Engineering and Physical Sciences Research Council

National Research Facility Annual Report: XMaS

Introduction

The NRF annual report showcases the NRF's performance, highlights, and challenges over the reporting period. The analysis should help the facility to reflect on the reporting period and to inform on their plans for the future. The report provides information for EPSRC and the High Level Group to gain insight into the operation of our facilities and is a useful tool to understand the individual NRF's missions and demonstrate their strategic importance to EPSRC. The annual reports are part of the monitoring and evaluation of NRFs to support facilities to ensure they are supported through the process for renewal.

EPSRC would like to work with the NRF community towards an open culture and encourage the facilities to provide transparent statements on the data and within the narratives in the annual report. Constructive reporting is valued as a positive approach by the High Level Group. It is important for facilities to understand that they will not be penalised for areas they can't control where evidence shows they have not met the targets. The key element the High Level group and EPSRC would like to see is that how the facility has considered and responded to these issues and identified appropriate and realistic plans to address them and improve the service. EPSRC acknowledges that each NRF is different, and each facility will have different strengths within their report.

Please note that this report uses calendar years to align with the reporting period. If any years have been impacted, e.g., by a grant starting halfway through the year, please note that in the appropriate places.

Report length and feedback

Please keep the length of the reporting to each section as defined. Any additional information can be placed in the appendix (e.g., full list of publications, meeting minutes from Advisory Board meetings), but this is not a requirement and does not count towards the page limit.

We expect the report and feedback from the High Level Group to be shared with your Advisory Group/Steering Committee and your EPSRC Theme Contact.

Estimated timeline

- Annual report submission deadline: 24 February 2025
- High level group assessment: end of March 2025
- Annual report feedback: April 2025

Section 1: Purpose and vision of the XMaS NRF

XMaS is the UK Collaborating Research Group (CRG) beamline at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, with a vision to provide a world-leading facility for the study of *materials science*. The higher-level objectives are detailed in Appendix A. The beamline remains an integral part of the UK's synchrotron radiation infrastructure and has been supporting UK materials scientists since 1997. XMaS provides a state-of-the-art facility, fully exploiting the capabilities of the ESRF lattice and delivers a brilliant X-ray beam with an operational energy range from 2.1 to 47 keV. A combination of techniques from X-ray diffraction to small angle X-ray scattering as well as X-ray absorption spectroscopy, techniques which underpin materials development at the fundamental and exploitation levels, are available to external users. XMaS has strong and evolving links with Diamond Light Source and there is frequent knowledge transfer between both facilities, exemplified by our new BAG access in partnership with B18. Co-development of software and sample environments support capability uplifts across both facilities with XMaS providing an essential mitigation route for Diamond users during the upcoming dark period associated with the Diamond upgrade.

The science portfolio on XMaS continuously evolves, embracing a broad spectrum of scientific disciplines under the generic theme of materials science and cutting across research activities in physics, chemistry, biosciences, healthcare, engineering, and energy. User driven multi-modal studies are performed across all energies and allow materials to be characterised in terms of composition (XAS, XRF, TXRF) as well as spatial ordering on local (XAS, WAXS, XRD), and larger (SAXS, XRR) length scales. There is an increasing focus on *operando* and *in situ* studies. A unique feature of XMaS is that these techniques can be applied to the same sample volume simultaneously (or within a short time) without changing the sample environment. Synchrotron studies are collaborative and XMaS provides an essential route for UK scientists to maintain, develop, and nurture links with international colleagues to increase the range, quality, and impact of their research. These partnerships ensure the future competitiveness, resilience, and creativity of the UK materials sector. This is aided by staff being involved in ISO committees and advisory committees at national and international levels to shape both infrastructure needs and plan scientific roadmaps.

Section 2: Quality and breadth of research that XMaS has enabled

Scientific excellence and impact

Scientific excellence and impact of the beamline are derived from the diverse and fascinating work of our users and the broad range of science that the users investigate.

Important scientific breakthroughs that have been supported by the facility

The ability to use a newly acquired Ge detector has allowed spectroscopic studies using high energies for the first time. An example is the exploration of Ba in corals skeletons, which can be used as a proxy to explore environmental changes.[1] Ba is believed to encode records of terrestrial run-off into the oceans but initial attempts using Ba L_3-edge XAFS were unsuccessful (Finch *et al.* 2010). The upgraded XMaS beamline enabled the user group to finally measure the Ba *K*-edge at 37.44 keV after waiting for over 15 years for a facility that could do it. In a study of disordered metal organic frameworks used for oxide catalysis, measurements of the EXAFS at the Ce *K*-edge (40.44 keV) and XANES at the Ce L_3-edge (5.7 keV) allowed the structure and valence of Ce to be quantified during the catalytic reactions. Such measurements at significantly different X-ray energies can now be done rapidly and easily by exploiting the source properties and suite of energy dispersive detectors.[2]

New methodologies that have been developed

2024 was a consolidation period at the facility where previous metrologies were further developed and made more user-friendly. In this reporting period, three main methodologies have been developed. First, the 7-element Ge detector from Mirion Technologies® was redesigned and, with the other new energy dispersive detectors (Si based Vortex ME4 and 1 mm Vortex-EZ) and a second fast XIA FalconX counting chain, has enabled spectroscopy studies across the whole energy range. Secondly, new modular flight tubes have been designed and installed on the SAXS rail to reduce background and interface with our 2D Pilatus3 S 1M detector. Finally, the KB mirror assembly was mounted and commissioning tests undertaken. Test experiments on geological samples showed that mapping the sample composition with a small beam 5 x 7 µm^2 [H x V] was possible.

The breadth of research areas that are supported, highlighting any new research areas

The scientific area of the research is identified by users in their end of run survey. Research areas in this reporting period are compared to the facility average in Figure 1. The breakdown on research area is in line with previous reporting periods.

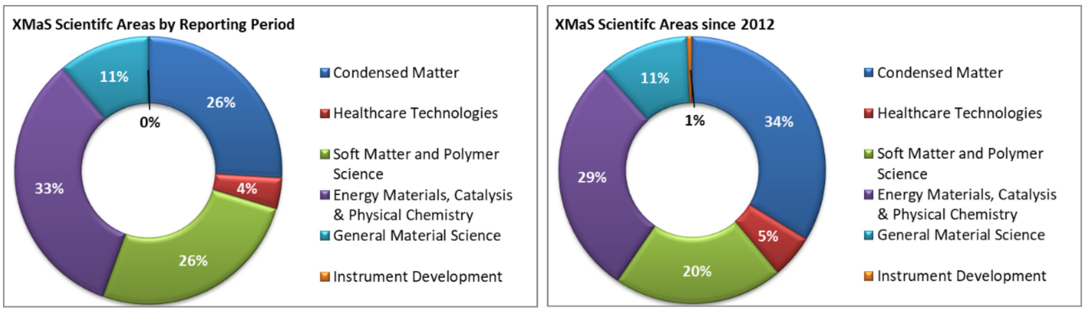

Figure 1: Research areas as reported by the users in their end of run survey. Data from this reporting period (left) compared with the facility average (since 2012, right).

[1] https://adrianfinchcouk.wordpress.com/2024/11/15/xmas-comes-early-unlocking-the-secrets-of-barium-in-corals-using-synchrotron-x-rays/

[2] Unpublished data from the Walton Group from Warwick Chemistry, 2024.

Publications

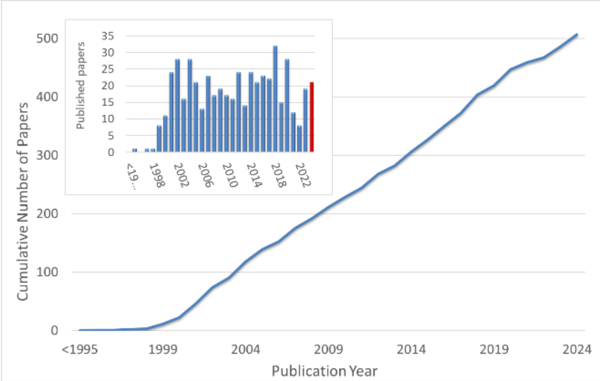

Figure 2: Cumulative output of the XMaS facility and (inset) the number of publications per year.

XMaS publications from 1995 are listed and continuously updated on our webpage with direct DOI links to all papers to facilitate ease of access. There is a direct portal for users to inform us of publications and we regularly search repositories to track publications. An annual reminder is also sent to the user community. 22 papers were published in 2024, a slight increase on the previous year (19). We note that during 2024 the cumulative output exceeded 500 publications as seen in Figure 2. The data show that the outputs are steadily recovering from the combined impact of the COVID pandemic and the ESRF shutdown. The publication rate is returning to ~0.7 research papers per experiment. Since 2020, a steady increase in the field-weighted citation impact factor has been observed which, for 2024, is 1.31. Some 50% of the recent outputs are reported in the top 10% of journals as defined using CITESCORE and 14% of the output are within the top 10% most viewed publications worldwide. On average, there are 38 views[3] per paper. Outputs continue to span a very broad spectrum of research areas and are highly collaborative. In 2024, 82% of outputs had international collaborations and 5% were the result of academic-corporate collaborations. Further details are provided in appendix B and three publications are detailed below:

Incommensurate charge density wave order in U_2Ti: X-ray diffraction (XRD) from a single crystal of U_2Ti was used to characterise a two-step phase transition from a parent hexagonal structure to an incommensurate charge density wave (ICDW) state below 71 K before a lock-in transition to the predicted commensurate Peierls-like charge density wave (CCDW) state at 43 K. The signature of the ICDW transition was seen weakly in thermodynamic and transport measurements but the XRD was crucial to confirm these findings, which may occur more widely in other systems but elude detection. The work highlights the collaboration between XMaS staff and scientists at the University of Edinburgh.

Colloidal Atomic Layer Deposition on Nanocrystals Using Ligand-Modified Precursors: Atomic layer deposition (ALD) is a method to grow thin coatings on materials one single atomic layer at a time. To characterise the resulting films, the combination of techniques available on XMaS, namely high-resolution powder X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) were used. XRD was employed to pin down changes to the crystalline structure of the nanocrystals or metal oxides upon growth of the coatings. XAS was used to track the structural evolution of the coatings as more ALD cycles were performed. The paper highlights the power of the multi-modal capabilities available at the facility.

Integration Of Solution-Processed $BaTiO_3$ Thin Films with High Pockels Coefficient on Photonic Platforms:
Ferroelectric materials such as barium titanate (BTO) are widely used in photonic devices as it has high Pockels coefficients and is thermally and chemically stable. The electro-optic properties of ferroelectric thin films are dependent on their crystal phase, so we characterised their crystalline structure using wide angle X-ray scattering under grazing incidence and showed that the solution-based growth methods yielded films with a tetragonal phase and high texture, making that fabrication route an excellent alternative to more traditional and expensive processes. The work is a close collaboration between XMaS and groups from Belgium, Finland and Spain.

[3] Views are generated from usage data in Scopus. The metric is the sum of abstract views and clicks on the link to view the full text at the publisher's website.

XMaS CASE STUDIES:

Dinosaurs, Dentists and Dragons

A.R.H. LeBlanc, A.P. Morrell, S. Sirovica, O. Addison – for more information contact Aaron LeBlanc, Faculty of Dentistry, Oral & Craniofacial Sciences, King's College London, UK. Aaron.leblanc@kcl.ac.uk

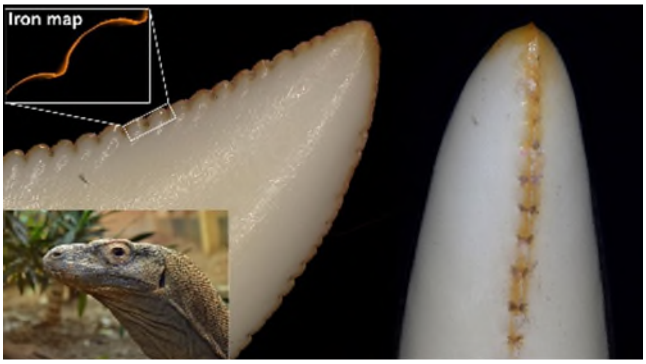

Figure CS1. Komodo dragon teeth have iron-coated serrations, as revealed through X-ray Fluorescence at the ESRF (inset). Image of Komodo dragon courtesy of Charlotte Ellis (ZSL).

As the largest living lizards, the Komodo dragons of Indonesia use jaws lined with serrated, blade-shaped teeth to subdue their prey. They also make excellent models for understanding how extinct animals with similarly blade-shaped teeth - such as meat-eating dinosaurs - might have used them to hunt. Our recent research[4] investigated the cutting prowess of Komodo dragons using state-of-the-art techniques at XMaS to look at the chemistry and structure of the thin veneer of enamel coating their teeth. We then compared these with alligator and crocodile teeth, and finally a sample of fossil meat-eating dinosaur teeth from the Cretaceous period.

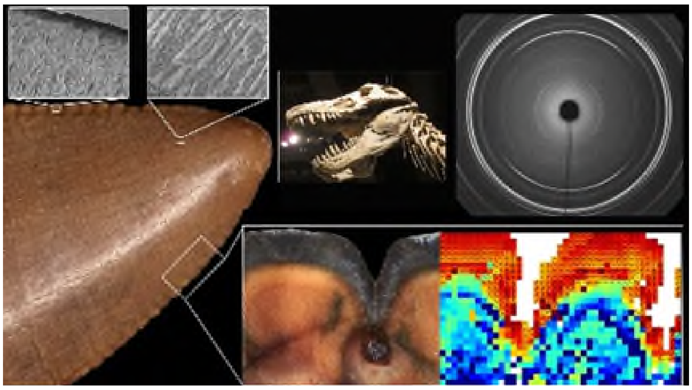

Figure CS2. Tyrannosaur serrations are capped in enamel that has a different structure than the rest of the tooth (SEM images in top left). Using diffraction (top right) across thin sections of tyrannosaur serrations revealed the structural complexity of the serration enamel, both in terms of crystallite orientations, and degree of texture (hot colours in the texture heat map in bottom right).

Our team of palaeontologists, dentists, physicists, and materials scientists combined expertise to devise a series of synchrotron experiments investigating the chemistry and structure of the enamel that coats the teeth of reptiles. We carefully sectioned fossil and modern reptile teeth into thin wafers and subjected them to elemental (X-Ray Fluorescence) and structural (X-ray Diffraction) imaging to reveal previously hidden adaptations. What we discovered was surprising: Komodo dragons have an iron-rich coating along the serrated edges of each of their teeth (Figure CS1). This coating, rich in iron oxides that stain the cutting edges and tooth tips orange, protects these parts of each tooth from wearing too quickly thus maintaining a sharp cutting edge. Iron-enriched enamel is a feature we classically associate with rats, beavers, and shrews, but not the teeth of lizards or other reptiles. Our findings led us to look more closely at the teeth of alligators and crocodiles: reptiles that lack the blade-like teeth of Komodo dragons but have sharp cutting edges to their teeth. Here too we discovered iron-enriched enamel along the cutting edges. Could the serrations of meat-eating dinosaur teeth harbour similar adaptations?

Unfortunately, our XMaS experiments revealed that iron seeped into all the inner parts of fossilised teeth over millions of years making it difficult to determine if dinosaurs were also able to reinforce their serrated teeth with iron in life. However, using diffraction, we showed a different, but equally impressive adaptation hidden within the teeth of meat-eating dinosaurs. Meat-eating dinosaurs altered the structure of the enamel itself along their serrations. The enamel of each tyrannosaur serration is made of tight spirals of mineral crystals, imparting a higher resistance to tooth wear along the cutting edges of their teeth compared with the more regular, columnar enamel structures found elsewhere on each tooth (Figure CS2).

These findings demonstrate that, while their teeth may look similar on the outside, meat-eating reptiles can evolve different and unexpected ways of maintaining a cutting edge.

[4] A.R.H. LeBlanc *et al.*, Nature Ecology & Evolution 8, 1711-1722 (2024).

Magnetic X-Ray Reflectivity Insights into Interlayer Coupling Phenomena in Thin Film Multilayers for Spintronics.

D. Rianto, B. Nicholson, L. Bouchenoire, Y. Choi, P. Kuświk, T.P.A. Hase, D. Atkinson – for more information contact Del Atkinson, Department of Physics, University of Durham, UK. del.atkinson@dur.ac.uk

Spintronics, the interactions between magnetism and electronics in magnetic multilayers, underpins magnetic data storage and hence cloud computing. Interlayer coupling, where two magnetic layers are coupled through a nonmagnetic (NM) layer, such as Cr or Ru is a key phenomenon in spintronics, crucial for data reading and sensor technologies. Pt is a key NM spintronic material but, coupling through Pt remains poorly understood. It has been proposed that coupling originates from proximity-induced magnetization (PIM) in Pt, where spin polarization arises due to hybridization with an adjacent ferromagnetic (FM) layer. Whilst PIM is recognized as an interfacial effect, its role in interlayer coupling remains largely unexplored.

In this study we obtained experimental evidence linking PIM to interlayer coupling by determining the PIM profile under varying magnetic fields. The ability to control the incident polarisation and the XMaS sample environments were key to the successful experiments. Figure CS3 shows the sample design and corresponding hysteresis loops that reveal a transition from double-step to single-step switching of the magnetization reversal as the Pt thickness decreases and the interlayer coupling strength increases. The depth-dependent magnetization was measured using element specific X-ray resonant magnetic reflectivity (XRMR). Figure CS4 shows the reflectivity and the magnetic asymmetry data along with fits allowing the chemical and magnetic profiles to be determined. Figure CS5 presents the extracted magnetic PIM profiles during magnetization reversal. At -51 mT, the PIM peaks are fully saturated and aligned. As the field increases (12 mT), the lower PIM peak (green) weakens, indicating an in-plane rotation. At 18 mT, the lower Pt PIM peak fully reverses, followed by the upper PIM peak (yellow), until both saturate again at 51 mT.

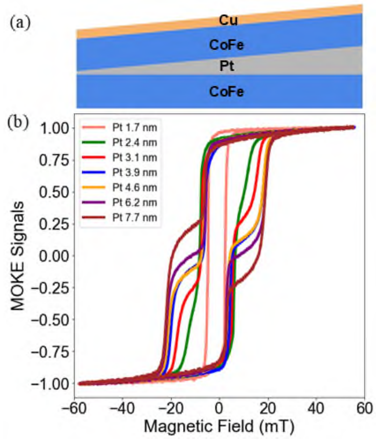

Figure CS3: Schematic of the sample and measured hysteresis loops for different Pt thicknesses measured by Magneto-Optical Keer Effect (MOKE).

Our findings highlight the effectiveness of XRMR in probing depth-dependent PIM behaviour at CoFe/Pt interfaces. The observed reversal of PIM provides clear evidence of interlayer coupling and the links between them. This finding has crucial implications for spintronic applications, particularly in controlling magnetization reversal and spin-orbit torque switching.

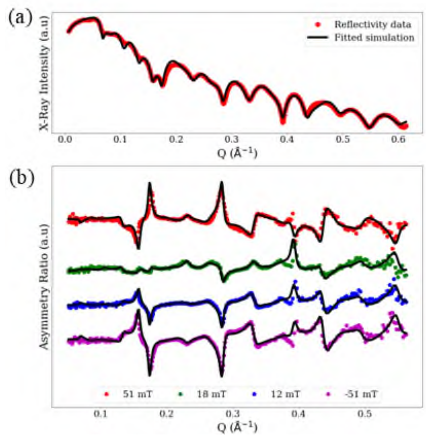

Figure CS4: (a) Specular reflectivity and (b) spin asymmetry data for four different applied magnetic fields.

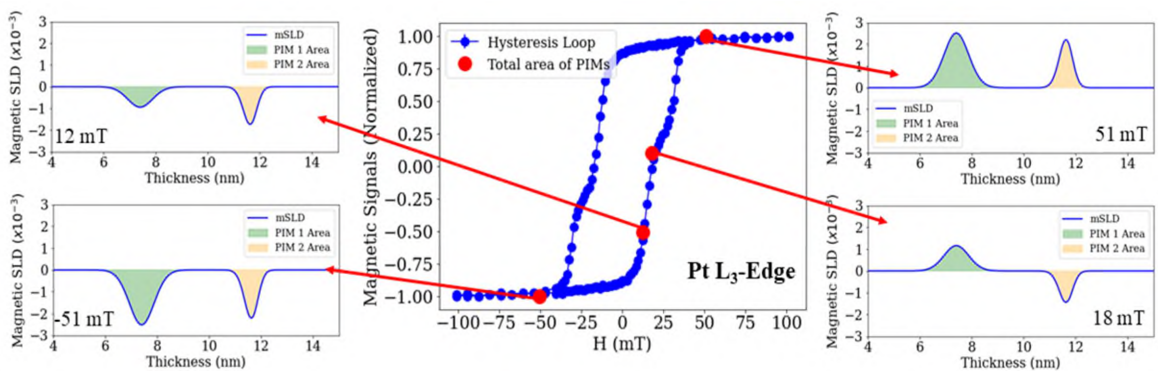

Figure CS5: Magnetic profiles of Pt proximity-induced magnetization (PIM) as a function of film thickness. The profiles are obtained at four magnetic fields. The hysteresis loop, also measured at the Pt L_3-edge, probes the Pt magnetic moment.

Unlocking New Insights into Arsenic Contamination with XMaS

J. Biswakarma, M. Matthews, J.M. Byrne, University of Bristol, UK. jagannath.biswakarma@bristol.ac.uk

Every day, millions of people unknowingly consume water contaminated with arsenic, which increases their risk of skin lesions, cardiovascular diseases, and developmental disorders. In Southeast and Central Asia alone, over 100 million people depend on groundwater sources that exceed safe arsenic limits. Arsenic mainly exists in two forms in natural environments: arsenite (As(III)) and arsenate (As(V)). As(III) is more toxic and mobile, making its presence in groundwater a significant concern. Traditionally, scientists believed that arsenic remained highly toxic and mobile in low-oxygen environments, like those found in Southeast Asia, making water treatment efforts challenging. It was widely assumed that As(III) could only be oxidized to As(V) in oxygen-rich environments. However, our research presents groundbreaking evidence that naturally occurring iron minerals along with organic compounds can transform the toxic arsenite into a less toxic form of arsenic, offering new hope for improving water safety.

Our team, which also included H. Forrester, and K. O'Neill, conducted high-resolution X-ray absorption spectroscopy (XAS) to investigate how arsenite (As(III)) interacts with green rust sulphate, a naturally occurring mixed-valent iron mineral. Using X-ray Absorption Near Edge Structure (XANES) spectroscopy, we made a surprising discovery: As(III) was partially oxidized even in the absence of oxygen. Furthermore, we found that it was fully converted to the less toxic arsenate form (As(V)) when citrate, a common organic compound found in soil, was present. XMaS' advanced X-ray techniques, including X-ray absorption near-edge structure (XANES) and extended X-ray absorption fine structure (EXAFS), provided unparalleled insights into arsenic and iron transformations at the molecular level [5]. Unlike conventional methods, which often rely on indirect measurements, XMaS enabled us to directly observe chemical/speciation changes. This capability was crucial in revealing how iron minerals act as natural arsenic detoxifiers, offering a new perspective on arsenic mobility in groundwater. Such findings are particularly relevant for flood-prone regions like Assam, where seasonal water fluctuations impact arsenic contamination levels.

Our findings challenge existing paradigms by showing that arsenic oxidation can occur without oxygen, driven by natural iron mineral transformations. If these processes are widespread in nature, they could help explain why arsenic behaves differently in certain groundwater systems, potentially reducing contamination risks. Furthermore, the study highlights the role of organic matter in enhancing arsenic transformation, paving the way for future nature-based, low-cost water treatment solutions.

Figure CS6. Dr. Jagannath Biswakarma (centre) helping children understand the groundwater quality in his hometown Assam, India.

This research effort has direct applications for communities reliant on groundwater, Figure CS6. Understanding the role of iron minerals in controlling arsenic mobility can guide the design of more effective remediation strategies and inform policies aimed at ensuring safe drinking water supporting regions struggling with arsenic pollution. This work aligns with the UN Sustainable Development Goals 6: Clean Water and Sanitation and reinforces the UK's role in addressing critical environmental challenges and most notably in tackling global water crises, water security and public health.

With growing concerns about climate-driven changes to groundwater quality, this study underscores the importance of continued investment in synchrotron-based research to solve pressing environmental challenges. The ability of XMaS to provide molecular-scale insights was critical in achieving these findings, which demonstrated the value of UK-funded large-scale research facilities in driving transformative discoveries. We are grateful for the support of XMaS and EPSRC in making this research possible and look forward to further interdisciplinary efforts in safeguarding global water resources.

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[5] J. Biswakarma et al., Environ. Sci. Technol. Lett. 11, 1239-1246 (2024)

Section 3: Usage, user focus, and non-scientific impacts

Statistics on usage and the range of users

User statistics are, in the main, derived from access protocols at the ESRF, which collect information required by French law. The data are captured at the level of an institution, not PI or group, which limits the analysis that can be performed. It should be noted that synchrotrons worldwide report and publish user statistics that relate directly to users as *individuals* making use of a facility and generally do not differentiate between unique and returning users or the status of an individual. As our data are included in ESRF outputs, it follows the standardised reporting metrics.

XMaS allocates very little beam time for *internal* users with the vast majority of beam time allocated directly by the external review committee. There is no "in-house" time reserved for facility personnel. Thus, we identify *external* users as those that have had time allocated via independent peer review panels and have subsequently attended an experiment on the beamline. Note here unique users *include* students and PDRAs. The total user statistics are provided for the past five years in Table 1. Note that the facility was shut down for the ESRF upgrade during 2020 and limited user access was possible through 2021 due to the COVID pandemic.

Year	Unique users			Repeat users	Total inc. repeat
	% internal	% external	Total excl. repeat		
2020	0	0	0	0	0
2021	1	99	60	21	81
2022	0	100	100	26	126
2023	4	96	102	22	124
2024	3	97	96	22	118

Table 1: Total users of the facility for the past five years.

A further breakdown of user visits based on identified unique users from 2020-2024 are presented in appendix C for context.

More details, but with data based on total user visits, are provided in Table 2 below. Again, we report users as *individuals* making use of the facility. We capture internally, from end of run surveys, the number of students and PDRAs that have used the facility along with direct users from industry. However, we do not capture or characterise ERC users. The latter is due to two factors: first, whilst the definition is relatively well-known in the UK is less clear for international users and secondly the formal employment status of an individual is not pertinent to the application process for the award of beamtime either through the ESRF or UK routes. In the table we include in the classification of *Academics* users those who were based at central facilities and research institutions as we do not know the formal status of many international research institutions. We also track the number of new users as a KPI and, in this reporting period, it was 41% well aligned with historical trends. Following a request in feedback from the 2023 annual report, we have also investigated how the new users are split between students, PDRAs and academics. For 2024 the split of new user was 47% students, 34% PDRAs and the remaining 19% academics. Historical data is presented in appendix D with the KPIs.

Year	Doctoral students	PDRAs	Academics	Industry	Total	% international
2020	0	0	0	0	0	0
2021	35	19	27	0	81	16
2022	40	28	58	0	126	15
2023	46	29	50	1	125	25
2024	41	16	61	1	118	32

Table 2: Users breakdown based on total user visits to the facility for the past five years.

The user data covering this reporting period is fully consistent with statistics from previous years. The total number of users is roughly constant with students making up ~35% and PDRAs ~20% of the total. We believe that having >50% of students and PDRAs as users shows that the facility makes a valuable contribution to training the next generation of researchers. Expansion of industrial users is more difficult. We are attempting to track experiments with industrial collaborators, but this relies on users informing us in end of run surveys. In 2024, 11% of experiments had an industrial link, down from the previous reporting period which was 15%. We plan to highlight in future newsletters output which has an industrial impact. End of run surveys also provide details on the breadth of the user community with research areas for each experiment identified by the users and reported in section 1, Figure 1.

An alternative metric for user base breadth can be gleaned from publication statistics. Using the ASJC default classification scheme in Scopus we can identify output as spanning the topical areas shown in Figure 3. The data shown covers the period 2020-25 and it should be noted publications may count in more than one topical area.

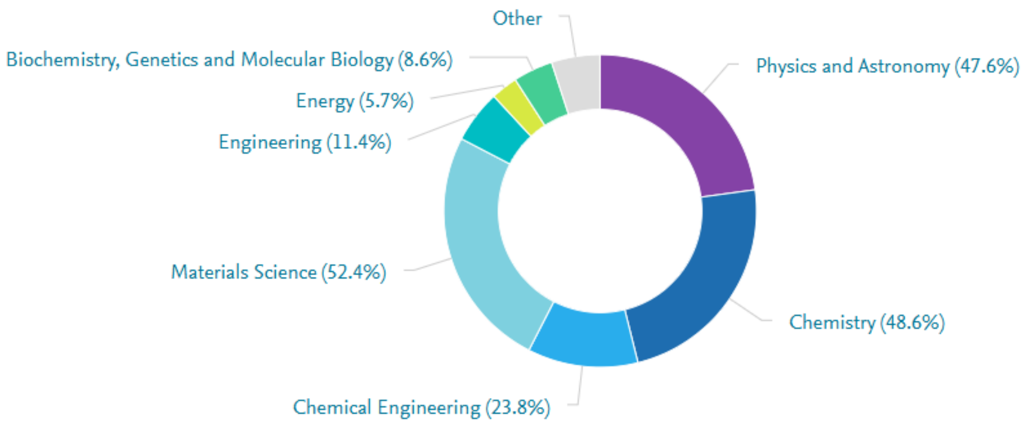


Figure 3: Research breadth as identified by publications using the Scopus research themes.

Service demand

Access to the facility is governed by a Collaborating Research Group contract with the ESRF which stipulates that 30% of the full flux beam time is allocated through public ESRF review panels in a worldwide call. The remaining beam time is available only to the UK community and allocated through our independent Peer Review Panel and assessed on scientific merit only. Beam time is scheduled in six-month allocations using all electron bunch modes of the ESRF. User calls are in April and October for scheduling some six months later. It is not possible to provide a chart showing demand and capacity monthly, but Figure 4 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 for the UK CRG time is returning to pre-pandemic levels whilst worldwide demand remains strong. In all cases, the trend to longer *in situ* or *operando* studies continues.

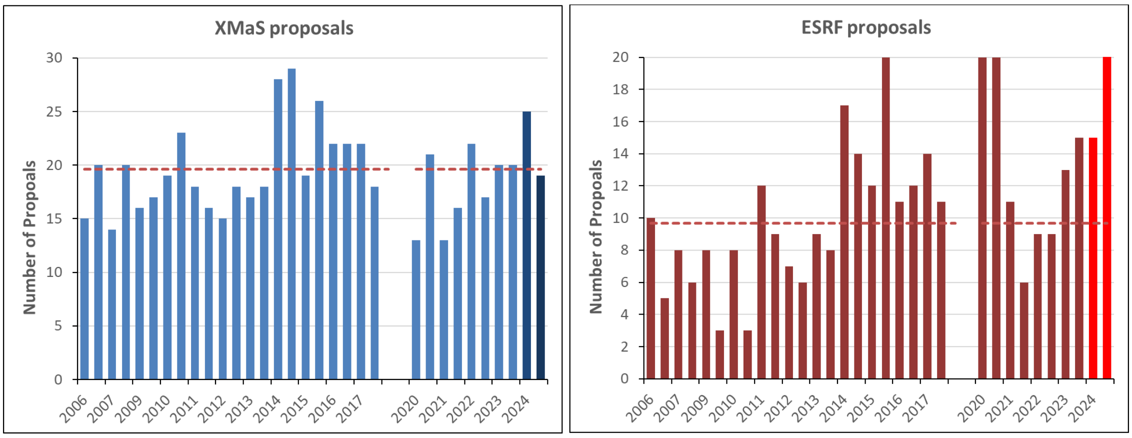


Figure 4: The number of proposals submitted. Proposals through the UK access (left) and international applications through the ESRF (right). Dashed lines are the averages calculated prior to the ESRF upgrade with the current reporting period statistics highlighted.

We can also analyse demand based on experimental shifts requested to those available. A shift is defined as 8 hours of experimental time. Analysis based on shifts provide a more nuanced demand metric as *in situ* and *operando* studies require a longer time to complete. UK proposals submitted in October 2023 and April 2024 were delivered in this reporting period. A total of 622 shifts were requested in these two calls against an available 237 shifts, a subscription rate of 2.62 and a rejection rate of 62%. We note that the PRP regularly comments that most applications have strong scientific merit and would warrant beam time. The same analysis on proposals submitted through the ESRF shows a total of 451 shifts requested against an availability of only 95 shifts: a subscription of 5.1 and a rejection rate of 79%. Historical statistics on service demand are presented in appendix C. A new Block Allocation Group or BAG route has been initiated in this reporting period in partnership with Kent and Diamond. BAG statistics will be reported from 2025.

In addition to the synchrotron beamline, XMaS also provides access to our "offline" facilities (the diffractometer hosted on a fixed tube X-ray micro-source and the facilities for electrical characterisation). These activities are handled *ad hoc* by the beamline staff. Often, this instrumentation is used in tandem to provide support for some of the experiments scheduled on the main beamline.

Uptime

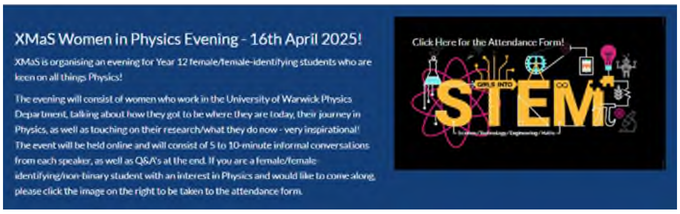
During this reporting period, the uptime of the facility was 94.3% with a total downtime of 5.7%, 3.3% of which was related to failures at the facility and the remaining 2.4% associated with external factors. Historical data are provided for context in appendix C.

Training, outreach, skills, and non-scientific impacts

The facility aims to report and monitor impacts according to the San Francisco Declaration on Research Assessment (DORA).

Activities to promote the facility beyond its core user base: In this reporting period, we focused our activities on highlighting the capabilities of XMaS to user communities beyond our core user base at both the ESRF and the wider UK community. The former was through a dedicated webinar "All the things you wanted to know about XMaS but never asked" hosted by the ESRF but aimed at a world-wide audience. In addition, we also delivered the Christmas lecture to the Physical Sciences staff and users at Diamond. We also reach out to the wider community through our X-feed (@XMaSBeam) with each experimental team encouraged to provide a photo and short description of their activities.

Public engagement activities run by XMaS: The annual XMaS scientist experience attracted over 60 applications, and we took 16 young women to the facility in June. We have also initiated a new online "XMaS Women in Physics Evening". Both activities are aimed at fostering discussions on careers for the next generation of female scientists. The 10th edition of the *XMaS Scientist Experience* was launched in December 2024. Similarly, staff members are also engaged with outreach activities in local schools answering 'what is a scientist? and what does a scientist at the ESRF do? They also host public tours of the ESRF and XMaS.



Societal & economic impacts: The work highlighted in our case studies enclosed herein also generated impact and outreach beyond conventional academic output. Articles across the mainstream media as well as vlogs were prepared by our users.


News Opinion Sport Culture Lifestyle

The Guardian

Environment Climate crisis Wildlife Energy Pollution

Reptiles

This article is more than 3 months old

Komodo dragons have iron-coated teeth, scientists find

Reptile's teeth found to have covering that helps keep serrated edges razor sharp and resistant to wear

Oscar Allan

Komodo dragons are the largest living reptile, growing to more than three metres in length and weighing 80kg on average. Photograph: Charlotte Ellis, Zoological Society of London

With their huge size, venomous bite and the fantastical connotations of their name, Komodo dragons seem like the stuff of legend.

Collaborations: XMaS retains strong and close links with other facilities and beamlines. A long-standing relationship exists with sectors 4 & 6 at the Advanced Photon Source (APS) in the US with their beamline scientists actively undertaking experiments at XMaS and being Co-Is in grant applications. We also have a strong and deepening relationship with Diamond, sharing the Energy materials BAG with B18 and considering options for a Catalysis BAG in the near future. XMaS is an acknowledged route for mitigation during the upcoming Diamond dark period.

External Visits: During October 2024, Prof Gianluigi Botton, CEO of Diamond Light Source, visited along with the new ESRF Director General, Prof. Jean Daillant. A few weeks later, delegates from the UK Embassy in France also visited with Jeremy Lumb (Head of Science & Innovation, West Europe) and Matthias Meheust-Kemp (Science & Technology Officer) being accompanied by Helen Beadman (Associate Director from STFC Programmes Directorate).

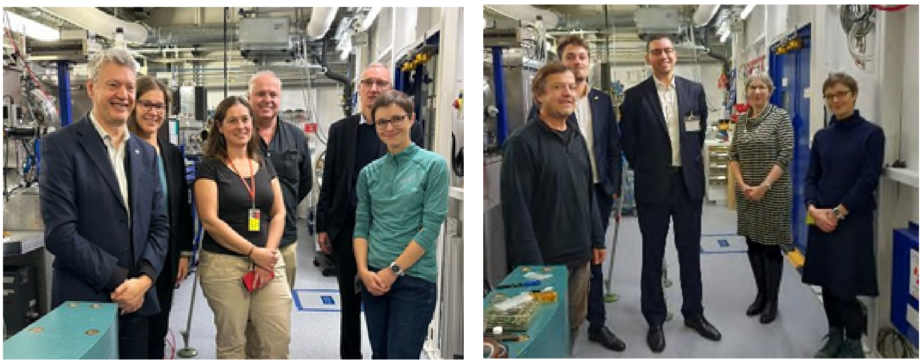


Figure 5: Visitors in the XMaS experimental hutch with members of the XMaS team.

Website: www.xmas.ac.uk

The facility website is hosted at the University of Warwick with its own uniform resource locator (URL) within the *.ac.uk* domain. The number of hits from distinct IP addresses to the facility website is shown in Figure 6. The web-traffic is regular with an average daily access rate of 208 hits. The website is actively updated and maintained, and we are building depth and links through the "user support" section, where links to inhouse and external developed content are provided to aid data visualisation, data reduction and data analysis.

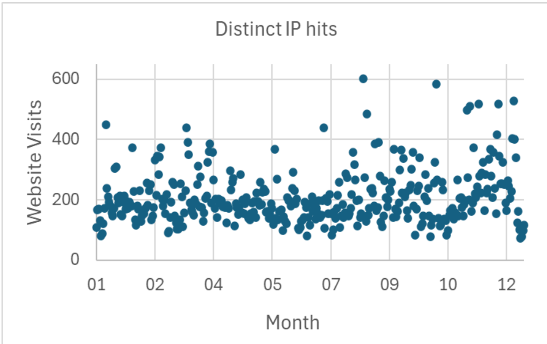


Figure 6: Daily website visits from distinct IP addresses during 2024.

User satisfaction

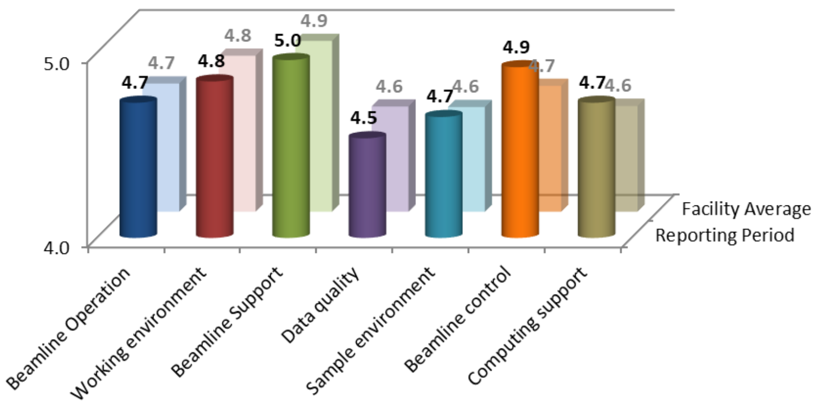


Figure 7: User survey results for the reporting period (foreground) with historically averaged data in the background.

For each experiment, the PI is required to complete, on behalf of the experimental team, an end of run survey scoring different factors of operational performance out of 5 (Figure 7). A direct follow-up with users occurs whenever the satisfaction is lower than expected or when issues are identified specifically in the free form text boxes which accompany the survey.

Our return rate for 2024 was 93%. User satisfaction in this reporting period is in line with the historical average and is positive. No complaints were received. We are immensely proud of the beamline support scores which were also highlighted by the external ESRF quinquennial review panel who noted in their report the *"stellar levels of user satisfaction."* Examples from the free form comments from users over the reporting period include:

> *"Whole experience very positive, although the experiment itself was challenging."*
>
> *"For future SAXS experiments, ensuring compatibility of the data with analysis software like SASView would aid in understanding the data quality during the course of the experiment."*
>
> *"The beamline scientist support was outstanding and underpinned the experimental success."*
>
> *"The beam suffered from long term position drifts and better beam monitoring tools are necessary. The stages were not very stable and routines that merge 2D data in batch mode, would be useful."*
>
> *"The support from the local contact was fantastic and went above and beyond to ensure the experiment ran, and we are grateful for their help."*
>
> *"We want to thank the beamline staff for their skills, explanations, and kindness, especially with inexperienced users, or those not yet experts in the technique!"*
>
> *"Our local contact went above and beyond, often staying beyond working hours and being accessible on weekends to promptly address our queries. The atmosphere at XMaS is unique; other beamline scientists who are not local contacting sharing advice and showing genuine interest in our work."*
>
> *"We just want to comment on the outstanding dedication of our local contact. Their help was indispensable, giving up their weekend and evenings to help teach and train students."*
>
> *"The beamline worked exceptionally well, and its capabilities are impressive. I had waited 15 years to perform an XAFS experiment at the Ba K edge, and it was a pleasure to complete such an experiment. The Ge detector was super and worked well. I would definitely come again!"*

We note the slightly lower satisfaction scores in 'data quality' and some specific comments on this matter were received. We are striving to address this through improvements in beamline systems to reduce background and stability, funded through recent capital calls, and expect to see improvements when we transition to the new ESRF standard BLISS control system. BLISS provides greater flexibility in controls and standardisation in data format and handling. 2D data reduction has also been developed and is now deployed for users.

Section 4: Effective management

Cost recovery

UK access to synchrotron radiation is provided through the ESRF and Diamond Light Source 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.

Year	Running Costs	Grants	Other Academic	Students	Industry	% Recovered
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%
2023	£1,141,944	£0	£0	£0	£0	-
2024	**£1,411,511**	**£0**	**£0**	**£0**	**£0**	

Table 3: Additional income through other funding sources.

The change in running costs in 2024 is associated with the start of the next operational funding period and reflects the total NRF costs divided equally over the 5 years. The cost for shift delivered on XMaS in 2024 was £4,200 as compared to the cost per shift for public beamtime at the ESRF of €6,700 and £5,263 at Diamond Light Source.

Cost recovery covering some staff expenses and instrument development has 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 (2013-2016), ADVENT (2017-2020) and OpMetBat (2022-2025). 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 user community. A further follow-up project, HyMetBat has been funded and will provide some funds to the facility in 2025. The funds have contributed marginally to the actual running costs of the facility.

Some cost recovery is also achieved from our 11 commercial licences, generating a few k£ per annum. Following renegotiations between the Universities and the staff who developed the designs, much of this is returned to the original IP holders. The remainder is reinvested into supporting the NRF staff activities. Further cost recovery can only feasibly be achieved by direct investment from industrial users. This access mechanism is handled through the ESRF but its uptake is traditionally low in the physical sciences.

Risks

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

1. Operational Risks, including specific risks to UK users accessing an international facility
2. Financial Risks
3. Data Risks
4. Projects

The Risk Register is reviewed, circulated, and discussed at each Project Management Committee (PMC) meeting, although it is updated more frequently as part of the day-to-day management of the facility. The discussions and input from the PMC have helped to define and evolve the risk register and keep it relevant and responsive to operational challenges. Monitoring the changing risk profile regularly has enabled project completion deadlines and targets to be agreed upon as well as highlighted several areas of action. The PMC uses the risk register to effectively stress-test current operations, help in the prioritisation of projects as well as ensure short, medium, and long-term risks are appropriately managed and mitigated against within a suitable staff-workload model. A copy of the latest risk register is provided in appendix D.

The risk register was used to identify operational risks and improvements that would benefit from additional funding available through the recent EPSRC Capital Call.

Summary of Risk Register

The general trend over the reporting period is that risks were mainly remaining unchanged. No major changes were made, reflecting the *steady state* of operations during 2024. An executive summary against the main headings is provided here:

Operational Risks: The biggest risks to operations are either outside of the control of the facility (ESRF/EPN campus shutdown) or are difficult to directly mitigate (failure of main infrastructure or staff loss). Operationally risks have remained unchanged, with mitigating obsolescence and ensuring sufficient staff resource is available the main factors. A review of risk assessments and requirements was conducted in 2024 with updated paperwork to be delivered in 2025 in compliance with both French and UK needs.

Financial Risks: The project is exposed to currency fluctuations with major commitments required in euros. During 2024 both inflationary pressures and the £:€ exchange rate were stable and within budgeted expectations. At the time of writing however, we note increased uncertainty in both factors due to the recent change in US government. A new risk was added in 2024 relating to cost-of-living allowances and maintaining salaries commensurate with those at the ESRF. We will be conducting a review during 2025 to recheck benchmark values and assess if salary costs are appropriate. The risk here directly relates to retaining and recruiting the best possible staff.

Data Risks: Accessing and retaining data within a secure portal are paramount. The data policy of XMaS follows that of the ESRF and we have implemented additional training for users regarding the risks of single sign-on on public computers. No significant changes occurred in 2024, although a transition to the new control system BLISS is required to mitigate obsolescence and control limitations.

Project Risks: The facility is balancing a portfolio of projects, from sample environments to better beam definition and mitigating obsolescence. Risks have remained flat but additional pressures on available staff resource need to be managed so that new projects associated with the recent EPSRC Capital calls can be delivered. Risks remain centred on finalising delivery. The risk register is used to prioritise projects and available resources.

XMaS KPIs and SLAs

During the reporting period and as part of the recent funding allocation the KPIs and SLAs for 2024-2029 were revised. RAG levels were agreed based on historical data and operational expectations. The revised descriptors of the KPIs are presented in the table below:

Description of KPI	Red	Amber	Green
A) The number of university research groups that have made use of the XMaS beamline in 12 months. [All beamtime]	<30	30-50	>50
B) The number of new users that have made use of the beamline expressed as a percentage of the Total Number of Users within 6 months.	<25%	25%-35%	>35%
C) The uptime of the beamline within 6 months as a percentage of the Total Available Time within that period.	<90%	90%-95%	>95%
D) The number of user complaints received within 12 months.	>2	1	0
E) The number of research outputs expressed as a Total Number for a calendar year.	<10	10-15	>15
F) The total number of publicity and/or outreach activities that the facility performs in 12 months.	<2	2	>2

Table 4: The revised XMaS KPIs and their associated RAG levels.

Service Level Agreements (SLAs)

- Requests for beamtime will have decisions made within 20 working days of the PRP meeting subject to knowledge of the ESRF review process. In 'exceptional' cases users will be informed if these benchmark times are going to be exceeded and an explanation provided.
- Facility users will be fully supported by a dedicated facility staff member during experimental time.
- The facility will respond to all user enquiries clearly and quickly in line within 5 working days for emails and 2 working days for telephone enquiries.
- The facility will respond to user complaints within 10 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.

For this reporting period, all service levels were met. The KPI metrics are reported for 2024 in Table 5.

KPI	2024
A) The number of university research groups that have made use of the XMaS beamline.	49
B) The number of new users that have made use of the beamline expressed as a percentage of the Total Number of Users within 6 months.	43%
C) The uptime of the beamline within 6 months as a percentage of the Total Available Time.	94%
D) The number of user complaints received within 12 months.	0
E) The number of research outputs expressed as a Total Number for a calendar year.	22
F) The total number of publicity and/or outreach activities that the facility performs.	4

Table 5: Performance report against KPIs for the reporting period 2024.

Two of the KPIs were just in the amber range. The uptime of the facility was negatively affected by some storage ring failures at the ESRF (2.5%) but mainly by a higher-than-normal incidence of beamline downtime during the first half of 2024. Two experiments were principally affected, one through an insufficiently sized beam-stop which caused too much stray scattering to be measured and secondly another experiment experienced some communications problems. The former is being addressed through the recent EPSRC capital call by developing a better beam stop and the latter will be rectified when the facility switches to the new ESRF standard controls system BLISS sometime in 2025/26. The uptime of the facility for the second half of 2024 was 97%. The number of user groups was also slightly lower than historically expected. We do not believe this is related to demand (see user statistics) but instead reflects the increasing number of *in situ* and *operando* experiments, which take longer, limiting the total throughput of users. To test this hypothesis, we determined the average number of groups per experiment which was 1.6 compared to the recent historical average of 1.7. We suggest that this metric may, in fact, be a better KPI and will be proposing this at the next PMC meeting.

Graphical representations of the new KPIs, mapped to historical statistics, are presented in appendix D for completeness.

Improvements and future plans for XMaS

The XMaS facility works closely with its user community to plan and prioritise future capabilities and needs. A free-form box is available on the end of run survey form for users to request or suggest improvements. Future plans are always a balance between developing capabilities to enhance the user experience whilst recognising that new developments put extra demands on facility staff. The Project Management Committee (PMC) is appraised of upcoming works and helps to prioritise activities. In the past year we have focused on:

BAG Access: A so-called "Block Allocation" access mechanism in the area of energy materials is now active on XMaS and is run by a PI at the University of Kent (Dr. Maria Alfredsson). Aimed at materials underpinning batteries, fuel cells, photovoltaics, etc., the new BAG provides regular and speedy access to core XAS spectroscopy for rapid assessment without the need for individual beamtime applications by the PIs. The focus is on conventional, *ex situ* XAS experiments at room temperature and a fast throughput of samples. The XMaS BAG works in close collaboration with the Energy materials BAG at Diamond providing an essential capacity resource to the UK. XMaS will consider a Catalysis BAG in 2025 but we are aware of the risk of balancing BAGs with conventional access routes.

User Experience – Data analysis: Central to an efficient beamline is the ability to visualise and reduce data. This is especially true in diffraction measurements using our suite of 2D detectors. Routines and protocols have been developed to display and plot data in 3D, and we are working with colleagues at Diamond to deploy the Diamond-developed "*msmapper*" and plot data in 3D reciprocal space using the UB matrix coded with the data collection. In addition, we continue to develop protocols for FAIR data repositories. A unique digital object identifier (DOI) is assigned to each experiment and automatically generated. The facility is working with users and the ESRF in more seamlessly incorporating the metadata and moving to h5 file architectures to make the data more FAIR compliant. This transition will be an integral part of the BLISS migration which will occur through 2025 and for which preliminary work is ongoing using the offline facility.

PDRAs: Two PDRAs were appointed in 2024. Their fields of expertise are in soft matter energy materials (Dr. Rachel Kilbride) and the reactive properties of actinide thin films for nuclear fuel applications (Dr. Florence Legg). Their skills will complement the core team and provide new insights and knowledge transfer into the facility. Over the course of their contract, they will develop new sample environments as well as work with users to develop new analysis tools and routines.

Capital Call: The EPSRC capital call has come at a propitious time allowing the facility to address obsolescence and re-invigorate core capabilities. These include a complete overhaul of the Off-line X-ray Source returning the system to the original flux and incorporating in-vacuum motors to facilitate future alignment and optimisation. An overall upgrade of our cryostats will restore capability and provide long terms facility resilience: our 1.8 K system will be repaired allowing use with our 4 T magnet. A new compressor will provide additional resilience along replacement temperature sensors. On the beamline a new diamond beam position monitor and amplifiers will provide real-time beam position information. Upgrades to slits and beam-stops assemblies will, during 2025, help reduce background which is essential for the study of weakly scattering systems. We will also add to our strain and stress capabilities by investing in a razorbill strain cell for hard condensed matter and a stress rig for soft matter materials. Supporting spectroscopy, we will develop an engineering solution to enable the heavy 7-element Ge detector to be positioned quickly and easily. A key design criterion will be ensuring that spectroscopy and scattering experiments can be performed simultaneously.

Sample Environments: Working with our community the facility will always retain the ability to react to user needs and develop or integrate bespoke sample environments or modify existing system to allow new multi-modal experiments to be undertaken.

Additional information: The XMaS Newsletter

XMaS activities are widely disseminated in our annual newsletter which is written for a scientifically interested reader. The newsletter highlights both the range and breadth of science undertaken as well as showcasing the facility's capabilities. The 2023 edition of the newsletter was released in March 2024 and circulated widely.

- Beamline Updates Details of new software developed at the facility that allows a quick, straightforward visualization and reduction of 2D scattering patterns (PyXscat) was released through the ESRF GitHub Data analysis tools. New capabilities in a sample environment for GI-WAXS studies of energy materials and our new fast scanning of the monochromator and KB mirrors were described.
- Magnetic Profiles in rare-earth transition metal thin films (Appl. Phys. Lett. 123, 122403 (2023)): Exploiting the ability of XMaS to control the beam polarisation and apply magnetic fields allowed the non-uniform Gd distribution and magnetization profiles within GdCoFe alloy thin films to be determined.
- New Molecules for evaporated organic solar cells (APL Mater. 11, 061128 (2023)): The successful transition to non-fullerene acceptors (NFAs) in organic solar cells is still pending for vacuum-thermal evaporated (VTE) OSCs, not least because most NFAs are too large to be evaporated without breaking. GI-WAXS data from NFA BTIC-H molecule show their potential and is a starting point for molecule design of suitable NFAs for VTE OSCs.
- Structural study of organic thin films for optoelectronic devices using with GI-WAXS (Langmuir, 39, 12099-12109 (2023)): The morphology and crystalline structure of diketopyrrolopyrrole derivatives were explored using GI-WAXS and specular diffraction to reveal information on the degree of crystallinity and the molecular packing in spin coated OSC films, critical parameters for the future development of organic optoelectronics.
- A different story of AI: Amelogenesis Imperfecta: X-ray diffraction was used to study the genetic disorder *Amelogenesis Imperfecta* that affects the formation of enamel on teeth. Mapping using small beams revealed the crystallite orientation close to the inner enamel and cuspal areas and how it was influenced by the disease.
- *Centipede* statistical polymer under nano-confinement (Journal of Colloid and Interface Science, 653, 1432 (2024)): X-ray reflectometry data were used to support mechanical studies on the frictional properties of functionalised n-dodecane copolymers under nano-confinement. The results suggest it will be possible to tailor the polymer structures tailoring the interface structures and hence their nanotribologial properties.
- 2D Quasicrystal from self-assembled polygonal nanocolumns (Nat. Chem. 15, 625-632 (2023)): A diffraction study of the first reported columnar liquid crystal made up of a T-shaped molecule which due to the tendency of the three incompatible but connected parts of the molecule tend to nanophase separate and drive a quasi-periodicity through the optimisation of the molecule packing.
- Sugar alternatives for processing radioactive waste (J. Non-Cryst. Solids 608, 122240 (2023)): Spectroscopic data were recorded from simulated high-level waste slurries to be used in the Hanford Waster Treatment and immobilization plant. The element specific XANES and EXAFS data allowed the structure and valence of the constituent components to be determined despite the complex chemical matrix. New pathways that allow the assessment of alternatives to sucrose in HLW feeds that could improve efficiency were investigated.
- Transforming bio-diesel waste into green hydrogen and chemicals (ACS Catal. 12, 14492 (2022)): The role of Ni in PtNi electrocatalysts in the production of green hydrogen was explored using EXAFS and XANES.
- Observing the incorporation of small heteroatoms into palladium metal (ChemCatChem 15, e2023008, 9 (2023)): Exploiting the tender X-rays available on XMaS, XANES studies of Pd were used to explore the effect of different PdC, PdH and PdN structures formed during catalysis action. The stability of the structures formed on Pd/Al_2O_3 were studied *in situ* during thermal cycling up to a 600°C
- Speciation and characterisation of Se in Pt-Pd-substitute pyrite: A spectroscopic investigation of the valence and chemical environment of Se in pyrite compounds was conducted as part of a broader study of extracting critical elements such as Pt and Pd from sulphide deposits.

The 2024 version is currently being finalised with an anticipated release date of March 2025.

Appendices and Supporting Information

Appendix A: Purpose and vision of XMaS

A photograph of the current XMaS experimental hutch is shown in Figure A1. The beam enters from the right and passes through monitors and shaping optics before interacting with the sample mounted on the diffractometer which is to the left of the picture.

Figure A1: Panoramic photograph showing the experimental hutch of the XMaS facility. The beam enters from the right and proceeds via a series of in-line beam conditioning optics to the diffractometer (left).

The beamline characteristics include:

Characteristic	Specification
Source	ESRF 0.86 T Short Bend dipole magnet
Bending Magnet Fan acceptance	2 mrad (H) × 0.2 mrad (V)
Double-crystal monochromator	Si (111) flat crystal pair with cryogenically cooled crystals
Energy Resolution	1.5×10^{-4} at 10 keV
Energy ranges	
Focused monochromatic	2.1 – 47 keV
Unfocused monochromatic	2.1 – 47 keV
Focusing mirrors	Pair of interchangeable 1.2 m-long Pt or Cr-coated Si mirrors with controllable toroidal shape
Source Focusing	1:1
Harmonic Rejection Mirrors	0.5 m flat Si mirrors with three stripes: Pt, Cr, and Si
Usable flux at the sample:	
Focused monochromatic	10^{13} photons per second per (0.1% bandwidth) at 10 keV
Unfocused monochromatic	~10^{12} per second
Typical beam sizes (FWHM) at the sample position:	
Focused monochromatic	80 µm (H) × 80 µm (V)
Unfocused monochromatic	10 mm (H) × 2 mm (V) (maximum)
KB focused	~5 µm (H) × 7 µm (V) (smallest)

Table A1: The main source characteristics of the XMaS facility.

User statistics are collated by the ESRF user office, which we have also had access to since 2001. Cumulative plots of scheduled hours, number of user visits and number of experiments are shown in Figure A2. The data are consistent over the entire reporting period from 2021. A slight increase in the number of experiments and user visits corresponds to more short experiments. Since the EBS and Covid shutdown, experiments have reverted to the standard 18 shifts due to the increased *in situ* and *operando* studies resulting in cumulative data trends similar to the earlier operating periods where 18 shifts allocations were more common.

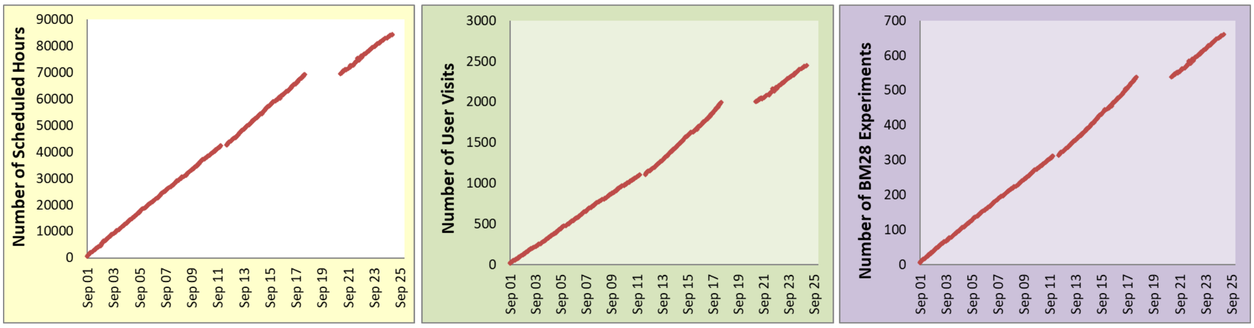


Figure A2: Historical performance metrics for XMaS including the number of scheduled hours (left), the number of user visits to the facility (centre) and the number of individual experiments performed on the beamline (right).

The vision of the facility is distilled into our high-level objectives which are reviewed annually by the external Project Management Committee:

- 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.
- Engage and communicate with the UK materials community.
- Train early career scientists and students in advanced X-ray methodologies.
- Operate the facility safely, efficiently, sustainably, and resiliently within a framework of equality, diversity, and inclusion (EDI).

Appendix B: Quality and breadth of research that XMaS has enabled

Details of new methodologies that have been developed over the past year on XMaS

Mirion® 7-Element Ge Detector: With the higher energy of the source, there was a clear need for an energy dispersive detector to allow EXAFS and XANES studies at technologically relevant X-ray adsorption edges, such as the Ce K edge. A new Mirion® 7-element Ge detector (Figure B1) was purchased but there were significant issues both with the stability of the sensor and the position of the refill port. After discussions with the manufacturer and a retroactive plan being agreed the detector was repaired and adjusted. In this reporting period we have successfully incorporated it into the counting chains and several user groups have used it. Due to its weight, there are still issues to be resolved in how to mount it efficiently and ensure it can be used easily – this is a project for the upcoming year.

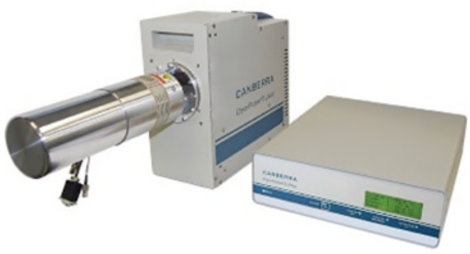


Figure B1: The Ge energy dispersive detector now routinely available for users.

New SAXS rail and flight tubes: To facilitate grazing incidence small and wide angle scattering new, modular flight tubes have been designed and commissioned. The flight tubes mount directly onto our SAXS rail (Figure B2) and can be filled with He or evacuated. The flight tube size is matched to our 1M detector and allows us to access a greater Q-range with lower background than previously.

Figure B2: The new flight tubes installed on the SAXS rail providing new capabilities for GI-WAXS and GI-SAXS.

KB Mirror commissioning: The KB mirrors, manufactured by IDT, were installed and commissioned on the beamline in 2024. The entire system rotates into the beampath with normal focused beam passing unhindered through the chamber. The KB mirrors themselves interact with the unfocused beam. Beams of some ~5 x 7 µm^2 (H x V) in size with a flux of ~10^9 photons/sec are easily obtained with a depth of focus at the same position of a few mm (Figure B3).

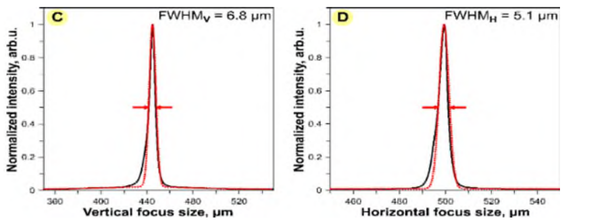


Figure B3: Commissioning studies showing the KB focused micro beams that can be focused at the sample position.

Gas Handling system: The gas handling system, designed in partnership with the UK Catalysis Hub, has been finalised and components procured during 2024 (Figure B4). The system will deliver a range of gases to sample environments and later to the ion chambers. It incorporates a mass spectrometer and will interface directly into the beamline controls.

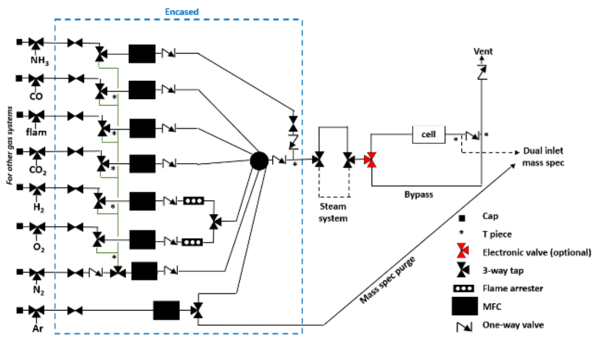


Figure B4: Schematic of the gas and mass-spec system for sample environments.

Publication Metrics

Our deep dive into the publication metrics is undertaken using data available through SCOPUS and the SciVAL portal. In the following pages, a report covering publication metrics from 2019-2024 is provided. Here we summarise some metrics from the reporting period, 2024. First, we present the publication topics in Figure B5 derived from 2024 publications

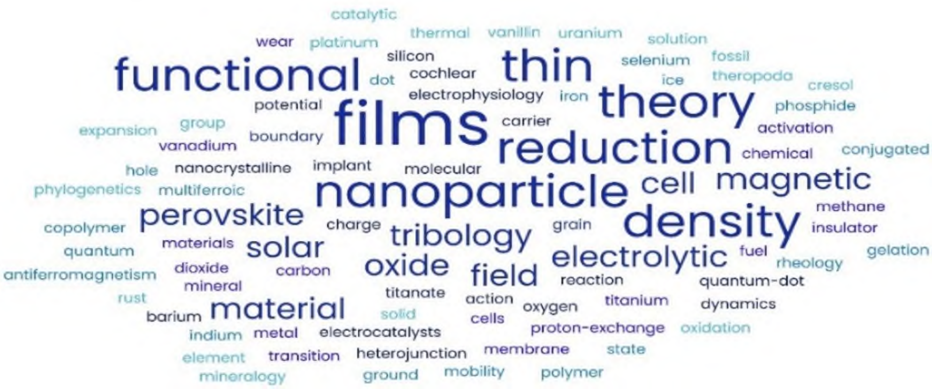


Figure B5: Word cloud derived from publication topics from 2024.

XMaS impact can be further studied by analysing the authors and their institutes from the publications. The total number of authors on the publications from 2024 was 213, with 201 of those authors being unique (only named on one publication). These authors are affiliated with a total of 103 institutions, (see Figure B6 for their geographical locations), with 69 of those institutions being unique.

Figure B6: Geographical location of institutes on XMaS publications in 2024.

We can also analyse the type of institution (academic, government (including central facilities) and corporate) as well as if a particular paper can be readily assigned to one of the UN global sustainability goals. These metrics are presented in Figures B7 and B8.

Figure B7: Percentage of publications readily identified with UN sustainability goals.

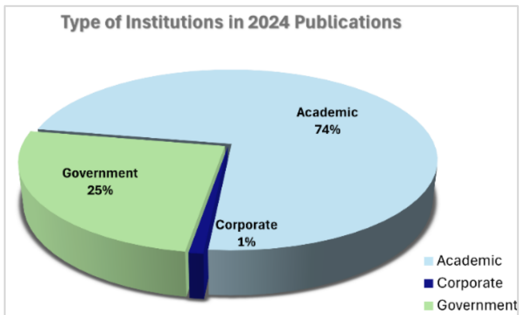
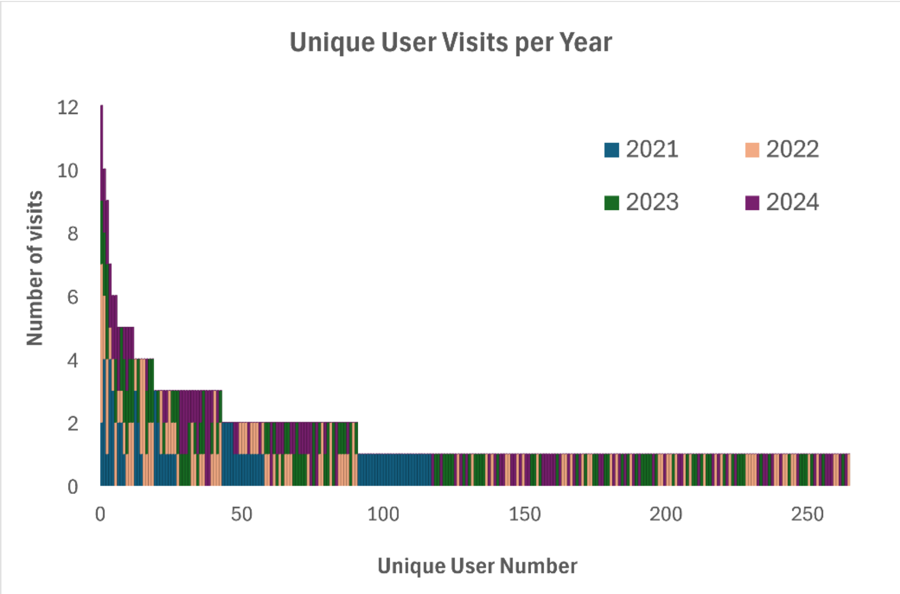


Figure B8: Types of institutions in the 2024 publications.

Appendix C: Usage, user focus, and non-scientific impacts

Statistics on usage and the range of users

A further breakdown of user access to the facility is provided here. A total of 264 unique users have been identified spanning the period 2021-2024. For each identified user, we track both the number of times they visited the facility per year and the number of shifts used by them. The data for 2021-2024 are presented in Figure C1 below. To note there were no users to the facility during 2020.



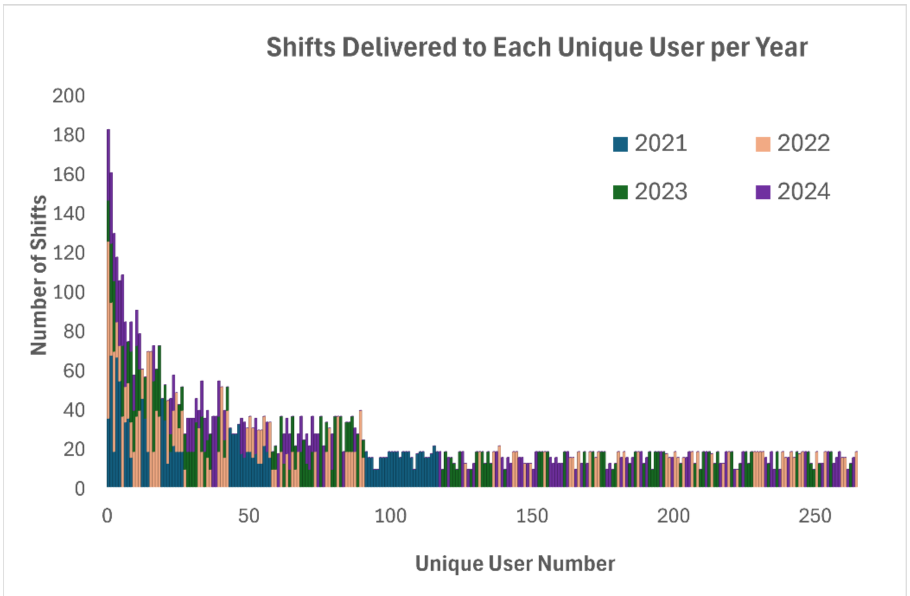


Figure C1: Access to the facility by unique users per year in terms of number of visits (top) and shifts (bottom).

Given the large number of students and PDRAs that use the facility it is not, surprising, that most users participate in only a single experiment. Some 66% of unique users attended once, 18% twice, 9% three times and only 7% were regular repeat users across the four years. The high repeat visits are from PIs of groups that make regular use of the facility. The data are clear, however, that the facility welcomes a large user community with no single set of users dominating access.

A detailed breakdown based on the 96 unique users for this reporting period is presented in Figure C2:

Figure C2: Access to the facility by unique users for 2024 in terms of number of visits (left) and shifts (right).

The trends noted across the four years are repeated here: 80% of users attended one experimental session, 16% two and only 3% three.

We are exploring the similarities and differences with a similar analysis performed using unique users within publications rather than those who attended beamtime. This is work in progress and would provide a complementary but different view of the impact of the facility.

Service demand: Subscription

Unlike the majority of beamlines at synchrotrons worldwide, XMaS assigns all available beamtime to user calls. Exceptions are made for critical commissioning and interventions, but there is no "in-house" time reserved for facility staff. Facility staff are expected to apply for beamtime through the public calls. This approach maximises the available shifts that can be delivered to users and minimises the number of proposals that need to be rejected. Scheduling constraints and equipment availability sometimes means that experiments are delayed, but we present here the subscription rate, and the associated acceptance (rejection) rate based on each proposal call. The data are presented separately for both access routes.

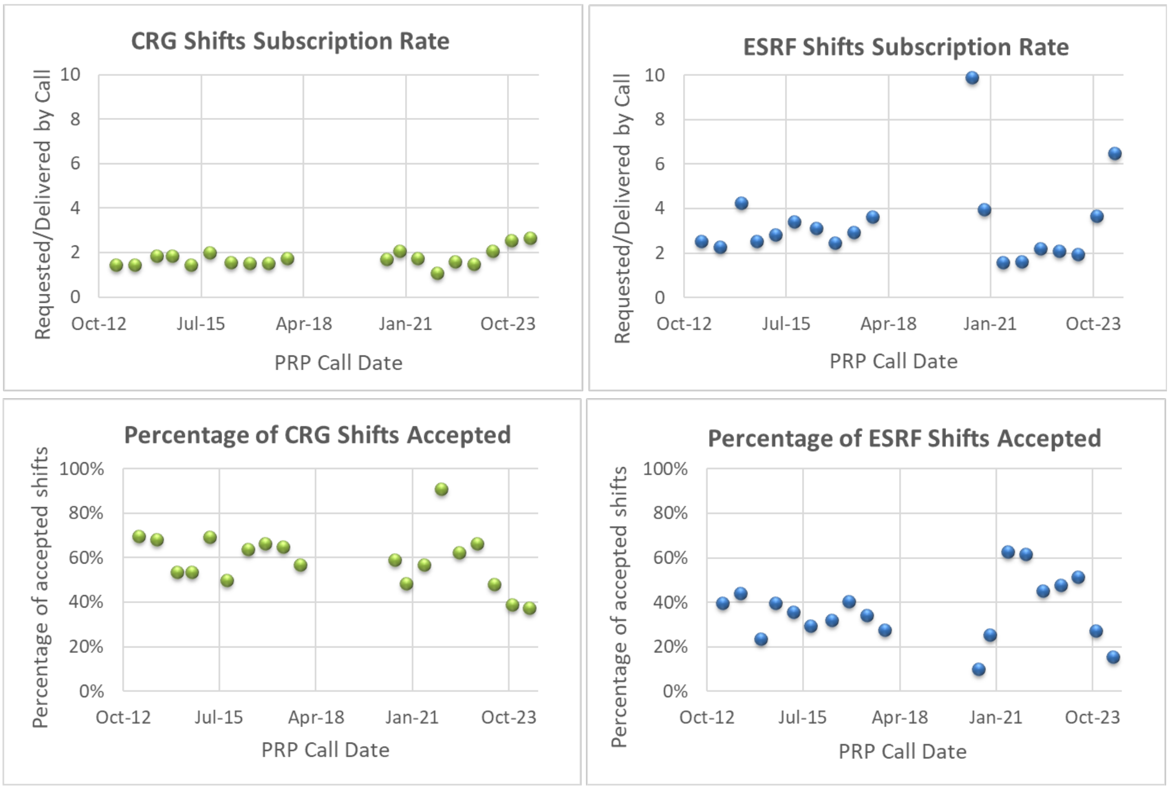


Figure C3: Subscription rates (top) and the concomitant acceptance rates (bottom) for the UK CRG access (left) and ESRF public calls (right) based on shifts.

Experience on XMaS and other synchrotron beamlines around the world suggest that subscription rates of between 1.5-2 are optimal. At this level, the best science is undertaken whilst allowing PIs a reasonable chance of beamtime and ensuring long-term research planning. Subscription rates of 3-4 are generally assumed to be unsustainable. Likewise, anything less than 1 shows facility capacity is not being exploited fully.

Facility Uptime

The ESRF, and hence XMaS, is operational 24 hours a day during ESRF storage ring operations. Figure C4 shows the operational efficiency of the facility as a function of time. In terms of downtime, this can be due to beamline failures or downtime beyond the control of the facility. The latter includes failures of the storage ring (ESRF) and user issues such as samples not being ready or last-minute cancellations due to external factors.

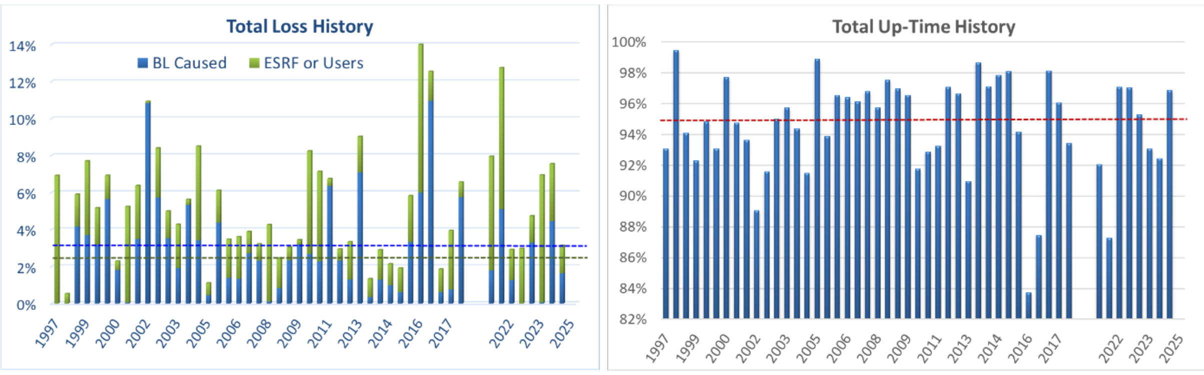


Figure C4: Downtime or loss as a function of time separated by cause (left) and the corresponding total uptime (right). Data are presented on a 6-month reporting period.

The dashed lines in Figure C4 are the averages derived from data prior to the ESRF shutdown and provide a benchmark for operations with the new storage ring. There were obviously some issues with the ramp-up, and the manufacturing issues associated with shipped Ge detector. Howsoever, with the detector now operational (2024) we are now operating with the same degree of uptime as before.

Appendix D: Effective management

KPIs and SLAs

New KPI metrics, based on all beamtime for all users and mapped to historical data are shown in the Figures D1 and D2 below.

A) The number of university research groups that have made use of the XMaS beamline.
B) The number of new users that have made use of the beamline expressed as a percentage of the Total Number of Users within 6 months.
C) The uptime of the beamline within 6 months as a percentage of the Total Available Time.

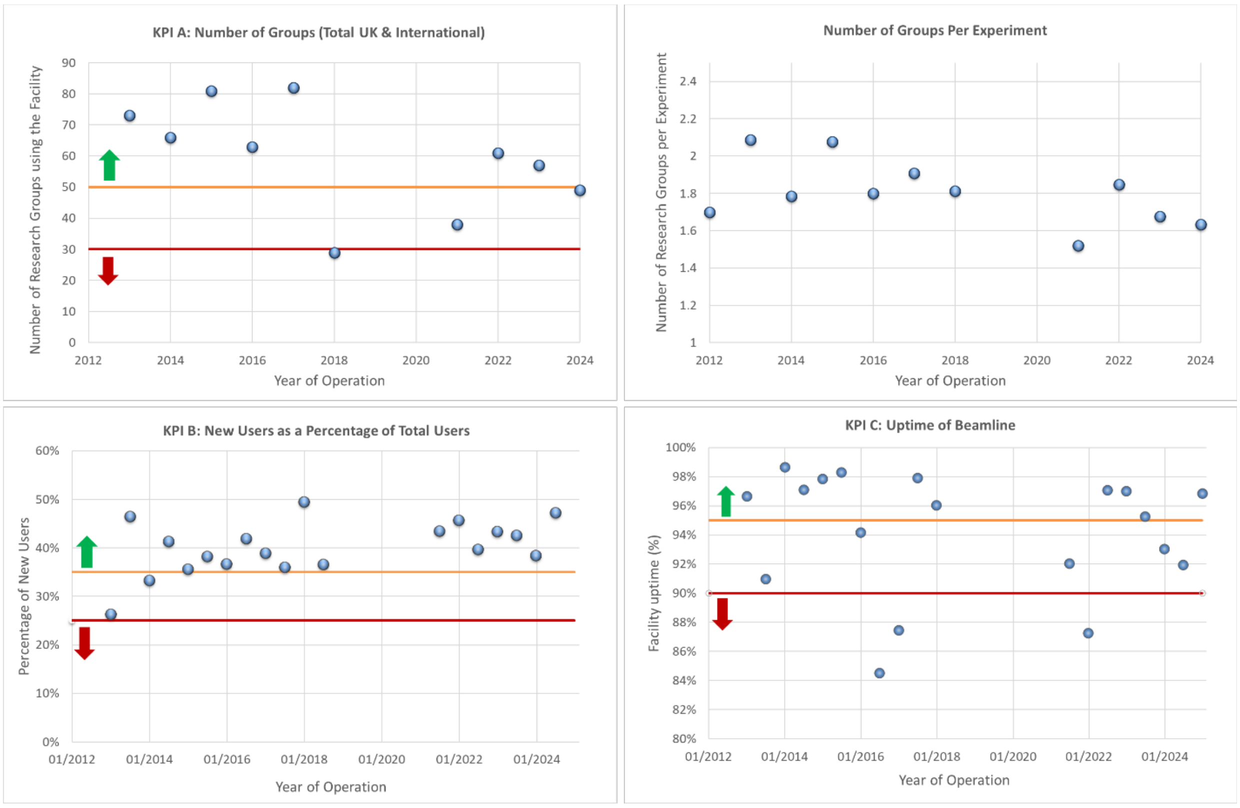


Figure D1: KPIs A, B, and C as a function of time. The orange and red lines represent the RAG thresholds for each KPI.

KPI D: There have been zero complaints against the facility over its entire operation

E) The number of research outputs expressed as a Total Number for a calendar year.
F) The total number of publicity and/or outreach activities that the facility performs.

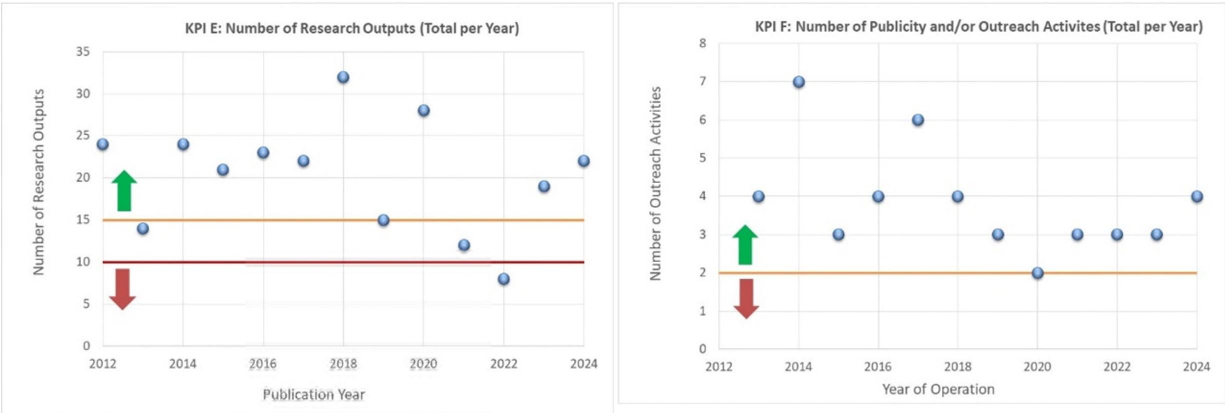


Figure D2: KPIs E and F as a function of time. The orange and red lines represent the RAG thresholds for each KPI.

As an additional metric, and as requested by the HLG in 2023 the breakdown of new users into students and PDRAs is shown in Figure D3 below:

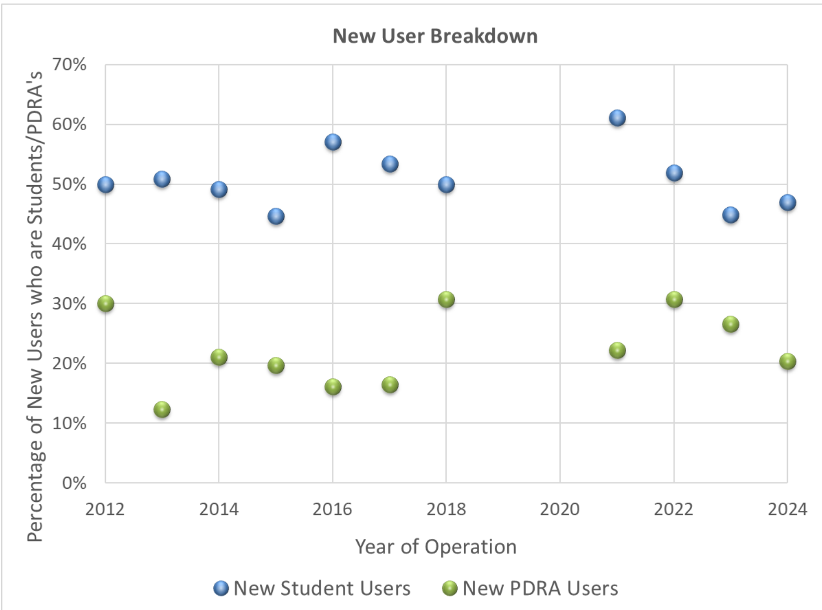


Figure D3: The percentage of new users (KPI B) that are students (blue) or PDRAs (green).

Risk Register

The latest version of the Risk Register is appended in the following pages.