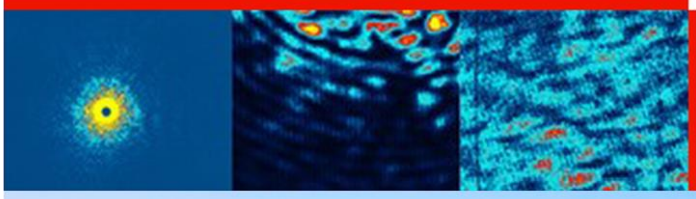

REXS2022

RESONANT ELASTIC X-RAY SCATTERING

28th June to 1st July 2022

Paris, campus Pierre et Marie Curie

Amphitheatre 25

Abstract Booklet

Information

https://www.synchrotron-soleil.fr/en/events/rexs2022

Overview

Following the success of the past editions (NSLS2 2019, DESY 2016, Oxford 2013, Aussois 2011), **the 5th international conference on Resonant Elastic X-ray Scattering** is hosted in Europe again.

The goal of the conference is to bring together the expanding REXS community, to share recent scientific achievements, reporting on current experimental capabilities, and discussing future challenges and opportunities. Particular attentions are focused on multimodality and x-ray coherence in REXS. A series of introductory lessons are dedicated to students and non-experts on the first day of the conference, as well as tutorials during the conference. A tour of SOLEIL is possible.

Topics are including:

- Electronic orderings, magnetism, interfacial phenomena, quantum materials, soft matter, phase transitions and inhomogeneity;
- Symmetry, topology, artificial structures, reduced dimensionality, structure and dynamics;
- Coherence, imaging, nanodiffraction, reflectivity, polarization and energy analysis (REXS in RIXS);
- Instrumentation development, multimodality….;
- Theory and simulation, modeling and data analysis;
- New possibilities using coherence based on diffraction limited sources and XFELs;
- New possibilities using laboratory experiment such as HHG.

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Bienvenue à REXS 2022

Après le succès des éditions précédentes (NSLS2 2019, DESY 2016, Oxford 2013, Aussois 2011), la 5e conférence internationale sur la diffusion élastique résonante des rayons X (REXS) est à nouveau organisée en Europe.

L'objectif de la conférence est de rassembler la communauté REXS en pleine expansion, de partager les réalisations scientifiques récentes, de rendre compte des capacités expérimentales actuelles et de discuter des défis et opportunités futurs. Une attention particulière est portée sur la multimodalité et la cohérence des rayons X dans REXS. Une série de cours d'introduction est dédiée aux étudiants et aux non-experts le premier jour de la conférence, ainsi que des tutoriels pendant la conférence. Une visite de SOLEIL est organisée.

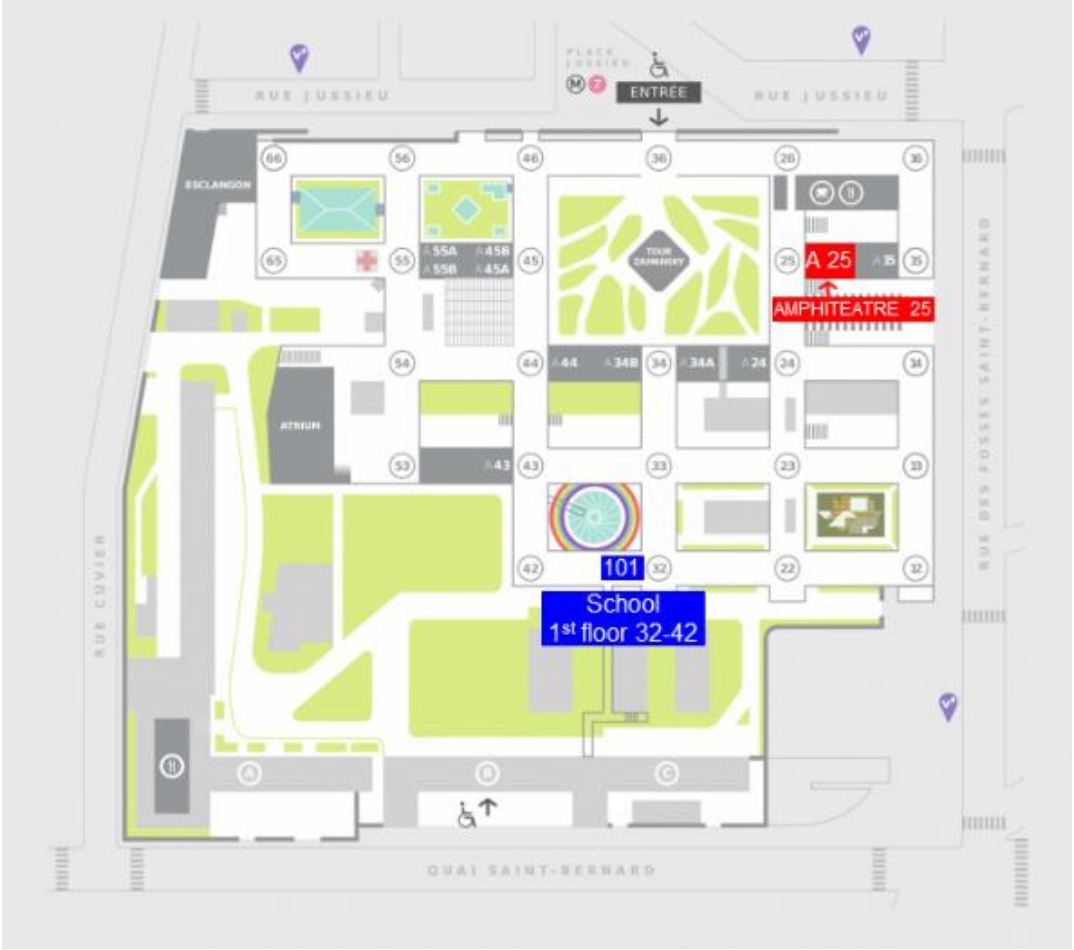
Les sujets abordés comprennent :

- Ordres électroniques, magnétisme, phénomènes interfaciaux, matériaux quantiques, matière molle, transitions de phase et inhomogénéité ;
- Symétrie, topologie, structures artificielles, dimensionnalité réduite, structure et dynamique ;
- Cohérence, imagerie, nanodiffraction, réflectivité, polarisation et analyse de l'énergie (REXS dans RIXS) ;
- Développement d'instruments, multimodalité... ;
- Théorie et simulation, modélisation et analyse des données ;
- Nouvelles possibilités utilisant la cohérence basée sur les sources à diffraction limitée et les XFELs ;
- Nouvelles possibilités utilisant des expériences de laboratoire telles que le HHG

Practical information

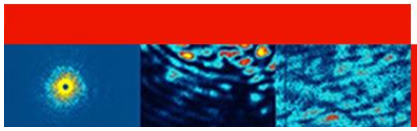
Access to conference

Information on how to access the conference can be found on the event's website https://www.synchrotron-soleil.fr/en/events/rexs2022. The main part of the conference will be at the Amphitheatre 25 (in red in the scheme below). The school on Tuesday morning will be in room 101, first floor of the 32-42 corridor (in blue in the scheme below).



Currently, there is no sanitary restriction in France, and you will not be asked for a health pass.

Eduroam is available everywhere on the campus, but specific wifi login will be distributed during the welcoming for those who needs it. To use them, you are accepting the rules http://www.actesreglementaires.sorbonne-universite.fr/_resources/statuts-RI/sorbonne-universite-reglement-interieur.pdf. Please select the network **congress, o**pen your browser, when redirected to the authentication portal, enter your login and password. If your browser doesn't redirect you automatically, enter this address : https://congres-wifi.sorbonne-universite.fr.



REXS2022

RESONANT ELASTIC X-RAY SCATTERING

Program
Link : https://www.synchrotron-soleil.fr/en/file/13962/download?token=QGGyTeln

Welcome: You will be given a conference badge at the welcome desk situated at the patio close to Amphiteatre 25. You will have to wear it during the 4 days of the conference.

Break and lunch: Will be provided with disposable dishes, so do not hesitate to bring your cup and water bottle to avoid too much waste.

The poster session
The poster session will take place throughout the conference at Jussieu. It will be possible to put the posters in landscape or portrait format from Tuesday to Friday.

Oral presentation
The contributed oral presentation will be 20 minutes long with additional 5 minutes for questions while the invited talks will be 30 minutes long with additional 5 minutes for questions. For the presentation, you will be able to use your own computer (HDMI or VGA connection) or upload your presentation on a conference laptop (windows, ppt and pdf) before the start of your session.

Half day at SOLEIL
To access the SOLEIL site (L'Orme des Merisiers - Saint-Aubin, 91192 Gif-sur-Yvette), you will need to present an ID at the Reception.
Registration for the visit of SOLEIL is closed. If you finally wish to come, please send us an email as soon as possible. A bus transfer is organized from the campus of Jussieu and back to it. If you don't remember your choice, please have a look here.

Tutorials at SOLEIL
There are 3 tutorials organized on the SOLEIL site on 29 June 2022 (L'Orme des Merisiers - Saint-Aubin, 91192 Gif-sur-Yvette). One on FDMNES, one on DYNA and one on MagStREXS. Please find the description of the tutorial here, and register for one tutorial by filling this table with your tutorial choice.

If you dine at SOLEIL on 29 June, you must present your conference badge at the cash desk of the staff restaurant.

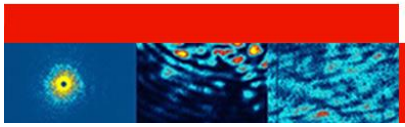
Conference dinner
The conference dinner will take place on a boat on Thursday 30th from 7pm to 11pm. Please find here the list of the participant. If you change your mind and would like to come, do not hesitate to let us know. The departure and arrival are from 'port de la bourdonnais' https://www.bateauxparisiens.com/en/practical-info.html.

For any question, please contact us: David.massot@sorbonne-universite.fr, nicolas.jaouen@synchrotron-soleil.fr, Emmanuelle.jal@sorbonne-universite.fr

Program at a glance

	Tuesday June 28th		Wednesday June 29th	Thursday June 30th	Friday July 1rd	
09:00 – 09:40	Collins	School	09:00 – 09:35	Ueda	Hesjedal	Mitrano	09:00 – 09:35
09:40 – 10:20	Joly		09:35 – 10:00	Huang	Vodungbo	Wang	09:35 – 10:00
10:20 – 10:50	Break		10:00 – 10:35	Scagnoli	Büttner	Peng (v)	10:00 – 10:35
10:50 – 11:30	Lefèvre		10:35 – 11:05	Break	Break	Break	10:35 – 11:05
11:30 – 12:10	Beutier & Jal		11:05 – 11:30	Subias-Peruga	Ramakrishnan	Wermeille	11:05 – 11:30
12:10 – 12:50	Mazzoli		11:30 – 12:05	Soldo	Geck	Sears	11:30 – 12:05
12:50 – 13:55	Registration + Lunch		12:05 – 12:30	Grunder	Steadman	Beutier	12:05 – 12:30
13:55 – 14:00	Intro		12:30 – 14:00	Lunch	Lunch	Conclusions + Lunch	12:30 – 14:00
14:00 – 14:35	Eisebitt		14:00 – 14:35	Transfert to SOLEIL	Pancaldi		14:00 – 14:35
14:35 – 15:00	Flewett		14:35 – 15:00	Visit	Schick		14:35 – 15:00
15:00 – 15:25	Bombardi		15:00 – 15:25		Rahn		15:00 – 15:25
15:25 – 15:50	De Santis		15:25 – 15:50		Jal		15:25 – 15:50
15:50 – 16:20	Break		15:50 – 16:20	Tutorials FDMNES by Joly DYNA by Grenier & Jal MagStREXS by Bereciarta	Break		15:50 – 16:20
16:20 – 16:55	Skjærvø (v)		16:20 – 16:55		McCarter (v)		16:20 – 16:55
16:55 – 17:20	Misawa		16:55 – 17:20		Leveillé		16:55 – 17:20
17:20 – 17:45	Hoell		17:20 – 17:55		Maznev		17:20 – 17:55
later			later	Dinner at SOLEIL Back to Paris	Social Dinner		later

Sponsors



REXS2022

RESONANT ELASTIC X-RAY SCATTERING

Detailed program

Tuesday 28th of June	
School room 101 - 1st floor of corridor 32-42	
09:00 – 09:40	Steve Collins *Introduction to Resonant Elastic X-ray Scattering*
09:40 – 10:20	Yves Joly *X-ray Matter Interaction for REXS*
10:20 – 10:50	Break
10:50 – 11:30	Christophe Lefèvre *Contrast methods using REXS*
11:30 – 12:10	Guillaume Beutier & Emmanuelle Jal *X-ray Resonant Magnetic Scattering*
12:10 – 12:50	Claudio Mazzoli *Evolution, applications and opportunities*
REXS 2022 – Amphitheatre 25	
12:00 – 13:55	Welcome and Lunch
13:55 – 14:00	Intro
14:00 – 14:35	Stefan Eisebitt *REXS accessing magnetization dynamics: Following the birth of topological structures and some surprises when looking into the depth*
14:35 – 15:00	Samuel Flewett, *Numerical Treatment of Resonant Elastic X-Ray Scattering – Towards the Understanding of Complex Magnetic Structures*
15:00 – 15:25	Alessandro Bombardi *A New Webtool to Simulate Magnetic Scattering*
15:25 – 15:50	Maurizio De Santis *In situ resonant x-ray scattering at the French "CRG-IF" beamline at ESRF*
15:50 – 16:20	Break
16:20 – 16:55	Sandra Skjærvø (v) *Recurring dynamics of magnetic texture in an artificial square ice close to AFM transition*
16:55 – 17:20	Ryusuke Misawa *Magnetic quadrupole order in chiral antiferromagnet probed by circularly-polarized resonant x-ray*
17:20 – 17:45	Armin Hoell *Anomalous Small-Angle X-Ray Scattering: Basic Aspects and Structure Analysis of Bimetallic Nanoparticles*

Wednesday 29th of June	
Oral presentation– Amphiteatre 25	
09:00 – 09:35	Hiroki Ueda *Conical spin order with chiral quadrupole helix in CsCuCl3*
09:35 – 10:00	Xinchao Huang *Controlling core-hole state through an X-ray cavity*
10:00 – 10:35	Valerio Scagnoli *X-ray three-dimensional magnetic imaging, the future is brilliant!*
10:35 – 11:05	Break
11:05 – 11:30	Gloria Subias-Peruga *Complementary Neutron and Resonant Magnetic X-ray Scattering Study to Reveal the Magnetic Ground State of* $La_{1.5}Ca_{0.5}CoO_{4\pm\delta}$
11:30 – 12:05	Yvonne Soldo *In Situ Surface Resonant X-Ray Diffraction Coupled With Ab Initio Calculations: A New Method To Unravel The Charge Distribution At The Electrochemical Interface*
12:05 – 12:30	Yvonne Grunder *In-situ surface resonant x-ray diffraction elucidating the charge Reorganization at the Adsorbate Covered Electrode Surface*
12:30 – 14:00	Lunch
Visit to SOLEIL	
14:00 – 14:35	Transfert to SOLEIL
14:35 – 16:00	Visit of the Beamlines: Cristal, Hermes, Nano, Sextants, Sims
16:00 – 16:30	Break
16:30 – 18:00	Tutorials • FDMNES by Yves Joly • DYNA by Stéphane Grenier & Emmanuelle Jal • MagStREXS by Pablo Bereciarta
18:30	Dinner at SOLEIL

Thursday 30th of June	
Oral presentation– Amphiteatre 25	
09:00 – 09:35	Thorsten Hesjedal *3D skyrmions in In-Plane Fields*
09:35 – 10:00	Boris Vodungbo *Laser-induced ultrafast demagnetization and perpendicular magnetic anisotropy reduction in a $Co_{88}Tb_{12}$ thin film with stripe domains*
10:00 – 10:35	Felix Büttner *Time-Resolved Coherent X-Ray Imaging: Resolving Emergent Dynamics at the Nanometer Scale*
10:35 – 11:05	Break
11:05 – 11:30	Mahesh Ramakrishnan *Observation of Magnetoelectric Octupoles in h-YMnO$_3$ by Resonant Soft X-ray Diffraction*
11:30 – 12:05	Jochen Geck *Resonant reflectivity studies of the LaAlO3/SrTiO3 interface*
12:05 – 12:30	Paul Steadman *Measuring Hysteresis With Soft X-ray Scattering: A Word Of Caution*
12:30 – 14:00	Lunch
14:00 – 14:35	Matteo Pancaldi *Light and Magnetic Vortices: The Experimental Evidence of Magnetic Helicoidal Dichroism*
14:35 – 15:00	Daniel Schick *Laser-driven resonant magnetic scattering in the soft-X-ray range*
15:00 – 15:25	Marein Rahn *Topology, Colossal Magnetoresistance, and Complex Magnetic Domains in Eu5In2Sb6*
15:25 – 15:50	Emmanuelle Jal *Unravelling the Transient Depth Magnetic Profile of an Iron Thin Film thanks to X-ray Resonant Magnetic Reflectivity*
15:50 – 16:20	Break
16:20 – 16:55	Margaret McCarter (v) *Structural Chirality of Polar Skyrmions and Vortices Probed by Resonant Elastic X-ray Scattering*
16:55 – 17:20	Cyril Léveillé *Synthetic Antiferromagnet Materials Studied by Soft X–ray Magnetic Resonant Scattering*
17:20 – 17:55	Alexei Maznev *Transient Gratings Or Impulsive Stimulated Scattering Spectroscopy: From Acoustics and Thermal Transport To Dynamics Of Nanoscale Magnetization Patterns*
19:00 – 23:00	Cruises Social dinner

Friday 1st of July	
Oral presentation– Amphiteatre 25	
09:00 – 09:35	Matteo Mitrano *Probing the Finite-Momentum Spectrum of a Light-Induced Superconductor*
09:35 – 10:00	Xiaocui Wang *Ultrafast manipulation of the NiO antiferromagnetic order via sub-gap optical excitation*
10:00 – 10:35	Yingying Peng *Observation of charge order beyond superconducting regions of cuprates and orbital order in 1T-TiSe2*
10:35 – 11:05	Break
11:05 – 11:30	Didier Wermeille *XMaS Reborn*
11:30 – 12:05	Jennifer Sears *Resonant X-ray Measurements of Magnetism in RuCl3*
12:05 – 12:30	Guillaume Beutier *Coherent diffraction imaging at space-group forbidden resonant reflections*
12:30 – 14:00	Conclusions and Lunch

Oral Presentation

Abstracts

REXS accessing magnetization dynamics: *Following the birth of topological structures and some surprises when looking into the depth.*

Stefan Eisebitt

Max Born Institute
Max-Born-Str. 2a, 12489 Berlin, Germany

ABSTRACT

Magnetic Skyrmions are spin textures which behave as quasi-particles and are characterized by a specific topology. Some types of skyrmions do exist in suitable thin magnetic multilayer film systems at room temperature, and they can be generated and efficiently moved laterally by spin-polarized current pulses. I will discuss how magnetic skyrmions can be generated via laser pulses instead of current pulses at unprecedented speed, with the topology change completed after 300 ps. Insight into the laser-induced formation mechanism comes from pump-probe resonant scattering experiments at a free electron x-ray laser tracking M(x,y,t) in comparison with atomistic spin simulations. Local topology fluctuations in a transient high temperature phase are identified as the key element for this topological phase transition - a mechanism that may be applicable to phase transitions with a net change of topology in completely different material systems as well. [1]

Thin magnetic films and stacked multilayers or heterostructures thereof are common sample systems to generate magnetic functionalities, such as all-optical magnetization switching or hosting structures like the skyrmions mentioned above. Even simple “single layers” typically contain growth-seed and cap layers. On a prototypical GdFe layer with a Ta cap layer and Pt seed layer, we demonstrate that time-resolved access to the magnetization *depth* profile M(z,t) after optical excitation is possible via broadband resonant elastic scattering in the soft x-ray region around 150 eV photon energy. Here, TMOKE spectroscopic information at a laser-driven HHG source is utilized in conjunction with polarization-dependent magnetic scattering simulations. [2,3,4] We resolve the transiently evolving magnetization depth profile *within* the 10 nm thickness of the GdFe layer. Unexpectedly, we observe a faster demagnetization of the ferrimagnetic GdFe layer at the interface to the seed layer, i.e. away from the side where the infrared pump laser is incident on the sample cap – illustrating the importance of depth-resolved information when trying to understand optically induced ultrafast dynamics in systems with heterogeneity on the few nanometer scale.

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[3] M. Hennecke, D. Schick, T. Sidiropoulos, F. Willems, A. Heilmann, M. Moerbeck-Bock, L. Ehrentraut, D. Engel, P. Hessing, B. Pfau, M. Schmidbauer, A. Furchner, M. Schnuerer, C. von Korff Schmising, and Stefan Eisebitt, “*Ultrafast element- and depth-resolved magnetization dynamics probed by transverse magneto-optical Kerr effect spectroscopy in the soft x-ray range*”, Physical Review Research (accepted, 2022)

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Numerical Treatment of Resonant Elastic X-Ray Scattering – Towards the Understanding of Complex Magnetic Structures

Samuel Flewett[1], Nicolas Jaouen[2], Erick Burgos-Parra[3], Cyril Léveillé[2], Nicolas Reyren[4], Vincent Cros[4],

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4. *Unité Mixte de Physique, CNRS, Thales, Université Paris-Saclay, Palaiseau, 91767, France*

ABSTRACT

We present work towards developing an efficient numerical framework for the analysis of REXS data in magnetic multilayers with an arbitrary magnetization direction. The problem of theoretical analysis of specular reflectivity curves from magnetic multilayers was largely resolved 20 to 30 years ago[1-3], however the generalization of this work to the off-specular scattering produced by magnetic domains remains a work in progress. We report on work in this direction, where at present we are capable of modelling the resonant scattering from an arbitrarily magnetized multilayer in the distorted wave Born approximation[4], permitting success in determining the hybrid domain wall profile in CoPd stripe domain samples, and resolving ambiguity in PEEM images from novel in-plane domain structures[5]. Working with multilayers, we have had some especially interesting results occurring due to interference effects when moving off the multilayer Bragg angles where measurements have been traditionally performed in order to maximize the signal to noise ratio.

Our current efforts in this line of investigation follow two main directions: Firstly, the attempts at determining the limits of sample complexity for which REXS can be considered a useful technique[6], and secondly, the full inclusion of roughness effects in our simulation code in order to model the diffuse scattering background. With respect to this first problem, the most complex structures will be candidates for vector field tomography, however this is extremely time intensive, thus providing us with the motivation to present REXS as a viable technique for such situations – especially those where substantial a-priori information about the magnetic structure is available. Regarding the question of the background noise, the magnetic scattering signal from complex magnetic morphologies is more dispersed in reciprocal space than in the case of stripe domains, meaning that simple subtraction of the diffuse background is no longer practical. Its incorporation therefore in our simulation model is a necessary step prior to tackling the inverse problem – the ultimate goal of this work.

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3. Z. Q. Qiu and S. D. Bader, Rev. Sci. Instrum. **71**, 1243 (2000).
4. S. Flewett et al. Phys. Rev. B **103**, 184401 (2021).
5. M. Cascales et el. In Preparation (2022)
6. M. Grelier et al. In Preparation (2022)

A New Webtool to Simulate Magnetic Scattering

Alessandro Bombardi

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ABSTRACT

The complexity of the magnetic scattering processes can be extremely intimidating for people wishing to use x-rays to determine long range magnetic ordering using x-rays but not familiar with the technique. Despite many references and textbooks are available e.g. [1], the occasional user of the technique has not many tools at her disposal that can be used before, during or after an experiment to simulate the data or analyze the results. In the relative small community of techniques experts many developed their own tools and are not keen to distribute software, as usually the process involves looking after different operating system versions, without considering upgrades, updates and bug tracking.

A better approach is to make use of Kubernetes virtual containers, centralize the software apps to follow more easily their life cycle and grant access to the user via web interfaces or REST API.

A beta release of the MaRS (temporary name) software is now available for the users of I16 in the Diamond intranet as a web app and it allows the users to define the geometry of their experiment, and the magnetic structures in their system of interest using the same conventions adopted by Basireps[3] and Isodistort [4,5]. The software allows to simulate Non resonant magnetic scattering and resonant scattering in the dipolar approximation as well as simple corrections for geometrical factors. Polarization of the incident and outgoing beam and the polarization of the final beam can be included in the simulations.

MaRS can be used either using a symmetry-based approach to the description of magnetic structures, what allows for a reduction of the number of degree of freedoms needed to describe the magnetic structure or in a more “brutal” way without any symmetry consideration.

After a beta test phase, we plan to make the software available on internet. Possible improvements include a generalization of the software to nonmagnetic ATS scattering including higher rank tensors, as well as going beyond the dipolar-dipolar approximation.

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In situ resonant x-ray scattering at the French "CRG-IF" beamline at ESRF

M. De Santis[1], L. Martinelli[1], G. Renaud[2], A. Bailly[1], Y. Joly[1], V. Langlais[3], X. Torrelles[4], V. Heresanu[5], G. Sitja[5]

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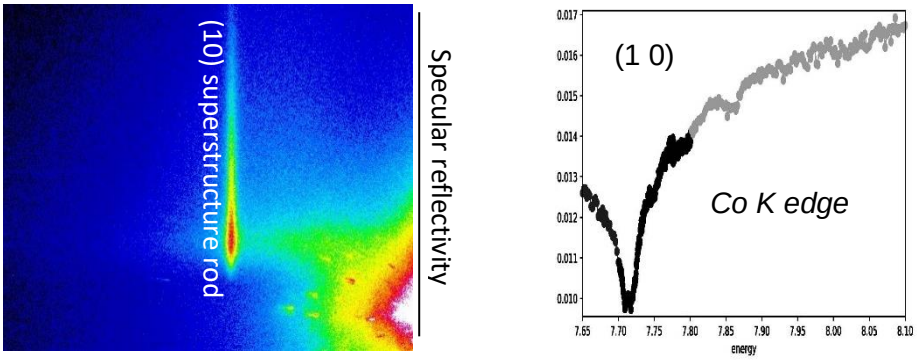
ABSTRACT

We show two examples of resonant x-ray scattering experiments performed *in situ* on the INS2 end-station of the BM32 beamline at ESRF. In the first one the inversion parameter of thin cobalt ferrite films grown on Ag (001) by oxygen-assisted MBE is found. In spinel structure this parameter quantifies the distribution of divalent and trivalent cations on tetrahedral and octahedral sites, and strongly influence the electronic and magnetic properties of the ferrite. Measuring grazing incidence resonant x-ray diffraction intensity versus energy of several spinel peaks at the iron and cobalt k-edges and comparing with theoretical calculations performed with the FDMNES code, we could find that cobalt occupies mostly octahedral sites, resulting in an inversion parameter of 0.88(5).[1] In the second experiment we studied Co-Pt core-shell nanoparticles self-organized on an ultrathin aluminum oxide on $Ni_3Al(111)$, a template with a 4.1 nm hexagonal surface lattice. Co and Pt were subsequently deposited on the template layer seeded with a few Pd atoms per unit cell. Bimetallic nanoparticles organize at the corner of the oxide surface cell giving sharp peaks in the small angle x-ray scattering pattern. The analysis of the RXD measured at the cobalt K edge on these SAXS features evidences then a core-shell structure.



GISAXS of 0.15 nm Co on alumina template (Pd seeded), and RXD of the (10) reflection at the Co K

These examples demonstrate the capabilities of BM32 for *in situ* resonant scattering studies. At short term, they will be improved with the installation of a crystal analyser

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Recurring Dynamics Of Magnetic Texture In An Artificial Square Ice Close To The AFM Transition

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ABSTRACT

Artificial spin systems are magnetic metamaterials consisting of nano-sized single-domain magnets that can exhibit collective behavior, similarly to bulk materials [1]. We chose the prototypical square geometry, known to order antiferromagnetically by dipolar interaction below the Neel temperature [2], which in our case is ~357K. X-ray Photon Correlation Spectroscopy (XPCS) under coherent soft illumination in the Resonant Elastic X-ray Scattering regime allows us to access the magnetic texture dynamic of the artificial spin ice. We discover an intriguing recurring magnetic texture in the vicinity of the antiferromagnetic ordering phase transition, evidenced by distinct double-peak diffraction patterns in the detector time series, intercalated with typical AFM (single-peak) ones. The recurring double-peak positions shows a distribution in length and angle from the AFM point (0.5, 0.5) at temperatures around the AFM phase transition. We discuss possible scenarios for the origin of the recurring double-peak pattern, being either of commensurate (AFM domains) or incommensurate origin. Especially the latter scenario would suggest that thermal magnetic moment dynamics in artificial spin ices could be fundamentally more complex than previously assumed.

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Magnetic quadrupole order in chiral antiferromagnet probed by circularly-polarized resonant x-ray diffraction

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ABSTRACT

The concept of multipole, which characterizes angular properties of the physical objects, scalar, vector, and higher tensors, is of great benefit to understanding physical phenomena in various quantum materials. Atomic multipole has long been investigated from the interest of their spontaneous ordering in *d*- and *f*-electron systems, which often dominates their electronic properties. This concept is nowadays extended to a cluster consisting of several atomic sites in crystalline solids. When multipole moments of adjacent clusters in a crystal are arranged in a uniform (staggered) manner, such a state can be regarded as ferroic (antiferroic) order of cluster multipoles.

In this study, we investigate circular dichroism observed in resonant x-ray diffraction at the Cu L_3 edge in a chiral antiferromagnet, $Pb(TiO)Cu_4(PO_4)_4$, which shows ferroic order of magnetic quadrupoles below the Néel temperature (T_N = 7 K) [1]. At temperatures above T_N, space-group-forbidden reflection 100 is observed due to the anisotropic tensor of susceptibility (ATS) scattering [2]. With decreasing temperature, the reflection intensity shows substantial circular dichroism below T_N, where the magnetic scattering overlaps. We found the correlation between the sign of the circular dichroism and that of crystallographic chirality. In addition, the reflection intensity depends on the product of poling magnetic and electric fields, to which the magnetic quadrupole responds [1]. The circular dichroism observed in this study is interpreted as the interference between the ATS and the magnetic scatterings [3]. This finding shows that the interference in resonant x-ray diffraction makes it possible to probe both the chirality and the magnetic quadrupole order in the chiral antiferromagnet.

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Anomalous Small-Angle X-Ray Scattering: Basic Aspects and Structure Analysis of Bimetallic Nanoparticles

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ABSTRACT

This talk will elaborate the advantages of anomalous SAXS (ASAXS) in the structural analysis of nanostructured multicomponent materials (1,2). Details and strategies necessary to measure anomalous small-angle scattering reliable will be emphasized.

Tailor-made mono- and bimetallic nanoparticles (NPs) are of great interest in e.g., catalysis, as sensor materials, and analytical assays. Here, we will focus on NiCu NPs. A facile and efficient methodology is developed for the solvothermal synthesis of size-tunable, stable, and uniform NiCu core-shell NPs for various applications in catalysis. Their diameter can be tuned in a range from about 6 nm to 30 nm, and the Ni:Cu ratio is adjustable in a wide range from 1:1 to 30:1. The NPs are structurally characterized by a method combination of complementary methods: transmission electron microscopy, ASAXS, X-ray absorption fine structure, and X-ray photoelectron spectroscopy (3). We focus on the ASAXS method and its ability to analyze nanostructure details and their compositions at once.

The X-ray K-absorption edges of the two elements Ni and Cu are nearby (8333 eV and 8979 eV). Consequently, the strong variation of the anomalous scattering behavior in the energy range between 8 keV to 9 keV is used for this special ASAXS investigation.

ASAXS excluded the hypothesis of a bimetallic core-shell structure and evidenced a core-shell-shell nanostructure. The outer shell having the lowest electron density is found to be NiO, while the inner core is Cu and Ni alloyed. That was proved to be valid for all particle sizes and Ni:Cu ratios. The inner shell is pure Ni.

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Conical spin order with chiral quadrupole helix in $CsCuCl_3$

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ABSTRACT

Resonant X-ray diffraction is a powerful technique to disentangle electronic degrees of freedom that strongly correlate with each other in materials, based on its sensitivity to electric monopoles (charge), magnetic dipoles (spin), and electric quadrupoles (orbital). When these multipoles order in a chiral way, using circularly-polarized incident X rays is beneficial to distinguishing enantiomers with opposite chirality through circular dichroism on diffraction intensities sensitive to the multipoles [1].

Here we present a resonant X-ray diffraction study at the Cu L_3 edge on the multi-chiral crystal $CsCuCl_3$ [2], exhibiting helical magnetic order in a chiral lattice. By using the unique capability of resonant X-ray diffraction with circular polarization, we investigated the chiral arrangement of electric quadrupole moments, ascribed to the unoccupied Cu^{2+} 3*d* orbital, and that of spin moments. While the arrangement of electric quadrupole moments is well explained by the reported chiral crystal structure [3], that of spin moments is found as not simple as in the previous report [4]. Detailed investigation reveals additional sinusoidal components on top of the helical order, thus a longitudinal conical (helical-butterfly) structure. The out-of-plane component can emerge due to spin-orbit interaction since the quantization axis of the Cu 3*d* orbitals is off the basal plane, suggesting a strong correlation between orbital and magnetism even in $S = 1/2$ systems [5].

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Controlling core-hole state through an X-ray cavity

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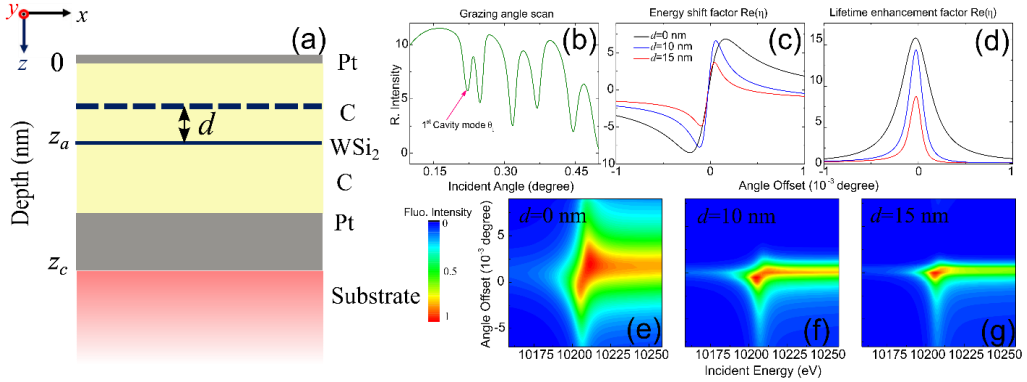
ABSTRACT

The dynamics of such core-excited states determine the application range of modern x-ray scattering and spectroscopy techniques, e.g., its elastic radiative pathway gives the resonant elastic x-ray scattering (REXS), its inelastic radiative pathways give the resonant inelastic scattering and emission spectroscopy. In general, the core-hole state is considered an intrinsic property because the relaxation pathways are usually hard to be manipulated. It is well-known that the decay process of an atom depends on the environment (PDS), PDS confinement in cavity is known as cavity-QED effect. Even though at hard x-ray energies, our group has recently demonstrated that the lifetime and energy of the core-hole state can be controlled simultaneously via an x-ray planar cavity [1], and a quantum model is recently built to show how the x-ray cavity modify the PDS and enhance the REXS pathway. The core-hole lifetime enhancement Γ_c and energy shift Δ_c can be considered to be linear to the cavity strengthening factor η. That is to say

$$\Gamma_c \propto \mathrm{Re}(\eta), \text{ and } \Delta_c \propto \mathrm{Im}(\eta), \quad (1)$$

where the linear relation depends on two constants of the atom number density and the resonant scattering length. Note here that η can be connected directly with PDS via the Green's function.

In our previous study, η was controlled by choosing different cavity orders and angle offset $\Delta\theta=\theta-\theta_1$, and the atomic layer exactly locates at the middle of the cavity (d=0 nm). Im(η) and Re(η) as a function of the angle offset at the 1st order of the cavity mode are depicted at Figs (c) and (d) (black lines), and the fluorescence 2D map in Fig. (f) shows clearly the linewidth broadening and energy shift. Recently we found that the PDS has a specific distribution inside the cavity based on our quantum theory [2], in this case η shows different dependence with the angle offset when the atomic layer is at different positions as shown in Fig. (c)-(d), and resulting in remarkable differences in the fluorescence map as shown in Figs. (e)-(g). Moreover, when the atomic layer is moved largely away from middle, Re(η) shows asymmetric Fano profile, which is an evidence of multi-mode field quantization that has not been realized at x-ray regime. This is the first attempt to map the PDS distribution inside the cavity, which will pave a new way to control core-hole state and facilitate new physics for x-ray cavity-QED and core-level spectroscopy.



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X-ray three-dimensional magnetic imaging, the future is brilliant!

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ABSTRACT

Over the last years, we have worked towards developing methods to fabricate and characterize three-dimensional magnetic structures. Specifically, we have combined X-ray magnetic imaging with new iterative reconstruction algorithms to achieve X-ray magnetic tomography and laminography [1-4]. In a first demonstration, we have determined the three-dimensional magnetic nanostructure within the bulk of a soft $GdCo_2$ magnetic micropillar and we have identified the presence of magnetic singularities (Bloch points) of different types [1, 3] and closed vortex loops [5]. Subsequently, we have used the flexibility offered by the laminography geometry to perform time-resolved measurements of the magnetization dynamics in a two-phase micrometer size GdCo disk. Therefore, X-ray magnetic three-dimensional imaging, with its recent extension to the soft X-ray regime [6], has now reached sufficient maturity that will enable to unravel complex three-dimensional magnetic structures for a range of magnetic systems.

In this presentation, I will first give an overview of our recent results and review the current shortcomings of the magnetic tomography technique. Finally, I will discuss how diffraction-limited storage ring source, together with state-of-the-art instrumentation, will allow three-dimensional magnetic nanotomography to thrive.

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Complementary Neutron and Resonant Magnetic X-ray Scattering Study to Reveal the Magnetic Ground State of $La_{1.5}Ca_{0.5}CoO_{4\pm\delta}$

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ABSTRACT

The magnetic ground state of a $La_{1.5}Ca_{0.5}CoO_{4.02}$ single-crystal has been studied combining neutron diffraction and resonant magnetic x-ray scattering (RMXS) techniques [1]. Our compound is a bit overdoped (nominal $Co^{+2.54}$ mixed valence) due to a slight excess of oxygen content, as deduced from x-ray absorption and emission spectroscopies [2]. The room temperature structure is orthorhombic *A*2*mm* with two nonequivalent compressed and expanded CoO_6 ordered into a checkerboard pattern in the *ab* plane and with a charge segregation of 0.4(1) e- [3]. Three single-crystals from the same boule have been investigated exhibiting the paramagnetic to antiferromagnetic phase transition at $T_N \approx 52K$.

Neutron diffraction measurements only detected one type of magnetic contribution ascribed to either k_1 = (1/2, 0, 1/2) or k'_1 = (0, 1/2, 1/2) propagation vectors as the single-crystal was twinned. On the other hand, RMXS experiments could successfully detect (1/2, 0, 1/2), (1/2, 0, 0) and (1/2, 0, 1) magnetic peaks. Despite their onset temperatures being the same (≈55K), a different thermal behavior is observed between (1/2, 0, 1/2) and (1/2, 0, L) (L = integer) reflections whose intensities peak at different temperatures, suggesting the coexistence of two magnetic phases, one of them hidden to neutron diffraction. The intensity of the (1/2, 0, 1/2) magnetic reflection is at least ten times larger than that of the (1/2, 0, L) (L = integer) ones. In addition, the RMXS spectral shape clearly concurs with the contributions of only high spin Co^{2+} showing no trace of the Co^{3+} participation in the magnetic order for characterizing any of the two magnetic phases. The polarization analysis discloses the same orientation of Co magnetic moments for all three magnetic orders, being aligned along one of the orthorhombic *a* (or *b*) axes with a small tilt (≈3º) into the *z* direction.

We conclude that the magnetic ground state of $La_{2-x}Ca_xCoO_{4\pm\delta}$ compounds strongly depends on the oxygen content. Our $La_{1.5}Ca_{0.5}CoO_{4.02}$ single-crystal with slight oxygen excess (as interstitial oxygen) exhibit a bulk magnetic structure with double *a* (or *b*) and *c* axes with respect to the crystallographic orthorhombic cell. However, samples without the disorder produced by the presence of interstitial oxygen adopt a magnetic structure where only the *b* axis gets doubled. This latter magnetic structure found by RMXS in our compound is likely due to the presence of oxygen vacancies near the surface as a minority phase.

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In Situ Surface Resonant X-Ray Diffraction Coupled With *Ab Initio* Calculations: A New Method To Unravel The Charge Distribution At The Electrochemical Interface

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ABSTRACT

Electro-catalysts make it possible to accelerate electrochemical reactions, with important applications in several fields, such as energy storage, chemical synthesis, biosensors, water electrolysis.

The electro-catalytic activity is largely influenced by the charge distribution at the electrochemical interface, the few Angstrom thick metal-liquid interface region where the exchange of charges takes place. Understanding the involved mechanisms is of paramount importance. It is above all a question of being able to characterize the structural and electronic properties of the catalyst surface and of the charge distribution in the solution. Nevertheless, unlike for the atomic structure characterization, there is currently no experimental method to specifically probe the electronic structure at this interface.

We present here a new approach, which allows the direct experimental measurement of the charge distribution at the electrochemical interface. This was achieved by combining experimental and theoretical approaches, i.e. coupling *in situ* experiments of Surface Resonance X-Ray Diffraction with first-principle simulation of the measured spectra. FDMNES, recently extended for the simulation of surface resonant diffraction experiments [1], has now been developed for the electrochemical interface description, to consider the presence of the electrolyte facing the crystal and the effect of the applied external electric field [2].

We have chosen to study the archetypal Pt(111) system in an acid medium. Platinum is a widely used electrocatalyst, particularly in the field of low temperature fuel cells and water electrolysis. In the potential region where no adsorbed molecules are present, we could determine the charge distribution on each of the metal surface layers and the distance separating the metal from the oppositely charged disordered ionic plane in the solution. We could reveal the presence of an electric dipole over the two outermost platinum layers [3].

Our results demonstrate the potential of this original way to unveil the electronic densities at the electrochemical interfaces, a challenging topic for the understanding of the electrochemical reactivity.

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In-situ surface resonant x-ray diffraction elucidating the charge Reorganization at the Adsorbate Covered Electrode Surface

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ABSTRACT

The presence of specifically adsorbed anions can significantly affect the electrochemical reactivity of a metal electrode which is of major interest for galvanic deposition, etching, corrosion and electrocatalysis. In-situ surface x-ray diffraction has enabled an atomic/molecular-level understanding of the interface under reactive conditions, including its potential and time dependence, to be developed. While information about the atomic structure of the electrode surface in electrochemical in-situ cells has been widely investigated, insight into the charge distribution and the structure of the electrolyte at the interface is still lacking. Advances in these directions offer possibilities in elucidating atomic scale models of the electrochemical interface and thus will help to establish structure-stability-reactivity relationships.

A fundamental understanding of the nature of the charge transfer, especially the influence of the applied potential and the screening by the electrolyte, is a major goal in electrochemistry to better understand electrochemical processes and charge transfer during adsorption and deposition. [1]

A combination of in situ resonant surface X-ray diffraction studies and self-consistent DFT calculations has allowed us to gain site specific information about the charge distribution at buried interfaces is a promising tool. [2-5]

The charge distribution and bonding mechanism for the adsorption of bromide anions onto a single crystal Cu(001) electrode surface could be assessed. A comparison between the experimental and modeled data gives detailed information about the charge distribution at the interface and the bonding of specific adsorbates, predicting a charge rearrangement rather than charging of the atoms involved and a surface dipole moment situated at the metal surface. [4]

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Visit of SOLEIL

There will be four groups to visit 5 beamlines each with the schedule below:

	14h35-14h50	14h50-15h05	15h05-15h20	15h20-15h35	15h35-15h50
Group 1 N Jaouen	CRISTAL	HERMES	SIXS	SEXTANTS	NANO
Group 2 M Sacchi	SEXTANTS	NANO	HERMES	CRISTAL	SIXS
Group 3 JM Tonnerre	HERMES	CRISTAL	NANO	SIXS	SEXTANTS
Group 4 G Beutier	NANO	SIXS	SEXTANTS	HERMES	CRISTAL

Simulation of REXS with FDMNES

Yves Joly

Institut Néel, CNRS et UGA, 38042 Grenoble, France

The tutorial is devoted to the *ab initio* simulations of resonant X-ray diffraction spectra using the FDMNES[1] code. The participants will first learn the basics to perform simulations in simple cases, with their own laptop. Analysis versus polarization conditions (in and out), transition channels (electric dipole, quadrupole, magnetic dipole) will be performed. The sensitivity of the spectroscopy, on spectra and azimuthal scans will show the contribution of the different terms. We will also show how the extraction of the spherical components of the scattering tensors can give information on specific projections of the density of states on the absorbing atoms. Relation to the magnetic and spatial symmetries will be evocated. Effects of self-absorption and birefringence will also be simulated.

Examples at K edges in magnetite, V_2O_3 and L_{23} in CuO will illustrate all this for non-magnetic and magnetic studies. Eventually on demand, examples from the participants could be addressed.

Participants must have their laptop. A specific package with documentation, in-data files and the FDMNES executables for Mac OS, Windows 32, Windows 64 and Linux are provided[1]. They must nevertheless have their own software to plot spectra (Origin, Kaleidagraph, …). Participation to the School the first day of the workshop would be helpful.

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Using MagStREXS To Determine Magnetic Structures Based On REXS Diffraction Data

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ABSTRACT

Resonant Elastic X-ray Scattering (REXS) is a powerful technique that has been successfully employed to study many different phenomena in solids and thin films [1-3]. One of these well-established applications is the characterization of magnetic structures, being possible to collect different types of REXS data to obtain information about a magnetic phase: the intensities of a set of magnetic reflections, the full linear polarization analysis of a magnetic reflection, or the azimuthal dependence of its intensity. However, the analysis of this type of data can be extremely complicated, especially for the non-expert in the field.

MagStREXS is a crystallographic software dedicated to the determination of **Mag**netic **St**ructures through **R**esonant **E**lastic **X**-ray **S**cattering, and it is under development since mid-2017 at beamline P09 [4] at PETRA III (DESY). The aim of this program is to facilitate this type of analysis and also to provide tools for the preparation of these magnetic diffraction experiments.

In order to be fully systematic, MagStREXS takes advantage of some concepts and tools developed within magnetic crystallography for the description and study of magnetic structures.

In this tutorial, these basic ideas on magnetic crystallography will be presented, together with the steps required to use MagStREXS for the determination of a magnetic structure based on REXS magnetic diffraction data. The whole process will be illustrated with several examples to show the main features implemented in MagStREXS.

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Dyna tutorial

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[2] *Sorbonne Université, CNRS, Laboratoire Chimie Phyisque Matière et Rayonnement, LCPMR, Paris*

ABSTRACT

Dyna is a simulation program for reflectivity of x-rays and optics, aimed at determining structural, magnetic and electronic stackings in ultrathin multilayers. Among so many programs in the field, Dyna has several specificities: it includes anomalous, magnetic and anisotropic components in the index of refraction; it simulates reflectivity either versus angle, or versus x-ray energy, with arbitrary incident and out-going polarizations; it simulates Kerr and Faraday spectra, and transmittance through thin layers. All the simulations can be simultaneously fitted against one model. The program integrates a toolbox to create charge and magnetic factors from tables. Dyna is an on-going free and open-source project, under Python + Qt, or Matlab environments. Dyna was also designed for pedagogical aims, making easy to slide parameters for on-the-fly effects. The tutorial includes a presentation of the X-ray Resonant Reflectivity technique, and its formalism [1]. Attendees can then either follow a tutorial on an actual system illustrating the sensitivities of the technique or bring their own data.

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3D Skyrmions In In-Plane Fields

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ABSTRACT

Magnetic skyrmions are 2D magnetization swirls that stack in the form of tubes in the third dimension. In out-of-plane applied magnetic fields in chiral bulk magnets, the skyrmion tube lattice phase only exists in a narrow window of the temperature-field phase diagram. In contrast, in confined thin plates, the skyrmion stability region is greatly enhanced and dominated by the skyrmion surface state. For thin plates, the breaking of translational symmetry at the two surfaces becomes energetically dominant, providing an exotic stabilization mechanism for skyrmions. The surface state is represented by a unique 3D skyrmion structure with modulated skyrmion helicity angle along the tubes, named the surface twist effect. Later, this twisting effect was also confirmed in semi-infinite systems, i.e., at the surface of a bulk chiral magnet [1,2], suggesting that this is a universal skyrmion stabilization principle.

Based on the idea of the surface twist originating from translational symmetry-breaking, the existence of other boundary 3D states seems plausible. The recent advances in 3D magnetic characterization techniques stimulated a broad study of skyrmions in the field in-plane geometry, i.e., in geometrically confined systems with the field applied perpendicular to the confinement direction. Such a confinement can be experimentally realized either in thinned-down samples, i.e., in a double-confined geometry, or on a well-defined side-face of a bulk chiral magnet, i.e., in a single-confined geometry. Indeed, for double-confined chiral magnets, the field-in-plane skyrmion phase appears to be more stable than the field-out-of-plane phase. On the other hand, for semi-infinite systems, in-plane skyrmions can survive at the very top surface, leading to a largely broadened phase pocket [3]. These experimental observations strongly hint at the existence of an exotic skyrmion side-face state, which is not simply due to a boundary confinement effect.

In this talk, we will use REXS for the 3D characterization of magnetic skyrmions in bulk samples and confined geometries, focusing on their surface stabilization.

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Laser-induced ultrafast demagnetization and perpendicular magnetic anisotropy reduction in a $Co_{88}Tb_{12}$ thin film with stripe domains

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ABSTRACT

Since its discovery by Beaurepaire and coworkers in 1996 [1], the phenomenon of laser induced ultrafast demagnetization has attracted world-wide attention and created an entirely new research field in magnetism named femtomagnetism [2]. Following 25 years of ongoing experimental and theoretical research, the underlying mechanisms of the rapid decrease of the magnetization of a ferromagnetic film on the femtosecond time scale after a femtosecond optical excitation remains intensively debated. The scientific challenge to explain this magnetization dynamics with its associated energy and angular momentum transfer between the electron/spin system and the crystalline lattice occurring on a sub-picosecond time scale is at the base of this strong interest.

In this presentation, we describe a time resolved X-ray resonnant magnetic scattering (TR-XRMS) experiment on amorphous $Co_{88}Tb_{12}$ thin films with magnetic stripe domains conducted at the free-electron laser FERMI. Although several femtomagnetism studies have already be n performed on ferrimagnetic Co-Tb [3], a material system of great technological relevance for future all optical magnetic data storage [4], experiments describing the evolution of magnetic domain structures in rare earth–transition metal alloys following an ultrashort optical pulse are still scarce. Recently, Fan et al. performed a TR-XRMS study on $Co_{88}Tb_{12}$ samples using a tabletop high harmonics source but their analysis remained limited to the first magnetic diffraction order at the N edge of Tb (155 eV) [5]. In the present work [6], we complement their findings using different probe beam energies and deepen the analysis by using an experimental setup that allows us to record the first and third magnetic diffraction order simultaneously. With this, we are able to explicitly monitor the pump-induced evolution of the periodic magnetic structure, i.e., the change of domain size and domain wall width with the highest accuracy up to 120 ps.

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Time-Resolved Coherent X-Ray Imaging: Resolving Emergent Dynamics at the Nanometer Scale

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Nanometer-scale textures, such as stripe domains and magnetic skyrmions, are ubiquitous in materials in which interactions compete at different length scales. Remarkably, such textures can exist even in a perfectly homogeneous underlying material. Since their energy is translationally invariant, they can move within the hosting material. It is of great fundamental and applied interest to image the emergent dynamics of such textures, for example to uncover their quasi-particle equation of motion or to investigate their interactions with ever-present defects in the underlying material.

However, the grand challenge in such studies is that they require exceptional spatial and temporal resolution, often beyond the reach of established imaging techniques.

Here, I will discuss two scenarios in which holographically-aided coherent x-ray imaging has allowed us to uncover previously inaccessible physics of emergent spin textures at the nanometer scale.

The first example is the confirmation of the particle-like character of magnetic skyrmions up to GHz frequencies[1]. For this purpose, we imaged the gyrotropic relaxation trajectory of a magnetic skyrmion after exciting the skyrmion with a magnetic field pulse. The sequence of images showed clearly that the skyrmion retained its shape during this motion, such that the dynamics is accurately described by the center of mass trajectory. This justifies a quasi-particle description of the skyrmion. Remarkably, our masked-based coherent imaging approach allowed us resolve fine features in the trajectory with sub-3 nm resolution, thereby discovering a large inertia term in the skyrmion equation of motion.

The second example is the direct imaging of thermal fluctuations between highly degenerate magnetic stripe domain states[2]. Such fluctuations are very common in nature, especially in disordered or imperfectly ordered systems at the nanometer scale. Yet, it is notoriously difficult to access fluctuating states, especially by direct imaging, because contrary to the first example, pump-probe techniques cannot be employed. The challenge can be traced back to a fundamental dilemma between temporal and spatial resolution. I will show that coherent imaging can overcome this dilemma, by allowing to identify the underlying state of a scattering pattern at much lower photon count as required for the reconstruction of a real-space image. This approach, which we coin Coherent Correlation Imaging, disentangles spatial and temporal resolution and allows us to uncover an intricate network of more than 30 recurring magnetic states, which form clusters due to the particular nature pinning in the class of perpendicular magnetic systems that we investigated.

I will conclude by showing recent results of CCI applied to data from the EuXFEL and by demonstrating that even sub-5 nm spatial resolution in x-ray magnetic imaging is in reach.

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Observation of Magnetoelectric Octupoles in h-$YMnO_3$ by Resonant Soft X-ray Diffraction

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ABSTRACT

Magnetoelectric multipoles are localized ground-state entities which simultaneously break parity and time-reversal symmetries[1]. We investigate the symmetry forbidden (0,0,1) Bragg reflection in hexagonal $YMnO_3$ below T_N using resonant X-ray diffraction (RXD). While the reflection primarily originates from an antiferromagnetic canting of the Mn^{3+} spins perpendicular to the hexagonal plane, we also observe changes in the spectral shape for different temperatures. Using *ab initio* calculations based on the FDMNES package[2] and phenomenology, we argue that this observation is a result of the interference between scattering from the magnetic dipole and parity-odd atomic multipoles localized on Mn^{3+} ions[3]. We also find that the most dominant multipole is an antiferromagnetically ordered magnetoelectric octupole (denoted $\langle G^3_3\rangle$-$\langle G^3_{-3}\rangle$ in the figure). This study also demonstrates a novel method to investigate exotic magnetoelectric multipoles using RXD.

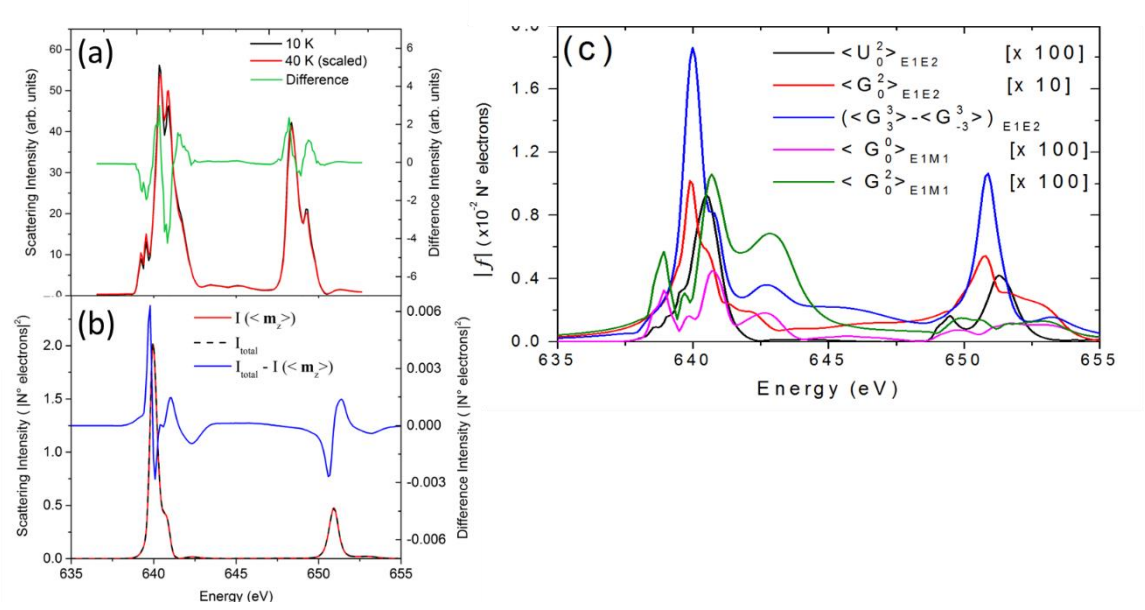

Figure: (a) Experimental and (b) calculated spectra and their difference profiles showing interference with multipoles; (c) multipolar form factors contributing to the (0,0,1) Bragg reflection in h-$YMnO_3$.

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Resonant Reflectivity Studies Of The $LaAlO_3/SrTiO_3$ Interface

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We present a resonant reflectivity study of the charge and orbital reconstructions in $LaAlO_3/SrTiO_3$ (LAO/STO) heterostructures. The interface between the two insulators hosts a two-dimensional electron liquid (2DEL) of high mobility, which is famous for its gate-tunable superconductivity, gate-tunable Rashba coupling, an exceptionally large spin-to-charge conversion efficiency as well as correlations and magnetism. Although these properties hold great potential for applications in new devices, their microscopic origins remain unclear. One reason for this uncertainty is that the electronic structure of buried interfaces is very hard to probe.

Here we combine the unique electronic sensitivity X-ray absorption with the exquisite interface sensitivity and depth resolution of x-ray reflectivity to achieve just that. More specifically, we examine the electronic reconstructions in the charge and orbital sector at the buried LAO/STO interface. The obtained depth profiles with atomic layer resolution reveal a pronounced temperature dependence of the 2DEL. We also discover a high-charge density of the 2DEL of at least 0.5 electrons per interfacial unit cell, which, as we show, is also significantly affected by the presence of oxygen vacancies.

Measuring Hysteresis With Soft X-ray Scattering: A Word Of Caution

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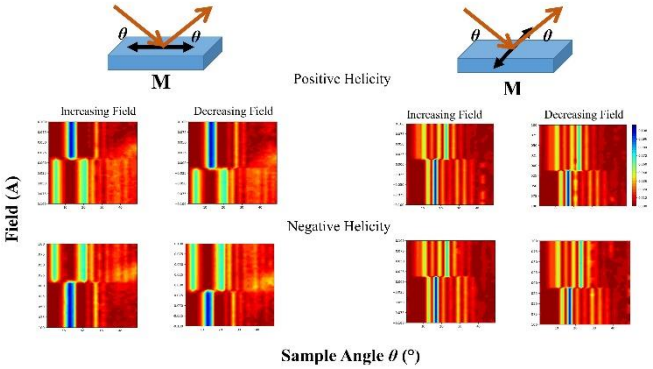
ABSTRACT

Soft X-ray scattering is a powerful technique for measuring the hysteresis cycle in thin films.[1,2] Advantages over other methods include element sensitivity and depth dependence. Direct comparisons between soft X-ray scattering and absorption with circular polarisation could lead to misinterpretations of the data due to the interference of the scattered photon are intrinsically non-linear in nature. Recent work on a simple magnetic thin film where the magnetisation was switched either parallel or perpendicular to the scattering plane (always parallel to the surface) has revealed some surprising results where all the principal polarisations of incident light were used i.e. linear horizontal and vertical with circular left and right. Results from vertical linear polarisation demonstrate a strong linear component when the magnetisation is switched perpendicular to the scattering plane with strong dependence on the strength of the imaginary structural scattering factor. Furthermore, with circular polarisation, the hysteresis in the scattering plane can lead to strong non-linear effects producing six unique classes of hysteresis curves due to interference between the charge and magnetic scattering. The ability to measure hysteresis out of the scattering plane with circular polarisation (not possible with absorption) is also shown. In addition, this rather unusual hysteresis loop does not switch with helicity. All the behaviours of the hysteresis loops can be reproduced to first order using calculations based on electric dipole transitions.[3,4]



Two main results using circular polarisation are shown on the left. The 2D plots show reflectivity versus applied field and incident angle. The two different measurement geometries are shown at the top roll with field either parallel or perpendicular to scattering plane. Each row below represents one helicity. Results with applied field perpendicular to scattering plane show hysteresis *behaviour without helicity reversal.*

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Light and Magnetic Vortices: The Experimental Evidence of Magnetic Helicoidal Dichroism

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ABSTRACT

The use of light beams possessing orbital angular momentum (OAM) is rapidly becoming a tool for manipulating physical systems and probing their properties, even in extreme ultraviolet range. The wavefronts of such beams develop a distinctive "corkscrew" shape determined by an azimuthal angular dependence of $\exp(i\ell\phi)$ for the electric field phase, which is associated with an OAM of $\ell\hbar$ per photon [1]. In this framework, it has been theoretically predicted that OAM beams should allow for novel kinds of dichroism experiments, paving the way for new spectroscopic tools in the fields of orbital physics and magnetism [2]. In particular, after the scattering of an OAM beam from magnetic structures featuring a non-uniform magnetization, like magnetic vortices, the far field intensity profile encodes the vortex symmetry in a way that depends on the sign and value of ℓ, giving rise to magnetic helicoidal dichroism (MHD) [3].

During the talk, I will show the experimental verification of this effect carried out at the DiProI end-station [4] of the FERMI free-electron laser, using p-polarized 52.8 eV photons (matching the Fe M-edge) and measuring the resonant scattering in reflection geometry at Brewster angle. Well-defined OAM values were imposed on the beam by using spiral zone plates [5], and the sample consisted in a 15 µm wide Fe-Ni disk, whose shape was designed to form a clean remanent magnetic vortex with reconfigurable clockwise (CW) or counter-clockwise (CCW) circulation. The MHD for opposite OAM values (in particular $\ell = \pm 1$) was obtained by taking the difference divided by the sum of two scattered intensity images collected for CW and CCW magnetic vortices [6]. The measured patterns well compare with the results of numerical simulations, and the effect has been proven to have the right symmetry for representing a proper MHD signal. Moreover, we also performed preliminary time-resolved measurements, to understand what kind of information can be gathered from MHD when applied to the detection of ultrafast magnetization dynamics, especially for non-uniform complex spin textures.

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Laser-driven resonant magnetic scattering in the soft-X-ray range

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ABSTRACT

Time-resolved resonant magnetic scattering in the soft-X-ray range is a powerful tool for accessing the spatially-resolved and element-specific spin dynamics in magnetic materials. So far, this photon-hungry technique has been limited to large-scale facilities. However, upgrades to diffraction-limited storage rings supporting only X-ray pulses beyond 100 ps and the shift of X-ray free-electron lasers towards attosecond pulses aggravate the competition for beamtime in the picosecond time window, which is of utmost relevance for magnetism research.

Here, we present the development of a lab-based instrument providing sufficient photon flux for resonant scattering up to 1.5 keV photon energy covering the soft-X-ray resonances of transition and rare-earth metal atoms. Our setup features the mandatory tunability in energy- and reciprocal-space combined with sub-10 ps temporal resolution exploiting the broadband emission of a laser-driven plasma X-ray source, which can be monochromatized to about 1 eV bandwidth by a reflection zone plate.

We benchmark our approach against accelerator-based soft-X-ray sources in a series of resonant magnetic scattering and spectroscopy experiments: (i) we probe the time-resolved evolution of the magnetic and structural Bragg peaks of an antiferromagnetically-coupled Fe/Cr superlattice at the Fe *L*-edges [1]; (ii) we characterize the lateral domain formation of a Gd/Fe superlattice by magnetic small-angle x-ray scattering (SAXS) in transmission at the Fe *L* and Gd *M*-edges; (iii) we enable white-light x-ray magnetic circular dichroism (XMCD) at the Fe *L*-edges utilizing ferromagnetic thin-film polarizers.

Our laser-driven approach enables a variety of resonant elastic scattering techniques on a laboratory scale and combines high availability with maximum flexibility in sample handling as well as environmental and excitation conditions. The temporal resolution below 10 ps is well suited to access photoexcited dynamics of, e.g., coherent magnons and phonons, de- and remagnetization processes, including domain dynamics and all-optical magnetic switching.

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Topology, Colossal Magnetoresistance, and Complex Magnetic Domains in $Eu_5In_2Sb_6$

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ABSTRACT

The axion insulating state is a paradigm of topological correlated matter which has been particularly difficult to demonstrate in real materials. We found that the non-symmorphic Zintl compound Eu5In2Sb6, which has previously attracted interest due to its extraordinary thermoelectric and colossal magnetoresistive properties [1], may provide an unprecedented platform to explore and engineer the effects of band topology in narrow-gap magnetic insulators [2,3]. While previous demonstrations of axion insulating states required the growth of artificial heterostructures or were limited by ionic disorder, Eu5In2Sb6 yields high-quality crystals with robust and reproducible physical properties.

Using neutron scattering, resonant elastic x-ray scattering, muon spin-rotation and bulk measurements, we clarify how the combination of co-planar glide symmetries and large Eu2+ magnetic moments produces an unusual two-step ordering process. At T_N = 15 K, the material first forms a complex non-collinear weak Ising-ferrimagnet, which we identify as a trivial insulator. Below T_Z = 7.5 K, this phase is continuously displaced by a growing volume fraction of a compensated antiferromagnetic arrangement that may have axion insulating character. This discovery also implies the presence of a solitonic antiferromagnetic domain structure on the mesoscale, which demonstrably couples to charge transport and, due to the net magnetization of some domains, should be highly susceptible to manipulation. This will potentially open up a platform to engineer interfaces of trivial and non-trivial insulators on the mesoscale.

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Unravelling the Transient Depth Magnetic Profile of an Iron Thin Film thanks to X-ray Resonant Magnetic Reflectivity

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During the last two decades, a variety of models have been developed to explain the ultrafast quenching of magnetization following femtosecond optical excitation [1,2,3]. These models can be classified into two broad categories, relying either on a local or a non-local transfer of angular momentum [3]. To distinguish those local and non-local effects we can measure the magnetization depth profile with femtosecond resolution, thanks to time-resolved x-ray resonant magnetic reflectivity [4, 5]. In this presentation, I will show how, from our experimental results gathered at the free electron laser FLASH, we can unravel the dynamics of the transient inhomogeneous depth magnetic profile of an Fe layer after optical excitation.

First our experiment on a polycrystalline Fe sample reveals two distinct dynamics at different time scales for the structure and the magnetization. Until one picosecond, the magnetic signal is quickly evolving while the structural one stays more or less constant. After that, the magnetic signal is slowly coming back to equilibrium while the structural one changes periodically. For this structural signal, we observe a maximum dilation of 2Å followed by a coherent damped oscillation of the thickness of the sample. This dynamic is due to stresses that are generated by the rapid increase in temperature and might be enhanced via magnetostrictive effects.

Second, the quantitative analysis of our magnetic reflectivity data allows us to retrieve the inhomogeneous depth magnetic profile for different delays after the optical excitations. Close to the bottom interface there is an overall reduction of the demagnetization. When comparing this result to simulation we can directly show that both local and non-local phenomena [6] take place at the same time scale and that there is probably a contribution from spin currents that could carry the magnetization beyond the magnetic layer [7].

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Structural Chirality of Polar Skyrmions and Vortices Probed by Resonant Elastic X-ray Scattering

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ABSTRACT

An escalating challenge in condensed-matter research is the characterization of emergent nanostructures such as ferroelectric and ferromagnetic skyrmions. Their small length scales coupled with complex, three-dimensional polarization or spin structures makes them demanding to trace out fully. Resonant elastic x-ray scattering (REXS) has emerged as a technique to study chirality in spin textures such as skyrmions and domain walls. It has, however, been used to a considerably lesser extent to study analogous features in ferroelectrics. Here, we present a framework for modeling REXS from an arbitrary arrangement of charge quadrupole moments, which can be applied to nanostructures in materials such as ferroelectrics. With this, we demonstrate how extended reciprocal space scans using REXS with circularly polarized x-rays can probe the structure and chirality of polar skyrmions and vortices in $PbTiO_3/SrTiO_3$ superlattices, as well as complex structures that emerge in multiferroic $BiFeO_3/TbScO_3$ superlattices. This technique can be extended to study ordered electric or magnetic phases in similar systems.

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Synthetic Antiferromagnet Materials Studied by Soft X–ray Magnetic Resonant Scattering

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Soft ferromagnetic (FM) materials are widely used in data storage technology due to small size of magnetic bit allowing high reliable storage capacity and our capabilities to control/read at microscopic scale in the GHz regime. Synthetic AntiFerromagnetic (SAF) systems are made of FM films with an antiferromagnetic coupling. SAF materials have been proposed for future magnetic devices since they emit less stray field, are thermally more stable and have a higher storage density. Moreover, the AF coupling between two ferromagnetic films composing a SAF could lead to an enhanced domain wall velocity that is linked with chiral stability or to the stabilization of small AF skyrmions with no transverse deflection while moving[1]. It has been recently demonstrated that the amplitude and sign of the circular dichroism in X-ray resonant magnetic scattering (XRMS) give direct information on the type (*i.e.* Néel or Bloch) and on the chirality (clockwise or anticlockwise) of the domain walls in ferromagnetic films[2]. In this contribution, we demonstrate that the same approach is also valid for SAF system[3]. It allows us to extract chirality information about the spin spiral optimized magnetic texture. We also report XRMS dichroic signal's temperature dependence that indicates the temperature evolution of the different magnetic interactions at play (*i.e.* magnetic anisotropy, interfacial chiral interaction and exchange interaction) through significant modifications on the spin textures stabilized in such SAFs. Last, we show the agreement of simulations performed with a distorted wave Born approximation (DWBA) with the specular and off-specular experimental data which can become a powerfull tool to retrieve samples 3D magnetization profile.

Figure 1 : (Left) Cross section of a calculated magnetic configuration of spin spirals antiferromagneticaly coupled in a bilayer (from W. Legrand et al. Nat. Mater. **19**. 34 (2020)) (Right) Corresponding experimental diffraction pattern at an angle that corresponds to half of the Bragg angle.

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Transient Gratings Or Impulsive Stimulated Scattering Spectroscopy: From Acoustics and Thermal Transport To Dynamics Of Nanoscale Magnetization Patterns.

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ABSTRACT

Laser-induced transient grating (TG) spectroscopy, sometimes also termed impulsive stimulated scattering, is a variation of non-collinear four-wave mixing, in which two short optical pulses of the same wavelength are overlapped in the sample to produce a spatially periodic material excitation whose dynamics are monitored via diffraction of a probe beam [1,2]. This technique has been used to study a wide range of phenomena, from the propagation of acoustic waves and thermal transport to charge-density waves and dynamical behavior of proteins. It has also been employed in materials science as a tool for accurate measurements of elastic properties and thermal diffusivity and commercialized for metal interconnect metrology in semiconductor industry. The advent of free electron lasers made it possible to expand the TG technique into EUV and x-ray spectral ranges [3,4]. In this talk, I will provide a brief historical overview of the TG spectroscopy and describe recent EUV TG experiments at FERMI with the probe wavelength tuned to the M_{23} edge of Co, including the recently reported observation of transient nanoscale gratings of magnetization [5].

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Probing the Finite-Momentum Spectrum of a Light-Induced Superconductor

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Ultrafast optical excitation, especially when resonant to specific lattice modes, has recently emerged as a powerful means to control and induce new functionalities in quantum materials[5]. One of the most ambitious goals is to selectively drive structural or electronic degrees of freedom to bring about nonequilibrium superconductivity at temperatures far above the equilibrium critical temperature T_c. While this phenomenon has been observed in a variety of systems ranging from copper oxides[6,7,8] to organic molecular metals[9,10], the microscopic physics of these dynamics is still largely unexplored. By focusing on the paradigmatic example of light-driven $La_{2-x}Ba_xCuO_4$, I will show how the newly developed technique of time-resolved resonant inelastic X-rays scattering (trRIXS)[11] provides an unprecedented route to probe the finite-momentum excitation spectrum of these transient phases[12,13]. Furthermore, I will discuss how trRIXS experiments could reveal transient pairing dynamics induced by a light-driven renormalization of the spin fluctuation spectrum[14].

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Ultrafast manipulation of the NiO antiferromagnetic order via sub-gap optical excitation

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ABSTRACT

Wide-band-gap insulators such as NiO offer the exciting prospect of coherently manipulating electronic correlations with strong optical fields [1]. It has been shown that in charge-transfer insulators sub-gap optical excitation can be coupled to low-energy bosonic modes, yet the identification of these bosonic modes currently remains unknown [2]. We use the prototypical charge-transfer insulator NiO to investigate the ultrafast manipulation of the antiferromagnetic (AFM) order via sub-gap optical excitation. Using time-resolved resonant x-ray reflectivity (Fig. 1a) at the FLASH free-electron laser (FEL) [3], we observe x-ray magnetic linear dichroism (XMLD) line shape changes at the Ni 2*p*1/2-3*d* resonance (*L*2-edge, Fig. 1b) and the reduction of the upper band-edge at the O 1*s*-2*p* resonance (*K*-edge, Fig. 1c). Comparing the transient XMLD line shape to ground-state measurements [4] allows us to determine a spin temperature rise of 65±5 K for time delays longer than 400 fs while at earlier times a nonequilibrium spin state is formed (Fig. 1b). The transient XMLD line shape at the Ni *L*2-edge demonstrates a significant reduction of the AFM order in NiO. At the O *K*-edge, we identify the formation of mid-gap states during the first 200 fs and a band-gap reduction lasting at least up to the maximum measured time delay of 2.4 ps (Fig. 1c). The split-beam normalization scheme (Fig. 1a), thanks to the implementation of a multiple x-ray beams experimental setup [5], enables us to eliminate the intensity and photon-energy fluctuations inherent to selfamplified spontaneous emission (SASE) FELs.

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Observation Of Charge Order Beyond Superconducting Regions Of Cuprates And Orbital Order In 1T-$TiSe_2$

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ABSTRACT

Charge orders are considered as a leading competitor of high-temperature superconductivity in the underdoped cuprates [1]. On the other hand, overdoped cuprates are widely regarded as conventional Fermi liquids without collective electronic order. This is challenged by our recent discovery of a reentrant CO in heavily overdoped Bi2201 beyond the pseudogap phase [2]. However, the presence of CO in overdoped regime is far from consensus and it remains a question whether CO is ubiquitously present in extremely overdoped cuprates. Determining the doping and temperature coverage of CO can disentangle the relations of superconductivity, pseudogap, and CO phases, which is critical to understand the high-temperature superconductivity. In this talk I will present our recent resonant X-ray scattering studies which reveal that charge order is the dominant order outside the superconducting dome of $La_{2-x}Sr_xCuO_4$ [3]. We find that the CO exists in the extremely overdoped regime and over a wide temperature range from 10 K to 300 K. Our results reveal that CO is distinct from the pseudogap phase ending at x=0.19. Our findings require a reassessment of the prevailing picture of the overdoped cuprates as weakly correlated Fermi liquids.

I will also show our recent resonant X-ray scattering experiments on the layered Van der Waals compound 1T-$TiSe_2$ [4]. Besides the conventional charge order, we reveal orbital order in this weakly correlated, quasi-two-dimensional material, which is consistent with our first-principles calculations. Our results demonstrate the essential role that orbital degrees of freedom play in $TiSe_2$, and their importance throughout the family of correlated Van der Waals materials.

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XMaS Reborn

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ABSTRACT

XMaS [1] is a diffraction and spectroscopy beamline which has been operating at the European Synchrotron Radiation Facility (ESRF) in Grenoble since 1997. It is a designated National Research Facility for UK and International users. Following the construction of a new magnet lattice at the ESRF, the EBS (Extremely Brilliant Source) upgrade, the *XMaS* beamline has been completely rebuilt to take advantage of its new 0.86 T short dipole source. The improved cryogenically-cooled monochromator and two new toroidally-focusing mirrors (Pt- and Cr-coated Si substrates) deliver an extended operational energy ranging from 2.1 to 40 keV into a beam spot of 50 µm (H) x 80 µm (V) (FWHM) at the sample. The upgrade gives an increase in brightness of about two orders of magnitude. Most beam conditioning devices have also been upgraded and a suite of new detectors commissioned. Simultaneously, the original Huber diffractometer was thoroughly refurbished and its detector arm doubled and strengthened. These improvements allow now a rapid switching between high resolution XRD or REXS and techniques using 2D detectors, such as RSM, time-resolved XRD or (Bragg)CDI. In this presentation, we explore the new beamline capabilities to study topical materials in hard condensed matter using REXS.

XMaS' features allowing high magnetic fields (4 T), low temperatures (sub-10 K) and high resolution x-ray diffraction to be deployed simultaneously have enabled the field-induced modulated states in the ferromagnet PrPtAl to be explored [2]. By applying the magnetic fields along specific crystallographic directions, a single modulated magnetic fan state was found for the first time. This fan structure has been modelled and explained by extending quantum orderby-disorder (QOBD) theory to include local moments and anisotropy.

XMaS was used to investigate the effects of strain and thin film thickness on the structural and magnetic properties of epitaxial thin films of the prototypal J_{eff} = ½ compound Sr_2IrO_4. REXS shows that the magnetic correlation length in Sr_2IrO_4 thin films strongly depends on the film thickness, whereas it is completely independent of their strain state [3]. This can be used as a finely tuned dial to adjust the out-of-plane magnetic correlation length and transform the magnetic anisotropy from two-dimensional (2D) to three-dimensional (3D) behavior by increasing the film thickness, opening new routes toward the stabilization of superconductivity in Sr_2IrO_4.

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Coherent diffraction imaging at space-group forbidden resonant reflections

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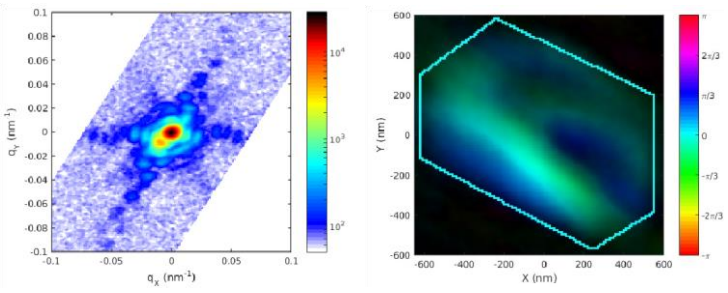
On one hand, coherent diffraction imaging (CDI) in Bragg geometry has emerged as a unique 3D microscopy of nanocrystals thanks to 3rd generation synchrotron sources. Away from absorption edges and at space-group allowed reflections, it provides not only the electronic density, but also, encoded in the phase, the atomic displacement field with respect to the mean lattice, which in turn reveals crystal strain, defects and domains [1–3]. On the other hand, some crystal structures have crystallographic reflections which are forbidden by the space-group symmetry but can nevertheless be observed at a suitable X-ray absorption edge, due to the anisotropy of the tensor of scattering (ATS) [4]. They are several orders of magnitude weaker than allowed reflections, but the absence of Thomson scattering allows the observation of various electronic phenomena related to electronic orders (magnetic, charge, orbital), static and dynamic atomic displacements.

The new generation of synchrotron sources, such as the ESRF “Extremely Bright Source”, opens opportunities to perform CDI on such weak reflections. Here we report on the measurement of the (115) forbidden reflection of a GaN nanopillar at the Ga K edge. Sufficient statistics could be obtained in a total accumulation time of ~30 minutes for an entire rocking curve to retrieve the phase of the scattering function. Such measurement at high temperature would provide an image of the inhomogeneity of thermal motion in the crystal [5], which would be particularly interesting close to surfaces, inversion domain boundaries [3] and crystal defects. This proof-of-principle experiment demonstrates that forbidden reflections are a new opportunity for CDI with the new synchrotron sources.



Left: (HK0) slice through the reciprocal space map around the (115) forbidden reflection. Right: 2D image of the complex scattering function in the basal plane as obtained from phase retrieval (the modulus and the phase are encoded by the brightness and the colour, respectively). The bright hexagon is a guide to the eye.

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Poster

Abstracts

udkm1Dsim – a Python toolbox for simulating 1D ultrafast dynamics in condensed matter

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ABSTRACT

The investigation of electronic, magnetic, and structural dynamics in solid-state physics has made great progress during the last decades due to the increasing availability of ultrashort electron and light pulses in a broad spectral range from THz to hard X-rays at large-scale facilities as well as in the laboratory. One of the major goals of these experiments is to follow the coupling of different degrees of freedom on the relevant time and length scales. In order to understand and interpret such experimental data, scientists rely on a pool of simulations for modeling and fitting, which are available as software toolkits or as published formalisms. The implementation of these formalisms or the usage and adaption of available external software packages are very time-consuming and each piece of software covers only a very limited aspect of real time-resolved scattering experiments. To that end, the need for a generic, modular, and open-source toolbox that allows for combining different functionalities is obvious.

The *udkm1Dsim* toolbox [1] allows for creating arbitrary one-dimensional (1D) structures made of crystalline and/or amorphous layers, including stoichiometric mixtures, typically on the nanometer length scale. These 1D structures hold all relevant material information such as structural, elastic, thermal, magnetic, and optical parameters. The toolbox allows for calculating thermal, structural, and magnetic dynamics on these 1D structures utilizing an *N*-temperature model (NTM) and multi-layer absorption formalism, a linear masses-and-springs model, as well as an interface for user-defined magnetization dynamics, respectively. Different types of light-scattering theories can be applied to retrieve the static as well as the transient response from these sample structures due to the above-mentioned dynamics, similar to real pump-probe experiments. Currently, kinematical and dynamical X-ray theories, which can also include polarization-dependent magnetic scattering [2], are supported. With that, the generally non-linear dependence of the actual observable (scattered light intensity) and the physical quantity of interest (temperature, strain, magnetization, ...) can be revealed. This includes also methods to apply realistic instrumental broadening to the simulated results for better comparison with experimental data.

The *udkm1Dsim* is freely available at
github.com/dschick/udkm1Dsim
and its documentation at
udkm1Dsim.readthedocs.org

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REXS and magnetism at *XMaS*

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ABSTRACT

XMaS [1] is a diffraction and spectroscopy beamline which has been operating at the European Synchrotron Radiation Facility (ESRF) in Grenoble since 1997. It is a designated National Research Facility for UK and International users. Following the construction of a new magnet lattice at the ESRF, the EBS (Extremely Brilliant Source) upgrade, the *XMaS* beamline has been completely rebuilt to take advantage of its new 0.86 T short dipole source. The improved cryogenically-cooled monochromator and two new toroidally-focusing mirrors (Pt- and Cr-coated Si substrates) deliver an extended operational energy ranging from 2.1 to 40 keV into a beam spot of 50 µm (H) x 80 µm (V) (FWHM) at the sample. The upgrade gives an increase in brightness of about two orders of magnitude. Most beam conditioning devices have also been upgraded and a suite of new detectors commissioned. Simultaneously, the original Huber diffractometer was thoroughly refurbished and its detector arm doubled and strengthened. These improvements allow now a rapid switching between high resolution XRD or REXS and techniques using 2D detectors, such as RSM, time-resolved XRD or (Bragg)CDI.

In this poster, we illustrate the new beamline capabilities using a few examples in magnetism using REXS and magnetic x-ray reflectivity.

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New developments at the COMET instrument from Sextants Beamline in Soleil, towards higher repetition rates and better resolution

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Abstract:

Many current forthcoming applications of magnetic materials involve heterostructures or alloys containing magnetic and non-magnetic elements. X-ray Resonant (Coherent) Scattering is the technique of choice to probe such phenomena thanks to its element-selectivity and spatial sensitivity.SEXTANTS [1] is a beamline of the SOLEIL synchrotron, covering the 50-1700 eV energy range dedicated to soft x-ray scattering. The resolving power exceeds 10^4 and maximum flux on the sample ranges from 1×10^{14} (100 eV) to 2×10^{13} (1000 eV) ph./s/0.1% bw. The beamline main objective is the investigation of the electronic and magnetic properties of solids using three scattering techniques: resonant inelastic x-ray scattering (RIXS), x-ray resonant magnetic scattering (XRMS) and coherent x-ray scattering (CXS), the last one including also imaging via Fourier transform holography (FTH) [2].

The COMET instrument [3] from SEXTANTS beamline combines the coherent imaging of magnetic domains with extreme conditions applied to the sample environment (magnetic field up to 900 mT, temperature 30-400 K, RF pumping) [4-8]. The detector part of COMET was recently upgraded: while the classic CCD PI-MTE is kept in service, we added two new detectors, a 2D c-MOS high repetition rate (50 Hz) detector [9, 10] and a double delay line MCP [11] for later time resolved experiments (a new fs pump laser is under construction and will be in service at the end of the year, being available for the XMRS and CXS stations). The distance between the sample and the individual detectors is tunable and the switch between the three detectors can be done within minutes.

Fourier transform holography (FTH) is a lensless imaging technique which uses a known reference in the sample to retrieve the object of interest in one single step of calculation (*i.e.* it does not require an iterative method), overcoming the phase problem inherent to other techniques such as coherent diffraction imaging and ptychography. In the case of an extended reference, a linear differential filter is applied, and the object can simply be obtained by calculating the inverse Fourier transform. This approach is known by the name of HERALDO. While in classical holography the resolution is limited by the size of the reference hole, with HERALDO this limit is overpassed.The new COMET setup permits closer sample to detector distances, increasing the maximum angle collected by the detector, which results in sub 10 nm reconstructed pixel resolution. Recent CMOS (Complementary Metal Oxide Semiconductor) 2D sensor now rivals the performance of state-of-the-art photon detectors for optical application, combining a high-frame-rate speed with a wide dynamic range. We will show a comparison of holographic images, recorded alternatively with the new CMOS and the classic CCD, taken for the same sample conditions. We would also like to point out that a future 6000 x 6000 pixels CMOS detector is under development and will be tested at SOLEIL. These new developments, initiated at the SEXTANTS beamline in collaboration with the SOLEIL detector group, are commercially available and already find application beyond synchrotron, as for example at FEL [10] or HHG x-ray base sources.

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Perturbated inter-site transition in honeycomb α-Li_2IrO_3 via ultrafast orbital excitation

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ABSTRACT

Honeycomb α-Li2IrO3 has drawn significant attention in recent years as a candidate for the realization of Kitaev quantum spin liquids (QSL) [1,2]. After long-range order in α-Li2IrO3 was discovered and thus ruled out the likelihood of a QSL ground state, external perturbation on the honeycomb 5d-system has risen as a new path to explore Kitaev physics [3–7]. Optical spectroscopy and X-ray studies have revealed dimerization of α-Li2IrO3 under high hydrostatic pressure, where oxygen-mediated inter-site hopping is blue-shifted and broadened [7]. Because of the interference between two Ir-O-Ir hopping pathways in the edge-sharing IrO6 octahedra, the oxygen-meditated inter-site transition is often considered a measure of bond-directional Kitaev interaction in honeycomb iridates [7,8]. Structural perturbation such as hydrostatic pressure, however, might affect all the couplings schemes simultaneously and complicate the underlying physics. In the paper, explore the 5-d honeycomb Kitaev system via orbital excitation through ultrafast laser pulses and time-resolved RIXS (tr-RIXS) spectroscopy.

Time-resolved RIXS (tr-RIXS) experiment was carried out at the SwissFEL Bernina beamline at Paul Scherrer Institute (PSI), Villigen, Switzerland. A hard X-ray RIXS spectroscopy setup design inspired by MERIX [9] was built and commissioned for the first time. The inelastic scattering signal was collected perpendicularly to the incident hard X-ray to suppress elastic scattering. Spherical Si(844) diced silicon crystal analyzers and a JUNGFRAU detector [9] were positioned in a Rowland's geometry to resolve the collected inelastic scattering in energy. The incident X-ray energy for probing RIXS spectrum is chosen at Iridium L_3 ($2p_{3/2}\rightarrow 5d$) edge (11.2145 keV). A Ti:Sapphire laser of 1.55eV, 35 fs in FWHM and 20 mJ pulse energy were frequency doubled (3.1eV) and synchronized with the hard X-ray to perform optical pump X-ray probe tr-RIXS experiment.

Tr-RIXS spectrum showed a non-equilibrium signature of perturbated inter-site transition (around 1.28 eV energy loss) in the honeycomb α-Li_2IrO_3 after t_{2g}-e_g orbital excitation, suggesting the presence of electron in e_g orbital perturbated the inter-site hopping between two neighboring Ir atoms.

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ALBA XMCD&XRMS beamline BOREAS, present status and vision

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ABSTRACT

BOREAS beamline 29 at ALBA Synchrotron Light Facility is a soft X-ray beamline dedicated to polarization-dependent spectroscopic investigations of advanced materials, enabling techniques such as x-ray magnetic circular and linear dichroism (XMCD, XMLD), and soft x-ray resonant scattering (including reflectometry, gisaxs, holography or transmission coherent diffraction imaging) [1,2]. The beamline provides a rather broad photon energy range (80 eV to above 4000 eV) with full polarization control for experiments at two endstations for spectroscopy and scattering approaches, both implementing high field (6 and 2 Tesla) and low temperature capabilities (4-380 K and 18-400K). This allows atomic level investigation of magnetic and electronic properties of quantum materials, among which ferromagnets, antiferromagnets, superconductors, ferroelectrics, multiferroics or topological insulators. Investigated samples have the form of isolated atoms, nanoparticles and powders, organic molecules, Van-der-Waals layers, thin films or bulk specimens. Operative since mid 2012, along the past few years we have largely enhanced the instrumentation available with notably: i) a state-of-the-art Scanning Tunneling Microscope, ii) a full surface preparation technique chamber with Molecular Beam Evaporation, LEED/Auger, ion sputtering and high temperature annealing, iii) an Argon-filled Glove box. All capabilities are now completed, fully commissioned and interconnected to the x-ray endstations via an iv) ultra-high vacuum radial distribution chamber. In this contribution, we will provide details on the available instrumentation emphasizing scattering experiments, highlights of recent experiments, and outline some ideas for the future upgrade of the instrumentation in the frame of ALBA II future upgrade (diffraction limited storage ring) and the evolution of the beamline scientific context and scope.

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2. Details of the beamline and its instruments are available at https://www.cells.es/en/beamlines/bl29-boreas.

Laser-Induced Magnetization Dynamics Studied by tr-XRMS at FEL Sources

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ABSTRACT

The availability of sub 100 fs short and highly intense free-electron laser (FEL) pulses enables studying ultrafast laser-induced demagnetization (LID) [1] in nanoscale domain networks of magnetic thin films employing, e. g., time-resolved resonant magnetic scattering (tr-XRMS). We present a systematic study on LID of Co/Pt-multilayer thin films at the FELs FLASH (DESY, Hamburg) and FERMI (Elettra, Trieste), for which we designed a beam-stop–photodiode, blocking the transmitted FEL pulses while monitoring their intensity [2], and a pair of in-vacuum Helmholtz coils, providing pulsed magnetic fields to generate different magnetic domain networks [3]. Our results from varying both intrinsic (film thickness and domain size) and extrinsic parameters (pump fluence, pump polarization and magnetic field) support microscopic theory of LID that explicitly considers electron-phonon and electron-magnon scattering for spin angular momentum conservation on ultrafast time scales [4, 5]. We observe laser-induced permanent domain reconfigurations accompanying LID if a magnetic field is applied and reveal their shot-by-shot dynamics conducting single-shot XRMS [3].

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MagStREXS: A Crystallographic Software To Analyze Magnetic Structures Using REXS Diffraction Data

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ABSTRACT

Resonant Elastic X-ray Scattering (REXS) is a unique element, site, and valence specific probe that allows studying a wide range of charge, spin and orbital orderings in solids and thin films [1-3]. Combining elements of diffraction and spectroscopy, this technique has been successfully applied to investigate different phenomena, also magnetic ground states of multiple materials.

Concerning magnetic structure determination, REXS is complementary to neutron techniques. Several situations make it essential: when the involved magnetic species present a neutron absorption cross-section that is too large, like Eu, Dy, Gd… [4], when the magnetic moments cannot be unambiguously determined with neutron experiments [5], or when more than one magnetic species are involved.

Different types of data can be collected in a REXS experiment to characterize a magnetic structure, but in most of the cases the analysis of these experimental data is highly complex and no crystallographic software has been developed to enable users to perform this analysis.

MagStREXS is a crystallographic software dedicated to the determination of **Mag**netic **St**ructures through **R**esonant **E**lastic **X**-ray **S**cattering. It is under development since mid-2017 at beamline P09 [6] at PETRA III (DESY) and is based on CrysFML, a library developed to facilitate the creation of crystallographic software that includes also some functionalities especially oriented to deal with magnetic structures. The aim of this program is to facilitate this type of analysis and also to provide tools for the preparation of these magnetic diffraction experiments.

In this poster we will present an overview of MagStREXS, its current status and the main features that have been implemented in the software until now.

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Magnetic helicoidal dichroism with XUV light carrying orbital angular momentum

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The interaction of polarized light beams, ranging from infra-red to hard-x-rays, with magnetic materials defines the rich set of analytical tools used in magneto-optics and it is also widely employed for studying magnetization dynamics in time-resolved experiments. Light polarization is associated with a spin angular momentum (SAM) of value S=0 for linear polarization and S=±1 for circular polarization, the latter imprinting a well-defined handedness on the photon beam. It is less common to exploit the orbital angular momentum (OAM) of value L carried by light beams possessing a well-defined handedness imparted by a helical wavefront. One important difference between SAM and OAM is that the latter can carry a topological charge $|L|>1$, with additional potential for new kinds of light-matter interaction. After finding many applications in the visible range, OAM beams with ultra-short pulse duration (also called *light springs*) and XUV wavelengths became available recently at high-harmonic generation (HHG), synchrotrons and free-electron laser (FEL) sources, widening considerably the range of experiments that can be envisaged.

We analyzed theoretically the interaction of OAM beams with magnetic structures featuring non-uniform magnetization, in particular of XUV beams with magnetic vortices. We predicted that the far field intensity profile encodes the vortex symmetry in a way that depends on the sign and value of L, an effect deriving from the inhomogeneous modification of the regular reflectivity coefficients by the local magnetization [1]. We named this effect Magnetic Helicoidal Dichroism (MHD). As for magnetic circular dichroism, MHD can be observed by inverting the sign of either the orbital momentum or of the magnetization, i.e. by switching the handedness of either the light spring or the magnetic vortex.

We obtained a first experimental evidence of MHD by measuring L-dependent scattering from permalloy magnetic vortices at the FERMI FEL source [2]. The 100 fs XUV pulses were tuned at the 3p-to-3d resonance of Fe (~23 nm), enhancing magneto-optical effects at XUV wavelengths and providing element selectivity. The experimental results match well our theoretical predictions, confirming the potential of the new toolset provided by MHD for studying the laser-triggered ultrafast dynamics of complex magnetic materials.

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Particle- and Phase-selective X-ray spectroscopy with Micro- and Macrobeams: The Case of $(SmS)_{1.19}TaS_2$ Nanotubes

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ABSTRACT

During the nanotube (NT) synthesis additional unwanted phases often occur (platelets, amorphic content, etc.) [1,2] and it is hard or even impossible to disentangle the information about the NTs from the data achieved by macroscopic methods. The purpose of this study is to show the advantages of the DAFS (Diffraction Anomalous Fine Structure) spectroscopy and microbeam XANES techniques in the analysis of NT powders containing a sufficient number of different phases. The DAFS technique, based on the measurement of the diffraction peak intensity in the vicinity of the X-ray absorption edge, brings additional information about the tubes in the powder mixture. Contrary to conventional XAFS (X-ray absorption Fine Structure) spectroscopy, DAFS allows to measure the XAFS-like signal from a certain phase or crystallographic site separately by choosing the proper diffraction peak, thus providing phase- and site-selectivity [3]. Microbeam spectroscopy allows one to focus the X-ray beam on a certain microparticle and perform a single-particle XANES analysis.

NTs have several diffraction features, that distinguish them from the conventional 3D crystals and single 2D layers, that are based on the same structural units/layers (Carbon nanotubes vs Graphite, etc). Due to the lack of the out-of-plane symmetry diffraction patterns of the NTs usually don't show the distinct reflections of the *h*0*l* and 0*kl* type, that distinguish them from the bulk particles; contrary to the single 2D layers the multilayered NTs show the reflections of 00*l* type due to diffraction from the basal planes. These 00*l* and *hk*0 reflections can be used to get information about the NTs using the DAFS technique from NT powder.

In order to understand the growth and stability of SmS-TaS_2 NT a set of powders were synthesized by the chemical vapor transport method (CVT) [2] at different temperatures (800, 825, 850, 875, 900, 925, 975, 1050 C). XRD and electron microscopy have shown that the NT abundancy falls down with temperature. The shape of the DAFS spectra also changes: the intensity of Ta L_3 'white' line decrease with temperature. The microbeam XANES measured on single SmS-TaS_2 nanotubes also shows higher Ta L_3 'white' line intensity in comparison to the powder. Such dependence of 'white' line intensity on NT abundancy can be explained by the difference in the interaction of SmS and TaS_2 layers in planar bulk SmS-TaS_2 crystals and SmS-TaS_2 NT. In the bulk SmS-TaS_2 crystals (usually defined as $(SmS)_{1.19}TaS_2$) it was found that SmS layer act as a donor of electrons for the TaS_2 part [4]. In the NT due to the curvature of the layer, the number of the SmS units is smaller than in the bulk crystals, thus SmS part donate less electrons. Therefore, in NT there should be more Ta 5d band vacancies in comparison to bulk, thus providing a more intense Ta L_3 'white' line in XANES spectra.

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In-Situ X-ray Diffraction and Imaging Beamline at PETRA III: status and prospects

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ABSTRACT

The In-situ X-ray diffraction and imaging beamline P23 at the PETRA III (DESY, Hamburg) operates currently with one experimental hutch. A second hutch operated by a joint KIT/DESY cooperation and dedicated to novel hard X-ray microscopy techniques will go into operation at the beginning of 2023. The scientific case of the beamline is concentrating on the physics and chemistry of systems dominated by low dimensional and confinement effects, with an emphasis on in situ and operando techniques.

The spectroscopic type undulator source and X-ray optics provide up to 10^{13} photons/sec into variable spot sizes down to one micrometer in the energy range 5-35 keV. Optionally, the energy can go higher up to 50 keV. The optical layout comprises an LN_2-cooled Si(111)/Si(311) double-crystal monochromator, horizontally deflecting plane and collimating mirrors and adjustable sets of compound refractive Be lenses in the optical and as well as experimental hutches. The experimental hutch is equipped with a heavy-load 5+2 circle diffractometer (HUBER), which can carry sample cells with up to 150 kg in horizontal scattering mode and up to 15 kg on the Eulerian cradle in the vertical mode. The experiment instrumentation pool is designed for multiscale analysis of bulk and nanostructured materials and devices: heating chambers, flow LHe-cryostat, piezo-based position stages, and an Andor optical spectrometer are available for the users. An in situ pulsed laser deposition chamber will become available on request for user projects starting September 2022.

The beamline allows the application of XAS and anomalous X-ray scattering techniques over the entire range of X-ray energies. Starting in the second half of 2022, the new CRL-based focusing system in the experimental hutch will be capable of holding focused micrometer beams on the sample in the energy range from about 6 keV to 25 keV.

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Thank you for your participation!