National Research Facility Annual Review 2020-2021

Timeline 2021/22:

- Reporting Period for this Annual Report: **1st September 2020 – 31st August 2021**
- Deadline for Annual Reports**: 11th February 2022**
- Assessment by Panel**: February/March 2022**
- Feedback to Facilities: **March/April 2022**

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)

1) Value Proposition

The XMaS beamline has been supporting the UK materials science community since it began operations at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France in 1997. In the period 2015-2021 the ESRF has delivered a €150M facility upgrade, the Extremely Bright Source (EBS), bringing its scientific users a first-of-a-kind, low-emittance, high-energy synchrotron light source. To take advantage of the unique opportunities provided by this new source, XMaS has also undergone an extensive upgrade through 2019 and 2020 to deliver a state-of-the-art facility that fully exploits the capabilities of the new ESRF machine. Despite being impacted by COVID, in terms of access and supply chain delays, the complete rebuild of the beamline was completed only a few months behind the originally planned schedule. The new facility delivers a much brighter X-ray beam with an extended operational energy range, which now reaches beyond 40 keV, thereby enabling new activities in materials research, particularly in terms of *operando* experiments. The XMaS science portfolio continues to evolve and embraces a broad spectrum of scientific disciplines under the generic theme of materials science, cutting across research themes in physics, chemistry, biosciences, healthcare, engineering, and energy. XMaS forms an integral part of the UK's synchrotron radiation (SR) infrastructure which includes the ESRF and the Diamond Light Source (DLS).

The main objectives of the facility are to provide the UK materials science community with access to a state-of-the-art X-ray facility (source and experimental equipment) and to facilitate training for early career scientists, including postgraduate and undergraduate students, in advanced scientific methodologies. XMaS delivers X-ray characterisation methodologies across a range of temporal and spatial length scales and, by the development and use of novel sample environments, enables increasing use of *operando* studies allowing correlations between structure and functional properties to be determined. To this end, and following a strong user drive, a new micro focusing capability is currently being added which will facilitate the high-resolution spatial mapping of new materials. 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 in partnership both with 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.

2) Scientific Excellence

Figure 1: A view of the completed EH1 cabin during a user's experiment.

During the reporting period, operations as well as access to the XMaS facility have been severely impacted by the COVID pandemic. Supply chain problems caused a delay in the completion of the beamline upgrade and meant that the final commissioning runs took place in the early part of this reporting period. Test experiments were performed throughout the autumn of 2020, which allowed us to benchmark the new source, test the updated beamline capabilities and identify further optimisation pathways that needed to be developed. As expected, the complete rebuild of the beamline from the source to the diffractometer itself resulted in some minor issues that were identified and fixed through this commissioning stage. By the December 2020 ESRF shutdown, XMaS was able to plan for the return of scheduled user operations, which began on the 27th January 2021 in the completed experimental cabin (figure 1). The new capabilities of the beamline were published in a "NewsFlash" to the user community in March 2021. Unfortunately, the COVID pandemic has continued to impact operations with access to the ESRF campus for users not being possible until late September 2021. Onsite access was again suspended towards the end of 2021 due to the rise in OMICRON case numbers. Thus, for this reporting period all experiments were run in "remote mode" with onsite staff heavily involved and users controlling the experiment remotely where possible. Within this reporting cycle we successfully delivered 15 user experiments.

The research output and scientific highlights we report here derive, in the main, from data collected prior to the shutdown of 2017 (although data collected at the APS as part of a mitigation strategy to minimise impact to some users has resulted in several papers, one of which is covered by this reporting period).

A summary of the outcomes covering the 2020-21 reporting period are presented here, grouped around challenge themes:

Energy research: *Research areas include photovoltaics, battery materials and catalysis but also storage of radioactive materials relevant to the nuclear industry. Performing operando experiments enabled by the development of bespoke sample environments continues to offer new insights into the relationship between structure and functional properties.*

In situ extended X-ray absorption fine structure (EXAFS) spectroscopy was measured at the Cl and S K-edges on XMaS as part of a study to explore MeOH solvent mixtures in the preparation of Pd/TiO_2 catalysts (ChemCatChem 13, 1–14 (2021)). This experiment, in combination with data obtained on B18 at DLS, was able to show that the formation of acid catalysed by-products could be reduced whilst maintaining the Pd catalytic ability, thereby minimizing process steps as well as optimising catalyst selectivity. Both of these issues are important objectives for delivering sustainable and green energy solutions.

Functional materials *underpin a range of emerging technologies and important insight into structural properties can be gleaned from studies of these materials using combinations of XAS/WAXS/XRR and diffraction in sample environments optimised for operando experiments.*

Exploiting the flexibility of the diffractometer, reflectometry and grazing incidence small angle X-ray scattering (GI-SAXS) were used *in situ* to explore the thermal stability of nano-pillars of Cu/W multilayers deposited on a Si substrate using ion beam deposition (ACS Appl. Mater. Interfaces, 13, 5, 6795–6804 (2021)). The combination of grazing incidence with energy dispersive X-ray (EDX) spectroscopy allowed the observation of diffusion processes within buried layers and demonstrated that the in-plane compressive residual stress and defect population results in low thermal stability of the multilayers. The experimental metrology shows how novel combinations of advanced experimental methods can be employed to obtain insights into the temperature-dependent stress and diffusion mechanisms within buried layers of nanostructured materials.

X-ray reflectometry studies on XMaS also underpinned a detailed study of the structure of hybrid nanoparticle-lipid multilayers (Biochimica et Biophysica Acta (BBA) - General Subjects 1865(4) 129542 (2021)). Here poly(amidoamine) (PAMAM) dendrimers with either a hydrophilic amine or a hydrophobic C_{12} chain surface termination on the 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) multilayers were studied for the first time. The experiment provided further understanding on drug delivery, as such lipid multilayers provide a model system for studying dendrimer-membrane interactions in which the dendrimers cause membrane thinning and structural disorder which depend on dendrimer size, surface chemistry, and dosage.

XMaS beamtime (performed on beamline 4-ID-D at the APS, as arranged with the APS during the XMaS shutdown) exploited resonant magnetic scattering and circular dichroism to explore the correlation between induced magnetisation and spin transport at the interface between a heavy metal (Pt) and a ferromagnetic alloy separated by thin Au layers (Appl. Phys. Lett. 119, 152401 (2021)). The subject of much debate in the literature, the use of Au to modify the induced moment and elemental specificity allowed the authors to show that the induced moment is highly relevant in interfacial spin transport and related spintronic phenomena, in marked contrast to previous studies. Under the same collaborative framework with the APS, but this time on sector 6, AC electric field driven *operando* synchrotron X-ray diffraction studies were performed on patterned thin films of $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) (Appl. Phys. Lett. 119, 202903 (2021)). The study focused on the effect of substrate clamping by investigating 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 which had been released from its substrate and whose functional properties showed a recovered bulk-like response.

XMaS' capabilities, allowing high magnetic fields (4 T), low temperatures (sub 10 K) and high resolution diffraction to be deployed simultaneously enabled the field-induced modulated states in the ferromagnet PrPtAl to be explored (Phys. Rev. Lett. 126, 197203 (2021)). By applying the magnetic field along specific crystallographic directions, a single modulated magnetic fan state was found for the first time and explained by extending quantum order-by-disorder (QOBD) theory. A different study exploring UAu_2 exploited the facility's ability to use resonant scattering and polarisation analysis at the U M_4 edge to investigate a novel magnetic structure (PNAS 118,49, e2102687118 (2021)). An identical temperature dependence for both the charge density wave modulation and magnetic modulation shows that UAu_2 hosts a robust non-Fermi liquid behaviour within a magnetically ordered state, not previously observed.

Controlling corrosion with naturally occurring corrosion scales is, potentially, a more environmentally sustainable alternative to current approaches. *Operando* grazing incidence X-ray diffraction and electrochemical measurements were performed on a corrosion scale composed of $FeCO_3$ crystallites using a custom-made environmental cell (ACS Appl. Mater. Interfaces, 13, 58193 (2021)). By simultaneously performing grazing incidence XRD and electrochemical impedance measurements, it was possible to correlate directly the structure to the functionality of the material. The results show that many other studies underestimate the passivation effectiveness and that these naturally occurring $FeCO_3$ scales are, unfortunately, not a tenable solution for corrosion protection.

Beyond the challenge themes, and focused on researchers in the art conservation and heritage science fields, XMaS data feature heavily in chapter six of Spectroscopy, Diffraction and Tomography in Art and Heritage Science 2021. The chapter covers the basics of diffraction and draws examples and case studies from buried treasure, chemical mapping of parchments, enamelled metal, synthetic corrosion protocols, pigments, monitoring changes in real time, coating, geology, and ancient cosmetics.

In addition, new methodologies exploring the resolution limits in Bragg coherent diffraction imaging (BCDI) for small sample volumes at high scattering angles have been proposed by XMaS staff (J. Synchrotron Rad. 28, 538-549 (2021)). Although not possible on XMaS itself, the use of (B)CDI is growing as upgraded synchrotron sources have led to increased coherence in the X-ray beams that are produced. In this work, Compton scattering, which is generally neglected in diffraction experiments, is shown to introduce significant background when the scattering volume is small and for high energies/low-Z materials. Under such conditions, the Rayleigh (coherent) and Compton (incoherent) contributions at Bragg peaks become comparable with a deleterious impact on the achievable resolution in the reconstructed object as the incoherent scattering blurs the higher-order Fourier terms in the data.

XMaS science continued to be singled out for inclusion in the ESRF's publications during this reporting period with two articles in the current 2020 issue of the ESRF Highlights. In the section on "Complex systems and biomedical sciences", the work of C. Dressel *et al.* on "*Helical Networks of π-Conjugated Rods – A Robust Design Concept for Bicontinuous Cubic Liquid Crystalline Phases with Achiral* $Ia\bar{3}d$ *and Chiral* $I23$ *Lattice*" originally published in Adv. Funct. Mater. 2004353 (2020) was presented. This work describes a design concept of liquid crystalline phases with cubic symmetry in which helical networks of π-conjugated rod-like molecules form two ranges of achiral double network phases with a spontaneous mirror symmetry broken triple network phase between them. In "Energy Materials", research exploring "*Pd-*$LaFeO_3$ *Catalysts in Aqueous Ethanol: Pd Reduction, Leaching, and Structural Transformations in the Presence of a Base*" authored by S. Checchi *et al.*, (ACS Catal. 10, 3933-3944 (2020)) showcased the capabilities of the beamline in which X-ray absorption spectroscopy and *in situ* X-ray diffraction were used to investigate the reaction mechanism of Fe-doped CeO_2 as a possible new electrode material for lithium-ion batteries. As well as XMaS studies appearing in the Highlights publication, collaborative work using nano-beam diffraction on ID01 and XMaS staff expertise was described in an ESRF Spotlight on Science on understanding heat-harvesting devices exploiting magnetism which had originally been published by P. Evans *et al.* in Sci. Adv. 6, 40 (2020).

The work of Prof. W. Briscoe's group in Bristol, in partnership with Procter and Gamble, on surfactants was also a highlight in the ESRF public outreach. This study, which focuses on the physical phenomenon known as stick-slip friction, results in a squeaky noise while washing the dishes. In Japan, this noise is known as 'kyu-kyu' and appears when there is physical contact of the human fingertip sliding across a wet lubricated surface (or dish). There is an accompanying video on YouTube.

The 2020 XMaS Newsletter was replaced by the XMaS Newsflash that described the significant upgrades made to the beamline during the long shutdown and announced the reopening of the facility for users. This was circulated in March 2021. The 2021 XMaS Newsletter is nearing completion and delivery is expected for release during the spring 2022. It will be detailed in the next annual report.

New Methodologies

Over the reporting period, the beam delivery system and diffractometer commissioning were finalised. All critical beamline components are now installed and available. These include:

- in-vacuum ion chambers (Dec. 2020),
- new Harmonic Rejection Mirrors (Mar. 2021),
- new GISAXS rail (Apr. 2021),
- new Lambda 750k CdTe detector (Dec. 2020),
- new Pilatus3 S 1M detector (Apr. 2021),
- in-vacuum Phase Plates (Dec. 2020).

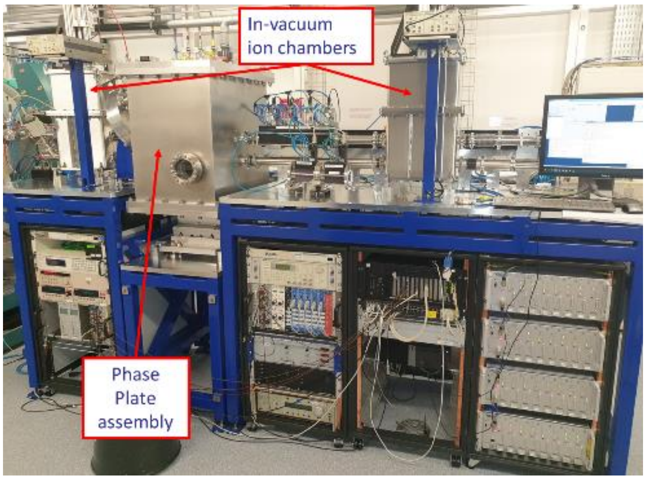

Figure 2: The beam delivery system showing the installed ion chambers and in vacuum polarisation assembly. The two delivery pathways are also visible, with the focused monochromatic beam path the upper and the unfocused beam the lower pipe that run horizontally across the image.

The beam delivery system (figures 1 and 2) is now fully completed and operational with two beam-paths (for focused and unfocused monochromatic beams). A calibration wheel containing elemental foils as well as two in vacuum ion chambers allow rapid spectroscopy studies to be performed across the entire energy range (with the high energy cut-off significantly extended from 15 to about 40 keV as part of the upgrade programme). The automatic gas handling and transfer system is delayed as the gas delivery system needs to be rehoused due to the new KB mirror project. However, the ion chambers can be individually dosed prior to experiments.

The phase plate assembly, now fully operational, allows for circular polarisation from 3 to 15 keV. The flipper mechanism for 50 Hz helicity switching is yet to be fully commissioned, and ongoing work is required to understand the observed spectral features of the phase retarders with the new beams.

Harmonic Mirrors

With the higher magnetic field source, there are significantly more harmonics in the monochromated beam than prior to the upgrade. The original harmonic mirror vessel needed redesign to allow the unfocused beam path clearance and we used the opportunity to upgrade the harmonic mirrors themselves. Higher tolerance Si mirrors, each 60 mm wide, have been purchased with three coatings and fitted on new mirror mounts with upgraded actuators. The new system allows an increased mirror angle of up to 8 mrad on the focused beam and the three stripes ensures no absorption edges interfere with the beam flux and caters for the full operational energy range of the beamline.

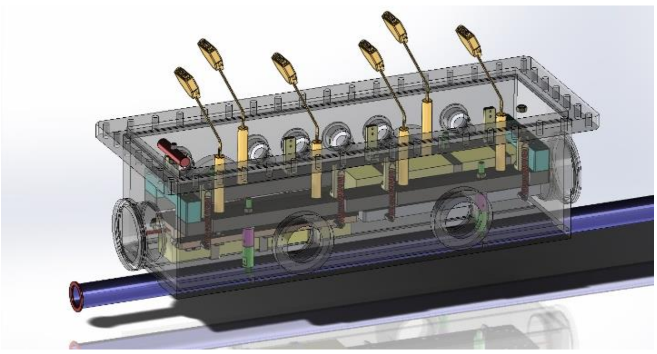

Figure 3: The CAD drawing of the new Harmonic Mirrors showing the unfocused beam pipe running below the harmonic mirror vessel itself.

Detectors

The suite of new 2D detectors, including the Lambda 750k and the Pilatus3 S 1M, have all been fully integrated into the counting and control systems. These allow for rapid scanning of reciprocal space volumes and allow crystallographic changes and phase transitions to be mapped as a function of external parameters including temperature, magnetic and electric fields, stress and strain. This added capability has significantly increased the data volumes recorded in experimental sessions, but the local network and computing resources are responding well to the extra demands. Over the coming year, new software and routines will be deployed locally to allow users to make decisions on the full data sets recorded during experiments.

Remote Access

During this reporting period, remote user access was granted via the systems deployed by the ESRF. The control computers could be accessed through remote.esrf.fr (Guacamole) and data transfer was routed through the Globus network. The users worked with their local contact, communicating through online platforms. Remote access is increasingly being deployed at synchrotron facilities but due to the complexity of the experiments that most users perform on the XMaS beamline, such access is not sustainable in the long term. Remote operations put more strain on already limited staff resources, with staff efforts over the second part of the reporting period devoted to delivering user results with less time available for ongoing developments and commissioning.

Technical Upgrades

Combined SAXS/WAXS Configuration

The SAXS rail has been re-machined to allow the new Pilatus3 S 1M detector to be remotely positioned with sample to detector distances ranging from 0.4 to 2.6 m (figure 4 top). At the maximum extent, the new SAXS capabilities facilitate studies down to 0.013 Å^{-1} which corresponds to real space length scales of some 50 nm, with the exact limit being energy dependent. Simultaneous wide angle scattering (WAXS) can be made in high resolution using a point detector, or the Pilatus3 300k or Lambda 750k 2D detectors.

The configuration shown in figure 4 allows combined SAXS/WAXS. Grazing incidence SAXS/WAXS is possible with a suitable sample holder mounted on the versatile theta axis of the diffractometer, which can also house various sample environments to facilitate *in situ* and *operando* studies. Including the XMaS spectroscopy chamber extends the capabilities even further to allow simultaneous SAXS/WAXS and XAFS studies. At energies approaching 30 keV, the SAXS configuration can be used for pair distribution function (PDF) studies by placing the Pilatus3 S 1M detector close to the sample position.

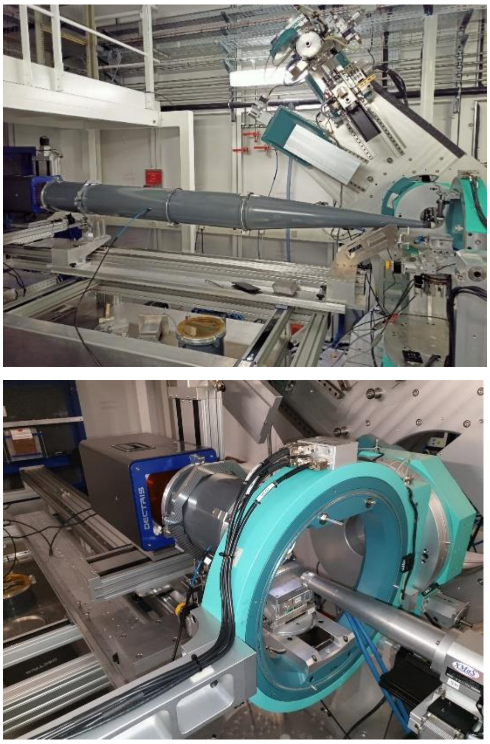

Figure 4: The double 2θ arm and detector configured for combined SAXS/WAXS studies. Top optimised for combined SAXS and WAXS studies and bottom for grazing incidence WAXS studies.

The X-ray energy can be easily changed across the full range, this allows the SAXS/WAXS/XAS and PDF studies to be performed under identical sample conditions. This is a unique capability on XMaS for the UK community to exploit.

New Stress-Strain Sample Environment for Ferroelectrics

In partnership with Electrosciences Ltd. and under the umbrella of the EU-EMPIR programme ADVENT, the new stress-strain sample environment reported on in the last report has been further modified over the past year. As well as being able to apply uniform stress (200 MPa) to samples whilst simultaneously measuring strain and polarisation, additional optical transmission/inspection functionality has been incorporated in the newest version. The cell now enables studies of ferroic samples with the added interrogation of the optical properties of the sample whilst driving the crystal with field, temperature or stress, for example. The new capabilities have opened up studies of novel piezoelectric materials (published in January 2022) and the cell is also currently being developed for commercialisation under an EPSRC Impact Acceleration Award.

KB Microfocus System

A tender to build and construct a KB mirror assembly was awarded to IDT in the spring of 2021. After detailed considerations and ray tracing we have decided to place the system on the unfocused beam path. The current design of the system is shown in figure 5 where the KB mirror can be easily positioned into the beam but crucially, allows normal operations using the focused beam to be unimpeded.

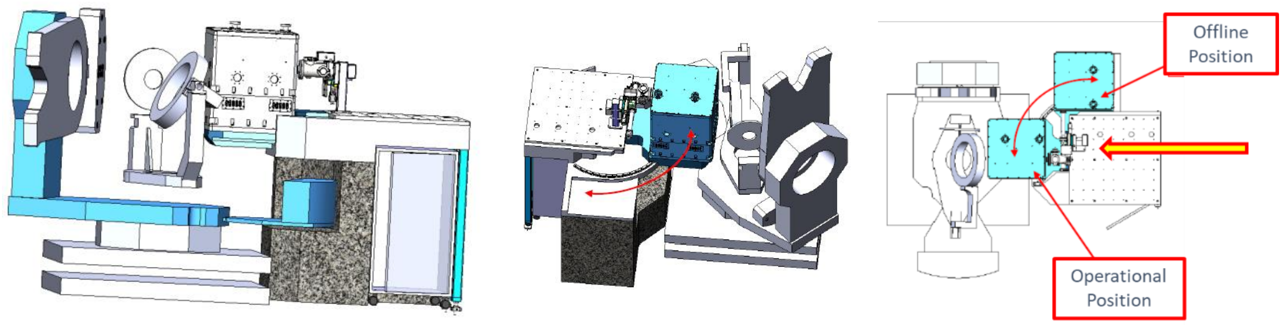

Figure 5: The IDT designed KB mirror system envisioned for the beamline. To maximise flexibility, the system will be retractable and can be positioned to the side of the main axis when the focused beam is in use.

At the time of writing, we are approaching the final design review of the proposed system, but it is envisioned that a beam of less than 10 x 10 μm^2 will be possible with a flux of some 10^9 photons/sec. The mirror mount is designed to enable the beam size to be controlled remotely from a maximum 10 x 1 mm^2 down to the smallest possible size. The new added capability will allow users to spatially map out the structural properties of a material sample whilst it is undergoing a functional process; charging/discharging of a battery material or operation of a catalyst material would be typical examples. Care has been made in the final design to ensure that we minimise the constraints to other operational modes that are employed on XMaS but also retain a degree of flexibility. The system is planned to be available for users from the April 2023 proposal call.

Communication Channels

Communications beyond the direct XMaS user community is through our website and Twitter. The facility regularly provides updates on current users of the facility and their experients along with information on beamline upgrades, application deadlines and other content of general interest through its twitter account @XMaSBeam, which now has 748 followers.

3) 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 is a list of the publications associated with the XMaS NRF published in peer reviewed literature over the past 3 years. Comparison with historical metrics is provided in section 10 (KPIs). The 2021 ESRF highlight publications from XMaS are marked (*).

2021

(*) Al Kindi M, Joshi G, Cooper K, Andrews J, Arellanes-Lozada P, Leiva-Garcia R, Engelberg D, Bikondoa O, Lindsay R.
"Substrate Protection with Corrosion Scales: Can We Depend on Iron Carbonate?".
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DOI: 10.1021/acsami.1c18226

Bikondoa O, Carbone, D,
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J. Synchrotron Rad. 28, 538-549 (2021).
DOI: 10.1107/S1600577521000722 Open Access

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"*Microscopic piezoelectric behaviour of clamped and membrane (001) PMN-30PT thin films*"
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(*) Brandt LR, Salvati E, Wermeille D, Papadaki C, Le Bourhis E, Korsunsky AM,
"Stress-Assisted Thermal Diffusion Barrier Breakdown in Ion Beam Deposited Cu/W Nano-Multilayers on Si Substrate Observed by in Situ GISAXS and Transmission EDX".
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DOI: 10.1016/B978-0-12-818860-6.00011-8

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(*) O'Neill CD, Abdul-Jabbar G, Wermeille D, Bourges P, Krüger F, Huxley AD.
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(*) Tierney GF, Alijani S, Panchal M, Decarolis D, Briceno de Gutierrez M, Mohammed KMH, Callison J, Gibson EK, Thompson PBJ, Collier P, Dimitratos N, Crina Corbos E, Pelletier F, Villa A, Wells PP.
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4) Impact

In 2021, impact activities have still been severely curtailed by the COVID-19 pandemic and the myriad of local travel and social distancing regulations. These continued to hamper travel and restrict face-to-face activities.

Training Courses and Workshops: The 2021 XMaS User Meeting planned to take place in Liverpool was cancelled due to COVID. It should have been the first gathering of the XMaS user community since the ESRF long shutdown. Moving the meeting online was a possibility, but there was general apathy amongst the user community for another online event. We are planning the next User Meeting to be an in-person event during the summer of 2022.

Activities to promote the facility beyond its core base: In 2020, a brief “NewsFlash” was produced and circulated to over 600 potential users, online through Twitter and also to other stakeholders prior to the Spring beamtime proposal call. The short document highlighted the delivered uplifts in capability, capacity and techniques that the rebuilt beamline can offer to users in normal operations. In addition, a more targeted mail shot to principal investigators in the hard condensed matter physics community also preceded the Autumn beamtime proposal call.

Figure 6: The cover of the XMaS 2021 NewsFlash circulated to users and interested parties.

Throughout the reporting period, updates about the XMaS upgrade have been posted regularly on twitter through @XMaSBeam. For example, the work conducted on XMaS led by Briscoe’s team (University of Bristol) in collaboration with Procter and Gamble received a lot of attention on social media when published on the ESRF YouTube channel.

Facility Staff Training and Career Development: Staff training has been through online courses at the ESRF and the universities. All staff had their annual Personal Development Review, which covers all aspects of training and career development.

Public Engagement: Due to COVID restrictions, it was not possible to host the XMaS Science Gala at the University of Warwick 2021, nor run the Scientist Experience. Summer internships during 2022 are planned for the successful winners of the 2020 competition. The 2022 edition of the Scientist Experience was launched at the end of November 2021 and received over 7,000 impressions on twitter on first announcement, including a retweet by the Deputy Ambassador of the British Embassy in Paris who visited the beamline a few weeks earlier.

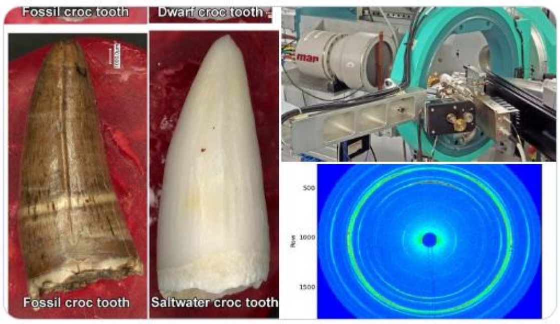


Figure 7: Societal impact example from XMaS.

Examples of Societal & Economic Impacts: Science highlights disseminated through social media, which enthused the general public included studies of crocodile teeth (figure 7) and the outreach work from the ADVENT project. An online interactive presentation is currently in development which highlights the work from that project.

5) Cost Recovery

UK access to synchrotron radiation through the ESRF and DIAMOND 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 supported it. XMaS is currently funded with the same user access model and there is, therefore, limited scope to generate direct cost recovery. 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. Unfortunately, over this reporting period the facility was still in "start-up" mode, which coupled with the ongoing COVID pandemic has meant that we yet to realise the efficiency uplifts expected.

Cost recovery covering some staff costs and instrument development have been secured through European funding in partnership with the University of Liverpool. The EMPIR funded ADVENT project has provided funds to cover some staffing costs and ensured that additional capabilities could be developed. The development of new sample environments and metrologies that occurred as part of this project as detailed in section 2, are now freely available for the wider XMaS user community. The funds have only contributed marginally to the actual running costs of the beamline.

Access and travel restrictions have further severely impacted attempts at cost recovery. During this reporting cycle we used a cancelled experiment to work with Finden Ltd., a UK SME specialising in advanced characterisation and expert analysis, to obtain industrially relevant data in preparation of an industrial case study which will be available in 2022.

Year	Running Costs	Grants	Other Academic	Students	Industry	Other*	%
2018							
2019		ADVENT (EU) £124489					
2020							
2021							

*give examples below

Future Plans and Issues

Some cost recovery is achieved from commercial licences, generating several 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.

Efforts continue to develop our industrial portfolio of capabilities and we aim to finalise it before any upgrade to DLS to ensure that critical business continuity for UK industries that require access to synchrotron studies can be maintained. We plan to reserve 2 days per 6-month operational cycle to develop these case studies as and when COVID protocols and backlogs allow.

6) Users

There has been no user access since 2018, 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. This necessarily impacted both the number and type of experiments that could be performed and placed a large burden on the facility staff. 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 has created a back-log of experiments that were approved by the review panel, but were subsequently delayed, and are now scheduled to take place in the first half of 2022.

The user statistics for the CRG access route time during 2021 are shown 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

Table 2: User statistics over the grant period. Here the "year" refers to the calendar year and not the reporting period.

The users in 2021 came from 15 UK and 3 international research groups with **43%** of user visits from new users. The breakdown on scientific area for the reporting period, as identified by the users themselves, is compared with the facility average in figure 8.

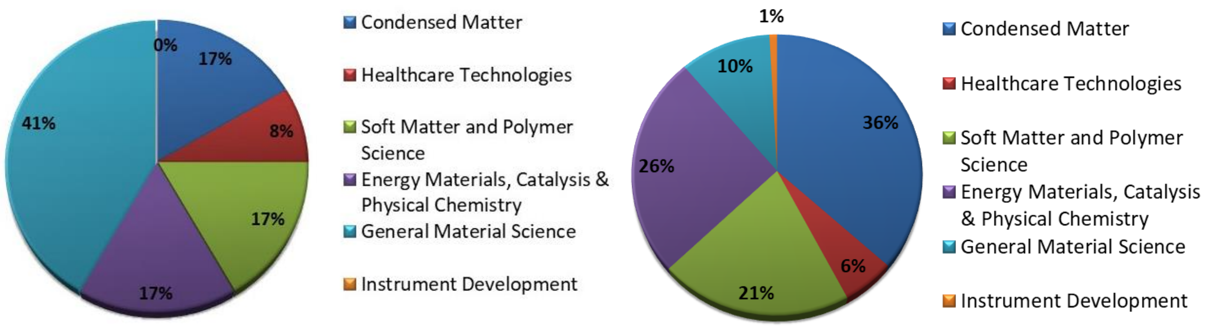


Figure 8: Research areas as reported by the users in their end of run survey. Data from this reporting period (left) compared with the facility average (since 2012).

Offline Facilities: Access to the offline facilities was also suspended for general users due to the travel restrictions. Over this reporting period, access has been reserved for studies to commission the stress-strain cell and measure ferroic samples as a function of temperature for the ADVENT project. The uptime of the facility (limited by available staff resource) has been ~80%, of which all available time was exploited.

Future Plans and Issues: 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 in the energy materials area, with XAS spectroscopy requiring shorter beamtime allocations. To facilitate this, and to grow the collaboration with DLS, we are creating a "BAG ACCESS" mechanism where groups submit samples to a community access round. Working in partnership with B18 at DLS, beamtime will be allocated to the most appropriate facility. This will ensure sample environments and beamline characteristics (energy, spot size, etc.) can be fully optimised for the community as well as ensure best practice is shared and common analysis and data reduction methodologies developed.

7) User Surveys/Satisfaction

Access to XMaS has only been possible since 27th January 2021, and then only for remote use. The ramp-up of user operations was complicated by the need to run in remote mode meaning complex experiments, which required dedicated user input, were not possible. Such remote operations put more strain on already limited staff resources, with efforts over the second part of the reporting period devoted to delivering user experiments. The users clearly appreciated these efforts with the maximum survey score reported along with free form text:

> "The beamline scientist was outstandingly dedicated, helpful, and knowledgeable, which ensured the success of the experiment. The organisation from the beamline was excellent. It is wonderful to have such outstanding colleagues at BM28."
>
> "The support from the beamline staff was excellent so that the process was as smooth as it could have been."
>
> "There were a few issues with beamline components, but the staff were great at resolving these quickly."
>
> "We are very grateful for how well things were run, including the help and support from the beamline staff."
>
> "Our local contact was very supportive and helpful, remaining cheerful throughout despite the mono failure that occurred following a thunderstorm. They were at the beamtime on the weekend and stayed till late on several occasions to help us run overnight scans. They were very knowledgeable with the handling and mounting of the samples and came up with an ingenious method to mount many samples at once, ensuring that we get the most out of our allocated beamtime shifts."

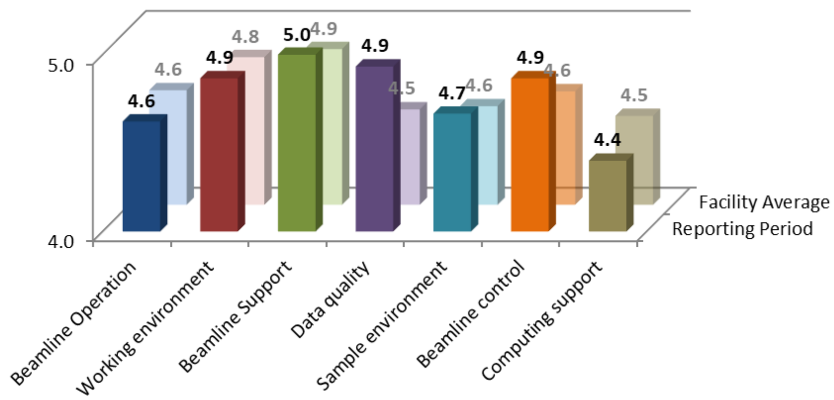


Figure 9: User feedback on facility operations over the reporting period. The current cycle is compared with the historical average from data obtained since 2012.

All users are required to submit an end of run survey from which the user satisfaction survey results are derived. We have 100% response and report here in figure 9 the average scores from the UK CRG beamtime award, compared to the total averages derived since 2012.

As seen in figure 9, the user satisfaction scores are in excellent agreement with the historical average of the facility.

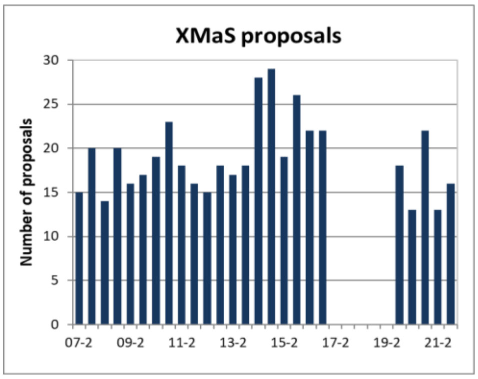
Particularly noteworthy is the jump in the "data quality" which we interpret as evidence of the improved beam quality derived from the new source and enhanced delivery. However, "computing support" is still the lowest score, as it has been historically. With the increased use of 2D detectors and subsequent increase in data set size, we are aware that data handling support is a key area for us to develop in order to enable users to obtain the maximum output from the experiments. HKL mapping in 3D was one area that users were keen to be developed and codes have now been written to project data into the relevant reciprocal space zones. This will help users process and visualise data more rapidly, especially as we return to onsite user engagement. To further provide resource, two PDRAs have been appointed and will work with users from the spring of 2022 to provide closer and more tailored user support in data management, reduction, and processing.

In terms of improving the feedback mechanism, we are working with the project management committee (PMC) to refresh these survey questions to allow more targeted and specific feedback in the future.

8) 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 and assessed on scientific merit only. Beamtime is scheduled in six-month allocations and where possible, all electron bunch modes of the ESRF lattice are used. However, since the EBS upgrade there have been some problems with the beam flux and stability in the lower bunch settings. The lower-than-expected electron ring current delivered by the ESRF machine in these modes means that they cannot be scheduled for user experiments, thereby limiting the number of available shifts that the facility could deliver.

It is not possible to provide a chart showing demand and capacity on a monthly basis, but figure 10 shows the number of proposals received through the two separate access routes as a function of time. We note that despite the added uncertainty on how the ESRF would be operating, a good number of proposals were submitted through both the XMaS and ESRF routes in 2021. Although lower than before the dark period, the dip in proposal submissions is anecdotally similar to that at other central facility beamlines that perform complex experiments. There is still, however, a slight drop in demand and we attribute this to several factors (i) a backlog of *in situ* and *operando* experiments that require on-site users, (ii) knowledge that complex experiments that require on-site user input were unlikely to be possible and (iii) the continuing uncertainties in travel and access to the facility due to COVID.



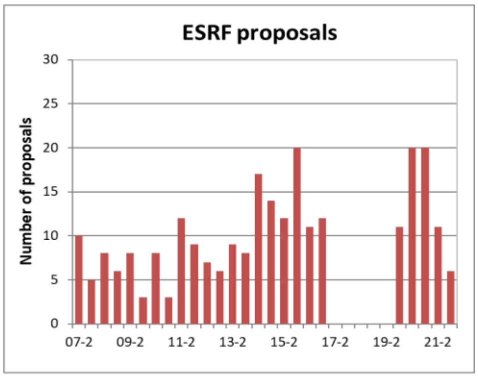


Figure 10: The number of proposals submitted to the XMaS NRF and reviewed by the independent review committees as a function of time. UK based proposals (left) and international applications through the ESRF (right).

Oversubscription rates can be calculated from the ratio of the total number of requested shifts to the total number of shifts delivered. Historically, the rate is ~2.4 for applications through the XMaS route. The international oversubscription rate was steadily increasing and now approaches 4. It is difficult to accurately determine the oversubscription rate during this reporting period as only a subset of proposed experiments could be accommodated. As a rough estimate, the oversubscription was approximately 1.5 for the CRG time although the statistics are rather unreliable. We expect a return to oversubscription rates of between 2 and 3 when COVID restrictions ease, and on-site *in situ* and *operando* experiments become feasible. Direct engagement with the current user community is planned through the upcoming User Meeting as well attracting new users through face-to-face in person interactions at Diamond, Catalysis Hub, and the Faraday Institution meetings in which our new PDRA appointments will play an important role

Remote access to the “offline” facilities was not possible in this reporting cycle as staff resource was diverted to support remote access on the synchrotron beamline. However, the offline X-ray facility was used continuously as part of the ADVENT project.

9) Risks

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

1. Operations
2. Financial
3. Ongoing Projects
4. COVID

The Risk Register is reviewed, circulated, and discussed at each project management meeting. 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 2020/21. 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 on a monthly basis 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 a clearer strategy regarding Brexit and orders. The project management committee uses the risk register to more effectively stress-test current operations as well as ensure short, medium, and long-term risks are appropriately managed and mitigated. In addition, the risk register has been used to review the submitted proposals to the beamline, in order to identify particular science communities whose usage has declined over the past few years. As an example, this information identified Hard Condensed Matter Physics as an area in which beamtime applications had declined and we therefore made efforts to reach out to this community in 2021 to make them aware of the diverse set of experiments that can be performed at XMaS which relate to this science area.

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

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

From December 2018 to August 2020, the ESRF upgraded its magnetic lattice (EBS upgrade programme) and was shut down with no user operations possible. We exploited this “dark time” to undertake an extensive capital upgrade and rebuild of the XMaS beamline ready for a planned full user operational cycle in late 2020. COVID-19 however had a direct impact on the upgrade timelines with supply chain delays and constrained access to the ESRF site for both staff and contractors. Local lockdowns and COVID protocols through 2021 required projects to be completed sequentially with fewer resources deployed at any given time. XMaS was only able to accept remote users from January 2021. As with other central facilities, users could not travel to the ESRF for the duration of the reporting period and only experiments that could be done remotely and handled by the beamline team have been scheduled. Last minute changes and cancellation of some experiments were inevitable as shipping, access to samples, as well as ongoing beamline project delays impacted the schedule. When this occurred, commissioning activities were brought forward to utilise the available synchrotron beam for facility development.

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 the following **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 full historical record of KPI and SLA data is maintained on our webpage and is updated quarterly in standard operating periods and reviewed every six months by the project management committee. Two service level agreements were unfortunately not met in this reporting period: the number of research outputs and the number of publicity activities delivered. Delivery of outreach and facility events was impacted as the limited staff resource was necessarily diverted to deliver remote user operations. In-person XMaS events are planned for summer 2022 as and when COVID restrictions ease.

Key Performance Indicators

A) **The number of Individual Researchers and University Research Groups visits**: The facility hosted 39 remote user "visits" from 13 UK and 3 international University groups over this reporting period. These statistics cover all access modes and are compared with the historical data in figure 11. The requirement for remote access, sample availability and continuing commissioning necessarily reduced the amount of time that could be devoted to user operations and the impact of these constraints are reflected in the data.

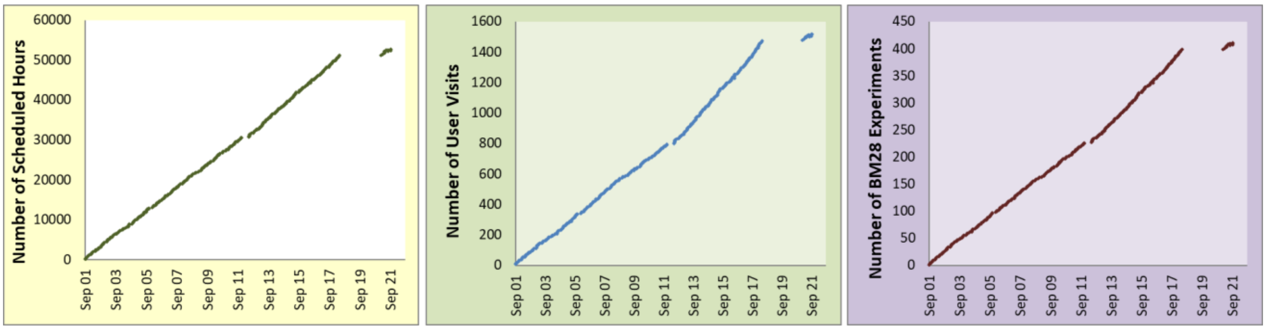


Figure 11: Historical performance metrics for XMaS including the number of scheduled hours (left), the number of user visits to the facility (centre) and the number of individual experiments performed on the beamline (right).

B) **Number of user complaints: XMaS has received zero (0) complaints over its lifetime of >20 years**.

C) **Uptime of the facility: 91.3%:** In this reporting period, the downtime losses were still predominately associated with ESRF storage ring failures (5.1%) with a further 3.7% associated with problems arising on the beamline. Both these numbers should reduce to pre-EBS levels as the upgrades "bed-in".

D) **The number of research outputs**: Over the reporting period there were a total of 11 published papers with the cumulative output exceeding 450 (figure 12). The publication rate has understandably dipped in this reporting period. We note that there is typically a year or two delay between beamtime and a resulting publication. The dark period (figure 10) will therefore be evident in the output statistics through 2021-2023. This explains the missed SLA, but we expect that research outputs will pick-up again towards the end of 2022 as newly recorded data are prepared for publication. Output in high impact journals continues to grow and is now over 45% in journals with an impact factor > 7 but also including APL and Scientific reports. Approximately 70% of the papers are co-authored with XMaS staff. There are also many conference and seminar presentations, which are more difficult to capture, and not included in our SLA reporting.

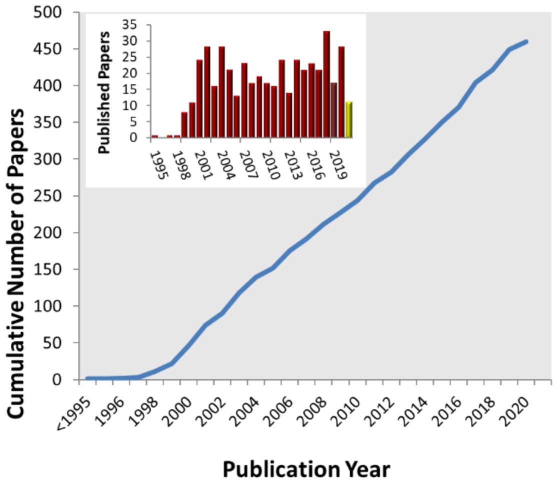


Figure 12: Publications from XMaS in peer reviewed journals.

Service Level Agreements

COVID-19 has impacted the SLAs. However, we are the first beamline at the ESRF to have an equality, diversity, and inclusivity (EDI) statement and regular updates on twitter and the website have kept the user community up to date with the changes on the beamline and the evolving needs and requirements for beamtime and access to the ESRF. The situation remains constantly under review and is subject to any changes in French law or directives from the ESRF safety office.

11) Links

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 with Prof. Andy Dent (Deputy Science Director at DLS) reviewing the facility as part of the latest quinquennial review conducted by the ESRF. A DLS science group leader (Prof. Chris Nicklin) sits on our Project Management Committee (PMC), along with Prof. Sean Langridge, the head of the *ISIS* Diffraction and Materials Division. XMaS directors likewise sit on, and have chaired, DLS review panels and Prof. Tom Hase is currently chair of the DLS Science Advisory Committee. 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 any 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. 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) and Faraday Institution 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 developing the understanding of material function in the working environment that drives advances in catalysis and battery technologies. Prof. Andy Beale (UK Catalysis Hub) sits on our PMC and is also helping to develop our industrial interactions. We are also engaged with the Royce Institute which is now advertising our proposal round calls to its science community. PDRA appointments to XMaS will focus on providing new data reduction and analysis pathways and by working with multiple groups they will enable the sharing of best practice and help to facilitate and grow the non-expert user community.

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.

12) Improvements and Future Plans

A newer and brighter XMaS is back in operation after what has amounted to a comprehensive rebuild of the entire beamline. This rebuild was necessary to take full advantage of the EBS upgrade, but also to update many of the beamline components which dated from the original construction phase (1994-97). The beamline now delivers a focal spot which is some 25 times smaller but with the same photon flux. XMaS can do everything it could before the upgrade, but in an improved manner with the exception of the white beam mode, which should become available again in a few years. The energy range has been extended with X-ray energies up to 40 keV now being reachable: opening up new and exciting experimental possibilities for materials research.

Optimisation in Data Reduction and Visualisation

From the user feedback and recognising the increasing trend in the type of user attending beamtime, the development of suitable software for data reduction and "on the fly" analysis is becoming increasingly important. To date we have been limited in the amount of staff resource we have been able to direct to these projects. The appointment of two post-doctoral staff in the areas of spectroscopy and small angle scattering will provide the resource to tackle this. As well as bringing new scientific expertise in both soft matter and geochemistry, the researchers will work with the users to develop data reduction and modelling routines. They will reach out to other facilities and beamlines to bring the current state-of-the-art software ideas to augment the XMaS suite of tools. By acting as a single point of contact for many users, they will be able to facilitate the sharing of best practice and, in the short term, identify areas for improvement. By the end of 2022, we hope to have a new section of the website developed and routinely accessed by users. The priority will be in the areas of soft matter and spectroscopy.

Facility Access

As well as the new BAG access route described in section 6, through 2022 we will develop industrially relevant case studies to attract new industry users to, either buy beamtime through the ESRF, or work with UK academics on relevant projects. As travel restrictions are now slowly being lifted, we will make an increased effort to publicise the capabilities of the upgraded beamline to potential new users. The new PDRAs will also attend UK conferences and give seminars at UK Universities to raise the profile of the facility and engage with young researchers and new academics to expand and grow the XMaS user community.

Facility Management

A new customer relationship management database is in development for deployment through 2022/23. This will 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 beamtime and publications ensuring better compliance with fair data practices.

Equality, Diversity and Inclusion:

As stated in section 10, XMaS is the first beamline at the ESRF to have an Equality, Diversity and Inclusion statement. "The XMaS facility will implement transparent policies and procedures to guarantee that access is based on scientific excellence only. 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. If you have any questions about accessing the facility at any stage of the application or experimental processes, please do not hesitate to get in touch." 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

Beam Delivery Optimisation

With the versatile diffractometer, the success of the facility is dependent upon the quality of the beam delivered to the sample. The quality of the beam has a complex interdependency on the components used to define and shape the beam, together with external factors such as temperature stability and vibrations.

Vibrations: With the small, higher brightness beam now delivered on XMaS, vibration of any optical component leads to aberrations in the beam spot, especially at high energies. A systematic study of vibrations is being completed with the aim to reduce or remove sources of vibrations and deliver a more stable beam. Our current efforts are focused on components in the optics hutch but will move to those pieces of equipment housed in the main experimental hutch during the summer 2022 shutdown.

White Beam and Electron Orbit Monitor: The beam quality and stability is ultimately defined by uncertainties in knowledge of the incident white beam into the beamline delivery system. Thus, the XMaS team is in the process of installing a new white beam orbit monitor to precisely determine the position and profile of the beam incident on the monochromator. This piece of equipment will facilitate the alignment of the two main optical elements of the beamline, the monochromator and the toroidal focusing mirrors, and make any diagnostics easier. Accurately locating the beam position with respect to the electron orbit in the storage ring is critical in defining the polarisation of the beam using the phase retarders further down-stream. Both a photodiode and a 2D beam viewer will be mounted on the chamber. A CAD drawing is reproduced in figure 13. Delays in fabrication and assembly occurred due to the COVID pandemic, and so it has not been available to date. Installation is foreseen during the ESRF summer shutdown in 2022.

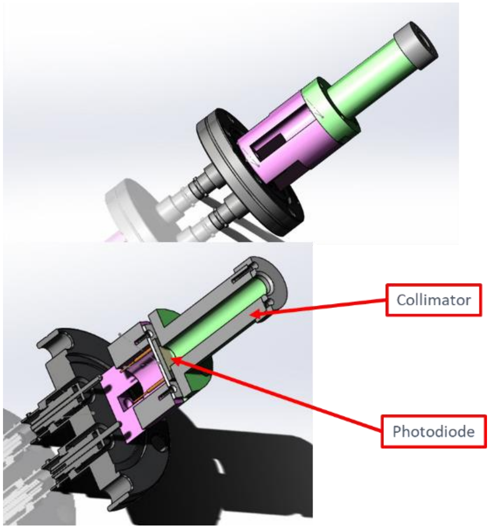


Figure 13: CAD drawing of the photodiode and collimator for the white beam orbit monitor.

Beam Position: Due to the brilliance of the new X-ray source and the quality of the new XMaS optics (cryogenically cooled monochromator with two Si (111) crystals and platinum and chromium coated bendable Si toroidal mirrors), the beam spot size is now 25 times smaller than before. It is thus critical to be able to bring the focused beam to the same position at the sample and to monitor its position, shape and/or intensity over the course of an experiment. This is even more critical during experiments requiring a change in energy. A redesign of the current beam position monitor is necessitated by the positioning of the KB mirror assembly. We are taking this opportunity to review additional beam diagnostics and to evaluate new electronics options in order to determine the most appropriate solutions.

Gas Delivery: The gas delivery system, to both samples and ion chambers, remains to be integrated within the envelope of the new KB mirror support. The system, for the remotely controlled dosing for automatic filling of the ion chambers and to deliver dedicated gases to the sample environment, has had to be moved due to the KB mirror mounting block. The bulk of the gas delivery infrastructure is in place, and with the installation of the KB mirror, the final components of the gas delivery system will be installed during the spring of 2023. Currently gas can be manually loaded, and operations are mainly unaffected but requiring more user interventions during experiments.

Detector Mounting and Slits: Even though the double 2θ arm of the diffractometer is fully functional, plans are underway to improve the switching between point (0D) and 2D detectors. A new versatile mounting for the 2D detectors is being developed (figure 14). By incorporating a slit, the background is reduced and when fully closed, the slit provides protection from the main beam inadvertently striking the detector and damaging it. This will mitigate the risks of any accidental damage to the detector components.

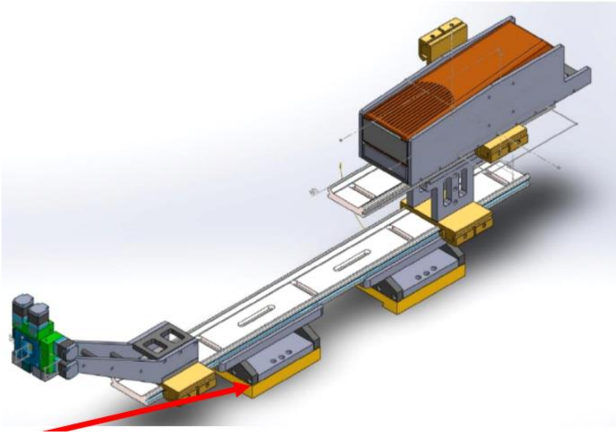


Figure 14: CAD drawing of the versatile detector mount design for the suite of XMaS 2D detectors.

Ge Multi-element Detector and Fast Counting Chains: For spectroscopy users, there is an identified need for a multi-element detector and faster counting electronics at high energy. Fast counting chains have been ordered and will be integrated into the acquisition electronics during the spring of 2022. The XMaS team has evaluated several germanium detectors, and a workshop will be held to canvas user's thoughts in the summer of 2022. We will work closely with the Diamond spectroscopy village to ensure knowledge transfer and to leverage expertise and support. The new spectroscopy capability is expected to be operational in 2023.

13) The XMaS Website

The NRF's website is www.xmas.ac.uk. The webpage is currently being refreshed and restructured to reflect the changes on the beamline and the new capabilities and will include a new section with clearer signposting dedicated to industrial users and access exploiting the industrial case studies once they are complete.

The host server at the University of Warwick is providing web analytics. The views over the reporting period are presented in figure 15. Excluding search engines, the website receives on average 67 page views per day.

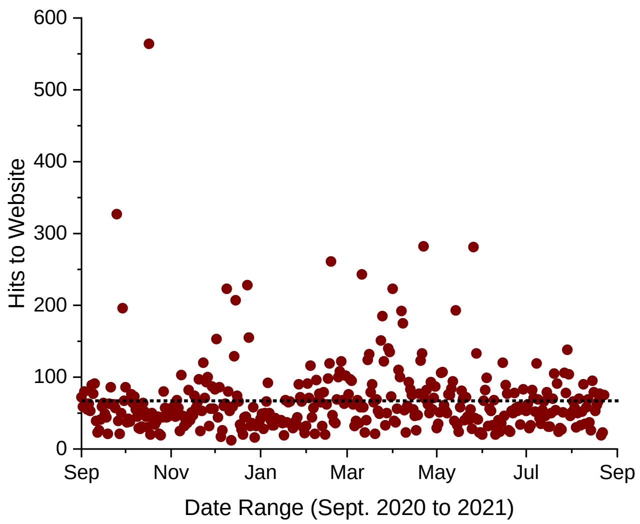


Figure 15: Distinct website views per day over the reporting period. The dotted line indicates the average of 67 page views per day.

14) Case Studies

1. Looking for the perfect squeak

The work of Prof. W. Briscoe's group in Bristol, in partnership with Procter and Gamble, on surfactants was featured in the ESRF public outreach. This study, which focuses on the physical phenomenon known as stick-slip friction, results in a squeaky noise while washing the dishes. In Japan, this noise is known as 'kyu-kyu' and appears when there is physical contact of the human fingertip sliding across a wet lubricated surface (or dish). You can watch the accompanying video here.

2. Tackling the UK's Plutonium Stockpile Problem

In this study, led by Professor Neil Hyatt from the University of Sheffield Energy Institute and Department of Materials Science and Engineering, the team demonstrates how a glass ceramic material could immobilise contaminated plutonium residues, arising from early research and development activities. Using data taken at XMaS, an extremely bright X-ray microscope at the European Synchrotron Radiation Facility in France, the Sheffield team developed an atomic scale model to understand how chlorine was bonded within the glass. They were then able to determine the solubility threshold for chlorine in the silicate glass material and show that it exceeded the worst-case expectation for the treatment of plutonium residues. The important impact of this work is to show that these plutonium residues could be immobilised within the glass ceramic material, without needing any prior treatment to remove the chlorine contamination. You can read the article here.

3. The Power of X-rays in Materials Science

We have been working with Futurum to prepare an educational resource/article. The aim of Futurum is to inspire young people aged 14-19 to pursue careers in STEM. We have worked with them to present an overview of the facility and how it is used to explore materials challenges through a collection of science highlights from our users. As well as making the work of the facility accessible, it also includes school-based activities that teachers can use to plan lessons focusing on materials science and the X-ray techniques used to study them. The article will be circulated globally through social media and is an open access resource that will target teachers and school students.