

**Session IX - Large European Neutron Facilities, September 11, Thursday****L29****INSTITUTE LAUE-LANGEVIN - INSTRUMENT AND INFRASTRUCTURE UPGRADES,
THE SCIENCE STRATEGY AND NEW RESEARCH OPPORTUNITIES****M. Johnson***Institut Laue Langevin, Grenoble, France
johnson@ill.eu*

The comprehensive Endurance upgrade programme was completed in 2024. With a budget of 50+ M€, about 30 projects have been delivered, including neutron guide systems, new and upgraded instruments, sample environment and data and software services. More intense neutron beams combined with more efficient detector systems provide major new capability for measuring ever smaller samples, including in extreme sample environments, and weaker signals. In addition, significantly shorter measuring times facilitate parametric studies and increase throughput and, therefore, overall capacity. Thus the upgrade programme as a whole, supported by ongoing and new pro-

jects, ensures that research capability at the ILL will continue to be world leading for the next decade, offering new opportunities for cutting-edge science. In this context, the ILL has elaborated a science strategy to optimise the use of its state-of-the-art scientific infrastructure over the next decade and enhance the delivery of societal impact with neutrons.

The Endurance programme, ongoing and new projects, and the science strategy will be presented, including recent science highlights, and set in the context of future reactor operation, given the recent, excellent decision that ILL will now operate at least until the end of 2033.

L30**DIFFRACTION AT MLZ****M. Hofmann***Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich (TUM), Garching, Germany*

The Heinz Maier-Leibnitz Zentrum or in short, the MLZ, is a cooperation between the Technical University of Munich (TUM), the Jülich Centre for Neutron Scattering (JCNS) and the Helmholtz-Zentrum hereon. This cooperation is the scientific umbrella for the exploitation of Germany's sole neutron source FRM II in Garching close to Munich. As such it is responsible for the installation and operation of all the positron and neutron scattering instruments installed at FRM II [1].

Besides a brief introduction of the facility at large, this presentation will focus primarily on the diffraction suite of

instruments of MLZ. In particular I will highlight recent developments and upgrades in the existing instrumentation as well as new diffractometers, which will be part of the user program once the FRM II restarts after a longer shutdown period in early 2026. In addition, I will also show some scientific highlights from experiments in energy materials, the life sciences as well as alloy development, of which many were also done in close cooperation with scientific groups from the Czech Republic.

1. <https://mlz-garching.de/englisch/about-mlz.html> .

ESS NEWS AND FIRST SCIENCE OPPORTUNITIES

Řremysl Beran^{1,2}

¹*Czech Academy of Sciences, Nuclear Physics Institute, Hlavni 130, Rez, 25068, Czech Republic*

²*European Spallation Source, ERIC, PO Box 176, Lund, 22100, Sweden*

premysl.beran@ess.eu

The European Spallation Source (ESS) [1], located in Lund, Sweden, is nearing completion and represents a significant advancement in neutron science research. Designed to be the world's most powerful neutron source, the ESS has achieved several significant milestones in its construction. The high-energy proton linac, responsible for driving the spallation process, has been successfully tested, and critical components such as the neutron target station and instrument infrastructure are now close to hot commissioning. The facility's technical complexity and scale, incorporating cutting-edge technologies in accelerator physics, neutron optics, and detection systems, reflect its ambition to transform the way neutrons are harnessed for scientific exploration. As construction progresses, ESS has transitioned into a new operational phase, focusing on the commissioning of its first suite of instruments and preparing them for experimental research and the users. An update on the status and the near prospects will be presented.

The "first science" opportunities at the ESS will validate the performance of the initial instruments, including LOKI, ODIN, DREAM, and others, marking the beginning of scientific operations and the user program. Each of these instruments is tailored to address specific scientific chal-

lenges. For instance, LOKI, a small-angle neutron scattering instrument, will provide insights into nanoscale structures and dynamics, enabling research into soft matter, polymers, and biological systems. ODIN is designed to perform high-resolution neutron imaging, making it ideal for investigating structural properties in engineering materials and complex natural systems. DREAM leverages neutron diffraction techniques to study atomic arrangements and phase transitions in materials critical to energy and quantum technologies. By conducting the first experiments, the ESS will establish baseline operations for its instruments and demonstrate the unprecedented capacity of its neutron beamlines. Here, it is equally important to underline the contributions of early users and the broader user communities, whose expertise, feedback, and collaborative research will be vital to refining the ESS's capabilities and ensuring its impact on scientific advancement across various fields. The way to get involved will be depicted.

1. K.H. Andersen, et al., The instrument suite of the European Spallation Source, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, **957**, (2020) 163402.



Session X - Neutron Science in Czech Republic I, September 11, Thursday

L32

NEUTRON DIFFRACTION LABORATORY IN ŘEŽ AND ITS USER PROGRAM

G. Farkas, V. Ryukhtin, P. Milkula, Ch. Hervoches, O. Levytska, P. Strunz and J. Šaroun

*Nuclear Physics Institute, v.v.i., Czech Academy of Sciences, Husinec–Řež, čp. 130, 250 68 Řež
saroun@ujf.cas.cz*

The neutron diffraction laboratory in Řež is part of the Centre of Accelerators and Nuclear Analytical Methods (CANAM) – a large research infrastructure hosted by the Nuclear Physics Institute of the CAS. It is one of the few European facilities providing the scientific community with neutron scattering methods and thus helping to fill the current gap in the availability of neutron beams. The laboratory equipment consists of five neutron diffractometers in the thermal neutron channels of the 10 MW research reactor LVR-15 (operated by Research Centre Řež, Ltd.), four of which are used for experiments mainly in the field of materials research and offered to external users within an open access programme. The TKS-400 instrument is dedicated to in situ thermomechanical loading experiments for studying deformation mechanisms in metallic materials. For this purpose, it has been equipped with a 20 kN uniaxial stress rig designed in-house, with current heating, as well as a small stress rig in an Eulerian cradle for analysing the evolution of lattice strain components in highly textured materials. Another instrument, TKS-100, is used for non-destructive mapping of residual stresses in bulky samples, with precise positioning enabled by a robotic arm. The powder diffractometer MEREDITH helps to solve vari-

ous problems of structure analysis where neutrons provide valuable complementary information, in particular on evolution of magnetic ordering or site occupation by atoms of similar proton numbers. Phase transformations can be observed in situ within a wide thermal range of about 10 to 1300 K using a closed-cycle He cryostat or vacuum furnace. This suite of instruments is complemented by the high-resolution small-angle scattering diffractometer MAUD, which is particularly well suited to studying microstructural features such as porosity or precipitation within the size range of approximately 50–2000 nm. Although there is no dedicated instrument available for neutron imaging, it is possible to perform neutron tomography with a monochromatic beam at the MEREDITH instrument, with a field of view of up to 4x4 cm² and a resolution of < 0.2 mm.

In recent years, the facility has offered around 300 instrument days per year as part of its open access programme, most of which have been allocated to experiments proposed by external users. Applications for experiments are welcome at any time, provided they are feasible and scientifically relevant. These are evaluated by a selection panel comprising internal and external experts.

L33

CZECH NEUTRON ASSOCIATION - ESTABLISHMENT, MISSION, AND OBJECTIVES

Milan Klicpera¹, Jan Šaroun², Petr Čermák¹, Pavel Strunz², Dominika Zákušná³

¹*Faculty of Mathematics and Physics, Charles University, Prague*

²*Institute of Nuclear Physics, Czech Academy of Sciences, Řež*

³*Faculty of Mathematics and Physics, Charles University, Prague*

We are reaching out to inform you about the establishment of a new professional association - the **Czech Neutron Association (Česká neutronová asociace, z. s.)**, founded to unite, support, and represent the community of Czech users of neutron radiation.

The Association's mission is to:

- Bring together researchers and institutions using neutron radiation across disciplines.
- Promote the potential and results of research based on neutron methods.
- Facilitate dialogue between the scientific community, the public, and government authorities.
- Represent the interests of the Czech neutron community in European and other international institutions and structures with relevant thematic focus.

We believe that the Czech Neutron Association will significantly contribute to the coordination of national neutron infrastructure, strengthen international cooperation, and facilitate access for Czech researchers to world-class experimental facilities and expertise.

Membership in the Association offers the opportunity to participate in the development of neutron research in the Czech Republic, engage in joint scientific initiatives, and become part of a representative platform for neutron-based science at both national and international levels. More information about the Association's activities, its statutes, and the membership application will be presented during Struktura 2025; and can be found at neutrons.cz.

Committee of the Czech Neutron Association.

RESIDUAL-STRESS DISTRIBUTION IN COMPONENTS FABRICATED WITH INVOLVEMENT OF ADDITIVE MANUFACTURING

Pavel Strunz^{1,*}, Josef Izák², Štěpán Jedlan³, Olena Levytska¹, Josef Hodek⁴, Gergely Németh^{1,5}, Jan Šaroun¹, Radim Kocich^{2,6}, Marek Pagáč⁷ and Kostyantyn Tuharin^{1,8}

¹*Nuclear Physics Institute of the Czech Academy of Sciences, Husinec—Řež 130, 250 68 Řež, Czech Republic; levytska@ujf.cas.cz (O.L.); nemeth@ujf.cas.cz (G.N.); saroun@ujf.cas.cz (J.Š.); tuharin@ujf.cas.cz (K.T.)*

²*Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896, 616 00 Brno, Czech Republic; 183119@vutbr.cz*

³*Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Prague, Czech Republic*

⁴*COMTES FHT a.s., Dobřany, Czech Republic*

⁵*Paul Scherrer Institute—PSI, 5232 Villigen, Switzerland*

⁶*Faculty of Materials Science and Technology, VŠB-Technical University of Ostrava, 17. Listopadu 2172/15, 708 00 Ostrava, Czech Republic; radim.kocich@vsb.cz*

⁷*Faculty of Mechanical Engineering, VŠB-Technical University of Ostrava, 17. Listopadu 2172/15, 708 00 Ostrava, Czech Republic; marek.pagac@vsb.cz*

⁸*Faculty of Mathematics and Physics, Charles University, Ke Karlovu 2027/3, 121 16 Prague, Czech Republic*

**strunz@ujf.cas.cz*

Additive manufacturing opened new possibilities in fabrication of components. However, at the same time, it introduced new tasks for metallurgists and materials engineers as the microstructure of the components prepared by additive manufacturing is significantly different than the microstructure of the conventionally fabricated components. One of the characteristics largely influenced by additive manufacturing is the residual stress distribution. Residual stresses play a crucial role in determining the performance and lifetime of engineered components.

Some examples taken from the field of materials fabricated by additive manufacturing are shown. Residual stresses were measured using neutron diffraction in these demonstrations. The use of neutron diffraction is indispensable for the measurement of residual stresses in the bulk of the material. It is a non-destructive method; therefore, the sample can be later used for other examinations.

The impact of manufacturing strategies on the development of residual stresses in Dievar steel is presented. Two fabrication methods were investigated: conventional ingot casting and selective laser melting (SLM) as an additive manufacturing process. Subsequently, plastic deformation in the form of hot rotary swaging at 900°C was applied. Microstructural and phase analysis, precipitate characterization, and hardness measurement—carried out to complement the investigation by neutron diffraction—showed the microstructure improvement by rotary swaging. The study reveals that the manufacturing method has a significant effect on the distribution of residual stresses in the bars. The results showed that conventional ingot casting resulted in low levels of residual stresses (up to ± 200 MPa), with an increase in hardness after rotary swaging from 172 HV1 to 613 HV1. The SLM-manufactured bars developed tensile hoop and axial residual stresses in the vicinity of the surface and large compressive axial stresses (-600 MPa) in the core due to rapid cooling. The subsequent thermo-

mechanical treatment via rotary swaging effectively reduced both the surface tensile (to approximately $+200$ MPa) and the core compressive residual stresses (to -300 MPa). Moreover, it resulted in a predominantly hydrostatic stress character and a reduction in von Mises stresses, offering relatively favorable residual stress characteristics and, therefore, a reduction in the risk of material failure. In addition to the significantly improved stress profile, rotary swaging contributed to a fine grain ($3\text{--}5\text{ }\mu\text{m}$ instead of $10\text{--}15\text{ }\mu\text{m}$ for the conventional sample) and increased the hardness of the SLM samples from 560 HV1 to 606 HV1. These insights confirm the utility of rotary swaging as a post-processing technique that not only reduces residual stresses but also improves the microstructural and mechanical properties of additively manufactured components.

Residual stresses were also measured in samples manufactured by two different AM technologies within one component: the bottom half prepared using either Laser Powder Bed Fusion (L-PBF) or Direct Energy Deposition (L-DED), and the second half of the component vice versa, i.e. using L-DED or L-PBF, respectively. A combination of fabrication by different additive technologies is not a commonly used procedure in practice. Cubic regions ($25\text{mm} \times 25\text{mm} \times 25\text{mm}$) of 316L steel were printed either by L-PBF or by L-DED on the steel substrate and afterwards finished to a height of 50 mm by the second technology. The aim was to determine the residual stresses that each technology introduces into the samples and a comparison with FEM prediction: the stresses measured by neutron diffraction are to be used for validation of the FEM model, which will be applied as an optimization tool in the combination of AM production methods.



L35

VALIDATION OF CONTOUR CUT MODEL FOR RESIDUAL STRESSES IN AM-REPAIRED SIMULATED DEFECT BY NEUTRON DIFFRACTION

Josef Hodek, Štěpán Jedlan, Martin Ševeček, Jan Šaroun, Olena Levytska, Michal Brázda, Antonín Prantl, Pavel Strunz

Institute of Physics, Czech Academy of Sciences, Řež

This study validates the accuracy and reliability of the Contour Cut Method (CCM) for residual stress assessment using neutron diffraction (ND) in a critical case — the repair of a simulated defect in a 316L component by Laser-Directed Energy Deposition (L-DED). CCM combines finite element modeling (FEM) with a series of precision cuts to recover residual stress data.

A strong agreement was observed between ND and CCM results. Neutron diffraction measurements along the

sample's central line revealed local stress maxima and minima, with the highest tensile stresses located in the L-DED region and the central part of the substrate.

The demonstrated correlation supports the applicability of CCM as a reliable technique for residual stress evaluation in various industrial contexts.

L36

PUMP-PROBE NEUTRON INELASTIC SCATTERING EXPERIMENTS.

J. Kulda

*Institute Laue-Langevin, CS 20156,38042 Grenoble Cedex 9, France
kulda@ill.fr*

The neutron and, more recently, X-ray spectroscopy have been standard workhorses for investigations of condensed matter dynamics at atomic resolution. Nevertheless, the inherently weak interaction of both probes with matter, accompanied by the tiny flux densities of neutron beams and by the huge X-ray photon energy as compared to the energy scale of elementary excitations in condensed matter, have limited their implementation to simple scattering, leaving no options for analogies to optical experiments with coherently split beams.

Experiments using synchronized pulsed X-ray and laser beams to investigate the time evolution of non-equilibrium states of condensed matter, both in the structural and in the magnetic domains, are quickly becoming routine at XFEL (X-ray Free Electron Lasers) beams exhibiting picosecond time-structures, accompanied by extreme transversal coherence (e.g. [1]). With neutrons the progress is slower, but reports on successful attempts of time-resolved work have appeared recently as well [2,3] and, after all, a dedicated pump-probe setup has been developed and tested at the SNS Hyspec spectrometer at the ORNL [4].

In this presentation we shall recall the basic principles of scattering theory based on time-dependent correlation

functions and review the present state of neutron experimental techniques addressing transient processes in matter, their principal limitations and development opportunities.

1. Y. Lee, K. Y. Oang, D. Kim, and H. Ihee, "A comparative review of time-resolved x-ray and electron scattering to probe structural dynamics," *Structural Dynamics*, vol. **11**, no. 3. AIP Publishing, May 01, 2024. doi: 10.1063/4.0000249.
2. M. Wang et al., • "Optically Induced Static Magnetization in Metal Halide Perovskite for Spin•]Related Optoelectronics," *Advanced Science*, vol. **8**, no. 11. Wiley, May 02, 2021. ' doi: 10.1002/advs.202004488.
3. Y. Wang et al., • "Monopolar and dipolar relaxation in spin ice Ho₂Ti₂O₇," *Science Advances*, vol. **7**, no. 25. American Association for the Advancement of Science (AAAS), Jun. 18, 2021. doi: 10.1126/sciadv.abg0908.
4. C. Hua, D. A. Tennant, A. T. Savici, V. Sedov, G. Sala, and B. Winn, • "Implementation of a laser.neutron pump.probe capability for inelastic neutron scattering," *Review of Scientific Instruments*, vol. **95**, no. 3. AIP Publishing, Mar. 01, 2024. doi: 10.1063/5.0181310.

Session XI - Neutron Science in Czech Republic II, September 11, Thursday

L37

EXPERIMENTAL DETERMINATION OF CRITICAL RESOLVED SHEAR STRESSES BY NEUTRON DIFFRACTION

G. Farkas¹, A. Ludwik², M. Wroński², P. Kot³, A. Baczmański²

¹Nuclear Physics Institute ASCR v.v.i., Czech Academy of Sciences, Řež

²AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland

³NOMATEN Centre of Excellence, National Centre of Nuclear Research, A. Sołtana 7, 05-400 Otwock-Świerk, Poland

This study investigates the plastic deformation mechanisms of AZ31 magnesium alloy using *in-situ* neutron diffraction and Crystallite Group Method (CGM). *In-situ* neutron diffraction enables measurement of the stress tensor for specific grain families within a polycrystal by determining lattice strains from diffraction peaks associated with the same grain family, observed from multiple orientations and hkl reflections. Tracking the evolution of the stress tensor makes it possible to experimentally determine the Critical Resolved Shear Stresses (CRSS) and to characterise the hardening behaviour of different slip and twinning systems.

Tensile tests were performed along the rolling direction (RD), while compression tests were conducted along the normal direction (ND), and at 30° (ND30) to the ND, allowing assessment of the anisotropic mechanical response. The CGM allowed direct determination of grain-level stresses for preferred crystallographic orientations, leading

to unambiguous CRSS values and, notably, an improved estimate for the basal slip system from the ND30 test, compared to previous findings [1]. These experimentally derived CRSS values, along with the evolution of Resolved Shear Stresses (RSS), were used to validate and calibrate the Elastic-Plastic Self-Consistent (EPSC) model adapted for hexagonal crystal structures. The combined experimental-modelling approach enhances understanding of plastic anisotropy in AZ31 alloy and improves the predictive capability of the EPSC framework for magnesium alloys subjected to complex loading conditions.

1. Kot, P., Wroński, M., Baczmański, A., Ludwik, A., Wroński, S., Wierzbowski, K., Scheffzik, C., Pilch, J., Farkas, G., 2023. A novel method of experimental determination of grain stresses and critical resolved shear stresses for slip and twin systems in a magnesium alloy. *Measurement* **221**, 113469.

L38

INVESTIGATIONS OF MAGNETIC VORTEX LATTICES AND SKYRMIONS USING NEUTRON SCATTERING

V. Ryukhtin

Nuclear Physics Institute ASCR v.v.i., Czech Academy of Sciences, Řež

Neutron scattering can be very efficiently used for studying of magnetic vortex lattices (VL) (or flux-line lattices (FLL)) in unconventional superconductors. Actually, very first experimental evidence of VL existence after their theoretical prediction by Abrikosov [1] was conducted by means of neutron scattering [2] in Nb. Exploring of small angle neutron scattering (SANS) for direct observation of FLL [3] got “second - breath” with discovering of high-Tc superconductors (HTSC), which are all of type-II and with higher upper critical field H_{c2} . SANS is exceptional tool for establishing the values of HTSC.

Sr_2RuO_4 , an isostructural of the high-Tc material $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, is the first 2D perovskite oxide that exhibits superconductivity without copper [3]. Unlike $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, however, it exhibits Fermi liquid behavior in its normal state. Sr_2RuO_4 then became an attractive material to

probe the mechanism of high-Tc superconductivity, and also to study p-wave superconductivity since it has a simple band structure compared to Uranium based systems, another p-wave superconducting family. To this date, however, some groups still claim that there is no credible evidence of p-wave superconductivity of Sr_2RuO_4 . Here, some first results of FLL in Sr_2RuO_4 measurements conducted at KWS-3 SANS facility are reported.

The measurements of dynamics of skyrmion lattice using neutron spin-echo technique is reported as well. Skyrmions are vortex-like magnetic structures, created in helimagnet (here was used single crystal MnSi). According to recent theoretical studies the lowest-energy excitations of the system are the so-called ‘phason’ modes of the skyrmion lattice. Their dispersion curves for the propaga-



tion vector ($\mathbf{q}_z$) parallel to the magnetic field are expected to be asymmetric along the strings of the skyrmions, indicating that the magnetic excitations have different q dependencies along $+\mathbf{q}_z$ and $-\mathbf{q}_z$. This prediction was tested by a Spin-Echo technique that is sensitive to these low-energy excitations and to their momentum and it was showed that an asymmetric magnetic dispersion is present in the skyrmion state [4].

L39

NOVEL PYROCHLORE-LIKE STRUCTURE IN RARE-EARTH IRIDATE SINGLE CRYSTALS

F. Hájek¹, D. Staško¹, K. Vlášková¹, J. Kaštil², M. Henriques², M. Klicpera¹

¹Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5, 121 16 Prague 2, Czech Republic

²Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic
filip.hajek@matfyz.cuni.cz

The rare-earth $A_2\text{Ir}_2\text{O}_7$ pyrochlore iridates ($A = \text{Y}, \text{Pr-Lu}$) constitute a family of materials revealing a plethora of novel and exotic properties. The geometrically frustrated pyrochlore lattice hosts Ir^{4+} ions displaying strong spin-orbit coupling comparable to electron correlations. In combination with crystal field effects and important f - d exchange between the rare-earth and iridium sites, various magnetic and topological phases emerge. Among others, the topological phases include the topological Mott insulator [1], axion insulator [2] or Weyl semimetal [2,3] and the magnetic phases include the fragmented spin ice state with monopole-like excitations [4] and spin liquid states [5, 6].

The following work is focussed on the magnetic and structural properties of the $A = \text{Nd}$ single crystal analogue. In contrast to previous works, e.g. [7], where $\text{Nd}_2\text{Ir}_2\text{O}_7$ adopts the pyrochlore structure, the present single crystals display a different, unusual crystal structure, attributed to a new Pb-based synthesis method. Magnetic properties, including two magnetic transitions at 41 K and 8 K, demonstrate notable similarities for the two crystal structures. The non-pyrochlore structure found using X-ray diffraction is analysed and compared to the pyrochlore structure, with a focus on the Ir pyrochlore-type tetrahedral sublattice with octahedral O^{2-} crystal fields found in both crystal lattices. The full crystal structure contains two Ir sublattices, three Nd sublattices and one Pb sublattice with a high degree of disorder in the form of vacancies. The magnetic structure,

1. A. A. Abrikosov, Zh. Eksp. Teor. Fiz. (1957) **32** 1442.
2. D. Cribier, *et al.* in Progress in Low Temperature Physics, (1967), **5** 161.
3. T. M. Riseman, *et al.* Nature (London) 396, 242 (1998).
4. Soda, M., *et al.* Asymmetric slow dynamics of the skyrmion lattice in MnSi. Nat. Phys. 19, 1476–1481 (2023).

fundamentally tied to the tetrahedral lattice in the pyrochlore case, is examined in the non-pyrochlore samples employing neutron diffraction.

1. Y. Otsuka, T. Yoshida, K. Kudo, S. Yunoki, Y. Hatsugai, *Sci. Rep.*, **11**, (2021), 20270.
2. X. Wan, A. M. Turner, A. Vishwanath, S. Y. Savrasov, *Phys. Rev. B*, **83**, (2011), 205101.
3. X. Liu, S. Fang, Y. Fu, W. Ge, M. Kareev, J.-W. Kim, Y. Choi, E. Karapetrova, Q. Zhang, L. Gu, E.-S. Choi, F. Wen, J. H. Wilson, G. Fabbris, P. J. Ryan, J. W. Freeland, D. Haskel, W. Wu, J. H. Pixley, J. Chakhalian, *Phys. Rev. Lett.*, **127**, (2021), 277204.
4. E. Lefrançois, V. Cathelin, E. Lhotel, J. Robert, P. Lejay, C. V. Colin, B. Canals, F. Damay, J. Ollivier, B. Flk, L. C. Chapon, R. Ballou, V. Simonet, *Nat. Commun.*, **8**, (2017), 209.
5. M. Kawai, J. Friedman, K. Sherman, M. Gong, I. Giannakis, S. Hajinazar, H. Hu, S. E. Grefe, J. Leshen, Q. Yang, S. Nakatsuji, A. N. Kolmogorov, Q. Si, M. Lawler, P. Aynajian, *Nat. Commun.* **12**, (2021), 1377.
6. Y. Machida, S. Nakatsuji, S. Onoda, T. Tayama, T. Sakakibara, *Nature* **463**, (2010), 210.
7. H. Takatsu, K. Watanabe, K. Goto, H. Kadowaki, *Phys. Rev. B* **90**, (2014), 235110.

L40

MAGNETIC STRUCTURE AND EXCITATIONS IN THE ANTIFERROMAGNET $\text{Na}_2\text{BaMn}(\text{PO}_4)_2$

David Svitak¹, Nikolaos Biniskos¹, Michal Stekiel², Bruce Normand³, Kari Schmalzl⁴,
Andreas M. Läuchli³, Flaviano Jose dos Santos³, Petr Cermak¹

¹Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics

²Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ)

³PSI Center for Scientific Computing, Theory, and Data

⁴Jülich Centre for Neutron Science (JCNS) at Institut Laue Langevin (ILL).

The investigation of geometrically frustrated systems with antiferromagnetically (AFM) ordered spins attracts attention due to their potential to stabilize exotic quantum states, such as a spin liquid state, which holds promise for applications in quantum computing. Here we present our study of the triangular AFM compound $\text{Na}_2\text{BaMn}(\text{PO}_4)_2$ [1,2], which has an unusually high spin $S = 5/2$. In contrast, the isostructural compound with Co ($S = 1/2$) [3] has been studied extensively, as lower spin systems are typically more favorable for the formation of quantum spin liquids. We use single crystal neutron diffraction and inelastic neutron scattering to determine the magnetic structures and spin excitations for magnetic fields applied in the basal plane and along the c -axis of the trigonal symmetry. At zero magnetic field, the system undergoes two magnetic transitions at around 1.25 K (AFM2) and 1.1 K (AFM1). The out-of-plane incommensurate component k of the magnetic propagation vector $(1/3, 1/3, k)$ changes significantly in these two AFM phases, which suggests non-negligible interlayer couplings.

Depending on the direction of the magnetic field, $\text{Na}_2\text{BaMn}(\text{PO}_4)_2$ shows several field-induced transitions. These transitions cause changes in the magnetic propagation vector before the system reaches the spin-polarized state. By combining neutron diffraction, low-temperature

specific heat, and dc magnetization, we establish temperature-magnetic field phase diagrams for both field directions. Using ab-initio calculations and Monte Carlo simulations, we determine the exchange interactions, anisotropy parameters, and the phase diagrams. Our combined experimental and theoretical study shows that $\text{Na}_2\text{BaMn}(\text{PO}_4)_2$ is mainly a 2D system, with very weak 3D coupling that only acts as a “witness” to what happens in two dimensions. The separation between the two zero-field transitions (AFM1 and AFM2) depends on the XXZ nature of the anisotropy and the 3D coupling. The gap in the dispersion of the fully polarized phase is influenced by the XXZ anisotropy, single-ion anisotropies, and the magnetic field. Finally, we compare our results with the Co ($S = 1/2$) and Ni ($S = 1$) [4] counterparts and discuss their similarities and differences.

1. J. Kim, et. al., Journal of Physics: Condensed Matter, 34, p. 475803 (2022).
2. C. Zhang, et. al., Phys. Rev. B, 110, p. 214405 (2024).
3. N. Li, Q. Huang, et. al. Nature Communications, 11, p. 4216 (2020).
4. N. Li, Q. Huang, et. al. Phys. Rev. B, 104, p. 104403 (2021).

L41

INFLUENCE OF METAL OXIDE DEPOSITION ON MAGNETIC DISTRIBUTION AND COMPOSITION OF SUPRAPARTICLES

R. Conan^{1,2}, V. Müller², S. Müssig², K. Mandel², D. Zakutna³

¹Department of Inorganic Chemistry, Charles University, Prague, Czechia

²Department of Chemistry and Pharmacy, Friedrich-Alexander University Erlangen Nürnberg (FAU), Erlangen, Germany

romain.conan@natur.cuni.cz

The development of multifunctional materials, which integrate multiple functional components, is a rapidly evolving field with significant implications across various technologies [1-2]. Colloidal nanocrystals are exceptional building blocks for constructing complex architectures in random or controlled assemblies [3-4]. By co-assembling different types of nanocrystals into larger colloidal particles, particularly at the mesoscale, novel supraparticles can be engineered. These supraparticles, typically micrometers in size

and composed of functionalized nanoparticles and molecular building blocks [5], combine the properties of their constituent nanocrystals while maintaining their colloidal stability [6]. Recent interest in these materials stems from their versatility and broad applicability. For example, incorporating magnetic nanoparticles into supraparticles offers diverse applications, including magnetic separation, hyperthermia, drug delivery, and magnetic imaging. Furthermore, the inclusion of non-magnetic functional metal



oxide ligands (e.g. Al_2O_3 for catalysis, ZnO for semiconductors, TiO_2 for photocatalysis) can further expand the potential of these innovative supraparticle systems [7–9].

Thus, our contribution aims to comprehensively explore the impact of the Atomic Layer Deposition (ALD) process of metal oxides on the magnetic signal, structure, and composition of iron oxide supraparticles. Through detailed Mössbauer analysis, we will demonstrate the oxidation-shielding properties afforded by specific metal oxides. Finally, using the Small-Angle Neutron Scattering with incident beam Polarization (SANS POL) we will reveal the absence of intra-supraparticle structural displacement during the ALD process, along with increased internal ordering and a significant reduction in the magnetic “dead layer” size.

L42

MAGNETIC MORPHOLOGY OF MULTISHELL NANOPARTICLES

Š. Hricov¹, O. Kaman², I. Dirba³, N. J. Steinke⁴, D. Zákutná^{4,5}

¹Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague 2, Czechia

²Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6, Czechia

³Technical University of Darmstadt, Karolinenplatz 5, 64289 Darmstadt, Germany

⁴Institut Laue-Langevin, 71 Avenue des Martyrs CS 20156, 38042 Grenoble, France

⁵Department of Inorganic Chemistry, Faculty of Science, Charles University, Hlavova 8, 128 00 Prague 2, Czechia

Magnetic nanoparticles (MNPs) are of high research interest due to their unique physical properties, which lay the foundation for various applications, ranging from biomedical diagnostics and therapeutic interventions to high-density data storage systems and environmental remediation processes. Broadly known and well-studied materials of this class are iron oxides MNPs. Among other research interests, they have been heavily exploited for their heating

abilities via magnetic fluid hyperthermia. This process is a cornerstone for innovative cancer treatment therapies, which aim to localise tumour elimination. However, we propose a novel candidate material, the $\gamma\text{-Fe}_3\text{N}$. It possesses unprecedented magnetic properties, essentially surpassing the well-established iron oxide MNPs [1], having larger saturation magnetization, leading to better heating performance in hyperthermia. As a result, the required

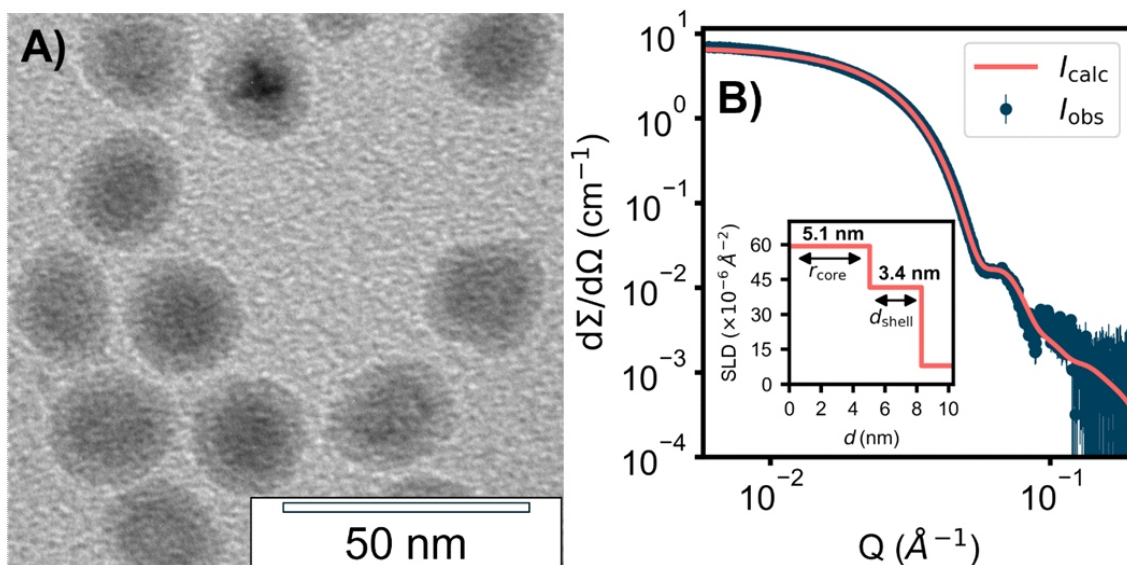


Figure 1. A TEM micrograph of passivated $\gamma\text{-Fe}_3\text{N}$ MNP, B SAXS curve recorded on dispersion of passivated $\gamma\text{-Fe}_3\text{N}$ MNP.

therapeutic temperatures for tumour ablation can be achieved with a less concentrated MNP dispersion, thereby reducing the dose needed. Nevertheless, due to the nano-sized crystals, the $\gamma\text{-Fe}_3\text{N}$ is air sensitive, which results in massive oxidation. Thus, a robust surface protection must be realised. While considering the potential biomedical applications, we propose a silica encapsulation procedure to hinder $\gamma\text{-Fe}_3\text{N}$ oxidation and to establish biocompatibility, together with possibility to form aqueous dispersions. To successfully grow a silica layer, we have chosen a route of $\gamma\text{-Fe}_3\text{N}$ surface passivation, which we present in this contribution, together with insight into magnetic behaviour of complex core@shell MNPs. The bright-field transmission electron microscope micrographs (**Figure 1: A**) and small-angle X-ray scattering (**Figure 1: B**) show well-defined core@shell MNP morphology of the passivated nanoparticles with a mean particle diameter of 17.2(2) nm. Nevertheless, the macroscopic magnetization measurements revealed unexpected behaviour leading to a decrease in saturation magnetization and the presence of exchange bias at 5 K. To further explore, the complex mag-

netic nature of this material was disentangled by probing magnetic scattering fluctuations using the magnetic small-angle neutron scattering with incident beam polarization at the D33 instrument at ILL [2]. Finally, we will disentangle the magnetic morphology contributions from the magnetic core and shell part of passivated $\gamma\text{-Fe}_3\text{N}$ MNPs and discuss the resulting magnetic response of the presented MNPs in detail.

1. I. Dirba et al., J. Phys. D: Appl. Phys, 56, 025001 (2023). doi: 10.1088/1361-6463/aca0a9.
2. Š. Hricov et al., Unmasking the Complex Core-Multishell Morphology of Magnetic Nanoparticles. Institut Laue-Langevin, proposal No. DIR-297 (2023). doi: 10.5291/ILL-DATA.DIR-297

This work was supported by the Czech Science Foundation (22-10035K) and the AMULET project, co-funded by MŠMT and the EU (CZ. 02.01.01/00/22_008/0004558). We also acknowledge the Institut Laue-Langevin for beamtime and financial support.

Session XII - September 11, Thursday

L43

LAUEDB: A DATASET FOR LAUE PATTERNS

Štěpán Venclík, Tomáš Červeň, Jan Kříž, David Sviták, Petr Čermák

Charles University, Prague, Czech Republic

Laue diffraction is a widely used technique for orienting single crystals and a routine procedure during sample preparation for many scientists. Over the years, a variety of software tools have been developed to assist in interpreting Laue patterns [1, 2]. Despite significant progress in image processing and pattern recognition, a robust and fully automated solution for indexing Laue patterns has yet to be achieved.

In recent years, **machine learning** has emerged as a promising approach to tackle this challenge [3]. However, the development and validation of more advanced algorithms are currently hindered by the lack of annotated experimental datasets. As a result, all training and testing are still conducted exclusively on synthetic data.

LaueDB aims to bridge this gap by creating a **dataset of oriented X-ray and neutron Laue patterns** that could

serve as a training and evaluation dataset for both classical and machine learning approaches.

We plan to utilise the Automatic Laue Sample Aligner (ALSA) [4] to create the initial dataset, capturing a large number of patterns for each sample crystal, as well as collaborate with research infrastructures to develop a submission pipeline for patterns created during routine sample orientation. In addition, existing tools and algorithms for peak finding and Laue indexing will be compared.

1. Esmeralda Laue Suite (<https://code.ill.fr/scientific-software/esmeralda>).
2. Clip4 (<https://clip4.sourceforge.net/>)
3. Purushottam Raj Purohit, R. R. P., Tardif, S., Castelnau, O., Eymery, J., Guinebreiere, R., Robach, O., Ors, T. & Micha, J.-S. (2022). J. Appl. Cryst. 55, 737-750.
4. ALSA (<https://charlesautomata.cz/alsa>).