Mid-Range Facility Annual Reporting Template

1. Background:

EPSRC Mid-range Facilities are research facilities that provide resources to the Engineering and Physical Sciences research community on a scale where there is limited availability in the UK for reasons such as:

- The relative cost of the equipment;
- Dedicated kit in every University is not needed;
- Particular expertise is needed to operate the kit or interpret the results;
- Progress is enhanced by sharing information or software.

The EPSRC Mid-range facilities are mainly supported through 5 year contracts and underpin research across the EPS landscape.

In 2014 EPSRC developed a new strategy for renewing and refreshing the Mid-range Facilities portfolio. A regular process for the submission and assessment of Mid-range Facility Statements of Need has been put in place which provides research communities with the opportunity to suggest new Mid-range Facilities. Statements of Need for newly proposed facilities are then assessed and tensioned against the Statements of Need submitted by existing facilities whose contracts are coming to an end. The next Statement of Need call will be released in spring 2017.

2. Annual Reporting Process

During the 5 year contract period for each facility, EPSRC wishes to support the facilities in providing an optimal service to their users. To assist with this EPSRC has an annual reporting process for the Mid-range Facilities where the performances of the existing Mid-range facilities are assessed by an experienced panel which includes representatives from the EPSRC Capital Equipment Strategic Advisory Team:

As part of the assessment process this annual reporting template has been provided and this year must be filled in by **all** Mid-range Facilities that have an ongoing contractual arrangement with EPSRC. The relevant EPSRC contract managers will also be invited to provide a short summary of their interactions and experience with the facility.

After the panel meeting, the assessment of the panel will be fed back to the facilities to enable them, together with their steering committee and EPSRC contact, to ensure the best possible service is provided to the user community.

This year the annual reports will also provide input into a report that EPSRC is currently commissioning on the economic impact of EPSRC supported equipment and an analysis of the broader impacts and benefits of the Mid-range Facilities.

Timeline 2016:

- Reporting Period for this Annual Report: **1st October 2015 through to 30th September 2016**
- Annual Reporting Template Released: **29th July 2016**
- Deadline for Annual Reports**: 31st October 2016**
- Assessment by Panel**: December 2016**
- Feedback to Facilities: **January 2017**

Annual Report for EPSRC Mid-Range Facilities

Facility: XMAS Beamline at the ESRF

Address: XMaS (BM28) ESRF - The European Synchrotron, CS 40220, 38043 Grenoble Cedex 9 France

Directors: Prof. Chris Lucas (University of Liverpool) and Dr. Tom Hase (University of Warwick)

Facility Manager:

Description of the Facility (max. 1/2 page)
The XMaS mid-range facility is a synchrotron x-ray beamline embedded in the heart of the European Photon and Neutron (EPN) Science Campus in Grenoble, France and is managed by the Universities of Liverpool and Warwick. The beamline is part of the European Synchrotron Radiation Facility (ESRF) which forms part of the EPN along with the other European institutes including the European Molecular Biology Laboratory (EMBL) and the Institute Laué-Langevin (ILL) neutron source. The original beamline was conceived primarily as a tool to study magnetic materials, hence the acronym **X**-ray **Ma**gnetic **S**cattering (XMaS). The beamline has been supporting users since 1997 but has a far broader remit than magnetic scattering and supports active research groups in over 49 UK universities (representing over 400 independent researchers) and covers research in materials science, physics, chemistry, soft condensed matter as well as biomaterials and healthcare. The facility is an enabling tool serving the materials science community (including academic researchers, national research laboratories and industry) – hence its rebirth as the UK's **X**-ray **Ma**terial **S**cience beamline at the ESRF. It plays a major role in underpinning interdisciplinary projects and contributes directly to societal challenges such as energy storage and recovery, the digital economy and advances in healthcare technologies as well as contributing to the UK research infrastructure. The objectives of the facility are to provide access to the UK materials science community to a state-of-the-art x-ray facility (machine and experimental equipment) and to provide training for early career scientists as well as postgraduate and undergraduate students in advanced scientific methodologies, all nestled within a vibrant international environment.

Contract Period and Costs
Contract Term: 5 Years Start Date: 18th September 2012 End Date: 18th September 2017 Total cost: £ 6,150,850 Total capital cost: £ 1,425,325 Spend on track? **YES**. The budget being reported at our upcoming project management meeting in November 2016 will show that we are 80% through the project with an expenditure level of 75% with several commitments outstanding at ~3% of the budget line. However, spending priorities may need to change to accommodate future upgrade plans and to take into account the uncertainty in the financial market surrounding Brexit which has resulted in a recent ~10% change in the €:£ exchange rate, increasing our exposure and risk to euro-based commitments (ESRF contract etc.).

Key Performance Indicators (KPIs) and Service Level (SLs) (max. 3 pages)

The following describes the activities on the facility covering the period 1st October 2015 through to 30th September 2016 [Quarters 13 through 16]. As per contract both KPIs and SLs are monitored quarterly and reviewed by our project management committee.

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

Service Level Agreements (SLs)

- 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.

To summarise, during the reporting period all KPIs and SLs have been exceeded. A list of current quarter KPIs as well as full historical data is maintained on our webpage (www.xmas.ac.uk) and is updated quarterly.

A) The number of Individual Researchers and University Research Groups visits.

There have been **114** individual researcher visits from a cumulative total of **52** UK and **11** International research groups in the reporting period and funded through the mid-range facility route. An additional **44** researcher visits from **6** UK and **15** international groups have accessed the facility through the ESRF public access route. These statistics are in line with user visits covering the lifetime of the mid-range facility (from 2012), in which we have hosted a total of **439** individual researcher visits from **149** UK research groups and **69** international research groups.

B) Uptime of the beamline in the previous 12 months

The uptime of the facility during the reporting period was only 83.5%. This is above our service level agreement, but significantly below our internal target of 95% (our average historical operating uptime). The increased downtime in this reporting period was due to independent and unforeseen events which had significant impact on our user program. In Q14 our new Ketek fluorescence detector was found to be defective mid-way through an experiment which then necessitated cancelling a further experiment at short notice. This meant that we could not reschedule an alternative experiment although we endeavoured to do so. We also had a failure of the He line to our Joule-Thomson cryostat. During the short Q16 operating period, the commissioning of the cryogenic monochromator experienced delays which resulted in the postponement of 1 week of beamtime into Q17. We also had a failure of the beam-shutter which impacted on the uptime in this quarter. Outside of these unfortunate instances our uptime has been 97% with dips in performance, a combination of facility instrumentation failures, user sample problems and external causes, such as failures in the synchrotron storage ring over which we have no control (Figure 2).

We have carefully reviewed the underpinning reasons behind the recent downtime. Our analysis revealed a fundamental design flaw in the Ketek detector as sold and we have worked closely with the manufacturer (who has admitted the fault). We have now received an updated model with a substantial discount on a second unit as compensation. Our beam-shutter has a mean time between failures (MTBF) of ~2-4 years. This was deemed too short at the start of the mid-range facility operating cycle and the units re-designed to have a MTBF of >10 years. The shutter that failed was the last of the old design and the newly designed unit is now installed with a further unit as a spare. Further commissioning of the monochromator has been postponed until a reduced user mode at the end of 2018 – this will ensure the maximum number of users can be accommodated through the remainder of the project.

C) Number of user complaints: XMaS has received zero (0) complaints in the last 12 months and for the lifetime of the facility.

D) The number of research outputs: There were 22 published papers in 2015 and as of 1st October 2016, currently 19 for 2016 (both exceeding our SL of 15). In addition, there are also a large number of conference and seminar presentations given by our staff and users which are more difficult to capture. Figure 1 shows the annual and cumulative output of peer reviewed papers from the facility. We rely on users informing us of publications and make every effort to capture this important metric, and have recently surveyed our users to ensure that this is as up-to-date as possible. Our publication record is comparable to, or even exceeds that, of similar beamlines at both the ESRF and DIAMOND. The research output of XMaS is rated highly by the ESRF management with highlights appearing often in their outputs. The director of research, Harald Reichert, states "*It is my pleasure to confirm that the UK CRG beamline BM28 (XMaS) contributes substantially, and on a competitive basis to the scientific output of the ESRF when compared to ESRF's public beamlines and to other CRGs doing similar work.*" Prof Andy Dent (Interim Physical Science Director at Diamond) states "*on similar beamlines at Diamond, which usually have 1 week long experiments, the typical publication rate is somewhere between 12 and 20 high quality publications. Often these experiments are complex projects which require more than one visit in order to merit a publication in a top journal.*"

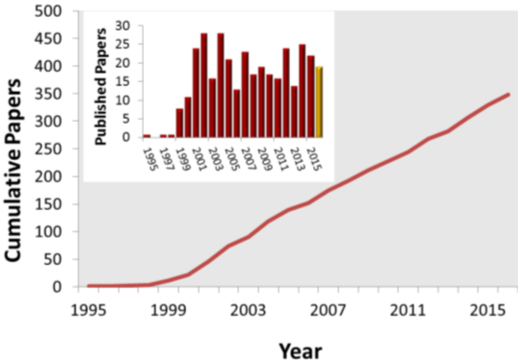

Figure 1: Cumulative outputs of peer reviewed publications. Inset, annual output as of 1st Oct. 2016.

Comparison with past performance: The KPIs reported above are in line with the previous reporting period as illustrated in Figure 2:

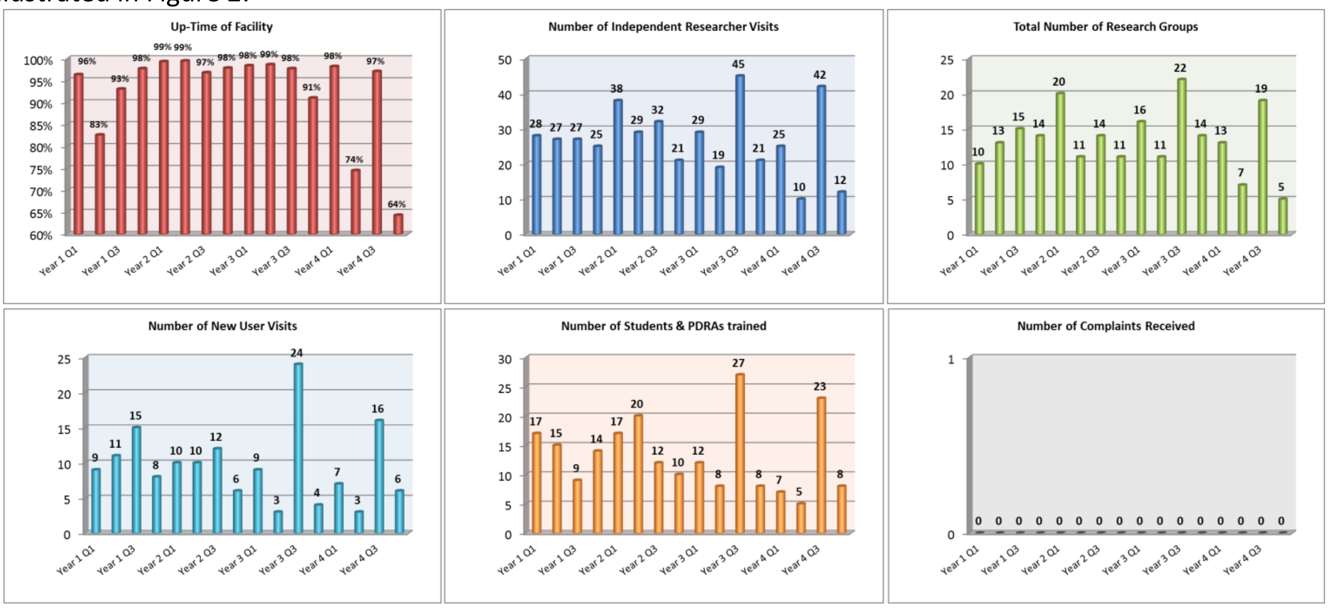

Figure 2: KPIs as a function of facility time displayed by operational quarter.

Access Requests

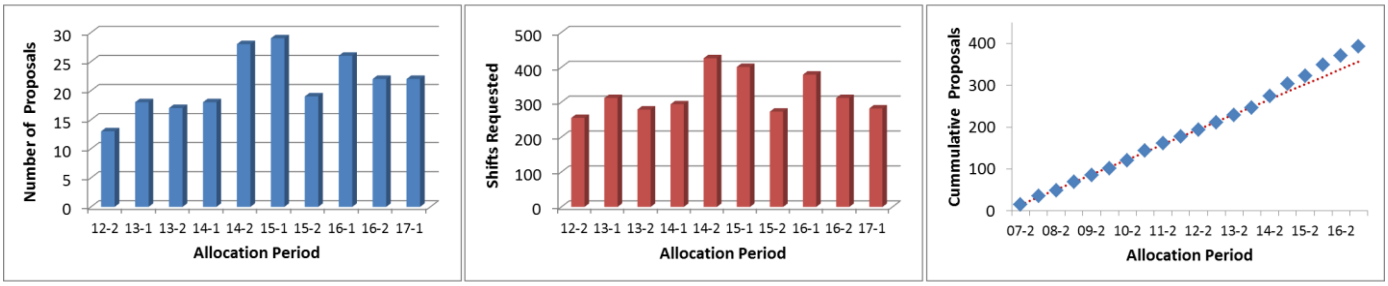

Figure 3: User access requested for the facility in terms of proposals (left) and shifts (centre). The cumulative number of proposals is shown on the right.

Although not a designated KPI of the facility, the demand for the facility can be gleaned from our application data which, for the lifetime of XMaS as a mid-range facility, is shown in Figure 3. In the last reporting period covering primarily allocation periods 16-1 and 16-2 we maintained a healthy request for beamtime which was on a par with the last few years, maintaining the increased proposal rate observed from ~2013. In proposal round 16-1 we again received over 25 proposals and the facility remains oversubscribed by a factor of ~2:1 when commissioning and development time is taken into account. Unlike other beamlines at the ESRF we schedule operations for *all* ESRF modes, significantly increasing the amount of synchrotron radiation beamtime available to our users. Over the same reporting period the beamline also received a total of **31** proposals (16-1 & 16-2) with a further 11 in 17-1 for the ~8 experiments allocated *per annum* via the ESRF (this allocation is part of the contract with the ESRF). This extremely high number corresponds to an oversubscription rate of ~4:1, with the quality of science being ranked very highly at the ESRF peer review panels and showing the international esteem in which the facility is held.

Historical metrics

As a mid-range facility, XMaS has successfully increased both the number of users and experiments that we have been able to accommodate (Figure 4). This has been due to increasing use of 9 shift experiments and efficiency gains in terms of configuring the beamline and sample environments.

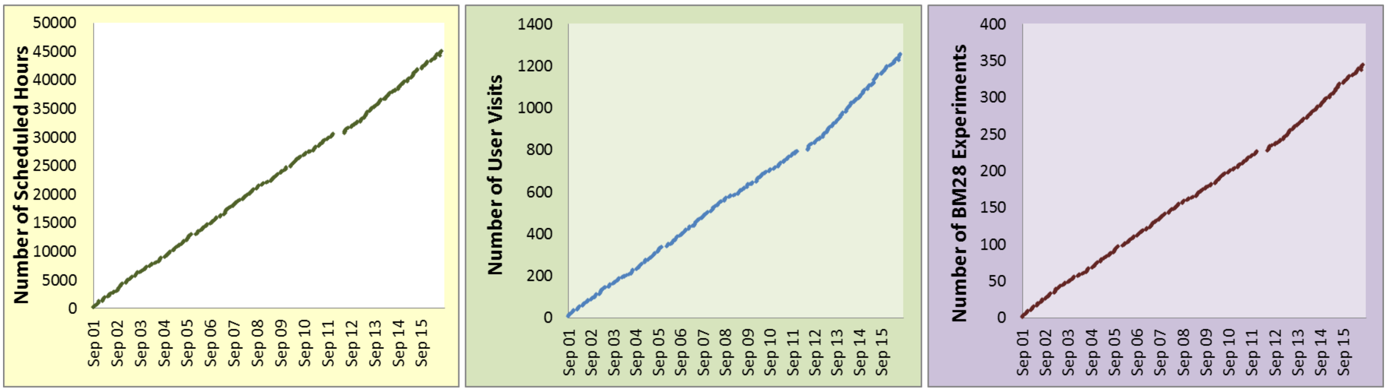

Figure 4: Historical performance metrics for XMaS including the number of scheduled hours (left), the number of user visits to the facility (centre) and the number of individual experiments performed on the beamline (right).

Offline Facilities

In addition to the synchrotron beamline, XMaS has developed a range of "offline" facilities exploiting previous capital investments. These include a magneto-transport laboratory for material characterisation under electric and magnetic fields without x-rays, as well as a high brightness x-ray source for x-ray diffraction, reflectometry and simple SAXS experiments. For the x-ray lab we had a total of **15** user visits covering **11** proposals with **4** proposals being handled as remote, or "mail-in" experiments handled by the on-site team. **8** proposals were received for the characterisation laboratory with 16 user visits. We are aware of 3 papers being submitted from this work, but there is a time lag towards publication for these new capabilities. Of the total possible shifts, the x-ray facility operated at 54% capacity with the characterisation lab at 22%. Any increase in these loads must be weighed against increasing impact on staff resource whose primary responsibility remains with the beamline itself. We will continue to monitor access requests and develop the management of remote requests in the future. A direct link to the XMaS facilities through the core capabilities support of the Advanced Material Research programme at the University of Liverpool has been put in place as part of a recent successful EPSRC equipment bid.

Users (max. 1 page):

Our user statistics are derived from the data generated by the ESRF access protocols and by independent user feedback provided at the end of each experimental session. As part of the contract with the ESRF we provide 30% of the available beamtime for public access. The KPI data returned below pertains to the 70% mid-range facility time with the numbers in parenthesis describing the ESRF publicly allocated time where appropriate.

Summary of Key User statistics:

Number of user visits: **89(23)** from **44(16)** user groups**;** Number of new users: **32(15);** student visits: **34(8)** and PDRA visits: **10(7).** Of these user visits 6% were from non-academic institutions including Diamond Light Source, AWE Aldermaston, the Swiss Light Source and the EU Institute for transuranic studies. Figure 5 shows a heat map of the user groups for the XMaS proposals for the reporting period. We have also received proposals from the Warwick Manufacturing Group as part of the advanced materials catapult. We are exploring partnerships with the catalysis hub at the Research Complex at Harwell and more recently with the nuclear decommissioning authority, the US Navy, Electrosciences Ltd. and the Surrey 5G centre. During the reporting period we also provided proprietary beamtime for Johnson Matthey.

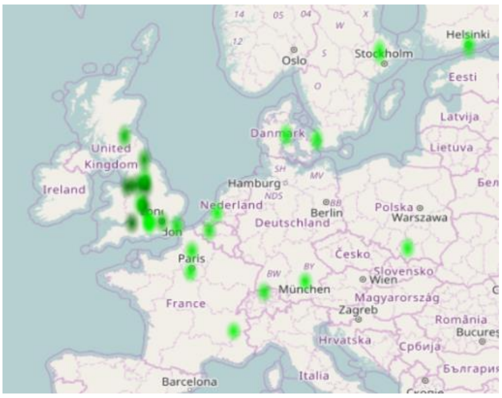

Figure 5: Heat-map of the geographical spread of our users and their collaborators in this reporting period.

Third Party Activities

XMaS was part of the recently completed EMRP funded *Nanostrain Project* which explored multiferroic materials under applied electric fields with cycling rates of up to 1 MHz. The collaboration, led by the National Physical Laboratory (NPL), brought together several of the EU metrology labs along with industrial partners including IBM (New York) to explore strain mediated transistor devices to replace current CMOS technology and overcome the current energy crisis in Si-based devices. This activity continues to be highlighted in several trade magazines and other online resources. Our users often work with third parties such as British Petroleum and Siemens, we now ask the users to give specific details in their end of run surveys on such engagement activities.

User feedback

End of run surveys returned by our users provides additional information about performance. These metrics, which are summarised in Figure 6 for the current reporting period, are scored out of 5, with 5 being the highest score. The data in this review period are consistent with the facility average. We recognise that the lowest performing metric is in computing support and will be devoting additional effort in the next reporting period to improving this.

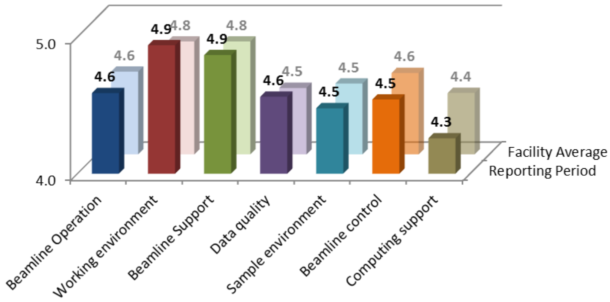

Figure 6: User feedback on facility operations covering the reporting period.

User Research Areas

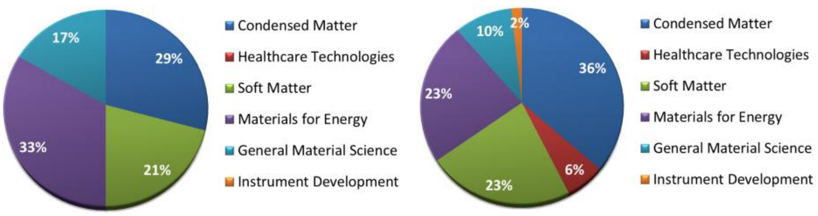

Figure 7: XMaS Experiments by research area as reported by our users for the current reporting period (left) and total mid-range facility time (right).

The science supported on XMaS covers a much broader range of challenges than are normally found on an SR beamline. Due to our multidisciplinary user community, which is stretched across Physics, Chemistry and Materials disciplines within the UK science base, there is a strong mapping to many of the science and technology areas that underpin EPSRC's remit. The user research profile continues to evolve, as seen in Figure 7, with new research areas, such as energy materials, strengthening during this period. The lack of research in healthcare-related research is due some of this activity being rescheduled into the next reporting cycle. XMaS remains in a unique position whereby the best practices of one community have been shared, adapted and implemented by others, to the benefit of all users, and wider afield through our international collaborations.

Scientific Excellence (max. 2 pages): For the reporting period, please provide examples on how the facility supports scientific excellence in the UK.

XMaS has a long history of engaging both with recurrent users as well as encouraging new users and this allows us to continually expand our scientific remit. Over the last ten years or so we have made considerable efforts to extend the operational energy range into the tender regime (2.4-5 keV). This opened up new user communities (particular within chemistry and catalysis) interested in spectroscopic and scattering experiments at the S, Cl and P edges, as well as opportunities for resonant x-ray diffraction studies at the Ru and Pd L edges and the Ir M edges. Being open to such developments is at the heart of the operational ethos of the beamline. Examples include recent developments for *in-situ* and *in-operando* characterisation under a range of external stimuli (applied electric and magnetic fields, humidity, etc.). We continue to expand our capabilities through development of new metrologies and techniques including simultaneous measurements of several data channels at rates up to 1 MHz (Rev. Sci. Instr. 86, 103901 (2015) and J. Appl. Cryst. 49, 1501 (2016)) and extending the polarisation control using phase plates. A newly designed (GI)-SAXS/XRR system has been commissioned and provides enhanced and more efficient operations in this growing area of research and also allows simultaneous WAXS measurements (Cryst. Eng. Comm. 18, 5448 (2016)). We have also recently used the white beam capabilities to open up new experimental paradigms (Angew. Chem. Int. Ed. 55, 1 (2016)). In terms of scientific excellence, a sub-set of the current research activities are presented below, grouped around challenge themes:

Energy research: Issues with Energy supply can only be solved through continuing materials development and understanding of fundamental processes. Research in this area covers photovoltaics, battery materials and catalysis. Experiments have utilised grazing incidence x-ray diffraction to investigate the effect of nanoparticles on the crystallisation and surface morphology of the commercially important polymer blends (Sci. Rep. 5, 10633 (2015) and Adv. Func. Mater. 4934 (2016)) as well as how surfaces evolve under ionic exchange (J. Phys. Chem. C, 120, 3360-3370 (2016)). New partnerships have been built both with academics (individual users as well as the catalysis hub at the Research Complex at Harwell) and industrial (Johnson Matthey) user communities interested in the chemistry of catalysis (J. Am. Chem. Soc., 137, 4151 (2015)). These studies exploit our *in-situ* EXAFS and XAS capabilities (J. Synchrotron Rad., 22, 1426 (2015)) at x-ray energies in the range 2-15 keV.

Fundamental studies of magnetic materials remain a key research area of the beamline in which a range of experiments can be performed exploiting the high magnetic fields and low temperature environments which are unique to the facility (Phys. Rev.B. 93, 195427 (2016) and IEEE Trans. Magn. 52, 4500104 (2016)). Fundamental studies on the magnetic order in PrPtAl provided the first clear experimental observation of 'order by disorder' (Nature Physics, 11, 321 (2015)) and users have also investigated charge density waves in the high temperature superconductor YBCO (Nature Commun., 6, 10064 (2015)).

New functional materials underpin a plethora of emerging technologies, ranging from mobile-phones to computer displays, and studies of these important materials will continue to be carried out using combinations of XAS/WAXS/XRR and diffraction in sample environments optimised for *in-operando* conditions (temperature, humidity, applied fields etc.). We have a growing user community focussed on understanding the properties of soft matter systems including polymers and carbon nanotubes (Polymers 92, 239 (2016)). Safeguarding the environment and the preservation of heritage artefacts remain important research areas. Experiments will continue to understand corrosion mechanisms on a range of heritage artefacts (Talanta, 132, 760 (2015), Heritage Science, 3, 14 (2015), Corros. Sci., 91, 220 (2015)) as well as spent nuclear fuel rods (Faraday Discuss., 180, 301 (2015)).

In the area of **healthcare**, there have been studies of dental and bone materials (Micron 83, 48(2016)) and recent experiments have used a model system to mimic how nanoparticles enter cells and their subsequent impact on human anatomy (Adv. Colloid. Interface, 218, 48 (2015)) as well as how Cu ions act as a contraceptive in an IUD device (Bioelectrochemistry 110, 41 (2016)). There have also been studies of photonic materials that could be used in the next generation of medical imaging detectors (Nature Photonics, 9, 843 (2015)).

From the above limited set of examples, it is clear that XMaS is truly interdisciplinary with outputs impacting across a wide range of scientific disciplines. Our research activities are frequently singled out in the ESRF's publications, (ESRF Highlights 2015: – Abdul-Jabbar *et al.* ''Complex modulated magnetism in PrPtAl''; Sherborne *et al.* ''Combining hard and soft XAS to characterize the deactivation pathway of an immobilized transfer hydrogenation catalyst'' as well as in ESRF Spotlights: - Grünewald *et al.* ''X-ray colour provides direct 3D information in crystallographic texture measurements''). We continue to disseminate the beamline activities in our annual newsletters and we are currently editing the 2016 newsletter (available Feb. 2017) which will be disseminated widely (>800 copies) and sent to all UK physics departments and most UK chemistry departments. In addition we also send copies to many international facilities and all of our previous users. Here we include a summary of the content of the current 2015 newsletter:

- **XMaS Scientist experience** – tackling gender inequality in physics (Lampard *et al. Materials Today 18, 356-357 (2015)*): *A report on the first XMaS scientist experience trip which showed female A-level students that a STEM career was both aspirational and attainable through interacting with the staff at the EPN campus.*
- **Complex modulated magnetism in PrPtAl** (*Nature Physics 11, 321 (2015)*): *The paper summarises a diffraction study of the complex low temperature phase transition between ordered and disordered magnetic states in PrPtAl. The data describes the first experimental evidence of the so-called "order-by-disorder" phase transition.*
- **Copper oxide layers are odd** (*Nature Communications 6, 10064 (2015)*): *A report on charge density waves observed in YBCO which have been shown to have a well-defined structure which is leading to new understanding of the role of the Fermi surface in these materials and high-T_C superconductors more generally.*
- **Dynamic magnetoelectric analysis at XMaS** (*McMitchell et al.*): *A summary of the sample environment and metrology upgrades that have been developed as part of the Nanostrain Project. Simultaneous measurements of crystal structure, polarisation and laser interferometry are described at rates up to 1MHz.*
- **Ferroelectric characterisation of PZT ceramics as a function of temperature**: *A report on the dynamical electric response of PZT ceramics as a function of temperature using the XMaS offline sample characterisation laboratory. The data shows a suppression of the polarisation at low temperatures which depends on the frequency and magnitude of the E-field.*
- **Area detector goes 3D** (*Angew. Chem. Int.Ed. 55, 1-6 (2016)*): *A paper describing the use of white beam Laue diffraction from bundles of carbon fibres. New metrologies using an energy dispersive 2D area detector are demonstrated with potential metrologies being developed for rapid 3D reconstruction of polycrystalline materials.*
- **Organic –Inorganic x-ray detectors** (*Nature Photonics 9, 843 (2015)*): *New materials for low cost, high resolution, flat panel detectors that can be used for radiography are proposed. The paper describes GI-WAXS studies of blends of organic and inorganic materials.*
- **Model membrane systems for studying nanoparticle cellular entry mechanisms** (*Soft Matter 12, 3877-3887 (2016)*): *An x-ray reflectivity study of how nanoparticles interact with model membrane structures and how these interactions modify the energetic process associated with membrane fusion.*
- **Potential hazards of long-term nuclear waste storage** (*Faraday Discuss. 180, 301-311 (2015)*): *Work describing the use of high intensity x-rays to mimic the effect of radiation fields on nuclear fuel rods which causes UO_2 to become water soluble, an important issue when considering the long-term storage of spent nuclear fuel rods.*
- **Activation and deactivation of an immobilised transfer hydrogenation catalyst** *(J. Am. Chem. Soc. 137, 4151-4157 (2015)): An in-situ measurement of the deactivation/reactivation of a commercial immobilised catalyst at the K and Cl edges using XAS. Structural changes are observed through the catalytic cycle and give insight into catalyst operation.*

A full and up-to-date publication list is maintained on our web-page. Work at the facility has produced 22 published peer reviewed papers in 2015 and currently 19 (and counting) in 2016:

Abes M, *et al.* Phys. Rev. B 93, 195427 (2016)
Barrows AT, *et al*. Adv. Func. Mater. 26, 4934-4942 (2016)
Collins SP, *et al.* Acta. Cryst. A 72, 197-205 (2016)
Grayburn RA, *et al*. Bioelectrochemistry 110, 41-45 (2016)
Greasley SL, *et al.* J. Colloid Interface Sci. 469, 213-223 (2016)
Grünewald TA *et al.* Angew Chem. Int. Ed. 55, 1-6 (2016)
Heeley EL *et al.* Polymers 92, 239-249 (2016)
Heeley EL *et al.* J. Polymer Science, in press (2016)
Hussain H *et al.* J. Phys. Chem. C 120, 7586-7590 (2016)
Khan MA *et al.* Micron 83, 48 (2016)
Kuschel T *et al.* IEEE Trans. Magn. 52, 4500104 (2016)
Lilliu S *et al.* CrystEngComm 18, 5448 (2016)
Lucas CA *et al.* J. Phys. Chem. C 120, 3360-3370 (2016)
Richardson SJ *et al.* Nanoscale 8, 2850-2856 (2016)
Sironi B *et al.* Soft Matter 12, 3877-3887 (2016)
Sisson N *et al.* J. Phys. Chem. C 120, 16100-16109 (2016)
Strempfer J *et al.* AIP Conference Proc. 1741, 030017 (2016)
Vergentev T *et al.* J. Appl. Cryst. 49, 1501-1507 (2016)
Vita F *et al.* Soft Matter 12, 2309-2314 (2016)

O. Bikondoa, ''X-Ray Photon Correlation Spectroscopy for the Characterization of Soft and Hard Condensed Matter'', Chapter 3 in 'X-ray and Neutron Techniques for Nanomaterials Characterization', Eds Challa S.S.R. Kumar, Springer Berlin Heidelberg, ISBN: 978-3-662-48604-7 (Print) and 978-3-662-48606-1 (Online).

Publications for the general public:

PCR	How new battery tech could help smartphones consume 100 times less power
ComputerWeekly.com	Reinstating Moore's Law: a next-generation transistor for mobile technology
ITProPortal	Could piezoelectrics solve the smartphone battery conundrum?
NPL	Nanostrain provides hope for battery drain

Impact: Training, Outreach and Societal Impacts (max. 1 page): For the reporting period please provide evidence of the broader impact that the facility has through its outreach and training activities.

The XMaS project transfers knowledge to a broad range of society through interactions with its users and the public as well as facilitating new experimental metrologies and techniques. It provides hands on training to the next generation of material scientists - last year we trained 47 new users and supported 59 student/PDRA visits.

Promoting XMaS to the wider public:

Figure 8: Competition winners partaking in the Synchrotron@School programme.

In 2016, with the help of an additional £18k from the Widening Participation fund of Warwick University, we repeated our outreach activity (XMaS Scientist Experience) tackling the gender bias in Physics. We also organized two additional Science Galas [~330 members of the public interacting with over 30 exhibitors] which were held at both the Universities of Liverpool and Warwick in partnership with our STEM collaborators. This year, 16 winners from around the country were taken on a life changing trip to the EPN campus where they participated in the Synchrotron@School program – Figure 8. The aim of the XMaS Scientist experience is to encourage young women to consider careers in STEM by showing them possible job opportunities and introducing them to inspirational role models in an international setting. The trip received a lot of attention on social media (@XMaSSchoolTrip) as well as blogs on the WISE Campaign, plotr, Science grrl and girlmuseum. We have formed strong partnerships with these organisations as well as STEMettes, BIG BANG, Uppsala University, CERN, IGGY, Ogden Trust Network and the National Science Centres in addressing the gender balance problem. The activity was publicised on the ESRF website and also featured in the local newspaper *Le Dauphiné Libéré*. Emmeline Poole was impressed by the familiar environment at the facility: "*I thought it would be bigger and less accessible and instead we've had the opportunity to discuss with scientists and we've been very close to the instruments too*". Another aspect the girls appreciated was life as a scientist. For Tayma Ferriera, "*you think scientists will always be working alone and instead it is the opposite as their work takes them to travel around the world sharing their results with other scientists, and that aspect surprised me*". The girls will be presenting their experiences at the upcoming science galas which will also launch the 2017 competition. The Scientist Experience featured in the renewal of the IOP Juno champion status and Silver Athena Swan awarded of the Warwick Physics Department as well as in the Silver Athena Swan application of the School of Physical Sciences at the University of Liverpool. It is also currently being prepared as a public engagement case study for the Royal Society as well as being publicised in the wider literature.

Users from XMaS featured in *'24 hours at the X-ray Factory'* which was published as an article and accompanying video in Nature (Nature, 531, March 2016). It took a 24hr look 'behind the scenes' of the science being performed at the ESRF and featured our user group from the University of Sheffield. More generally, ~3,000 members of the public visit the ESRF annually and our on-site staff conduct tours highlighting the importance of the users' research.

Actions taken to develop the User community:

As well as hosting an annual user meeting, producing an annual newsletter and having a presence on the web and social media (@XMaSBeam) we also sponsor UK meetings to promote our activities and build new collaborations:

25th May - **User Meeting**: *Opportunity to see how XMaS operates as a mid-range facility and interact with the on-site team. Summary of new technical developments were presented and discussions of how the beamline can help users and their science were conducted. There was an interactive session on The future of XMaS and the ESRF upgrade.*

3rd November - **X-ray & Neutron Scattering in Multiferroic and Ferroelectric Materials Research Workshop IV**. *These workshops are designed to bring together experts from the multiferroics, magnetoelectrics and ferroelectrics communities with neutron and synchrotron facility users to present the latest developments in this field. The meetings are organised by the Smart Materials & Systems Committee of the UK's Institute of Materials, Minerals and Mining and Electrosciences Ltd. and the XMaS beamline.*

We also encourage exploratory studies from new user communities to be instigated through in-house research collaborations and are open to designing, building and commissioning new sample environments to facilitate new opportunities for the wider community. The capabilities of XMaS are presented at focused meetings, such as at DIAMOND and other SR facilities, where we engage with the wider SR community.

Impact: Economic Impact (max. 1 page): Please provide evidence of the economic impact that the facility has had.

Examples of where work supported by the facility has led to wealth creation and/or attracted inward investment:
It is difficult to track directly the economic impact of the research undertaken on the facility as this is often several stages removed from the fundamental studies that are performed. We actively ask our users for details of industrial collaborations associated with beamtime and this is logged in our database. The interactions are with central facilities as well as national and international companies including in the last year, ABB, Siemens, British Petroleum, the Nuclear Decommissioning Authority, the US Navy, Electrosciences Ltd. and the Surrey 5G centre amongst others. Inward investment has been through proprietary beamtime purchased through the ESRF by Johnson Matthey.

Information on projects which have led to the development or improvement of products and procedures:
The beamline staff are involved with ISO/TC 201 and, in particular, the subgroup SC 10. We are represented on the BIS committee - UK standardisation committee on surface chemical analysis which mirrors TC 201 and are working with our international partners to define the new ISO and hence British standards on the analysis of x-ray reflectometry (XRR) and x-ray fluorescence (XRF) spectroscopy. This covers both SR and lab-based sources.

Information on collaborative projects with industry that have been supported by the facility:
XMaS has continually evolved to meet a broad range of scientific challenges and this has required continual development of both sample environments and beam conditioning components. For example, a new optical microscope to observe x-ray excited light from materials has been developed to study the spatial variations in materials without the need for nano-focused beams with high power density (Heritage Science 3:14 (2015). To date XMaS currently holds 9 licence agreements with 3 different companies which have resulted in over £1M of sales:

1. X,Y,Z cryostat carrier for Huber 512/410 Eulerian cradle maintaining 40 micron diffractometer sphere error with sub-micron precision in X, Y & Z. Huber Diffraktionstechnik GmbH & Co, Germany.
2. In-vacuum "Tube Slit" assembly enabling slit screen to be mounted within a few mm of sample. Huber Diffraktionstechnik GmbH & Co, Germany.
3. In-vacuum slit screen, Huber Diffraktionstechnik GmbH & Co, Germany.
4. In-vacuum x-ray polarization analyzer. Huber Diffraktionstechnik GmbH & Co, Germany.
5. 4 Tesla superconducting magnet for Huber 512/410 cradle configuration. American Magnetics Inc. Oak Ridge, TN, USA.
6. Piezo diffraction stage for incident beam polarisation conditioning (phase plate). National Physical Laboratory, London, UK and Huber Diffraktionstechnik GmbH & Co, Germany.
7. 1.5 Tesla electromagnet for Huber 512/410 cradle configuration, Huber Diffraktionstechnik GmbH & Co, Germany and Advanced Research Systems, PN, USA.
8. In-vacuum magnetic x-ray beam attenuators and control electronics, Huber Diffraktionstechnik GmbH & Co, Germany.
9. High side-load actuator for UHV environments, Huber Diffraktionstechnik GmbH & Co, Germany **[new in 2016]**

Related publications that have industrial or international co-authorship:
Within the last reporting period, 77% of the publications have international co-authorship, and 44% are co-authored with collaborators at central facilities. In addition, two papers within the healthcare field have potential impact in therapeutics:- Grayburn RA, *et al*. Bioelectrochemistry 110 41-45 (2016) (with the Gynecological Outpatient Clinic and IUD Training Center, Ghent) and Khan MA *et al.* Micron 83 48 (2016) (in partnership with Birmingham Children's Hospital NHS Foundation Trust and the Mark Holland Metabolic Unit, Salford Royal Foundation NHS Trust).

Information on any additional funding or leverage that has been received:
Within the framework of the *EMRP Nanostrain Project* we leveraged additional funding for a 2 year PDRA position – the PDRA now has a position at the University of Lyon. The success of the *Nanostrain* Project has resulted in a submission of a follow-up EMPIR JRP program "*Metrology for advanced energy-saving technology in next-generation electronics applications*" and this is currently under review with a decision due in January 2017. A further £18k was received to support out outreach activity from the University of Warwick Widening Participation fund as well as £10k from the Physics Departments of Liverpool and Warwick. The facility supports the recently funded EPSRC program grant EP/N032128/1 "Skyrmionics: From Magnetic Excitations to Functioning Low-Energy Devices". XMaS is also part of the materials characterisation suite that is being developed at Liverpool University and is part of the infrastructure which underpins a successful equipment bid to EPSRC (EP/P001513/1) for x-ray diffraction capabilities.

Details of any other activities that have involved industrial participation:
Large collaborative projects that we are developing are closely aligned with energy materials and our partners include the 5G centre at the University of Surrey, IBM Zurich, the US Naval labs and Electrosciences Ltd. We are also working on expanding our green chemistry and catalysis research programs in partnership with British Petroleum, the catalysis Hub at RAL and Johnson Matthey.

International Interactions (1/2 page): If relevant please provide information on any international interactions the facility has had or supported.

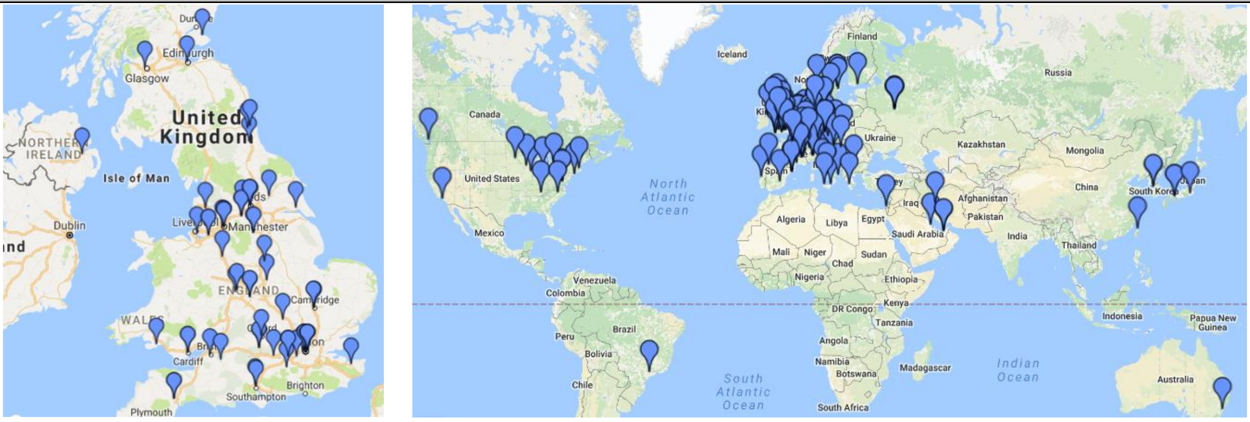

Figure 9: Reach of the XMaS facility since it began supporting UK materials researchers and their collaborators.

XMaS provides the UK science base with direct access to the EPN campus, placing EPSRC-funded science at the forefront of European research. Access to EPN support facilities (including the Partnership for Soft Condensed Matter) is guaranteed through our ESRF contribution and comes with no additional cost. Synchrotron studies tend to be international in nature and the facility is well placed to facilitate and foster strong international collaborations, greatly enhancing the research, impact and training quality for the UK community. Our user community and its collaborators extend around the world (Figure 9) and in the past reporting period **77%** of our publications had international co-author(s). The facility has a strategic partnership with sectors 4 and 6 of the Advanced Photon Source in the US in the development of new x-ray metrologies and sample environments. We are currently exploring partnerships with the Australian Synchrotron through the Universities of Warwick and Monash alliance and the United Arab Emirates synchrotron user organisation in hosting scientists on XMaS. We are actively involved in the European Synchrotron Users Organisation and are looking to host several PhD students through Marie-Curie networks with "INSIDE" being submitted in January 2017.

Improvement (max. 1 page): Please indicate steps that have been taken to improve the access, user experience and ensure the long term sustainability of the facility.

In 2009, the ESRF launched an ambitious Upgrade Programme (UP) aimed at providing enhanced capabilities across the facility. The final stage of the UP involves the design and implementation of a new ultra-low emittance lattice storage ring to be constructed and commissioned within the existing storage ring tunnel (EBS project). This will be completed in 2020 and result in one of the brightest synchrotron facilities in the world. The upgrade is well-timed for the XMaS facility which is also in need of updates and upgrades after nearly 20 years of operation. Following consultation with our users we will upgrade our current source to a high field 0.86 T short bend magnet. The proposal was contained in a CDR presented to the ESRF Strategic Advisory Committee which fully approved the CDR. The higher magnetic field increases the available flux at energies above 20 keV by several orders of magnitude. The new source size ~(30 x 80 μm) will be significantly smaller than the current focused spot size (300 x 600 μm) but with a comparable flux – Figure 10. Geometrically the source will move ~3 m upstream so it will be necessary to upgrade the focusing mirror(s) as well as extend the experimental hutch which will allow us to move the diffractometer and minimise beam aberrations. Such a hutch extension also allows additional beam defining and conditioning elements to be incorporated increasing our operational efficiency and allowing rapid switching between experimental configurations and higher user throughput. As the majority of experiments require a small angular divergence and beam size the more brilliant source increases usable flux for most users by at least an order of magnitude. Further increases in the S/N ratio are derived from the reduced background and the stability of the source.

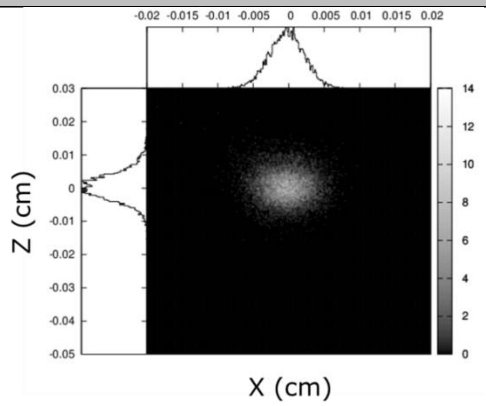

Figure 10: Ray-tracing of the new source through a new mirror shows the expected spot size at the new focal position.

Post EBS upgrade, the beamline will have more than an order of magnitude gain in usable flux at conventional energies as well as having a smaller focal spot and access to higher energies.

For the user community the newly upgraded beamline will enable higher sample throughput, open up studies of weakly scattering systems as well as emergent phenomena more generally. The high energy and brightness will allow new insights into quantum critical behaviour as well as facilitating studies of confinement and proximity in magnetic and superconducting materials. Advances in simultaneous studies allow the direct correlation of functional properties with structure on timescales up-to 1 MHz. Newly combined (GI)-SAXS/WAXS and XRR metrologies allows the structure to be measured across a wide range of length scales simultaneously. The higher brightness enables more systems to be studied *in-operando* and on relevant timescales allowing the study of ionic migration in battery systems and photovoltaics. The well-defined and small beam facilitates experiments on small samples or on localised regions of larger samples. Structural studies will be more spatially resolved enabling individual domains and their temporal evolution to be studied under external stimuli. Such activities provide new insights into phase transitions and the emergence of new functional properties. New mirrors will allow continuous and tuneable energy operations from 2.1 to ~40 keV. This transforms studies of new catalysts and green chemistry more generally – being unique in probing the same sample volume across this entire energy range and within the same sample environment. Thus, reactions can be followed on a site-by-site basis and in real time. An upper energy of ~40 keV allows experiments to access the K edges of the rare earths as well as enabling new studies on the L edges of the transuranic elements (exploiting XMaS's operational licence). The higher energies also facilitate experiments on buried interfaces in more complex sample environments. Studies of solid-liquid interfaces relevant to electrochemical processing become possible. The smaller horizontal divergence enables the front-end Be window to be thinned further, significantly increasing the useable flux at low energies. Finally, the new lattice will greatly facilitate polarisation studies due to the better defined beam positions and more efficient phase retarders leading to the development of new polarisation studies such as SAXS/WAXS from chiral systems.

We recognise that upgrading our capabilities is a continual process and have recently purchased two new Ketek fluorescence detectors and continue to develop sample environments. In response to the changing nature of our users, who are becoming less “expert synchrotron users”, recent efforts have concentrated on data reduction, visualisation and processing (*esaproject*). It will be important to improve such provision as well as update our control protocols during the upgrade to maximise the impact of using the XMaS facility in the future.

Strategic Fit (max. 1/2 page): Please provide evidence on how the facility fits the strategic priorities of EPSRC and state any actions taken / will be taken to align the facility with these strategic priorities.
Much of the scientific programme at the XMaS mid-range facility is contained within the Physical Sciences remit of EPSRC, but the facility is also an important component of the research infrastructure that underpins the wider materials science communities across the UK and their international collaborators. Although originally conceived as a facility to probe magnetic materials and hard condensed matter, the flexibility of the original design coupled with technological developments has enabled an ever broadening range of scientific challenges to be addressed. The demonstrable ability to adapt to the changing scientific challenges and landscape shows that the facility remains flexible to the strategic requirements of EPSRC and other UK stake holders. The principal aim of the XMaS facility is to support world-leading research, discovery and innovation by providing a set of unique materials research capabilities to the UK science base. As well as contributing to future communications technologies (5G centre collaboration) we provide creativity within the science base to stimulate innovative solutions through advanced materials research driving new processes, products and sustainable solutions. The materials research portfolio is an efficient resource, providing a sustainable asset to support design, build and test the next generation of transformative technologies across a range of relevant length-scales. Our plans facilitate and support the development of new storage and generation technologies for future energy options and new metrologies to reducing energy consumption, as exemplified through the Nanostrain Project, as well as provide a proving ground for advanced materials with novel chemical, physical or mechanical properties for health-related applications. Thus, the balance of science that is performed at XMaS encompasses both long-term discovery-led research and shorter term impact cases that contribute to the development of a productive (creativity within the science base to stimulate innovative solutions), connected, resilient (materials research and resource efficiency to enable sustainable use of assets and infrastructure engineering to design, build and test across length-scales, generation, storage and transmission technologies for future energy options and reducing energy consumption and demand) and healthy (developing, characterising and processing advanced materials with novel chemical, physical or mechanical properties, for health-related applications) nation. The combination of a world class photon source, continual innovation in photon techniques, high quality technical and scientific support and a strong international user community has maintained the beamline at the leading edge of materials characterisation. The continuing development of novel sample environments enables XMaS to maintain a diverse scientific programme cutting across the challenge themes and complements as well as strengthens UK-based facilities. As materials discovery continues apace it is evident that the XMaS beamline has an important strategic role in providing fundamental and technologically relevant atomic-scale information to researchers in the physical and life sciences. Due to the location of the XMaS facility at the ESRF, which itself is part of the larger EPN campus, there is a natural environment for UK researchers to adopt an international approach and form collaborative projects. ***In a post-Brexit landscape it is essential that UK scientists are able to maintain, develop and nurture links with international colleagues and facilities.*** XMaS will play a key role in maintaining engagement with EU collaborators and provide an access point for UK users to experience the ESRF and develop collaborative projects both at the ESRF and ILL that go beyond the capabilities of the XMaS beamline. This has been proven repeatedly during the 20 years of XMaS operations.