING with hard X-rays was observed in 1991 [1]. Scattering of coherent X-ray by disordered materials produces characteristic far-field interference pattern called speckles. Speckles encode instantaneous distribution of scatterers in a material. With advent of modern synchrotron sources that provide X-ray beams with high degree of coherence coherent scattering emerged as a powerful tool to study structure and dynamics of disordered materials. Recent upgrade of the ESRF lattice to a new Hybrid Multiple Bend Achromat [2] have improved the coherence of the beam and boosted the coherence scattering techniques [3]. In this talk I will cover the X-ray photon correlation spectroscopy [4] (XPCS) and coherent diffraction imaging [5] (CDI) – two techniques that allow probing dynamics and structure of materials at nano and down to angstrom length scales. It will be demonstrated how new EBS source advances the XPCS in the studies of concentrated protein solutions [6] and of metallic glasses under high pressure [7,8]. Recent progress in CDI will be discussed in particular for investigation of crystallization of $CaCO_3$ microparticles. At the end new challenges and future prospects will be outlined.

ACKNOWLEDGEMENT Beatrice Ruta and Federico Zontone are acknowledged for fruitful collaboration.

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S-10

Azimuthal Integration for Powder Diffraction and Rietveld Refinement

Zdeněk Matěj [1,*]

16.10.2024, Wednesday
16:30 – 17:00

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Topic 3
Synchrotron sources

THE MOST PREVALENT powder diffraction geometry at the accelerator based X-ray sources nowadays is the transmission geometry with a flat area detector positioned in the forward direction. While this experimental setup does not provide the highest angular resolution, it is straightforward to implement. It takes advantage of intensive X-ray diffractions at lower scattering angles and, by utilizing large, fast area detectors, delivers sub-millisecond time resolution with robust signal strength and decent angular resolution.

Rietveld refinement is a widely recognized method for analyzing X-ray and neutron powder diffraction data to determine the crystal structure and micro-structure of crystalline materials. Among the various Rietveld software options, only GSAS II & EXPGUI and MAUD offer an "all in one solution," including Rietveld refinement, detector calibration, and azimuthal integration (AZINT). Other software, such as FullProf, TOPAS, Jana2020 or MStruct, require pre-integrated data. However, as AZINT auto-processing becomes more common and its reliability is improving at light source facilities, AZINT data can also be imported into these programs. This contribution describes the common geometrical notation and physical corrections for flat detector data, including polarization, solid angle, sample, and air-absorption corrections. Detector corrections, such as the parallax effect and the finite thickness of the detector sensor, are also briefly discussed. Numerous specialized software options for AZINT are available, including fit2d, PyFAI [1], diffpy.srxplanar [2], Nika, and the AZINT-module [3]. These tools offer various parameters and options, such as detector calibration, intensity corrections, pixel-splitting, normalization, error modeling, and correlation between neighboring powder pattern bins [2]. The contribution focuses on the interoperability of the AZINT and Rietveld software with emphasis on the correct interpretation of AZINT-reduced data in Rietveld software analysis, highlighting common issues and potential critical mistakes.

References

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S-11

From Molecular Dynamics Simulations to Diffuse Scattering Maps

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16.10.2024, Wednesday
17:00 – 17:30

Topic 3
Synchrotron sources

Modern materials often exhibit a considerable portion of structural disorder, playing a key role in their functionalities. In order to characterize local atomic arrangements and short-range correlations one has to study the shape of Bragg lines and the distribution of diffuse scattering below and between them. To extract information from experimental data one has to compare model-based intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices by a variety of approaches ranging from *ab-initio* DFT methods via molecular dynamics (MD) to phase-field models based on the Landau formalism. Alternatively, one may retrieve the displacement pattern without making assumptions on its origin by reverse Monte-Carlo (RMC) modelling [1]. The focus of this year's lecture will shift from algorithms for efficient calculation of the total and energy-resolved scattering cross-sections [2] to strategies in atomic-scale modelling of crystalline systems. Emphasis will be put on the complementarity between *ab-initio* techniques (DFT) and molecular dynamics (MD), combining the predictive power of DFT for the interaction potentials and the ability of MD to handle large size boxes of 10^5-10^6 atoms with realistic representation of atomic motion and lattice distortions. The key features will be illustrated by experimental results and simulations on the popular ferroelectric compound barium titanate ($BaTiO_3$) [3-6].

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S-12

ASTRA Beamline at SOLARIS: XAS in the Tender and Hard X-ray Range

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16.10.2024, Wednesday
18:00 – 18:20

Topic 3
Synchrotron sources

ASTRA is a bending magnet beamline for X-ray absorption spectroscopy (XAS) at the 1.5 GeV SOLARIS synchrotron in Krakow (Poland). The beamline was built as a interantional cooperation of SOLARIS with Hochschule Niederrhein University of Applied Sciences (Germany), the Physics Institute of Bonn University (Germany) and the Synchrotron Light Research Institute (Thailand). ASTRA is a compact and user friendly beamline without mirrors and without - in this case unnecessary - radiation safety hutches. With no windows down to the exit flange of the vacuum double crystal mochochromator, the beamline was specifically designed as a 'work horse' for XANES/EXAFS measurements at 1-15 keV, including the tender and part of the hardenergy range of X-rays. Therefore, measurements at the K absorption edges of important 'low Z' elements such as K, Ca, Cl, S, P, Si, Al and Mg are feasible. Besides, ASTRA's energy range also includes K-edges of heavier elements up to Se, L-edges of elements up to Bi and some M edges of elements including U, which allows investigation of a variety of highly application relevant materials. XAS can be applied to both crystalline and amorphous materials, liquids and samples in the gas phase, at ASTRA either in transmission or fluorescence mode, i.e. spectra of samples in any state of matter with high and very low concentration of elements of interest can be recorded. Furthermore, spectra of functional materials in dynamic sample environments (in situ and operando) can be acquired (besides catalytic studies e.g. structural investigations of anode/cathode material during (dis)charge of batteries). The beamline is equiped with an X-ray camera, facilitating appropriate sample positioning for XAS with higher data quality and more reliable results. The measurements are controlled by the specialized program AstraLibra with a user friendly interface and advanced functionalities. As the most recent development it is worth to mention that Raman spectrometer and microscope was installed to the beamline. It enables obtaining complementary information to XAS simultanously.

Acknowledgement The further development of the ASTRA beamline for measuring at low photon energies and installation of the spectrometer for high energy resolution fluorescence detection was supported within the EU Horizon2020 programme (952148-Sylinda).

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S-13

The Revealing of Ni2Fe-OH Layered Double Hydroxide Magnetic Characterization using the powerful XAS/XMCD Methods

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16.10.2024, Wednesday
18:20 – 18:40

Topic 3
Synchrotron sources

The transition-metal complexes are of the great interest due to their variety of unique phenomena associated to the electron configuration changing. The Ni_2Fe-OH layered double hydroxide (LDH) material constituted of mixed divalent and trivalent metal hydroxide layers with anionic species between them is in the focus of our study. The cation size and the content, ratio and ordering, as well as the interlayer distance of intercalated magnetic ions, essentially effect on electric and magnetic properties to be varied [1]. From the previous study with magnetometer methods, in contrast to Ni_3Fe LDH with different cation ratio, it turned out that Ni_2Fe demonstrates several intriguing magnetic behaviors over a wide temperature range: cluster spin glass, long-range order, and coexistence of two magnetic phases at low temperatures. To unravel unexplored magnetic properties of materials at sub-electron scale, the one of the most powerful and available options called the X-ray Magneto-Optical Spectroscopy XMCD method [2] can be used. This technique is very sensitive to chemical and orbital selectivity, what is the crucial advantage. It allows to probe the magnetic moment of one specific atom, and the specific shells for which the magnetic orbital and magnetic spin moments can be measured qualitatively and quantitatively independent. The spectral analysis allows one to extract the Hamiltonian parameters using the so-called sum-rules and simulation methods, especially for complex signals, while the oxidation states variation is seen directly from the measured spectra.

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S-14

TEM and Synchrotron Study of Precipitates in Al-based Alloys

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16.10.2024, Wednesday
18:40 – 19:00

Topic 3
Synchrotron sources

In this study, a combination of Transmission Electron Microscopy (TEM) and synchrotron radiation was used to analyse the structure of Al-based alloys after various heat treatment processing. Analysis of synchrotron diffraction data showed that the Al matrix structures exhibited only spherical precipitates of the $Al_{12}(Fe,Mn)_3Si$ phase with a diameter of approximately 100 nm. It is well known that these precipitates do not contribute to the strengthening of the alloy. However, mechanical testing demonstrated significant differences between the ultimate strengths of the annealed samples. Unlike the synchrotron data, TEM observations in reciprocal space revealed additional fine precipitates, indicated by typical streaks in the diffraction patterns. These streaks arise from Laue condition relaxation phenomena. After setting of specific diffraction conditions, rod-shaped precipitates of the Mg_5Si_6 phase, with a diameter of 3 nm, were also identified and documented in imaging mode. These precipitates were coherent with the Al matrix and responsible for alloy strengthening.

The goal of this contribution is to briefly emphasize the complementary nature of TEM and synchrotron methods. The importance of combining data from both methods for a comprehensive structural analysis is underscored. On the other hand, while both rely on diffraction phenomena, they can sometimes yield different results due to the distinct ways in which electrons and photons interact with matter. This point is further concisely highlighted by the clear differences in information gain obtained from each method.

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Part IV

Neutron sources

N-01

The Institut Laue Langevin: a World-leading Neutron Facility for the Next Decade of Science and Innovation

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17.10.2024, Thursday
8:30 – 9:15

Topic 4
Neutrons sources

NEUTRONS are a unique and ubiquitous probe of matter, materials and processes that deliver cutting-edge, impactful science and innovation. ILL has just completed a a major upgrade programme, Endurance, which spanned the period 2016 – 2024 with a budget of more than 50 M€. About 30 projects have been delivered including neutron guide systems, new and upgraded instruments, sample environment and scientific data and software services. Endurance as a whole ensures that research capability at ILL will continue to be world leading for the next decade, offering new opportunities and perspectives for excellent science, both for academia and industry. The ILL and its Endurance programme will be presented along with examples of new science that highlight how improved instrument performance enables new research opportunities.

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N-02

Neutrons for Structural Biology at ILL

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17.10.2024, Thursday
9:15 – 9:45

Topic 4
Neutron sources

THE INSTITUTE LAUE-LANGEVIN (ILL) is a European research facility that provides the world's most intense, continuous neutron beams, particularly for low-energy neutrons used to study the structure and dynamics of macromolecular complexes. Small-angle neutron scattering (SANS) enables the study of the structure of macromolecules and their complexes in solution at low resolution. Neutron reflectometry (NR) focuses on interactions between biological species, such as proteins or viruses, and lipid bilayers that mimic biomembranes. In contrast, high-resolution neutron macromolecular crystallography (NMX) offers detailed insights into hydrogen bonding networks and surrounding water distribution, both of which play crucial roles in enzyme mechanisms and ligand binding.

Significant new capabilities are being developed for structural biology at ILL, including upgrades to the instruments and services for sample preparation (such as crystal growth, perdeuteration of proteins, and natural lipids), as well as flexible beam time adapted to the needs of the biology community.

Although neutrons are not the most widely used analytical probe in this field, they provide unique and complementary insights due to their sensitivity to light atoms (particularly hydrogen) and the ability to vary contrast by hydrogen-deuterium substitution. In this presentation, I will provide an overview of the new developments at ILL and illustrate their application in structural biology with recent examples from selected instruments.

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N-03

Applications of Pulsed Reactor Neutrons

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17.10.2024, Thursday
9:45 – 10:30

Topic 4
Neutron sources

SCIENTIFIC RESEARCH in general and condensed matter studies in particular have always benefited from the development of large-scale scientific infrastructures. Starting with the first X-ray tubes – coincidently around the same time as Alzheimer's disease was identified – and all the way to modern synchrotron radiation sources, neutron sources, and powerful lasers, research approaches based on nuclear physics have been playing a significant role in the investigations of both hard and soft condensed matter. The peculiar properties of neutrons, power of synchrotrons, innovations in optical spectroscopy, including Raman, have their own niche in studies of the chemical composition and structure of condensed matter that possesses a high level of order or disorder – order that is the most important property of structure and disorder that is believed to be one of the foundations of life.

The legacy of the Frank Laboratory of Neutron Physics (FLNP) of the International Intergovernmental Organization – Joint Institute for Nuclear Research (JINR) lays for more than half a century in applying the results of nuclear physics using the pulsed reactors in particular, for materials and life science research. Our researchers and their collaborators use neutron scattering and complementary methods for aiding a design of new materials and advancing existing materials to fulfil the needs of state-of-the-art applications. The advances achieved over past decades developed to an extent that our scientists employ diffraction approaches to successfully characterize the physical properties of a wide range of materials that assemble a base for further advancements. The presentation will show examples where unique material properties have been easily studied with neutrons, while the unique nature of neutrons has allowed to look inside non-transparent composites or revealed invisible magnetic structures. Particularly interesting illustrations will document how neutrons grant to determine the distribution of water or hydrogen-rich components. The latter permits one to study not only hard condensed matter, but also the soft matter, biomaterials and life science applications in general. This will be presented in the context of structural studies of lipid membranes and their changes due to the environmental and compositional changes related to various functions as well as disfunctions. Our observations based on the neutron scattering experiments keep proving to be important even for studies on amyloid toxicity and the molecular mechanism of Alzheimer diseases, to mention but one last example.

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N-04

Exogenous Lung Surfactant for Drugs Delivery: A View through Scattering Techniques

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17.10.2024, Thursday
11:00 – 11:30

Topic 4
Neutron sources

Lung surfactant (LS) is a lipoprotein film lining the alveoli of the lung that reduces the surface tension at the air-liquid interface. LS is composed of lipids (90 wt.%) and specific surfactant - associated proteins (10 wt.%). The absence of LS due to prematurity, or its damage, is treated with exogenous LS in neonatal medicine, and promising results are also obtained in ventilated Covid-19 patients. Curosurf (Cur), an extract of porcine lung tissue, is clinically used as a replacement surfactant. Structurally, Cur is a mixture of uni-, oligo-, and multilamellar vesicles. The use of an exogenous LS to deliver other relevant drugs to the lungs is a promising strategy for combined therapy. Combining techniques of small-angle X-ray and neutron scattering (SAXS and SANS) we investigated structural changes of exogenous LS (Cur) induced by selected drugs: N-acetylcysteine with anti-inflammatory and antioxidant properties, polymyxin B (PxB) peptide antibiotics [1] mainly used to treat infections by resistant Gram-negative bacteria, and a corticosteroid budesonide [2]. In lung infection, the bacterial endotoxin, lipopolysaccharide (LPS), interferes with LS and alters its structure and function [3]. Small- angle neutron diffraction (SAND) on the stacks of aligned bilayers of LS model system free of proteins deposited on a silicon wafer and hydrated in vapor allowed unraveling the effect of both, LPS and PxB on the lipid bilayer thickness. Our structural findings accurately reflect the situation with a native lung surfactant, as confirmed by a recent in vivo study [4].

Acknowledgement SAXS experiments were performed at BL11-NCD beamline at Alba Synchrotron with the collaboration of Alba staff. SANS experiments were performed at PAXY instrument of LLB CEA Saclay; SAND at D16 spectrometer of ILL, Grenoble. Experiments were supported by projects APVV-17-0250 and VEGA 1/0305/24.

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N-05

Budapest Neutron Centre - Science at a Medium Size Reactor with Examples on Structural Studies of Ionic Liquids

17.10.2024, Thursday
11:30 – 12:00

Topic 4
Neutron sources

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The lecture gives an overview of the research with neutrons at the Budapest Neutron Centre, describing the most popular techniques and instruments for neutron scattering, imaging and elemental analysis with neutrons. Examples of applications of neutron scattering methods in various fields of materials science and cultural heritage science, carried out at BNC, are briefly presented.

The second part of the talk describes current results on application of small angle neutron and X-ray scattering for better understanding the mixing behavior and structural features of aqueous and non-aqueous solutions of ionic liquids.

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N-06

Neutron Scattering in the Czech Republic from Intermetallics to Oxides

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18.10.2024, Friday
8:30 – 9:15

Topic 4
Neutron sources

The lecture focuses on the development of the Czech neutron community, involvement in national and international neutron infrastructures, and traditional and new topics studied by Czech scientists using neutron scattering. Several examples of neutron scattering studies will be included, focusing mostly on nuclear and magnetic structures and magnetic excitations in intermetallics and oxide materials.

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N-07

Vibrational Properties and Mass Transport in Thermoelectric Materials studied by Neutron Spectroscopy

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18.10.2024, Friday
9:15 – 10:00

Topic 4
Neutron sources

THERMOELECTRIC MATERIALS (TEM)s are widely known for their application in Peltier elements for cooling purposes of high-performance electronics and in power generators converting excess and waste heat into electricity. The later application is believed to form an important contribution to future global energy supply as a green energy source. Today, it is an indispensable part of spacecrafts operated by NASA and ESA, such as for the Voyager, Cassini-Huygens and recent Mars missions, to name a few.

The performance of a compound as a TEM is determined by its electronic and heat transport properties. Whereby, the electronic properties of a TEM should correspond to those of a semiconductor and the heat transport should be as low as possible in order to achieve optimum performance. Therefore, a lot of effort is put into reducing the heat transport through lattice vibrations leaving the electronic contribution unaffected.

There exist some basic strategies to achieve this goal which all target a reduction of the TEM's sound velocity and of the lifetime of its heat carrying acoustic phonons. Apart from their obviously successful functioning, the mechanisms behind the impaired thermal transport need to be investigated and understood on a microscopic scale.

We will present strategies for tailoring materials for optimal TEM performance, discuss their effects on the physical properties of the materials, and introduce neutron scattering techniques that are best suited for their experimental study. Inelastic neutron scattering, e.g. time-of-flight and three-axis techniques, is particularly suitable for investigating the vibrational dynamics in solids on microscopic scales, as the energies of neutrons with wavelengths of the order of atomic distances ($\sim$Å) correspond to the energies of lattice vibrations (meV). This enables excellent resolution in momentum and energy for the study of heat carrying phonons. Specialized neutron spectrometers such as backscattering and spin-echo instruments achieve resolutions high enough ($\sim \mu$eV) to follow relaxation processes like mass diffusion and the lifetime of vibrational excitations.

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N-08

Representation Analysis of Magnetic Structures: Theory and Practice

18.10.2024, Friday
10:00 – 10:30

Topic 4
Neutron sources

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Representation analysis of magnetic structures is a powerful method applied to predict all possible orderings of magnetic moment in crystalline compounds defined by a magnetic wave-vector k. It derives from the mathematical theory of group representations and developed from the pioneering work of Bertaut [1]. By using character tables and through representation analysis it is possible to calculate all the possible sets of configurations of the magnetic moments allowed by the symmetry properties of the crystal structure hosting the magnetic atom and identify the possible magnetic space groups. The method is therefore based on the fact that some of the symmetry properties of the crystallographic structure are maintained in the magnetic ordering. In particular, all the symmetry elements of the crystallographic space group G_0 that leave k invariant constitute the little group G_k. Hence, the representations describe the symmetry properties of a magnetic moment under all the symmetry operations forming the little group G_k.

In summary, the outline of my presentation will include a brief theoretical introduction to this method, practical examples of how to apply it, illustrations of software resources and selected representative cases.

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N-09

Disentangling Anisotropy Contributions in Mn-mixed Ferrite Nanoparticles

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18.10.2024, Friday
11:00 – 11:20

Topic 4
Neutron sources

Tailoring magnetic nanoparticles (NPs) by choosing a suitable combination of size, shape, and material is the basis for realizing various technological (data storage, spintronics) [1], biomedical (magnetic hyperthermia, drug delivery) [2], or environmental applications. The macroscopic physical properties of magnetic NPs rely on magnetic anisotropy, and their understanding is fundamental to the design of magnetic materials for different applications. Nevertheless, magnetic anisotropy is influenced by the shape, crystal structure, surface effects, and interactions. To gain a comprehensive understanding of these properties, it is essential to investigate all the factors contributing to the total effective magnetic anisotropy. Conventional magnetic measurements like DC magnetization and AC susceptibility provide an overview of the macroscopic physical properties but do not reveal the detailed microscopic phenomena that drive these properties. This is where small-angle polarized neutron scattering (SANSPOL) comes into play, offering sub-atomic resolution and serving as a powerful tool for studying surface anisotropy[3] and microscopic phenomena. In this contribution, we will show the impact of the Mn-doping level in cobalt ferrite NPs (10 nm) on their magnetic properties. Nevertheless, the macroscopic magnetic responses of the Mn-mixed cobalt ferrite NPs were inconclusive and inconsistent with changing Mn content. However, we will demonstrate the versatility of SANSPOL and disentangle all anisotropy contributions of the total magnetic anisotropy of a series of Mn-mixed Cobalt ferrite NPs with different Mn content but the same shape, size, and surfactant and correlate it with their macroscopic response[4]. Ultimately, our work aims to clarify the complicated picture of magnetic anisotropy and offer insights into the design of magnetic materials.

Acknowledgement The authors thank ISIS Neutron and Muon Source for the provision of the beamtime (RB22206201). The authors acknowledge the assistance provided by the Advanced Multiscale Materials for Key Enabling Technologies project, supported by the Ministry of Education, Youth, and Sports of the Czech Republic. Project No. CZ.02.01.01/00/22_008/0004558, co-funded by the EU. DZ has been supported by Charles University Project No. UNCE/24/SCI/010, and MG by the Grant Agency of Charles University: GAUK 267323.

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N-10

Interaction of Magnetic Nanocarriers with Cell Membranes

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18.10.2024, Friday
11:20 – 11:40

Topic 4
Neutron sources

The interactions between cell membranes and smart magnetic nanoparticles (NPs) have been investigated by means of several complementary methods. Both native cell cultures and model lipid membranes have been exposed to the core@shell NPs that consist of magnetic Fe_3O_4 core ($D_{XRD} \sim 9$ nm) and thick shell of mesoporous silica ($t_{SEM} \sim 10$ nm). Neutron reflectometry and quartz crystal microbalance experiments have shown that supported lipid bilayers of DMPC (Dimyristoylphosphatidylcholine) have been untouched by the action of the NPs even after application of external magnetic field. The conclusions have been reconfirmed by the data obtained from in-vitro experiments employing native cell cultures, where confocal microscopy evidenced the NPs outside of the cell body with no significant cell membrane damage. The results are encouraging with respect to the biomedical application potential of the prepared NPs. Our NPs can be delivered to the place of action by external magnetic field and drugs accommodated in the pores of the NPs can be released upon stimuli. This mechanism may facilitate faster and more efficient treatment of diseases along with easy metabolization of the NPs from the intercellular space.

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N-11

Structural Investigations of Disordered Systems using Total Neutron Scattering

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18.10.2024, Friday
11:40 – 12:00

Topic 4
Neutron sources

Total neutron scattering has been traditionally employed to explore local ordering in liquids, utilizing diffuse scattering to develop molecular models, particularly Monte Carlo-style simulations, guided by experimental data. In recent years, there has been a surge in studies examining more complex systems, such as nano-confined fluids—fluids restricted within geometries like the pores of porous materials.

Mesoporous silica, MCM-41, for instance, has gained attention as a versatile material for various applications: drug delivery systems for ibuprofen, sustainable ethane separation from natural gas, and heterogeneous catalysis in benzene hydrogenation. In these systems, fluid-interface interactions are crucial, with the fluid molecules often filling the pores completely.

Interestingly, nano-confined fluids exhibit distinct macroscopic behaviours compared to their bulk counterparts. For instance, benzene's molecular mobility is significantly suppressed when confined within MCM-41. Moreover, some studies highlight the microphase separation phenomenon when miscible liquids like tert-butyl alcohol and toluene are confined. These macroscopic differences stem from molecular-level interactions, which total neutron scattering is uniquely equipped to probe. In this talk, I will present how wide Q-range total neutron scattering (0.01 to 50 $Å^{-1}$), as conducted at the NIMROD instrument at the ISIS Neutron and Muon Source, has revealed structural details of confined hydrocarbons such as benzene-d6, cyclohexane-d12, and cyclohexene-d10 in MCM-41. I will also touch upon studies of gases (e.g., oxygen, nitrogen, deuterium) in MCM-41, the structure of confined water, and the arrangement of molecules during reactions on Pt-doped MCM-41. The talk will include a brief introduction to total neutron scattering and highlight key findings from these studies, along with their broader implications.

Acknowledgement The author acknowledges ISIS Neutron and Muon Source for the provision of beamtime.

N-12

Small-Angle Scattering and Neutron Reflectometry Methods in the Study of Magnetic Nanoparticles in Magnetic Fluids and their Composites

Peter Kopčanský [1,*], K. Siposova [1], M. Karpets [1], M. Rajnak [1], M. Molcan [1], M. Timko [1], V. Lackova [1], N. Tomasovicova [1], L. Balejcikova [2], I. Safarik [3], V.I. Petrenko [4,5]

18.10.2024, Friday
12:00 – 12:20

Topic 4
Neutron sources

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The possibility of using neutron and X-ray scattering methods for structural investigations at the nanoscale will be discussed in detail, drawing on our extensive experience over the last 10 years. Namely, results from neutron reflectometry (NR) [1] and small-angle neutron scattering (SANS) for nanoscale characterization of magnetic nanoparticles (MNPs) in bulk and at interfaces will be presented. The structural analysis of various types of magnetic fluids (MFs), MNPs with bio-macromolecules (including magnetoferritin, amyloids, and magnetosomes), textile-based nanocomposites [2] with MNPs, and ferronematics (composite systems of liquid crystal (LC) with MNPs) will be described in detail during the presentation. Additionally, the interaction characteristics between surfactant/polymer molecules used in the stabilization of MFs were investigated, which is crucial for understanding the synthesis procedures of highly stable MFs with controllable properties. The effect of external magnetic and electric fields on the behavior of MNPs will also be presented based on neutron scattering data. Neutron and X-ray scattering methods have been used to study the clustering of MNPs in an LC matrix, particularly regarding the alignment of MNPs in different phases of LC [3]. The structure of all studied systems will be modelled according of neutron and X-ray data using appropriate methods and presented.

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Part V

Poster presentations

P-01

The Universal Anomalous Behaviour of As-S Glasses

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17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

The low temperature properties of the disordered solids differ from their crystalline counterparts. Single-crystals are characterized by cubic temperature dependence C_p, $k(T) \propto T^3$, in agreement with Debye's prediction for the specific heat and thermal conductivity at the lowest temperatures, respectively. The glasses are characterized by linear $C_p \propto T$ and square $k(T) \propto T^2$ temperature dependences below 1 K. These two features were successfully described by the tunnelling model (TM) [1], assuming that a group of atoms changes its conformation due to quantum mechanical tunnelling. The TM model successfully described the temperature dependence, but the question of what constitutes the tunnelling entities is still open. We recently discovered using DFT simulation, Raman spectroscopy, thermal conductivity and, specifically, that in As-S systems, the tunnelling entities can be larger ring-like and branchy-like nanoclusters [2,3]. The other anomalies in glasses are most significant at higher temperatures (2 K < T < 20 K) as an excess over the Debye continuum in the temperature dependence of C_p/T^3 called the boson peak. At the same temperature area, there is another anomaly in thermal conductivity manifested as a constant value, $k(T)$ plateau. Our recent analysis of $k(T)$ [3] based on the unique combination of the Soft Potential model (SPM) [4] and nanocluster approximation [3] shows that a ring-like S8 and other ring-like structures can be essential for the $k(T)$ plateau creation in the As_xS_{100-x}. The recent numerical simulations support our assumptions that chain-like and ring-like structures can be responsible for Boson peak creation [5].

Acknowledgement This work was supported by the Slovak Research and Development Agency Projects numbers APVV-18-0197, APVV-SK-BY-RD-19-0008, APVV-20-0324, APVV-22-0172.

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P-02

Evidence of Field-induced Berezinskii–Kosterlitz–Thouless Transition in Quasi-Two-Dimensional S = 1/2 Antiferromagnet Cu[C6H2(COO)4][C2H5NH3]2

Illia Kozin [1,*], R. Tarasenko [1], A. Orendáčová [1], E. Čižmár [1], R. Tarasenko [1], P. Danylchenko [1], V. Tkáč [1], M. Orendáč [3]

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17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

A METAL-ORGANIC compound $Cu[C_6H_2(COO)_4][C_2H_5NH_3]_2$ was previously identified as a quasi-2D spin $S = 1/2$ quantum antiferromagnet by means of susceptibility, magnetization and heat capacity measurements. An anisotropic exchange interaction was reported with a dominant intraplane coupling $J_1/k_B \approx 10$ K, forming a rectangular lattice characterized by anisotropy parameter $R = 0.4$. Prior investigation revealed no magnetic ordering down to 1.8 K [1].

Our study extended the former heat capacity research down to the lowest temperature 0.4 K in magnetic fields up to 9 T. A powder sample, in a form of a pressed pellet, was measured using a Physical Property Measurement System (PPMS) device equipped with ^{3}He insert. Again, no magnetic phase transition was evident down to the lowest temperature without an external magnetic field. However, round maxima in heat capacity shifted to lower temperatures in the presence of the magnetic field, attributing to the presence of a magnetic phase transition. Consequently, a magnetic phase diagram was constructed based on these in-field peaks, which showed reasonable agreement with Quantum Monte Carlo (QMC) simulations for the Berezinskii-Kosterlitz-Thouless (BKT) transition in a spin $S = 1/2$ Heisenberg antiferromagnet on an isotropic square lattice. Supplementary analysis of magnetic entropy released near the BKT transition confirmed the correspondence of the experimental data with theory, though, minor deviations from theoretical predictions were found, likely due to interlayer interactions.

ACKNOWLEDGEMENT The work was supported by the projects APVV-22-0172 and VEGA 1/0132/22.

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P-03

17.10.2024, *Thursday*
18:00 – 19:00

Topic 5
Miscellaneous

Sol-Gel Polyacrylamide Route: Optimization for Nanomaterials Preparation

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The purpose of this work was the optimization of the popular sol-gel polyacrylamide route synthesis method to produce LaMnO3 nanoparticles and its later application to the wider $REMnO_3$ (RE = Nd, Sm, Eu, Gd, Tb) and $Nd_{1-x}B_xMnO_3$ (B = Ca, Sr, Ba) systems. Additional task was to investigate structural and morphological properties of all samples.

Perovskite oxide structure materials (general formula - ABO_3, where A and B - cations of different radii) were selected due to their unique properties such as colossal magnetoresistance, tunable magnetic properties and narrow band gap (1.0 eV for $LaMnO_3$), which makes them excellent candidates for photocatalytic and photovoltaic applications. By procuring small, spherically shaped nanoparticles, it is possible to increase the surface area, which could potentially lead to increase of photocatalytic efficiency. Furthermore, though these materials are usually antiferromagnetic (AFM), by doping with bivalent cations, the magnetic properties can be changed to ferromagnetic (FM) due to the emerging superexchange interaction between Mn^{3+}-Mn^{4+} sites. The sol-gel polyacrylamide route was chosen due to capability to quite easily and without any expensive equipment obtain high purity nanoparticles with quite a narrow particle size distribution (in $LaMnO_3$ case - 10-40 nm interval), because of the construction of a polymeric carcass with tunable density. We investigated the relation between various synthesis parameters (monomer – linking agent ratio, choice of chelating agent, duration and temperature of annealing and glucose content) and phase purity as well as particle size of the obtained samples.

After optimization for the $LaMnO_3$ perovskite, the same synthesis parameters were applied directly to other $REMnO_3$ systems. After miniscule tinkering (changing the annealing temperature based on phase formation temperature), we were able to produce single phase materials in most cases. $NdMnO_3$ system was selected for solid solution preparation, due to low phase formation temperature and promising stability. Rietveld analysis was performed to determine the change in lattice parameters after incorporation of various amounts of bivalent cation (in the Ca, Sr cases from 0 to 100% and in Ba case 0 to 50% in 10 mol% increments.) Characterization techniques, like X-ray diffraction, Raman and FT-IR spectroscopies were used for polymer degradation assessment and structural investigation. Moreover, magnetometer measurements at low and room temperature were applied for magnetic property assessment and SEM for morphological analysis.

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P-04

XUV/X-ray Laser-induced Damage to Lead Iodide: Pulse Duration and Wavelength Effects

Alžběta Horynová [1,2,*], V. Hájková [1], Š. Jelínek [1,3,4], J. Chalupský [1], V. Vozda [1], L. Vyšín [1], J. Bulička [1,2], T. Burian [1], R. Dudžák [1,3], M. Krupka [1,2,3], Z. Kuglerová [1,4], J. Krása [1], M. Šmíd [5], N. Medvedev [1,3], L. Fekete [1], L. Juha [1,‡]

17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

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Lead iodide, a wide band gap semiconductor with a layered crystalline structure, is a material exhibiting interesting and useful behavior when exposed to either ionizing or non-ionizing radiation. Numerous related applications of lead iodide and its derivatives have been reported, including photography and radiography, detection of ionizing radiation, photovoltaics (solar cells), or imprinting of laser beams. The radiation-chemical study of lead iodide and derived materials also offers deeper insight into the general mechanisms of radiation damage in complex solids. As a heavy, high-Z material, lead iodide has been proven to be an optimal medium for ablation imprinting of focused X-ray free-electron laser (FEL) beams, see for example [1,2] and references cited therein. From damage patterns, physicists extract information on the beam and its interaction parameters (e.g., transverse distribution of fluence, focal spot size, pulse energy and peak fluence) [2] while chemists are interested in mechanisms of X-ray-laser induced decomposition reactions and phase transitions occurring in the irradiated material. At the extremely high dose rates typical for such sources, a key question arises whether the damage process is either thermal or non-thermal. Special attention should be paid to a possible interplay of thermal and non-thermal effects. In this contribution, results obtained for PbI_2 with focused beams of X-ray FELs and XUV capillary-discharge lasers are presented with attention to the role of photon energies and pulse durations. Experimental results are compared to computer simulations carried out by means of the hybrid code XTANT-3 (X-ray-induced Thermal and Nonthermal Transitions in matter) [3].

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P-05

The Effect of Budesonide on the Thickness of the Lipid Bilayer in the Model System of Pulmonary Surfactant

Rastislav Korfanta [1,*], N. Kučerka [1], B. Demé [2], D. Uhríková [1]

17.10.2024, Thursday
18:00 – 19:00

Topic 5
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PULMONARY SURFACTANT (PS) is a complex of lipids (∼ 90 wt.%) and proteins (∼10 wt.%) that are produced and secreted by the respiratory epithelium of the lungs. PS minimizes surface tension at the air-liquid interface of the alveolar space, which reduces the work of breathing. Thus, PS is responsible for gas exchange in the alveolar space and its damage or deficiency can cause respiratory distress syndrome (RDS). The condition is treated with the administration of exogenous pulmonary surfactant (EPS) obtained from animals, such as porcine Curosurf®. Due to the ecological and economic cost, the development of synthetic EPS is of urgent need. Recent approaches discuss the possibilities of combined therapy employing EPS as a drug delivery vehicle. Budesonide (BUD) is a non-halogenated corticosteroid with a broad anti-inflammatory effect on different types of cells. The combination of EPS and BUD was reported as an effective therapy for pulmonary inflammation and oxidative modifications resulting from RDS. Our SAXS/WAXS experiments on BUD/EPS have shown that BUD does not affect the lamellar packing of EPS; however, its effect on the lipid bilayer was less apparent [1].

We performed a small-angle neutron diffraction (SAND) experiment to determine the impact of BUD on the lipid bilayer. A PS model system composed of diC16:0PC/16:0-18:1PC/16:0-18:2PC/16:0-18:1PG = 50:24:16:10 wt.% mimics well Curosurf® concerning lung functions in an animal model [2]. Oriented lipid bilayers were hydrated from vapor at 97% RH. Four different D_2O/H_2O mixtures (100%, 70%, 40%, 8%) were used to vary the contrast between the lipid bilayer and water. The reconstructed NSLD profiles then give the thickness of the lipid bilayer, the water distribution profile, and the width of the bilayer–water interface [3]. The results obtained indicate non-linear changes in the thickness of the lipid bilayer with an increasing content of BUD.

ACKNOWLEDGEMENT SAND experiments were performed at the D16 spectrometer at ILL, Grenoble. Experiments were supported by project VEGA 1/0305/24.

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P-06

Textile/Iron Oxide Nanozyme Composites: Preparation, SANS/-SAXS Characterization, Modelling of Structural Arrangements and Environmental Technology Applications

Ivo Safarik [1,2,3,*], J. Prochazkova [2], M. Schroer [4], V.M. Garamus [5], M. Timko [1], M. Molcan [1], M. Rajnak [1], V.I. Petrenko [6,7], K. Zelena Pospiskova [3], P. Kopcansky [1]

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18:00 – 19:00

Topic 5
Miscellaneous

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Magnetic iron oxide nano- and microparticles (MPs) have a great potential in biochemical, biomedical, clinical, biotechnology and environmental applications. In the year 2007 the presence of intrinsic peroxidase-like activity similar to horseradish peroxidase was described; the term "nanozyme" was introduced to define nanomaterials with enzyme-like activities. Immobilization of (bio)catalysts to a solid carrier enables their simple separation from the reaction mixture and repeated application. Textile materials represent low-cost carriers applicable for immobilization of wide variety of molecules or particles. Cotton textile was modified by direct application of acid magnetic fluid or by microwave synthesized magnetic particles. Peroxidase-like activity of textile bound iron oxides enabled decolorization of selected organic dyes such as crystal violet. Cotton textile and cotton textile with MPs were measured by SANS and SAXS. Due to the different behavior of the experimental SANS curves for various samples by means of appropriate modelling it was concluded that addition of nanoparticles to textile changes the structural organization at nanoscale. At SANS curves two power laws regions could be seen which points out that there are two kinds of scattering objects in the samples. At intermediate q-region power-law behavior of scattering intensity close to -1 corresponds well to cylinder-like objects while in small q-region power exponent is -2.7 or -3.4 depending on the sample [1]. SANS and SAXS data give similar results about structural organization of textile and (nano)-particles. Sketch of the different behavior of MPs was proposed according to the analysis of SAS curves [1].

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References

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P-07

Different Ceramide Structures and their Effect on the Skin Barrier Model

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17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

The skin barrier is essential for human survival on dry land, it is located in the uppermost layer of the skin, in the stratum corneum (SC). SC consists of corneocytes that are surrounded by an oligolamellar lipid matrix. The main components of the SC lipids are ceramides (Cer), free fatty acids (FFA), and cholesterol (Chol). These lipids prevent excessive water loss from the body and the entry of undesired substances from the external environment into the body. Cer belong to the group of sphingolipids. By this time, 15 subclasses of Cer had been discovered. They are divided according to whether they contain sphingosine (S), dihydrosphingosine (dS), which is typical for eukaryotic cells, phytosphingosine (P), or 6-dihydrosphingosine (H) specific to the epidermis [1].

The aim of this work was to prepare simple model membranes containing a mixture of Cer (NS, NdS, or NP–type), FFA, and Chol and to find out whether Cer structure has an effect on the properties of the deposited thin films. The films, which served as skin barrier models, were deposited by spraying at different theoretical thicknesses of 3.7, 0.55, 0.073 (an approximation of SC lipid lamellae), and 0.008 μm, respectively. The effect of annealing (heating the samples over the melting temperature and subsequent cooling down) and the presence of water during annealing were also studied. The periodic structure of samples, the conformational order, and the molecular arrangement of the lipids in the samples were investigated using X-ray diffractometry, Raman microspectrometry, and Fourier transform infrared spectroscopy.

References

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P-08

Textural Zoning of Phenocrysts and Groundmass in Dikes of Porphyritic Rocks

17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

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Intrusive rocks provide a unique opportunity to study the mechanisms of spatial movement and crystallization of magma in individual stages of development. Intrusive porphyry rocks support additional information about the evolution and conditions of crystallization taking place in the deep development of the parental magma that is contained in the zoning of the feldspar phenocrysts. The knowledge obtained may provide a key to the interpretation of complex magmatic systems with a significantly more complicated history. This thesis utilizes petrological and mineralogical methods to study three different dyke systems in the western part of the Bohemian Massif. Quantitative textural analysis, X-ray powder diffraction and microanalytical methods are used to study granite, syenite and diorite porphyry and their K- feldspar and plagioclase phenocrysts. Textural records of the porphyry rocks of the three dyke systems and crystallographic-chemical records of their feldspar phenocrysts suggest a mechanical flow accumulation taking place within the dyke at all three locations, but with different characteristics of magma flow rheology. The records also suggest different deep developments and crystallization conditions of the parent magmas of the studied dyke systems.

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P-09

An X-ray Absorption Spectroscopy Investigation of Irradiation-induced Structural Modifications and Damage Recovery in Nd2Zr2O7 Pyrochlore

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17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

The physicochemical properties of complex oxides are significantly impacted by the ordering and disordering process when they are subjected to severe conditions such as high temperature, high pressure, or ion irradiation. Both long-range and local atomic level disordering affects structural transformation in these materials, but short-range ordering plays an essential role in the response of pyrochlore ceramics submitted to ion irradiation and other severe conditions. Understanding the order-disorder phase transformation in pyrochlores has attracted attention due to the appearance of unconventional ordering at different length scales. Electronic excitation (100 MeV I^{7+}) induced crystalline to amorphous phase transition in $Nd_2Zr_2O_7$ pyrochlore synthesized through three steps solid-state sintering method was investigated. The synchrotron X-ray diffraction, along with Raman spectroscopy and X-ray absorption spectroscopy experiments conducted on pristine and irradiated pyrochlore, showed an increase in the rate of amorphization with ion fluence.

XRD results indicate that the specimen is amorphized with minor traces of defect fluorite structure on irradiation at the highest fluence of 5×10^{13} ions/cm^2. The significant changes in the Nd-L_3 and Zr-K edges of X-ray Absorption Near Edge Structure (XANES) spectra confirm strong local distortions and modifications in the short-range ordering upon irradiation. Extended X-ray Absorption Fine Structure (EXAFS) data reveals that the different local coordination environment of Nd and Zr cationic shells supports the phase transformation as observed by the XRD. The increasing value of DWF for all interatomic distances and observed the higher values of Nd-O distance for the sample irradiated at the highest fluence compared to the pristine pyrochlore structure indicate the occurrence of disordering at anionic sublattice. In-situ synchrotron XRD results reveal that defect fluorite structured is recovered upon thermal annealing of irradiated specimen at 400 C. No initial pyrochlore structure is recovered up to highest temperature of 1000 C.

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P-10

Analysis of Magnetic, Structural, Morphological Properties of CoFe2O4 Nanoparticles in Three Shape Modifications and Investigation of their Hyperthermic Effect

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17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

Magnetic $CoFe_2O_4$ nanoparticles, approximately 15 nm in size and synthesized in three distinct morphological modifications, were prepared using thermal decomposition techniques. These highly crystalline nanostructures were extensively characterized by various analytical methods, including X-ray diffraction (XRD), superconducting quantum interference device (SQUID) magnetometry, X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM), to evaluate their magnetic, structural, and magnetothermal properties. The sample morphology was confirmed by TEM, which verified the shape modifications induced by alterations in synthesis parameters, specifically the oleic acid-to-sodium oleate ratio. Structural analysis via XRD confirmed the formation of the cobalt ferrite structure, while magnetic property evaluation using SQUID magnetometry revealed high values of saturation magnetization and coercive field strength. The particle size distribution, as determined by SQUID magnetometry and XRD measurements, was found to be consistent across both techniques. The elemental composition, particularly the ratio of Co to Fe atoms within the inverse spinel structure of $CoFe_2O_4$, was investigated and analyzed using XPS. Given the high coercivity of the studied systems, magnetothermal response measurements were conducted, with results indicating significant potential for these nanoparticles in magnetic particle hyperthermia applications.

Acknowledgement This work was supported by the Slovak Research Agency under the contracts No. 09I03-03-V04-00177 - Magnetic nanosystems as hyperthermic agents for magnetic fluid hyperthermia – NANOTERM.

P-11

Modelling Angular Resolution of the Instrument P21.2 at Synchrotron Source PETRA III

17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

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The angular resolution in the case of angular dispersive X-ray (XRD) diffraction in transmission geometry is significantly influenced by parameters such as the size (cross-section) and divergence of the photon beam, its degree of monochromaticity, the dimensions, geometry of the sample, and the arrangement of the experiment. This work focuses on characterizing the angular resolution of the instrument P21.2 at the PETRA III synchrotron radiation source in DESY Hamburg (DE). The characterization of angular resolution was performed for an experimental setup corresponding to XRD diffraction in transmission geometry using a two-dimensional (2D) detector VAREX XRD4343CT.

In the first part of the work, a series of 2D diffraction records were analyzed, which were obtained on a calibration sample of LaB_6. The distance between the reference sample and the 2D detector was systematically varied in the range from 460 to 1800 mm. The photon beam energy was 81.8 keV, its size was 1×1 mm, and the sample thickness was 1 mm. A relationship between the angular width of diffraction maxima of the LaB_6 reference sample as a function of the diffraction angle and the distance between the sample and the 2D detector was determined by fitting the measured data.

In the second part of the work, attention was given to the theoretical modelling of the experimentally acquired data. A simple model describing a single-scattering event of diffracted photons based on kinematic diffraction theory was proposed. Based on numerical simulation of the model using a Monte Carlo method, theoretical profiles of angular resolution were calculated depending on the parameters used in the diffraction experiment. The obtained results indicate very good agreement with experimental data.

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P-12

FATRA software - The Fast Train Review Application

17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

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FATRA (Fast Train Review Application) is a tool that helps researchers analyze data from scientific cameras by providing an easy-to-use interface for visualizing and reviewing large datasets. It specifically addresses challenges associated with accessing data from Shimadzu cameras at the European XFEL facility, but its flexibility allows it to be applied to any type of camera or research facility. This software is integrated with Karabo framework (https://github.com/European-XFEL/Karabo), and leverages PyQT for a user-friendly interface. Key features of FATRA include real-time monitoring, layback, and offline analysis capabilities, as well as exporting data to videos for further review.

Acknowledgement This work was performed within the HORIZON-EIC-2021-PATHFINDEROPEN-01-01, MHz-TOMOSCOPY project, Grant agreement: 101046448. www.tomoscopy.eu

P-13

Time-resolved in situ X-ray Diffraction Monitoring of Instantaneous Mechanochemical Synthesis of Nickel-Copper Sulfide Composites

17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

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METAL SULFIDES have been used in various fields due to their excellent physicochemical properties [1-2]. There are many synthetic pathways to reach these compounds [3]. Among them, the mechanochemical synthesis is environmentally sound [4]. By just high-energy ball milling elemental precursors, it is possible to initiate the self-sustaining reaction [5], an instantaneous synthesis route to yield the desired compounds [6]. In this work, nickel-copper sulfides composite was successfully synthesized within 15 seconds via MSR (Mechanically induced self-propagating reaction). The process was performed at BESSY-II synchrotron, and X-ray data was collected in situ during milling. Time-resolved in situ monitoring of the mechanochemical processes, including X-ray diffraction, is a hot topic today [7]. The process was followed for a longer time to study the effect of time on the morphology of the composites. The XRD analysis reveals that the milling of Ni:Cu:S stoichiometry 1:1:2 leads to the formation of NiS, NiS_2, $Cu_{1.8}S$ and Cu_2S. The SEM analysis has shown the presence of micrometer sized agglomerates, which is a natural consequence of milling under dry conditions [8]. Energy disperse X-Ray analysis revealed that the content of nickel, copper and sulfur are 24.42%, 23.56% and 52.03%, respectively, thus confirming the desired stoichiometry of the product.

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P-14

Instrument Resolution Function of 2D XRD Setup at the P21.2 Beamline at Synchrotron Source PETRA III

17.10.2024, Thursday
18:00 – 19:00

Topic 5
Miscellaneous

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The systematic study of reciprocal space resolution of two-dimensional X-ray diffraction (2D XRD) setup implemented at the P21.2 beamline is presented. Beam size, sample thickness and sample-to-detector distance were identified as key parameters, mostly affecting reciprocal space resolution. Few series of 2D XRD patterns were taken on powder LaB6 standard sample with a monochromatic photon beam having energy of 81.84 keV. Beamsize (square profile) was set to four distinct sizes 0.1, 0.3, 0.5 and 1.0 mm. Sample thickness was set to 0.4, 1.0, 1.5 and 2.0 mm. Sample-to-detector distance was changed from 460 to 1800 mm. Scattered photons were acquired by 2D detector VAREX XRD4343CT (2880×2800 pixels, pixel size 150 μm× x 150 μm, 16 bit intensity resolution). Altogether 144 patterns were acquired and used in analysis. Each 2D XRD pattern was azimuthally integrated, and its peak profiles were analyzed with pseudo-Voigt function. Instrument resolution function, *i.e.* variation of the peak full-width at half-maximum with Bragg angle 2θ was investigated as a function of the beam size, sample thickness and sample-to-detector distance.

Acknowledgement The authors are grateful for the financial support received from the project VEGA 1/0638/24. Part of this work was funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V03-00034.

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