Book of Abstracts

Wednesday, 11 December 2024 - Friday, 13 December 2024

Institut Laue-Langevin, Grenoble (France)

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14:30	Interplay between structural and magnetic chiralities in NiCo2TeO6	BEAUVOIS, Ketty
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16:30	Exploiting Advanced Polarised neutron and X-ray synergies to reveal magnetic structure and dynamics in spin caloritronics	MANNIX, Dan
16:50	Crystal structure and absence of magnetic order in single crystalline RuO$_2$	KIEFER, Lara
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Friday, 13 December 2024

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time	title	presenter
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14:50	Polarised neutrons for users at ESS	LEE, Wai Tung
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Coffee break and posters (15:30 - 16:00)

Single-crystal polarized neutron opportunities at the ILL - Chadwick amphitheatre (16:00 - 17:00)

Introductory lectures

Polarized neutron diffraction as a supreme probe of atomic-scale magnetism

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Polarized neutrons are an essential tool in the study of magnetic materials at the atomic scale, providing information which in some cases cannot be obtained if only unpolarized neutrons are employed. In this talk I will introduce the different ways in which polarized neutron diffraction can be performed and the corresponding information that can be obtained. I plan to cover the techniques of uniaxial polarization analysis, XYZ polarization analysis, the half-polarized beam technique, and spherical neutron polarimetry. The strengths of these techniques will be illustrated by examples.

Unravelling complex ordering phenomena with polarised x-rays

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A key feature of the synchrotron light that helps us to unravel the properties of the materials is the ability to generate, control and analyse the polarisation of the photons in a wide energy range [1,2,3] This feature of the synchrotron beam offers the opportunity to enhance different element of the light-matter cross section and to apply it to a variety of synchrotron-based techniques exploring materials at different lengths and energy scales.

The dominant term in the x-ray diffraction cross section do not modify the polarization of the scattered photons, however in resonant condition or when a more comprehensive model of the scattering process is used, the light-matter cross section can modify in a well-defined manner the polarisation state of the diffracted photon and an analysis of the final polarisation state of the diffracted photons can be used to distinguish different scattering processes, and to access different physical properties of the system under investigation [4].

For this reason, the x-ray polarisation is often used to investigate ordering phenomena, to solve magnetic structures [5,6], to establish their chirality [6], and, when combined with the spatial resolution capability of the synchrotron beam, to map different types of domains [7,8], the same approach can be readily transferred to the study of excitations, where energy and momentum are transferred [9].

In the same manner the photoelectron emitted using polarised light can be used to investigate topological magnetic textures and domain patterns in few nanometres of quantum materials[8] complementing the spatial resolution achievable with diffraction.
In this seminar I will introduce the polarisation of the light in relation to the investigation of chirality and non-collinearity and I will discuss the opportunities offered by this property.

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[8] Ueda et al, Nature volume 618, 946 (2023)

Historical accounts

Historical account of polarised neutron techniques development at Grenoble

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Since the first polarised neutron experiment carried out with the diffractometer DN2 in the reactor Mélusine, a tremendous work has been performed at Grenoble to develop polarisation neutron techniques.

At the ILL, among the first generation of instruments, there was only one using polarised neutrons, built by the team working at Mélusine. The extraordinary step brought by the high-flux reactor opened a field of opportunities and motivated brillant scientists, engineers and technicians to develop techniques and tools for exploiting polarised beams.

We shall present an account of the main projects that have paved the way to the polarised neutron techniques that are today proposed on 40% of the instruments and representing 25% of the total beamtime, with an emphasis on the techniques which are more relevant to Flipper's participants.

Frustrated magnetism

Polarized neutron studies of a Kitaev candidate spin liquid

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Samarium (Sm, element 62) is a singular element to study with neutron scattering. It has a very large neutron absorption, a magnetic form factor that peaks at high Q, and often a low magneto-crystalline anisotropy due to the limited basis of single-ion states. We use polarization techniques to study the ground state of Kitaev candidate SmI_3, a 2D honeycomb material that is similar to other rare earth tri-halides where dipole-dipole interactions can become involved. Our experiments were carried out at D3 using a hybrid setup with a Heusler monochromator and the "liquids" area detector, and using very short wavelengths in order to minimize the absorption and access high Q. The large $\Delta\lambda/\lambda$ at these wavelengths allows us to calibrate the polarization by measuring the peak shape. Using this approach, we find that the ground state of SmI_3 contains quantum fluctuations that depolarize the beam, and we characterize their time and length scales at 50 mK by comparing these results to muon spin rotation studies. We also show that the single-ion wavefunctions of SmI_3 contain ingredients for Kitaev-type interactions, by characterizing the crystal field scheme and magnetic form factor with D3 and Panther.

A triangular lattice Ising model candidate

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Rare earth trihalides are gaining attention in the field of quantum matter for their potential to exhibit exotic ground states due to interacting magnetic moments with competing interactions or geometrical frustration. Compounds such as YbBr3 and ErBr3 exemplify this interest with their unique 2D honeycomb structures where magnetic anisotropy can be tuned by varying the rare-earth ion, enabling the study of 2D magnetism in various regimes including XY, Ising, and Heisenberg limits. These attributes make rare earth trihalides versatile systems for probing the fundamental physics of 2D magnetism.

In contrast, early rare earth halides with a 3D UCl3-type structure have a honeycomb-like topology in the ab-plane. We have investigated a cerium trihalide that display an antiferromagnetic ordering wave-vector of k=(1/3, 1/3, 1/2). Recent single crystal diffraction and spherical polarimetry studies have further elucidated the magnetic properties of this system. The cerium sublattice splits into two orbits, and we find the compound to be a triangular lattice Ising model candidate. These findings highlight the complex interplay between 1D and 2D magnetic behaviors in rare earth trihalides, enriching our understanding of magnetic anisotropies and order parameters in quantum materials.

Spin-lattice coupling in the spinel $GeCo_2O_4$

Author: Edmond Chan[1]

Co-authors: Arno Hiess [2]; Ketty Beauvois [3]; Laura Chaix [1]; Manila Songvilay [1]; Ursual Bengaard-Hansen [2]; Virginie Simonet [1]

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Normal spinels AM_2O_4 crystallize in the cubic space group Fd-3m at room temperature. The magnetic ions M form a pyrochlore sublattice, consisting of a network of corner-sharing tetrahedra prone to magnetic frustration. Complex magnetic ground states arise in these spinel compounds from a strong competition between magnetic interactions beyond the third neighbor [1-5]. In this talk, we focus on $GeCo_2O_4$, which orders at TN = 23 K into a complex antiferromagnetic structure characterized by the propagation vector k = (½ ½ ½) [3-5]. The magnetic ordering is accompanied by a cubic to tetragonal structural transition [3,4], which partly releases the magnetic frustration through magneto-structural effects. Moreover, elastic constant studies using ultrasound velocity measurements reported acoustic anomalies (in particular, in the C44 elastic constant related to the transverse acoustic phonons) at the magnetic transition, possibly associated to the structural distortion, thus suggesting a coupling between the magnetic excitations and the acoustic phonons [6].
In this context, we have studied in detail the dynamics in GeCo2O4 and particularly focused on the coupling between spin and lattice degrees of freedom in the dynamical regime. We have performed inelastic neutron scattering on IN5 [10], which shows an interesting excitation spectrum around the Brillouin zone center, with acoustic phonons crossing gapped spin waves. Such crossing may hide the presence of hybrid excitations as previously evidenced in the hexagonal multiferroic YMnO3 [7-9]. We have tested this hypothesis and used longitudinal polarization analysis on THALES and IN20 in order to separate the nuclear and magnetic contributions to the inelastic neutron scattering cross section in GeCo2O4. The presence of a novel mode was evidenced in the nuclear scattering. It follows the dispersion of a magnon and disappears above TN, suggesting a spin-lattice hybrid excitation. However, the intrinsic nature of this mode remains unclear and will be discussed in this talk.

Novel insight into $Tb_2Ti_2O_7$ Flavor modes and mixed dipolar-quadrupolar phases

Author: Sylvain Petit[1]

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$Tb_2Ti_2O_7$ has remained an enigma in condensed matter physics, and more specifically in the field of frustrated magnetism, for about two decades [1]. This material evades long-range order down to temperature as low as 20 mK and its ground state exhibits puzzling diffuse magnetic scattering [2,3]. Its low energy spin dynamics includes, on the one hand, an exciton located at about $\hbar\omega$ = 1.5 meV, which shows a significant dispersion [4]; on the other hand, Tb_2Ti_2O7 also hosts an exotic low energy collective mode (≈ 0.3 meV), which is believed to be a hybrid dipolar-quadrupolar mode [5,6].

Using polarized inelastic neutron scattering measurements, I will present a review of the characteristics of this low-energy mode, its dispersion, the evolution of its spectral weight in the Brillouin zone and its temperature dependence. I will then describe RPA simulations, based on a Hamiltonian, which includes both dipolar and quadrupolar couplings [7], yielding spin dynamics which compare quite well with those data. The best set of couplings suggest that $Tb_2Ti_2O_7$ is one of the very rare examples of quantum spin ice, yet very close to several ordered phases, especially a planar antiferromagnetic dipolar phase and a purely quadrupolar one [8,9].

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Magnetically frustrated dynamics on the Cairo pentagonal lattice; $Bi_2Fe_4O_9$

Authors: Andrea Kirsch[1]; Emma Ynill Lenander[1]; Jakob Lass[2]; Kim Lefmann[1]; Pascale Deen[3]

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The octahedrally and tetrahedrally coordinated Fe3+ (S=5/2) ions in Bi2Fe4O9 form a quasi two-dimensional Cairo pentagonal lattice (Pbam). Combined with predominantly antiferromagnetic interactions, this leads to a strong frustration with Tn=245 K while $_{CW} = -1670$ K in a fairly unexplored geometry. The magnetic structure for T<Tn can be indexed with k=(½, ½, ½) with a noncollinear magnetic structure of Fe1 and Fe2 moments, 2 different sites, and an interpenetrating pattern of fourfold spin rotations, a very novel magnetic state.

Previous measurements studying the low-lying excitations, 0–30 meV, in the ordered phase were measured on small single crystals (> 0.6 g). Beauvois et al. (PRL2020) argues that no anisotropy is required while Duc Le et al. (PRL2021) indicates an easy-plane single-ion anisotropy. Accordingly, Beauvois find the acoustic AF mode is not gapped while it is for Duc Le.

We have synthesized a 2.35 g, high quality single crystal of Bi2Fe4O9 and are re-examining the magnetic excitations. Already at energy transfers below 10 meV we see distinct discrepancies between our data and previous data in the ordered phase using CAMEA and EIGER (PSI). Our data show a clear double spin gap, that allows us to differentiate axial and planar anisotropy scenarios. Additionally, we have measured inelastic neutron scattering on IN20 (ILL) with polarization analysis, which has enabled us to study the nature of the anisotropic fluctuations for the different magnetic excitations. All this has been modelled in SpinW with very good agreement.

Multiferroics

Unveiling the Influence of Local Magnetic Distortions in Ho-Doped Langasite: A Complementary Approach Using Polarised Neutron Diffraction and Angular Resolved Magnetisation Techniques

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In this presentation, we will explore the complex magnetic behaviour of Ho-doped langasite ($[La_{1-x}Ho_x]_3Ga_5SiO_{14}$), focusing on understanding how local structural distortions influence the ising-like Ho3+ moments and ultimately the macroscopic magnetoelectric properties. The study leverages complementary experimental evidence, combining polarised neutron diffraction and angular-dependent magnetisation measurements to precisely determine the atomic site susceptibility tensor and reconcile it within the constraints of the local-ionic and global symmetries. The analysis incorporates a novel framework that models the orientations of the Ho3+ ising axes, along with symmetric rotations around the trigonal C_3 axis that restore the global $P312$ symmetry, despite the presence of broken local C_2 symmetry. The conclusions provide insights into the interplay between local distortions, magnetic anisotropies and macroscopic magnetic and magnetoelectric behaviour, underscoring the importance of polarised neutron diffraction in resolving subtle magnetic features that are otherwise obscured in complex materials such as multiferroics and other systems with strong spin-lattice coupling.

Exploring Ferrotoroidic Order in $LiNi_{0.8}Fe_{0.2}PO_4$

Authors: Adheena Painganoor[1,2]; Navid Qureshi[1]; Paul Steffens[1]; Rasmus Toft-Petersen[2,3]; Niels Bech Christensen[2]

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Ferrotoroidicity is the fourth ferroic order characterized by the simultaneous breaking of both time and space-reversal symmetries [1]. The intrinsic magnetoelectric effect associated with this order makes it interesting for energy-efficient memory devices. The ability to pole and control ferrotoroidal domains could prove important for non-volatile and high-density data storage applications. [2]

Lithium orthophosphates, $LiMPO_4$ (M= Mn, Ni, Co, Fe) are a family of antiferromagnets that crystallize in the olivine crystal structure (orthorhombic space group Pnma) and exhibit a magnetoelectric effect below their ordering temperature [3]. The distinguishing factor among these compounds is the preferred orientation of magnetic moment. For instance, in $LiNiPO_4$ and $LiFePO_4$ the magnetic moments are aligned along the c and b axes respectively [4]. For the stoichiometric compounds, the form of the magnetoelectric tensor (α) which connects the electric polarisation to the applied magnetic field is determined by their magnetic point group [5]. Additionally, this family of compounds is notable due to their potential to support ferrotoroidal order. The non-zero off-diagonal elements in α in M=Fe, Co, and Ni suggest the possible existence of ferrotoroidic order [2] which was experimentally confirmed in $LiCoPO_4$ [6].

In this study, we focus on the ferrotoroidic order in the mixed compound $LiNi_{0.8}Fe_{0.2}PO_4$, where Ni sites are doped with Fe. Previous research on this compound identified a distinct low-temperature magnetic phase due to the combined effect of exchange interaction and mismatched anisotropy. Initially, the magnetic moments align along the b-axis below 25 K similar to $LiFePO_4$. However, below 21K they rotate towards the a-axis, a direction different from the easy axes of both parent compounds. In this phase, where we expect four domains, the strength of magnetoelectric coupling is increased by 100-fold [7].

Using spherical neutron polarimetry, we investigated the ferrotoroidic order in $LiNi_{0.8}Fe_{0.2}PO_4$ giving us direct insight into the magnetic domain distribution and poling behaviour under crossed magnetic and electric fields. Our results suggest mixed-anisotropy ferrotoroidal systems to be a promising route towards next-generation storage devices.

References

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Single-crystal investigation of $YBaCuFeO_5$ by spherical neutron polarimetry

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The low ordering temperatures of most non-collinear spiral magnets critically limits their implementation in devices. The layered perovskites $LnBaCuFeO_5$ are a rare case of frustrated oxide family that has raised great expectation as promising high-temperature spiral magnets and chiral spin-driven multiferroic candidates. Though a novel mechanism ("*Spiral order by disorder*") seems to account for the extraordinary thermal stability of their presumed spiral order, such order was alleged on the basis of neutron data on powder samples. Thus far, it has not the support yet from single-crystal studies able to lift ambiguity. A $YBaCuFeO_5$ single crystal has been grown with enough Cu/Fe disorder to stabilize the incommensurate magnetic phase up to T_S ca. 200 K. Here, we unveil the features of its magnetic structures by spherical neutron polarimetry and single-crystal neutron diffraction, demonstrating the non-collinear chiral nature of the magnetic domains in the singular incommensurate phase. It is thus finally proved that such phase is spiral in our crystal, and therefore also in those compositions of this perovskite family where T_S values well above room temperature have been reported. Yet, this study also illustrates critical features of relevance to the search for high-temperature magnetoelectric response induced by the spiral phase.

Chirality

Neutron diffraction in $MnSb_2O_6$: Coupled chiralities in a polar magnet

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Multiferroic materials have been intensively studied these last decades for their interesting physics and their promising magnetoelectric applications [1]. Materials having a crystallographic chirality are particularly interesting in the sense that their structure can couple to magnetism an display novel magnetoelectric coupling mechanisms. This is the case of $MnSb_2O_6$ which crystallizes in the noncentrosymmetric $P321$ space-group. The Mn^{2+} magnetic ions are arranged in a triangular motif in the (ab)-plane, where the magnetic moments are dephased by 120° and follow a cycloidal modulation along the c-axis [2]. The respective sense of rotation of the spins, the so-called magnetic chiralities are directly linked through Heisenberg interactions to the structural chirality, defined as the helical winding of super-super-exchange pathways along the c-axis. This compound was predicted to have a unique ferroelectric switching mechanism, but the magnetic ground state remained ambiguous [2,3]. By a combination of unpolarized and polarized neutron diffraction techniques, we have extensively studied both the nuclear and magnetic structures of $MnSb_2O_6$. We have notably used polarized neutrons to perform Schwinger scattering, sensitive to structural chirality, and spherical neutron polarimetry, sensitive to magnetic chirality, and found out a complex mixture of chiral structural and magnetic domains. We subsequently propose a mechanism leading to electric polarization based on coupled structural and magnetic chiralities [4].

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[4] E. Chan *et al.* Phys. Rev. B **106**, 064403 (2022)

Interplay between structural and magnetic chiralities in $NiCo_2TeO_6$

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$NiCo_2TeO_6$ crystallises in the $R3$ space group where the displacements of the O1/O2 oxygen atoms in the triangular plaquettes lead to left-handed and right-handed structural chiralities [1]. This compound is particularly interesting because an anomaly was observed in the dielectric susceptibility at T_N suggesting the presence of magnetoelectric behaviour [2]. A long-range magnetic order (magnetic space group $R3.1'(00\gamma)ts$) develops below 52 K consisting of ferromagnetically coupled a-b layers of Ni^{2+} that rotate along c with an incommensurate propagation vector k = (0, 0, 0.211) [2]. It is not yet clear if the magnetic helix echoes the feature of two helices of opposite handedness where the globally preferred chirality emerges as a difference between the displacements or if it presents a single chirality. Therefore, we probed the structural and magnetic chiralities using polarized neutrons on the D3 diffractometer at the ILL, following the successful methodology from our previous work on a langasite compound [3]. We studied two $NiCo_2TeO_6$ single crystals, one of each structural chirality. Spherical neutron polarimetry and Schwinger scattering were exploited to deduce the magnetic and structural chiralities, respectively, while our complementary X-rays results yield information concerning the coupling of those two quantities. Our findings constitute an important step towards the understanding of the magnetoelectric properties of this compound.

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Chiral magnetic structures probed by SANS & GISANS

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Chiral magnetic structures in single crystals and thin film structures probed by polarization-analyzed Small Angle Neutron Scattering (SANS) & Grazing-Incidence-SANS are often connected to complex analysis procedures and require the development of individual magnetic models. Additionally, precise data-reduction protocols are needed to distinguish sample scattering from instrumentational effects. The more involved the different interactions in one sample system, the more care has to be taken for a comprehensive understanding as function of, e.g., magnetic field, electric field, temperature, and further parameter sets. The key to a broad understanding then can be given by the comparison of various analysis methods.

Here, I will provide two examples on the complexity of magnetic (GI-)SANS data analysis on different materials: (i) a ferromagnetic/superconducting thin film with temperature dependent chiral magnetic domain walls, and (ii) a magnetoelectric single crystal with chiral magnetic phases depending on temperature, magnetic, and electric field. For study (i) we will compare polarization-analyzed GISANS data on Nb/FePd thin films with perpendicular magnetic anisotropy with results from CD-XRMS, and evaluate our conclusions together with information gained by Density Functional Theory (DFT) [1]. In study (ii), we present the dependence of magnetic chiral phases occurring in the magnetoelectric single crystal $Ba_{2-x}Sr_xMg_2Fe_{12}O_{22}$ [2] as function of temperature and magnetic field.

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Magnetic Fluctuations in FeSi

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Our research focuses on the magnetic properties of FeSi, particularly investigating the potential presence of magnetic chirality through neutron spin-dependent scattering experiments. FeSi, which crystallizes in the P213 space group, shows a distinct increase in bulk magnetic susceptibility with temperature, peaking around T = 500 K. Despite this, it exhibits no long-range magnetic order across the entire temperature range. However, magnetic fluctuations are observed at ambient and higher temperatures. This study expands on previous work exploring the magnetic behaviour of FeSi and the related compound MnSi, which also belongs to the P213 space group. MnSi has been shown to demonstrate a skyrmion lattice phase, a unique magnetic state with chiral fluctuations, which we aim to compare with FeSi.

Using polarized neutron beams and xyz-polarization analysis on the IN12 triple-axis spectrometer, we conducted a detailed examination of the magnetic fluctuations in FeSi. We aimed to determine whether chiral magnetic scattering is an intrinsic feature of crystals with the B20 structure, a crystal structure known for its non-centrosymmetric properties. We measured the differences in neutron scattering intensities for distinct spin configurations and applied flipping ratio corrections to enhance the accuracy of our results. While magnetic fluctuations were observed, the analysis showed only a small chiral component, suggesting that chirality is not a pervasive magnetic feature in FeSi, unlike in MnSi.

Our findings' comparison with the magnetic fluctuations in MnSi provides insights into FeSi's magnetic behaviour that could have a significant impact on the scientific community. It may help explain the enhancement of the topological Hall effect observed in Mn(1-x)Fe(x)Si alloys. These results contribute to understanding the complex magnetic ground states in materials with non-centrosymmetric crystal structures.

Smart materials

Synergy between structure and magnetism in magnetic shape memory alloys

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Ferromagnetic Shape Memory Alloys (FSMAs) are a group of active materials that undergo martensitic transformations induced by temperature, stress and/or magnetic fields, which result in large recoverable mechanical deformations. Their fast response and high energy density makes them ideal candidates for implementation in sensors and actuators. The magnetic properties of FSMAs depend on the interactions between the magnetic moments of atoms that, in turn, depend on the atomic positions within the lattice. Here we present a combination of powder neutron diffraction experiments in a series of polycrystalline samples of 6-element FSMAs with varied Fe content, where the alloys present actuation at temperatures around 370 K. Their atomic site occupancies, the ratio c/a and, therefore, the maximum achievable deformation are calculated for each alloy. Based on the atomic site occupancies and additional measurements of the saturation magnetization in each sample, the influence of the structure and atomic site occupancies on the magnetism in these samples is presented. This study is complemented by single crystal polarized and non-polarized neutron diffraction experiments in one of the samples used for the powder neutron diffraction measurements, from which a single crystal was grown. Together with the atomic site occupancies in the single crystal, the analysis of the polarized neutron diffraction measurements provides us with information about the magnetic moment distribution in each atomic position present in the unit cell of the single crystal. Finally, the element-specific magnetic moments contribution to the magnetism of the alloy are depicted via X-ray magnetic circular dichroism (XMCD) measurements. The combination of the polarized neutron diffraction and XMCD measurements allows us to unravel element and site-specific magnetic moment distributions in the alloy.

Exploiting Advanced Polarised neutron and X-ray synergies to reveal magnetic structure and dynamics in spin caloritronics

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Spin caloritronics a currently a science highlight due to their potential exploitation in the next generation of spintronics applications. The magnetic materials and interfaces at the core of spin caloritronics of materials combine both spintronic and thermoelectric functionalities by interconversion of charge, spin, and heat currents. A prominent example is the spin Seebeck effect (SSE), where the generation of a net spin current is understood in terms of thermal excitation of chiral magnons and converted into a charge current by the inverse spin Hall effect [1]. We present new insights into the physics of the prototypal spin caloritronic compounds, i.e. the rare-earth compensated ferrimagnets Gd3Fe5O12 and Tb3Fe5O12, by exploiting the synergies of polarised neutron and photon methodologies. Polarised inelastic neutron scattering and RIXS experiments identify the chiral magnons involved in the SSE thermoelectric conversion. In addition, recent polarised neutron Lamor diffraction experiments results are presented that could eventually lead to the measurements of the Q-dependent magnon lifetimes in the vicinity of the magnetisation compensation temperatures of this class of materials. Polarised soft X-ray diffraction studies was exploited to reveal new magnetic phase transitions in thin films of Tb3Fe5O12. Finally, ultrafast pump-probe experiments, combined with polarised resonant X-ray scattering, have been used to characterise the heat, phonon and spin dynamics currents in thin films spin caloritronic heterostructures [3].

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Crystal structure and absence of magnetic order in single crystalline RuO_2

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RuO_2 initially attracted interest in the field of catalysts and microelectronics, but the recent report of antiferromagnetic order occurring above room temperature and its identification as an altermagnetic state boosted activities on this material [1,2,3].
The combination of spin splitting otherwise characteristic for ferromagnetic order with the linear magnon dispersion of an antiferromagnetic system may open the path to applications in spintronics and magnonics [4].
However, even the occurrence of magnetic order in RuO_2 was recently questioned by muon and neutron experiments as well as by DFT calculations [5-7] and it was proposed that magnetic order only occurs in the presence of vacancies [5].

We, therefore, performed polarized and unpolarized neutron diffraction experiments on RuO_2 crystals that were characterized by magnetization and electrical conductance measurements as well as by X-ray diffraction [8].
Single crystals were grown by chemical vapor transport using two different transport molecules. In addition a powder sample was obtained by annealing a commercial compound.
The neutron experiments were performed on D9, D3 and IN12 and the crystal structure was investigated on a Bruker D8 venture diffractometer. We were not able to confirm the proposed structural distortion in our crystals down to 2K. There are no superstructure reflections [3] breaking the symmetry of the rutile-type structure in the X-ray and long-wave length neutron experiments. Such peaks are observed for short neutron wave lengths but can be attributed to multiple diffraction. The amount of ruthenium vacancies is below a few per cent in our crystals. Polarized neutron experiments do not indicate magnetic Bragg reflections for the proposed propagation vector of $\vec{k}$=(0,0,0) [3]. Even magnetic order with a five times smaller ordered moment than what is claimed [3] would have yielded significant intensities in our experiment. This antiferromagnetic order can be ruled out in our stoichiometric samples [8].

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Magnetic structure of Mn_3Sn

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Mn_3Sn is one of the first antiferromagnetic compounds to exhibit an anomalous hall effect. Mn_3Sn is a frustrated Kagome metal with a broken time reversal symmetry leading to a non-zero Berry curvature, which in turn leads to a large and controllable anomalous Hall effect.

Depending on the exact stoichiometry of the sample, two main types of Mn_3Sn occur. One type exhibits a temperature dependent phase transition into a non-commensurate magnetic structure at around 280K, a structure which no longer breaks time reversal symmetry and hence does not display an anomalous hall effect.

The magnetic structure is essential for understanding the properties of this material. However, despite years of research, the exact structure remains a topic of debate. Using polarimetry, we here settle the debate, by identifying the exact magnetic structure of Mn_3Sn

In this work, we present our D3 polarimetry data and D23 diffraction data, along with our preliminary findings.

Multipolar order/moments

Detection of magneto-electric multipoles

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The fundamental interaction between the neutron dipolar field and the magnetization density surrounding the scattering ion, lies at the heart of magnetic neutron diffraction. However, if the ion resides in an environment which breaks both time and spatial inversion symmetry, the current formalism for magnetic diffraction does not fully account for all the possible scattering mechanisms arising from the asymmetry of the magnetization density cloud of the scatterer [1].
In our work [2,3], we have extended the theory of magnetic neutron diffraction to include these effects. Drawing analogies from the magneto-electric (ME) phenomena and standard magnetic neutron diffraction, developed a framework to calculate the associated ME form factor, size of the ME multipoles and the ME propagation vector from density functional theory (DFT) calculations.
Furthermore, we have identified several material systems, which can not only host these ions but also display an ordered arrangement of these magneto-electric multipoles. Alongside our DFT calculation of the corrections to the scattering amplitudes and form factor of these multipoles, we used spherical neutron polarimetry to provide evidence for the interactions between neutrons and the long-ranged order of these magneto-electric multipoles in CuO.

On the unusual microscopic magnetisation of some rare-earth and actinide based intermetallic compounds

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To identify commonalities and differences we will compare the unusual microscopic magnetisation of some rare-earth- and actinide-based intermetallic compounds with exotic electronic quantum properties. To this end, we revisited previous results obtained from polarised neutron diffraction for Flipper 2024.

For the intermediate valance compound YbAl3 the field induced magnetic moment is well-described by a Yb3+ free-ion form factor plus a small temperature-independant positive conduction electron polarisation [1]. Similarly, the magnetic moment on the cerium site in the low-charge carrier-density Kondo system CeNiSn is well described with Ce3+ free ion form factor but here a small magnetic moment on the nickel site needs to be added [2]. The situation changes in the itinerant antiferromagnetic system UGa3 in which the orbital contribution to the magnetic moment changes on entering the antiferromagnetically ordered state [3]. Similarly in the normal state of the plutonium-based superconductor PuCoGa5 we observed a form factor significantly different from a conventional Pu3+ ion [4].

Our results demonstrate that not a single theoretical model is applicable to all such intermetallic systems. The microscopic information obtained by polarised neutron diffraction remains invaluable to understand the magnetic ground state of such compounds which is at the origin of a large spectrum of electronic quantum phenomena.

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Superconductivity

Hidden Magnetic Texture in the Pseudogap Phase of the High-Tc Superconducting $YBa_2Cu_3O_{6+x}$

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Despite decades of intense investigations, the origin of the enigmatic pseudogap phase of high-Tc superconducting cuprates remains an unsolved mystery. In the last 20 years, condensed matter physicists discovered that this mysterious phase hosts symmetry breaking states such as an intra-unit cell (or q=0) magnetism preserving the lattice translational (LT) symmetry and breaking the time-reversal and parity symmetries [1]. This q=0 magnetism gives rise to magnetic scattering on top of nuclear Bragg peaks and is interpreted in terms of loop current (LC) patterns accompanied by anapoles (or polar toroidal moments) [1]. It is followed, upon cooling, by an additional incipient charge density wave breaking the LT symmetry. However, none of these states can (alone) account for the partial gapping of the Fermi surface.

Our recent polarized neutron diffraction measurements in $YBa_2Cu_3O_{6+x}$ single crystals with different hole doping levels [2,3] reveal a novel hidden magnetism that breaks LT symmetry and that may be crucial to elucidate the pseudogap puzzle. This short-range magnetism (with typical correlations over 5-6 unit cells) is carried by the CuO2 layers and settles in at T*. Distinct from the q=0 magnetism, the related magnetic signal appears at the planar wavevectors of the form q=(0.5,0) and (0,0.5), yielding a (2x2) quadrupling of the magnetic unit cell within the [a,b] plane (q=½ magnetism). The associated magnetic moment is strongly anisotropic, predominantly pointing perpendicular to the CuO2 planes, which is consistent with the picture of a LC state as the microscopic origin of the q=½ magnetic correlations. Finally, the q=½ magnetism vanishes in the overdoped regime, following the doping dependence of the pseudogap [3].

We discovered that the q=0 and q=½ magnetisms could be embedded within a single complex and highly spread-out chiral magnetic texture of LCs consisting in an anapole vortex-like pattern accounting for the q=½ magnetism binding larger ferro-anapolar domains of the q=0 magnetism. Such a magnetic texture is consistent with the recent proposal of LC supercells, breaking the LT symmetry and able to account for the pseudogap opening [4]. The existence of such broad entities reveals an unexpected aspect of the pseudogap physics that may modify our understanding of this state of matter.

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Search for orbital magnetism in the kagome metal CsV_3Sb_5

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Kagome metals of the AV3Sb5 types with A={K,Cs,Rb} are under the spotlight recently due to their non-trivial topological Z^2 nature and their strongly correlated electronic phases at low temperature reminding the ones of High-Tc superconducting Cuprates. For instance, CsV3Sb5 exhibit both a charge density wave phase below 94K with a 2x2 doubling of the unit cell and a superconducting phase below 2.5K [1]. These materials also show strong anomalous Hall effect, but no spin ordering has been found in these compounds both by muon spin spectroscopy and neutrons diffraction. To explain this without relying on spins the possibility of an chiral flux phase / orbital magnetism coming from a chiral flux pahse, emerging alongside the charge density wave, has been theoretically proposed [2,3]. This phase would be similar to the current loop phase predicted in cuprates which can explain the weak magnetism found at [1 0 0] in several cuprates and at [1/2 0 0] in YBaCu3O7-x [4]. To check for the presence of this orbital magnetism in Kagome materials we carry out neutrons diffraction experiment on IN22 triple-axis spectrometer at ILL. Most models predict this chiral flux phase to produce magnetic intensity at M1=[1/2 0 L] or M2=[1/2 1/2 L] reciprocal space positions with L={0,1/2} [2,3]. We investigated both positions by polarised neutrons diffraction. For the first one, no magnetic signal has been observed ruling out the possibility of having a magnetic moment larger than 0.01 uB by vanadium atoms. However, measurement on M2 do not exclude the possibility of a magnetic signal corresponding to a moment of 0.02 ± 0.01 uB by Vanadium atoms. This show that current models have to be refined whether toward a lowering of the expected magnetic moment or toward a different orbital magnetism pattern giving rise to magnetic intensity at different reciprocal space positions to be compatible with our measurements. This work has been experimentally challenging and went close to the limit in precision obtainable with polarised neutron in a reasonable measurement time, Our results are on the process of being published in Physical Review B [5].

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Molecular magnetism

Multi-Technique Experimental Benchmarking of the Local Magnetic Anisotropy of a Cobalt(II) Single-Ion Magnet

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A comprehensive understanding of the ligand field and its influence on the degeneracy and population of d-orbitals in a specific coordination environment are crucial for the rational design and enhancement of magnetic anisotropy of single-ion magnets (SIMs). Herein, we report the synthesis and comprehensive magnetic characterization of a highly anisotropic Co^{II} SIM, $[L_2Co](TBA)_2$ (L is an N,N -chelating oxanilido ligand), that is stable under ambient conditions. Dynamic magnetization measurements show that this SIM exhibits a large energy barrier to spin reversal $U_{eff} > 300K$ and magnetic blocking up to 3.5 K, and the property is retained in a frozen solution. Low-temperature single-crystal synchrotron X-ray diffraction used to determine the experimental electron density gave access to Co d-orbital populations and a derived U_{eff}, $261cm^{-1}$, when the coupling between the $d_{x^2-y^2}$ and d_{xy} orbitals is taken into account, in very good agreement with ab initio calculations and superconducting quantum interference device results. Powder and single-crystal polarized neutron diffraction (PNPD, PND) have been used to quantify the magnetic anisotropy via the atomic susceptibility tensor, revealing that the easy axis of magnetization is pointing along the N–Co–N′ bisectors of the N,N′-chelating ligands (3.4° offset), close to the molecular axis, in good agreement with complete active space self-consistent field/N-electron valence perturbation theory to second order ab initio calculations. This study provides benchmarking for two methods, PNPD and single-crystal PND, on the same 3d SIM, and key benchmarking for current theoretical methods to determine local magnetic anisotropy parameters.

The results of the work are published in [1].

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Open-shell borazine: synthesis and magneto-structural relationships

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Borazine ($B_3N_3H_6$) is a heterocyclic compound made of alternating boron and nitrogen atoms, known as the "inorganic benzene" because the C=C and B=N bonds are isostructural and isoelectronic. Despite such similarities with benzene, the borazine ring has very different electronic properties due to significant differences in electronegativity between the boron and nitrogen atoms.
We synthesized the first example of borazine functionalized by nitroxide free radicals: the N,N',N"-tris(4 Bromophenyl))-B,B',B"-tris((2,6-dimethyl-4-(N-tert-butyl-N-oxyamino)phenyl)borazine (simplified as Borazine-B-Tris-Nitroxide), in order to study whether the nitroxide radicals could be coupled via the borazine ring and comparatively with other π-conjugated systems.
We will show that the molecule exhibits crystalline polymorphism that differently affects the magnetic properties of these systems. Two phases were isolated and their magneto-structural investigated. To explore where the unpaired electrons are localized in the crystal we completed this work with the mapping of charge and spin densities using high-resolution X-ray and polarized neutron diffractions.
All together, these studies help to rationalize for the first time.the relationships between structure, magnetic properties and exchange interactions involving the borazine core.

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Topological materials

Diffuse SANS signatures of the DMI

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The antisymmetric Dzyaloshinkii-Moriya interaction (DMI) arises in systems with broken inversion symmetry and strong spin-orbit coupling. In conjunction with the isotropic and symmetric exchange interaction, magnetic anisotropy, the dipolar interaction, and an externally applied magnetic field, the DMI supports and stabilizes the formation of various kinds of complex mesoscale magnetization configurations, such as helices, spin spirals, skyrmions, or hopfions. A question of importance in this context addresses the neutron scattering signature of the DMI, in particular in polycrystalline bulk materials and random nanoparticle assemblies, where the related magnetic neutron scattering signal is diffuse in character and not of the single-crystal diffraction-peak type, as it is e.g. seen for a skyrmion lattice in the B20 compounds. In this talk we discuss (i) the effect of the DMI in spherical FeGe nanoparticles on the randomly averaged magnetic neutron scattering observables, more specifically on the spin-flip small-angle neutron scattering cross section, the related chiral function, and the pair-distance distribution function. Additionally, (ii) recent theoretical results regarding the diffuse scattering signatures of two types of stable hopfions in the SANS observables are presented, and (iii) experimental data for the less well studied microstructural defect-induced DMI are discussed.

Solving Multi-q Incommensurate Magnetism in a Europium Triangle Lattice Material

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Recently, centrosymmetric lanthanide metals have been the subject of intense research due to the discovery of skyrmions in materials such as Gd_2PdSi_3, $GdRu_2Si_2$, $Gd_3Ru_4Al_{12}$, $EuAl_4$, and $EuNiGe_3$. In this talk, I will present work on a europium triangle lattice compound in this family. Through spherical polarimetry using CRYOPAD at ThALES and polarized SANS measurements at D33, we demonstrate the existence of one single-q cycloidal and two multi-q vortex lattice states with unusually low symmetry propagation vectors. These unusual propagation vectors motivated the development of new SANS data visualization and analysis tools. I will also discuss how these states are deeply intertwined with the electronic structure of the material, and what insights this may provide for the design of new multi-q materials.

Polarized neutron instrumentation

Polarized Neutron Capabilities of the HYSPEC spectrometer at SNS

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The HYSPEC spectrometer at the Spallation Neutron Source combines time-of-flight spectroscopy with focusing Bragg optics, facilitating both unpolarized and polarized neutron scattering experiments. Polarization analysis of scattered neutrons is achieved using a multi-channel array of 960 FeCoV-based supermirror polarizers, spanning 60 degrees horizontally and ±7.5 degrees vertically. The sample region is highly configurable to support various polarization optics. An elevator/oscillator system allows for swift transitions between unpolarized, half-polarized, and full polarization analysis modes, enhancing flexibility and convenience. The current polarization capabilities at HYSPEC are demonstrated through recent polarized elastic and inelastic scattering studies on several magnetic materials. Particularly, I will showcase the results of a linear XYZ-polarization study on the antiferromagnetic and paramagnetic states of an MnO single crystal subjected to uniaxial pressure along the [110] crystallographic direction.

Polarised neutrons for users at ESS

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Polarised neutrons have long been used to study magnetism. Polarisation analysis also provide a complementary tool to deuteration in the determination of coherent and single-particle motions in soft matter studies. In addition, Neutron Spin Echo has been used extensively in the studies of dynamical processes in soft matters. In fundamental physics, the search for the neutron electric dipole moment and the study of symmetry violation are two examples that use polarised neutrons. To meet the coming user demand, twelve of the fifteen ESS instruments [1] under construction aim to offer polarised neutrons for user experiments. They include an imaging instrument (ODIN), a SANS instrument (SKADI), two reflectometers (ESTIA, FREIA), three diffractometers (DREAM, HEIMDAL, MAGiC), and four spectrometers (BIFROST *, CSPEC, MIRACLES, T-REX). In conjunction with in-kind contributions and instrumentation grants, the ESS Polarisation Project will support eight of the eleven instruments to incorporate polarisation analysis capabilities [2]. An update of the project will be presented alongside examples on the use of polarised neutrons in both magnetism and soft-matter studies.

* See presentation by Kristine M. L. Krighaar

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Polarisation analysis concept for the BIFROST spectrometer at ESS

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The BIFROST spectrometer at the upcoming neutron source ESS in Lund (S) will be a game-changer for the study of quantum materials, such as frustrated magnets, quantum magnets and superconductors. The spectrometer utilizes a multiplexing backend on an indirect geometry time-of-flight (ToF) front end. The primary spectrometer enables an unprecedented polychromatic sample flux exceeding $7 \cdot 10^9$ n/s/cm^2 at 2 MW accelerator power, with a bandwidth of 1.7 Å, whilst retaining a primary spectrometer resolution $\Delta E_i/E_i$ of 4 \%, common in cold neutron spectroscopy. The multiplexing backend consists of 9 Q-channels, each containing 5 fixed analyzers probing a scattered neutron energy range of 2.7 to 5.0 meV. The analyzers utilize the graphite crystal mosaicity combined with position sensitive neutron detectors to gain continuous energy sensitivity, resulting in a back-end energy resolution considerably better than on a classical Triple Axis Spectrometer.

For the study of quantum materials, use of the technique of neutron polarisation analysis will yield additional and crucial information about the structure and dynamics in the materials. However, the wide angular coverage of BIFROST presents a technical challenge to implement polarisation analysis. Futhermore, for many quantum materials studied on BIFROST, polarisation analysis will be used together with high magnetic fields. Together with the requirements imposed by the time-of-flight nature of the instrument, a polarising supermirror based wide-angle analyzer is the only suitable method that is currently available.

In this work, we present current work in progress on McStas simulations of BIFROST together with the design concept of polarisation analysis. The concept consists of a V-cavity polarizer[1] and a device that can perform neutron wide-angle polarisation analysis in an applied field. The analyzer design follows a recent proposal with polarising supermirrors, bent into the shape of a logarithmic spiral [2]. This would reflect neutrons with the unwanted polarisation direction, and let them be absorbed in the BIFROST radial collimator. Hence, neutrons with the desired polarisation direction would continue undisturbed into the BIFROST analyser-detector system. This setup is compatible with having a high-field magnet on the sample position.

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Posters

Spin-density studies of the multiferroic metal–organic compound $[NH_2(CH_3)_2][FeIIIFeII(HCOO)_6]$

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Metal–organic frameworks combining two or more properties have been the focus of interest of several research groups in the last few decades. A good approach to achieve this combination has been the design of perovskite-like metal–organic frameworks where a three-dimensional network made of metallic centres linked through organic ligands, which presents magnetic order, also accommodates counterions responsible for electric order. One of these examples is the mixed-valence iron(II)–iron(III) formate compound [NH2(CH3)2][FeIIIFeII(HCOO)6].
Previous results revealed that upon cooling, the magnetic moments of the Fe(II) and Fe(III) sublattices do not order simultaneously: the magnetization of the Fe(II) sublattice increases faster than that of the Fe(III) sublattice because of the larger value of the saturation magnetization of the latter.[1] Unpolarized neutron diffraction measurements at 2 K with no external field revealed some discrepancies in the saturation value of the magnetic signal on the Fe(III) sites and in the ferromagnetic moment along the c axis. These discrepancies could be related to the actual distribution of magnetic moment, since unpolarized neutron diffraction gives information on the magnetic moment localized only on the magnetic ions. Polarized neutron diffraction allows an analysis of the magnitude of the spin density over magnetic and nonmagnetic ions (the organic ligand and the counterion), which can give a clue to explain the low saturation on the Fe(III) sublattice and the correlation with the physical measurements.
The present study also contributes to the understanding of the magneto-electric behaviour of this compound, giving insight into the role of metal disorder in the origin of the structural phase transition, which is responsible for its antiferrolelectric order, and into the influence of spin-density delocalization on its magneto-electric properties, allowing a discussion of the alternative explanations given so far for its electric properties at low temperature. [2]
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Spin-resolved electron density on a tri-radical borazine

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The first experimental electron density study of a borazine core was conducted by Guzman et al.[1]. This study allowed for the analysis of charge delocalization (Figure 1.b) in the core of an unsubstituted borazine and confirmed the very low aromaticity of this core compared to a benzene ring.\\\\
Recently, the D. Luneau team focused on the magneto-structural properties of radicals based on a borazine core by performing substitutions on the boron atoms, thereby enabling the study of the influence of these substituents on the borazine core [2]. This work led to the synthesis of new compounds, including a tri-phenyl borazine (B, B', B"-trimethyl-N, N', N"-triphenylborazine) and an open-shell (nitroxide radical) borazine (Figure 1a). In collaboration with our team, a charge density study was conducted on the tri-phenyl borazine using the Hansen and Coppens multipolar model [3]. From a magnetic perspective, spin density maps derived through maximum entropy methods based on polarized neutron diffraction data (ILL Grenoble) collected on a borazine with nitroxide radical groups provided key insights. On the one hand, no intramolecular couplings were observed (no spin density on the borazine core), but inter-molecular ferromagnetic couplings between nitroxide radicals located on parallel layers were identified (Figure 1.c).\\\\
To further analyze these couplings, we are currently refining the experimental electron density, which will serve as a starting point for joint refinement using polarized neutron and high-resolution X-ray diffraction data with the spin split model [4]. This study will allow us to map the spin-resolved electron density of the tri-radical borazine and perform charge integration using Bader's theory, thus leading to a more precise analysis of the influence of nitroxide radicals on the borazine core and its crystalline magnetic behavior.

Understanding the magnon dynamics in $LuFeO_3$ for magnonics applications

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Magnonics is a multidisciplinary field of research focusing on the study and application of magnons in information processing and technology [1]. Magnons can carry the spin information through thermally generated spin-wave spin currents over the large distances [2]. Insulating antiferromagnets (AFMs) are promising for next-generation high-density and high-speed spintronic applications due to their negligible stray field and ultrafast spin dynamics [3]. Especially, non-collinear AFMs with high magnon velocities corresponding to terahertz frequencies are greatly appreciated [1, 4]. In view of the technological prospects LuFeO3 has attracted the attention [4]. We report here the magnon dynamics based on the inelastic neutron scattering studies performed on the single crystal of LuFeO3. The measured magnon dispersions along the (011) matches well with the simulated results obtained using the Holstein-Primakoff theory for the present antiferromagnets. Our analysis including the simulated and experimental results revealed that magnon propagates into such material with supersonic velocities of more than 20 kms−1. This source of short wavelength magnon carriers opens the new prospects for terahertz antiferromagnetic magnonics and logic devices at terahertz frequencies.
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A two-dimensional square-lattice compound with Jeff = 1/2 magnetic moments

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The interplay between the quantum effects from low-dimensionality and the spin-orbit coupling leads to exotic ground states with unusual excitations. Among the diverse 2D spin systems, the S = ½ 2D square lattice has piqued the curiosity of researchers due to its connection with the High-Temperature Superconductivity (HTSC). Studying the Crystal electric field (CEF) and spin-orbit coupling (SOC) effects in a Jeff = ½ 2D square lattice magnets is one of the recent fundamental interests in condensed matter physics. While a few transition metal-based square lattice materials exist, the experimental exploration of rare-earth magnetic materials with a perfect 2D square lattice structure is very limited. Herein, we report the structural, magnetic, heat capacity, and electronic structure studies of Bi2REO4Cl (RE = Yb, Er), which constitutes a structurally perfect 2D square lattice with rare-earth magnetic ions. The magnetization and heat capacity data analysis confirms that both the Yb3+ and Er3+ ion host the spin-orbit driven Jeff = ½ state at low temperatures. The Curie-Weiss temperature for the low-temperature region in the case of Bi2YbO4Cl and Bi2ErO4Cl comes out to be -1 K and -2.1 K, implying the presence of antiferromagnetic (AFM) coupling between the magnetic moments. The heat capacity measurements for Bi2YbO4Cl reveal a broad peak at 0.3 K, suggesting the development of short-range correlations. In contrast, Bi2ErO4Cl exhibits magnetic long-range order at 0.47 K. Our first-principles calculations based on density functional theory provide further insight into the crucial role of spin-orbit coupling and magnetic anisotropy of the spins.

A diffuse scattering in a single crystal of $Cd_{0.9}Zn_{0.1}Te$

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Semiconductors with composition A1−xBxC find widespread applications in solid-state devices due to their tunable bandgap. Cd0.9Zn0.1Te is a very attractive ternary semiconductor material for x-ray and gamma-ray detectors. Single-crystal diffuse scattering provides very detailed information about the local structure. We have measured diffuse scattering in a single crystal of Cd0.9Zn0.1Te using a state-of-the-art laboratory diffractometer. Cd0.9Zn0.1Te single crystals were grown by the vertical Bridgman method in graphitized quartz ampoules from stoichiometric charges of high-purity (6 N) source components. A small amount of In (~1017 at/cm3) was added to the charge. As a result, the Cd0.9Zn0.1Te single-crystal ingot with a diameter of 20 mm and a length of 60 mm was obtained. A large-box atomistic simulation of a model crystal is used in conjunction with Monte Carlo modeling and the Kirkwood potential. A combination of structural relaxation in the presence of the dopant and thermal motion results in good qualitative agreement between the computed diffraction patterns of the model crystal and the measured x-ray patterns. The atoms are shown to displace predominantly in ⟨1,1,1⟩ and ⟨1,0,0⟩ type directions. So, we show that state-of-the-art laboratory equipment allows to record single-crystal diffuse scattering in addition to the Bragg peaks, making this technique accessible in a laboratory setting.

Acoustic Instabilities of $CuFe_2O_4$

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Motivation

The tetragonal distortion in spinel structures, such as $CuFe_2O_4$, $CuCr_2O_4$, and $NiCr_2O_4$, has garnered significant attention due to its profound influence on structural and magnetic properties [1]. Among these, $CuFe_2O_4$ is unique as it is ferromagnetic at room temperature. The tetragonal distortion in $CuFe_2O_4$ has been explained using semicovalent bonding [2] and the Jahn-Teller effect [3]. The transition from a tetragonal to a cubic structure upon heating has been the subject of ongoing research. Bertaut [4] initially proposed a transition temperature of 760℃, but subsequent studies by Miyahara and Ohnishi [5] using high-temperature X-ray diffraction and heat analysis corrected this value to approximately 400℃. This transition occurs below the magnetic Curie temperature, highlighting the coupling between structural and magnetic properties. Additionally, Takei et al. [6] and Forrer et al. [7] observed anomalies near 390℃, consistent with this structural phase transition. These findings motivate further studies on $CuFe_2O4$ to understand its temperature-dependent structural transitions, magnetoelastic coupling, and associated changes in elastic constants. Such investigations provide key insights into the material's fundamental physics and potential applications in magnetostrictive and multiferroic devices.

Findings and future plan

$CuFe_2O_4$ demonstrates complex structural and acoustic transitions driven by temperature variations. The tetrahedral structure transitions to a cubic phase with increasing temperature as evidenced by X-ray diffraction. Elastic neutron scattering reveals temperature-induced changes in the Lorentzian scale and width. The scale decreases with increasing temperature, while the width broadens, indicating evolving elastic properties. These trends align with fitting models, confirming the consistency of our interpretation.
Inelastic neutron scattering along $\mathbf{Q} = [1, \bar{1}, 0]$ at room temperature reveals the relationship between the Lorentzian peak position and the acoustic rate. The acoustic rate, defined by the Lorentzian peak position, is directly linked to the elastic constant c_{11}-c_{12}. Shifts in the Lorentzian peak position and width with increasing temperature provide insights into the softening of elastic constants, with our fittings confirming these trends.
Future experiments will refine the understanding of these transitions, expanding measurements of elastic constants and exploring scattering along additional directions. These efforts aim to advance knowledge of the interplay between structural, acoustic, and magnetic properties in $CuFe_2O_4$.

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Spherical neutron polarimetry at MAGiC

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Spherical neutron polarimetry has been routinely established using Cryopad [1], measuring in zero-field the full polarization tensor for single Bragg peaks. This is a precise tool perfectly suited for monochromatic instruments at reactor sources. How to achieve this goal at ESS and at pulsed sources in general with polychromatic beams?
There are two feasible solutions. Since such experiments are essentially not limited by flux, a straightforward solution for pulsed sources would be to use the Cryopad as a sample environment at instruments that are already equipped for longitudinal polarization analysis.
Here we consider an alternative approach based on a precession technique [2,3] that can be fully adapted to a pulsed, polychromatic neutron beam to cover a large section of the reciprocal space in time-of-flight Laue diffraction. Since this method accepts the non-precessing component for polarization analysis, it applies as well to inelastic scattering. In order to make use of the full wavelength band, the $\pi/2$-flipper, which initiates the precession mode, needs to be ramped in time according to the neutron's wavelength and its time-of-flight. A common phase of the precession angle at the sample is not a necessary requirement but can be favorably achieved by an additional spin-echo setup. For an instrument like MAGiC at ESS, spherical polarization analysis can be a straightforward extension of the existing setup for longitudinal polarization analysis. We are considering this potential upgrade for the MAGiC instrument and present a relatively simple scheme how to modify the magnetic field setup for the incoming beam to enable spherical polarimetry. Full simulations of the polarized neutron transport not only demonstrate the feasibility of spherical polarimetry but also its excellent performance.
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Mysterious incommensurate Dy^{3+} magnetic ordering in $DyFeO_3$. Spherical neutron polarimetry study

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$DyFeO_3$ is the only known rare-earth orthoferrite with an incommensurate magnetic ordering of the rare-earth element without an external magnetic field [1,2]. $DyFeO_3$ establish the ordering of the Fe^{3+} sublattice, according to the Γ4 representation (magnetic space group $Pb'n'm$) below T_N = 645 K. Below the spin-reorientation temperature T_{SR} ≈ 65 K magnetic moments rotate into the Γ1 ($Pbnm.1$) Fe^{3+} structure with symmetry forbidden ferromagnetic component, making it suitable for spherical neutron polarimetry studies.

Our unpolarized single crystal neutron diffraction (IN12, ILL) measurements show the temperature evolution of $DyFeO_3$ satellites at zero magnetic field below 4 K [3]. It is worth comparing it with $TbFeO_3$ [4] which orders incommensurately in a solitonic lattice in the applied magnetic field (~ 3 K and H > 1 T). Both show long modulation periods ($DyFeO_3$ 280 Å and $TbFeO_3$ 340 Å) and higher order satellites ($DyFeO_3$ up to 7^{th} order, $TbFeO_3$ up to 11^{th} order). However, in $DyFeO_3$ the intensity ratio between satellites suggests triangular modulation ($1/n^2$), while for $TbFeO_3$ it is square-like (1/n), where n is the satellite order. $DyFeO_3$ and $TbFeO_3$ have different modulation vector directions, [00l] and [0k1], respectively. The formations of incommensurate order in $DyFeO_3$ and $TbFeO_3$ are of first-order and second-order type, respectively.

The incommensurate magnetic order of Tb^{3+} in $TbFeO_3$ is reported as the solitonic lattice [4], while for Dy^{3+} magnetic ordering in $DyFeO_3$, three models are proposed in the literature: (i) spin density wave [1], (ii) elliptical-based helical ordering [1], and (iii) spin density wave on the top of commensurate ordering [2]. Our half polarization analysis on $DyFeO_3$ [3] shows no magnetic chirality term and our spherical neutron polarimetry analysis supports the spin density wave ordering model over the helical ordering model (both measured on TASP, PSI). Surprisingly, we observed a high value of the Pxz component of the polarization matrix measured on magnetic satellite peaks, in contradiction with all models proposed in the literature [1,2]. According to the Blume-Maleev equations, the Pxz component arises from nuclear-magnetic interference, however, high values of the Pxz term were observed for (001)±q and (003)±q satellite peaks, which are pure magnetic as (001) and (003) commensurate peaks are nuclear-forbidden. Spherical neutron polarimetry data were collected very recently and we are working on the model of the Dy^{3+} magnetic ordering in $DyFeO_3$.

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D007: a new instrument for neutron diffuse scattering with polarization analysis

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The ILL is finalising the construction of the D007 neutron diffuse scattering spectrometer. The instrument makes use of neutron polarization analysis to provide a clean and unambiguous separation of the magnetic, incoherent, and structural contributions to the scattering. It replaces D7, which made major contributions in the study of frustrated magnetism, short-ranged order and the dynamics of soft matter. D007 represents a major upgrade over its predecessor, with calculations predicting more than a ten-fold increase in the flux without a major change in the resolution [1]. The instrument will offer improved capabilities over D7, which was used to measure diffraction from liquids, powders, and single crystals. Time-of-flight spectroscopy, previously possible but challenging on the old D7, will now be viable due to the flux boost and cleaner thanks to the installation of frame-overlap suppression.

D007 received its first neutrons in 2024, with initial measurements qualitatively confirming the predictions. Further development is proceeding with the installation of the new chopper system for spectroscopy and new two-dimensional position-sensitive detectors, and with technical issues discovered during initial tests being resolved. The instrument will be finished and introduced into the user programme in 2025.

This contribution will introduce the layout and instrument goals for D007, describing the upgrades over D7, and will present the results from the preliminary measurements to test its performance.

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D3 - The polarised hot neutron diffractometer

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With its long and successful history, D3 is a reference in polarized neutron diffraction. D3 is a hot neutron two-axis diffractometer (mainly) dedicated to magnetic studies in single crystals using polarised neutrons. D3 offers 3 main configurations:

- In the high magnetic field, half-polarised option precise magnetic form factors are measured which can be modelized to describe the ground state of the magnetic ions. Accurate 3-dimensional magnetisation densities in real space are extracted, which evidence fine details of the magnetic order. Local susceptibilities can be also determined. A number of magnetic materials, ranging from metallic alloys to molecular magnets, as well as superconductors are routinely investigated with this technique.
- The spherical polarimetry mode (Cryopad), with polarisation analysis, allows one to unambiguously determine complex (antiferro)magnetic structures, often indistinguishable by unpolarised approaches. In the cases of e.g. multiferroics, unique information is extracted about the character and population of magnetic domains. Finally, Schwinger scattering assesses the coupling of magnetic and structural chiralities. Topological magnetic materials, chiral magnets, multiferroics and other magneto-electric systems are among the main topics addressed by this technique.
- A multi-detector covering a 20° angular range, along with vertical polarisation analysis, broadens the use of D3 beyond single crystals. It allows measurement of liquids, amorphous and powders, as well as diffuse scattering in single crystals, making possible e.g. the separation of coherent and spin-incoherent scattering in hydrogenous liquids, or detecting magnetic diffuse features in frustrated systems.

Over the years, D3 has proved very useful in all areas of magnetism: superconductors, GMR, multiferroics, chiral magnets, magnetic shape memory alloys, magnetocaloric compounds, molecular magnetism… Due to its unique capabilities, D3's impact is often decisive in the understanding of fundamental phenomena. In recent years, new trends have been identified towards hot topics like topological materials, multipolar orders, or altermagnets. Together with the exceptional capabilities of the instrument, the improvements made in data analysis make D3 a precious tool accessible for a broad user community.