Engineering and Physical Sciences Research Council

XMaS Annual Report

Timeline 2022/23:

- Reporting Period for this Annual Report: **1st September 2021 – 31st August 2022**
- Deadline for Annual Reports**: 20th February 2023**
- Assessment by Panel**: March 2023**
- Feedback to Facilities: **April 2023**

Facility Name: XMaS the UK Materials Science Beamline at the ESRF
Directors: Prof. Tom Hase (University of Warwick) and Prof. Chris Lucas (University of Liverpool)
Start/End Dates: 15th November 2018 through 14th November 2023
Funds awarded: £6,909,720: split between Liverpool (£3,427,966) and Warwick (£3,481,754)

Value Proposition

XMaS is an integral part of the UK's synchrotron radiation (SR) infrastructure and has been supporting UK materials scientists since 1997. Following the recently completed European Synchrotron Radiation Facility (ESRF) upgrade, XMaS has undergone extensive modifications to deliver a state-of-the-art facility fully exploiting the capabilities of the new machine. It delivers a much more brilliant X-ray beam with an operational energy range from 2.1 to 40 keV. The upgraded facility is more versatile, providing a combination of techniques from X-ray diffraction to small angle X-ray scattering as well as X-ray absorption and emission spectroscopy. The science portfolio on XMaS continues to evolve, embracing a broad spectrum of scientific disciplines under the generic theme of materials science, cutting across research in physics, chemistry, biosciences, healthcare, engineering, and energy. XMaS provides access to tender X-ray spectroscopy (2-4 keV), which is very uncommon and in high demand, especially for application to materials such as batteries and catalysts as well as in heritage and environmental research. The new high energy capability (25-40 keV) opens up *operando* experiments as well as accessing technologically important X-ray absorption edges. Building on the new enhanced capabilities, XMaS is able to deliver the correlative characterisation that is needed to understand ever more complex and heterogeneous materials and devices under technologically relevant conditions.

XMaS has strong links with the Diamond Light Source (DLS). It has been operational throughout the development of the DLS beamline portfolio and there is frequent transfer of expertise between both facilities. Most synchrotron studies tend to be collaborative, and, in the post-Brexit landscape, it is essential that UK scientists can maintain, develop, and nurture links with international colleagues to increase the range, quality, and impact of their research. XMaS plays a pivotal role in this by providing a key access point to the ESRF, enabling UK users to develop international collaborations with both academic institutions and industry. These partnerships ensure the future competitiveness, resilience, and creativity of the UK materials sector, which relies on the development, characterisation, and exploitation of novel functional materials. The overall objectives of the facility are:

- Deliver internationally leading science based on X-ray metrologies across a range of temporal and spatial length scales;
- Implement and develop instrumentation needed to keep the UK at the forefront of materials science;
- Attract world-class researchers to the facility and the UK;
- Train early career scientists and students in advanced X-ray methodologies;
- Operate the facility efficiently, sustainably, and resiliently within a framework of equality, diversity, and inclusion.

Scientific Excellence

During the reporting period, operations at XMaS were still impacted by the COVID pandemic with the OMICRON variant causing difficulties in travel and access to samples. However, in partnership with the ESRF and with user co-operation, it was possible to support onsite access and some 30 user experiments were successfully delivered.

The replacement of the ESRF lattice and corresponding beamline upgrades from late 2018 through to the gradual resumption of user operations during 2020 naturally has impacted the number of published outputs from the facility during this reporting period. Historically, we note that there are typically several years between an experiment and publication. This timeline will have been further impacted by the COVID pandemic. However, here we summarise the scientific excellence as collated from research publications grouped around challenge themes:

Energy research: *Catalysis, Chemical Reaction Dynamics, Energy Storage, Fuel Cells, Materials for Energy Applications, Nuclear and Photonic materials*

The charge distribution and bonding mechanisms at polarized solid–liquid interfaces remain a topical and fundamental challenge in electrochemistry. In situ resonant surface X-ray diffraction studies were performed on XMaS, supported by self-consistent DFT calculations, to assess the charge distribution and bonding mechanism at the electrochemical active interface during the adsorption of bromide anions onto a single crystal Cu(001) electrode surface (J. Phys. Chem. C 126, 9, 4612–4619 (2022)). The results concluded that charge reorganization within the interface atoms occurred, rather than a charge shift between atoms. The data show the importance of considering the detailed charge distributions at interfaces within metal electrodes when modelling electrochemical reactions. Such information and the developed metrological approaches are key to understanding a wide range of energy materials including the next generation of battery materials and their response to charge/discharge cycling.

Physical Sciences: *Polymer Materials, Magnetism and Magnetic Materials, Multiferroics, Ferroelectrics, Electronic Structure, Spintronics, Skyrmions, Superconductivity, Surface Science, Supramolecular Chemistry, Chemical Engineering*

A joint study using XMaS, as well as I22 and I16 at Diamond, used a combination of GI-SAXS, powder SAXS together with WAXS to show that liquid-crystalline columns with long-range helical order can form by spontaneous self-assembly without the inclusion of any chiral chemical groups or dopants (Nat. Comm. 13, 384, 1-11 (2022)). The resulting structure of counter-rotating staircases form a complex lattice with *Fddd* symmetry with a total of 8 columns per unit cell (4 right-, 4 left-handed) can be characterised by an “antiferrochiral” structure. In selected compounds, such a configuration allows close packing of fluorescent groups reducing their bandgap and giving them promising light-emitting properties.

In magnetism, significant research has focused on understanding spin-transport in spintronic systems. In ferromagnetic (FM)/non-magnetic (NM) thin-film systems, “spin-pumping” formalisms are used to explain the correlation between magnetic precession and damping as spin polarised currents traverse the interface. The effect is enhanced when the FM thin films are layered with heavy metals, such as Pt. XMaS sample environments facilitate studies exploiting resonant magnetic scattering to explore the spin transport across such interfaces. A recent review paper

(J. .Appl. Phys. 131, 170902 (2022)) highlights new experimental observations including recent XMaS studies that require conventional theories to be extended after compelling evidence of a role played by proximity-induced magnetism (PIM) which hitherto has been ignored. Contributing to the ongoing scientific debate was an experiment studying the enhancement of damping in $Co_{25}Fe_{75}$/SL/Pt multilayers in which a nonmagnetic spacer layer (SL) of either Au or Cu was used to modify the interface coupling between the FM and the heavy metal (Phys. Rev. B 105, 094433 (2022)). Element specific X-ray magnetic reflectivity and X-ray magnetic circular dichroism at the Pt and Au L_3 edges were used to determine layer orientation and moment distribution. The Pt PIM and the damping both fall rapidly, with a relationship between damping and PIM that depends on the spacer layer. The PIM observed in the Au layer showed a complex dependence on the layer thickness, suggesting some hybridization with the Pt. This work was chosen as an APS highlight. Resonant reflectivity was also used in conjunction with vibrating sample magnetometry to characterize field driven and spin orbit torque driven magnetization reversals in a CoFeTaB/Pt bilayer (Phys. Rev. B 106, 094429 (2022)) in which the Pt PIM plays an important role. Soft X-rays tuned to the Co L_3 edge (I10 at DLS) studied the magnetisation within the bulk of the FM layer, with experiments tuned to the Pt L_3 edge performed on XMaS focusing on measuring the size and extent of the interface Pt PIM.

Exploiting the ability to control magnetic, electric, and optical properties in (multi)ferroic materials has not only revolutionised condensed-matter physics but also presages future cutting-edge solid-state devices and technologies. The highest and most effective couplings are realized in ferroic materials. Experiments using the XMaS offline source with a custom co-developed sample environment was used to show that the ferroelectric domains in perovskite $Pb(In_{1/2}Nb_{1/2})O_3$–$Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ (PIN-PMN-PT) domain-engineered crystals can be manipulated by electrical field and mechanical stress. Associated with the domain reversals, a transformation from an opaque polydomain structure into a highly transparent monodomain state occurs (Adv. Mater. 2106827, 1-8 (2022)). In thin films of perovskite relaxor-ferrolectrics such as PMN-PT, the application of stress or electric fields drives the system through a complex structural phase transition driven by domain reorientation. AC electric field driven *operando* synchrotron X-ray diffraction on patterned device structures was used to investigate the piezoelectric domain behaviour under an electric field for both a clamped (001) PMN-PT thin film on Si and a (001) PMN-PT membrane released from its substrate (Appl. Phys. Lett. 119, 20, 2903, (2021)). In the clamped film, the substrate inhibits the field-induced rhombohedral (R) to tetragonal (T) phase transition resulting in a reversible R to Monoclinic (M) transition with a reduced longitudinal piezoelectric coefficient d_{33}. Releasing the film from the substrate results in recovery of the R to T transition and restoration of a large d_{33}. The data highlight the subtle relationships between the strain fields and the resulting ferroelectric properties of these technologically important materials.

Focusing on outreach an accessible publication, complete with activity sheets for schoolchildren, was prepared in partnership with Futurum. The article covers vignettes from user science as well as describing the facility. Activity sheets are designed to explain the science and methodologies employed using readily available objects. The sheet was widely shared online and through social media.

Science performed on XMaS continued to be singled out for inclusion in the ESRF's publications during this reporting period with an article in the current 2022 issue of the ESRF Highlights. In the section on "Electronic structure magnetism and dynamics", the work of C. D. O'Neill *et al.* on "*The observation of Kondo charge accumulation*" originally published in PNAS 118, 49, e2102687118 (2021) was presented. This work describes the complex magnetic and structural ordering in UAu_2. Below the Néel temperature, T_N, the system weakly orders magnetically with a sinusoidal modulation. The low background and good signal to noise ratio enabled the magnetic and charge diffraction peaks to be measured as a function of temperature down to ~4 K. The data suggest that the magnetic ordering is accompanied by an incommensurate Kondo state which has an ordering temperature well below T_N.

OpMetBat

XMaS, through the University of Liverpool, is a partner in the Joint Research Project within the European Partnership on Metrology "Operando metrology for energy storage materials" – OpMetBat which was launched in 2022. The project focuses on the development of new battery materials and specifically on improving the performance, lifetime, safety and cost of energy storage technologies. Innovation is currently hampered by the inability of industry to characterise the chemistry of new batteries under *operando* conditions. The project will build a metrological framework supporting traceable operando characterisation of state-of-the-art battery materials under dynamic charge / discharge conditions and establish a good practice guide for *operando* spectroscopy and diffraction methods.

New methodologies that have been developed

The XMaS vision, building on our new enhanced capabilities, is for the facility to deliver the correlative characterisation protocols needed to understand ever more complex and heterogeneous materials and devices under technologically relevant conditions. This approach requires multimodal studies to enable materials to be characterised in terms of composition (XAS, XRF, TXRF) as well as spatial ordering on local (XAS, WAXS, XRD, xPDF), and larger (SAXS, XRR) length scales. The approach has driven co-developments of sample environments and increasingly in simultaneous deployment of different X-ray techniques.

Spectroscopic Studies: XAS Developments at Beamline Energy Limitations Si <111> Mono

The facility uses a Si <111> monochromator and, over the reporting period, we have been working with users to test operationally the cryogenically cooled system across the entire energy range using XAS studies. Alfredsson (Kent) studied a NaP standard at the P K edge (2.146 keV) with data collected in fluorescent yield (fig. 1, left). At the other energy extreme, a SmCe catalyst was measured in transmission at both the Ce (40.443 keV) and Sm (46.834 keV) K edges by Walton (Warwick) (fig. 1).

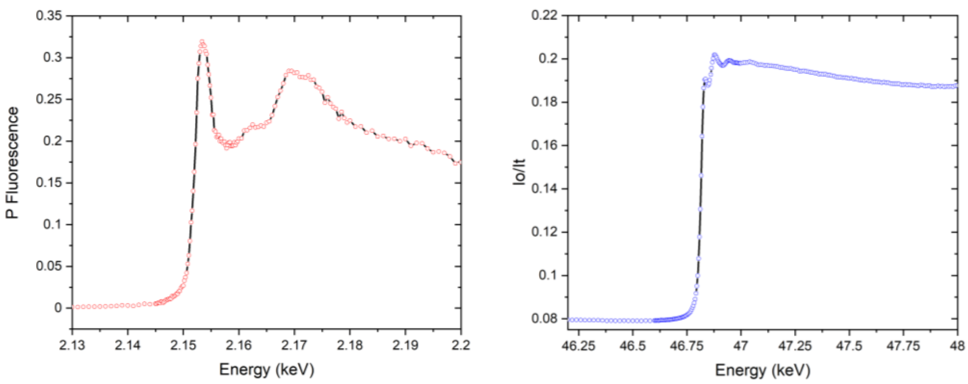

Figure 1: XAFS spectra recorded from a NaP standard at the P K edge (left) and a SmCe catalyst recorded across the Sm K edge.

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KB Mirror

In the last Annual Report, we detailed the decision to add micron-sized beams to the facility through a new KB system. Over this reporting period, the technical designs for the system were finalised (fig. 2) and manufacturing is nearing completion. Preliminary works at the facility have been completed, and delivery of the system is expected during the spring of 2023 for user operations from autumn 2023. Unfortunately, some delays have arisen with shipping due to Brexit and new VAT regulations in France.

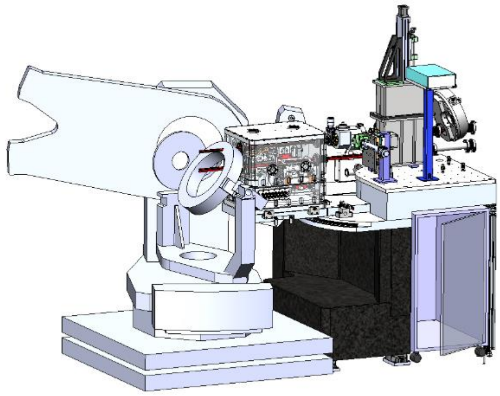

Figure 2: The final optimised design of the IDT KB mirror system.

The system will be housed on the unfocused beam path but will not impede normal focused beam operations as this beam will pass uninterrupted through the final housing. Beam sizes down to sub 5 x 5 μm^2 are expected.

Total Reflection X-ray Fluorescence (TXRF)

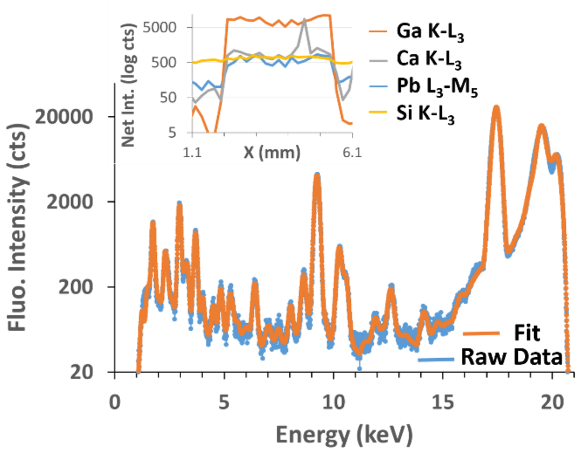

Figure 3: TXRF spectra of ICP multi-elemental standard solution IV; 5 µl droplet, 1 µg/L on quartz carrier with (insert) selected elemental distributions across the dried droplet residue. Incident energy: 20.2161 keV; counting time: 300 s (insert 10 s).

The versatility of the XMaS diffractometer, coupled with the low background, and the ability to perform high resolution scans at grazing incidence have enabled the facility to add Total Reflection X-ray Fluorescence to the suite of techniques available to users. This technique exploits standing waves from a reflector to excite small amounts of analyte (fig. 3). Environmental monitoring and the ability to quantify ultra-trace levels allow statutory limits for elements such as lead (Pb) in the environment including both water and particulate matter to be determined. Initial experiments exploited the two detector arms to facilitate sample alignment and fluorescent measurements. Efforts during these proof-of-principal experiments focused on aligning the fluorescent detector with the dried sample residues. Extrapolating data such as that shown in fig. 3 suggest a limit of detection of picograms of material is possible on XMaS. User data have been incorporated into both the revision and creation of new ISO standards (within TC201). The facility has been a round-robin partner within the COST Action ENFORCE TXRF, and Smart Solutions srl in developing TXRF methodologies for the study of particulate matter on filters.

X-PDF and Spectroscopy

X-ray Pair Distribution Function (X-PDF) is another technique that is exciting users with the new high energy capabilities at the facility. Although normally measured at energies in excess of 60 keV, an energy of 40 keV can still yield good data. XMaS also has the advantage of both a high energy resolution, due to the double crystal monochromator, as well as a high angular resolution, through using the diffraction configuration. The higher Q resolution results directly in a slower dampening of the PDF spectra. As an initial test, a CeO_2 standard powder was measured at 40 keV using the high energy CdTe 2D pixel detector mounted on the detector arm and combined using the ESA software (fig. 4). The data can potentially be collected up to Q_{max} > 30 $Å^{-1}$ and analysis by colleagues from the ESRF shows that the spectra can be fitted to standard models across multiple length scales.

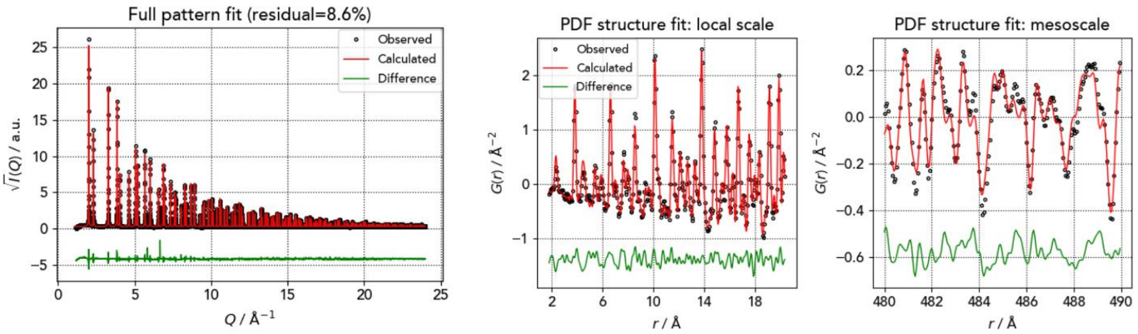

Figure 4: Processed diffraction pattern from a CeO_2 standard as a function of scattering wave vector (left). Fits (lines) to the data (points) in both the XRD and radial functions (G(r)) show the data fit to expected parameters at both the local and mesoscale.

A key to delivering a user program in X-PDF in the future is reducing the background and managing the data sets from the 2D detectors. The data collection proceeds via recording a series of 2D images as a function of scattering angle and reducing the data set to a collated powder diffraction pattern for further processing. In collaboration with colleagues from the Swiss-Norwegian beamline (SNBL) at the ESRF, new conical tungsten beam stops have been designed to specifically reduce the background. In addition, fig. 5 shows the newly designed and commissioned helium filled flight tubes of various lengths that can be used to further reduce air scatter.

One of the unique opportunities offered by XMaS is the ability to potentially perform X-PDF and spectroscopic scans on the same sample under the same conditions. This multimodal capability is currently being developed for the user community as we continue to refine the data handling and reduction challenges.

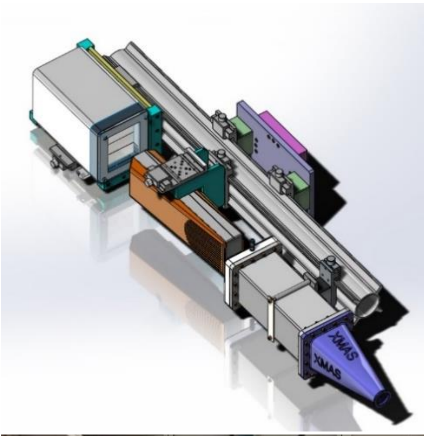

Figure 5: The low background system designed to interface with the 2D detectors (top) and mounted on the 2θ arm (bottom).

Linkam Sample Stage for WAXS/SAXS Experiments

Two Linkam sample stages have been integrated to the beamline: a single cell calorimetry stage (DSC-600) and a temperature-controlled capillary cell (HFS600-CAP) (fig. 6). The DSC-600 accommodates small sample pans that can contain either liquids, powders or soft matter and is designed for scattering experiments (WAXS and SAXS). The HFS600-CAP stage takes 1.7 mm diameter capillaries. Both stages operate between -195 °C and 600 °C with heating/cooling temperature ramps up to 130 °C per minute. To support users and enhance data collection efficiency we have developed a python-based software tool to extract the data from the proprietary Linkam control software in a format more suitable for our users and for further integration into the XMaS data streams. The cells can be used offline without beam if needed.

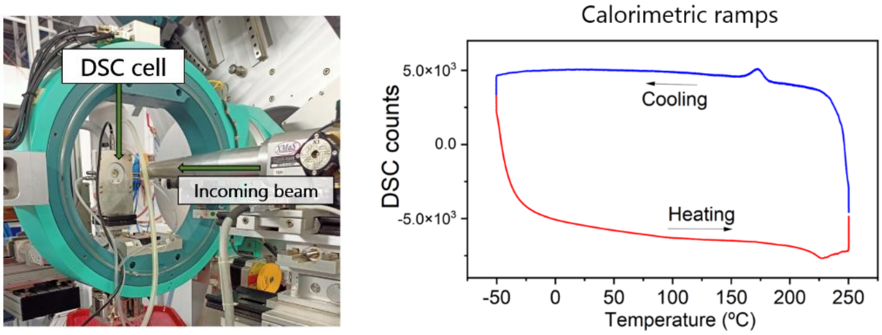

Figure 6: A Linkam DSC-600 calorimetric cell mounted at the beamline and configured for SAXS/WAXS experiments (left). An example of a calorimetric ramp obtained from a polymeric sample (right).

White Beam and Electron Orbit Monitor: The beam quality and stability are ultimately defined by uncertainties in knowledge of the incident white beam into the beamline delivery system. A new monitoring system is onsite and is ready to be installed when a suitable window in the operational schedule can be identified. It will facilitate alignment of the two main optical elements of the beamline, the monochromator and the toroidal focusing mirrors, and make any diagnostics easier. We note, however, that the experience gleaned over the past year is that the new EBS source is stable and so operations are not significantly impacted. We have prioritised user access to the facility over the past year rather than taking time out of the schedule for this installation, and instead delaying a few projects to make a more targeted intervention where several upgrades can be installed simultaneously.

Scientific Excellence Case studies

XMaS Newsletter: XMaS activities are widely disseminated in our annual newsletter which is written for a scientifically interested reader. The 2021 version was available from March 2022 and circulated widely (> 600 copies). A summary of the new beamline capabilities and upgrades was presented along with a series of user research highlights:

- **Novel in-situ stress rig reveals origins of giant piezoelectric effect** (Adv. Mater. 2106827, 1-8 (2022)): *Results from the ES1500 multifunctional stress rig to explore the crystallographic and optical changes in PIN-PMN-PT perovskites.*
- **Quantum order by disorder revealed under magnetic field** (Phys. Rev. Lett. 126, 197203 (2021)): *Observation of quantum order by disorder through two modulated spin density wave states invested with resonant elastic X-ray scattering under applied magnetic field.*
- **Substrate protection with sweet corrosion scale: Mind the gap** (ACS Appl. Mater. Interfaces 13, 48, 58193–58200 (2021)): *Exploration of the corrosion protection of steels afforded by iron carbonate scale using in situ diffraction in a custom sample environment under electrochemical cycling.*

Figure 7: Front page of the 2021 XMaS Newsletter.

- **Wolfram's copper blisters** (ACS Appl. Mater. Interfaces 13, 5, 6795-6804): *Study of nano-multilayers of Cu/W studied using GISAXS as a function of temperature.*
- **Dendrimer interactions with cell membrane models** (Biochimica et Biophysica Acta (BBA) - General Subjects 1865, 129542 (2021)): *X-ray reflectivity study of lipid layers combined with dendrimers of varying concentration and positive charge.*

The 2022 XMaS Newsletter is being finalised and will be released mid-February 2023 and available online. It will be detailed in the next annual report.

Publications

A full list of the publications is maintained on our website. We track publications by direct engagement with our users, an online submission portal through our website and regular searches of Web of Knowledge. Herewith, a list of the publications associated with the XMaS NRF published in peer reviewed literature over the past 3 years. Comparison with historical metrics are provided in section 10 (KPIs). The 2022 ESRF highlight publications from XMaS are marked (*). Publications that have been prepared for a wider audience are marked (†).

2022

Burn DM, Fan R, Inyang O, Tokaç M, Bouchenoire L, Hindmarch AT, Steadman P,
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2021

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2020

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Impact

During this reporting period, impact activities were still being somewhat impacted by the COVID-19 pandemic and the myriad of local travel and social distancing regulations, particularly in France.

Activities to promote the facility beyond its core base: As COVID eased, we began to make an increased effort to publicise the capabilities of the upgraded beamline to potential new users. The deadlines and details for proposal submission were also published on the website of the Royce Institute. Our staff and PDRAs are reaching out directly and individually to potential user groups as well as attending conferences and meetings including:

- ESRF User meeting
- 23rd International Mineralogical Association General Meeting in Lyon, France.
- Winter school on Molecular Simulations (MolSim2023).
- International Conference on the Science and Technology of Synthetic Metals (ICSM-2022), Glasgow.
- Physical Aspects of Polymer Science (PAPS 2022), London.
- International Conference on Resonant Elastic X-ray Scattering (REXS 2022), Paris.
- International Workshop on Advanced Techniques in Actinide Spectroscopy (ATAS 2022) & Workshop on Speciation, Techniques and Facilities for Radioactive Materials at Synchrotron Light Sources (AnXAS 2022), ESRF, Grenoble.
- Dissemination of the Futurum article for more general readers and school students.

Public Engagement: **Scientist Experience:** Our annual nationwide competition for Year 12 female students to come to XMaS and the ESRF as part of a four-day trip was able to run for the first time since the pandemic. We had a larger response than ever before, and the standard of those entries was exceptional. We found it hard to pick out winners, taking 18 girls rather than the planned 16! In Grenoble the girls spent two days touring the ESRF facility, taking part in the ESRF Synchrotron at Schools session and talking to lots of female scientists based at the ESRF, gaining the inside track on how far Physics can take you as a career. The competition remains a wonderful way to take learning out of the classroom and into the real world. We have just launched our 2023 competition, so if you know someone who fits the brief or have contacts with Science Teachers, please encourage them to submit an entry.

Figure 8: The 2022 XMaS Scientist Experience participants at the ESRF

Examples of Societal & Economic Impacts: Following on from the Advent project £40k was awarded under the EPSRC IAA scheme to develop a novel stress cell in partnership with the company Electrosciences Ltd. A follow up application for InnovateUK funding to commercialise this product is under consideration. XMaS has a strong track record in commercialisation of products developed on the facility. 2021 also saw the publication of the REF2021 results and we are aware of at least one impact case study where the original research was performed on the XMaS beamline.

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Cost Recovery

UK access to synchrotron radiation is provided through the ESRF and DIAMOND and follows the "free at point of use to the best science" model. The Elsy report, submitted to BEIS in 2017, stress-tested this access mechanism in an independent review of National Large Facilities at Harwell and strongly supported it. XMaS is currently funded with the same user access model and there is, therefore, limited scope to generate direct cost recovery through user access. The upgraded facility has been designed with increasing efficiency as a key driver, ensuring that we can support more users and therefore be more sustainable by reducing the cost per user/experiment.

Cost recovery covering some staff costs and instrument development have been secured through European funding in partnership with the University of Liverpool. Through Horizon2020, the European Metrology Programme for Innovation and Research (EMPIR) has funded several projects in which the facility has been a partner – Nanostrain, ADVENT and OpMetBat. These projects have provided some limited funds to cover staff costs (60%) associated with the project work and ensured additional capabilities could be developed (40%) which are now freely available for the wider community. The funds have contributed marginally to the actual running costs of the facility.

Year	Running Costs	Grants	Other Academic	Students	Industry	% Recovered
2018	£1,741,944	£0	£0	£0	£0	
2019	£1,741,944	ADVENT: £124,489	£0	£0	£0	4%
2020	£1,141,944	£0	£0	£0	£0	
2021	£1,141,944	£0	£0	£0	£0	
2022	£1,141,944	OpMetBat: £103,417	£0	£0	£0	5%

Table 1: Additional Income through other funding sources.

Future Plans and Issues

Some cost recovery is achieved from commercial licences, generating a few k£ per annum which is reinvested into the NRF. Further cost recovery can only feasibly be achieved by direct investment from industrial users. This access mechanism is handled through the ESRF.

Users

There has been no user access since 2018 mostly due to the ESRF shutdown for its EBS upgrade, with first users on this grant only accessing the facility since January 2021. Unfortunately, with the resurgence of COVID cases, travel to France and access to the ESRF facility was limited to staff members only. To maximise the uptime of the facility and to generate the highest impact to the user community, we prioritised and triaged experiments that *could* be performed without users travelling to the facility. This necessarily created a back-log of experiments that were approved by the review panel, but were subsequently delayed, and scheduled to take place in the first half of 2022. Unfortunately user access was then further complicated by the Omicron wave.

The user statistics requested have been compiled from the CRG access route and are shown below in table 2:

Year	Student	RA	Academic	Industry	Other	No. Repeat	No. unique
2019	0	0	0	0	0	-	-
2020	0	0	0	0	0	-	-
2021	26	14	18	0	0	19	39
2022	31	22	52	0	0	10	80

Table 2: User statistics over the grant period. We report the statistics by calendar year and not the reporting period.

The CRG users in 2022 came from 34 UK and 16 international research groups with **37%** of user visits from new users. For the remaining ESRF allocated time, there was an additional 36 users from 11 UK and 2 international groups of which 14 were students and 9 PDRAs. The percentage of these users who were new to the facility was 39%. Historical trends and a further more detailed breakdown of our user statistics can be found on our website.

The breakdown on scientific area for the reporting period, as identified by the users themselves, is compared with the facility average in fig. 9.

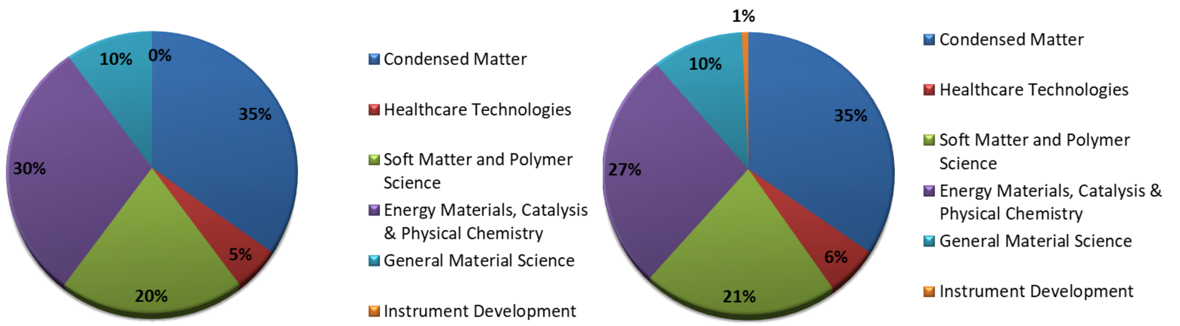

Figure 9: Research areas as reported by the users in their end of run survey. Data from this reporting period (left) compared with the facility average (since 2012, right).

Future Plans and Trends: Growing and sustaining the user community is a priority for the future. A clear trend over the last few proposal rounds is for more proposals to make use of the co-modalities offered. XAS spectroscopy requiring shorter beamtime allocations is best accommodated in a “BAG ACCESS” mechanism where groups submit samples to a community access round.

User Surveys/Satisfaction

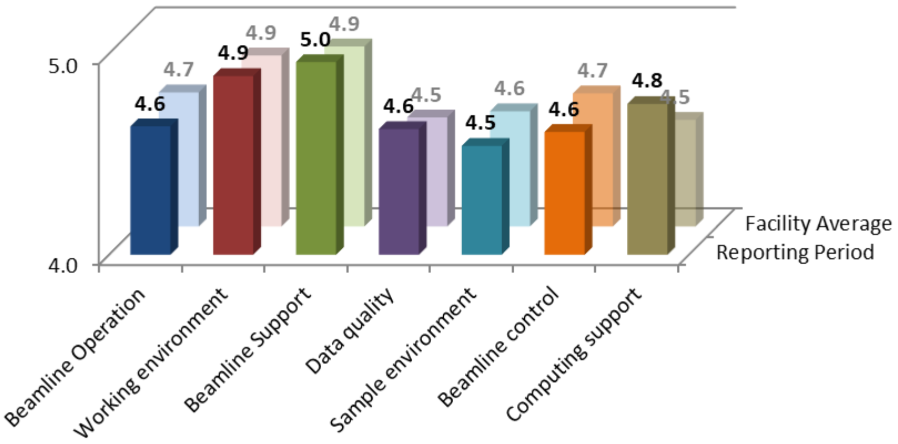

Figure 10: User survey results for the current reporting period (foreground) with historical averaged data in the background.

The principal investigator for each experimental run at the facility are asked to complete, on behalf of the experimental team, an end of run survey scoring against operational performance as shown in fig. 10. Our return rate is over 90% and direct follow-up with the users occurs whenever the satisfaction is lower than expected. We note the user satisfaction is in line with the historical average and is generally very positive. Some free form comments from users over the reporting period include:

“Excellent support from beamline scientists.”

“The support from beamline scientist was excellent. He made sure we had everything we needed and responded to all our requests with highly professional and efficient assistance.”

“Our local contact went above and beyond to help us collect all our data. They travelled to the facility on Sunday and Monday (bank holiday) to change our samples and were quick to reply to our messages and emails even when offsite.”

“We want to express our appreciation to the beamline scientists for their great help and support in this tricky experiment.”

“The beamline scientist was extremely helpful and outstandingly dedicated, which made the experiment a success.”

“The beamline scientist was enthusiastic and resourceful in equal measure and integral to the success of the experiment.”

“Excellent support, as always, from the beamline staff.”

“Beamline support and facilities excellent, outstanding support from local contact and exciting data. Wow the beamline is something everyone should come and see. What an amazing work the local team has done, and data quality has improved significantly.”

“Beamline staff were incredibly helpful, which made for a very productive session, thank you again. Experiments were successful and all equipment worked as intended.”

“Excellent support was given from our local contact who worked extremely hard to get our experiment to work.”

Service Demand

Access to the facility is governed by a Collaborating Research Group (CRG) contract with the ESRF. This contract stipulates that 30% of the full flux beamtime is allocated through ESRF review panels in a worldwide call. The remaining beamtime, which is available only to the UK community, is allocated through our independent Peer Review Panel (PRP) and assessed on scientific merit only. Beamtime is scheduled in six-month allocations and where possible, all electron bunch modes of the ESRF filling are used. However, since the EBS upgrade, there have been some problems with the beam flux and stability in the 16- and 4-bunch modes, limiting the number of available shifts that the facility could deliver to users. It is not possible to provide a chart showing demand and capacity monthly, but fig. 11 shows the number of proposals received through the two separate access routes as a function of time. We note that the number of proposals submitted is slowly returning to pre-pandemic levels as the research community returns to full capacity. This trend mirrors what has been seen at other beamlines and facilities over the past year or so.

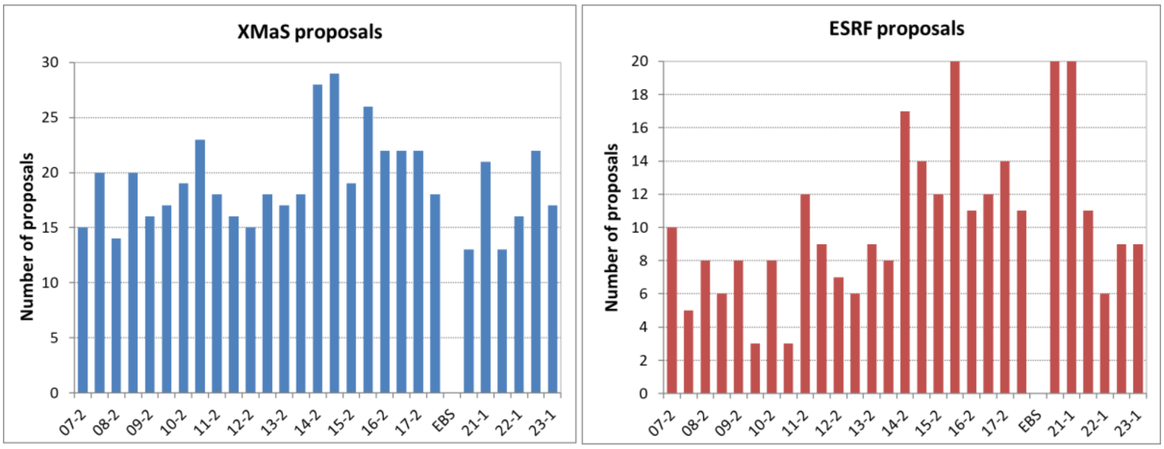

Figure 11: The number of proposals submitted to the XMaS NRF and reviewed by the independent review committees as a function of time. UK based proposals (left) and international applications through the ESRF (right).

Demand for the facility can be gleaned from the application statistics. Figure 12 shows the demand of the facility since 2013. We plot the ratio of the requested to available shifts in the left panel of fig. 12. A ratio of over 1 means that there is more demand than we can meet, and we cannot accommodate all user requests and have to reject some proposals. The right-hand panel of fig. 12 shows the percentage of shifts applied for that were rejected. We note that the PRP regularly comments that the vast majority of applications have strong scientific merit and, in most cases, would warrant beamtime. We aim for a rejection rate of between 30-50%. This ensures that only the best scientific challenges are addressed whilst at the same time not discouraging users from applying for time. The open data points in fig. 12 correspond to the statistics dominated by COVID where some experiments were not possible due to remote working and access rules. This necessitated some accepted experiments having to be deferred as well as last-minute scheduling to accommodate both operational and user needs. Some experiments also needed to be given more beamtime than requested due to some inefficiencies with fully remote working. Such actions have skewed the statistics but even so, the average demand has remained at a manageable level.

Unfortunately, we cannot provide the same statistical analysis of the ESRF applications from our international colleagues, but the rejection rate is more than double that for the UK CRG time and approaches 80% in some application rounds.

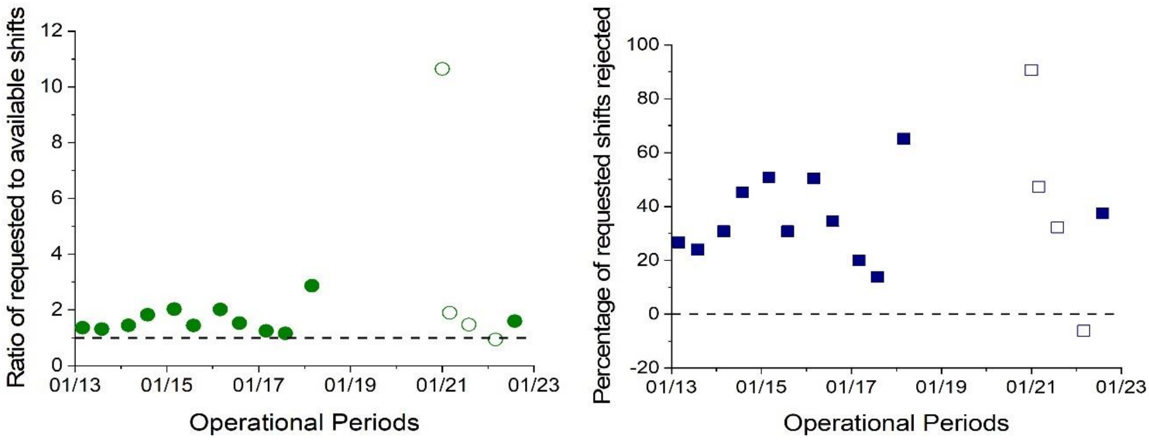

Figure 12: The demand for the facility represented by the ratio of requested to available shifts (left) and the same information but presented as the percentage of requested shifts that could not be accommodated. The open symbols on both plots are data that are compromised due to COVID.

We aim to continue to grow the user community in the future. In preparation of the Statement of Need, direct engagement with the Diamond community was achieved which we will develop as the Diamond dark period approaches. Direct engagement with the current user community is planned through the upcoming User Meeting (May 2023) as well through face-to-face in person interactions at meetings at Diamond, Catalysis Hub, and the Faraday Institute.

Remote access to the "offline" facilities (the diffractometer based on a fixed tube X-ray micro-source and the facilities for electrical characterisation) restarted in 2022. Often this instrumentation was used in tandem to provide support for some of the experiments scheduled on the beamline. One extended programme of experiments resulted directly in a publication: P. Finkel *et al*. *"Simultaneous Large Optical and Piezoelectric Effects Induced by Domain Reconfiguration Related to Ferroelectric Phase Transitions",* Adv. Mater. 2106827, 1-8 (2022).

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Risks

A risk register is maintained for the facility and reviewed every two months. It consolidates the risks into:

1. Operational Risks
2. Financial Risks
3. Data Risks
4. Ongoing Projects
5. COVID

Following feedback from the management committee and the HLG, the Risk Register was updated to include a new risk category focusing specifically on risks associated with Data. This caused us to refine our Data Policy and enhance underlying data access and storage provision.

The Risk Register is reviewed, circulated, and discussed at each project management meeting, although is updated more frequently as part of the wider management of the facility. The discussions and input from the management committee have helped to define the risk register and keep it relevant and responsive to the regularly changing operational challenges during 2021 and into 2022. Most risks remain at the same level, but obviously, the COVID situation has necessitated dynamic management of several risks, which has helped the facility and the management committee to mitigate supply chain delays and to prioritise limited resources.

Monitoring the changing risk profile monthly has enabled project completion deadlines and targets to be agreed upon as well as highlighted several areas of action, which include updating Health and Safety documentation and developing clearer operational strategies. The project management committee uses the risk register to effectively stress-test current operations as well as ensure short, medium, and long-term risks are appropriately managed and mitigated.

At this time, the risk register is not made public through our website, but the latest version is always available upon request and is appended to this report.

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Key Performance Indicators (KPIs) and Service Level (SLs)

XMaS operates under the following **Key Performance Indicators (KPIs)**:

A) The Number of Individual Researchers and University Research Groups ["users"] that have made use of the XMaS beamline in that Period. This should be expressed as a Total Number for that period.

B) Number of User Complaints received during the period. This should be expressed as a percentage of the Total Number of User Approvals made within the period.

C) The Uptime of the beamline within the period. This should be expressed as a percentage of the Total Available Time within that Period.

D) The Number of research outputs. This should be expressed as a Total Number for the period.

and **Service Level Agreements (SLAs)**:

• Requests for beamtime will have decisions made within 20 days of the PRP meeting subject to knowledge of the ESRF review process. In 'exceptional' cases Users will be informed by the service operator if these benchmark times are going to be exceeded and an explanation provided.

• Facility Users will have access to facility staff for assistance on site.

• The facility will be operational and available for use for 80% (eighty percent) of the maximum possible operational time.

• The facility will train all new Users in the safe and effective use of the beamline.

• The facility will perform a minimum of 2 (two) publicity activities per year.

• The facility will generate a minimum of 15 (fifteen) research outputs per year.

• The facility will respond to all User enquiries clearly and quickly in line within 5 (five) working days for emails and 2 (two) working days for telephone enquiries.

• The facility will respond to User complaints within 10 (ten) working days.

• The facility will treat all proposals equally, fairly and in confidence.

• The facility will treat all Users equally and fairly.

• The facility will uphold high standards of integrity in all operations and in contact with Users.

A) **The number of Individual Researchers and University Research Groups visits**: The facility hosted 75 user "visits" from 28 UK and 10 international University groups over this reporting period. These statistics cover the CRG access and can be compared with historical data in fig. 13.

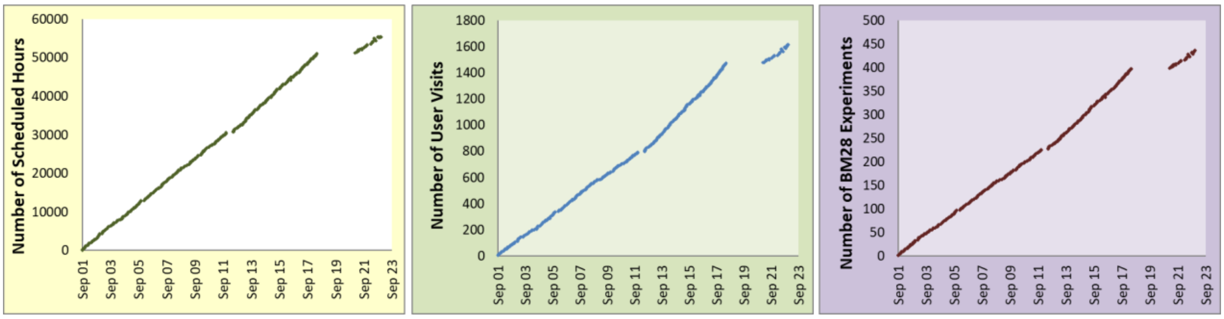

Figure 13: Historical performance metrics for XMaS including the number of scheduled hours (left), the number of user visits to the facility (centre) and the number of individual experiments performed on the beamline (right).

B) **Number of user complaints: XMaS has received zero (0) complaints over its lifetime of > 25 years**.

C) **Uptime of the facility: 93.4%:** In this reporting period, some time was lost due to an electrical trip and concomitant impact on the operation of the monochromator. This arose due to a power surge from a thunderstorm affecting the ESRF electrical supply.

D) **The number of research outputs**: Over the reporting period there were a total of 9 published papers with the cumulative output exceeding 460 (fig. 14). The publication rate has understandably dipped in this reporting period. We note that there is typically a year or two delay between beam time and a resulting publication. The dark period and the impact of COVID will therefore be evident in the output statistics throughout 2019-2023 and explains the missed SLA. We expect that research outputs will pick-up again during 2023 as newly recorded data are prepared for publication. Approximately 60% of the papers are co-authored with XMaS staff. In addition to peer reviewed publications, there are many conference and seminar presentations, which are more difficult to capture, and are *not* included in our KPI reporting metric.

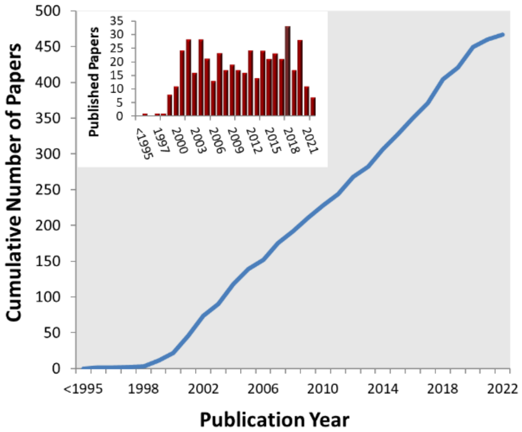

Figure 14: Publications from XMaS in peer reviewed journals.

Service Level Agreements

All SLAs have been met. The 2021 newsletter was disseminated in March 2022 and regular updates are communicated on the webpage and through twitter. Direct engagement with the user community arose through the preparation of the Statement of Need and associated meetings.

Links

The UK has been at the forefront of synchrotron radiation (SR) provision for decades, building the world's first dedicated SR facility in 1981. Third generation machines (pioneered by the ESRF and DLS) increased the flux and beam quality, greatly enhancing the impact of SR across the physical and life sciences. Now, new technologies deliver diffraction-limited sources, hugely increasing the brilliance and coherence of the X-ray beams. These transformative designs are redefining the SR landscape with all major facilities upgrading - the ESRF upgrade was completed in 2021, the Advanced Photon Source (APS) in 2023-24 and DLS in 2027-29. SR facilities have a range of beamlines catering to their user communities and these are built up to be complementary, both within and between facilities. Access is based on peer-reviewed scientific excellence, with the ESRF limiting UK access to 10%, aligned to the UK's budget contribution. XMaS provides UK access to the ESRF over and above this limit. DLS has commissioned its beamline suite with XMaS operational and, as such, XMaS, DLS and the ESRF together constitute the UK research infrastructure for SR. As an integral component of the UK Synchrotron Radiation infrastructure, XMaS naturally has strong links with the Diamond Light Source (DLS) and has been operational throughout the development of the DLS beamline portfolio. DLS executives are fully cognisant of the capabilities of XMaS and the recently submitted (January 2023) National Statement of Need for the XMaS beamline was partly coordinated through the DLS user base. A DLS science group leader (Prof. Chris Nicklin) chairs our Project Management Committee (PMC). Representing the complementary neutron scattering community, Prof. Sean Langridge, the head of the ISIS Diffraction and Materials Division is also a member of the PMC. XMaS directors likewise sit on, and have chaired, DLS review panels and Prof. Tom Hase is currently chair of the DLS Science Advisory Committee and attends Diamond Board meetings. There is a free flow of information about current capabilities and opportunities for collaboration. Access to XMaS is already part of the DLS mitigation strategy for the future DLS upgrade and its concomitant dark period.

Beyond Diamond, XMaS also has strong links with sectors 4 and 6 at the Advanced Photon Source (Argonne National Laboratory, US). These links have been developed over many years, including knowledge transfer on sample environments and metrologies for magnetic and high-resolution diffraction. XMaS users were granted some access to beamline 4-ID-D during the recent ESRF shut-down and XMaS looks forward to reciprocating and hosting some APS users during the planned APS upgrade which begins in May 2023. We are also developing close contacts at beamline 4-ID at the National Synchrotron Light Source-2 (Brookhaven National Laboratory, US). The engagement with other facilities is built on long-standing collaborations and mutual trust and support. We fully expect this to continue and develop further in the years ahead.

XMaS has been working closely with key stakeholders at the UK Catalysis Hub (Research Complex @Harwell) to provide sample environments that exploit the unique ability to access both tender (2-4 keV) and hard (20-40 keV) X-ray photons interacting with the same sample volume. The focus here is on developing sample environments for operando experiments, which are crucial for the understanding of material function in their working environment that drives advances in catalysis and battery technologies. Prof. Andy Beale (UK Catalysis Hub) sits on our PMC and helps to develop our industrial interactions. We are also engaged with the Royce Institute which advertises our proposal round calls to its science community.

Industrial and non-academic collaborators include: APS, AXO Dresden, BP, DLS, ElectroSciences, EU Institute for transuranic studies, Futurum, Huber, IBM, Mary Rose Trust, NPL, Nuclear Decommissioning Authority, PragmatIC Printing, P&G, PSI, Siemens, Surrey 5G centre, Swiss Light Source, US Navy, Vienna Fine Art Museum and the Advanced Materials Catapult (WMG). Third party activity has been through EMPIR-funded projects including Nanostrain, ADVENT and recently OpMetBat. XMaS is also involved in standard developments through the ISO TC201 "surface chemical analysis" committee and the COST action CA18130 "ENFORCE TXRF". XMaS supports users with a current EPSRC grant portfolio conservatively in excess of £200M and in applying for fellowships and international research programmes. Our users, often with industrial partners, are involved in several Centres for Doctoral Training, either funded directly through EPSRC or at a university level.

Of course, XMaS benefits tremendously from being part of the ESRF and based at the European Photon and Neutron (EPN) campus in Grenoble, France. The EPN campus is an international science hub hosting the ESRF and the world's most intense reactor neutron source, the ILL, along with joint partnerships. In normal times, it hosts a staff of 1500 people, including 500 scientists and postgraduate students, and typically welcomes more than 8000 guest researchers every year. There is strong interaction between XMaS and the ESRF. Prof. Chris Lucas has sat on and chaired several beamline review panels and ESRF upgrade steering groups. The XMaS beamline scientists engage in day-to-day interaction with the broad EPN international scientific community, for example benefiting from the technical expertise both at the ESRF and the ILL in the development of novel sample environments. Users to XMaS become part of this international community often developing new scientific ideas that lead to collaborative projects involving scientists from across Europe and beyond. Many of the UK driven experiments have international collaborators, some of whom also apply for time directly through the ESRF international route. XMaS staff are heavily involved in developing international standards through the ISO TC201 and BSI CII-60 committees and have worked with international partners with the COST action CA18130 (ENFORCE) to define terminologies and obtain reference spectra needed for total reflection X-ray fluorescence (TXRF). The benefit of these interactions are difficult to quantify but provide huge knowledge transfer to and from the facility and are of crucial importance in maintaining the scientific competitiveness.

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Improvements and future plans

Facility Access

We are continuing to plan for a BAG access route in "energy materials" in partnership with Diamond and the B18 beamline. We are finalising the capabilities and routine measurements that we can provide and that would provide additional capabilities to the UK community. The BAG route will be available from the October 2023 call. We recognise the continuing need to develop industrially relevant case studies to attract new industry users for proprietary research, or to work with UK academics on relevant projects. Unfortunately, our efforts in 2022 were hampered by Brexit related import problems.

Facility Management

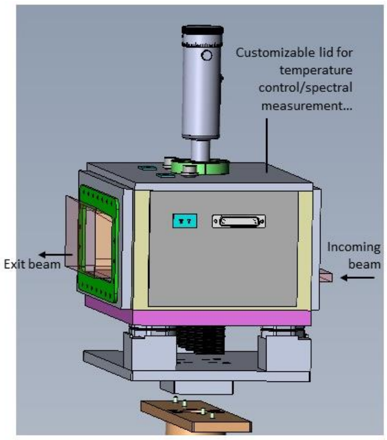
A new customer relationship management database is in development for deployment through 2022/23. This would replace our current limited database and ensures GDPR compliance. Enhanced reporting and annual data checks with users will ensure the most up to date and relevant metrics can be gleaned for the management committee. The new tool will ensure more targeted interactions with sections of the user community and allow better communication channels to be maintained. It will also consolidate data linking users to beam time and publications ensuring better compliance with fair data practices.

XMaS is committed to implementing its published EDI policy. In partnership with the ESRF Safety Office, we will endeavour to ensure that the facility can accommodate any user, but this may require an individual needs assessment. We continue to monitor the EDI requirements and needs of our users through the project management meetings and update policies whenever they are needed.

Technical Upgrades and Equipment Developments

New sample environments for WAXS/SAXS experiments

A challenge for soft-matter studies and SAXS/WAXS studies in general is background signals arising from the various apertures and windows, which are inherent in the beamline and many of the sample environments. Over the reporting period, we have designed and successfully tested different sets of apertures and windows to continue to reduce the background and improve the signal to noise ratio for measurements on samples with low scattering power.



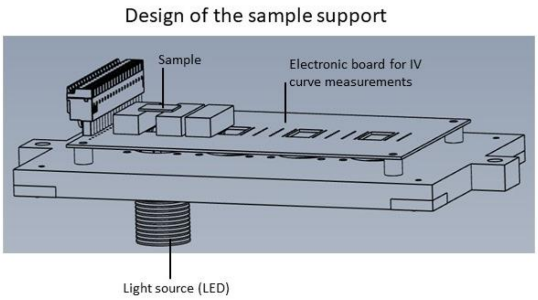


Figure 15: A new GIWAXS chamber for energy materials with an integrated sample support for simultaneous measurements of functional properties in situ and operando.

Following user requests, a new enhanced multipurpose GIWAXS chamber for energy materials and organic electronics is being designed (fig. 15). This new chamber will allow combined and simultaneous *in situ* and *operando* structural (scattering) and spectroscopic (UV-visible-IR) studies. It has been co-designed with user input especially to study photo-induced degradation of high-efficiency organic solar cells but will also be suitable for a range of material science challenges including organic transistors.

Detectors

Detector technologies continue to evolve, especially in the field of 2D and energy dispersive detectors. The new extended high energy range of the beamline facilitated spectroscopic studies up to 50 keV (fig. 1). To access these energies, Ge based detectors are needed. To increase efficiency, both in terms of count rates and solid angle intercepted, detectors with multiple sensing elements are an advantage. Tests measurements were made on the beamline using a borrowed 4-element Ge system and we have now placed an order for a 7-element Ge detector from Mirion Tech. (Canberra).

Figure 16: The FalconX electronics unit from XIA.

To fully exploit the new detector, as well as process higher count rates with lower noise, two new 8-channel FalconX digital X-ray spectrometers have been purchased and integrated into the beamline controls (Fig. 16). These high-performance systems support a count rate up to 4 x 10^6 counts per channel. We are also exploring upgrade options across our suite of Si based detectors to take advantage of Si detectors with a greater dynamic range and increased sensor thickness. New detectors are being purchased through the latest EPSRC capital equipment call.

Gas Delivery

The gas delivery system, for the remotely controlled dosing and automatic filling of the ion chambers and sample environment, was originally planned to be positioned where the KB mirror assembly is now located. Final engineering is only possible once the KB mirror mounting block is installed which is now due in the summer of 2023. The bulk of the gas delivery infrastructure is in place, and with the TDR completed for the KB mirror, we have been designing the final integration of the gas system on the beamline. Currently gases can be loaded manually, and operations are mainly unaffected but do require more interventions during experiments and limit the ability to change energy automatically.

Fast Energy Scanning

Scanning the incident energy quickly is now routine on many spectroscopy beamlines and greatly increases throughput and time resolution. The XMaS monochromator is optimised for scattering experiments, but faster scanning is possible with some updates to the hardware. We are actively scoping this possibility during 2023 but are mindful that we need to retain stability for other experimental configurations.

Software Developments

Data processing – mapping to q

Advances in data processing continue as the facility consolidates the improvements delivered through the upgrade period. 2D detectors have routinely been employed for SAXS/WAXS studies, but they are now being more routinely used in diffraction. Each pixel in the recorded image corresponds to a unique position in reciprocal space. Each image therefore intercepts a plane in reciprocal space and thus, scans of the diffractometer map out a volume of reciprocal space. Software codes are being developed both in-house and with users to compile Python scripts to visualise and reduce such data sets, mapping the results in reciprocal space zones or in terms of reciprocal lattice units as illustrated in fig. 17.

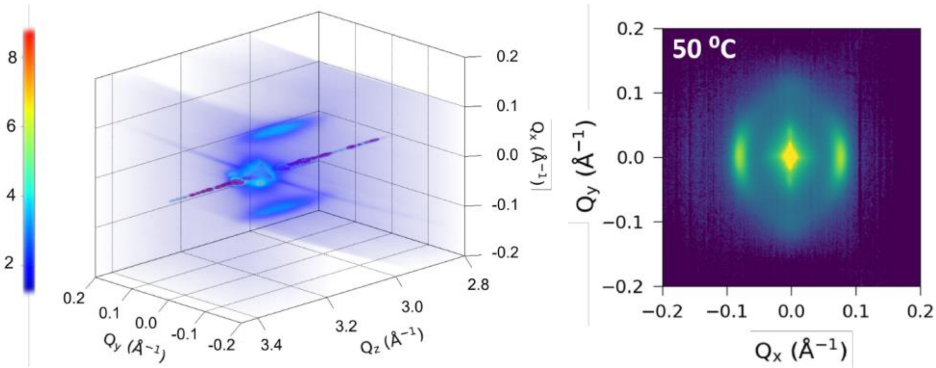


Figure 17: Reciprocal Space Volume reconstructed from a series of 2D images taken during a rocking curve of the (002) Bragg peak in $DySrO_3$ (left). Projection onto (Qx – Qy) wave vectors, giving a Reciprocal Space Map (RSM) around the same reflection (right). Taken from Dorin Rusu's thesis, University of Warwick (2021).

Data handling, visualisation and analysis tools

An ongoing concern in many scattering experiments is the background introduced through air scattering, environmental windows, sample holders, etc. To maximise signal over noise, this parasitic contribution needs to be reduced to a minimum. However, it is often not possible to remove it completely and the background is mingled with the measured scattering signal. Background subtraction is generally done during post-experiment data treatment and can be very challenging. It can even compromise the usefulness of the data, which if not addressed during the experimental time reduces the impact of the experiment and the beam time.

To help users and the wider data strategies, we have developed a software tool (PyXScat) for visualisation and online background correction/subtraction of scattering data recorded using a 2D detector (fig. 18). PyXScat provides a route to evaluate whether the experimental background is within tolerance and the data exploitable. The program can operate online and access "live" data in real time or be used as a post-experiment processing tool. PyXScat has been written in Python, has a graphical user interface, is light (requiring just standard and some ESRF packages) and easily customisable for other experimental configurations or requirements. The full code will be available for users soon. We have also implemented several Jupyter notebooks (based on Python) to help users handle data taken at the beamline or control some lab hardware. The Jupyter notebooks are fully commented with explanations on how to use them and require a minimum of programming. These notebooks use packages that can be run on the ESRF cluster, for which users have access during their experiments. We plan to populate a XMaS Gitlab repository very soon with all the software tools we develop and make it publicly accessible.

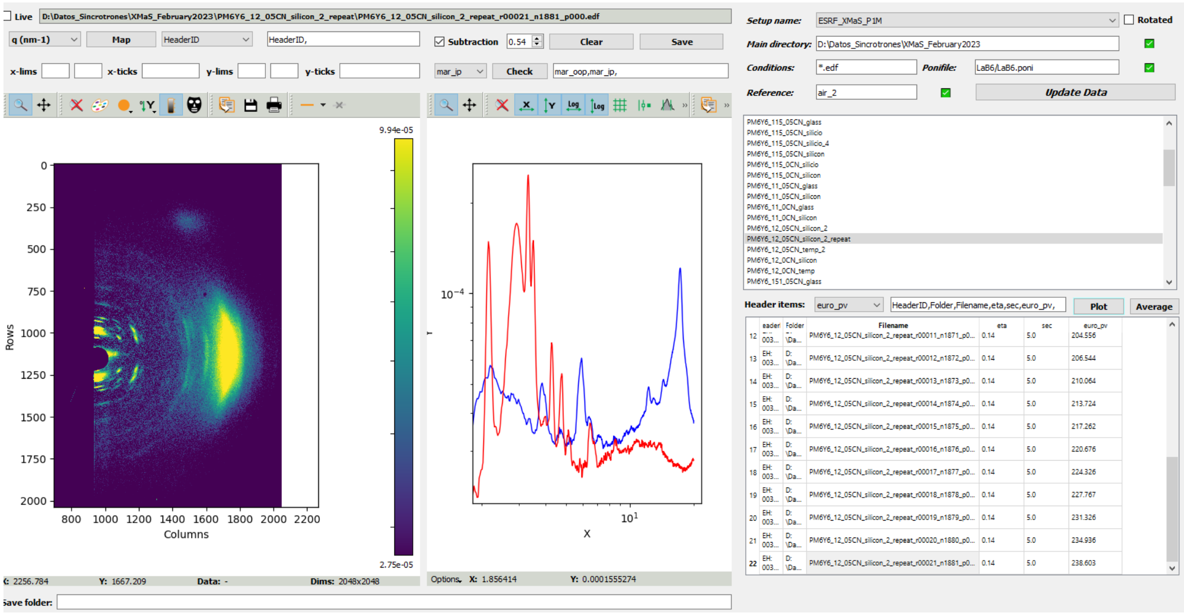


Figure 18: Snapshot of the PyXScat software GUI. A typical GI-WAXS diffraction pattern recorded is shown on the left panel. The curves in the middle panel show a linear cut along the vertical (blue line, integrating along the columns on the image) and horizontal (red line, integrating along rows) reciprocal space directions. Information about the angular positions, counting times and other parameters registered during the experiment are shown on the bottom right panel.

Updated Data Policy

Over this reporting period, we have updated our Data Policy. The XMaS National Facility aims to ensure that all data collected at the facility, including the beamline and offline facilities, are compliant with the FAIR (**F**indability, **A**ccessibility, **I**nteroperability, and **R**eusable) principles. Users of the facility are encouraged to provide suitably informative metadata to enable FAIR data handling.

As a Collaborating Research Group of the ESRF, the data policy of the XMaS facility follows that of the wider Data Policy for Public Access of the ESRF. Acceptance of this policy is a condition for the award of beam time. Deliberate infringements of this data policy may lead to denial of access to raw data or metadata and/or denial of future beam time requests at the ESRF, as well as actions of the ESRF in the court of law. XMaS and the ESRF will provide curation of results over the long term on a best effort basis. Neither XMaS nor the ESRF can be held liable in the case of unavailability or loss of data or results.

The ESRF (subject to the data protection legislation of France) acts as the custodian of all raw data and metadata collected on XMaS. The metadata will be stored in the ICAT metadata catalogue which can be accessed online to browse and download (meta)data. The experimental team will have sole access to the data during a three-year embargo period, renewable if necessary. Experimental teams can release their data before the end of the embargo period by creating a DOI for a publication or by sending a request to dataportal-feedback@esrf.fr. After the embargo period, the data from publicly funded research will be released under a CC-BY-4 licence with open access to everyone. XMaS data will have a DOI created automatically with high level metadata such as Title, Authors, Abstract, Beamline made public as soon as the experiment has been completed. This information shall be available via the persistent identifier landing page on the web. Any publications related to XMaS data must cite the persistent identifier of the experiment and that of the data in their publication.

Website

The NRF's website is www.xmas.ac.uk. The webpage has been refreshed and restructured to reflect the changes on the beamline and its new capabilities. Clearer signposting and a more logical layout have been developed and there is now a section dedicated to industrial users.

Web analytics are provided by the host server at the University of Warwick. Excluding search engines, the website receives on average 69 page views per day. The views over the reporting period are presented in fig. 19.

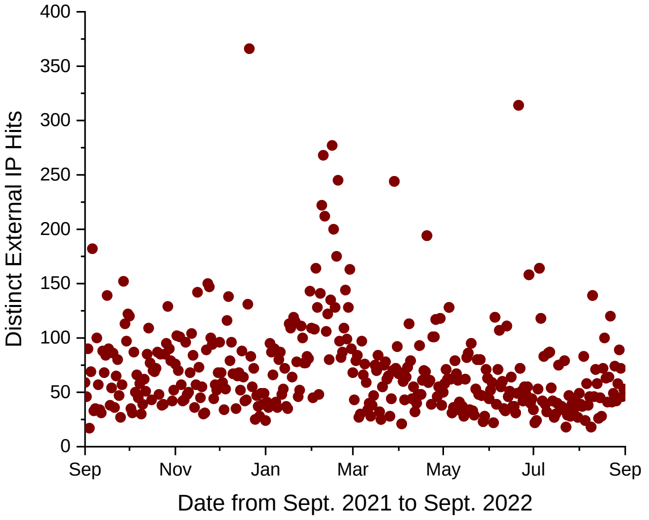
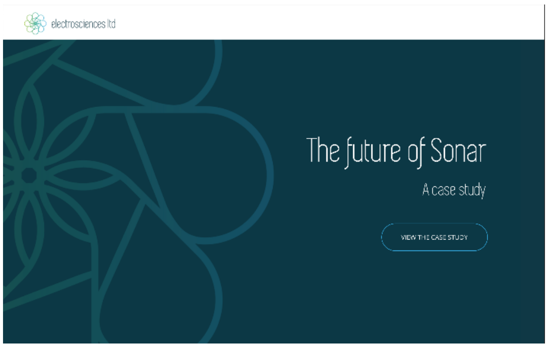


Figure 19: Distinct website views per day over the reporting period.

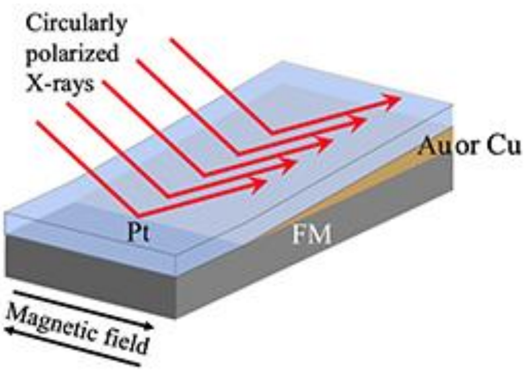
Case Studies

The Future of Sonar: *A case study from Electrosciences*



Electrosciences Ltd have developed and commercialised a new multipurpose and multifunctional stress-strain rig. This tool was co-developed with our collaboration partners the University of Liverpool and the XMaS beamline at the ESRF (European Synchrotron Radiation Facility), with early research support from the European Commission and the Office of Naval Research Global. The new rig allows users to characterise the electromechanical response of novel systems to stress, electric field, load, and temperature whilst simultaneously being scanned by an X-ray beam.

APS Science Highlight: *Understanding the Flow of Spin Currents across Interfaces*



User science performed on beamline 4-ID-D at the Advanced Photon Source, Argonne National Laboratory as part of the mitigation of the XMaS dark period was selected as an APS science highlight. Resonant magnetic scattering and dichroism using circular polarised light was used to explore the induced interface magnetic moment and its orientation. Conclusive evidence for a direct correlation with the magnetic damping in an adjoining ferromagnet was presented. Both the extent and size of the induced moment was determined in the experiment which was originally published in Appl. Phys. Lett. 119, 152401 (2021).

25 years of world-class science on XMaS: *Seeing is believing at the X-ray Materials Scattering facility*

The completion of the XMaS renewal coincided with the 25th anniversary of the XMaS facility which was highlighted by UKRI on its website as part of the "how-we-are-doing/research-outcomes-and-impact" section.

From tooth fillings to the Mary Rose, the UK's X-ray Materials Scattering (XMaS) user facility allows scientists to explore the secrets of materials. 2022 marks the 25th anniversary of the operation of the UK's XMaS user facility at the European Synchrotron Research Facility (ESRF) in Grenoble. It has been directed for all that time from Warwick and Liverpool University Physics Departments.