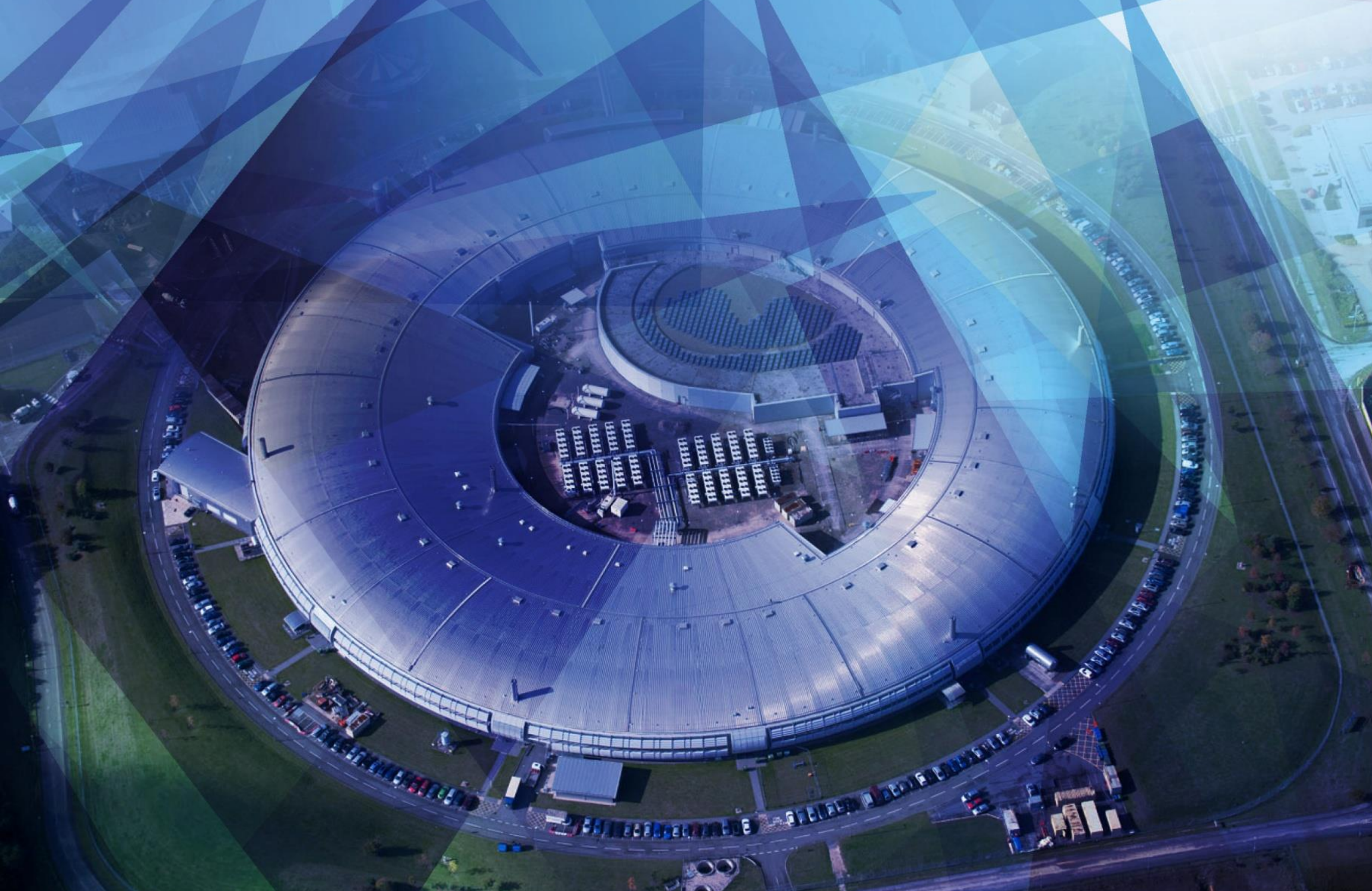
A 10-Year Vision for Diamond Light Source

Diamond Light Source Ltd

October 2015



Foreword

The Diamond Light Source has been operational for 8 years, providing brilliant beams of light to probe the structure and composition of matter in the most incisive fashion, from the life sciences and medicine, through materials for energy and computing, to the environment, earth sciences and cultural heritage. It underpins research and innovation from more than 8000 scientists, mainly from UK universities and industry, with over 90 companies already paying for its services. Every year over 900 PhD students gain experience and training in state-of-the-art experimental and analytical techniques, and Diamond also supports training programmes for apprentices and extensive outreach to the public. It is a key component of the Harwell Campus, which brings together other central facilities of international standing, in partnership with UK universities as one of the leading centres for research and innovation in the world. However, the development of synchrotron technology proceeds at a blistering, relentless pace, with orders of magnitude improvement in brightness of sources, optical components and detectors. If Diamond is to continue to provide world-class facilities, and enable the academic and industrial communities it serves to remain competitive, it must continue to upgrade its technical capability: standing still will lead to decline and ineffective exploitation of significant investment in this facility. This document outlines a Vision for the scientific and societal challenges that synchrotron science will serve over the next 10 years, and the enabling technology that should be developed to meet these challenges. It presents a strategy to establish Diamond sustainably as a world-leading centre for synchrotron science, particularly in areas of excellence at UK universities, research institutes and in industry, and a cornerstone of a world-class site for scientific discovery and innovation at Harwell. It is based on extensive consultation within Diamond as well as discussion with external, international experts who have also advised on priorities for the various upgrade projects. It takes into account developments at other facilities in Europe, particularly the ESRF in which the UK also has a share.

Diamond Management *October 2015*

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EXECUTIVE SUMMARY

- *Diamond Light Source is the UK's national synchrotron light source and provides world-class facilities for scientists from universities and industry, both in the UK and internationally to advance knowledge in virtually all fields of research. It is a limited company, owned 86% by the UK Government via the Science and Technology Facilities Research Council (STFC) with the remainder funded by the Wellcome Trust. At the heart of the facility is a particle accelerator, where electrons travel close to the speed of light emitting electromagnetic radiation, primarily as X-rays, but also ultraviolet and infrared light. These brilliant beams of light are used to reveal the structure and chemical character of a very wide range of materials down to atomic scales. Such information is essential in understanding and developing the properties or processes for a very wide range of systems, from biomolecules and catalysts, through electronic devices and high performance engineering alloys to astrophysics and archaeology. The work that Diamond supports has an increasingly high impact on some of the key challenges for our society, from healthcare and the environment, to more energy efficient devices and transport. It also plays a key role in underpinning research and fuelling innovation for industry. Diamond has a strong commitment to train the next generation of scientists, engineers and technicians, ensuring they develop the skills and experience to exploit both Diamond and other world-class research facilities in the UK.*

- *Since user operations began at Diamond in 2007 its performance, capability and capacity have improved, in some cases dramatically: the beam current and reliability have risen steadily; the number of operational beamlines now stands at 25, with a further 8 planned for completion by 2018; in the 2014/15 Financial Year there were over 3500 unique users who made nearly 5000 on-site user visits and more than 2700'remote' visits; over 90 companies pay for access to beamtime. Published outputs are in line with other facilities of this size at this stage of operation, and many of these are of very high impact; during 2014, Diamond ranked in the top 3 facilities in the world for depositing structures in the Protein Data Bank.*

- *The fast, relentless, pace of the development of technology for synchrotron facilities offers wholly new opportunities for science further into the future. Diamond wishes to take full advantage of these opportunities to continue to support UK research and innovation at a world-class level. It is also timely to reflect on whether the structure and operating model for Diamond, which was set up for the design and construction of the facility, is still most appropriate as it enters a new stage of its lifecycle, with full-blown operations and an expectation to deliver world-leading or world-class science across its beamlines. Diamond has consulted internally and externally to develop a 10-year Vision of the scientific and societal challenges to which it should rise, together with a Vision of the technical development required to meet those challenges.*

- *The vision for Diamond is to be: a world-leading centre for synchrotron science, particularly in areas of excellence at UK universities, research institutes and in industry; a cornerstone of a world-class site for scientific discovery and innovation at Harwell. This vision has five goals:*

  - *to be a world-leading user facility engaged in synchrotron research and innovation;*
  - *to maximise the scientific, economic and societal impact of Diamond;*
  - *to ensure the long-term sustainability of Diamond as a national facility;*
  - *to engage and inspire the general public through promoting an understanding of and enthusiasm for science;*
  - *to continuously plan for Diamond's technical and scientific future.*

- *This document outlines a vision for science and its contribution to the solution of societal challenges enabled by access to a world-class synchrotron. It also presents the technical developments that will enable such advances, comprising: a brighter, more reliable source and the launch of a project to establish a scientific case and technical design for a new lattice for the storage ring – 'Diamond II'; upgrades to current beamlines to maintain or even make a step change in competitiveness – as well as proposals for additional new beamlines; development and implementation of new technology for detectors, optics and metrology and for sample environment; significant enhancement of what is currently possible for data storage, transfer and analysis; improvements in the degree of effectiveness of automation and higher throughput methods. The choice of upgrade projects is the result of a rigorous process of prioritisation against the strategic aims of Diamond, which eliminated many other proposals and ranked the remainder.*

- *Diamond's most valuable asset is a highly motivated and skilled workforce and future success will depend critically on continuing to attract such people in a very competitive market and to make the most of their talents through continued development, and the provision of a stimulating working environment, effective management and strong leadership. This is also a very valuable source of highly trained people for the UK knowledge-based economy so Diamond will continue to develop its programmes for outreach and training, as part of the national infrastructure to attract and develop the next generation of scientists, engineers and technicians.*

- *The performance of Diamond has been significantly enhanced through support laboratories and other integrated facilities, most of which have been established in partnership with UK universities and industry. This is starting to play an increasingly important role in providing integrated solutions to yet more complex scientific problems, and should be developed further where appropriate. The greater Harwell Campus should also be exploited to a greater extent, through more effective scientific and technical links, for example with ISIS and the CLF, and further strengthened by increasing the number of strategic partnerships with universities to establish Harwell truly as a campus in spirit as well as name.*

- *From its inception, Diamond embraced the vast potential the facility has to engage and excite public audiences as well as to inspire the next generation of scientists. In addition, our communications programme ensures that effective and tailored dissemination of information is facilitated to the 7,000 strong members of the user community and growing with the addition of new beamlines and capabilities.*

- *A delivery plan for the vision and strategy, with details of budget profiles for resources and the evolution of the operating model as Diamond approaches full-blown operations with a complete suite of beamlines, is described in a complementary document for the Diamond Board and stakeholders.*

1.0 INTRODUCTION

1.1 A Vision and Strategic Plan for Diamond

The **Diamond Synchrotron** has been operating as a user facility for synchrotron science since 2007. It provides brilliant beams of light, mostly in the X-ray region of the spectrum, serving a suite of beamlines that provide some of the most incisive means in the world to study the structure and chemical character of materials from bulk components used in engineering down to the atomic length scales required to understand the origin of disease or chemical catalysis at a molecular level. The generic nature of the probe means that it can be applied to almost all areas of scientific research and innovation, from the life sciences and medicine, through chemistry and condensed matter physics, through to engineering, processing and the environment.

The initial suite of 7 beamlines that were offered initially has since grown to 25, and 8 more will be completed by 2018. A significant number of these beamlines are technically world-class or world-leading, served by a machine (and sources) whose brightness and reliability is at least on a par with other facilities of comparable energy. The user community has also grown from strength to strength, with over 8000 user visits per annum in the last year, and over 90 companies accessing the facility to date. This has led in turn to strong outputs, with burgeoning publications in high-impact journals, and a strong showing in the recent REF2014 exercise – including a significant number of 'impact' highlights. Such achievements are presented in greater detail in section 3 of this document.

Diamond also plays a key role in training scientists, engineers and technicians in developing and exploiting the very latest technology for science and innovation: each year over 900 PhD students come to perform experiments, some of whom are also part of numerous CDTs supported by the Research Councils in partnership with Diamond. Additionally, Diamond's strategy is to part-fund at least two students per operational beamline with different universities, which will lead to ~ 70 studentships in steady state. Such activities, together with the very extensive outreach programme that involves over 6000 members of the public every year, from placements for school children to open days and other public events, are also outlined in section 3.7.

The success of all of these activities depends on Diamond maintaining world-class facilities and attracting world-class staff to work there. However, the pace of technical development in synchrotron science is very rapid and relentless, so if Diamond is to continue to support UK research and innovation at an internationally competitive level, it must continue to develop: standing still is simply not an option if the UK has any aspiration to maintain its strong position in sciences for which synchrotron measurements play an essential role. Furthermore, the organisation and operating model for Diamond was largely established when it was still under construction; now that the facility is approaching full-blown operations with many more beamlines and staff scientists, and much greater demand from users for support services, it is timely to reflect on what will be the most effective operating model for the future. The Diamond Board therefore requested Diamond management to present a strategy for its future, and to do so within the first 2 years (2014-2015) of appointing a new CEO, Andrew Harrison.

This document presents a vision for the scientific and societal challenges that could be met through synchrotron science for up to 10 years hence, together with the technical developments required to meet those challenges most effectively. It also presents a 5-year strategy to enable Diamond to deliver that vision, as well as fulfilling its mission in other areas, including education, training and public engagement. This extends well beyond the technical evolution of Diamond, and includes changes to the nature and scope of operations at Diamond and in partnership with other institutes and organisations, both on the wider **Harwell Campus** and further afield.

The process of developing a strategy is also very timely with respect to the UK Government Comprehensive Spending Review in 2015: we are submitting clear, justified proposals for support for future developments. Indeed, our initial preparations to develop a strategy have already proved very useful in preparing our submission to the BIS 'Capital Consultation Exercise' last July 2014. [1]

1.2 The Strategic Planning Process

The development of a 10-year vision and a 5-year strategy for Diamond was launched by the Diamond Executive team in February 2014, and took the following course.

- Diamond staff were engaged through group leaders in the Science and Technical Division, to develop a 10-year Vision of the scientific and societal challenges to be met through synchrotron science and the technical development required to meet those challenges (*February – April 2014*)
- These scientific and technical visions were refined through presentation and discussion between groups: scientists developing their visions inspired by new technical possibilities; technical groups considering new ways to meet scientists' demands and priorities. This process also identified strengths and weakness of the Diamond operating model and ideas for the evolution of the future scope of Diamond activities, for example collaboration with other facilities, and initial discussions were held with the Diamond Science Advisory Committee (SAC) (*April-May 2014*).
- Scientific and technical groups drew up and presented their priorities to management who made an initial assessment of global priorities and presented them to Diamond staff (*June 2014*).
- A science-focussed 10-year vision was drawn up, led by internal 'Science Champions', together with proposed technical developments for an external meeting, based around SAC and the Diamond Industrial Science Committee (DISCo) but with additional external experts and representatives of key UK Research Councils and the Wellcome Trust (comprising a total of over 55 external people) (*July-September 2014, with the 'Vision' meeting taking place on September 30th and October 1st*).
- The scientific and technical priorities were refined based on feedback from the Vision meeting and this provided the basis for prioritisation of resources for the various upgrade and developmental projects to match various levels of strategic ambition. Many proposals were eliminated at this stage to leave the projects outlined later in this document, each designated 'option 1' and 'option 2' according to priority. Discussion was also held about the evolution of future operation and scope of Diamond. Benchmarking with other synchrotron sources undertaken. (*October-December 2014*).
- The Vision and Strategy Document was discussed with the Diamond Board, Science Advisory Committee and other representatives from STFC and Wellcome Trust on January 26th 2015. Further revision of the document was carried out following their recommendations, and the resource profiles were also developed further to ensure that they were consistent with existing commitments and short-term plans for essential upgrades and maintenance. A delivery plan for this vision and strategy which outlines both the resources required and the evolution of the operating model as Diamond makes the transition to 100% operations, is described in a complementary document for the Diamond Board and stakeholders (*September 2015*)

[1] https://www.gov.uk/government/consultations/science-and-research-proposals-for-long-term-capital-investment

2.0 BACKGROUND AND CONTEXT

2.1 Synchrotron Radiation and Diamond Light Source

Synchrotron radiation has provided a uniquely powerful tool to explore the structure, composition and excitations of materials for decades, first at beamlines parasitic to facilities for high energy physics and then at dedicated, 2nd generation facilities, pioneered by the UK at the world's first dedicated user facility, the **Synchrotron Radiation Source** (**SRS**) at the **Daresbury Laboratory** (**DL**) (first operational in 1981). Such centres have since evolved further through the introduction of insertion devices to the electron beam in 3rd generation facilities, first at the **European Synchrotron Radiation Facility** (**ESRF**) in Grenoble (first operational in 1994), which generate yet brighter radiation. This radiation is primarily in the X-ray region of the spectrum and reveals the nature of materials in a variety of ways.

- The coherent scattering or diffraction of X-rays provides *the* primary source of atomic and molecular structural information over length-scales from sub-nanometre to almost a micron; the fact that X-rays can be polarised means that they may also reveal the magnetic structure of materials.
- X-rays may be absorbed by materials through the excitation of electrons in a manner that is characteristic of the elements they contain, as well as the way they are bound chemically and their magnetic environment. Such excitation may lead to ejection of electrons from the material, providing a very powerful means of exploring the electronic character of solids, or a fingerprint for molecular species, for example transient compounds during a chemical reaction.
- All of these insights may be provided with very high spatial resolution at the sample with highly focused and brilliant X-ray beams in uniquely powerful beamlines.

Synchrotron radiation may also be generated from the infrared (IR) to the ultraviolet (UV) region of the electromagnetic spectrum, providing a further range of tools that have reinforced its position as an essential part of the research infrastructure in all developed countries – either based in those countries, or accessed through international partnerships. Understanding the structure, composition and dynamics of materials underpins all areas of research in the physical and life sciences, from structural biology and chemistry, through physics to earth sciences and engineering. This provided a compelling case for the UK to establish its own 3rd generation source to serve the increasing needs of both academia and industry beyond the capacity of the ESRF – as well as to tailor it to the specific needs of these research communities. It was natural that the **Wellcome Trust**, the world's leading biomedical charity, joined the UK government (then through CCLRC, now **STFC**) in establishing a new facility – the Diamond Light Source **-** as a Joint Venture in 2002 with shares of 14% and 86% respectively.

The initial phase of construction of Diamond – Phase I – was completed on time in 2007, with 7 beamlines operating for the user community. At the time the storage ring had the lowest emittance of any 3rd generation source. Phase II of construction (2007-2013) provided 15 further beamlines and Phase III will run until 2018, ultimately delivering a total of 33 beamlines. Throughout the period of operations the beam current and reliability have ramped up (**Figure 1**), while delivering more experimental shifts (**Figure 2**) and attracting and supporting increasing numbers of users. This includes a very significant component of industrial users, and right from the start Diamond established an advisory body for industrial access and development **- Diamond Industrial Science Committee** (**DISCo**) **-** which draws on senior figures or key users from across all relevant industrial sectors, and has proved very effective in advising Diamond how best to develop its facilities for the needs of industry. Over 90 companies have now made use of Diamond through the proprietary access mode, with additional companies coming to Diamond through peer review. Some of the developments demanded by industry, such as high-throughput methods, have also benefitted the university community. We expand on both the academic and industrial achievements together with some other performance metrics in section 3 of this document.

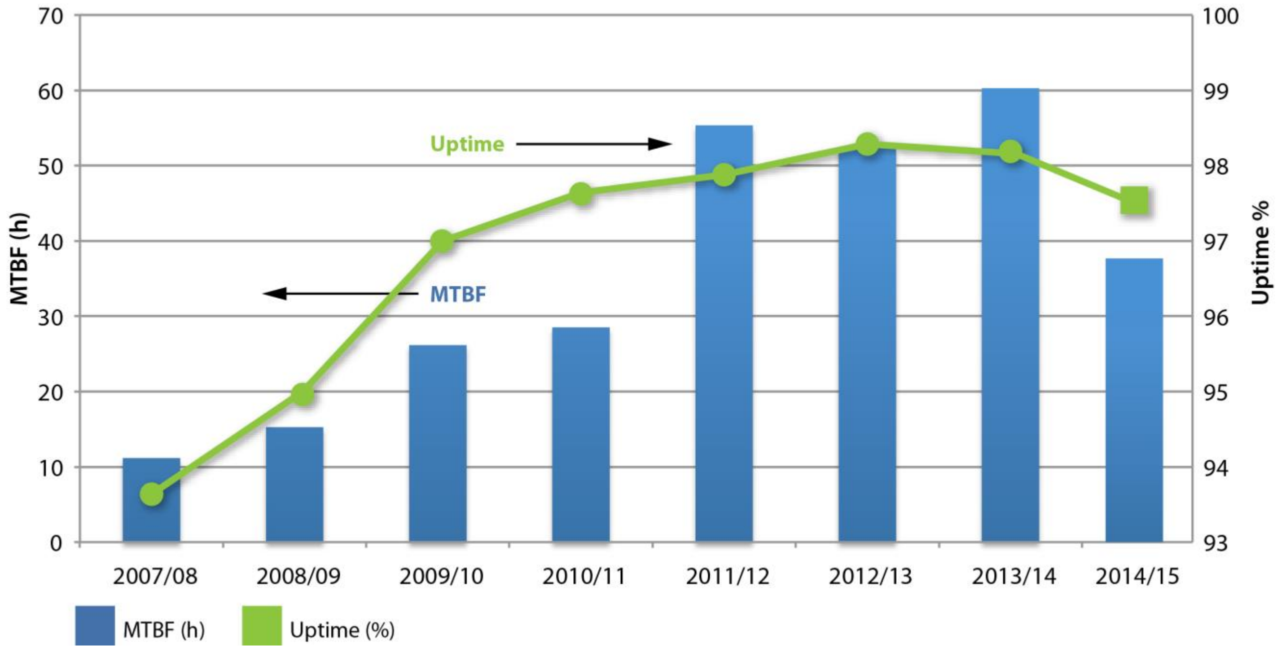

Figure 1 *Evolution of the Mean Time Between Failures (MTBF) and percentage up-time for the synchrotron beam with the number of years of operation, starting in 2007. Data include beamline start-up days but exclude special beam conditions (low alpha mode). Note that the reduction in performance in the last year recorded here was due to a failure in the storage ring for which long-term mitigating action has been taken.*

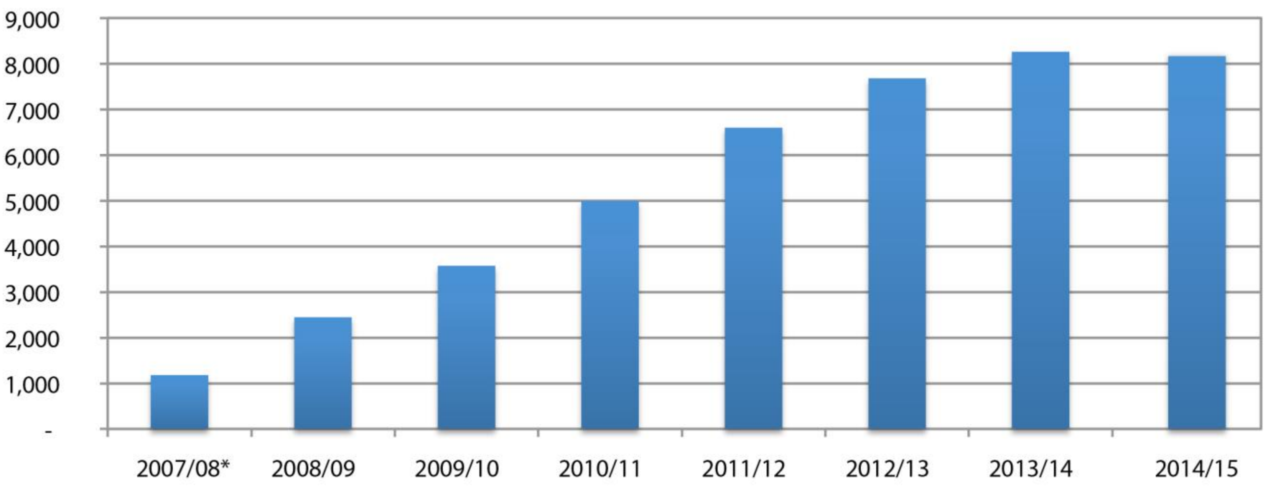

Figure 2 *Delivery of shifts by Financial Year for both Peer Review and Proprietary access (*07/08 data is for Jan07-Mar08 (inclusive))*

Diamond is organised into three Divisions – Science, Technical, and Finance and Corporate Services – together with the CEO's office. The Science Division is led by two Directors – one for Life Sciences and one for Physical Sciences – and the other two have a Director each. The four Directors and the CEO comprise the Management team. Within the Science Division, the beamlines are clustered into Villages which either have a scientific or technical coherence, and are each facilitated by a co-ordinator. The number of staff employed by Diamond is ~ 550 (summer 2015), and it is planned that this will rise a little more as additional staff are needed to support some of the Phase III beamlines that remain to be constructed.

A summary of the beamlines that are currently available is presented in **Table 1**, which also indicates through colour-coding the way in which they are organised into 'villages' for operational reasons. The same colour coding is also used in **Figure 3** which displays the location of beamlines around the Diamond ring while **Figure 4** presents the timetable for beamline construction, past, present and future.

Diamond's beamlines: current operational status April 2015

Beamline Name and Number	Main Techniques	Energy / Wavelength Range	Status
I02 - Macromolecular Crystallography	Macromolecular crystallography (MX), Multiwavelength Anomalous Diffraction (MAD)	5 - 25 keV	Operational
I02-1/I02-2 - Versatile MX (VMXi/VMXm)	Versatile macromolecular crystallography (VMX)	10 - 25 keV	**Construction**
I03 - MX	MX, MAD	5 - 25 keV	Operational
I04 - MX	MX, MAD	5 - 25 keV	Operational
I04-1 - Monochromatic MX	MX, Fragment Screening (XChem)	13.53 keV (0.9163 Å - fixed wavelength)	Operational
I05 - ARPES	Angle-Resolved PhotoEmission Spectroscopy (ARPES)	18 - 240 eV; 500 eV	Operational
I06 - Nanoscience	X-ray Absorption Spectroscopy (XAS), X-ray photoemission microscopy and X-ray magnetic circular and linear dichroism	First harmonic circular: 106 - 1300 eV; Linear Horizontal: 80 - 2100 eV; Linear Vertical: 130 - 1500 eV	Operational
I07 - Surface and Interface Diffraction	Surface X-ray diffraction, Grazing Incidence X-ray Diffraction (GIXD), Grazing Incidence Small Angle X-ray Scattering (GISAXS), X-ray Reflectivity (XRR)	6 - 30 keV	Operational
B07 - VERSOX: Versatile Soft X-ray	Spectroscopic and scanned-probe imaging	50 - 2800 eV	**Construction** / End station commissioned at I09
I08 - Scanning X-ray Microscopy	Scanning X-ray microscopy	250 eV - 4.2 keV	Operational
I09 - SISA: Surface and Interface Structural Analysis	XPS (including HAXPES), X-ray Standing Waves (XSW), Near Edge X-ray Absorption Fine Structure (NEXAFS), energy-scanned photoelectron diffraction	Hard X-rays: 2.1 - 18+ keV (currently 2.35 - 18+ keV) Soft X-rays: 0.1 - 2.1 keV (currently 0.1 - 1 keV)	Operational
I10 - BLADE: Beamline for Advanced Dichroism Experiments	Soft X-ray resonant scattering, XAS and X-ray magnetic circular and linear dichroism	500 - 1600 eV	Operational
I11 - High Resolution Powder Diffraction	High resolution and time resolved X-ray powder diffraction including dynamic and non-ambient conditions; Long Duration Experiments (LDE)	EH1: 6-25 keV (2.1-0.5 A) LDE: 25 keV (0.5 A)	Operational
I12 - JEEP: Joint Engineering, Environmental and Processing	Imaging and tomography (phase and attenuation), single crystal diffraction, powder diffraction, energy dispersive diffraction, high-energy small angle scattering	53 keV - 150 keV monochromatic or continuous white beam	Operational
I13 - X-ray Imaging and Coherence	Phase contrast imaging, tomography, full-field microscopy (under commissioning), coherent diffraction and imaging (CXRD,CDI), ptychography and photocorrelation spectroscopy (XPCS) (under commissioning), innovative microscopy and imaging	Imaging branch: 8 - 30keV Coherence branch: 7 - 20keV	Operational
I14 - Hard X-ray Nanoprobe	Scanning X-ray fluorescence and X-ray Spectroscopy, ptychography, small and wide angle scattering	5 - 25 keV	**Construction**
I15 - Extreme Conditions	Powder diffraction, single crystal diffraction	20 - 80 keV monochromatic focused minimum beam size restrictions for E> 30 keV White beam for special applications	Operational
I15-1 - X-ray Pair Distribution Function (XPDF)	X-ray Pair Distribution Function (XPDF)	40, 65, and 76 keV	**Construction**
I16 - Materials and Magnetism	Diffraction/scattering, spectroscopy	2.7 - 15 keV	Operational
B16 - Test beamline	Diffraction, imaging, reflectometry	4 - 20 keV monochromatic focused 4 - 45 keV monochromatic unfocused White beam	Operational
I18 - Microfocus Spectroscopy	Micro XAS, micro Extended X-ray Absorption Fine Structure (EXAFS), micro fluorescence tomography, micro XRD X-ray Absorption Spectroscopy (XAS)	2.05 - 20.5 keV	Operational
B18 - Core EXAFS	X-ray Absorption Spectroscopy (XAS)	2.05 - 35 keV	Operational
I19 - Small-Molecule Single-Crystal Diffraction	Small-molecule single-crystal diffraction	5 to 25 keV / 0.5 to 2.5 Å	Operational
I20 - LOLA: X-ray Spectroscopy	X-ray Absorption Spectroscopy (XAS), Energy Dispersive EXAFS (EDE), X-ray Emission Spectroscopy (XES)	Dispersive branch: 6 - 26 keV Scanning branch: 4 - 20 keV	Commissioning Under refurbishment
I21 - Inelastic X-ray Scattering	Inelastic X-ray Scattering (IXS)	250 - 3000 eV	**Construction**
B21 - High Throughput SAXS	Solution state small angle X-ray scattering	Currently 11-23 keV but set to 12.4 until variable camera installed	Operational
I22 - Small Angle Scattering and Diffraction	Non-crystalline diffraction: SAXS, WAXS, ASAXS, USAXS	3.5 - 20 keV	Operational
B22 - MIRIAM: Multimode InfraRed Imaging And Mircrospectroscopy	IR microspectroscopy and imaging, THz spectroscopy	Microscopy (μFTIR): 100 -10,000 cm-1 (100 -1 μm) Imaging (FPA): 900-4000 cm-1 (11 - 2.5 μm) Spectroscopy (FTIR bench): 5-15,000 cm-1 (0.6 meV -1.8 eV)	Operational
I23 - Long Wavelength MX	Long wavelength macromolecular crystallography	3 - 8 keV (1.5 - 4.1 Å)	Commissioning
B23 - Circular Dichroism	Circular dichroism	Module A: 125 - 500nm (for multiplates and films) Module B: 165 - 650nm (for solutions)	Operational
I24 - Microfocus MX	Macromolecular crystallography, MAD	6.5 - 25.0 keV	Operational
B24 - Cryo Transmission X-ray Microscopy (TXM)	Full field cryo soft X-ray imaging	2 - 10 keV	Commissioning

Table 1. *Diamond beamlines and status at the end of 2015. The colour for each line indicates the village to which the beamline belongs, defined in* **Figure 3***.*

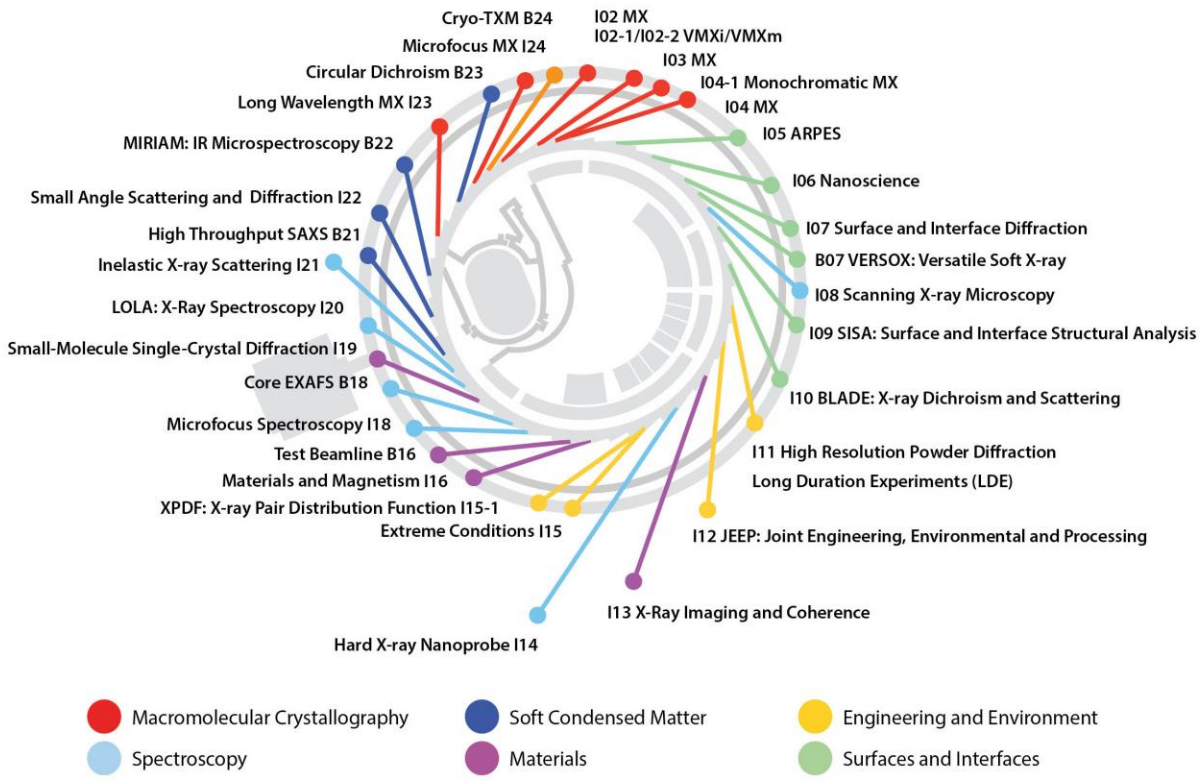

Figure 3. *Location of beamlines around the Diamond storage ring, and designation in 'Villages'*

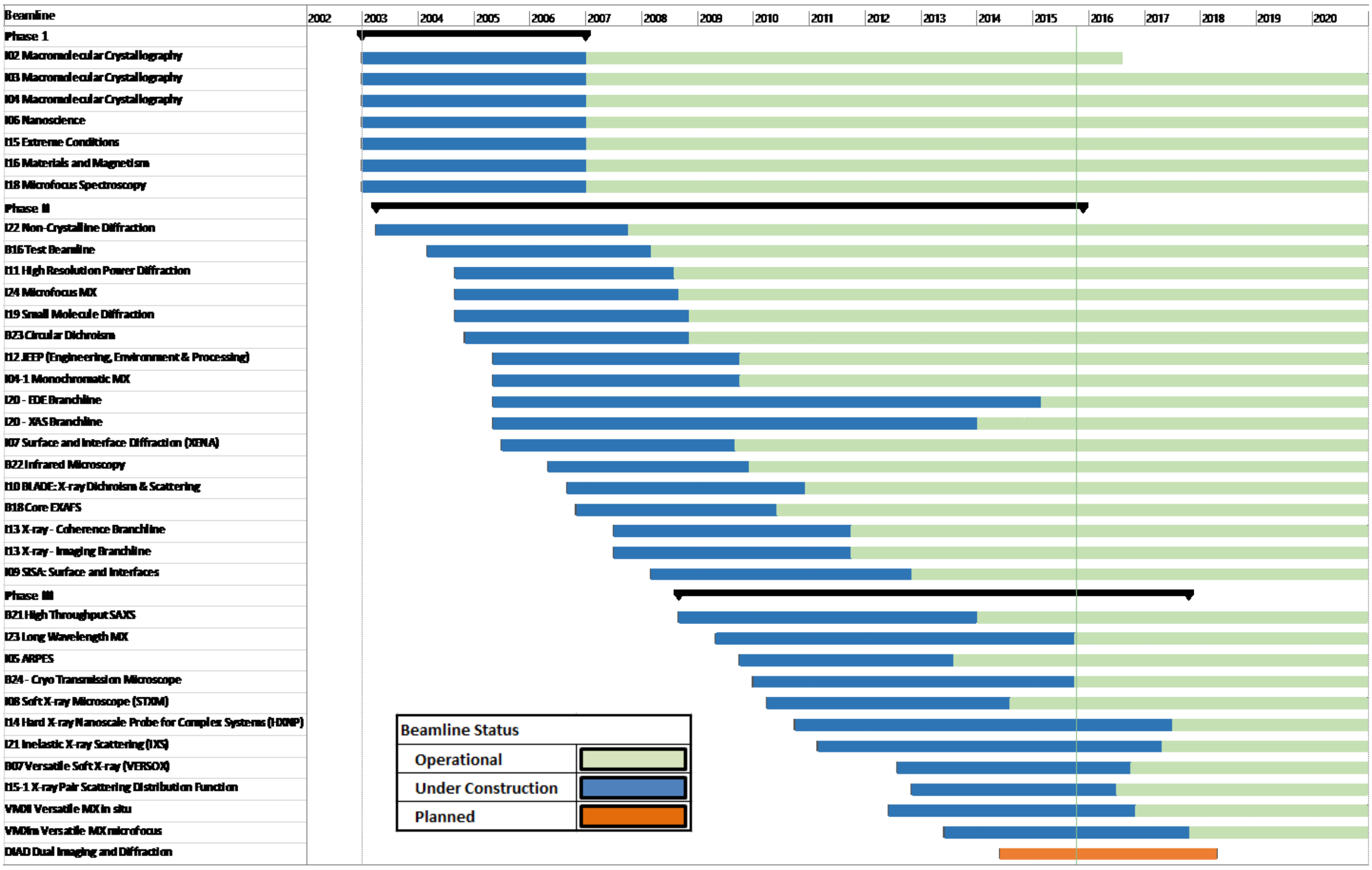

Figure 4. *Schedule for development of beamlines at Diamond for the three phases to date. Further information about beamlines is summarised in* ***Table 1***

A number of technical services have also been established at Diamond, both to support operations and to produce essential technical components. In house developments include advanced systems for electron beam diagnostics and control; insertion devices; a unified system for beamline control that is probably the most coherent in the world; metrology and correction of X-ray optics; advanced detectors, also in collaboration with **STFC Technology** at the **Rutherford Appleton Laboratory** (**RAL**) and Daresbury Laboratory. Diamond has also established the **Membrane Protein Laboratory** (**MPL**) [2] with **Imperial College London** and funding from the Wellcome Trust. The MPL is a research and training facility open to scientists worldwide, providing high throughput technologies for the production and crystallisation of membrane proteins in conjunction with Macromolecular Crystallography (MX) beamlines to determine their structure.

2.2 The Harwell Campus

Science campuses, which bring together large-scale science infrastructures with research groups from universities and industry, are increasingly seen as particularly effective and efficient organisation to tackle some of the most challenging and complex scientific problems, and then to apply the knowledge this generates into the innovation cycle [3]. Diamond is located within the largest science campus in the UK at Harwell [4] (**Figure 5**) which hosts several other national facilities and laboratories, several of which are world-class. The most significant among these for Diamond are the **ISIS Facility** [5] and the **Central Laser Facility** [6] (**CLF**).

– **ISIS** is the world's most productive pulsed neutron source, providing techniques to explore the structure and dynamics of materials that complement synchrotron X-rays, in particular for magnetic structures, the location of light atoms in materials and low energy excitations and dynamics (< 10 meV). There are also potential synergies in developing instrumentation, particular for sample environment, and in data analysis.

– The **CLF** develops and applies very specialised lasers, particularly with very high energy or short pulse lengths, with applications to physics, chemistry and biology that overlap strongly with activity in Diamond – for example in probing chemical reactions on the shortest timescales and studying biochemical and biophysical processes critical to life itself.

The potential to develop such synergies further was instrumental in an agreement between Diamond and RCUK to establish the **Research Complex at Harwell** [7] (**RCaH**) in 2006. This provides 5000 m^2 of laboratory space and offices to host groups from universities and industry who have secured funding for projects in both the physical and life sciences that exploit and develop one or more of these three facilities. It now hosts over 200 researchers in fields that include protein purification, structural biology, ultra-high resolution imaging, the dynamics of fast processes in chemistry and biology and catalysis; the last of these is supported through the EPSRC-funded Catalysis Hub that brings together groups from over 30 UK universities.

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[2] http://www.diamond.ac.uk/Beamlines/Mx/MPL.html
[3] https://www.gov.uk/government/speeches/speech-by-david-willetts-to-the-uk-science-park-association
[4] http://harwellcampus.com/
[5] http://www.isis.stfc.ac.uk/
[6] http://www.stfc.ac.uk/clf/default.aspx
[7] http://www.rc-harwell.ac.uk

Elsewhere on the site, there is the MRC **Mary Lyon Centre** [8] for mouse functional genomics, a **Biological Solid-State NMR Facility** [9] and several **STFC Technology** laboratories with which Diamond collaborates in the development of detectors and superconducting undulators.

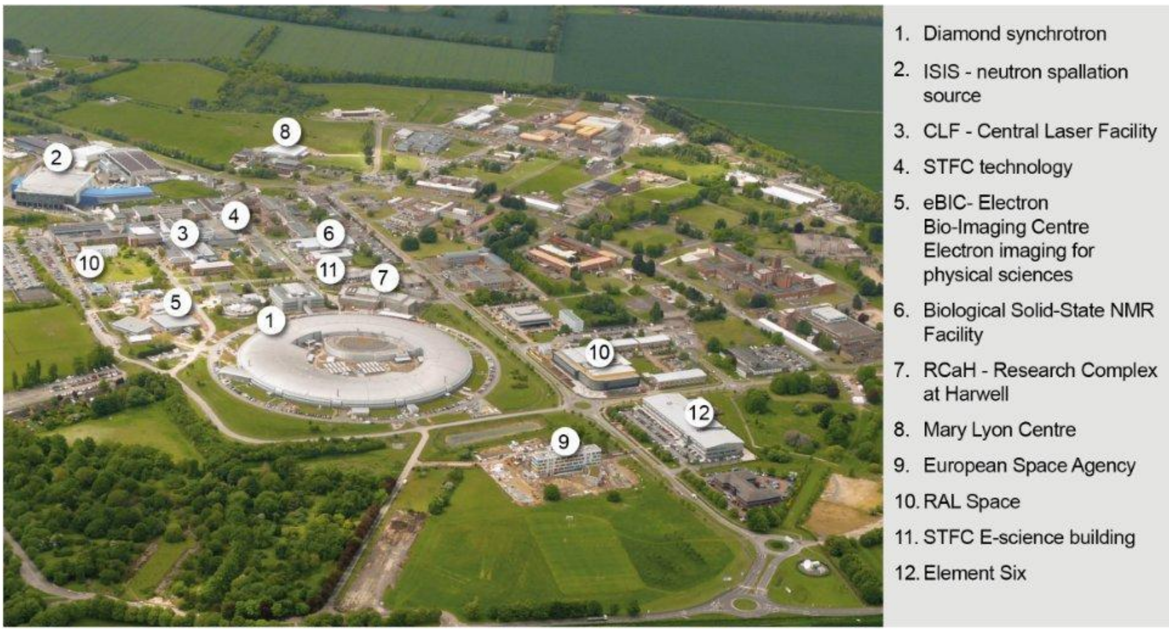

Figure 5. *The Harwell Campus, illustrating the facilities and laboratories it hosts (summer 2015)*

Most recently, construction is underway of a building that will house both the I14 Hard X-ray Nanoprobe beamline at Diamond and a national **Electron Microscopy Facility** (**EMF**). Within the EMF, **Johnson Matthey**, the **University of Oxford** and Diamond Light Source are collaborating on the creation of a state-of-the-art materials characterisation facility on the Harwell Campus, with Johnson Matthey and the University of Oxford both contributing cutting-edge microscopes from JEOL. The EMF will also house a National Facility for Cryo-Electron Microscopy - the electron Bio-Imaging Centre (**eBIC**) – with an additional two advanced electron microscopes being funded by **The Wellcome Trust**, **MRC** and **BBSRC**, in an initiative led by **Birkbeck College, London** and the University of Oxford. Some of the time on these microscopes will be provided as a national service, with the instruments run much in the same way as beamlines at Diamond. The co-location of these instruments at a synchrotron facility - in particular with I14 - will provide unique scientific opportunities. There will also be technical synergies between Diamond and the EMF in the development of methods to prepare and introduce samples, as well as in image analysis.

The Harwell Campus is also being developed through a Joint Venture between STFC, the UK Atomic Energy Authority (UKAEA), and Harwell Campus Developments Ltd, to attract significant activity and inward investment by industry. Prime factors in attracting such development include the existing and developing scientific infrastructure, a stimulating environment of scientists and engineers and highly-skilled technicians, and the growing university engagement with the campus. This venture is also developing some of the physical and social infrastructure on the campus to encourage relocation or growth of enterprises.

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[8] http://www.har.mrc.ac.uk/about/mary-lyon-centre
[9] http://www.bioch.ox.ac.uk/aspsite/index.asp?sectionid=oubsu

3.0 IMPACTS AND ACHIEVEMENTS 2007 – 2014

3.1 Scientific community and science

Diamond strives to attract and enable the best scientific groups to conduct excellent science and since it has opened the user base has grown very strongly (**Figure 6**) so that in the 2014/15 Financial Year, Diamond had over 3600 unique users, of which almost 1000 were PhD students; these users made almost 5000 user visits plus an additional 2700 'remote' visits for which samples were sent from the home institution and experiments followed, or even controlled remotely *via* the internet. Research undertaken at Diamond covers a broad spectrum, as illustrated in the chart of **Figure 7** for the 2013/14 Financial Year.

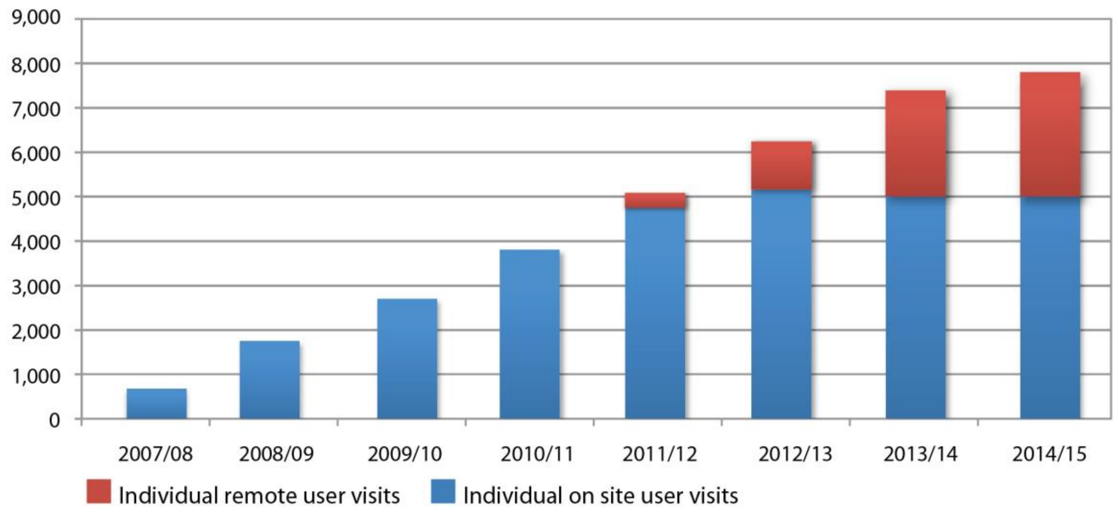

Figure 6. *Increase in the number of external user visit since operations began at Diamond.*

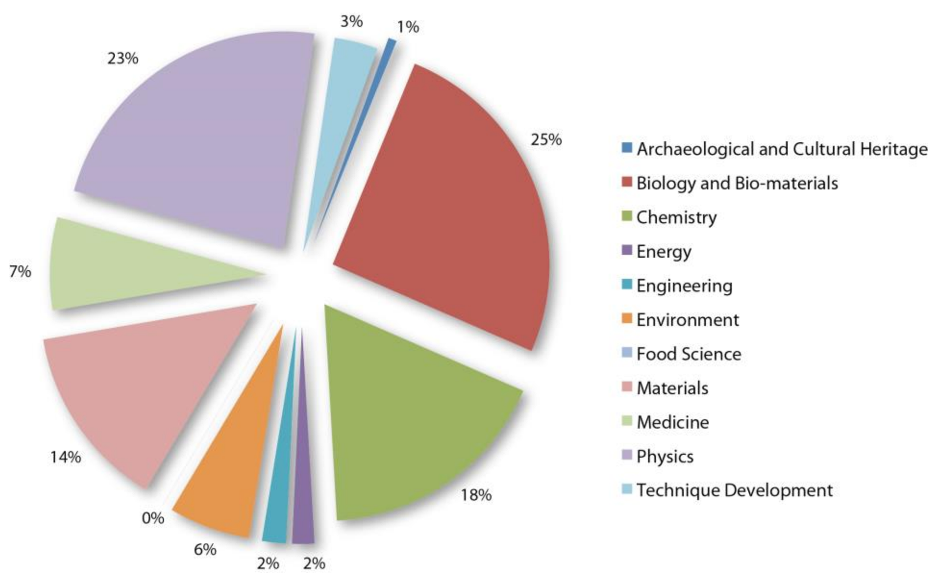

Figure 7. *Experimental Shifts awarded by main subject area for 2014/15 for peer reviewed proposals*

As the number of experiments performed at Diamond has increased so too have the number of publications. So far, over 4000 publications from Diamond users and staff have been logged in the Diamond publications database (**Figure 8**). In the life sciences a key measure of output is the number of structures deposited in the

Protein Data Bank (PDB): this has risen so strongly since operations began in 2007 (**Figure 9**), that in 2015 to date Diamond has deposited more structures in the PDB than any other national facility in Europe, and the total is currently in excess of 3000.

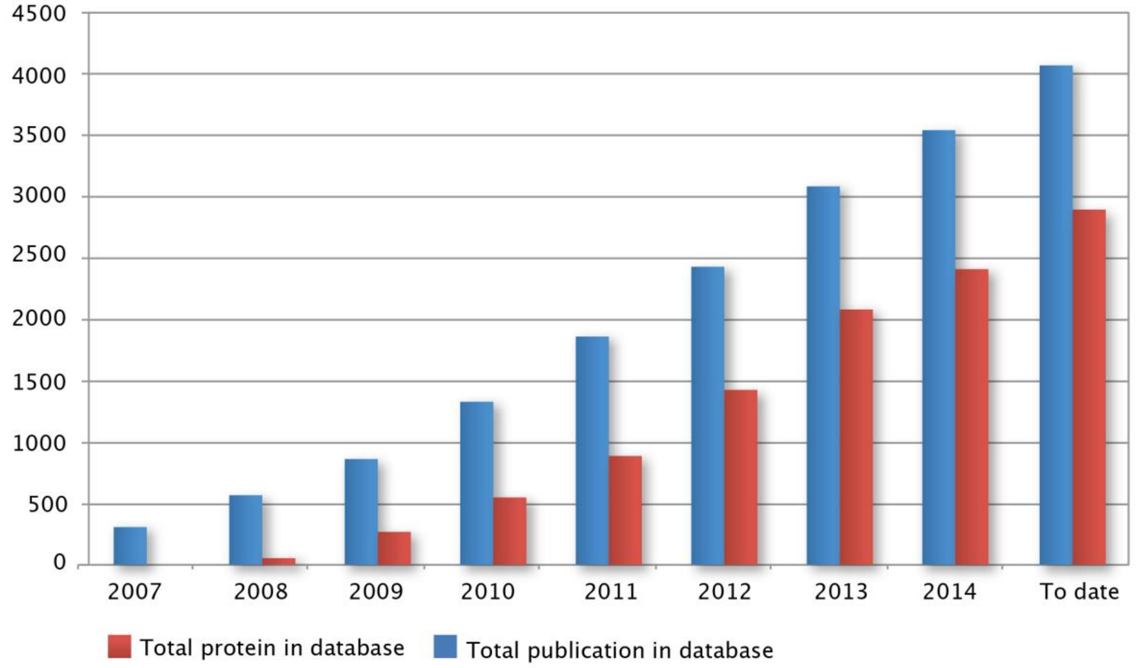

Figure 8. *Evolution with time of number of publications and structures deposited in the Protein Data Bank based on data taken at Diamond (red bars) since operations started in 2007.*

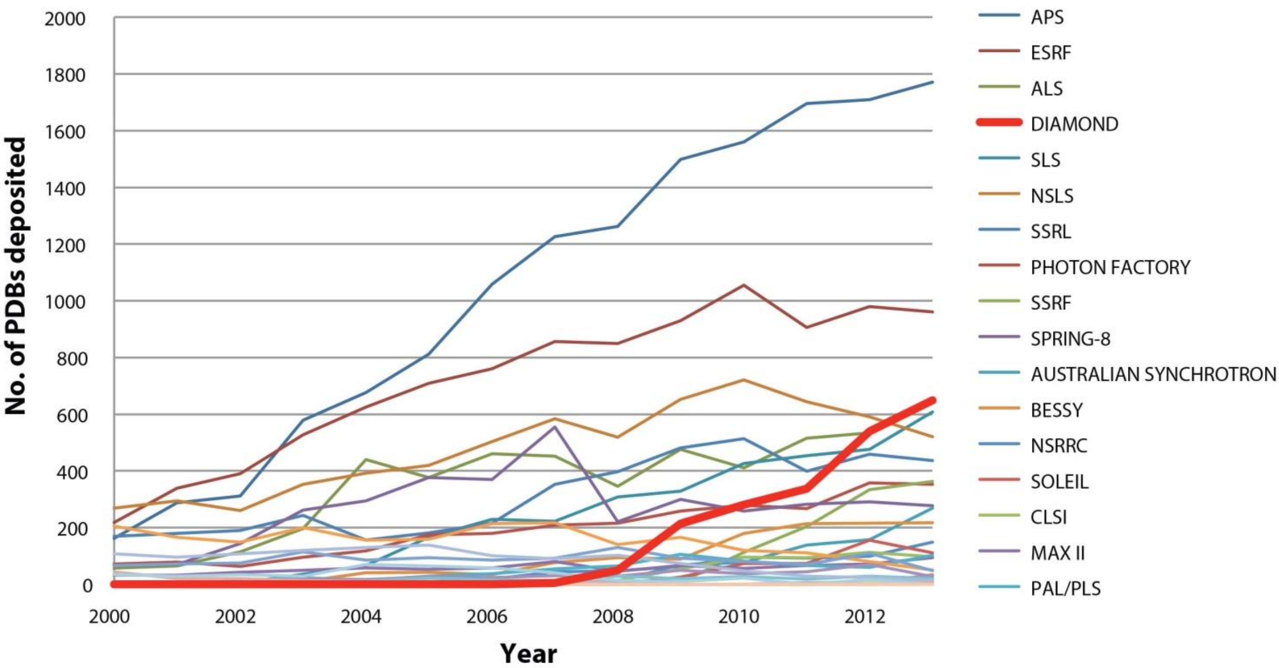

Figure 9 *Evolution of PDB depositions per annum for different synchrotron facilities.*

Behind these statistics there is a wealth of scientific achievement across a very wide range of science, and impacts on many of the grand challenges our society faces – in healthcare, advanced energy supply, environmental protection, food security, new materials and the next generation of industrial processing and computer technology. The diversity of science that Diamond supports draws together scientists from different backgrounds, from both industry and academia, cross-fertilising ideas and setting them off on new, unexpected lines of enquiry and discovery. There is evidence provided by the recent REF2014 exercise that research at Diamond is already starting to have an impact, and before it the SRS in Daresbury also made very significant impacts on societal problems, and innovation.[10]

Illustrative research highlights are given immediately below, while some of the outcomes of industrial research are presented in the following section (**3.2**).

Drug targets for inherited cancers [11]

In 2011, Scientists from Cancer Research UK's Paterson Institute within the University of Manchester succeeded in purifying a protein called PARG found in bacteria that could reveal new drug targets for inherited breast and ovarian cancers as well as other cancers linked to DNA repair faults. They used one of Diamond's protein crystallography beamlines (I04) to solve the structure of the protein.

New foot-and-mouth vaccine signals advance in global disease control [12]

Diamond's protein crystallography beamlines were used by the research team who developed a new methodology to produce a vaccine for foot-and-mouth disease virus (FMDV). In 2013, a collaboration involving Diamond, The Pirbright Institute and the universities of Oxford and Reading published first results on a synthetic vaccine that is made up of tiny protein shells designed to trigger optimum immune response. It is safer because it isn't based on live infectious virus. It is also engineered to be more stable, and so the need for a logistics cold chain is reduced. This research represents a step forward in the global campaign to control FMDV where it is endemic, and could reduce the threat to countries currently free of the disease. Crucially, this new structure-assisted approach to making and stabilising vaccine could also impact on how other viruses from the same family are fought, including polio.

Scientists unlock the structure elusive 'stress' protein [13]

Scientists working to design advanced medicines that are perfectly targeted to control the body's natural receptors made a major discovery in 2013 using Diamond's microfocus protein crystallography capabilities on I24. Heptares Therapeutics, a leading UK-based drug discovery and development company, was responsible for identifying the 3D structure of CRF1, the protein receptor in the brain which controls our response to stress. This discovery will help scientists to develop improved treatments for depression and anxiety. Furthermore, having identified the architecture of CRF1, scientists now have a template that can be used to accelerate research into other protein receptors that are known to be in the same 'family', including those that can be targeted to treat Type 2 diabetes and osteoporosis.

Tackling "hidden hunger" [14]

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[10] http://impact.ref.ac.uk/CaseStudies/search1.aspx

[11] Slade D, Dunstan MS, Barkauskaite E, Weston R, Lafite P, Dixon N, Ahel M, Leys D, Ahel I. The structure and catalytic mechanism of a poly (ADP-ribose) glycohydrolase. *Nature*, 477 (7366): 616-620 (2011).

[12] Kotecha A *et al*. Structure-based energetics of protein interfaces guides foot-and-mouth disease virus vaccine design. *Nature Structural & Molecular Biology*, 22: 788-794 (2015).

[13] Hollenstein K, Kean J, Bortolato A, Cheng RK, Dore AS, Jazayeri A, Cooke RM, Weir M, Marshall FH, Structure of class B GPCR corticotropin-releasing factor receptor 1. *Nature*, 499 (7459): 438-43 (2013).

[14] A.L. Neal, K. Geraki, S. Borg, P. Quinn, J.F. Mosselmans, H. Brinch-Pedersen, P.R. Shewry,

Scientists from Rothamsted Research and Diamond collaborated to devise a technique that allows them to pinpoint the exact location of multiple essential nutrients such as iron and zinc simultaneously in wheat grains. The research, which is ongoing, utilises Diamond's spectroscopy beamline I18 and offers hope for the acceleration of attempts at wheat biofortification, which can be used to increase the iron and zinc content of wheat products. This is important since some 1.3 billion people worldwide may be deficient in zinc, with clinical consequences including impaired immune responses.

Advances in industrial catalysts [15]
Scientists have been striving for many years to prepare porous solids within which they are able to mimic the sophisticated chemistry performed by nature. In 2010, researchers from the universities of Cardiff and Manchester succeeded in engineering crystals that are able to maintain their structure, providing a permanent porous matrix within which chemical reactions can take place. With this new porous crystal, made from an iron-containing compound called phthalocyanine, the group looked to nature to maximise its potential within the field of industrial catalysts. Diamond's single crystal diffraction beamline (I19) was used to establish that it is feasible to make porous crystals with the reactivity of hemoproteins and produce more effective man-made catalysts.

Spintronics potential for electronic materials [16]
The rapidly advancing field of spintronics, which involves the manipulation of electron spins in device technology, has led to big improvements in magnetic storage. However developing spintronic analogues of active electronic devices has proved much more challenging. A collaboration involving experimentalists and theorists from seven different countries in Europe and Asia have now shown that the semiconductor WSe_2 exhibits spin-polarised electronic states despite retaining bulk inversion symmetry. This research, which was done on the angle-resolved photoemission spectroscopy (ARPES) beamline (I05) and at MAX-III in Sweden, opens up the potential for a new class of materials in which spins can be controlled for possible logic applications.

Conserving a national treasure [17]
Henry VIII's warship, the Mary Rose, is the only 16th century warship on display anywhere in the world. Since 2008, scientists from the Mary Rose Trust, the University of Kent, Diamond and Daresbury have been bringing samples of the wood timbers to Diamond's spectroscopy and IR beamlines to enhance their knowledge of the conservation process to preserve the historic timbers. Now that the ship is drying in the new museum, samples are brought every six months so that any potential issues can be identified and addressed swiftly.

3.2 Industrial engagement

Iron and zinc complexation in wild-type and ferritin-expressing wheat grain: implications for mineral transport into developing grain, *J. Biol. Inorg. Chem.*, 2013, 18, 557–570.

[15] Grazia Bezzu, C., Helliwell, M., Warren, J.E., Allan, D.R., McKeown, N.B., Heme-Like coordination chemistry within nanoporous molecular crystals. *Science* 2010: vol. 327 no. 5973 pp. 1627-1630

[16] Riley J. M., Mazzola F., Dendzik M., Michiardi M., Takayama T., Bawden L., Granerød C., Leandersson M., Balasubramanian T., Hoesch M., Kim, T. K. Takagi H., Meevasana W., Hofmann Ph., Bahramy M. S., Wells J. W. and King P. D. C. Direct observation of spin-polarized bulk bands in an inversion-symmetric semiconductor. *Nature Physics* 10, 835 (2014)

[17] Schofield, E. Sarangi, R., Mehta, A., Jones, M., Mosselmans, F., Chadwick. A., Nanoparticle de-acidification of the Mary Rose *Materials Today* 14. 354 – 358 (2011)

With Diamond now firmly into its third phase of construction, the availability of new beamlines is allowing industrial usage to thrive. The scope for industrial research and development is greater than ever before allowing our clients to probe their systems of interest with greater resolution or under closer to realistic operating conditions. Much of the engagement with industry occurs via collaboration with university groups, indeed we estimate that approximately 25% of all experiments at Diamond have some industrial involvement, much of which establishes 'proof of concept' that leads to stronger involvement by industry. However, we have also set up a dedicated unit – the **Industrial Liaison Group** – to engage directly with industry.

The Industrial Liaison Group at Diamond raises awareness of the benefits of Diamond in the commercial sector and supports them to make best use of the synchrotron and associated facilities throughout their research programme. The team of scientists covers a wide range of specialisms including macromolecular crystallography, X-ray absorption spectroscopy, small angle X-ray scattering, X-ray powder diffraction and small molecule crystallography. The myriad of ways in which we support industrial scientists include running a mail-in service across a number of techniques, providing a full analytical service where we translate research problems into solutions, and collaborating on large research projects either through peer review or grant funded projects.

While the pharmaceutical sector is still the predominant user of Diamond beamlines (mainly for macromolecular crystallography), an increase in both usage and income is being seen throughout the physical sciences. Over 90 companies from a range of sectors as shown below have purchased beamtime through the proprietary (fee-paying) route, using a broad range of beamlines and techniques. The current level of proprietary use of Diamond beamlines is ~ 5%. However, an analysis of questionnaires sent to non-MX users accessing Diamond through peer review revealed that ~ 17% of the users had direct industrial involvement in the research undertaken at Diamond, with an additional 17% having indirect industrial involvement.

Diamond also engages with industry through the Diamond Industry Science Committee (DISCo), which has representatives from 12 different companies various industries including the pharmaceuticals and aerospace sectors.

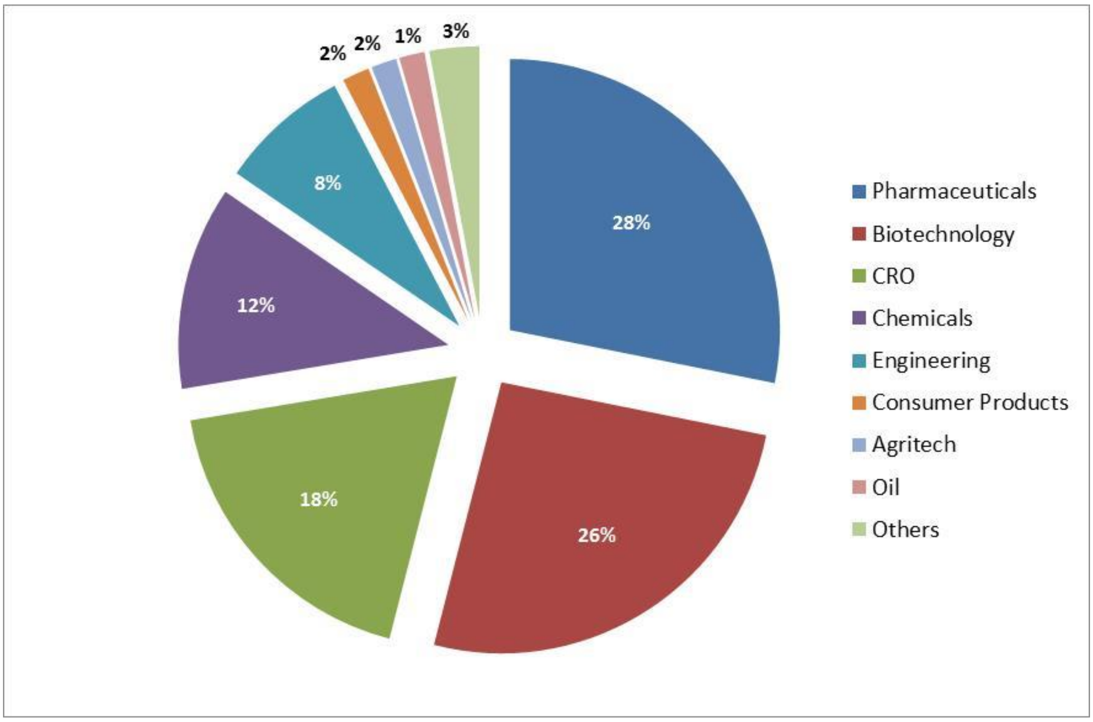


Figure 10 *Income by market sector 2014-15 where 'CRO' denotes 'Contract Research Organisation'*

Proprietary users of Diamond come from a wide range of sectors, as is illustrated in **Figure 10**, while **Figure 11** displays the growth in industrial income over the years, broken down into the physical and life sciences. It should be noted that the decrease observed in FY 2014/2015 compared to the previous year is primarily due to cancellation of experiments after the failure of the RF cavity in 2014; data for 2015 to date indicate that the delivery of such beamtime is recovering to the levels before the cavity failed.

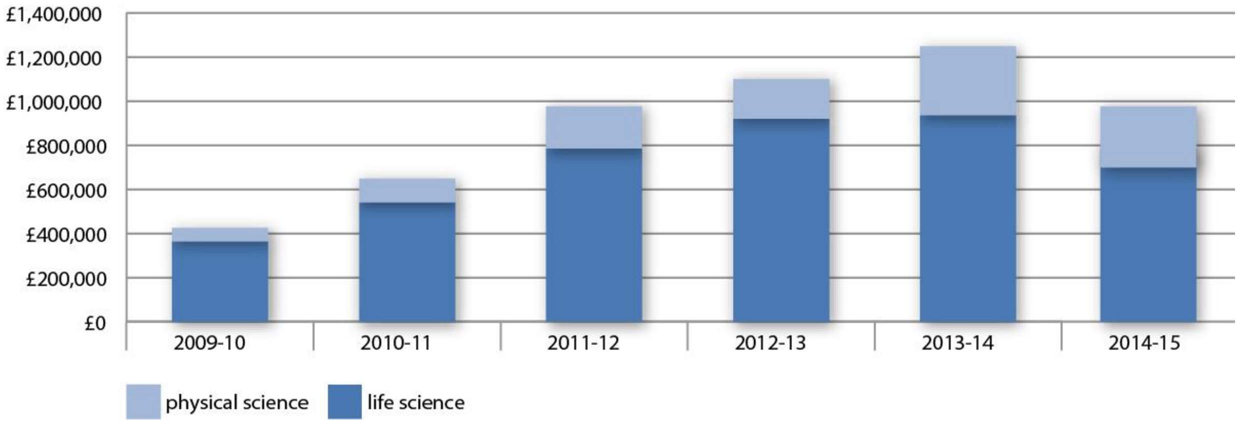


Figure 11 *Industrial income from beamtime sales by financial year showing the split between life and physical sciences. (The decrease in 2014-15 is due to RF cavity failure and subsequent cancellations of bookings).*

Two examples of scientific highlights since the start of Diamond operations are given below, with further examples in **Appendix 1.**

Drug Discovery

The industrial use of Diamond has, to date, been dominated by the life sciences sector, with around 75% of proprietary use by pharmaceutical and biotech users. Given the nature of Diamond's beamline portfolio it is not surprising that structural biology has been the primary usage by this market sector. Examples include the structural determination of serine racemase by Evotec using data collected at beamline I04, one of four tuneable MX beamlines at Diamond. Serine racemase is responsible for the synthesis of D-serine, an endogenous co-agonist for N-methyl-D-aspartate receptor-type glutamate receptors (NMDARs), the overactivation of which is involved in acute and progressive neurodegenerative diseases such as stroke, amyotrophic lateral sclerosis, and Huntington's, Alzheimer's and Parkinson's diseases. Another example comes from scientists at Heptares Therapeutics who used beamline I24 to reveal the complex structure of the vital adenosine A_{2A} receptor and show how xanthine-based drugs such as caffeine bind to their target. Adenosine A_{2A} receptors regulate the effects of neurotransmitters in the brain, cardiovascular and immune systems, and are of particular interest as a drug target for Parkinson's disease.

"GPCRs represent the single most important family of drug targets in the human body because they are central to so many biological processes. The design of drugs for GPCRs is hampered by the lack of structural information so access to a facility like the Diamond synchrotron is vital to our research. It has enabled us to solve the 3D structure of the adenosine A2A receptor in complex with caffeine and other xanthines as well as our own novel drug candidates."

Dr Andrew Doré, Senior Scientist at Heptares

In situ Catalysis

Catalysis is estimated to be involved in 90% of all chemical processes and in the creation of 60% of the chemical products available on the market, but still it is rarely analysed at the atomic scale. The need to understand catalysis at this level is driven by both economic and environmental concerns; therefore, there is a global interest in optimising the syntheses of new catalytic materials and in understanding the fundamental process of catalysis. A proper understanding of structure-property relationships plays a central role in the design and discovery of novel catalysts. In many cases, exploring the relationship between the structure of these new materials and their physical and chemical properties requires that measurements are carried out under exactly the same *in situ* conditions of temperature, pressure and atmosphere as the materials would experience in their performance environments.

Scientists from Johnson Matthey have used beamline B18 at Diamond to carry out X-ray Absorption Spectroscopy (XAS) measurements. The main goal of this experiment was to determine the types of platinum species present in representative current technology of fresh and road aged diesel vehicle emission control catalysts, obtained from registered UK car dealers in both non-coastal and coastal regions. Detailed analysis of the XAS data revealed the presence of a mixture of oxidic and metallic species in the fresh catalysts. In the road aged catalyst the Platinum was metallic in nature. Johnson Matthey were able to rule out the presence of toxic chloroplatinate species in the materials.

"We did this work on behalf of the International Platinum Group Metals Association and were able to conclude that there were no Pt-Cl bonds present in the samples. Working with Diamond gave our scientists access to world-class beamline facilities and staff"

Dr Peter Ash, Johnson Matthey Technology Centre

3.3 Technical and technique developments

Machine Performance

Over the 8 years since Diamond became operational, the number of hours of scheduled User Mode operation has built up to the nominal target figure of 5000 hours while at the same time there has been a significant improvement in reliability as shown in **Table 2**, and illustrated in **Figure 1**. Uptime represents the beam hours delivered as a percentage of scheduled hours while MTBF is the Mean Time Between Failures i.e. beam trips. The maximum current has also increased from the initial operation at 150 mA to the nominal 300 mA.

Year	Scheduled User Mode (h)	Uptime (%)	MTBF (h)	Max. current (mA)
2007-8	3495	93.7	11.2	150
2008-9	4305	95.0	15.3	250
2009-10	4728	97.0	26.2	275
2010-11	4728	97.5	28.5	200
2011-12	5064	97.7	55.4	300
2012-13	4872	98.3	52.4	300
2013-14	5088	98.2	60.3	300
2014-15	4944	97.6	38.6	300

Table 2. *Improvements over time to beam characteristics at Diamond*

During this time various other improvements have been introduced which enhance the performance of the facility – though it should be noted that the drop in MTBF in 2014-2015 arose from the failure of the one of the RF cavities followed by the slow process of conditioning the replacement to operate reliably as the current was brought back up to 300 mA. Stability has been improved by the introduction of fast-orbit feedback (Jul. 2007) and the top-up mode of operation (Oct. 2008). X-ray brightness has been enhanced through a reduction in vertical emittance from the nominal 27 pm-rad to 8 pm-rad (Oct. 2012). Some special modes of operation have also been introduced. A "low-alpha mode" was introduced (Apr. 2009) to produce short X-ray pulses (~ 3.5 ps rms) for time–resolved measurements as well for enhancement of the THz radiation on the IR beamline. A 156-bunch mode has also recently been made available.

Substantial changes to the ring have also been made in order to accommodate particular new beamlines. Extra quadrupole magnets were installed in long straights 13 (Aug. 2010) and 9 (Mar. 2011) to implement "double-mini beta" schemes which allow two narrow gap undulators to be installed in each straight section. A fast polarization switching scheme has also been made available on the I10 beamline (Aug. 2012).

The Diamond machine has thus developed considerably since initial operation in 2007. Further major improvements will however be needed to keep Diamond at the forefront of 3rd generation light sources, as detailed later in this document (section **4.2.1**).

Science Division

Diamond has the most advanced complete detector data acquisition systems for X-ray spectroscopy in the world as a result of long-term development programme started many years ago at the SRS. Quantum Detectors Ltd, which is jointly owned by STFC and Diamond, is now supplying the resulting Xspress3 systems to synchrotrons worldwide. Diamond has developed the highest performing double crystal monochromators in the world. These are now in use on four beamlines at Diamond and the principles that they employ are being adopted by commercial suppliers.

It is widely acknowledged that software development is one of the greatest ongoing challenges facing modern scientific user facilities. Soon after first users the decision was made to adopt a centralised high performance computing environment, a model now being widely adopted, and from the beginning Diamond decided to create a fully coherent and all-encompassing data acquisition system for all beamlines. The resulting Generalised Data Acquisition (GDA) system is unique worldwide and developing into a formidably competitive environment for carrying out synchrotron experiments. This system has been made Open Source and is therefore freely available for all facilities to adopt.

3.4 Skills for success

As a world-leading centre for synchrotron science it is critical that we maintain a highly skilled staff base, engage the user community with our work, and work with schools and universities to encourage and grow the next generation of scientists, engineers and technicians.

Developing our staff

Diamond staff are in general very highly skilled, with a diverse range of specialisms and are drawn from over 40 different countries. Of ~ 550 personnel (summer 2015), 45% are in the Science Division, 40% in the Technical Division with the rest in administrative and other supporting roles (15%). To ensure that we maintain our position as a global leader in synchrotron science, we support our staff to develop within their roles, and offer training which enables personal and professional advancement.

Our scientists are encouraged to undertake world-class research, and more than 15 hold professorships at universities around the UK. Diamond scientists hold UK grants to the value of ~£1.3M and collaborate with over 25 institutes and universities in the UK. A further £2M has been brought in from the European Commission in recent years to support transnational access and projects. These collaborations ensure that synchrotron science is at the heart of leading research, and that the expertise held by our scientists is shared and exploited as effectively as possible. Diamond is committed to equality, and to encouraging a diverse, fair and professional workplace. To this end, we are drawing up plans to be a member of the Athena SWAN Charter.

Creating skilled communities

Diamond relies on the scientific community being aware of, and engaged with, the techniques offered at Diamond in order to succeed. We must communicate our capabilities effectively, and ensure that the facility offers opportunities for users to build their knowledge of and skills in our techniques.

Every year, Diamond welcomes around 6,500 visitors on-site through outreach, communications and scientific event activities. About 50% of these visitors attend events which develop scientific and technical skills.

Our commitment to developing skilled researchers starts at the earliest stages of a scientific career. Diamond hosts an active programme of PhD studentships, currently co-funding over 70 active studentships, and maintains 100 collaborative partnerships with 32 Universities. Around 1000 PhD students had beamtime at Diamond in 2013/14. To further support young researchers, we work with Doctoral Training Centres, and run courses and events for PhD students.

Inspiring future scientists

Diamond's success is dependent on its skilled, dedicated staff and the user community around it. To safeguard this success in the future, the facility must ensure that young people are given opportunities to engage with our science and technology. Our work with future scientists and engineers starts with our schools programmes. For schools, Diamond offers a rare glimpse of how science works; an interdisciplinary, vibrant and diverse space in which talented people carry out vital research.

Our work with young people and University students goes beyond early stage career training – we aspire to build networks of skilled young scientists, who view the facility as a key partner long into their careers.

3.5 Key collaborations

As Diamond has grown, so it has forged alliances with a range of partners who bring complementary skills, experience and activity. The establishment of the MPL and the EMF has already been noted, but there are other very significant collaborations with UK universities and in international consortia.

Diamond and the **University of Manchester** (UoM) are collaborating to fund and operate a branch of the I13 Imaging and Coherence beamline. As a result of the collaboration the UoM have now placed a significant number of staff and students (~ 25) on the Harwell Campus, some of whom are located within the I13 external building, with most of the team based in the RCaH.

Diamond also has a number of joint appointments with UK universities including the Universities of Oxford, Leeds, Reading, York, UCL, Birkbeck and with STFC. New joint appointments are currently being progressed with several other universities, and Diamond is currently exploring other possible collaborations with other universities.

The UK is taking a leading role in the development of a new structural biology facility (**SFX**) at the European **X-ray Free Electron Laser** (**XFEL**), in Hamburg, Germany. At Diamond, as part of the Wellcome Trust and UK Research Councils funded strategic award, the UK XFEL Hub is being established to explore opportunities to exploit this facility. SFX brings together members of the scientific communities in some eight countries. Diamond is also an active partner, together with colleagues at Daresbury and in the wider user community, in a STFC-led review of the needs of UK scientists to access FELs in future

The UK XFEL hub will act as a focus for a number of activities including: development of hardware and software for SFX; provision of a sample environments lab to enable users to prepare samples for current liquid jet technologies at operating hard X-ray FELs; provision of a user access Programme for SFX/SPB and currently operating hard X-ray FEL facilities worldwide.

Diamond also collaborates with STFC in a variety of technical projects, primarily in detectors and precision engineering for beamline development and is in the process of exploring other areas in which it can work more closely with STFC on technical projects and to make better use of their technical expertise in areas such as cryogenics and magnets for sample environment. STFC provides services for data storage and networking and is currently discussing with Diamond how to collaborate more widely in data analysis through their Scientific Computing Department.

3.6 Health and safety

Since becoming operational Diamond's health and safety performance has developed as part of the organisation's commitment to continual improvement. The most notable indication of this progression is the transition from a three-star site at start-up to a five-star site in 2012, through the British Safety Council (BSC) Health and Safety Management System audit. Another of the fruits of Diamond's commitment to safety management has been sustainment of a low accident rate throughout its operational period. As part of this assurance review programme the site went on to achieve the BSC Sword of Honour in December 2013, an award designed to recognise excellence in safety management.

3.7 Engaging Society

From its inception in 2002, Diamond recognised the vast potential it has to engage and excite public audiences as well as inspire the next generation of scientists. Diamond's profile has continued rising as the facility has grown, helped by the successful delivery of the facility on time on budget and to specifications, as well as by a series of large scale events and media campaigns.

Diamond is committed to engaging the public with its vision and mission. Since Diamond was established, we have welcomed over 30,000 visitors, allowing direct access to some of the most inspiring scientists and research programmes in Europe. One of our strategic objectives is to 'To engage and inspire the general public through promoting science', in line with the UK Government's ambition to 'stimulate and sustain public discovery of science'. Implementation of the strategy includes some of the following areas as examples:

- **Education programme**. As part of our education programme, we welcome 2000 students each year to Diamond. Our events for schools include regular education open days, which give insight into the operation of the facility, and allow students to meet with our scientists and engineers. We also run subject dedicated days, and an innovative programme of special events delivered with key partners. Diamond plays a vital role in training young scientists and helping to get youngsters interested in science and engineering from an early age. We also hold placement schemes for undergraduate and school age students, enabling valuable hands-on training at the facility.

- **Public programme**. Regular events are organised for the public, with a weekend 'Inside Diamond' event 5 times per year, and small evening visits for community groups which promote open conversation between the visitors and our scientists and engineers. Around 1500 members of the public access Diamond each year through the regular open days. Since their introduction in 2009, over 6000 members of the public have visited via this route. We use our open days as a showcase for our users, with a science fair featuring research groups from around the region and beyond.

- **Offsite engagement**. Outreach and engagement at science festivals and cultural events is also an important part of our programme. Events in which we participated have been attended by over 100,000 visitors since 2009.

- **Media profile**. Diamond has had a strong media relations programme from the day construction started. The institute has made good use of international platforms such as the American Association for the Advancement of Science annual meeting to showcase our scientific outputs and capabilities, as successfully shown in our 2009 worldwide campaign which achieved a total audience reach of 78 million. Over 150 pieces of media coverage items on our scientific research were generated in 2012 alone through the various campaigns undertaken. Diamond has also been able to secure national high profile broadcast pieces like features on the BBC's Ten O'Clock News for its launch and several medical stories. In 2013, the new Foot-and-Mouth Disease Virus Vaccine received worldwide coverage, reaching 298 million people.

- **International**. Diamond has been a catalyst in mobilising Light Sources in Europe to work collaboratively under a Networking grant under Frame 7 EU funding to work together through joint press conferences, journalists' visits and briefing materials. In addition, Diamond provides management and financial administration for Lightsources.org, a global network of some 20 synchrotrons and free-electron-lasers. Internally, the communications and public engagement team provide the technical underpinning and editorial support for all communications software and web systems at Diamond, with the exception of the User Administration System.

Diamond is able to achieve all that it does, in terms of engaging with society, through the commitment of senior management, and a dedicated team of volunteers. One third of our staff help with these activities and they are supported through a tailored training and development programme. The facility also looks to forge partnerships with funding bodies, industry collaborators, museums, science centres and festivals so that external funding can be secured for specific projects and we can reach the large audiences that can be accommodated at external public events.

3.8 Environment

Diamond's environmental impact is in respect of the amount of electrical power it consumes, which to a large extent is inescapable given the operating parameters of the machine and the facility in general. This, together with some gas used for domestic heating, indirectly gives rise to the production of carbon dioxide emissions which are summarised in the table below.

	Year to 31st March 2014 tonnes	Year to 31st March 2013 tonnes
Carbon Dioxide Emissions arising from:		
Electricity Consumption	21,913	21,595
Gas Consumption	1,109	1,282
Total Carbon emissions	23,023	22,877
The emissions (tonnes) per user shift were	2.79	2.98

The emissions per user shift have fallen year on year reflecting improvements in efficiency as the number of shifts increases year by year, and a number of initiatives which have reduced our power consumption by ~15% compared with what would have been case had these actions not been taken.

These actions included the installation of variable speed drives (VSDs) on electric motors, the installation of sensors and LED lights on lighting systems and changes in operational parameters for the air handling units and domestic heating systems.

Our emissions have been further mitigated by the installation of a solar panel array which became operational in April 2013 and generated nearly 100MWh in its first year of operation. Further actions to improve our environmental impact will be constrained by the availability of capital funding but could include: the installation of further VSDs, in particular on the Dry Air Coolers; Helium gas recovery and liquefaction facility; the installation of further solar panels.

3.9 Cost savings and efficiencies

Although Diamond's operating costs inevitably increase as more beamlines become operational the relatively high fixed cost base of operating the facility means that the incremental costs of additional beamlines (and of increasing the number of shifts available from each beamline as its operation is optimised following "first user") do not increase proportionally with the increase in available shifts. This means that as more beamlines are added (and their operation optimised) Diamond inevitably becomes increasingly cost effective. This was recognised in the Phase III Business Case where a 45% increase in the number of beamlines was predicted to require only a 17% increase in operating costs. It is also illustrated by the data on cost per shift summarised in **Table 3**.

It should be noted that that the number of user shifts is only a proxy measure for output. The increasing application of automation, improved detectors and data analysis, and changes to modes of access are all contributing to further increases in output as well as improvements in the scientific outcomes. It is difficult to measure these further improvements, the impact of which will vary from beamline to beamline and science area to science area, but they can be illustrated by the fact that the number of MX shifts required in order to generate a protein structure for deposition in the PDB has fallen to little more than half of those required before the recent upgrades to the MX endstations.

	No of Shifts	Operating Costs (£ M)	Cost per Shift (£s)
2009/10 Actual	3,572	30.5	8,538
2010/11 Actual	4,996	33.5	6,705
2011/12 Actual	6,600	36.5	5,532
2012/13 Actual	7,683	39.8	5,180
2013/14 Actual[18]	8,264	42.5	5,144
2014/15 Actual	8,221	44.4	5,400
2019/20 Forecast[19]	12,642	54.9	4,343

Table 3. *Evolution of operating cost per shift at Diamond as the number of beamlines has increased*.

Since operations commenced Diamond has implemented a number of schemes to reduce its operational costs, many of which were associated with the environmental improvements referred to in section 3.8. These cost reduction schemes are summarised below in Table 4. There have been other exogenous changes to Diamond's cost structure since it began operations. These include the following:

- Increase in employers pension contributions (from 2010/11) - £0.8 M increase *per annum*
- Introduction of the CRC tax (from 2011/12) - £0.4 M increase *per annum*
- Reduction in business rates (from 2013/14) - £1.2 M saving *per annum*
- Increase in employer's NI contributions (from 2016/17) - £0.52 M s increase *per annum*

[18] Costs have been not been adjusted for the Business Rates rebate
[19] At 2014/2015 economics

Category	Action	Savings 2011/12 (£K)	Savings 2012/13 (£K)	Savings 2013/14 (£K)	Projected savings 2014/15 (£K)
Electricity Consumption Savings	Installation of light sensors, variable speed drives and resetting of various operational parameters	383	427	460	500
Gas Consumption Savings	Reducing water heating during summer months[20]	25	20	10	40
Liquid Nitrogen Consumption Savings	Retendering LN_2 contract and improving efficiency of distribution pipework	49	43	40	40
Manpower Savings	Bringing maintenance resource 'in-house' and introducing plant efficiencies	81	163	176	176
Total Savings achieved/projected from completed schemes (£K)		**538**	**653**	**686**	**756**

Table 4. *Summary of principal saving schemes for Diamond operations and their impact*.

[20] Necessary load testing of chillers - artificially increased gas consumption

4.0 A 10-YEAR VISION FOR DIAMOND

The scientific achievements of Diamond outlined in sections 3.1 and 3.2 illustrate the critical role that world-class synchrotron facilities play in developing and supporting key areas of the physical and life sciences and engineering and this will continue for the foreseeable future. While there have also been dramatic developments in recent years in other techniques - most notably electron microscopy (EM) - and keen anticipation of what FELs will deliver, their technical capability will only impact on a relatively small fraction of the portfolio of important science served by synchrotrons. It is therefore clear that if the UK is to remain competitive in addressing the most significant scientific and societal problems it should continue to have access to the very best synchrotron facilities, both in the UK at Diamond and at the ESRF where different beam characteristics offer complementary research opportunities. This vision for Diamond focusses on solving the scientific challenges that will be at the heart of UK scientific and industrial development over the next 10 years, and beyond, and defines how the technical and operational performance might be enhanced to meet these challenges. It also recognises that many of the most challenging scientific problems can only be solved through an integrated approach that brings together multiple techniques and teams of people with complementary skills and experience from universities.

Our vision for Diamond is therefore to be:

- A world-leading centre for synchrotron science, driving and supporting science at UK universities and research institutes that is regarded as internationally excellent, and enabling essential research and development for UK industry;
- A cornerstone of a world-class site for scientific discovery and innovation at Harwell.

The different scientific components of the Vision have been organised into 7 general areas and are presented in section 4.1, with further details provided in Appendix 2.

- Integrated Structural Biology
- Chemistry and Catalysis
- Soft Condensed Matter
- Biomaterials and Medicine
- Engineering and Materials
- Condensed Matter Physics
- Environment, Earth Sciences and Cultural Heritage

We describe the key technical developments that will be needed to meet these scientific challenges (section 4.2), as well as defining the wider infrastructure we might need to deliver our vision (section 4.3). It should be noted that delivery of the vision will depend on many other, non-technical qualities, from the excellence of our staff to the effectiveness with which we engage with our current and developing user communities. The present structure and operating model for Diamond was established at a time when it was preparing for construction. Now that it is approaching full operating strength, it is timely to reflect on whether this model is optimal for the delivery of science. It is also timely to reflect on the evolution of the way that science is pursued, with greater integration of different techniques, higher throughput and automation in some areas, and increasing demands in many areas for faster access to beam time and results. Some aspects of this are outlined in section 4.4, with further details provided in our description of the wider strategy proposed to deliver our vision in section 5. Finally, we indicate some of the key developments that are planned for other synchrotron facilities to provide a global perspective on what we propose (section 4.5).

4.1 Scientific Vision and the Role of Synchrotron Radiation

X-rays, IR and UV light generated at Diamond reveal the structure, composition and dynamics of matter with a spatial and temporal resolution that access details down to atomic and molecular levels revealing the most fundamental processes such as the motion of electrons or vibrations in molecules. They are unique analytical tools for the physical and life sciences and for tackling some of the most important technical and societal challenges that confront our society, now and for years to come. These challenges are embodied in the '8 Great Technologies', presented by the UK Government in 2013 [21] as an essential part of its economic strategy:

- Advanced materials and nanotechnology;
- Agri-science;
- Big data and energy-efficient computing;
- Energy and its storage;
- Regenerative medicine;
- Robotics and autonomous systems;
- Satellites and commercial applications of space;
- Synthetic biology.

Driving forward these technologies requires major technical advances for which synchrotron radiation will be an essential enabling tool – from antibiotic resistant bacteria to stronger, lighter alloys for more fuel efficient transport, and from the treatment of degenerative disease to quantum computers and the development of new synthetic strategies in chemistry as feedstocks have to adapt to the changing availability of hydrocarbons to protecting and maximising our vulnerable soil resources.

4.1.1. Integrated Structural Biology

Modern molecular biology really took off when the power of an atomic level description of DNA to explain fundamental aspects of genetics became clear. However biology is immensely complicated and it is now clear that to understand the workings of cells across all forms of life requires an in depth knowledge at the molecular level of the many complex structures involved. Deciphering the often weak and transient interactions between these structures and the diverse roles they play in the makeup and biological functions of cells is a unique strength of structural biology. Beyond this, structural biology is now expanding its reach towards the *in situ* cellular context, and aims to link to the traditional field of cell biology. Achieving a molecular description of life is now one of the grand challenges in biology, and will transform our understanding of disease processes, allowing a more effective definition of targets for drug design. More generally questions such as 'what is the molecular basis of memory?' can not only inspire a generation of researchers but might yield insights to drive whole new technologies – as an example one of the latest methods of DNA sequencing is based on pore-forming proteins (Oxford Nanopore Technologies Ltd). To realise this ambition requires increasingly sophisticated advanced methods, and continued technical developments.

Synchrotron radiation provides the definitive example of how highly efficient advanced infrastructure provided as an efficient dedicated user service and driven forward by technical and engineering advances has revolutionised our molecular understanding of biology. Specifically, macromolecular crystallography (MX) at third generation synchrotron sources has in recent years been responsible for the vast majority of protein

[21] https://www.gov.uk/government/speeches/eight-great-technologies

structures deposited with the PDB. These structures provide atomic details of enzymes, adhesion molecules, macromolecular complexes, membrane proteins and viruses, which have transformed our understanding of the molecular machinery of the cell. The remarkable level of automation achieved and improvement in speed and quality of data derived from increasingly small crystals has enabled studies of more difficult systems. Furthermore much of the work done at Diamond is now via remote data collection. This relentless focus on optimising productivity and the user experience we characterise as ‘the synchrotron model’ and is now being applied to optimise workflows at other beamlines (in both life and physical sciences).

The methods for integrated structural biology are described in more detail in Appendix 2, and include several synchrotron methods, including notably small angle scattering and X-ray microscopy, but increasingly electron microscopy is making a major contribution. We propose to provide tools for ordinary users to make the best use of the various techniques and also to roll out the synchrotron model to all other cutting-edge structural biology methods requiring advanced infrastructure, To this end we now offer cutting-edge electron microscopy at Diamond (see box).

A model for further integration? In April 2015 a high-end electron microscope was installed on a synchrotron hall floor for the first time – adjacent to I20 at Diamond. Before the end of June it was delivering a user programme and atomic detail structures, such as that shown to the right (GroEL, Birkbeck College).

However there is also the need to integrate the various methods if we are to achieve the goal of extending our study into more complex systems extending from subcellular organelles through to imaging of whole cells. To this end at Harwell a concerted effort is in place to enable exactly such a multidisciplinary approach, providing imaging, scattering and diffraction capability across the spectrum and extending to electron microscopy and tomography and super-resolution light microscopy. These methods are developing very rapidly and in the appendix we outline some of the expected challenges and opportunities over the next 5-10 years. Our ambition, by working closely with other infrastructures such as Instruct (see Appendix 2), is for Diamond to become the central player in an internationally leading centre, which will not only attract users from the UK and beyond to more effectively reveal the inner workings of the cell, progressing ultimately towards a full dynamic picture of living organisms, but also have strong links with chemists and clinicians to facilitate the effective application of the knowledge in medicine and biotechnology.

4.1.2 Chemistry and Catalysis

Chemistry plays a major role in many of the Global Grand Challenges identified by all of the UK research councils, in particular sustainability, health, enabling technologies and resilient economic growth, both in terms of fundamental understanding of chemical processes and in the development of new substances and technologies. In 2010, the International Council of Chemical Associations estimated that the chemical industry was directly responsible for approximately 5% of the world GDP and supported the employment of approximately 20 million people. It has been estimated that 90% of all chemical processes make use of a catalyst [22], and according to the North American Catalysis Society this translates, through their role in the fossil fuel cycle, to 35% of the world GDP being reliant on catalytic processes. The long standing goal of catalysis research is to enable new synthetic processes for the production of current materials or new substances. This result requires an integrated approach to the total catalytic process, focused on products, feedstocks, catalytic materials, and energy sources. Desired future efficiencies dictate enhanced selectivity, an effort that focuses on the catalytic materials themselves. In order to minimise consumption of non-renewable energy sources such as fossil fuels, it is important to develop processes that utilise alternative energy inputs. The ultimate dream is to have the knowledge required to be able to custom design the catalysts that are appropriate for enhancing whichever chemical processes need to be undertaken.

Research in chemistry and catalysis has greatly benefited from the use of synchrotron radiation facilities. The use of spectroscopy and scattering techniques has allowed the elucidation of the geometrical and electronic structures of the different species involved in chemical processes with the goal of relating this knowledge to their function. The development of high-brilliance third generation sources has taken us from the need to study model systems primarily under vacuum to enabling us to follow fast processes under *operando* conditions and under realistic reaction conditions of concentration, temperature, etc. Synchrotron facilities have enabled the study of chemical species at very different length scales, from the atomic structure (sub-nanometer) to the long range order structure or meso-scale, and time scales, from femtoseconds to days.

Nowadays, it is recognised that in most cases it is insufficient to investigate chemical processes with a single structural and/or analytical technique, and the evolving paradigm prescribes the application of multidisciplinary methods if the comprehensive insight required for knowledge guided process optimisation is to be obtained. This approach may perhaps lead to the ultimate experiment elucidating fundamental understanding of chemistry: observing single molecules at the timescale of an elementary reaction step, i.e. femtoseconds. Implementation of this multitechnique strategy can only be made possible by closer links with industry and academic researchers and the Catalysis Hub in the Research Complex at Harwell is seen as an exemplar and first step of this strategy. The need is for a fully integrated approach to the study of chemistry and catalysis using SR centred facilities. This will entail the development of better technologies such as faster and more sensitive detectors but these must be designed around sample environments which mimic industrial operating conditions. A whole system approach to study of catalysis combined with high throughput automation will allow optimal experiments to be carried out which shorten the path to development of commercially useful product. The long-term requirement of this approach may be to build a new beamline dedicated to chemistry and catalysis while the most fundamental studies may need new beam operating conditions to be developed to study reaction on the shortest timescales.

4.1.3 Soft Condensed Matter

Soft Matter is the name given to a diverse class of materials which has vast economic importance and which plays a central role in many of the grand societal challenges, including energy, healthcare, and the digital economy. Soft solids, typified by polymers, food and healthcare products all share one thing in common; that their structure changes over a range of length scales and this property is a vital factor in their value.

Development of improved materials will have a profound impact upon the generation, transport and storage of energy. Organic photovoltaics, for example, are destined to play an important role in reducing our reliance on

[22] G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, ed. Handbook of Heterogeneous Catalysis. (Weinheim, 2nd ed., 2008)

fossil fuels in turn helping to resolve the energy crisis. Success could lead to materials that could coat the outside of buildings potentially leading to some skyscrapers being net contributors to the National Grid. Gas storage materials, such as metal-organic frameworks and zeolites, are becoming increasingly important in the rise of the hydrogen economy. These could have a significant impact in helping combat climate change. The use of molecular materials with particular electron, magnetic or optical properties may lead to new materials for the digital economy.

Polymeric and gel-based materials are essential components for healthcare products. Society needs new and improved materials which can replace components such as heart valves and joints. There is a rapidly increasing need for synthetic materials to accelerate the healing of biological tissue and to develop new biosensors. One target is the creation of biomechanical and self-healing materials for use in hospital trauma recovery where, introduced as a patch, they will integrate with the natural tissue and provide a scaffold for future skin/muscle growth. Crucial to their application will be a detailed understanding of the self-assembly and reassembly processes on the molecular level.

Success in all of these visionary applications rests upon an understanding of the structure and behaviour of materials from knowledge at a molecular level and which then extends over all lengthscales: from the nanometre to the visible. In addition it is necessary to be able to probe the response of materials to changes over timescales which span millionths of a second to years. Synchrotron radiation provides a suite of tools which meet all of these requirements for knowledge. Furthermore, due to the penetrating nature of X-rays it is possible to study soft matter under operating conditions.

Future developments planned at Diamond for the study of soft matter, include brighter, more coherent sources, improved optics and X-ray detection together with continued software development for real time data evaluation and structural modelling. These will extend the range of length and time scales available in a single study. Smaller samples in complex systems will be studied which will make it possible to mimic real processing conditions where a soft solid may be a small but necessary component of a bigger system. The properties of many of these systems are often time and history dependent and difficult to reproduce precisely so it can also be important to combine many measurements – for example complementary probes of optical or mechanical properties – to build up a much more complete picture. The impact of SR in the study of soft solids has been profound, but only a tiny fraction of those who might benefit from using SR actually do so. Therefore an important part of our vision for the next decade is to make it possible for a much larger group of scientists and technologists to access SR by making the facilities simpler to use and much more efficient to operate.

Looking back across the past two decades it is clear that the impact of SR in the study of soft solids has been profound. However only a tiny fraction of those who might benefit from using SR actually do so. Therefore an important part of our vision for the next decade is to make it possible for a much larger group of scientists and technologists to use SR as a necessary part of their business model. This vision can only be realised by making SR facilities both simpler to use and much more efficient to operate which demands development of better sources, improved optics and X-ray detection together with continued software development for real time data evaluation and structural modelling. At the same time these development will allow studies under real processing conditions where a soft solid may be a small but necessary components of a bigger system. This will allow SR studies of soft matter at Diamond to simultaneously expand the impact upon industry and venture into new areas of discovery.

4.1.4 Biomaterials and Medicine

Many people are living longer than in the past and a fundamental challenge is to maintain wellbeing into old age. This is a key driver for today's frontier research in biomaterials and medicine. In practice this means attempting to find solutions to complex sets of diseases such as cancer, neurodegenerative diseases (including Alzheimer's and Parkinson's diseases), cardiovascular ailments, diabetes, and infectious diseases. All of these have a major impact on public health and society.

One area where there is an urgent need for improvement is the development of new/early investigation methods and instruments for diagnosis – e.g. biomarkers and imaging techniques. These naturally arise from fundamental research and may derive from advanced methods, key among them synchrotron measurements, which then allow translation into tailored diagnostic methods to bring these methodologies as close as possible to clinical application. Given the complex nature of these diseases there is now a significant focus on personalised patient treatment and so rapid and precise measurements as close to the bed-side as possible are required, meaning that methods need to be mapped to routine/affordable hardware. The role of SR is to provide essential structure based validation of the analytical methodologies that will be required for personalised medicine.

A further increasing area of activity is Stem Cell research, now a field of research in its own right. Although there are still thorny social issues to be resolved, synchrotron radiation, for instance IR microspectroscopy, might reveal early developmental cues at a single cell level.

At a more macro scale modern health research also addresses improvements in the replacement of organs or human tissue, using for example, bioactive scaffolding as well as regenerative approaches. For regenerative medicine stem cells are key and significant progress has been made, so it is now feasible to grow bone structure, skin or even, to some extent, organs. The high resolution X-ray imaging techniques developed at SR facilities will provide essential insight into the interplay between biological function and physical structure and permit the improvement of both aspects.

Finally, dramatic increases in the human population present challenges in ensuring future food supplies, prompting significant efforts in plant research, especially high resistance/high nutrition crop selection and transgenic modifications. More generally, plant biology is an extremely important field of fundamental research where there is a considerable role for integrated structural biology, for example in the crucial aspect of mimicking photosynthesis where biophysical models should be tested and developed through ultrafast dynamic experiments promised by state-of-the art SR studies.

In general, the understanding of biomaterials and biomedical tissues calls for high contrast imaging and quantitative microanalysis. This requires a facility such as Diamond that can offer a portfolio of techniques with high sensitivity and selectivity at different resolution and length scales ranging from subcellular to major organs. The length scales therefore span microns to sub-nanometres in often delicate or soft materials that push X-ray microscopy and scattering methods to their limits. Nanometre resolution is needed in 3D on samples that are sufficiently large to encompass to provide a genuinely representative context, for instance of an organ. Indeed whole system studies are much more desirable rather than studies of thin sections. A major challenge for Diamond is to develop detector systems with optimum signal to noise. Photon counting imaging detectors are therefore a long-term goal in studies of biomaterials. Finally for such integrative studies no single technique can tell the whole story and SR experiments must be complemented by other microscopy and spectroscopy studies, either *in situ* at the beamline or off-line, including at facilities elsewhere on the Harwell Campus such as in the Research Complex. The challenge is to make multi-technique approaches available concurrently with SR measurements. Such correlative methods would provide a considerable improvement for both imaging and spectroscopy. In almost all cases, measurements should be made under conditions as close to 'ambient' for living organisms or tissue as possible, requiring dedicated facilities for sample preparation or culturing and purpose-built equipment on beamlines to provide the correct, controllable sample environment.

4.1.5 Engineering and Materials

Excellence in the fields of engineering and materials is widely recognised as a key requirement for a society to remain economically competitive in the 21st century and in all developed nations, access to synchrotron radiation is an essential enabling technology. The discipline of engineering is concerned with understanding the creation and performance of useful objects across a range of length scale and times which span from the atomic scale to the properties of whole objects, e.g. turbine blades and times which span the impact of a shock wave in matter through to the long-term storage of nuclear waste or the integrity of civil engineering structures. Engineering concerns itself with the way that objects are made such as by casting or welding and also by the way that objects fail by cracking or corrosion.

Engineering materials are frequently structurally complex, spatially heterogeneous materials in which the properties of one component on one length scale will couple to the properties of another component at a different length scales: for example in fibre reinforced materials. In order to move from empirical methods of materials discovery to materials development by design, information is required at all significant lengthscales. This is a challenge ideally suited to synchrotron radiation.

Development of new materials underpins all strategies for meeting the energy challenges facing society. The need for new materials includes more radiation resistant materials for nuclear power, more efficient solar cells, fuel cells and lighter longer lived batteries. Functional applied materials will increasingly combine multiple properties for smarter utilisation. Advances will build upon the deeper understanding provided by condensed matter physics of these very complex materials. Outcomes are expected in denser data storage devices that need lower power. Additive layer manufacturing promises a paradigm shift in low energy manufacturing. Synchrotron radiation will be exploited to monitor the development of structure, strains and defects during the deposition process in order to enhance the chances of success and to gain competitive economic outcomes.

During the past two decades the use of X-rays for imaging and diffraction from the nano- to macro-scale has revolutionised the use of synchrotrons for engineering. The challenge of the next decade is to make these facilities more widely usable and to extend their use to circumstances that are ever closer to the point of application. Improvements are required in the available flux, automation, sample environment control, detectors and software to speed every stage of study. These changes will revolutionise the use of synchrotrons for engineering and materials. The primary opportunity for SR in the engineering rests in the increasingly efficient exploitation of *in operando* experiments which mimic manufacturing conditions. The next generation of photon counting high energy detectors will revolutionise the study of dynamic processes across a vast range of timescales (from µs to years). Increasingly, a multiprobe experimental philosophy will be needed which may in the next decade prompt the need for new beamlines or experimental endstations for dedicated studies of processes linked to particular manufacturing industries (e.g. pharmaceuticals, energy or transport).

4.1.6 Condensed Matter Physics

Research into the physics of solid matter carried out over the past century has revolutionised our society making possible all modern modes of communication and the digital world, as well as many devices that are now regarded as essential for medicine, transport and energy efficiency. Many of the leaps in technology that enrich our lives today were based on concepts that were often considered esoteric and overturned accepted models of nature at the time. Looking forward, we should anticipate that frontier research in condensed matter physics will continue to be a rich source of ideas and principles for tomorrow's technology.

Superconductivity is just one example of an area still ripe with promise. First observed more than 100 years ago, the phenomenon at low temperatures was explained in 1957 and since then has found uses in numerous applications, the most notable of which is found in MRI medical scanners. Superconductivity has also been observed at higher temperatures and applications for this are now emerging, but a coherent and universally accepted theory for this phenomenon is still elusive, and challenges remain in understanding and controlling the influence of imperfections on the performance of real materials. SR provides a particularly powerful probe of the subtle interplay between the principal forces at play in superconducting materials, controlling electronic, magnetic and structural behaviour, together with the chemical composition and role of defects. Increasing the speed with which new materials may be characterised and improving the resolution in space and energy with which the physics can be explored, in combination with theoretical insights, is *the* most promising route to understanding this phenomenon, and has provided several of the key insights on which our current understanding of the phenomenon is based. The rewards of success in fully understanding principles of room temperature superconductivity cannot be overstated, offering the tantalising prospect of vastly improved utilisation of energy in the plethora of superconducting technologies, and making new technologies, for example for high-speed computing, much more readily available.

The intellectual challenge of condensed matter physics is harder to explain. There is an infinite number of different ways in which atoms can be assembled into a solid and the resulting properties emerge from a subtle interplay between the precise position of individual components and their individual electronic properties. The key idea in the field is that when individual atoms are brought together then a collective behaviour emerges which can be radically different from that of the individual components. One frontier that is being explored in this field is the transformative influence of nanostructure or quantum fluctuations on such collective behaviour, providing evidence for the existence of new states of matter which touch upon some of the most profound outstanding problems in fundamental physics. Such matter may also have wholly new properties that could provide the basis for truly disruptive technology – for example the elements for practical quantum computers that will utterly transform the scale and scope of computational work in the future.

Testing the validity of theories requires experimental data and synchrotrons are key providers of the tools and techniques which not only help decide which theories are best but also give pointers to the need for new theories and hence applications. When Diamond Phase III is complete, the UK will have a suite of beamlines which are capable of studying the atomic, electronic and magnetic structure of materials across length scale which spans from nanoscale and interfaces through to device-scale objects. These beamlines will allow the behaviour of matter on timescales which extend down to ps and which provide a coherent link to the fs studies made possible at X-ray free electron laser facilities.

Studies of fundamental properties will link directly to studies of their technological application. Whilst the medium term practical objective is for steady improvements to existing technologies which will give the hardware to cope with ‘big data’ the long-term big vision is to replace what we have now by entirely new technologies, for example in quantum computing.

4.1.7 Environment, Earth Sciences and Cultural Heritage

The environmental and resource challenges facing mankind are increasing in number and in complexity. Demand for natural resources is surging, mineral and energy resources are depleted and soil, water and our atmosphere are threatened. The extreme versatility and unique capabilities of a synchrotron to provide definitive chemical and structural information on the most complex natural materials mean it is the most important facility for addressing these environmental challenges, underpinning the UK’s sustainable growth. The proposed technical developments at Diamond will improve, by an order of magnitude the spatial resolution, detection limits to realistic concentrations and acquisition times and provide a step change in scientific quality and output. At one extreme, fundamental questions about Earth and planetary evolution will be answered by the ability to undertake *in situ* experiments at very high P and T, while at the molecular scale the environmental processes and mechanisms involved in elemental cycling will be defined. The development of nano-scale analysis will provide the ability to interrogate the miniscule fragments of planetary and interstellar materials, including the intriguing possibility of products from the Mars return missions of the mid-2020s.

The identification of the speciation of a very wide range of anthropogenic and natural, inorganic and organic pollutants in contaminated brown-field sites, soils, aerosols and water is essential for their control and remediation. SR has already played an essential role in highly sensitive analysis of structure and elemental composition of phases in a wide range of environmental media although for the detection levels of some toxic elements are well above their lower toxicity limits. The latest challenge to the environment is the unknown effect of nano-materials. The new XAS-based and high brightness lattice developments will provide information at ppm levels and nm spatial resolutions that will allow validation for the models constructed to predict the production, transport and impact of pollutants, and define their effect (e.g. nanoparticles) on a cellular scale. Perhaps the UK’s most pressing challenge in this area is the understanding the fate of long half-life radionuclides (such as U, Np, Pu, Am, Se and Tc) in the engineered and natural barriers of a geological disposal facility which is essential for developing the safety case for secure, economic long-term storage of our legacy and future nuclear waste.

The search for new and secure supplies of strategic minerals/elements essential to UK manufacturing requires identification of new natural sources and innovative pathways of extraction, while minimising environmental footprints. Determining elemental coordination environments in low concentrations and undertaking bio- and chemical leaching *in situ* using XAS and tomographic chemical imaging techniques is vital to optimise the efficiency of mineral extraction. The UK’s future energy demand requires novel and innovative engineering techniques to extract new fossil fuel resources on untapped energy reservoirs such as shale gas and complex petroleum containing lithologies. This successful and environmentally sustainable exploitation requires the full understanding of the fine graining host rocks, their mineralogy and response to extraction techniques, using the unique combination of micro-diffraction and tomography that current and proposed beamline developments provide.

The power of synchrotron radiation to probe complex natural materials is exemplified by the ability to examine the mineral-fluid-microbial-organic-plant components in surface environments such as soils, perhaps our most valuable and vulnerable natural resource. The demands for food generation increases while soils become exhausted and polluted. Understanding the behaviour of nutrients and toxins in evolving soil systems is essential for their protection and sustainability, through managing agricultural practices and addition of amendments. The soft X-ray, imaging, nano-probes, tomography, micro-focus and environmental cell developments allow a holistic understanding of these multifaceted systems and the range of coupled biotic and abiotic processes that determine their fertility. For example, the role of bacteria and other organisms in biogeochemical cycling of both essential and toxic elements, as well as nanostructures, surfaces and interfaces in such processes.

Cultural Heritage. Finally, we wish to explore opportunities to work more widely in the field of cultural heritage, applying SR as a uniquely powerful tool to look deep inside valuable objects that may be very fragile or dense and opaque. The challenge in applying SR to cultural heritage does not primarily lie in development of new technologies but in using existing technologies in the most effective manner to answer 'cultural' questions. The long standing and highly productive collaboration between Diamond and the Mary Rose Project shows that the most important and frequently component is people who understand the opportunities afforded by SR and who also appreciate the multifaceted language of cultural heritage. The enabling step for this field is the establishment of trained staff and preparation laboratories and storage and sample environments to support users who are generally non-expert in SR methods, but who nonetheless represent a very important activity in the UK, both culturally and economically with wide public appeal.

4.2 A vision for technical development at Diamond

The sweep of science encompassed in our vision is very broad but it contains a number of common themes in terms of the types of measurements that scientists aspire to perform in future. There is an increasing need to study smaller samples, or regions of samples such as interfaces and defects that are inherently small, often over a wide range of length scales. There is also a compelling need to study materials in an environment that is yet closer to real operating, or *in situ*/*vivo* conditions – or to make samples in the beam itself. New areas of science will be opened up by measuring structure, composition, electronic or magnetic character much faster than is presently possible, enabling processes to be followed in real time, or for many more samples to be studied per day and then map structure-property relations far more extensively than is currently possible. It is also becoming increasingly important to integrate the results of experiments across beamlines and with other techniques, perhaps across facilities to tackle increasingly complex systems and materials; this will require new ways of handling workflows, and even of granting access to beamtime. And more data, taken more quickly will place unprecedented demands on our ability to handle and analyse information.

The range of technical developments that could have been proposed to achieve the vision as extensively effectively as possible was potentially immense, and outside the bounds of realistic future budgets and resources, so the various possible projects were prioritised as outlined in section 5.6 and designated '**option 1**' (essential, or 'must have' to retain or achieve world-class status), '**option 2**' (highly desirable to retain or achieve world-class status), and '**option 3'**, which were not considered any further. The projects that were retained are organised and presented below as steps in the measurement process, from the source, through the beamline (including the sample environment, optics and detectors) to data analysis, each of which is vital in transforming scientific ideas into knowledge and innovation. The key developments for each of these stages are as follows.

- **Improve the reliability and performance of the source**, first by upgrading Radio Frequency (RF) components to increase reliability, then developing brighter insertion devices to deliver higher photon flux to beamlines, and achieving greater stability of photon beams to better exploit higher repetition rate detectors. An extensive study will be conducted of options for a future lattice upgrade – 'Diamond II' - which could be envisaged leading to a reduction in the horizontal emittance of the storage ring (increase in brightness) by at least an order of magnitude early in the next decade. This must be matched by a compelling business case based on new scientific opportunities afforded by such an upgrade, together with a robust plan to minimise the impact on our user community of a long shutdown early in the next decade.

- The performance of beamlines can be transformed by new technology, so if Diamond beamlines are to retain their competitive edge and offer the most incisive tools to tackle the most challenging and significant problems, there needs to be a **vigorous campaign of beamline upgrades**; we also propose new beamlines or significant development of endstations that will open new areas of science, previously inaccessible at Diamond.

- Development and implementation of **key enabling technologies for detectors**, both in house and in collaboration with other laboratories and facilities, many of which will be crucial to exploit the full potential of brighter sources. Projects will be conducted to enable or produce: faster measurements, below μs and perhaps even down to ns timescales; higher-performance area detectors enabling faster collection rates or with much smaller pixel size, or different geometry or with higher efficiency for softer or harder X-rays; higher throughput spectroscopy measurements through detectors with greater count rate and effective energy resolution.

- Develop in-house facilities for **fabrication and metrology of optical components**, promising unprecedented spatial resolution of beamlines (ultimately < 10 nm over 10 years), and reducing risk of reliance on a small number of very specialised companies. This will also be essential for the full exploitation of future, lower emittance sources.

- Enable a much wider range of science to be performed at beamlines through significantly greater provision of equipment for **specialised sample environments**, particularly for *in operando* or *in situ* measurements, enabling systems to be studied during chemical and biochemical reactions and processes, or under the mechanical thermal and electrical loads experienced by engineering or electronic materials during manufacture or in use.

- Diamond is already reaching its limits in terms of **storage and analysis of increasingly vast quantities of data**, together with the means to make them available remotely to users and provide fit-for-purpose means of analysis. As data rates from detectors become ever faster, and increased automation speeds up throughput, so it becomes increasingly important to be able to visualise and analyse data sufficiently quickly to allow decisions to be made in real time and optimise the efficiency of experiments. The analysis of data sets will be increasingly integrated across beamlines and with other types of measurement, requiring new methods of handling workflows. Much greater use will be made of high performance computing for modelling and simulation of yet more complex systems, both for preparation and post-experimental analysis. Many of these challenges are common to other types of facilities and collaborative approaches should be sought.

Further details of what is envisaged in each of these areas are given in the following sections, as well as Appendix 3.

4.2.1 Sources

One of the main figures of merit for 3rd generation synchrotron light facilities is the horizontal emittance, to which the brightness and transverse coherence of the radiation are directly related (brightness and coherence being inversely proportional to emittance). When Diamond started user operation in January 2007 it had the smallest emittance of the medium-energy synchrotron light sources (2.7 nm), and the second lowest in the world, after the APS (2.5 nm) (**Figure 12**).

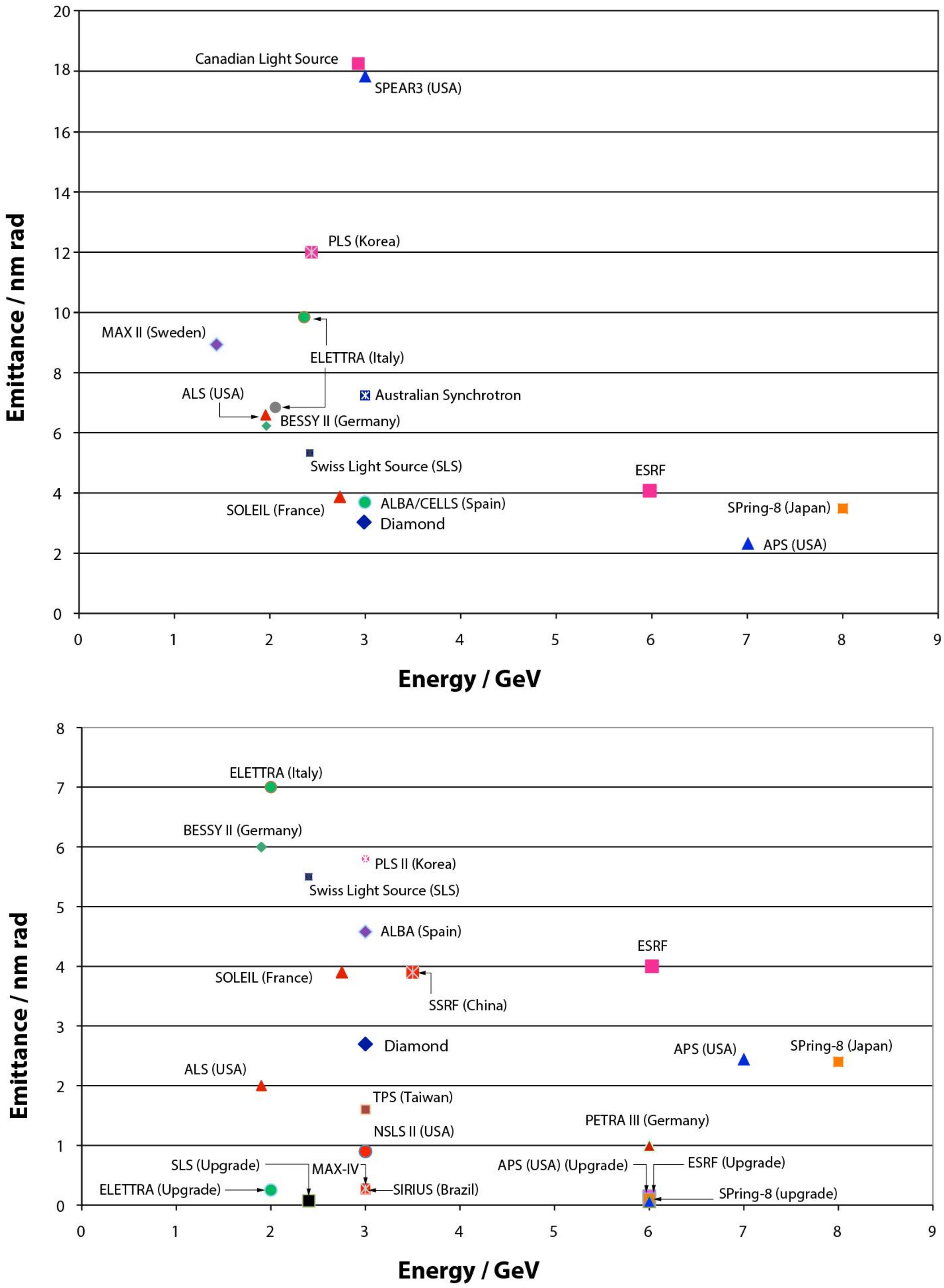


Figure 12. *Comparison of the emittance of 3rd Generation Synchrotrons (a) at the time Diamond came into operation and (b) the situation in 2014, together with indications of proposed or planned upgrades.*

There have however been significant developments in the field since then: PETRA-III came into operation in 2010 with 1 nm emittance and the ALS was upgraded from 6.3 nm to 2 nm emittance in 2013. More importantly, two new medium-energy machines are under construction with sub-nm emittance: MAX-IV in

Sweden will come into operation in 2016 with an emittance in the 230-330 pm range and Sirius in Brazil will come into operation in 2018 with an emittance of less than 280 pm, both of which are 3 GeV rings. Elsewhere, many facilities are proposing or studying upgrades that will reduce the emittance significantly: ESRF will upgrade in 2019-20 to a new lattice with ~140 pm emittance and studies are underway at most other facilities e.g. ALS, APS, ELETTRA, SLS, SOLEIL etc. Initial studies at Diamond have shown that a reduction in emittance by an order of magnitude or more might be feasible. Given the importance of radiation brightness, and transverse coherence, for many experimental techniques, it is clear that for Diamond to offer the most significant and exciting experimental opportunities into the next decade and beyond it must take advantages of such technical advances and plan for a similar emittance upgrade i.e. **Diamond-II**.

Physics options studies, followed by a detailed Technical Design Study and Science Case for Diamond-II should therefore be initiated in the near future. Preliminary studies based on a six-bend achromat concept indicate that the source brightness could be enhanced by a factor of 20-30 while at the same time significantly increasing the capacity for insertion device beamlines, which would re-position Diamond, early in the next decade, on the leading edge of light source development. In combination with upgrades to detectors and optics this will deliver the highest coherence flux in focal spots reaching down to 10 nm in size, enabling structure and chemical composition to be studied at unprecedented length and timescales. However, it will take at least five years to complete the technical design and carry out such an upgrade, and the case to proceed or not needs to take a holistic approach and assess the benefits – and possible disadvantages – for the entire beamline suite. The timing of any upgrade should also take into account downtime in other major facilities, particularly the ESRF around 2019, and even then careful thought needs to be given to how the needs of the UK community - both academia and industry - would be met in this period.

In parallel, it is essential that several other performance improvements are implemented in the short/medium term in order to fully exploit the existing facility. These address different aspects of performance of the source and are therefore not incompatible with a possible future Diamond-II.

- An **improved resilience and reliability** of the superconducting RF system is urgently needed. The reliability of the machine as a whole has been dominated since the beginning by that of the RF system. In normal operation, the RF has been responsible for more than half of all short duration beam trips, as a result of cavity vacuum events or various faults in the RF power source. In addition, a number of RF cavity failures have resulted in significant periods of reduced beam current and enhanced trip rates during the lengthy conditioning of a new cavity. The most recent cavity failure in early September 2014 has prompted a reconsideration of the longer term strategy for the RF cavities.

  Our plan for building greater resilience and reliability into the RF system is firstly to install **two additional normal conducting RF cavities**. As a by-product, this will also provide sufficient additional capacity to be able to run with 3 rather than 4 inductive output tubes (IOTs) per superconducting cavity in the event of a trip, which should assist in terms of overall reliability. To provide further resilience against failure of the superconducting cavities, and to allow the nominal beam current to be maintained even when the cavities are operating with reduced performance, the possibility of installing further normal conducting cavities will be considered.

  A second cause of unreliability has been the IOT-based RF amplifiers which supply power to the superconducting cavities. Furthermore, in the longer-term they will become obsolete, as the market moves towards solid-state RF technology. In the accelerator world, there is also a movement towards solid-state RF, which has been shown at SOLEIL in particular to be extremely reliable. As we already have a considerable number of IOTs, and the cost of solid-state RF is currently high, the strategy here is initially to introduce solid-state amplifiers for the additional cavities that are installed and over a longer period, as funding permits, migrate to solid-state RF.

- The conversion of one double bend achromat (DBA) cell of the storage ring into a double-double bend achromat (**DDBA**) allows an extra beamline to be built based on a high performance insertion device, which would not otherwise be possible (essentially converting a bending magnet port into an insertion device port). The DDBA conversion of Cell 2 in the storage ring is already going ahead as part of the implementation of the Phase III VMXm beamline (completion Aug.-Sep. 2016); a second cell for DIAD is also under consideration.

- Improvements in **brightness**, particularly at high photon energies, are being pursued through the development of a new generation of Cryogenic Permanent Magnet Undulator (**CPMU**), and its subsequent deployment to upgrade several key beamlines. Such devices would be simpler than superconducting undulators and their cryogenic systems are more cost effective. The project is underway and tests of the cryogenic system have successfully been carried out. The first device will be used to upgrade the I24 beamline (Mar. 2016).

- Various improvements in **electron beam stability** are needed. Firstly, it is now necessary to improve the vertical orbit stability in the frequency range > 100 Hz, partly as a result of the reduction in vertical emittance from 27 pm to 8 pm that was implemented in 2013, but also in view of faster detectors that are rapidly coming on the scene. Such demands can only increase further with Diamond-II. The approach will be to try to reduce the source of the disturbance, rather than embark on a major upgrade of the orbit feedback system. An investigation is therefore needed to determine where the significant contribution to beam motion in the 150-400 Hz range comes from, and to design and implement engineering solutions. The specific objective of this project will be to reduce the integrated vertical orbit motion (1 Hz – 1 kHz) from 10% to 3% of beam size (with 8 pm vertical emittance) by the end of 2017.

  Secondly, an improvement in longitudinal stability is needed. The majority of experiments that use the synchrotron photon beams cannot resolve the individual bunches in the storage ring, which are of the order of 5 mm rms in length (equivalent to ~17 ps in time). There are however experiments that do make use of the time structure of the radiation, and in this case the longitudinal stability of the electron bunch becomes important. The present level of stability of the bunches is of the order of 5.5 ps rms, however an improvement by an order of magnitude is requested. This will be achieved by means of an improvement to the "low-level RF" (LLRF) system which stabilises the amplitude and phase of the accelerating fields in the RF cavity. Diamond presently uses analogue LLRF systems, however in recent years digital systems have been developed at several labs, which not only provide greater stability, but are also much more flexible in their operation.

  Finally, a reduction in the disturbance of the electron beam during top-up is required. The injection of electrons into the Diamond storage ring, as with other synchrotrons, results in a small disturbance of the orbit of the stored electron beam, due to an imperfect cancellation of the series of "kicks" produced by the four injection kicker magnets. During top-up, injection occurs with beamline shutters open and hence this orbit disturbance can introduce unwanted artefacts in the experimental data, depending on the sensitivity of the beamline optics and method of data taking. Signals are available to gate-out these regular disturbances, however using these would disrupt experiments on many beamlines. The situation up to now has been satisfactory, but this is unlikely to be the case for all beamlines in the future, especially as beamline optics and detectors improve, and so effort is needed now to tackle the problem.

- Improvements in **photon beam stability** are needed for several Phase-III or upgraded beamlines in view of the continuing improvement in beamline optics and the push for increasingly smaller spot sizes at the sample. Although this will be improved by increases in the electron beam stability, it is also influenced by the stability of all the intervening optical components in the beamline and therefore needs a coordinated approach and the development of appropriate feedback systems. Such a project could lead to a feedback system being implemented on instruments such as the Phase III beamline VMXm by mid-2017.

Further highly desirable developments include the following.

- Increase in **beam current** from the present 300 mA. This would be desirable for many beamlines, however, this cannot be achieved with the current RF installation. Another superconducting cavity, or multiple normal conducting cavities, must be installed together with their associated RF plants. Any plan to increase beam current requires careful assessment, in order to maintain reliability (which is of higher priority than beam current) and resilience in case of catastrophic vacuum failure (which influences the type and location of any further cavity installations). To progress much above 350 mA will also require the installation of a 3^{rd} harmonic cavity in order to overcome the RF heating that results from the short bunches in Diamond.
- Development of **Super Conducting Undulators** (SCUs). SCUs will in principle provide a further increase in brilliance compared to CPMUs particularly at high photon energy. The projected improvement possible with the SCU currently under development by STFC (in collaboration with Diamond) is ~ 50% at 30 keV, however further gains are possible in principle in the longer-term with the development of Nb_3Sn technology. The R&D phase should be completed in 2015, at which point a strategic decision needs to be taken on whether to proceed with the construction of a full device.

4.2.2 Beamline development

Any ambitious synchrotron facility will aspire to installing beamlines that are at least world-class, if not world-leading when they are commissioned. However, the rapid speed of development of key components of beamlines, means that they rapidly become uncompetitive without regular upgrades to incorporate advances in technology, particularly to optical components, end-stations and detectors. Some of these upgrades will arise from in-house technical development, or collaborative projects with a significant in house contribution, as outlined in sections 4.2.3 and 4.2.4; others may be delivered through purchase of components developed and manufactured outside Diamond. We propose a programme to upgrade many of the older beamlines at Diamond to ensure that they remain competitive world-wide, and offer the very best opportunities to tackle the scientific and societal challenges of our vision. This process has already started: many of our older beamlines have already been upgraded through prioritised projects supported by our operating capital budget, and these have proved essential to ensuring that these beamlines have maintained Diamond at the forefront of what can offered to its users. A case in point is the programme of end-station and detector upgrades on our MX beamlines which have ensured that they have remained 'best in class' in the world and Diamond is now one of the most productive facilities in the world in this field. Priorities for continued beamline development would be informed by the expert beamline review process with the SAC, starting with a review of the proposals outlined briefly in Table 5, to establish 'must have' and 'highly desirable' options. Such development will also be constrained by the availability of expert technical support, so we envisage no more than 2-3 major upgrades being completed in any one year and this is the basis on which we have calculated the approximate resources and volume of activity associated with such upgrades expressed in Figure 16.

Beamline Name and Number	Future Developments	Science Benefits
I02/I02-1 - Versatile MX (VMXi/ VMXm)	Exploiting the latest detectors, insertion devices and optics. Leading development in software	Leading the world in study of the most challenging problems in structural biology to be tackled ahead of anyone else in the world,.
I03/I04/I04-1 – Macromolecular Crystallography	5-fold increase in flux through provision of CPMUs, upgrades to automation, optics, detectors and software.	Diamond retains world-leading position in protein crystallography. Increase capacity to match increasing user demand.
I06 - Nanoscience	Reorganised beamline layout for enhanced throughput. Ultra high-resolution (<5 nm) PEEM instrument.	Determination of electronic structure of individual nanostructured objects and more efficient use restoring world competitive status.
I07 - Surface and Interface Diffraction	New focussing optics to exploit advances in X-ray monochromators coupled to next generation detectors, automation and ultimately a new lattice for the storage ring.	New insights gained more swiftly into fundamental structural, electronic and magnetic properties, greatly accelerating and widening the scope for discovery of technological materials.
B07 - VERSOX: Versatile Soft X-ray	Endstations for the second branch of Versox will enable high throughput spectroscopy in the 1-2 keV for structure of materials containing relatively light elements ($Z \leq 14$).	Very significant extension of the range and impact of Diamond in the pharmaceuticals, formulation science and earth sciences (e.g. 20% of the earth's atoms have $Z \leq 14$).
I08 - Soft X-ray Microscopy	A new endstation offering full-field imaging down to 5nm resolution.	A ten-fold improvement in resolution will make the beamline a world leader in X-ray spectromicroscopy and benefit catalysis, earth and environmental science, biomaterials, and materials science.
I09 Beamline for Surface and Interface Analysis	New endstations for soft X-ray ARPES and surface science	Provide momentum resolved electronic structures of functional oxide thin films and buried interfaces. Removing the restriction imposed by soft X-rays for ultra clean surfaces in the study of electronic structure of complex materials – for example high-T_c superconductors – and buried interfaces. New capability for Diamond at the world's only two-branch, hard + soft energy beamline.
I10 - BLADE: Beamline for Advanced Dichroism Exp'ts	New detectors, endstations, improved sources and optics sources – and ultimately a new lattice for the storage ring	Accelerated materials discovery and new, faster insights into fundamental structural, electronic and magnetic properties
I11 – HRPD for energy and engineering materials research	New high energy detectors (area and linear) and upgrade optics to complement SCU source for energy and materials engineering research.	Greater penetration will strongly enhance energy research and engineering materials developments e.g. next generation battery materials, fuel cells, advanced alloys and nano-composites.
I12 - JEEP: Joint Engineering, Environmental and Processing	A multimodal facility to allow parallel measurements of nano- and mesoscale structure based on a new undulator	Greatly enhanced studies of: defects in engineering materials; deep earth processes; faster engineering processes slower processes in

	device and equipped with faster, high energy detectors with enhanced efficiency for kinetic measurements.	greater detail; soft materials at higher resolution, opening up new opportunities in chemical processing.
I13 - X-ray Imaging and Coherence	Full-field imaging to 5nm of electronic character in parallel with structure through: (i) upgrades to optics and detectors; (ii) greater coherence and brightness of Diamond-II.	This will make X-ray imaging a routine tool for science and bridge the gap between X-ray diffraction, and optical and electron microscopies.
I14 - Hard X-ray Nanoprobe	New mesoprobe branch for small angle scattering and pink beam imaging	Enables imaging SAXS of complex heterogeneous materials and provides new opportunities for studies currently not feasible e.g. scanning tomography of biological samples.
I15 - Extreme Conditions	Enable kinetic experiments through provision of faster, high energy detectors, renewed focusing optics, and second endstation for large-volume high pressure studies.	Studies of deep earth processes via access a much large part of the P-T phase diagram. Increased range of geological systems that may be studied.
I15 - XPDF	New high energy detectors, microfocus optics, and improved sample environments.	Maintain competitive status of one of the few beamlines worldwide dedicated to pdf studies for use by non-specialists.
I16 - Materials and Magnetism	New detectors, improved polarisation analysis, new monochromator and replacement of the 6 axis goniometer.	Maintain I16 as a world-leading beamline for study of fundamental structural, electronic and magnetic properties.
B16 - Test beamline	A large-object XRF endstation.	New applications in cultural heritage/ palaeontology.
I18 - Microfocus Spectroscopy	Procurement of world-leading XRF detectors. State of art detectors for XRD. New optics and rebuilt endstation, new CPMU source.	5 fold improvement in spatial resolution, 10 fold increase in speed. New insights in neurobiology, biomaterials, environmental science, catalysis and active materials. Huge increase in throughput.
I19 - Small-Molecule Single-Crystal Diffraction	Higher energy and spatial resolution detectors. New CPMU source, optics and monochromator.	Vastly accelerate discovery for energy materials and pharmaceuticals. Retain I19 as a world-leading facility
I20 - LOLA: X-ray Spectroscopy	New 4-bounce monochromator, new optics, source and detectors.	Making I20 the world-leading facility for ultradilute spectroscopy essential to tackle structural trace element analysis for biological, environmental and energy applications.
I21 - Inelastic X-ray Scattering	Polarisation analysis for RIXS.	Providing essential, detailed complementary magnetic measurements of excitations in functional materials
B21 - High Throughput SAXS	1-2 orders of magnitude increase in photon flux on SAXS beamline B21 through upgrades to optics.	World-class beamline to determine the structure of large biological macromolecules in solution to study ‘in vivo’ structure and assembly processes, and systems that defy attempts to crystallise.
I24 - Microfocus MX	5-fold increase in flux through CPMUs, with rolling upgrades to automation, optics, detectors and software.	Diamond and the UK retain their world-leading position in protein crystallography. Increase capacity in microfocus capability.

Table 5. *Proposed upgrades to beamlines categorised according to current Village membership, with the same colour code denoting village as in* ***Table 1***.

In addition to these essential upgrades to existing beamlines, we also propose to develop wholly new types of beamlines or new end-stations at existing beamlines that fill important gaps in our suite, and offer transformative opportunities for science. Polarisation of these projects would follow the procedures that have been developed for and well tested by the Phase I, II and III beamlines. Consultation with the user communities, industry and funding bodies is key, followed by rigorous review by the Diamond SAC. Requests for new beamlines will be constrained by the availability of insertion devices or bending magnets around the storage ring, or in competition with existing beamlines (although consideration should be taken of the opportunity for further insertion devices in the Diamond-II phase). Without further expansion of the technical groups who would be charged with the design, construction and installation of such beamlines, we will also be constrained in the number of new projects for the period 2015-2020, noting that Phase III will not be completed until 2018. However, given the long lead time for planning we believe it prudent to develop the scientific case and outline technical designs in the next 2 years for review and prioritisation with the aspiration to build 1-2 new beamlines a year beyond 2018. A provisional prioritisation of 'must have' beamlines has emerged through internal consultation and discussion at the Diamond Vision meeting of 2014, indicated by underlining of project descriptions in the following list.

- **Soft (0.25-5 keV) X-ray absorption spectroscopy** beamline to follow active species in real chemical and catalytic systems as reactions proceed. Consideration will be given to the need of expansion of capacity in the energy range 5-35 keV as part of this project.
- **SAXS/WAXS/USAXS diffractometer spanning unprecedented lengthscales**, from 0.1-10,000 nm, to study growth and properties of complex materials whose function depends on structure over a hierarchy of lengthscales.
- **Versatile, high-energy (40-60 keV) beamline spanning many timescales** (ms to years, extending the long-duration experiment model pioneered at I11) and combining SAXS, high resolution powder diffraction and high resolution imaging for functional materials and engineering processes whose performance may depend on a spectrum of dynamic processes.
- **High-throughput beamlines for rapid characterisation of complex, advanced materials**. A rate-limiting step in **materials discovery** is exploring the composition-property phase diagrams of multiple element, or multicomponent materials. It is proposed to equip key beamlines for the determination of chemical composition, structure, electronic and magnetic character with upstream endstations (leading contenders would include B07, I10, I16) to facilitate rapid scanning of phase space, aided by automation and rapid data handling and analysis.
- **New, multiple endstations on materials/engineering beamlines** to facilitate and provide huge efficiency saving for experiments requiring long set-up times (complement or adjunct to I11 and I15-1).
- **Enhancement of cryo-bioimaging facility**, correlative imaging of cryo-specimens with fluorescence microscopy, X-ray microscopy and electron microscopy will fully integrate an enhanced cryo-electron microcopy facility with Diamond's synchrotron activities. Given the huge expansion in the cabability of cryo-electron microscopy, we expect that the provision of two high-end microscopes in the national facility will be swamped by demand within the course of the coming five years. We predict that at least a doubling of capacity will be required. Funding for such instruments will be sought outside the capital budget of Diamond.
- **High resolution hard (3-15 keV) X-ray RIXS** to study electronic and structural excitations at real interfaces and inside 'dirty' materials – *i.e.* not prepared under very specialised, UHV conditions. A particular focus, reflecting research strengths in the UK, will be complex electronic materials containing heavy (4d and 5d) metals which have novel electronic transport properties, including superconductivity

- **Hard X-ray (2-10keV) PEEM to explore the electronic structure of buried objects –** bulk behavior of real, ‘dirty’ materials – i.e. below any surface impurity layers – and buried interfaces at unprecedented spatial resolution. This would be new beamline or side-station to I14
- **High field magnet facility (up to 40T, 0.08-2.0 keV)** to probe the fundamental physics in high temperature superconductors, antiferromagnets, and advanced functional materials such as multiferroics.
- **Facility for resilience in MX**: beamline enabling high-quality automated high throughput collection of data established at another synchrotron facility to ensure access for UK industry and academia almost 365 days per year.

It should be noted too that any new beamline, or new, independent endstation whose character is very different from the parent beamline, will require additional scientists and technical support for operations, typically at the level of 6 additional FTEs for each new beamline to exploit it effectively.

4.2.3 Detectors

Most of the major detectors currently in use at Diamond will need to be replaced or upgraded over a five to ten year timeframe in order to keep Diamond at the forefront of synchrotron radiation science. There is a need for faster, more efficient, and increasingly sensitive detectors which have improved spatial and energy resolution. A large fraction of these detectors do not yet exist but are being developed or will require a future development programme. This is too large a task for Diamond alone and therefore a strategic plan has been developed which spans all Diamond beamlines and which exploits the resources of the Diamond detector group, the STFC Technology Department, collaborations with other facilities and some university departments as well as through close customer-manufacturer relationships. Detector development is a key priority for all SR facilities worldwide and therefore in the context of Europe there exists a substantial opportunity for industry and facilities to collaborate within the framework provided by H2020 to make Europe the worldwide centre for detector development. Key areas in which detector upgrades are required are described below, all of which have been prioritised as ‘must have’ except for those presented under ‘other detectors’, which are ‘highly desirable’. Further details are provided in Appendix **A3.1**.

- **Higher performance area detectors.** It is arguable that the development of fast efficient area detectors has had the greatest impact of any technology outside of the rachet wall of a synchrotron facility and this continues to be the focus of the majority of detector development. Many detectors currently in use are not capable of counting all of the photons produced at the required speed and therefore detectors are needed that are better performing in terms of detection efficiency, maximum count rate and frame rate.
  The next generation MX, small molecule crystallography and SAXS beamlines benefit from detectors equipped to cope with a high photon flux and at much higher frame rates (around 1 kHz) with smaller pixels. These are being developed by a number of manufacturers and we expect to replace the entire suite of currently world-leading detectors on these beamlines over a 5-7 year period. These detectors will not only increase throughput, but they will provide higher quality data, extending the reach of the beamlines. Detectors for higher energies (>20 keV) currently lag behind those used in MX but will become available over a 1-3 year time period. Development of high energy detectors will allow the fabrication processes used in engineering and materials processing to be studied in real time and at atomic resolution. Extrapolating from the experiences gained by the introduction of new detectors and improved sample logistics in MX we would expect that throughput of materials sciences beamlines to be doubled as a result of such development.

Development of high resolution photon counting for X-ray microscopy would lead to a revolution in the field similar to that experienced within structural biology caused by the development of direct electron detection for electron microscopy.

- **Area detectors with different functionalities and geometry.** Whilst most highly performing photon-counting area detectors are based upon silicon sensors with 172 μm pixel size, there is a distinct need for detectors with different functionality. Small molecule crystallography requires energy windowed area detectors and smaller pixel size (a goal for many beamlines). Some such as the I13 imaging and coherence beamline could exploit detectors with very small pixel size, of the order of 15 μm. Furthermore detectors with novel geometries would benefit SAXS/WAXS beamlines and powder diffraction on I11 and the PDF branch of I15. A strategy is required of commercial procurement coupled to partnerships with STFC and other facilities for this area of development.
- **Detectors for time resolved experiments.** In-house and collaborative development projects will deliver area detectors with sub-microsecond time resolution and possibly down to the nanosecond range which will open the way to new experiments across material science (I11 and I12), in small angle scattering (I22), in IR (B22), and in X-ray photon correlation spectroscopy (I13). Microsecond time resolution may be achieved with hybrid technology area detectors by triggering, or pump-probe methods, but the duty cycle tends to be very low.
- **Better performing spectroscopy detectors.** Diamond has some of the best detector systems for spectroscopy of any facility but the detector is often the single factor that limits performance. In order to improve sensitivity and the throughput of the beamline there is a strong continuing need is to improve the count rate and effective energy resolution of these detectors. It is proposed to extend the performance of high energy detectors in an in-house and STFC development and to seek ways to encourage new suppliers to enter the market for germanium monolithic multi-element detectors. For XRF mapping, area detectors developed by Brookhaven National Laboratories and Australian Light Source are superior and we seek to buy them. Energy dispersive spectroscopy has been hindered for more than two decades by the lack of incident beam monitors: this is a development target for Diamond.
- **Improved soft X-ray area detectors.** This would bring enormous benefits both for diffraction, imaging and spectroscopy. The CCD cameras currently in use are limited in size and frame rate and if replaced would bring huge benefits to beamlines serving condensed matter physics, materials, life, and environmental sciences. The area detector used on the inelastic X-ray scattering beamline will be the single major barrier to performance. Diamond is collaborating with DESY and STFC in one project which should deliver a working prototype in two years. A long-term development project for high-resolution direct detection area detector will be sought with other facilities.
- **Other 'highly desirable' detectors.** Beam monitors are not completely satisfactory. More-compact beam stop monitors would be very valuable for small angle scattering beam lines. Other beam lines would benefit from more accurate beam position monitors able to withstand the beam power and also those with very little interaction with the beam when used permanently (i.e. thin devices). MX beam lines require, as soon as possible, beam position monitors for the use in feedback loops. An APD capable of working in the soft X-ray regime has been required by I08. Finally Bolometers could be improved for B22, as infrared detectors, and by I16, as very high energy resolution X-ray detectors.

4.2.4 Optics and metrology

The Optics and Metrology Group at Diamond provides essential and expert support to the Diamond beamlines in the design, testing and optimisation of beamline optics and the development of specialised optical systems.

Many optics used on today's beamlines are at the limit of the manufacturing capabilities of commercial vendors. The challenge over the next 10 years will be to produce optics that preserve the X-ray beam quality to allow experiments to be ready to exploit the upgrades to the Diamond source (DDBA and eventually Diamond-II) which will result in a lower emittance producing even higher brightness and more coherent X-ray beams and increased X-ray power density.

It is therefore important that Diamond has adequate infrastructure and expertise in place to enable Diamond beamlines to be at the forefront of science with synchrotron radiation. On the whole, Diamond's Optics and Metrology activities are highly competitive compared to other leading synchrotron institutes, with facilities and expertise that are world-class. We predict that over the next 10 years there will be requirements for nano focusing optics for producing focal spots below 50nm in size and highly coherent X-ray beams for imaging which will require stable optics able to retain the high coherence without introducing distortion of the wavefront.

The following improvements to technical capabilities are proposed for the field of optics and metrology.

- **A facility for fabrication of multilayer X-ray optics.** Diamond optics activities – and ultimately beamline performance - would benefit considerably from the establishment of a multilayer deposition facility in order to develop novel multilayer coatings. This development would allow at wavelength metrology to be used to optimise the fabrication of optics of unparalleled stability and accuracy under increasing heatloads. It would also reduce the risk of over reliance on a small number of commercial manufacturers of the optics.
- **Deterministic polishing of X-ray mirrors.** X-ray mirrors are extensively used at Diamond which are supplied by a small number of industrial companies. However, for some of our most technologically demanding components – for example nano-focusing, grating substrates there are very few suppliers. This is a significant risk to our supply, the products are very expensive and production times can be very lengthy. We propose to set up equipment at Diamond for deterministic polishing (ion-beam milling or preferential deposition), similar to those at facilities such as ESRF, NSLS-II and APS. Such a facility would let us achieve diffraction limited focusing of X-rays. Combined with at-wavelength measurements on beamlines, such that it would also open the possibility of fabricating optics for correcting wavefront distortions and for achieving the ultimate in nano focused beam size.
- **Advanced methods of optics modelling**. Geometrical ray tracing used for the design of optics fails when diffraction and coherence effects have to be considered. Therefore, wave-optics simulations of the propagation of partially-coherent radiation are essential. Diamond is already working on developing such methods and has established collaborations with other synchrotron facilities, but further developments are required.
- **Micro- and nano-focusing optics for X-rays.** An increasing number of beamlines at Diamond require micron and sub-micron beam sizes. For sub-100 nm beam sizes nano-focusing mirrors, zone plates, refractive lenses and multilayer Laue lenses are used. The multilayer deposition lab and a deterministic mirror polishing facility at Diamond would allow us to develop bespoke reflective nano-focusing optics whilst we collaborate with key international labs which excel in zone plates fabrication. Development work on refractive nano-focusing optics in silicon and diamond will continue. The diamond lens development is higher risk but preferred for its better efficiency. The long-term target over more than 10 years is to provide beams that approach 1nm in size.

Other optics and metrology projects

It is highly desirable to establish a **new Test beamline on an insertion device source**. This would provide X-ray beams with characteristics similar to the user beamlines to enable testing of coherence and diffraction limited optics as well as instrumentation at 'real' power density loads.

With the predicted demand for upgrading existing beamlines, we are also proposing **facilities for refurbishing** existing optics for higher performance. This will be supported by advanced modelling and *in situ* optics measurement methods.

X-ray crystal monochromators will also require development to cope with the high heat loads and to minimise wavefront distortion. Wavefront distortion may be caused by the imperfect polishing of the diffracting surface. An in-house silicon **polishing and etching facility** would be used for achieving the required surface finish.

4.2.5 Sample Environment

The best beamlines, supplied by a brilliant source are of little value if the sample cannot be put in the beam, or studied in a relevant state. There is therefore a critical need to match the capability of beamlines with equipment to provide appropriate sample environment, ranging from control of thermodynamic variables such as temperature, pressure and magnetic field, to exposure to reactive chemicals.

Internal and external consultation delivered the very clear message that Diamond must develop a much wider range of equipment for sample environment, and to do so in a co-ordinated manner that facilitates transfer between beamlines; standardisation of mechanical, electrical and software interfaces will also make it easier for external groups to develop their own equipment to bring to Diamond. The value of such standardisation has been demonstrated in MX where so-called SPINE standard pins have been adopted across Europe. The design, construction and support of new equipment will call on a range of resources, including existing in-house expertise in the technical division, on the beamlines, and through partnerships with university groups - as is already happening through the Catalysis Hub at the RCaH – and with other facilities at Harwell - for example expertise at the ISIS facility in cryogenics and high magnetic fields. Indeed in the area of macromolecular crystallography the engagement extends already to the European XFEL. Where gaps in expertise still remain, we would aim to employ a small number of additional engineers or technicians with key skills. Co-ordination of activity to ensure standardisation across beamlines, where appropriate, will be facilitated by bringing it together in proximate laboratories and workshops in Diamond, overseen by scientific co-ordinators in the life and physical sciences.

The following areas provide the richest opportunities, noting that there are individual projects within each category that are designated 'must have' and others as 'highly desirable'.

- ***in situ*** **studies of chemical reactions and catalysis**, requiring the delivery of precise amounts of gases or liquids at well-defined temperature and pressure, with post reaction analysis of products and byproducts. This may also require special provision of special procedures and facilities to handle hazardous chemicals, and complementary *in situ* measurements, for example optical (IR, Raman, UV/Vis) and NMR spectroscopy, integrated into the experimental control systems.
- **Facilities to study chemical and materials processing**, e.g. microfluidic reactors and stop-flow cells, electrochemical cells batteries during the charge-discharge cycle, additive manufacturing technology (e.g.

3D printing) and high-throughput methods to explore combinatorial processes, all with the range of complementary measurements required for *in situ* chemistry, above.

- Ensure that **all MX beamlines** are equipped with state of the art facilities for **routine, rapid throughput studies of yet more challenging samples**, e.g. sub-micron crystals, and to do so as part of a broader initiative to extend the boundaries of MX measurements at synchrotrons, FELs and electron microscopes. This will build on the existing support from the Wellcome Trust, BBSRC and MRC within the UK-based XFEL Hub project, and integrate with the bio-electron imaging centre activity.

- Establish facilities to **prepare and test the properties of new biomaterials**, starting with the provision of *in situ* conditions across appropriate beamlines, for example ambient temperature and humidity, or controlled stress (mechanical, chemical…).
- **Provision of extreme conditions of pressure, magnetic field, temperature or photon flux** to manipulate and explore the properties of materials and reactive systems. Specific projects include the provision of a new generation, compact yet 'high-volume' press to access new regions of parameter space for earth sciences, and fast, high energy lasers, in collaboration with the CLF on the Harwell campus, to explore reactive chemical states, or in combination with diamond anvil cells to explore elemental partition deep inside planets. Extend the range of complex electronic materials that may be studied through a dedicated high-field magnet (>20 T) that can be operated down to 1 K, essential for probing quantum magnets, topological insulators and a much wider range of multiferroics.
- Dedicated facilities to provide **secure and benign environments for artefacts in cultural heritage** studies where samples may be very valuable or fragile, and easily degraded with light or air or humidity, or stolen.

We will also develop a facility to handle medium level active materials at Diamond leading to a fourfold increase in the throughput of user experiments. In addition we plan to develop a capacity for in-situ experiments that would be world-leading and unique and which would give the UK nuclear community access to all useful beamlines at Diamond. Discussions have been held with the relevant nuclear advisory bodies within the UK and an outline application for funding is currently under consideration by the National Nuclear User Facility. Discussions are being held with other national facilities in this field (Culham, AWE Aldermaston), the atomic energy industry and energy companies.

4.2.6 Data handling and computing

Introduction

One of the defining features of many modern scientific facilities, from hadron colliders to gene sequencing factories, is the avalanche of data they generate. There is a dramatic increase in not only the overall data volume, but also the peak rates (velocity) of data collection and processing and the variety of the data from multiple and often interconnected experiments. Alongside this the expectations for simple, high quality, reliable software, and easy access to facility resources have grown. Already in many areas of synchrotron science IT has revolutionised the user experience and become a critical part of the experimental process. However as computing hardware and software continue to evolve and new experiment opportunities arise in Diamond an expansion of this investment will be essential to realise the potential of the facility. Furthermore, this mediation of IT between the user and the experiment shifts the scope of user expectations. No longer do most users come to Diamond to collect data points, they come to perform experiments, and often expect to receive real-time feedback to help optimise the experiment and the use of the facility. In other words “IT is the enabler of science - no IT, no science", however all software developments are science driven. From this basis, looking forward 5 to 10 years, the following are seen as the strategic IT challenges and opportunities: Automation, Remote Access, Detector Integration, Data Pipeline, Data Management and Post-Visit Analysis.

To address each of these challenges will be a substantial undertaking and will require investment in software, hardware and support infrastructure. For some challenges the cost of the software components will likely far exceed that of the hardware. Overall the ultimate data storage capacity or rate will probably not be limited by the available technology, but by the available funding. To put it bluntly we may have some hard choices to make about what data we preserve. Moore's law states that computing power doubles approximately every two years, however over the last few years Diamond data rates have doubled every 9 months (**Figure 13**). Were this to continue then in 10 years the repository would have increased from the current level of 2 PB to 2 Million PB or 2 ZB. In comparison the LHC had generated 75PB of data up to Feb 2013.

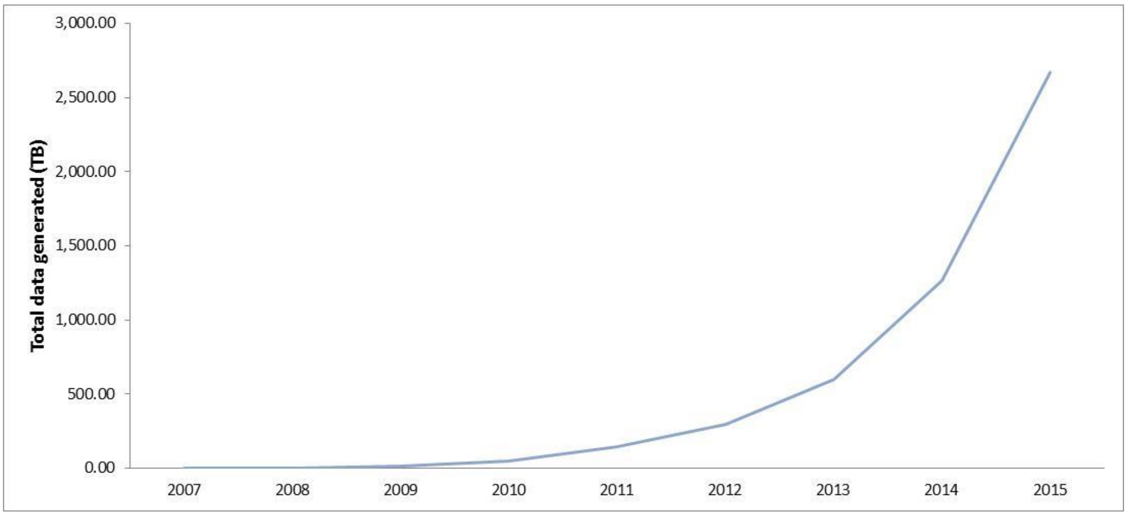


Figure 13. *Cumulative data stored for experiments performed at Diamond*.

- **Automation.** The value of the increased use of sample handling automation and analysis feedback loops has been proven in areas such as crystallography and BioSAXS. But further experimental station efficiency could be achieved using higher capacity robots and the automation of data taking and analysis feedback loops, building in greater intelligence. This will also increasingly be applied across other techniques. A second stage will be to automate the preparation of samples and loading of carousels offline. This requires investment in hardware infrastructure and in information systems to track the samples through the process. Automation of data taking requires the next generation of data acquisition software with close interactions with data analysis. In many areas of synchrotron science this level of on-line data analysis to inform the next step of the experiment is simply not yet available, the impact could therefore be considerable, and will extend to some of the more sophisticated physics experiments where data analysis of any complexity is done very much after the event.
- **Remote Access.** There is increasing demand for remote access, both during and after the experiment. Indeed the majority of MX data sets are already collected remotely. With fewer users coming to the facility, highly intuitive user interfaces will become increasingly important. We also need to work to build communication paths, to replace the direct face-to-face communication that happens when users come to site, otherwise we risk diverging from the true user needs. To fully realise this needs investment to provide a truly immersive experience, akin to that of a physical visit. This represents a substantial IT project and would require high bandwidth, utterly reliable, secure network connections. The logistics of

handling rapidly increasing numbers of unaccompanied user samples will require end-to-end sample tracking/warehousing.

- **Detector Integration.** Since Diamond was commissioned in 2007, the peak detectors data rates have increased from 10 MB/sec and are projected to be 6 GB/sec in 2015. This may flatten off over the next few years, but the challenge is still considerable. Computing technologies are managing these higher rates by increasing parallelisation, and this trend will continue. However a major issue of such systems is the management of complexity, since they rapidly become boutique and risk being 'bleeding edge'. Our approach is therefore to take advantage of commercial tools and systems where possible, keeping the parallel systems as simple and scalable as possible. However there is still a significant capital investment required, and specialist expertise to evaluate new products to assess their suitability in our environment and optimise them to achieve the required performance.
- **Data Pipeline.** As experiment efficiency and data volumes have increased, so has the pressure on providing data provenance and the value of the data. Experiment success can in general only be achieved by capturing information prior to measurements at the facility, be it sequence information or theoretical multiple scattering calculations, and using that effectively to design and assess the experiment. Advances, pioneered in Diamond in areas such as structural biology, have shown how influential to the experiment online data analysis can be. However there is still considerable scope for improvement even in the most developed areas of science. Furthermore as new opportunities arise from advances in computing hardware and new detector technologies, analysis tools and algorithms will need to be developed and be embedded in the experiment. We aim to provide well-maintained state of the art data analysis tools to prepare for, conduct and guide the experiment and help interpret the results. Collaborations with many institutions and groups such as research council funded CCPs and other facilities worldwide will be critical to exploit the latest data analysis developments.
- **Data management.** Diamond operates a coherent facility-wide data management policy and at the start of operations took the unprecedented decision to invest in long-term storage of all Diamond experimental data. This has been achieved with services and collaborations undertaken with STFC and other European facilities. For this to be really useful we need to capture the information associated with the experiment (meta-data) and not only the raw data. Indeed such data are essential if we are to attempt an integrated approach to bridge complex multi-technique and potentially multi-site experiments. Furthermore managing the complexity and quantity of experimental information generated is becoming beyond the capabilities of many of the research groups using Diamond. We therefore believe it is critical that Diamond lead the development of a service to enable all experimental facilities to be fully exploited by the best researchers.

- **Pre-Visit Preparation and Post-Visit Analysis.** Currently the immediate results produced during the experiment are processed within the synchrotron using software systems managed directly by Diamond, and are maintained by Diamond. The majority of users then take their raw or reduced data home for full analysis. However as we get an increasing number of remote users there is a switch in expectations, it becomes natural that the analysis, like the experiment, be conducted remotely. Furthermore when multiple experimental techniques are applied to a single problem the complexity of interpreting such experimental data tends to create a demand for computing resources, and software expertise that is beyond that available to most non-expert or infrequent users. Building on Diamond's position as custodian of user data we propose the development of integrated services, available transparently through Diamond. This should not only aim to provide state-of-the-art analysis after an experiment but also help to optimise the use of valuable time during an experiment, particularly for complex, multidimensional systems where it is not clear where in parameter space (position, energy/time and/or momentum) it might be most fruitful to look, guided by modelling or simulating the system in advance. This would be of particular value to new researchers and communities. We are working with STFC on developing HPC facilities focussed on Neutron and Photon Scientists' needs, recognising that this, 'data centric' science is significantly different to that of traditional HPC users. Ideally, where the processing takes place physically should be completely transparent to the user.

Summary

To remain world-class, and in some areas world-leading we will need to substantially expand our software activity, and we expect that the required additional IT hardware (disk farms and compute clusters) will need an additional data centre, of around 500kW capacity over the next 5 years. This need not be part of the present building and could be a shared resource with a partner organisation. Overall we expect to mitigate the substantial costs of the developments proposed, where possible, by working with partner organisations, particularly STFC.

4.3 Support laboratories and complementary facilities across the Harwell Campus

Support laboratories for sample preparation and characterisation at Diamond have already played an essential role in its success, from the range of in-house facilities for biology, soft matter, engineering materials and some aspects of chemistry and materials fabrication. Some of these, such as the Membrane Protein Laboratory are supported through substantial external grants held jointly with university partners. We propose to continue the development of such facilities, strengthening what we have or expanding into new areas, as outlined in the sections above on science visions and under 'sample environment'. Funding for this should continue to come from a combination of operating capital and external grants, with expertise brought in through collaborations with universities. We note however, that such facilities will add to the pressure on space. There is already a well-developed case to provide additional laboratories and offices in the proposal to build the 'Pod' extension, based on the demands exerted by developments for Phase III. Looking further forward it is likely that we will need yet further provision of such space, so we anticipate needing a second Pod extension beyond 2018.

We are also keen to participate fully in any appropriate development of other facilities on the Harwell Campus as part of a wider strategy to optimise its impact as one of the leading centres for scientific research in innovation in Europe, in partnership with UK universities and industry. This will involve both technical facilities, and the social infrastructure to make the campus a more attractive place to work and thus attract and retain even stronger staff.

We anticipate playing a strongly supportive role in the expansion of the **Research Complex at Harwell** and we are already fielding requests from university groups and industry to extend current projects in imaging, reactive chemistry and catalysis that will exploit our beamlines yet more effectively, and link them with activity at the CLF and the ISIS Facility. Other opportunities could include:

- **The Rosalind Franklin Institute**, a centre for the development of new physical techniques for the life sciences, led by the University of Oxford for a larger consortium of UK universities;
- A new **centre for data storage and analysis** led by STFC;
- An expansion of the **Electron Microscope Facility** to accommodate a larger number of microscopes that will be run as a national resource, drawing on the experience at Diamond in highly efficient operation of valuable instruments. The initiative for this would be taken by the user community and funding sought from UK research councils, perhaps also with appropriate industrial support;

- The XFEL Hub is part of a growing community of UK scientists who are developing ways to explore and exploit opportunities for science at FELs which may one day grow to an extent that a strong case could be made to establish a XFEL in the UK. Harwell would be a natural host for such a facility, providing an environment and workforce with directly relevant scientific and technical strengths and the opportunity to combine multiprobe measurements with crossed beams, involving Diamond or high energy lasers at the CLF.
- A national facility for **ultra high field NMR** which has been prioritised by the UK biological NMR community but is subject to funding prioritisation and further review with regard to a potential site.

Diamond will continue to look for opportunities to increase the presence of university groups on the Harwell Campus through establishing laboratories or outstations such as the one run by Manchester University that is proving so productive in developing and exploiting imaging techniques for engineering materials, manufacturing and processing and earth sciences. This is not only important for our technical development, but also raises the scientific and intellectual vitality of the campus as a whole, making it a much more attractive place for students, medium and long-term visitors and industrial engagement. We do not anticipate putting substantial resources of our own into such ventures beyond what we already plan for our technical upgrades. However, this has the potential to lever substantial matching funding from universities, as was the case for Manchester in the I13 building, in return for privileged access for a number of years to this beamline. The key point here is that the Harwell Campus offers a wonderful opportunity for universities to make the most effective use of their key resource – the most outstanding academics and postgraduates to be found anywhere.

We are currently discussing future strategic alliances of this type with other universities. However, we believe it is important to do this with a broader strategic mission in mind, beyond the mutual benefit that might flow from bilateral agreements between each university and Diamond or other facilities at Harwell. Scientific problems are becoming increasingly complex, and require increasingly integrated techniques and it would make sense if the development of the Harwell Campus was done in a coherent manner to establish world-leading capability in partnership with world-leading university groups. Coherent grouping of facilities and techniques is already increasing in the field of integrated structural biology, with the MPL, the Oxford Protein Production Facility, the Lasers for Science initiative in the RCaH and eBIC all clustered around Diamond.

Such development should be complemented by improvements to the infrastructure in and around the Harwell Campus, including more buildings for offices, laboratories and accommodation, and the development of space and buildings to stimulate social interactions, and enable meetings and discussion within the growing community of scientists and engineers, both staff and visitors. Initiatives to achieve this are being driven through the Joint Venture between STFC, UKAEA and Harwell Campus Developments Ltd, outlined in section 2.2.

4.4 Operating model and organisation of Diamond

Since first starting operating as a user facility just 8 years ago, the number of beamlines – and with them the number of scientists and technicians – has risen steeply, with 8 more set to become operational by 2018. In the light of this we need to reconsider the operating model across all Divisions. For example, since beamlines were first organised into Villages, they have grown significantly in number and range so it is timely to reflect on whether the current configuration is still the most effective. Furthermore, while the concept of villages still appears appropriate for operational purposes, it is not very conducive to communication of broader technical issues or science across the organisation and some complementary, transverse structure could be beneficial. Further, as Diamond scientists spend an increasing fraction of their time engaging in and delivering science, so the organisation needs to establish a more vibrant and pervasive science culture.

A second area where reflection on organisation – and also processes – is required at this stage in the evolution of Diamond is engineering support, both for projects and operations. Processes were originally set up for the design and construction phases of Diamond whereas there is now a mixture of demands on the teams involved in this area of work that include ongoing upgrades and operational maintenance. It is therefore timely to assess how best to prioritise, plan and execute such work.

During Diamond's first years of operation, there has also been an evolution in the way in which users engage or wish to engage with our facility, particularly in the following areas.

- An increasing number of users choose to send samples by courier and follow measurements remotely, particularly for MX beamlines, and we expect this to grow for other beamlines, small molecule crystallography, powder diffraction, SAXS and spectroscopy, for example. Such developments, in combination with increased automation could greatly increase our capacity to run samples, but do have a cost in terms of increased demand for technical support.
- The 'standard model' for applying for beamtime leads to very considerable delays between a scientist having the idea for the beamtime, and gaining access once a proposal has gone through the twice-yearly peer review process. Mechanisms have been established or evolved to provide faster access – although a small amount of time is allocated by rapid access, this is primarily by the BAG (block allocation group) method, common in MX experiments, where consortia of users are allocated blocks of time that they can use with some degree of flexibility, and this could be extended to some of the types of beamline outlined in the previous paragraph. However, there are many sorts of experiment for which the BAG model is not appropriate, and for these we will consider ways to allow researchers to make more efficient and more rapid use of scarce national facilities in a planned manner.
- There is also increasing demand for access to multiple beamlines, or even across facilities to bring to bear a battery of techniques to solve yet more complex problems. At present we achieve this to some extent within the BAG system, but a proper implementation is likely to require changes to the way in which beamtime is reviewed and allocated.

As Diamond has evolved, so has the number of projects running at any one time, with new beamline design and construction operating in parallel with upgrade projects, and both competing for technical resource with beamline operations. This increased pressure on resources and complexity calls for a review of the processes for planning and managing many aspects of technical development and support at Diamond.

All of these issues concerning the operating model and organisation of Diamond – and more – will be explored in greater detail in a separate document outlining the Delivery Plan for the Diamond Vision and Strategy.

4.5 Development of other major synchrotron facilities

The landscape of major synchrotron facilities throughout Europe and beyond continues to evolve. **Figure 14** summarises which of these have come on stream or closed over the period 1990-2050. However, this gives no idea of developments in brightness or other technical aspects of performance, and most of these facilities that are already running are also carrying out or planning significant upgrades to sources and beamlines. Such developments are summarised in **Table 6** for those facilities that have already drawn up plans or have active upgrade programmes.

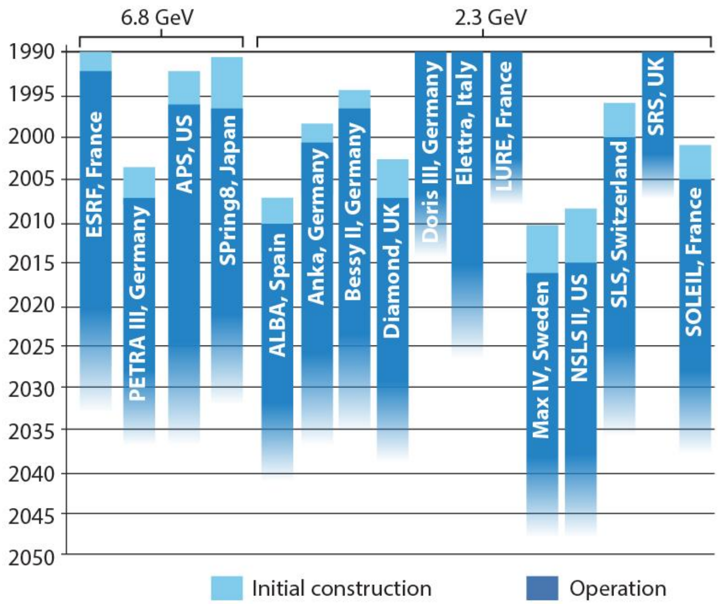


Figure 14: Evolution of major European synchrotron facilities together with leading facilities in North American and Japan.

Existing/New Low Emittance Facilities:

Facility	Energy (GeV)	Emittance (nm rad)	Operation date for users	Number of initial beamlines	Comment
NSLS-II	3	0.9	2015	7	29 beamlines operating by ~ 2018. Aims to have 60-70 beamlines in total
MAX-IV	3	0.2-0.33	2016-17	7	25 by 2026
SIRIUS	3	0.28	2017	13	
PETRA III	6	1	2009	25 (by 2017)	

Upgrades to Existing Facilities:

Facility	Energy (GeV)	Current Emittance (nm rad)	Emittance after upgrade (nm rad)	Proposed dates of lattice upgrade	Number of beamlines	Lattice upgrade status
Spring-8	8	2.4	0.1 (6 GeV)	TBC	57 (incl. 1 planned RIKEN beamline)	Preliminary design
APS	7	3.1	0.065 (6 GeV)	TBC	72	Preliminary design
ESRF	6	4	0.15	2018/20	46	Design fixed
Diamond	3	2.7	0.14-0.28	TBC	33 (by 2018)	Preliminary design
SLS	2.4	5.5	0.072	TBC – but likely 2020-2024	21 (incl. 1 under construction)	Preliminary design
ELETTRA	2	7	0.25	TBC	26	Preliminary design

Table 6. *Summary of machine characteristics for major synchrotron facilities, both current and planned*.

5.0 STRATEGIC GOALS AND OBJECTIVES

The Vision for Diamond – to be a world-leading centre for synchrotron science, and a cornerstone of a world-class site for scientific discovery and innovation at Harwell - has 5 strategic goals:

- to be a world-leading facility in synchrotron-enabled research and innovation;
- to maximise the scientific, economic and societal impact of Diamond;
- to ensure the long-term sustainability of Diamond as a national facility;
- to engage and inspire the general public through promoting science;
- to continuously plan for Diamond's technical and scientific future.

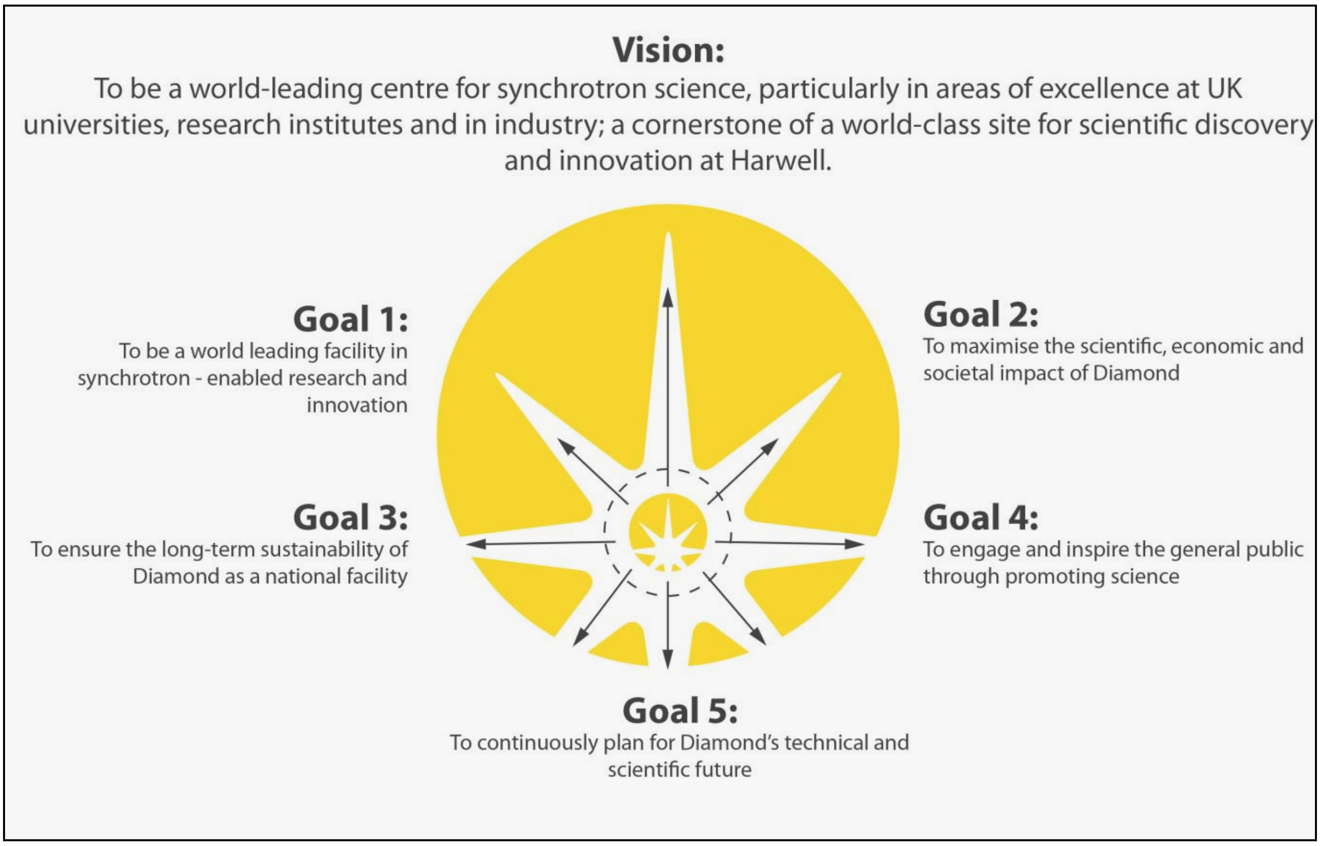


Figure 15. *The Diamond Vision and Strategic Goals*

Each of these goals has a set of strategic objectives, elaborated in the following sections. We also comment on the resources that will be required, together with a delivery plan to achieve these objectives, in section **5.6**.

5.1 A world-leading facility in synchrotron-enabled research and innovation

- **5.1.1 A highly reliable, high performance source of X-rays, UV and IR light.** To ensure that these beamlines are served by the highest performance beams, as reliably and for the highest percentage of time that is feasible. RF components will be upgraded to increase reliability, brighter insertion devices will be installed to deliver higher photon flux to beamlines, and feedback and control systems for the storage ring will be improved to provide greater stability of photon beams to better exploit higher repetition rate detectors. The case will be made for an upgrade to the storage ring to reduce the emittance by at least an order of magnitude - Diamond-II - and maintain the competitiveness of our source in the face of upgrades to other leading facilities across Europe; plans also need to be made well ahead of time to mitigate the effects of an extensive dark period on the user community during any such upgrade.

- **5.1.2 World-leading beamlines and analytical tools.** To ensure that Diamond offers beamlines that are world-class or world-leading in areas that match the UK's strengths in science and innovation in universities and industry, and appropriate to the character of the source. In parallel with the completion of Phase III, a programme to upgrade existing beamlines will be launched to maintain the performance of those that are already world-class, raise the game of those that have fallen behind through technical obsolescence, and offer transformative opportunities in areas not yet covered. A shortlist will also be drawn up for 4 additional, new beamlines or endstations to be constructed beyond 2018, working with the user communities to develop the technical designs and case for support. Priorities will be guided by the scientific vision and the opportunities provided by transformative technology; they will also be informed by expert review of the performance of the current suite of beamlines.

- **5.1.3 Exemplary technical and scientific support for experiments.** To ensure that we provide the very highest levels of scientific and technical support in preparing for and conducting of experiments at the facility. This will require establishing the following for all beamlines: adequate laboratories for sample preparation; coherent provision and support for sample environment through collaboration with universities and industry to enable all core scientific problems to be studied; extension of automation and high throughput methods to all appropriate areas of experimentation, together with workflows and software to make them efficient.

- **5.1.4 World-leading data handling and analysis.** To ensure that world-class sources and beamlines deliver world-class synchrotron-enabled science through state of the art data handling and analysis. A holistic approach is essential, providing methods of capturing all relevant information associated with an experiment, rapid visualisation and analysis tools to allow experimentalists to assess progress in an experiment and enable rapid, accurate decisions to be made to continue, and to ensure that there are no significant bottlenecks in post-experimental analysis. This is a very ambitious task that will require exceptional leadership and co-ordination to develop and implement an effective plan.

- **5.1.5. Recruitment and retention of the best talent.** Ensure that all areas of activity at Diamond that are essential to the delivery of world-class science are led or supported by highly motivated and skilled staff. This extends from front-line scientists, through technical innovation and support, to workers essential to maintaining physical and organisational infrastructure. Competitive terms of employment, a creative recruitment strategy, continued training and development, and the provision of a stimulating work environment are vital, together with clear organisation and leadership to make the most of individual talents. As Diamond continues the transition from construction to full-blown operations, and approaches a full complement of staff, it should review whether its organisation is still optimal. Communication between and across all levels of the organisation must be open and effective to ensure that: everyone understands top-level strategy and the challenges Diamond will face; operational difficulties are identified and tackled as soon as possible; lessons learned and best practice identified in individual projects is shared.

- **5.1.6. World-leading technology to underpin our science delivery.** To ensure that Diamond has early and secure access to the very best new enabling technology, either through in-house programmes where world-leading capability exists or can be developed, or through collaboration with key partners such as STFC Technology, selected synchrotron centres (and in some cases other types of central facilities, for example for high-energy physics) and specialised technology companies. Roadmaps will be developed over the next year – where they do not already exist – with such partners in the areas of: sources, detectors and optics. Transformative developments in most of these areas take considerable time, often over a decade or more, so plans should be long-term and discussions with potential funding bodies need to be centred on taking a long-term view.

5.2 Maximising the scientific, economic and societal impact of Diamond

- **5.2.1 Attract and enable the very best research groups in universities and institutes to Diamond**. Systematic reappraisal of scientific opportunity and identification of leading groups will be informed by regular exchange with the scientific community at many levels and through discussions with the UK Research Councils. Leading groups who do not yet use Diamond should be persuaded of the opportunities to be exploited either through wider, more effective communication or direct engagement. The current means of allocating beam time should be reviewed to identify more rapid yet rigorous ways of providing access, for example through more frequent panels, reducing the lag between application and allocation of time, or the establishment of programme allocations with rolling review for particular large groups.

- **5.2.2 Support even stronger engagement and support for UK industry.** To widen industrial participation at Diamond by gaining a larger share of existing industrial users in a highly competitive worldwide market and by seeking new users who currently do not use large facilities like Diamond in their research and development programmes. Enhanced staffing of the team is critical in achieving this goal and the staffing profile will develop over the next 5-10 years as new beamlines with new capabilities come online. Additionally, more strategic partnerships will be sought with industry, concentrating on those areas which will fit within and enhance the Government's industrial strategic plans. As appropriate, we will continue to work with other large science facilities, both on the Harwell campus and more widely, to provide a complete solution for our industrial users.

  5.2.3 Work in partnership with other organisations to help realise the full potential of the Harwell campus. Diamond will be pro-active in the development of the Harwell Campus, in partnership with STFC and other neighbouring institutes, with the Joint Venture and in partnership with universities and industry. Synergies with existing facilities should be explored more thoroughly, in particular with ISIS and the CLF, for example in software development and sample environment. A plan should be drawn up and implemented to develop the Research Complex at Harwell further, with a greater emphasis on industrial engagement. Embedded complementary laboratories such as the Electron Microscopy Facility will be firmly established in the next two to three years as an essential component of integrated solutions to problems in the life and physical sciences; further opportunities should be explored with other partners on the Harwell campus to establish other, appropriate large or meso-scale infrastructure where there is a clear advantage in co-location with synchrotron beams. Such developments must be done with the other organisations in and around the Harwell campus, with an eye on attracting new partnerships with universities and industry. Strenuous efforts should also be made to establish infrastructure at Harwell to make it more attractive for students and scientific visitors to spend longer periods of time on the site so that it develops a critical mass of leading or aspiring young scientists. Diamond will keep actively engaged with local and national government to persuade them that such developments will bring important benefits to the economy.

- **5.2.4. Build stronger collaborations at the European and international levels.** Synchrotron facilities across the world share common challenges, particularly in the development of technology to push back the boundaries of what can be measured. It is essential that a roadmap and a delivery plan for such requirements is developed, together with other types of facilities that share some common ground (for example FELs), starting with European facilities. Key areas include: detectors, nanofocusing and nanomanipulation; software development, particularly for higher through data analysis. Support for this will be sought from the European Commission together with other European facilities, while in the UK discussions should be held with appropriate industries and BIS to explore ways to engage more closely with industry for such development.

- **5.2.5. Ensure the widest possible dissemination of the scientific output of Diamond.** Diamond will disseminate its scientific achievements as effectively as possible as scientific publications, anticipating that in future they will all be made available through open access, and making provision for the financial consequences of this in partnership with universities and industry. It will develop the infrastructure and legal framework in agreement with its stakeholders to make data available in a suitable form and on a suitable timescale for wider exploitation.

5.3 Ensuring the long-term sustainability of Diamond as a national facility

- **5.3.1. Deliver value for money in all aspects of our operations.** To continuously demonstrate value for money to shareholders and stakeholders through evidence-based outputs and outcomes. Diamond will continue to ensure that it has the most appropriate KPIs for each of these groups and regularly communicates and discusses their values with its Board, with SAC and DISCo, with DUC and with the Research Councils. It will be committed to taking prompt, effective action to identify and correct for any sustained drop in performance.

- **5.3.2. Engage effectively with stakeholders at all levels.** To engage with the wider stakeholder community to ensure that Diamond responds to changing priorities and requirements and that stakeholders understand Diamond's evolving capabilities and resource requirements. Diamond will make sure that it is as well informed as possible, and has excellent opportunities to communicate and discuss such issues by ensuring that the various advisory bodies (SAC, DISCo, DUC and the various beamline working groups) that it has set up operate as effectively and transparently as possible. It will also continue to run regular public meetings to consult with the user community and communities of potential new users about new scientific opportunities.

- **5.3.3. Identify and access new income streams.** To maximise the use of funds through effective collaboration and securing additional 3rd party funding. Diamond will continue to seek and exploit funding opportunities with industry, universities, charities and government or EC funding bodies, as well as securing complementary funding from other facilities such as European synchrotron facilities in bids to EC H2020 funding.

- **5.3.4. Maintain operational infrastructure that is efficient and resilient.** As time goes on, the reliability and maintainability of the infrastructure that supports the Diamond facility, across the board from computer systems and networks to the water cooling and air conditioning plant, will become increasingly critical, due to ageing of components as well as obsolescence. A significant and continuing investment will therefore be needed to overcome deteriorating performance, and minimise beam interruptions and longer outages.

- **5.3.5. Ensure governance is fully transparent.** To demonstrate excellence in standards of corporate governance. Diamond recognises that in order to retain and nurture the enthusiastic support of its shareholders, users and other stakeholders it must be able to demonstrate its commitment to excellent standards of corporate governance. This can be achieved by providing a focus upon: an appropriate vision and strategy; effective mechanisms for assurance and accountability; a culture of openness and integrity; clear leadership and stewardship. The principal mechanisms for delivering the above are already in place and include: an effective Board supported by sub-committees for Audit & Risk and for Remuneration; stakeholder consultation, such as the Diamond User Committee and the Scientific Advisory Committee; regular reviews and audits, such as Gateway Reviews and Triennial (Governance) Reviews.

- **5.3.6. Maintain health and safety at the forefront of operations.** Diamond will continually review and align its health and safety objectives with its business objectives. The facility is moving towards accepting higher hazard experiments from its users in multiple scientific disciplines – for example in radioactive materials and high power lasers. As a scientific user facility, the broad strategy is to ensure that the health and safety systems are as leading as the science. This will continue to be achieved through the implementation of extensive training programmes, the employment of competent personnel and the development of suitable safety systems and facilities.

5.4 Engaging and inspiring the general public through promoting science

- **Strengthen educational activities for students at all levels.** Diamond will continue to consolidate its public engagement and education programme, ensuring that it meets the needs of education providers and takes advantage of emerging technologies that offer exciting prospects of reaching a variety of audiences with our messages. For example, new schemes for schools work experience and 12 month undergraduate interns will be launched, adding to our portfolio of activity. These schemes have been developed in collaboration with educators and students and will be evaluated and developed to ensure they meet the high standards that we set for all our engagement work.

- **Put public engagement and communications at the heart of the facility.** Embedding engagement at the heart of the organisation has been integral to the organisation and Diamond will continue to train and nurture scientists, staff and the wider user community in communications and public engagement. Diamond's relationship with external researchers is key to successfully raising the profile of the science that results from Diamond experiments. Through a proactive approach, the facility has built up a reputation for being a valuable channel through which scientists from a wide range of fields can disseminate their research via the media and face to face interactions with the general public. Diamond will continue with this approach as it is successfully helping us to build a reputation for inspiring scientific outputs and an increased level of public awareness in the UK and abroad.

- **Champion the importance of STEM Skills at all levels.** Diamond will actively strive for equality in all areas; this will include partnering with organisations that are helping to raise awareness of STEM subjects among girls and those from underrepresented groups.

- **Greater exploitation of opportunities to disseminate science at a global level.** Diamond will seek to maximise the opportunities presented by large international events such as the International Year of Light (2015) and awareness raising days that are relevant to the research that is undertaken at the facility. As an active member of lightsources.org, the facility maintains a global view of how light sources are engaging with the public and schools. This presents opportunities for us to adopt best practice and gives us inroads at important science meetings such as the annual AAAS Meeting in the USA and the World Conference of Science Journalists. The facility will continue to foster relationships with national and international organisations whose remit it is to bring the world's best scientific achievements to the attention of the public in exciting and engaging ways.

- **Ensure there is effective two-way communication at all levels of the organisation.** Core reputational issues such as health and safety, environmental impact, employee relations and impact on our local community are continually monitored and the facility encourages two way dialogue with all members of the public and the media who are interested in obtaining information on such matters. This will continue to be done in an open, transparent and informative way.

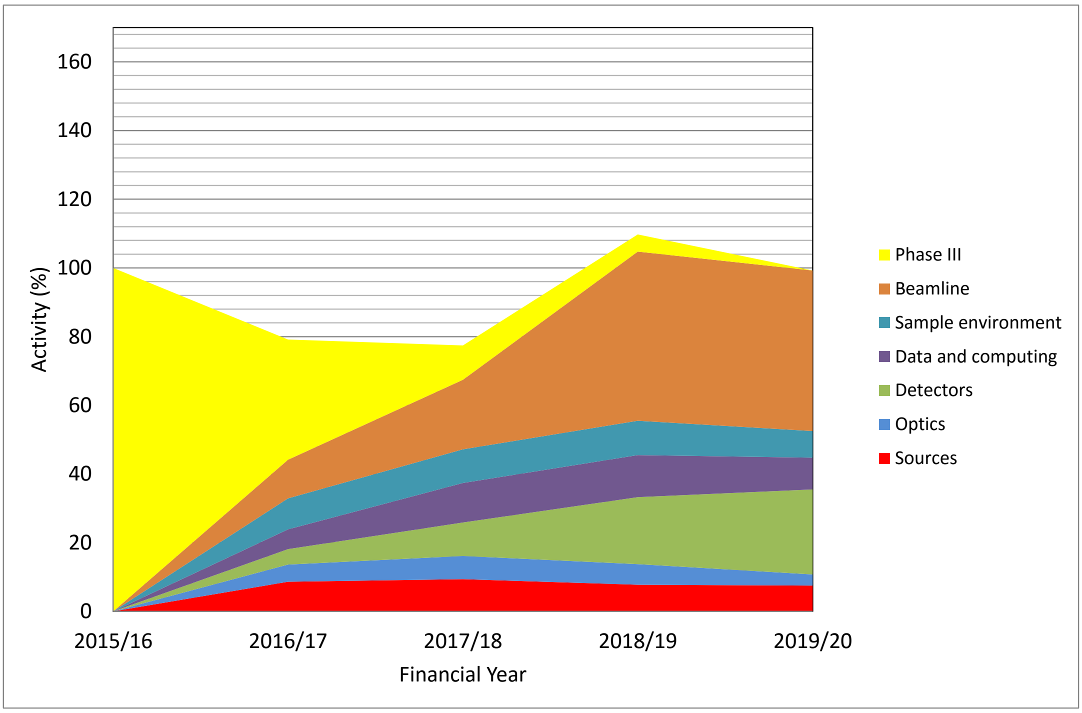
5.5 Continuously planning for Diamond's technical and scientific future

- **5.5.1 Ensure there is a clear planning cycle for delivery of activities.** Diamond will continue to develop its vision for science and technical development, and the strategy to achieve it, through periodic reviews and external consultation, with universities and industry. The vision will be updated at least every 5 years, and strategy every 3 years, though faster change may be needed if there are significant and unexpected developments in scientific challenges or enabling technology. It is therefore important that Diamond retains significant agility in being able to reprioritise developments.

- **5.5.2 Adapt the operating model to changing requirements.** The best operating model for Diamond for science and technical support must evolve as circumstances change or as the facility approaches a new phase in its lifecycle. Phase III will be complete by 2018, offering 8 more beamlines than at present, supported by many more scientists and technicians. An assessment should be made and action taken with regard to the optimal organisation of staff, particularly in the Science and Technical Divisions, as well as the balance between engineering and technical support for projects as opposed to operations.

5.6 Options, Resources and a Delivery Plan

Diamond has a mission to be a world-leading facility for science with synchrotron radiation, which in a rapidly developing field means that in order to enable the very best science its performance must continue to improve year on year. Other synchrotron facilities have ambitious development programmes planned for the near future, or already underway (section 4.2.1 and section 4.5): the Upgrade programme at ESRF, and the development of PETRA III at DESY and NSLS II at Brookhaven are already in full swing, while the new facility MAX IV in Lund will be available in 2016 and a lattice upgrade is planned at SLS in Switzerland by the end of this decade. In general, beamlines remain competitive without major upgrade for a finite time that depends on the type of beamline and may range from 10 years to significantly less. It should be anticipated that a facility the size of Diamond should plan to upgrade or replace of the order of 2-3 beamlines a year once it has reached steady state operations. It is equally important to continue to develop the supporting infrastructure and enabling technology, from sample environment to software.



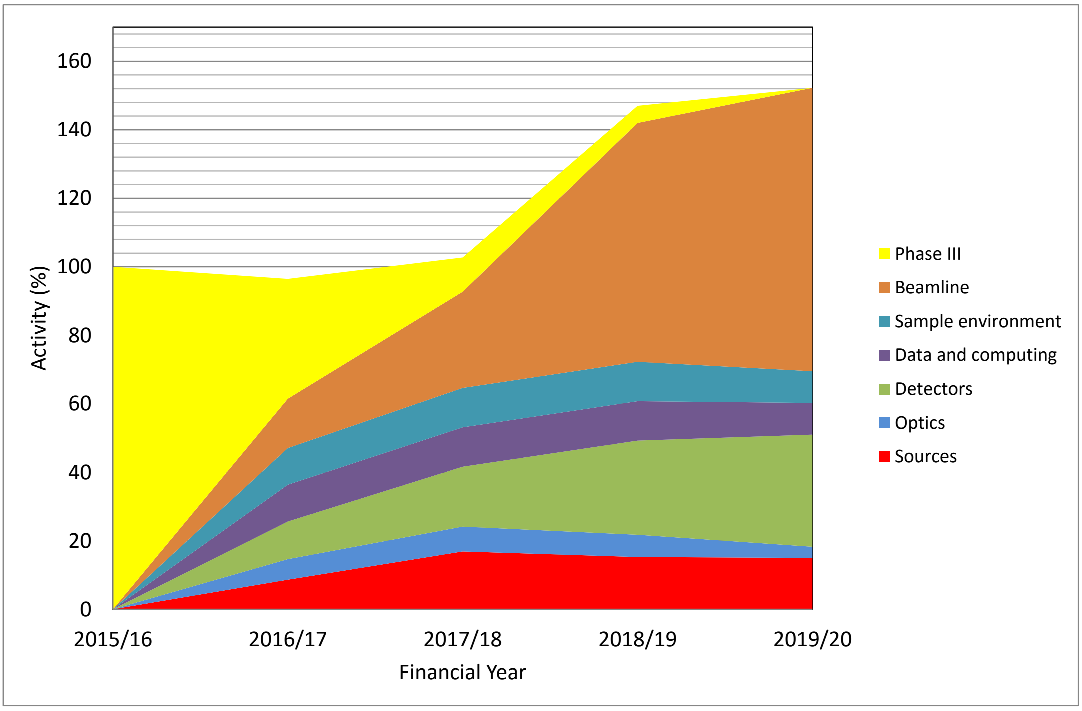


Figure 16. *Evolution of projects to continue to develop Diamond as a world-class facility for science at a synchrotron, scaled approximately to the magnitude of capital funding required. The upper graph (i) displays the highest priority projects (option 1) for: sources, beamline upgrades, enabling technology for detectors, optics and sample environment, and the provision of greater capacity and capability for data handling and analysis. It also displays a comparison with the funding for Phase III and the component of operating capital that is currently used to maintain equipment at an operational level. The lower graph (ii) shows the combination of the first and the second priority projects (option 2s), together with the level of capital funding to maintain current operations.*

The prioritisation process outlined in the Introduction (**section 1.2**), which drew on extensive internal and external consultation, identified particular technical upgrade projects that were judged to be essential to ensure that the UK scientific community in industry and academia continues to have world-class or world-leading facilities for science at a synchrotron and deliver high-impact science in areas of national strength and significance ('must have' developments, designated **option 1**). This process also identified a second set of projects ('highly desirable' developments, designated **option 2**) that would also bring very substantial improvements to the technical capability of capacity of Diamond, and with it further scientific opportunities. This prioritisation was also conducted with an eye on the availability of other facilities for these communities, particularly the ESRF, and further details of the screening and evaluation process is given in Appendix 4. Priorities for the different projects was outlined in section 4.2 for sources, detectors and optics, while all projects for sample environment and computing that were retained were designated to be of the highest priority; priorities for beamline upgrades should be discussed further through discussion with SAC, though we have made a preliminary division into 'option 1' and 'option 2' as a consequence of discussion and feedback from the 'Vision' meeting in autumn 2014. It should be noted too that an independent review process co-ordinated by RCUK came to very similar general conclusions about priorities for technical development in their Requirements Exercise of 2014[23]

Figure 16 illustrates schematically how the various types of project will be rolled out in the medium term, in approximate proportion to the scale of the capital funding required. This includes the development of sources, beamlines, enabling technology for detectors, optics and sample environment, as well as provision of greater capacity and capability for data handling and analysis. It also displays a comparison with the funding for Phase III and the component of operating capital that is currently used to maintain equipment at an operational level. The gradual ramp-up of such expenditure from FY 2015/2016 represents the fastest feasible launch of prioritised upgrades with reasonable levels of technical resource. In the longer term we also anticipate the replacement of some existing beamlines by different types of beamline as the portfolio of the science we support changes, or the balance of the user community moves. However, the priorities for this have yet to be set and will require several years of planning and prioritisation and no further capital resource will be required for this until at least 2018.

Likewise, the upgrade to the storage ring envisaged in the 'Diamond-II' project still requires extensive planning to produce technical options and an accompanying scientific case, weighing up the gains on some beamlines and in some areas of science, against potential losses in other areas. Any upgrade must also include a means of ensuring that scientific output does not suffer significantly from extended dark period when the work is done. The earliest likely start date for such a project is likely to be 2021, with a duration of 15 – 18 months. We also have initial estimates for the capital resource required both for the upgrade to the lattice (of the order of £M 60) , and for necessary upgrades to beamlines in response to lower emittance beams which will be more demanding, for example on optical components (higher heatloads for instance) – which is of the order of £M 10.

Finally, we also anticipate playing a role in the further development of the Harwell campus and the various large and medium scale facilities it hosts; such initiatives will be conducted in collaboration with STFC, and/or partnership with universities and industry

Some designs of Diamond II will offer the opportunity to provide a significant increase in the number of insertion devices and with them the potential number of beamlines at the facility. However, at present, the upgrade and development projects we propose are envisaged within a framework that includes the current

[23] http://www.rcuk.ac.uk/RCUK-prod/assets/documents/documents/ScienceRequirementsReportDec2014.pdf

number of beamlines. Nevertheless, we do envisage a need to increase the number of staff in some areas to increase what Diamond can deliver and optimise the return on capital. Additional staff will make the greatest impact in the following areas.

- Data handling and analysis, enabling Diamond to remain competitive or be a leader in managing and exploiting increasingly large and complex data sets, where additional expertise is at least as important as upgraded hardware and software; funding for this will be provided significantly through external grants and industrial income and some personnel may be provided through joint appointments with universities.
- A big factor in determining the quality and quantity of science delivered at a beamline is the level of expert scientific and technical support. Modest increases in staff on beamlines will have a very significant impact on productivity. Furthermore as beamline automation and remote operation becomes more pervasive although the overall productivity of the beamline is markedly increased, more beamline support is also required.
- Sample environments. The most frequent request from users in our consultation exercise has been for improved assistance with provision of sample environments which allow studies to be made under in-operando conditions. Investment in a few staff extra will be very effective in strengthening and exploiting the existing but as yet not-coordinated activities at Diamond and amongst our users. This activity will also have an immediate impact upon the service that Diamond is able to offer to UK industry.
- After improvements to the source, the single most important area for hardware development lies in detectors. In some cases Diamond has particular expertise that will enable it to develop world-leading technology – to varying degrees in collaboration with expert groups at other facilities or with specialised companies and this could be strengthened with significant effect by the appointment of a modest number of additional staff. It is also essential that there is at least adequate support to operate and maintain such detectors.

The capital required to deliver the key components of our Vision, options 1 and 2, is very much in line with what one would expect to maintain a world-class facility at at least a competitive level, with systematic upgrades of each beamline about once every ten years and matching upgrades to complementary infrastructure. By contrast, a failure to continue to invest at such levels will lead after a few years to a drop in performance relative to facilities abroad, and lost scientific opportunities for UK science and innovation. Further underfunding will lead to the rapid downward spiral in competitiveness and performance experienced by the SRS at Daresbury where a sustained period of underinvestment played a decisive role in its decline from the world-leading facility of its kind at that time.

Standing still is simply not an option for Diamond if it is to achieve its potential to deliver world-leading science for UK universities and industry for decades to come. This is true both of the technical development needed to maintain pole position among facilities internationally as well as the evolution of the structure and processes within the organisation as it approaches full-blown operations. Further details of organisational and operational changes (outlined briefly in section 4.4) and the resources required for new projects, operating costs and personnel will be presented in a separate Delivery Plan.

Appendix 1 - Further highlights of industrial use

Drug Development

Drug products are manufactured to an extremely high standard to maintain product safety when taken by patients. Specifications used throughout the manufacturing process cover not only the drug itself, but also the level of potential impurities (chemical, solvent, or polymorph), which are set to limits that are monitored by regulatory bodies to uphold safety and product quality requirements. X-ray powder diffraction is a key analytical technique in the pharmaceutical industry for characterising drug compounds. This is used throughout the development process to fingerprint compounds and quantify impurities.

GSK development scientists were working on the detection limit for the presence of a solvate within a manufactured drug batch. This limit was necessary to develop confidence that solvent in the process was kept to a minimum. The crystalline development form was produced by desolvation, but residual traces of a disordered/ poorly crystalline solvate remained, which required monitoring to maintain the regulatory specification. The poor crystallinity of the solvate broadens the diffraction peaks making it very difficult to quantify in low amounts. Using laboratory based diffractometers, the detection limit of this form in the mixture was 15% w/w and it was difficult to obtain improved detection from alternative techniques.

Diamond beamline I11 is designed to provide high resolution X-ray powder diffraction data (both spatial and temporal) with rapid data collection and the brighter source delivers exceptional count statistics. Using the high spatial resolution mode, the diffraction peaks measured were sharper and therefore better defined than those obtained using a laboratory source. The new diffraction pattern allowed for better discrimination of the two drug versions in the mixture lowering the detection limit to around 10%, with the potential to achieve 5%. Typical manufactured batches were found to contain less than 10% w/w solvate.

This experiment has shown that the manufactured batches contain a limited amount of the solvate material and that the current limit of detection is suitable for specification.

"Without the use of I11, we would not have been able to reach these detection limits that have led to greater understanding and control over the solvate material, thereby allowing us to have confidence in the reproducibility of our manufacturing process."
Dr Matthew Johnson, GlaxoSmithKline

Engineering Applications

For engineering applications, the key benefits to industry come from the much higher energy and flux of X-rays that are generated at synchrotrons. Larger penetration depths are achievable and times for data collection are much reduced, allowing engineers to extract more detail out of their studied systems than feasible using conventional facilities.

Advanced design approaches by engineers can solve complex real world problems; novel concepts are needed to push performance boundaries and greater scientific insight is often needed to fully realise the design. Increased insight can be achieved by improving the materials and processes used in the manufacturing route or measuring parameters such as stress and strain directly to validate computational models. Additionally, in the event of catastrophic failure of the engineering system, a forensic method is often needed to re-engineer the component or system. Diamond provides specialist analytical techniques for the atomic to microscale characterisation of materials ranging from high performance engineering components and devices through to diagnostic tools and drug delivery technologies.

For example high energy diffraction can be employed to measure the stress and strain to evaluate the mechanical performance of an engineering component or system in real time. Other applications of high energy diffraction include studying the residual stress and strain in a component that arises due to manufacturing processes by non-destructively mapping the strain profile in 3D or investigating failed components to determine the underlying cause, establishing routes to re-engineer the component for future requirements.

A recent industrial experiment was performed to characterise the autofrettage process and evaluate the effect of impact damage on gas cylinders manufactured by Luxfer Gas Cylinders which find application in high pressure, self-contained breathing apparatus used by fire fighters. The use of this non-destructive technique allowed the materials engineers to understand their processes in a more detailed manner and the results are feeding into the product development cycle.

"Luxfer Gas Cylinders are delighted with the excellent information obtained as a result of our collaboration with Diamond Light Source and the University of Southampton. The results achieved will assist greatly in the development of our lightweight composite cylinders."
Dr Warren Hepples, Luxfer Gas Cylinders Europe

Consumer Products

Innovation and sustainability are two of the key drivers for the consumer products industry in today's marketplace. With sustainability high on the consumer agenda and with rising raw material, water, and energy costs, the development of efficient and green products, packaging and processes is vital to long-term business success. Increasing demand for product performance, product security and shelf life make the development of innovative products and technologies vital. However, successful innovation requires a fresh approach, a good understanding of the science behind the product or process, and access to the widest possible variety of research and development tools. By adding a synchrotron facility to the researcher's armoury of analytical tools, a wide range of experiments relevant to the consumer products sector can be performed. These might include structural characterisation of dispersions, emulsions and partially ordered materials under controlled conditions; investigation of phase behaviour of self-assembled systems including surfactants, lipids and polymers or understanding structural changes associated with the use of additives e.g. rheological modifiers. Additionally, the packaging of materials is becoming ever more complex. Grazing incidence X-ray diffraction can be used to study structure, thickness and roughness of thin films and coatings; X-ray imaging can observe microscale features in bulk samples e.g. cracks and pores and small angle X-ray scattering can be used to develop novel polymer composite materials.

Hair care is a rapidly developing science. Consumers demand more from their products in terms of sensory perception and functionality. Rapid innovation into market is key to growth. Increased product complexity requires greater understanding of the interplay between components and an accurate description of the product microstructure and its rheological and dispersion properties are essential. Unilever researchers have used Diamond to demonstrate the stability and suitability of new technology in product formulations in both product and "in use" formats. I22 was used to investigate the product microstructure in diluted form. Working as an extended team, data was translated into understanding and communicated to the project team within just a few weeks of the original experiment. Consequently the project accelerated to a working prototype product which will undergo “in home trial” in late 2013.

“The excellent facilities, flexibility and “can do” attitude at the Diamond Light source aligned well with our project needs and objectives. Without this contribution we would not have our current best prototype option to hand. An excellent partnership which bodes well for the future.”

Dr Ian Tucker, Dr Cesar Mendoza, Dr Julia Li, Unilever R&D Port Sunlight

Appendix 2 - Science Visions

A 2.1 Integrated Structural Biology (Science Champion: Martin Walsh)

Introduction

One of the grand challenges in 21st century science is to bring together structural and cell biology so that functional biological systems can be dissected from the cellular level to the atomic level, providing an understanding of the system in time as well as space. This ambition would deliver fundamental biological insights which in turn would translate to impact in applications from energy and ecology to food security and health. The remarkable technological developments in structural and molecular biology methods in recent years suggest that elements of this ambition will be realised within the next ten years. Structural biology already provides detailed mechanistic information about biological macromolecules and complexes that underpins our understanding of biological processes in healthy and diseased cells. It has had enormous impact on biomedical research, as evidenced by recent Nobel prizes awarded for the structure of the ribosome (2009, the major antibiotic target) and the structure of the integral membrane GPCRs (2012, the protein class targeted by ~40% of all current medicinal drugs). This activity promises to recapitulate, at the molecular level, the survey of nature that, in the Victorian era inspired Charles Darwin to propose an integrated view of the development of life. This will represent another information-led revolution in biology. However many challenges persist at most stages in the endeavour, we often still struggle to decipher the precise details of how macromolecular machines carry out their functions and we certainly do not yet have the proper tools to synthesise the various levels of information to put them into the cellular/tissue context. Nevertheless this technology enabled science is advancing rapidly, but is entirely dependent on researchers having access to an increasingly broad range of cutting-edge instruments and software.

Macromolecular crystallography

Structural biology largely had its origins in the UK and the UK led the way in the use of synchrotron radiation for macromolecular X-ray crystallography (MX) with the provision of specialised beamlines at the first dedicated synchrotron light source (the SRS at Daresbury). Since then the UK has largely maintained its strength in not only MX but also NMR and EM. The early focus on MX developments at the UK synchrotron has helped, over a period of more than 30 years, to also drive hardware and software efforts in a community coordinated way across the whole field, extending to an involvement in the international community. Diamond has reinvigorated activity in this area and has already made notable achievements in particular through exploiting the properties of this new source to deliver highly stable microbeams to tackle more challenging samples of high biological relevance. Development of new software methodology, algorithms and the establishment of automatic data analysis pipelines has been a key part of this success as it enables users to truly capitalise on the step change introduced by automation developments and new detector technologies.

Over half of Diamond's users are currently from the MX community and the majority of macromolecular structures are determined by the technique. The sheer size of the community and the concomitant development of the technique through software and hardware innovations provide an excellent model for how centralised resources and coordination can move a whole scientific field forward. A crucial part of this success can be attributed to the software coordination started by the collaborative computing project CCP4 which has contributed to transforming MX software into a coherent, robust commercial quality package that has had a huge international impact. CCP4 has consolidated the software data structures, facilitated data exchange and acted as a framework into which innovative algorithms can be embedded. Now based at the Harwell campus CCP4, together with Diamond plus a newly formed collaborative software initiative for EM (CCP-EM), are tackling the challenges of getting the most out of the data that can be measured by high end instruments. At Diamond work is already well advanced on developing innovative algorithms and software in a new diffraction integration package DIALS and building cloud based tools (with CCP4) for users to measure, process and analyse their data in MX. Together with CCP-EM this represents the groundwork for the integration of tools, applications and services used across these principal techniques of structural biology. Laying the foundations for standards and data exchange are key to improved automated solutions and lessons learnt are being applied to nascent software initiatives for solution scattering, X-ray imaging and super resolution light microscopy.

On the instrumentation side Diamond MX beamlines are pushing the boundaries of developments with the world's first dedicated *in vacuo* soft X-ray beamline (I23), the first dedicated *in situ* microfocus beamline (VMXi) and an innovative submicron beamline (VMXm) to complement efforts in the XFEL field towards measurements from the tiniest crystals. At the same time we believe that the existing beamlines broadly satisfy the needs of a hungry user community by offering automated high-throughput capability for what has become routine (a euphemism for state of the art) structural biology investigations.

Current limitations in measurement signal-to-noise, exacerbated at lower X-ray energies, have led to novel *in vacuo* developments on I23 and these same principles will be taken forward in combination with experience from the cryoEM field to deliver new approaches to submicron MX on the VMXm beamline where signal-to-noise and radiation damage dominate. Indeed it is at the interface of MX, CryoEM and XFEL developments that Diamond sees the future of sample delivery and sample handling for the most challenging of structural biology problems. The rather brute force serial crystallography approach taken to date at the LCLS (the first operational hard X-ray XFEL, at Stanford) must be refined for use at Diamond and this provides strong motivation for a significant effort in sample preparation and presentation. This is aided by a large collaborative effort to exploit next generation light sources, in particular the European X-ray Free Electron Laser (XFEL). Again inspired by the success of the MX community in delivering highly robust, efficient and reliable state of the art automated beamlines the first dedicated high-throughput crystallography beamline (SFX) is in construction to exploit the emerging serial femto-second crystallography approach pioneered by the group of Henry Chapman at LCLS. The UK are key players in SFX, thanks to support from the Wellcome Trust, BBSRC and MRC and an XFEL-hub is being set up within Diamond that focuses on the development of sample environments and sample delivery together with the challenges of data management and data analysis for next generation synchrotron beamlines and light sources. The short-term goal of the hub is to facilitate the use of XFELs by the UK community, especially the SFX instrument when it comes on-line. The strong synergies which exist for exploiting diffraction from submicron crystals both at XFELs and synchrotrons and the challenges these bring will benefit from a concerted approach. The XFEL hub is envisioned to play a role in development and implementation of new algorithms for data analysis and delivering new sample delivery systems for a range of experimental techniques.

Scattering and spectroscopy techniques

In solution, small angle X-ray scattering (SAXS) for the biological sciences is the only biophysical technique that provides a complete, albeit resolution-limited, picture of the thermodynamic state. SAXS measurements are inherently weak, derived from the scattering difference between the biological macromolecule and solvent background. Nevertheless, the scattering is isotropic permitting a large number of redundant observations from ~10,000 billion macromolecules during a single exposure. The macromolecules are in a thermodynamic equilibrium where at any given moment, a molecule will occupy one of a limited number of structurally distinct states (ensemble). Although crystallography has contributed a wealth of structural data that provide snapshots of nature at atomic or near-atomic resolution a precise understanding of how these macromolecules actually function remains unclear in many cases. Macromolecules are thermodynamic entities that function not as static structures but as dynamic machines interchanging between a set of discrete structural states.

These discrete states are often not conducive to crystallisation and may not even be resolvable by electron microscopy (EM), thereby creating a blind spot in our set of scientific observations. Current and evolving SAXS technologies now provide the tools to remove this blind spot enabling structural biology to move from a technique dominated by statics (crystal structures) to a technique of dynamics.

SAXS has benefited tremendously from advances in the X-ray sciences and with the success of MX there is now a strong renewed interest in the complementary dynamic and structural data provided by the technique. New developments in Information Theory provide a path for resolving the structurally distinct states by SAXS. Here, SAXS measurements are made of the sample under slightly varying conditions, e.g., changes in salt concentration or temperature. Application of Information Theory to the collection of SAXS measurements reduces the measurements to a set of independent SAXS curves where each curve represents a resolution-limited member of the ensemble. Thus SAXS can provide a complete structural snapshot of the thermodynamic state and resolve the thermodynamic ensemble. With this information, structural biology can now understand the dynamics of macromolecular action. Computational approaches that energy minimise a prior crystal structure into a SAXS observed distinct state will link the static structural understanding of biology to the dynamics that are requisite to macromolecular function. Delivery of a dedicated high flux beamline for biological solution scattering will enable such experiments to be performed and can provide, for example, high throughput SAXS to detect microcrystallinity. As X-ray, and EM, diffraction techniques advance towards sub-micron beam sizes for microcrystal diffraction experiments, the ability to detect sub-micron crystal formation must be made efficient and reliable. High-throughput SAXS can readily screen for the presence of microcrystals that would otherwise be lost using visible light techniques. A measurement can be made within seconds thereby reliably triaging samples for submicron focussing capable diffraction beamlines. This further builds on the use of SAXS for the assessment of sample suitability for single crystal structural studies. Circular Dichroism (CD) has the potential to play a role here especially with the current developments in high throughput CD measurements at Diamond’s CD beamline B23. Building on developments to date, the provision of an energy dispersive CD capability would bring new opportunities to complement the information obtained from scattering in addition to enabling the technique to provide information to structural biologists on timescales that can be used effectively to feed into single crystal analysis.

Electron microscopy

EM is a natural extension of MX to encompass the study of cellular machines and is a key technique for studying large macromolecular assemblies and cellular machinery. As biomedical science moves from discovering the structures of individual proteins and small complexes towards integrating larger systems and understanding their function in the cell, the tools provided by 3D EM have become central to the field. EM is in a state of rapid development and recent developments in direct electron detectors, in particular, substantially enhance the power of the method to study cellular machines both *in vitro* and *in situ.* Indeed it is now possible in the case of the most favourable samples to determine a single particle structure in atomic detail (at ~3 Å resolution) for a large, symmetric and rigid biological assembly using state-of-the-art equipment. Illustrations of the power of the complex approach come for example from virus, proteasome, chaperone and ribosome structures, but it is now clear that the same level of understanding is required in the context of cells and tissues, and for transient complexes. To achieve this, the methods of multiscale imaging are key to integration of molecular and cellular information. The central role of EM was recognised some years ago by the community, who prioritised the establishment of a national facility for EM. Inspired by the success of the MX community in delivering specialised beamlines delivering cutting-edge science it was proposed that the EM facility should operate in the same way as a synchrotron beamline to deliver high end microscopes for the UK community to use effectively. The establishment of the facility will create a natural focus for software support, development and training, synergising with the activities in macromolecular crystallography and X-ray tomography already established at the Harwell campus. The success of this national EM facility depends on its usability for the structural, molecular and cell biology community and thus will build on the knowledge gained at Diamond in providing a highly complex set of instruments to a growing community of users through a facility running 24/7.

Many parallels exist between EM and MX, as the methods for both cutting-edge electron microscopy and electron tomography are highly specialised and require considerable training and expertise, even more so once data are collected. Challenges exist with providing the necessary tools for users to fully exploit the high-end microscopes and growing a knowledgeable user community can be championed by the National facility. Furthermore, as with MX, there is considerable scope for further technical developments, from detectors, through electron optics to sample presentation, which remains wasteful, and also opportunities to apply the same end-to-end workflow analysis to the software that has proved so effective in MX.

Other imaging techniques

The synergy of EM with photon-based techniques underpins our strategy for the life sciences. Beamlines currently in construction include a full-field cryo soft X-ray microscope for biology (B24). This beamline will complement EM, providing tomographic imaging of whole cells and tissue samples, typically prepared by high pressure freezing. Whilst the resolution that can be achieved is currently much lower than that offered by electron tomography the advantage is that even 500 eV X-rays, which provide spectacular contrast for vitrified hydrated biological specimens, penetrate the specimen much more effectively than electrons, so that whole eukaryotic cells can in principle be imaged, whereas either cryo-sectioning (which typically distorts the specimen) or cryo ion beam milling (which is in its infancy) are required to provide a sliver of the cell of interest. Alongside X-ray and electron imaging light microscopy is being revolutionised by the application to biology of advanced superresolution techniques to provide images of fluorescently labelled systems at resolutions that can approach that of X-ray microscopy. To fully utilise the information requires the further development of cryo-fluorescence microscopy (*e.g.* through the routine use of liquid nitrogen immersion lenses). Diamond will not only provide cryo fluorescent capability embedded in the B24 X-ray microscope, but is also, in collaboration with Oxford University, developing a state-of-the-art cryo-fluorescence super-resolution microscope to be embedded in B24 as an 'offline' user facility. In addition to the capability of B24, Diamond beamline I08 will provide a scanning transmission X-ray microscope spanning the soft to multi-keV energy range. While elsewhere we will explore how harder X-ray imaging capabilities (especially at I13) might be exploited in biology is being pursued. All of these instruments will be tightly integrated so that Diamond can become the centre for high resolution biomedical imaging in the UK.

Logistics, software and hardware

Developments in the automation of sample transfer at MX beamlines have played a transformative role in increasing the efficiency of use of synchrotron beam time while permitting biologists to address tougher problems by alleviating the burden of manual sample mounting and manipulation. Experience at Diamond in recent years with the implementation of fast exchange sample changers, creation of shorter user visits of just a few hours and extraordinary throughputs of several hundreds of crystals per day has now created the need for an extension of automation systems to address issues of sample and user management outside the beamline. Remote access is already playing a major part in alleviating the logistical challenges of bringing users through the doors and training them but a side-effect has been a greater demand on internal dewar shipping and management systems, not to mention the demands on staff to maintain, move and mount samples into the beamline sample robots. The trend shows little sign of slowing and the extensive use of automated shipping and handling systems will be key to MX and other life science beamlines in future.

The marrying of expertise in building instruments to measure data and in designing software to analyse that data has been the seed for a new generation of MX analysis software called DIALS (Diffraction Integration for Advanced Light Sources). DIALS aims to allow explicit modelling of the diffraction experiment to produce the best estimates of diffraction intensities and their errors in the context of a quickly evolving field. DIALS has been designed to analyse both synchrotron and XFEL diffraction data and can easily adapt to the implementation of new data collection schemes and the use of new detectors. Moreover it lends itself to efficient parallelisation so that data analysis times can keep pace with the sometimes shockingly fast data collection speeds (seconds or less) from Diamond beamlines using modern (> 100 fps) area detectors. Finally, it will also be adapted to work with electron diffraction data.

The adoption of commercial hybrid pixel counting detectors technology in MX has opened up new avenues of investigation in data collection methods. The ability to measure room temperature data using very high X-ray dose rates and detector frame-rates (100 fps) reduces the impact of radiation damage opening up new territory for *in situ* data collection. However the use of silicon-based sensors still limits the sensitivity above 20 keV and counting detectors suffer from count-rate limitations at the highest dose-rates. This problem will become even more acute as source brilliance increases. There remains a need therefore for technology that permits measurements at very high count-rates ($>10^7$ counts/pixel/second) with high sensitivity above 20 keV, especially since the potential value of higher photon energy, for instance in distributing radiation damage beyond the crystal volume for microcrystals in microbeams, is not yet fully understood.

Increased brightness and photon flux can aid in expanding the scientific capabilities of Diamond. Significant advances can be made through incremental upgrades to beamlines (improved and/or novel optics) and the Diamond machine via increasing the machine current to 500 mA. Improvements to current insertion devices such as use of cryocooled or superconducting undulators, as well as modifications to the lattice structure to allow additional insertion device beamlines to be constructed will ultimately pave the way for Diamond-II. This is expected to reduce by an order of magnitude the emittance of the machine. Careful analysis of the requirements of integrated structural biology will be needed to provide an opportunity to optimise the machine parameters, and the considerable down-time whilst the upgrade takes place presents a risk for the UK community. As the community moves away from the expectation that X-ray screening for MX will occur in their own laboratories Diamond might consider providing a state-of-the-art off-line source to mitigate some risks to the community.

Summary

At Diamond our overarching aim is to provide the infrastructure and technical expertise to enable an integrated approach for molecular and cellular structural biology combining multiple technologies and disciplines that spans determination of individual macromolecules at atomic resolution through to the cellular context as illustrated in Figure 1 (thanks to Dr Kay Grüenewald and Prof. Helen Saibil for the use of this figure).

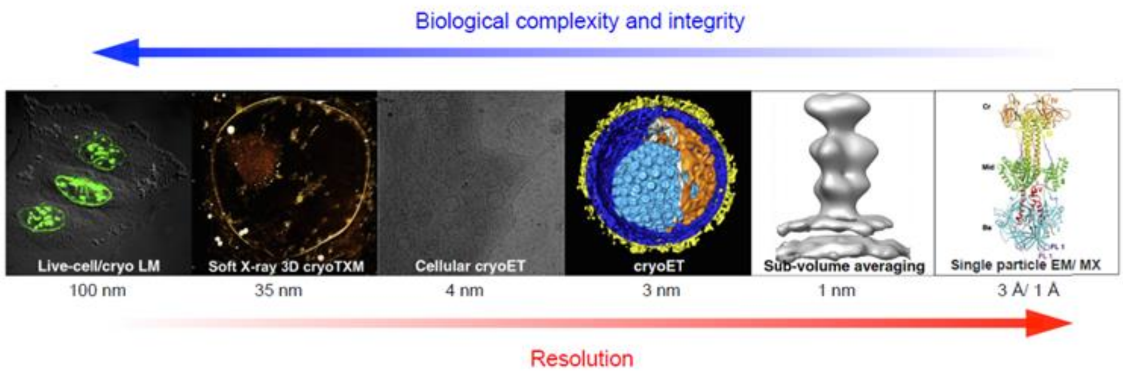


Figure A 2.1 *Integrated structural biology approach combining correlative light, soft X-ray cryo and electron cryo microscopy with high-resolution structure information and thus enabling the dissection of dynamic processes different levels of resolution and complexity. The biological process is visualised by LM (light microscopy), cryoTXM (transmission X-ray cryo microscopy), cryoET (electron cryo tomography), single particle cryo EM and/or macromolecular crystallography (MX).*

A core aspect of this vision is the development of new instruments and techniques that exploit the light generated by the Diamond synchrotron, as well as complementing these capabilities with other techniques that are integrated within Diamond. Specialised laboratories to tackle challenging biological problems have been pioneered in or adjacent to Diamond and aid delivery of these objectives. The membrane protein laboratory (MPL, a joint Diamond/Imperial College activity supported by the Wellcome Trust) provides a uniquely integrated synchrotron laboratory for the production and structure determination of membrane proteins as well as methods development. The joint development of *in situ* crystal characterisation between I24 and the MPL exemplifies how the integration of such facilities into Diamond drives both science and technology. The MPL has benefitted from the establishment of the OPPF-UK at Harwell (funded by the MRC and BBSRC), where expertise in the development of a range of technologies focused on exploiting robotics systems has enabled high-throughput production of recombinant proteins for structural studies to be pioneered. Bringing together the expertise of these core facilities is an essential part of delivering an integrated structural biology facility. Most importantly these facilities together are opening up structural studies of very challenging systems such as membrane proteins, once the domain of a few specialised groups, thereby empowering a broader community of molecular and cell biologists.

In summary capitalising on improved source capabilities through upgrades to beamlines and the build-up and integration of associated facilities both at Diamond and on the Harwell campus as a whole as graphically summarised below will allow structural biologists to confidently tackle biological systems in a cellular context. This project, to provide a world-leading centre for integrated structural biology is in-line with the ESFRI pan-European roadmap for science infrastructures, which features an infrastructure with exactly this remit, Instruct. Instruct is led from the UK (MRC are the lead support agency, and the Instruct Hub is currently based in Oxford) and the intention is, initially via an MOU, for Diamond and Instruct to work closely together to deliver outstanding infrastructure to UK and European scientists. Indeed it might be appropriate, in the medium term, for the Instruct Hub to relocate to the Harwell campus.

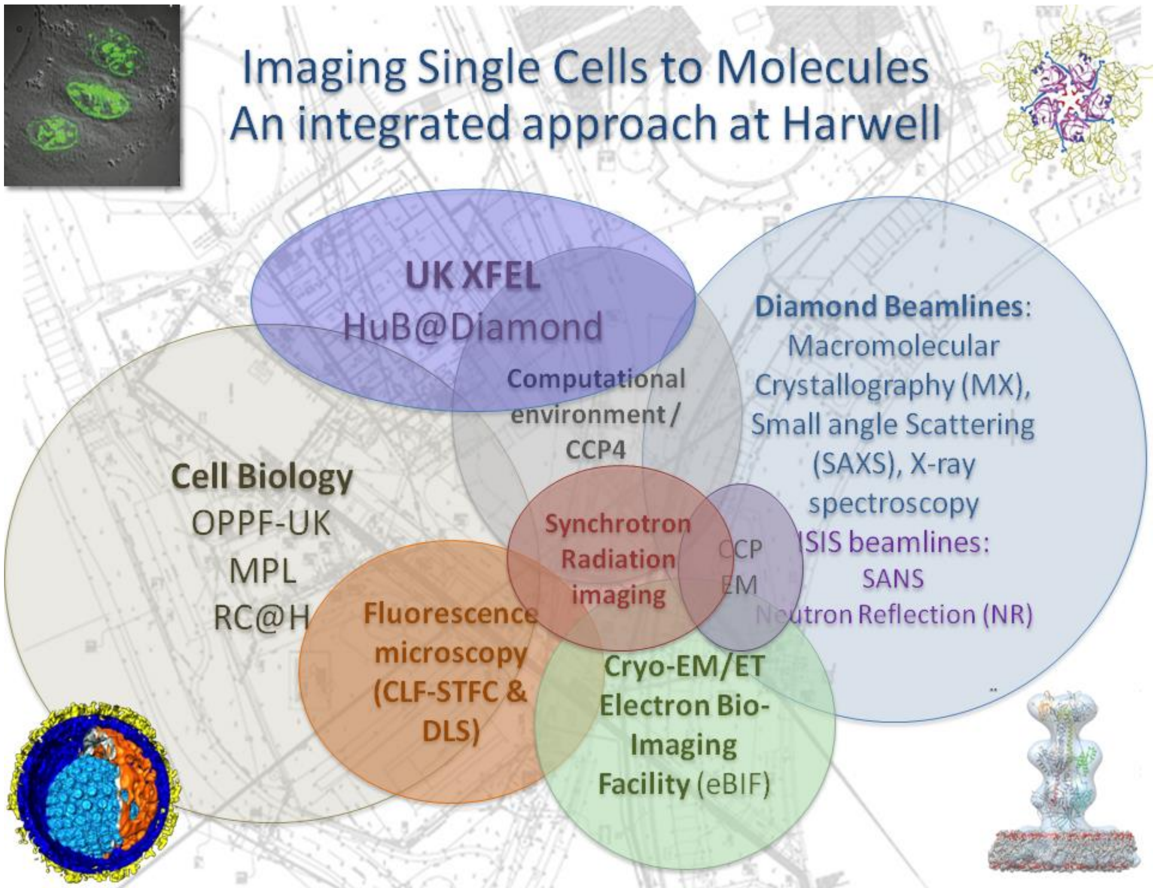


Figure A 2.2 *A summary of the infrastructure available at Harwell which provides a unique imaging platform for structural biologists*

Summary of Deliverables

The major infrastructure deliverables foreseen over the next five years are:

- Delivery of the VMX project which will provide a submicron variable focus beamline to generate the best data from the smallest of crystals (VMXm) and a dedicated tuneable microfocus beamline that will exploit *in situ* diffraction
- Phased upgrades of I24, I03, 4,4-1 optics, insertion devices to CPMUs delivering ~x5 increase in photon flux at the sample.
- Establish a new prototype MX facility to enable high performance automated collection of diffraction data through the delivery of a new dedicated MX beamline.
- Rolling upgrades of detectors for X-ray techniques (*circa* 1 per year)

- Upgrade of B21 to increase by at least an order of magnitude the photon flux at the sample
- Establish a state of the art off-line X-ray facility for MX and SAXS to provide close to full year-round access for structural biology users
- Establish a dedicated sample environments group to exploit new Diamond beamlines/sources (XFEL, EM, X-ray and super resolution light microscopy).
- Establish and develop the National facility for Electron microscopy, to become an integral part of Diamond's structural biology user infrastructure
- Continued development and implementation of automation hardware and software for Diamond beamlines and the EM facility
- Delivery of a diffraction limited source and associated high brilliance, high photon flux beamlines for cellular and molecular structural biology, using MX and solution scattering.
- Consolidation and enhancement of software developments for X-ray imaging techniques across Diamond.
- Establish the UK XFEL hub, and a plan for sustainability
- Investigate value of UK based hard X-ray Free Electron Laser
- Energy Dispersive CD Beamline for high-throughput structural biology applications

A 2.2 Chemistry and Catalysis (Science Champions: Sofia Diaz-Moreno and Georg Held)

Introduction

Chemistry plays a major role in many of the Global Grand Challenges identified by EPSRC, in particular sustainability, health, technology and growth, and resilience, both in terms of fundamental understanding of chemical processes and in the development of new substances and technologies. In 2010, the International Council of Chemical Associations estimated that the chemical industry was directly responsible for approximately 5% of the world GDP and supported the employment of approximately 20 million people. It has been estimated that 90% of all chemical processes make use of a catalyst [1], and according to the North American Catalysis Society this translates, through their role in the fossil fuel cycle, to 35% of the world GDP being reliant on catalytic processes. The long standing goal of catalysis research is to enable new synthetic processes for the production of current materials or new substances. This result requires an integrated approach to the total catalytic process, focused on products, feedstocks, catalytic materials, and energy sources. Desired future efficiencies dictate enhanced selectivity, an effort that focuses on the catalytic materials themselves. In order to minimise consumption of non-renewable energy sources such as fossil fuels, it is important to develop processes that utilise alternative energy inputs. The ultimate dream is to have the knowledge required to be able to custom design the catalysts that are appropriate for enhancing whichever chemical processes need to be undertaken.

Research in chemistry and catalysis has greatly benefited from the use of synchrotron radiation facilities. The use of spectroscopy and scattering techniques has allowed the elucidation of the geometrical and electronic structures of the different species involved in chemical processes with the goal of relating this knowledge with their function. The development of high-brilliance third generation sources has taken us from the need to study model systems primarily under vacuum to enabling us to follow fast processes under *operando* conditions and under realistic reaction conditions of concentration, temperature, etc. The use of synchrotron facilities has allowed the study of the structure of these chemical species at very different length scales, from the atomic structure to the long range order structure or meso-scale.

Nowadays, it is recognised that in most cases it is insufficient to investigate chemical processes with a single structural and/or analytical technique, and the evolving paradigm prescribes the application of multidisciplinary methods if the comprehensive insight required for knowledge guided process optimisation is to be obtained. The study of chemical processes by multiple techniques simultaneously under realistic conditions can deliver the full hierarchical characterisation of materials. To date the use of successful combinations of techniques such as XAS/DRIFTS/MS/UV-Vis, XAS/XRD/UV-visible/Raman, or SAXS/WAXS/Raman/UV-visible have proven to be very powerful for elucidation of reaction mechanisms and improving catalytic systems.

Below we highlight a selection of current research themes that are expected to continue to evolve over the next decade, and that are intimately related to the field of chemistry and catalysis. Some of the research themes will be also covered by others of the seven scientific areas identified as part of this exercise. This is for example the case of the Electrochemistry theme, as batteries, fuel cells and electrochemical sensors will be covered by the Materials and Engineering area.

[1] G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, ed. *Handbook of Heterogeneous Catalysis*. (Weinheim, 2nd ed., 2008).

Scientific Challenges

2.1 Catalysis

The outstanding challenge for catalysis research is the delivery of more efficient and selective chemical syntheses, with the maximum speed and the minimum amount of waste. To this end, current research efforts are focussed on designing sequences of catalytic reactions that do not require external intervention, such as those found in many biosynthesis pathways. Major development themes include (i) the formulation of independent mutually compatible catalysts that work in one-pot, where each catalyst in the mixture is responsible for an individual step in a multi-step reaction series whilst not interfering with other steps, and (ii) the development of switchable catalysts, that can be activated or deactivated by external methods, such as light, temperature etc., that would allow chemists to externally program multi-step syntheses.

Aside from efficiency and selectivity, another important issue relates to the sustainability of both the feedstock and the catalysts. Petrochemical feedstocks will need to be used for some time yet, but there is recognition that it is increasingly urgent for new alternative hydrocarbon sources to be found, such as biomass or engineered feedstocks. In addition, most of the catalysts in current use are formulated using precious metals. For reasons of cost and long-term sustainability it is increasingly important for traditional chemical processes that new catalysts are developed that either function with very low loadings of the precious metals, or that are based on less expensive and more abundant elements. One very promising development route in this area is the combination of traditional heterogeneous and homogeneous catalysts with very selective enzymatic synthesis mechanisms to facilitate the efficient coupling of biocatalytic reactions with more traditional chemocatalytic processes.

In order to develop highly selective, efficient and long lifetime catalysts, it is important to improve our understanding of the reactivation pathways and of the poisoning of the catalysts, together with the stereochemistry, formation and decomposition of intermediates that occur in the catalytic cycle. Structural techniques available at synchrotron facilities can clearly help address these questions by providing detailed characterisation of reactions under *'in situ'* conditions. Faster and more sensitive structural methods are continuously being developed, and are shaping up to be almost ideal tools to meet these objectives. Advances in theoretical approaches are also necessary in order to be able to rationally design catalysts with specific capabilities. Within the EPSRC research portfolio, catalysis is the only field of chemistry that is expected to grow over the next years.

2.1.1 Homogeneous catalysis

Looking specifically at the area of homogeneous catalysis, the major challenge is the development of robust materials that are able to operate in a wide range of conditions of temperature, pressure, pH, etc.

If more efficient and robust catalysts are to be synthesised, the structure of the catalysts in the reaction media needs to be properly understood, as well as the chemical interactions that occur with other species that can be found in the reaction media. If these fundamental investigations are to be of use to chemical engineers, it is particularly important that the investigated systems are operating under realistic conditions; the catalyst and reactants need to be present at realistic concentrations, and the reaction media needs to be representative of what is expected when the reaction takes place in the chemical plant. Taking these requirements to their logical conclusion means that ideally realistically sized reactors need to be used, as scaling can have an impact in chemical transformations.

Selectivity control can often be achieved in homogenous catalysis through molecular recognition. In these cases, the solvation of the ligand(s) and/or the cavities plays an important role in the reaction mechanisms and consequently a deep understanding of the solvation of the species involved in the reaction would help us develop more efficient catalysts.

In homogeneous catalysis a longstanding challenge is the separation and recovery of the catalyst following use. Although the aim is to use small quantities of catalysts, it is important to be able to recycle them and to ensure that they do not end up as part of the final product in the form of undesirable impurities.

2.1.2 Heterogeneous catalysis

Heterogeneous catalysis is essential to the majority of chemical industries as it underpins most chemical syntheses. The development of more sustainable chemical processes requires better catalyst formulations and the optimisation of these catalytic materials for specific applications. One of the major problems related to the operation of heterogeneous catalysis is the loss of catalyst activity with time-on-stream. Although still poorly understood this deactivation process is inevitable, but it can be slowed and some of its consequences can be avoided.

In spite of their industrial ubiquity, tuning the chemical properties of catalytic systems remains a real challenge due to the inherent complexity that derives from both reaction phase heterogeneity and sensitivity to various conditions (gas flow and composition, temperature, pressure). Current research in using metallic nanoparticles as catalysts for heterogeneous processes is showing a great amount of potential for future developments in this area. The surface structure of the catalytic site plays a very important role in the efficient of the catalyst, and in the particular case of nanoparticles the coordination of surface atoms can be substantially different from those in larger crystallites, which will greatly affect the function of the active site(s). Controlling the surface structure in nanoparticles will allow us to design function-specific coordination environments. Topical examples are the refinement of gas-to-liquid (GTL) processes involved in Fischer-Tropsch (FT) syntheses that are used to produce liquid hydrocarbons and finding suitable catalysts for refining biomass to fuel and/or fine chemicals. These processes have become increasingly important due to the decreasing availability of natural resources and the high price of fossil fuels [1,2]. Recent studies using mono- and bi-metallic nanoparticles with tailored shape and size are showing considerable promise for improving the efficiency of the process.

[1] “Chemistry - Developing Solutions in a Changing World”– EuCheMS report (2011)

[2] P. Frenzel, et al. “Biomass as Feedstock in the Chemical Industry - An Examination from an Exergetic Point of View”, Chem. Eng. & Technol 36 (2013) 233.

2.1.3 Chemoenzymatic synthesis

Biocatalysis is extremely selective, but is highly substrate specific, generally slow, and can only happen under tightly controlled conditions of temperature, pressure and pH. In addition, the sources of energy for enzymatic processes are frequently found to be very expensive or difficult to obtain. The current challenge is to design new catalysts and mechanisms that, maintaining the high selectivity achieved in biocatalytic processes, can be used under a wider range of conditions and at higher speeds, using alternative chemicals as energy source for the enzymes. Research in the field is currently focussed in chemoenzymatic synthesis, that combines the flexibility and robustness of the chemical synthesis with the high selectivity of enzymatic synthesis. This is becoming a real alternative for the production of complex carbohydrates. The strong life science foundations of Diamond Light Source will provide an ideal opportunity for building strong collaborative projects in this interdisciplinary field.

2.2 Atmospheric chemistry

Man-made changes to the earth’s atmosphere will remain one of the big challenges for the current and future generations of scientists and politicians alike. Air pollution in urban centres and associated health concerns [1], climate change, photochemical smog [2] ozone depletion caused by CFCs [3] and acid rain due to high sulphur emissions [4] have direct impact on humans and nature. Decades of research have shown that the complex interplay of chemical reactions that determine the atmosphere cannot be modelled accurately without thorough experimental characterisation of each of the key chemical processes.

While most of the important gas-phase reactions of small molecules in the atmosphere, such as the ozone cycle or NOx chemistry, are well-studied and understood, the chemistry of aerosols and larger volatile organic compounds (VOC) still requires significant fundamental research. Their impact on the near-earth atmosphere is of similar magnitude. Aerosols can act as nucleation centres for cloud formation or heterogeneous catalysts for reactions of trace gases, VOCs can adsorb on water droplets and form surfactant layers or dissolve and pollute rain water, they can react with trace gases and/or coalesce and form aerosols.

Recent developments in *in situ* X-ray spectroscopies now make it possible to measure concentration depth profiles of surfactants and solutes in droplets and jets of water and other liquids. The same technique also enables measuring the uptake of water on aerosol molecules.

[1] H. Altug, et al., Proceedings of the 8Th Conference on Environmental Science and Technologies, 609-625, (2012)
[2] T. Castro, S. Madronich, S. Rivale, A. Muhlia, B. Mar, Atmos. Env., 35 (10), 1765-1772, (2001); Jianzhong Ma, Xiaobin Xu, Chunsheng Zhao, Peng Yan, Advances in Atmospheric Sciences, 29 (5), 1006-1026, (2012)
[3] M. Shoeberl and D. Hartmann, Science, 251 (4989), 46-52, (1991); M. Piot and R. Von Glasow, J. Geophys. Res. Atmos., 64 (2-3), 77-105, (2009); S. A. W. Gerstl, A. Zardecki, H. L. Wiser, Nature, 294 (5839), 352-354, (1981)
[4] G. E. Likens, F. H. Bormann, N. M. Johnson, Environment, 14 (2), 33-35, (1972); X. J. Wen, C. Q. Duan, D. C. Zhang, Environmental Earth Sciences, 69 (3), 843-853, (2013)

2.3 Sustainable chemistry

In the area of sustainable chemistry, one of the main aims is to find novel uses for materials that are currently classed as waste products. This may require the development of new catalysts to process waste into biofuel or useful products. A highly topical research area is focussed on the potential use of carbon dioxide, a major waste product of the hydrocarbon fuel cycle, as a chemical feedstock for the production of other chemicals, materials or fuels.

Metal extraction and recovery (recycling) is another important goal within sustainable chemistry. New approaches need to be found where the metals can be extracted without damaging the materials in which they are contained. The main challenge in the medium term is the need to extract ever smaller quantities of metals out of solutions, as processes become more efficient, and being able to do this in a selective manner. This task requires the design of new chemical processes, which in turn requires detailed knowledge of the structure of metal ions in solution and their affinity for different ligands. Synchrotron radiation techniques play an important role in increasing the understanding of the local and medium range environments that will allow the development of more efficient and select methods for metal extraction.

A specific example of metal extraction and recovery is the need to improve our ability to efficiently reprocess spent nuclear fuel. This frequently involves the challenging issue of separating actinides from the lanthanide fission products, with very similar chemical properties.

2.4 Energy

Energy issues, both nationally and internationally, are among the most urgent and important global challenges. Synchrotron facilities have a key role in supporting this research theme, for example through improving our understanding of energy storage and efficiency and CO_2 mitigation, thus reducing our dependence on limited fossil fuel supplies for energy conversion. These are all recognised as major challenges and there is a strong expectation that these issues will be addressed in large part by new scientific developments and technological solutions. This research area has significant overlap with Materials research, but Chemistry plays an essential role in meeting the challenges in materials discovery and the fundamental understanding of the chemical processes required to develop new generations of solutions. This includes immediate energy-technology requirements and planned long-term programmes in for example, energy storage (batteries, hydrogen), energy harvesting (photocatalysts, photovoltaics) and energy utilisation (fuel cells).

The discovery of new materials for the next generation of devices is a major research topic, and the final goal is to increase the difference voltage in a redox couple. Similarly, novel materials that have potential as components in solid oxide fuel cells, oxygen generators and sensors, are under continuous investigation and this research significantly benefits from synchrotron radiation studies. One of the key targets for these materials is their ability to conduct oxygen ions at intermediate temperatures (500-750°C) whilst also maintaining compatibility with other components within the device. Synchrotron radiation facilities allow the study of these materials under *operando* conditions using techniques such as powder diffraction and spectroscopy in a routine manner. Future requirements are to better integrate sample environments with conventional lab methodologies (e.g. Raman spectroscopy) in order to ensure appropriate conditions are being replicated.

Studies of porous metal-organic framework (MOF) materials have attracted enormous attention owing to their potential for high capacity gas adsorption, in particular, for selective capture of harmful flue gases (CO_2 and NO_2). Single crystal diffraction allows *in situ* studies of the structure of microporous MOF materials as a function of gas loadings, while X-ray absorption spectroscopy allows the determination of changes in the electronic structure of the metal site. Understanding the causes of the different selectivities for different gases will help in the design of new materials tailored for specific functions.

2.5 Solution chemistry, crystallization

The interactions between the different species present in solution during a reaction affect strongly not only the rate of the reaction but also the resulting products. The solvated ion structure and their in-solution ion complexation can markedly affect the reactivity of an ion species, and the choice of solvent can dramatically change the yield of a given reaction. Understanding the structure of the different species in solution, including how the solvent structure changes over time and how is perturbed or modulated by the presence of the solutes, will help in optimising the conditions for which the reaction occurs. Synchrotron radiation techniques, in particular X-ray spectroscopy and X-ray pair distribution function methods (XPDF), will help deliver detailed insight into the molecular length scale structure of the solution. Combining the capabilities of these techniques allows us to move beyond the traditional picture of a continuous solvent solvating isolating solvent molecules.

Knowing the structure of a solution is also an essential step on the route to understanding how nucleation, the first step in crystallisation, is triggered. Improved knowledge in this area should allow us to improve the crystallisation process or stop it from happening. Traditional experiments are directed at determining the nucleation rate of a molecule of interest in several different solvents, but knowing the structure of the nanoscale nuclei at the time of formation will help identify the best conditions for nucleation to occur. It is still not known if molecules nucleate and build into a cluster with a single crystal form, the same as the bulk, or whether polycrystalline clusters, with competing conformations, form. This is expected to depend on the system under study and on a whole range of factors such as solvent, concentration, temperature etc…

Controlling the crystallisation process is essential for the chemical industry and in particular in pharmaceutical synthesis. Crystal purity is important, but other factors such as the shape and size of the crystal can impact the dissolution rate, which in turn changes the time profile of a drug dose. In order to control the crystallisation process we need to understand the structure of the interface between the crystal and the solution surrounding it and how this interface is stabilised by the solution environment. The addition of additives and the choice of solvent can have a very strong effect on the crystallisation process, but their role is still not completely understood.

The use of synchrotron radiation techniques such as small angle scattering, FTIR and diffraction can help to increase our knowledge about the nucleation and crystallisation processes, so more controlled methods can be developed.

2.6 Fundamental reaction studies

In-situ time-resolved XAS is a strong development in the UK using pump-probe methods with emission XAS as well as absorption measurements and this is a natural extension which will lead to longer term developments on FEL sources. This uses light activation on catalytic systems to obtain ps-ms structural determination of reaction pathway intermediates and investigation of conformational changes in photoactivated catalytic processes. Understanding these mechanisms is key for developing new catalysts and materials.

2.7 Electrochemistry

The defining characteristic of electrochemistry lies in the spatial separation of oxidation and reduction reactions and their control by application of a potential. This is useful both as a tool to better understand chemical processes and as an alternative route for production and processing. Electrochemistry finds wide application across chemistry and materials science and it is a core component of energy application because its use offers a practical route to obtain the maximum fuel efficiency. With the increased use of renewable power sources such as solar, tidal and wind where demand and supply cannot always be matched, there is an increasing need for efficient energy storage on scales ranging from domestic batteries to power stations. Thus development of suitable batteries is a high priority worldwide. Electrochemical solutions for transport applications are a key target in this area. Cheap and reliable alternatives to lithium ion batteries are highly desirable. After many decades of development, fuel cells are moving into the marketplace in transport and also for combined heat and power solution to domestic energy usage. The search for lower cost electrocatalysts whose reliability matches that of platinum based systems continues and is likely to continue for the foreseeable future.

Corrosion is estimated to cost ca 3% of GDP each year and is implicated in many safety critical applications such as the integrity of transport systems such as bridges and boats, the storage of nuclear waste and biomaterials (hip transplants). Corrosion is subject to many factors spanning from surface structure, materials microstructure, environmental factors such as stress and fluid flow. The ability of SR to study interfaces, materials and whole systems using soft through hard X-rays, diffraction, spectroscopy and imaging, makes it a particularly relevant tool in the study of corrosion.

2.8 Organometallics, Coordination and Supramolecular Chemistry

With the increasing interest in the synthesis of functional materials beyond what can be achieved with single molecules, new approaches in supramolecular chemistry are promising to revolutionise the properties of materials through the close control of their structures. By linking small molecules via intermolecular interactions such as hydrogen bonds, large supramolecular assemblies can be formed with structures that have been carefully tailored to perform the required, often highly specific, function. This bottom-up approach to the synthesis of nanoscale systems provides a variety of materials with applications ranging from biology to materials science [1]. Perhaps the most widely known supramolecular assemblies, due to their promising potential as gas-storage materials for energy applications, for gas sequestration and for the slow-release of pharmaceutical agents within the body, are the metal organic frameworks (MOFs) [2]. Another class of molecular framework material, covalent organic frameworks (COFs), dispenses with the metal component completely and the linker molecules are bound together via covalent bonds by additional organic components to form a framework [3]. These systems are attractive as the lack of a potentially toxic metal atom makes them more environmentally friendly. Other supramolecular assemblies, such as threaded rotaxane and catenane molecular systems, have the potential, due to their unique topological cavities, to exhibit unprecedented anion recognition, sensing and molecular machine-like properties, where the molecular movement of the rotaxane/catenane constituent parts are controlled by anion binding [4].

These, and the many other examples of engineered supramolecular systems, are steadily evolving into ever more complex structures and their structural characterisation is increasingly beyond the capabilities of most university based instrumentation. The use of X-ray scattering and X-ray spectroscopy techniques at Diamond, providing structural information from atomic to mesoscale length scale, are crucial for the directed design of these materials so that they are optimised for their specific function.

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[2] Metal–Organic Frameworks in Biomedicine, Patricia Horcajada, Ruxandra Gref, Tarek Baati , Phoebe K. Allan, Guillaume Maurin , Patrick Couvreur , Gérard Férey , Russell E. Morris, and Christian Serre, Chem. Rev., 112 (2), 1232–1268, (2012).
[3] Covalent organic frameworks, Andrew I. Cooper, CrystEngComm, 15, 1483-1483, (2013).
[4] Rotaxanes Capable of Recognising Chloride in Aqueous Media, Hancock, Laura M.; Gilday, Lydia C.; Carvalho, Silvia; Costa, Paulo J.; Felix, Vitor; Serpell, Christopher J.; Kilah, Nathan L.; Beer, Paul D., Chemistry-A European Journal, 16(44), 13082-13094, (2010).

2.9 Surface chemistry

Electron-based synchrotron techniques, such as photoelectron spectroscopy or electron-yield X-ray absorption spectroscopy, are inherently surface sensitive. Hence surface chemistry, i.e. chemical modifications that involve only a few layers of atoms near the gas/liquid-solid/liquid interface, has long been a subject studied at synchrotrons. It underpins a number of the subjects above, e.g. heterogeneous catalysis, electrochemistry, corrosion or atmospheric chemistry, but the scope of surface chemistry goes further. It also covers surfactant layers (gas – liquid interface) as well as self-assembled organic layers on solid surfaces, functionalised surfaces and novel graphene-like or graphene-based materials.

Surfactant layers of lipids or proteins may be used as simple model systems for bio-membranes to study their reaction to changes in their physical or chemical environments (e.g. freezing at oil-water interface). Self-assembled organic layers and functionalised surfaces are interesting models to study pattern formation, molecular recognition, or signal transmission between molecules. Such organic layers are also the basis of future electronic devices or sensors.

After a decade of intense research on graphene and its most unusual material properties, graphene derivatives and graphene-like materials, such as BN, have now moved into the centre of attention promising equally interesting findings.

Enabling technology and processes

As mentioned in the introduction section, it is nowadays recognised that in the chemistry and catalysis area, in most cases it is insufficient to investigate chemical processes with a single structural and/or analytical technique. As we want to study more complex systems, the application of multidisciplinary methods is necessary if the comprehensive insight required for knowledge guided process optimisation is to be obtained.

In order to make this possible at Diamond, we will need to invest not only in new technology and equipment, but we will also need to revise the work structure at Diamond and our scientific interactions within diamond and more widely with the rest of the Harwell Campus.

We envisage that for Diamond to really have the best chances to make a worldwide impact in this research area we will need to strengthen the collaborative bonds between the scientists working at Diamond Light Source and the very strong scientific groups working across the Harwell Campus, as well as Universities. In particular the synergy with the expertise available at the Research Complex at Harwell and Diamond will create a unique environment that can stimulate the advancement and understanding of chemical and catalytic processes. A good collaborative agreement with the Catalysis Hub will facilitate the development of state of the art equipment for the beamlines for the study of catalytic systems that will translate in high impact publications. This collaboration can thus parallel the underlying reasons that have enabled the Swiss Light Source to become a recognised centre of excellence in catalysis research through that facility's very strong partnership with the ETH Zurich. In addition, strong collaborations with the Dynamics and Structure Science Consortium at the Research Centre will be beneficial to build the expertise at Diamond in dynamics experiments (pump-probe) that will then be used for the future UK FEL experiments. This is the main goal to be achieved that will help to put the UK at the forefront of international chemistry and catalysis research.

Below are listed some of the technological and logistical aspects that will need to be looked at in order to achieve our goal for the next ten years.

3.1 Collaboration between diamond beamlines and with other facilities based at RAL

In order to achieve a multidisciplinary approach that will be needed to tackle many of the Chemistry and Catalysis challenges in the coming decade, we will need to facilitate access to many of the different techniques that available at Diamond and on the wide site.

If an experiment requires the use of several Diamond beamlines or even the use of off-line equipment available at diamond but not based on synchrotron radiation, a system should be available where the proposed experimental programme only needs to be judged once by a panel of experts in the field. If the experiment is considered good enough it would be advantageous that beam or facility time is then allocated to the project as a whole across all the different instruments. Ideally, this would be extended to other facilities on-campus such as those at the ISIS pulsed neutron and muon source, and the Central Laser Facility.

This will undoubtedly aid users to take advantage of complementary techniques and, within this framework, scientific collaborations inside Diamond and with scientists from other facilities will be encouraged.

This collaboration should also be extended to equipment availability. Although the requirements among the different facilities and even for different beamlines are very specific, sometimes equipment can be shared. This is for example the case with the lasers needed to perform fast time-resolved experiments at Diamond, where the most cost effective and convenient alternative to purchasing dedicated lasers for Diamond beam lines would be to ask the Laser facility at RAL to assist us. In those cases where equipment cannot be directly moved within diamond or to different facilities, the expertise should be in any case shared to avoid unnecessary duplication of effort.

3.2 Sample environment

The development of new sample environment equipment designed to specifically perform '*in situ*' experiments and under real conditions of pressure, temperature etc. should be considered a priority in order to address the challenges in the fields of chemistry and catalysis.

In addition, the ability to simultaneously use other analytics techniques such as Raman, IR, UV-Vis spectroscopies, mass spectrometry and NMR will make a difference when complex processes need to be understood.

These developments will only be possible if dedicated technical (engineers and technicians) and scientific teams are formed, and if dedicated laboratory space is made available to carry out the assembly and testing of the new instrumentation. Chemical reactions in particular require the control/determination of many parameters (e.g. temperature, concentration of reactants and products, pH, potentials, etc.) in addition to the typical beamline parameters. Diamond could make a real step-change if we could create an environment that allows the integrated control of such multi-parameter experiments. These will be different for every user, hence this can be only be achieved by a science-driven committed team of software engineers, who can react fast and flexibly to user demands.

It is also important to highlight that an increasing number of samples that are brought to Diamond to be studied, require sophisticated *in situ* sample preparation which cannot be provided at every beamline. Thus, the provision of a series of load locks with glove boxes and ex-situ facilities (chemistry laboratories) and *in situ* preparation facilities such as MBE, organic layer deposition, nano fabrication, etc., coupled with a number of non-synchrotron analysis facilities (STM/AFM, IR, SEM, TEM), will help avoid waste of valuable beam time on poorly characterised samples. A methodology needs to be put in place to transfer samples from any preparation facility to any analysis facility, including beamlines. In the case of samples that need to be kept under vacuum, a UHV sample storage and transfer system should be developed.

3.3 Sources and beamlines

The stability of the X-ray beam during an experiment, both in energy and position, is extremely important when following *in situ* processes. If a reaction is being studied and a structural change occurs, we need to ensure that the observed change in the experimental data is real and not due to spurious instabilities in the experimental equipment. Special attention needs to be paid to the stability of the X-ray beam delivered by the machine, but also to the stability of the beamline optics.

If the rate at what a chemical reaction can be followed is limited by the statistics, increasing the number of photons will help to allow the study of faster processes. However for most of the time, the experimental limitation rests with the detection method, and efforts should be devoted in developing detectors that can cope with the high flux of synchrotron beamlines (see section below).

Decreasing the emittance of the machine will be beneficial for diffraction and imaging techniques, as this will improve the temporal (µs – ns) and the spatial resolution (nm). This is particularly relevant for the study of the 3D structure of heterogeneous catalysts under *operando* conditions. The smaller source size will be translated in a smaller X-ray beam focal size at the sample. This in turn will allow the development of microreactor cells for the study of chemical processes in solution with smaller dead times and using considerably lower quantities of solutions. However we need to be cautious as samples will degrade faster due to the radiation damage produced by the higher brilliance of the X-ray beam.

It is important to highlight that any development in the machine will need to be followed by development of the optics in the beamlines. Better mirrors will be needed to preserve the lower emittance of the machine, and better cooling systems will be needed to be designed to ensure that the optics does not drift because of the higher power densities.

Another critical aspect of the machine operation that affects the study of chemical processes is the presence of top-ups to maintain the ring current in the ring. Currently, the experiment needs to be stopped during an injection, and if a time resolved experiment is being performed, temporal information is lost. Ideally, the injection should be transparent for the beamline, so we will be able to follow a reaction without interruptions. Alternatively, more flexible top-ups modes should be made available so the injection frequency can be optimised for the reaction length, or the synchrotron top-ups should be slaved to the operations at the experimental stations.

To optimise the performance of Diamond for pump and probe experiments, it would be greatly beneficial if the fill pattern of the synchrotron could be matched to the timing requirements of the experiments. This suggests a need for highly flexible scheduling of the machine-operating calendar.

3.4 Detectors

One of the main goals in the field of chemistry and catalysis is to follow processes in real time in order to elucidate the mechanisms and aiming to improve the processes. Typical time scales for chemical processes range from millions of years (e.g. astrochemical processes, rock formation) to femtoseconds (e.g. transition states). Therefore, Diamond needs to provide a mix of experimental stations for different timescales, most importantly: long-term (weeks – months; e.g. corrosion), medium-term (min – hours/days; e.g. catalyst activation, poisoning, slow biochemical reactions), fast (ms – min; e.g. adsorption/desorption at interfaces, surface modifications), ultra-fast (fs – µs; e.g. molecular motion; reactions; life times of excited states).

In order to achieve this, faster and more efficient detectors need to be developed. In the case of 2D detectors, fast frame rates up to MHz are the target for future detectors. Another important challenge is the improvement of the spatial resolution of these detectors. This will for example allow the structural study of heterogeneous catalysts in flow beds by full image X-ray fluorescence mapping while a reaction is taking place.

In the case of spectroscopy detectors, the improvement of the signal to background performance together with higher element density in multi-element fluorescence detectors will improve count rate capability. This in turn will allow the investigation of the structure of catalysts in real conditions of concentration. For example, modern generations of metalloenzyme-inspired polymer supported metal catalysts can promote organic reactions at ppb levels, e.g. allylic arylation in water. Equally, active catalysts can be poisoned by ppb levels of chalcogenides contaminants.

This development should come together with the improvement of incident intensity detectors, as they will need to be able to cope with the high flux required to study concentrations at the part per billion levels.

The research in chemistry and catalysis will also benefit from the development of more efficient high energy diffraction detectors. This will allow the study of reactions under more extreme conditions of pressure, temperature, etc… as the materials that can be used for the manufacture of the sample cells will not be limited by the penetration capabilities of lower energy photons.

3.5 Data Acquisition

The development of detectors able to run faster and with higher spatial resolution needs to be accompanied by the increase of data transfer rates and data storage capabilities.

When following a chemical processes, a large number of spectra will be collected, in particular if angular or energy dispersive methods are used. In those cases, the development of automatic data reduction and analysis software (batch mode) to handle large data volume will reduce significantly the time required to process the data and extract the required structural information. This needs to be achieved through either specific software developments or implementation of already exciting software packages into the Diamond computer systems, e.g. Dawn.

Time resolved chemical experiments also frequently required the simultaneous measurement and/or control of other data/parameters, e.g. temperature, pressure, pH, potential, gas-composition (GC, RGA), or optical spectroscopies, together with the X-ray measurements. This leads to a requirement for a data analysis framework that allows the temporal information between the measurements to be synchronised.

If a multidisciplinary approach is adopted for the study of more realistic and complex systems in chemistry, a coherence methodology to analyse the data obtained by using different techniques will be necessary to extract a consistent image, e.g. the combination of XANES, EXAFS and XPDF data analysis. Going beyond X-rays, the combined analysis of X-ray data with neutron scattering/spectroscopy will particularly enhance the study of chemical processes and catalysts.

A 2.3 Soft Condensed Matter – Physical Sciences (Science Champion: Nick Terrill)

Introduction

Soft Condensed Matter is a diverse field encompassing most of the major scientific disciplines and covering a number of the themes and grand challenges for EPSRC/RCUK. The focus of this report is the physical science aspects of Soft Condensed Matter. For biological aspects please see Integrated structural Biology (BioSAXS, CD) or Imaging (Cells, etc.).

The field is characterised by a multiplicity of experimental methods across all of the physical science disciplines, including imaging (I08, B22, B23 and I22), spectroscopy (B07, I08, B22 and B23) and diffraction/scattering (I07, I12, B21 and I22) techniques. The spectral range of the techniques spans from THz to UV and X-rays and thus fits well with what can be delivered by synchrotron sources.

The upgrade path ways discussed for the Diamond storage ring (low-emittance, high brightness or flux, diffraction limited source), should allow new science avenues to be explored. This calls for a planned upgrade of the relevant beamline capabilities in terms of beamlines, end stations, detectors, optics and sources.

Scientific challenges

A concise list of the main scientific drivers and of key developments foreseen in the field of soft condensed matter is reported here per thematic subject.

Energy : The harvesting of sunlight has the potential to revolutionise the way mankind generates electricity. At present however, only a small fraction (0.02% in 2008) of the world's total electrical power is generated using sunlight. Photovoltaic (PV) installations based on crystalline silicon are an increasingly popular way of generating electricity from solar-radiation; however such installations suffer from a relatively long pay-back time resulting from their high cost of manufacture. There is thus growing necessity to explore new materials that may display these properties. Multifunctional polymer systems (OPV) show great promise but there is a huge body of work to be done both spectroscopic plea and structurally to underpin the synthetic research already underway. Beamlines such as B07, I07, I08 and I22 will have roles to play understanding the charge transfer functionality and hierarchical morphology of the systems.

Application of bio-based nanocomposites may hold the key to building new generation wind turbines but understanding the properties and morphology of these new materials will be critical to their success again strengthened by the use of scattering.

Applying surface techniques to ionic liquids has great potential for trapping small molecules and may lead to useful sequestration of harmful greenhouse gases but much is left to be understood how the molecules interact with the surfaces.

Our need for energy generation is only one of the challenges which we face; storage is also an important problem to be solved especially with some of the renewable energy resources such as wind wave and solar where energy generation is variable. Fuel cell technology, where polymers will play a key role, will be essential in securing our energy future. Understanding the three-dimensional and surface structures of the polymer and colloid-based materials contained within fuel cells will be crucial in developing the next generations of this technology. The interaction of ionic liquids and other electrolytes at interfaces with metal electrodes in fuel cells/ batteries at nanoscopic scales will require imaging, XANES and micro-XRF to fully explore the systems to be developed.

Among the recent developments at MIRIAM there is the routine use of broadband (sub-)THz spectroscopy thanks to the intense Coherent Synchrotron Radiation from Diamond in low-α mode. THz microspectroscopy still needs to be explored in order to allow spatial resolution and spectra below 100 μm. This could open the research of molecular conformational changes/low energy modes, micro-MOF dynamics as well as far-IR imaging/tomography of C-based microstructures.

Healthcare Technologies : Transformative research in the area of polymer-based bionanotechnology, which we define as the application of synthetic polymers (man-made long-chain molecules) to solve important biological problems, will play an increasing role on a number of the Diamond beamlines over the next 5 to 10 years. The synthetic chemist's ability to manufacture new materials will allow the technologists to explore a whole range of medical application including lung surfactant replacement, skin graft, bone reconstruction and potentially new organ growth. The work will involve the integration of innovative polymer chemistry, state-of-the-art characterisation techniques, including multiple characterisation techniques at the synchrotron, and world-class bio-engineering to produce a paradigm shift in the fast-moving inter-disciplinary field of bionanotechnology.

Novel, wholly synthetic hydrogels based on the self-assembly of biocompatible block copolymer systems which form worm-like particles and which are readily prepared in concentrated aqueous solution could form the basis of future stem cell research however it is essential that the self-assembly process is fully understood from both the chemical and structural perspective. Both of these aspects will require use of the spectroscopy and diffraction beamlines at Diamond in the future.

Interface characterisation would benefit from CD Imaging in the field of semiconductors and data storage, nanomedicine and tissue engineering. The challenge resides in the development of micron spatial resolution with sensitivity to absorbance variation around 10^{-4} typical of CD materials.

As our knowledge of medicine improves our need for more sophisticated biosensors becomes essential. Many of the challenges in this area come from trying to understand the interaction of the biosensor with its surroundings and here spectral microscopy will play a key role in developing new systems.

Manufacturing the Future : The elucidation, over a large length scale range, of the hierarchy in new materials such as polymers together with biocomposites and ceramics is also dependent on simultaneous collection of USAXS/SAXS/WAXS data. Such continuity in measurement is essential for studying processes such as nucleation and growth phenomena as well as evolution of long range structural features during mechanical stress. The experimental field includes self-assembly in manmade materials mimicking nature and liquid crystals/supramolecular assemblies (photonic band gap materials), droplet interfaces e.g. aerosols, and particle growth or surface activity, combinatorial chemistry/product formulation as well as industrial processes.

These macromolecules are all around us, but their current application is limited. Synthetic polymer chemistry has now reached the stage where macromolecules are being made that can conduct electricity, mimic the function of simple muscles or interact with light. Self-assembly is the key to this new field where the molecule itself has its own blueprint which dictates the structures that they form. Both molecular/chemical (B22 and B23) and structural characterisation (I07 and I22) will be essential in exploring this new field. This is very much an interdisciplinary area where what we learn from biology can impact our ability to synthesise and manipulates new materials for our needs.

Similar to self-assembly systems, self-healing materials will soon be possible. These are likely to be soft materials which will need characterisation and development using synchrotron radiation as a means to elucidate where they perform well and how they fail.

Completely new opportunities arise from the ability to carry out CD imaging via spectroscopy analysis of chiral material e.g. thin film of polymers and biocomposites. The challenge resides in the development of micron spatial resolution with sensitivity to absorbance variation around 10^{-4} typical of CD materials.

Nano particles are now common however understanding of their activity and toxicity is still weak in many areas. Scattering and surface techniques will play an increasing role in understanding the systems and exploiting their potential in templated nanostructures, catalysis and other areas.

Quantum Technologies : Fourier Transform IR interferometry (FTIR) is an ideal probe for sub-eV quantum excitations. One advantage of SRIR is the broadband character, allowing the whole IR spectrum up to THz, and the microbeam brightness for a diffraction limited IR microanalysis e.g. of quantum dots/wells. High flux density of low energy IR photons is applied in the study of molecular crystals in DAC, and more generally it is key in the study of material under extreme thermodynamic conditions (microFTIR H/LT and/or HP). The current research at MIRIAM will need expanding into IR t-resolved detection for the dynamic study of quantum materials via implementation of pump-probe laser system at B22 e.g. on organic semiconductors/devices and magnetism.

Interface characterisation would benefit from CD Imaging in the field of semiconductors and data storage. The challenge resides in the development of micron spatial resolution with sensitivity to absorbance variation around 10^{-4} typical of CD materials.

Digital Economy : Molecular electronics will play an increasing role in our future and will call upon the both synthetic and manufacturing processes to work at ever smaller length scales. Characterisation of these new systems will only be possible with techniques that can operate at the same length scales including reflectivity, surface diffraction and electronic spectroscopy.

Other Areas
In situ/operando : This is a main research trend across beamlines with access to microbeams or enhanced reflectivity. Once more, dedicated sample set up arrangements, such as microfluidic devices, would be essential to develop this field, especially for industrially relevant processes.

A minimal list includes real catalysis (SAXS and IR), gel and colloids (SAXS/WAXS and CD) electrochemistry on thin films (IR), liquid-liquid reaction dynamics and microfluidic (CD, SAXS, IR), nanomaterial stress-strain and microanalysis (IR and SAXS), polymer chain dynamics during aggregation/crystallisation (CD and SAXS), Liquid Crystal dynamics (SAXS and CD), induced helicity in homochiral/racemic systems (CD), gas-solid microinteraction (IR).

Food safety and security: Feeding an ever-increasing population places great demands on food manufacture but also food technology and yet our understanding of some of our simple foods is still rudimentary. The technology associated with processing starch for example is basic. *In situ* measurement of real industrial processing using equipment as used in industry across a wide length scale range will be essential. The techniques used can also be applied to drug delivery systems and biofuel development.

Technical Innovations necessary to meet the Science Challenges

In order to enable the future scientific view, the necessary technical requirements are specified below in terms of beamline, sources, optics, end stations, detectors and software. A final part is dedicated to sample environment requirements.

Beamlines:

- Multi-length SAXS (Hierarchy) : New beamline with extended and overlapping q ranges giving access to length scales between 1 Å and 10 μm simultaneously.
- CD imaging: New beamline for correlated CD spectroscopy detection and spatial position in UV microscope.
- IR imaging/tomography : New high flux SRIR facility for full-field microspectroscopy via FPA detector.
- Soft Matter Liquid GiSAXS and Refractometer : Dedicated facility for studying soft matter and liquids in grazing incidence and reflectivity modes.

Sources

- IR imaging: New BM dedicated source and Front End geometry suitable for multibeam illumination of large Flat Panel Array detector (increase of IR flux of one order of magnitude and reduced X-ray heatload, dedicated front end and brightness increase of one order of magnitude).
- IR ultramicroscopy : Low E_c BM source providing more collimated beam for higher brightness (increase 100 times with respect to B22) and AFM detection at nm scale; n.b. development toward FEL with dedicated BM-like source (on spent beam dipole).
- Energy dispersive CD: Bright and low divergence microbeam generated at B23 essential.
- USAXS/GiSAXS/Reflectivity and SAXS tomography: Flux 10^{16}ph/sec brilliance >10^{20}ph/sec/mm^2/mrad^2 0.1%bw via cryo-cooled or superconducting undulators; pink beam from undulator; n.b. developments towards XFEL for lower divergence or parallel beam geometry.
- ASAXS: Extended energy range (from current 3.5-23 keV) to 1-50 keV.
- A general comment concerns the requirement of dedicated e-BPM at the actual source position of BM beamline in Diamond-II.

Optics

- SAXS: Multilayer mono or filters for undulator; variable control of beamsize including microfocus; improved DCD system for liquid surfaces.
- IR: Adaptive optics for sample illumination optimisation, source re-shaping, and mirror aberration corrections.
- CD: Design of energy dispersive CD optics.

Detectors

- CD: Active collaboration with Detector group needed for implementation of APD, spectroscopic and imaging CCD.
- SAXS: Energy resolving capability for pink beam with energy resolution 1-2 eV; time resolution to at least 1μs for dynamic measurements incl. speckle; in vacuum single photon counting and count rate matched to new ID sources; high dynamic range (matching count rate) and improved spatial resolution coupled to 10-50μm microbeam; n.b. time resolution toward ns for XFEL.
- IR: Single bunch discrimination for ns time resolution (signal gain expected 100 times with pulse detection); from LHe to LN_2 cooled (micro)Bolometer and HTSC edge detector, broadband RT Schottky diode array for t-resolved; n.b. development toward t-domain detection (E field and phase) for fs IR at FEL.

EndStations

- E-dispersive CD: New end station for high throughput CD via angular dispersion for simultaneous (and t-resolved) CD detection; spectropolarimeters to be designed custom.
- CD imaging: Correlated CD spectroscopy detection and spatial position in UV microscope.
- USAXS/GiSAXS/Reflectivity and SAXS tomography : Nanopositioning control and environmental stability (<0.1°C, humidity and atmosphere).
- IR imaging: Hardware and control of sample stage in 3D imaging/tomography; THz microspectroscopy via microbolometers; near field IR imaging via AFM detection fully exploited.
- T-resolved IR: Pump and probe implementation by coupling/synchronising lasers with SR bunch structure.

Software

- SAXS tomography: Real time reduction with visualisation tools in 3D.
- GiSAXS and Reflectivity: Theory and modelling effort for soft matter surfaces plus the tools to build model structures and compare scattering data with the theoretical systems.
- SAXS: Cluster computing for multi component model fitting of real systems; MD to calculate 2D and 3D models then FT to give scattering patterns.
- IR imaging : 3D and tomography spectroscopic image reconstruction; on line point spread function deconvolution of oversampled images as function of wavelength for spatial resolution retrieval (toward $\lambda/2$); on line chemometrics and digital staining via (un)supervised analysis of IR maps/spectra.

Sample environments

There are several requirements in this field which are in common among the SCM beamlines. For example T-controlled sample stages (e.g. microfurnace also allowing reactive gases), microfluidic devices development for dynamic analysis (including microincubator and stop-flow cells), tensile micromanipulator for material analysis under deformation. The general demand is for a dedicated engineering support for in house sample environment development (e.g. microsample environment), ideally as modular systems allowing combined techniques.

Wider views on Diamond's future

The first comment common to all the visions proposed is that new science and technology are only possible if the necessary manpower of scientists and engineers are allocated. It is evident that any proposal of this scale for any Diamond upgrade – or UK FEL project - is quite demanding in resources for design, implementation and commissioning. Moreover, full operation with scientific users accessing beamlines and off line instrumentation can only be productive by guaranteeing the proper scientific and technical support during operations.

Among the future scenarios to be considered there is the possible science driven evolution of) Diamond as a research facility offering a portfolio of techniques not only based on SR, as well as offering experimental know-how and analysis expertise (e.g. like the EM UK facility or the CLF). Clearly, this has implications on proposal review for not only SR based methods or multi-beamlines/techniques, as well as on the full time support needed beyond the beamtime for off line facilities, including sample preparation in the labs, post process data analysis, etc.

Diamond's profile should be widened beyond the "hi-tec giant microscope" and might better be described as a science hub where research/technological projects carried out at beamlines can be translated into scientific applications for the benefit of the wider community. Diamond should be more at the centre of the scientific research, taking due credit in the user/collaborative/in house success, with Diamond playing a scientific role e.g. in networks as the centre connecting users/research groups. Scientific collaboration and technical development with successful research groups should be encouraged/supported e.g. via joint research projects.

Stronger collaboration with the facilities available on the Harwell Campus/RAL to make Diamond a true science hub rather than just a facility provider should be actively encouraged. This could include i) further coordination/integration of e.g. biological activities on-site; ii) strengthening software modelling development on-site (photon science/applied theory groups for algorithms/simulations); iii) purpose built science institutes to exploit the unique capabilities and expertise offered on-site for the benefit of the scientific research of Diamond staff in collaboration with Universities and other Laboratories.

A UK FEL facility, ideally situated on the campus, will expand Diamond SAXS and IR research into e.g. ultrafast electronic processes and non-equilibrium dynamics. Basic IR FEL requirements: i) ~10 fsec bunch length fwhm for Coherent Synchrotron Radiation in the mid-IR and far-IR/THz (quadratic gain in flux with e-number per bunch $>10^8$); ii) low critical energy bending-magnet-like source for broadband emission (simultaneous multi-wavelength detection advantage of FT interferometers) iii) bunch current around 0.1 nC and repetition rate ideally 1 kHz (MCT IR detectors allow MHz response); iv) time-domain detection for electric field and phase detection (advantage in retrieving directly material absorbance and refractive index).

A 2.4 Biomaterials and Medicine (Science Champions: Gianfelice Cinque and Christoph Rau)

Introduction

The rationale for biomaterials and biomedical frontier research is nowadays motivated by the dramatic increase of world population and longer lifetime expectation. An objective is wellbeing and countering the effects of ageing over an extended lifetime. Among recent significant advances in the medical field, there is more focus on personalised patient treatment, complex illnesses and particularly those with major societal impact, e.g. cancer, multiple sclerosis, Alzheimer's and Parkinson's diseases, cardiovascular ailments and diabetes as well as serious inflammatory/infectious conditions. Special emphasis is given to the development of new/early investigation methods and diagnosis instruments – e.g. biomarkers and imaging methods – and to bring these methodologies as close as possible to clinical application. People's health research also concerns the replacement of organs or human tissue, using for example, bioactive scaffolding as well as regenerative approaches. For the latter significant progress has been made, being able to grow bone structure, skin or even -to some extent- organs. Fields of research in their own right are Stem Cells and Cancer. For Stem Cells the social impact is about to be addressed. For Cancer, the potential of research is not fully explored at the clinical level yet. Finally, dramatic increases in human population present challenges in ensuring future food supplies, prompting significant efforts in the research of plants, especially high resistance/high nutrition crop selection and transgenic modifications. More generally, plant biology is an extremely interesting field of fundamental research, for example in the crucial aspect of mimicking photosynthesis where biophysical models of e.g. energy transfer and ultrafast dynamic experiments are quite advanced.

Biomaterials and biointegration

Due to the ageing population and increasing expectance of life quality, biomaterials will play an increasingly major role. They are key to replacing parts of our body or to help repair processes as well as to prevent health degradation. Diseases such as osteoporosis are addressed with modern methods like injectable bone substitute or bone growth enhancing materials. Monitoring the bone growth under real conditions remains a challenge. Much effort is required for studying in detail the early stage of bone fracture. *In vitro* characterisation at single cell level (e.g. in osteocyte cultures) and in living conditions is biologically fundamental. The replacement of organs and other body parts such as defective/aged joints will ensure a high quality of life even at a late stage. Artificial hip joints become unstable with time, requiring improved methods for their embedding. Worth mentioning is the research in soft tissues and soft materials like skin, collagen, cornea, cartilage etc. and their artificial equivalent. Artificially grown tissue - such as blood vessels -should be monitored under the most realistic conditions. The challenge will be achieving three dimensional information, preserving the integrity of the tissue (radiation damage), as well as learning about its functionality. The acceptance or biointegration of engineered body replacement -stent and scaffolds- by the human body is another large area of interest. Other biomaterials will become a more important part of our daily life. An example would be glassy materials for tooth paste, helping closing crevices and cavities. Bioglasses and bioceramics will play an important role in the foreseeable future.

BioMechanics

In many medical areas the understanding of functionality of organs and biomechanics is often limited by the characterisation methods available. They are only partially covering the reality of the underlying processes. For example, the mechanics involved in the movement of a mouse knee is only partially understood; live material has never been investigated on the micron-lengthscale. In general the representation of soft tissue environment is very difficult, but would offer many new insights into hidden structures and mechanisms. Hearing research is currently limited by the knowledge of micromechanics in the Cochlea. Representing in three dimensions the membranes and cells involved in the hearing process is challenging since soft tissue (cells, membranes) and strongly absorbing material (bone) have to be imaged at the same time. It might be a dream for the future to apply Cochlear imaging for clinical application, the challenges are numerous and the most important one remains the radiation dose required to achieve the spatial resolution. The insight into biomechanics is of high relevance for the development and deployment of modern prosthesis, or synthetic tissue substitutes. One example is the study of tendon and their collagen constituents on a molecular level, in particular the correlation between molecular fibre orientation and stiffness development with ageing. In another area, insects are a viable model system in biomechanics, for example when studying aerodynamics or their respiration. Their vision system is relevant for the development of lightweight navigation systems in our daily life.

Plant science

With an increasing world population increasing levels of pollution and the prospect of climate change, securing the food chain becomes a major challenge. The investigation of water transport inside plants, the three-dimensional imaging of soft material and following the transport and distribution of trace elements remains a major task. This is only partially addressed today. The uptake and storage of nutrients in plants plays an important role for agriculture in polluted soil. The study of the accumulation of heavy metals is relevant for the food industry, as well as the biochemical effect onto bioremediation organisms, aiming to separate toxic elements from the nutrient crops. There is a growing interest in the application of non-destructive imaging techniques for biological materials. Reagent-free photon based imaging at molecular and atomic scale are potential methods to other technologies. They provide new insights into structure and functionality.

Stem Cells

Research on the therapeutic use of stem cells is highly important, given their potential for the production of differentiated human tissues and organs. There are numerous challenges in stem cell biology and regenerative medicine; i) maintenance of the stem cell phenotype; ii) reproducible control of cell differentiation; iii) quality control of cell population purity. Undifferentiated pluripotent stem cells can cause tumours in a human host. The current biochemical methods to follow such processes - utilising biological assays and chemical labels - are hampered by the limited number of known biomarkers, and their lack of specificity. Fluorescent or magnetic labels also have drawbacks, being potentially harmful to the cells or needing destructive analysis. Imaging in combination with microscopy/spectroscopy offers a potential alternative to monitor the differentiation process. They follow biochemical changes in the living cell, being reliable and relatively inexpensive. Pilot studies of stem cells, specifically for differentiation are required.

Cancer research and personalised medicine

Current research aims to improve the understanding of how cancer develops and spreads. Investigations address the large variety (>100 so far) of specific cancer types. This work provides a general foundation for other studies. Key areas of research include drug discovery/development and efficacy study *in/ex vivo*; prevention via early detection and automated imaging methods; surgery and radiotherapy including patient's follow up; improving outcome of patients (e.g. with aggressive cancer) with personalised medicine; clinical applications of new diagnostic methods. Currently the choice of chemotherapy agents and drug combinations is based on multicentre studies, resulting in the identification of anticancer drugs giving the best results for individual types of cancer. However, within each individual tumour, cells do not exhibit the same sensitivity and it is not clear yet how the best drug combination can be identified for each individual patient. A method to assess tumour cell sensitivity to chemotherapy is still required as well as *in vivo* tumour growth and survival assays, and *in vivo* molecular imaging and microspectroscopy.

Drug resistance, superbugs infections and antimicrobial resistance

Drug resistance is an increasing health problem in the population, with some bacterial pathogens now resistant to a wide range of available drugs. Too few new treatments are in development, and we need more diagnostics that will help us to match treatments with infections. This is particularly critical for pathogenic agents. They require the use of more specific antibiotics, for example the increasing resistance of bacteria to antiseptic and disinfectant. Such problems extend beyond human health: animals, particularly livestock, are increasingly being infected with antibiotic-resistant bacteria. Only a multidisciplinary approach will succeed in tackling the rise in superbug spreading and antimicrobial resistance. This research is overlaps strongly with structural biology, described elsewhere in this document.

Nanomedicine, nanoparticles and nanotoxicology

Nanotechnologies have an increasing importance for biology and medicine. Nanoparticles can be used for cancer treatment and research. They are susceptible to act as drug carriers or as co-factors in targeting the malignant parts. Some of them are suitable for imaging. A much more targeted drug delivery to the cancerous cells will help to overcome the traditional issues related to chemotherapy. Nanotechnology will be employed also into biomaterial technology. Nanoparticles have the potential to migrating to specific areas or implants, which is not necessarily the case for much larger cells. Also, the increased use of nanomaterials in industrial products gives rise to the question of their biological interaction with living organisms, and especially the impact on human health.

For biomedical and toxicological studies controlling the dispersion/transmission/diffusion of nanoparticles, and the interaction with biological fluids at single cell level are current challenges.

Summary

In general, the understanding of biomaterials and biomedical tissues calls for high contrast imaging and quantitative methods of microanalysis. Such research requires a facility offering a portfolio of techniques with high and specific sensitivity at different resolution. Different length scales from subcellular to major organs are involved. The sample environment for biological studies under real conditions is key. A multiple technique approach can overcome intrinsic limits of the probes used, and should complement in resolution, penetration depth and sample preservation.

For X-ray/VUV imaging the radiation damage is a challenge. This has been predicted to be the limiting factor for 'traditional' Sub-10 nm resolution with X-ray/VUV imaging methods. However this lengthscale appears to be interesting for biology. One of the recent trends in cell biology is *in vitro* studies in living conditions, e.g. in liquid environment.

Correlative microscopies provide a huge potential for developments, in addition to improving imaging and spectroscopy techniques. The combination of different methods is not always obvious, and needs to be investigated case by case. A 10 year framework is the right timescale to grow the corresponding interactions of Diamond with other facilities on the Harwell site and nearby. The work includes a common data analysis platform capable of rendering measurements made at different photon energies, from the IR to visible, VUV and hard X-rays.

An online/automated data analysis system for digital fast tissue imaging would be ideal. It should serve for multimodal imaging, combining the information of different techniques in a single image. New spectroscopical biomarkers drive the research for stem cell niches, identification in organs and quantitative classification of cancer cells at an early stage. This is develops together with a protocol for targeted personalised medicine. It is a diagnostic tool, influencing treatment of patients, meaning dose-time and cell response to specific chemotherapy before beginning patient treatment.

Summary of technical and instrumental development required to increase the impact of Diamond for Biomaterials, Medicine and Biology

The upgrade of the storage ring is central to future developments. It ensures Diamond's competiveness in respect to other lightsources. The reduced horizontal emittance impacts on the beam shape ('round beam') and degree of coherence (diffraction limited source).

Machine

In a simplified view one might distinguish between 'flux' and 'brilliance' relevant experiments. Intense photon flux is particularly important for full-field imaging/microscopy techniques, while increased brilliance will be of advantage for scanning and confocal micro-spectroscopy, coherent imaging and scattering based methods. While it is assumed that brilliance increase is essentially achieved through the machine upgrade, advanced radiation sources/new insertion devices will additionally provide increased flux.

Higher brilliance:

The upgrade of Diamond to a lower emittance provides increased sensitivity (e.g. trace elements), signal quality (signal-to-noise) and degree of coherence (phase contrast, higher resolution). This is particularly relevant for scanning and ultra-microscopy, micro-spectroscopy and coherence related imaging techniques. In particular:

- I08, I13-1, I14, I18: For the spectroscopy beamlines, the rounder beam and increased flux in the focal spot, for coherence experiments the increased coherent fraction. For both cases an increase of about a factor 100 is expected.
- Multi-length SAXS with extended and overlapping q ranges giving access to length scales between 1 Å and 10 micron simultaneously calls for higher brilliance
- B23 CD imaging i.e. CD spectroscopy detection and spatial position in UV microscope requires high photon flux density.
- For B22 the increased brightness SRIR will allow near field IR imaging at nanometric resolution and with molecular specificity (IR+AFM and/or SNIM).

Beam stability

Beam stability is a highly relevant aspect for preserving emittance and brilliance provided. This concerns not only the e- orbit (n.b. transversal vibrations and RF induced longitudinal movements), but also the radiation sources and the entire beamline optics and building support. Upgraded e- and X-BPM at the actual source position with wider bandwidth are a must for new radiation sources. This is applicable to all beamlines, but most sensitive are I08, I13, I14, I18, B22.

New radiation sources

Advanced radiation source technology enhances the beamline capabilities significantly. The increased diversity of devices available allows tailoring of beam characteristics to specific applications. High brilliance and flux provide access to new scientific domains: sub-10 nm, fast, dense etc. Cryo- and superconducting insertion devices provide increased flux and brilliance. The gain is about one order of magnitude in the energy range above 20 keV. This will give access to denser or larger specimens and give the opportunity to access the iodine edge, commonly used in medical research. For fast radiography at high energies and over a large field of view, other technologies may be developed. This is the case for example for 3-poles wigglers. Broadband sources for microspectroscopy are needed for low energy photons methods (VUV, UVCD, IR and THz). The possibility to use smaller ID gaps below 5 mm has to be investigated. This option provides significantly increased flux, too. In particular:

- I13-2: A cryo or superconducting ID for E>20 keV for larger and denser samples and to access iodine edge. Any advantage of such a device needs to be checked for the coherence branch.
- SRIR (B22) new source dedicated geometry suitable for multibeam illumination for full field microscopy (homogeneous illumination on 256x256 pixels FPA detector via effective flux increase 10 times); low critical energy SR source providing more collimated beam for higher brightness (increase 100 times with respect to B22) for near field IR+AFM;
- SRCD (B23): brighter and lower divergence microbeam generated by a new source for allowing energy dispersive CD at Diamond (time resolved CD).
- USAXS/GiSAXS and SAXS tomography: flux 10^{16}ph/sec brilliance >10^{20}ph/sec/mm^2/mrad^2 0.1%bw via cryo-cooled or superconducting undulators; pink beam from undulator; ASAXS: extended energy range (from current 3.5-23 keV) to 1-50 keV.

Detectors

Detectors should be developed further in the following areas: photon counting, fluorescence, time resolution. The efficiency of the detectors has to be optimised for fast detection and to minimise radiation damage at samples. Smaller pixel size photon counting devices may be useful for radiography as well as for microspectroscopy. Nanosecond time resolution for dynamic measurements incl. speckle should be achieved either by custom development (TimePix) or be purchased commercially. Energy sensitive 2-D detectors will be required for spectroscopic imaging and coherent imaging when using pink beam. Photon counting with energy selectivity (ideally 1-2eV) and high dynamic range will be critical. The count rate has to match the flux available with the new ID sources. Soft photon detection capabilities at Diamond in VUV, visible and IR (scintillation, luminescence, APD) has to be further developed by the detector team. In particular:

- Coherent imaging I08, I13-1: Further development based on EXCALIBUR system: Detector operational in accordance to all initial specifications (Energy selective mode, dead pixels, etc.), for ptychography. Adaptation of Merlin/EXCALIBUR design to TimePix chip required for fast data recording (in particular XPCS)
- Full-field imaging/microscopy I12, I13-2, I14: Coupled scintillation screen / visible light microscope detectors should be fully supported by the detector group. This includes the support of visible light optics, scintillation screens, commercial detectors etc (similar to the situation at the ESRF: T. Martin (scintillation screens) and C. Ponchut (optical systems). These detectors are also needed for I13-1.
- SRCD (B23) implementation of Avalanche Photo Diode detectors and spectroscopic imaging CCD allowing correlated CD spectroscopy detection and spatial position in a UV microscope;
- SAXS (I14, I22, B21): energy resolving capability for pink beam and time resolution <1 μs for dynamic measurements including speckle; in vacuum single photon counting and improved spatial resolution coupled to 10-50 microns microbeam.
- SRIR (B22): single bunch discrimination for ns time resolved pump-probe experiments (n.b. signal gain expected 100 times with pulse detection); from LHe to LN2 cooled broadband microBolometer and HTSC edge detector ideally allowing mid- to far-IR imaging.
- XRF microscopy (I08, I14, I18): Excellent solid angle acceptance and high count rate capability; Large multi element high solid angle silicon drift or Ge pixel detectors (>1sr solid angle at working distance > 25mm); Low background/High peak – valley for energy dispersive detectors (>7000:1) for study dilute concentrations found in biological samples; High count rate (>=2 Million counts per second per channel).

Sample environment

Dedicated sample environments have to be developed by Diamond to provide access for the *entire* user community to the science they are interested in. There are several requirements which are common among beamlines. Examples are; temperature controlled sample stages (e.g. microfurnace also allowing reactive gases), microfluidic devices development for dynamic analysis (including microincubator and stop-flow cells), tensile micromanipulator for material analysis under deformation. The level of Diamond's involvement in such a development has to be clarified. It could be envisaged that Diamond provides a standard set of sample environments, while more customised setups may be developed in conjunction with users, or may be the property of the research team? Dedicated engineering support for in house sample environment development allowing combined techniques would be useful. Likely, this type of development should be modular.

In order to enable the cryogenic capabilities fast, high precision nano-mechanical devices are envisaged:

- Fast low wobble rotation stages;
- Cryogenic systems (sample transfers, cryo sample mounts and low vibration mechanics);
- Cryogenic mounts suitable for high resolution tomography;
- Fast scanning stages (high resonance frequency stage operating at fast scanning rates with advanced feedback control).

Further science enablers

Multimodal imaging is key for biomedical research. Diamond's location means it has access to a multitude of imaging methods and facilities on the RAL site and Harwell Campus, including nearby Universities (e.g. Oxford and London). Diamond should strengthen its links to other facilities, aiming to be a true science hub beyond a facility provider. This could include i) further coordination/integration of e.g. biological activities on-site; ii) strengthening software modelling development on-site (photon science/applied theory groups for algorithms/simulations); iii) purpose built science institute to exploit the unique capabilities and expertise offered on-site for the benefit of the scientific research of Diamond staff in collaboration. It would be useful to create a forum for all Diamond beamlines involved in imaging. Diamond should become an intellectual centre for imaging, offering experimental knowhow and analysis expertise. In particular for multimodal imaging and sample environments:

- Ability to transfer samples between instruments and beamlines – development of suitable common sample environments (e.g. suitable for IR and XRF spectroscopy techniques, or suitable for electron microscopy and XRF)
- Development of fiducial marker systems for imaging and registration across instruments – Development of shared expertise in lithographically patterning substrates, holey substrates, dyes and markers.
- Development of wet cells and flow cells
- Shared expertise and laboratory infrastructure for cryogenic sample preparation (high pressure plunge freezing, sectioning)

Radiation damage and non-destructive methods are central subjects for biomedical imaging. One part of the research should be dedicated to radiation damage. It determines resolution limits, probe sensitivity or specificity, and therefore the kind of science which can be addressed.

Centralised support facilities for common aspects like sample compartment will help increase the efficiency of the different beamlines. This is the case for sample preparation (cutting, freezing etc.). Diamond has to discuss a standard for sample holders.

Last but not least data acquisition and data analyses capabilities will need to be improved:

- Fast automated alignment of samples.
- Reduction of no of projections through advanced algorithms.
- Dose fractionation to reduce overall dose in 3D (particularly scanning based modes).
- Fast data workflows for on-the-fly data processing.
- Higher software reliability. Scanning microscopy based tomography is much slower than full field.
- Mean time between software failures should > 72 hours.
- XRF tomography algorithms and visualisation (multi element, combined visualisation, attenuation corrections).

A 2.5 Engineering and Materials (Science Champion: Chiu Tang)

Existing programmes of Engineering and Materials (E&M) research at Diamond are playing a vital role in addressing societal grand challenges, in particular in the areas of Energy, Health & Welfare, Security and Transportation. For instance, improved structural integrity and performance in materials engineered for mechanical components or structures such as those in the transport and construction industries are important in the improvement of public safety and the reduction of running costs. New materials to enable the development of high sensitive sensors and scanning probes for airport security, hospital screenings and domestic applications will improve our health and security. With the decline of the world's reserve of fossil fuels and escalating cost per unit power, more research is needed to develop economically viable and safer alternatives as well as sustainable renewable sources such as high power battery materials, next generation of nuclear reactors and high efficient photovoltaic mediums.

The E&M research activities will continue in the next decade to seek new information, to make new discoveries and to obtain new results for the testing of existing or new theories and hypotheses using existing Diamond beamlines and support facilities. More opportunities will be available in the near future for new E&M science using new beamlines (Phase III and upgrades), including the next generation of detectors and sample environments which will probe deeper into the materials structures and capture the dynamics of physical properties and their behaviours (real-time changes). The science is interdisciplinary and will include engineers, metallurgists, materials scientists, computer scientists, physicists and chemists. With the appearance of new classes of materials such as nano-structures, superalloys and composites, multiferroics, photovoltaics and others, the wealth of knowledge, materialistic and technological gains will be available to address the societal challenges mentioned above.

Engineering

Structural integrity and performance of materials under operational conditions such as mechanical loading and *in situ* (hostile) environments (temperature, high pressure and corrosive, etc.) will be the main challenge for E&M research using principally high resolution diffraction, imaging and high energy scattering and tomography. These include the following key research areas:

Fatigue and fracture: This large area encompasses the broad topic of structural integrity concerning the weakening of materials caused by repeatedly applied or direct loads. The detrimental effects can lead to catastrophic failures of materials in engineering components or structures. A particular focus of the work has been in the area of contact mechanics and fretting fatigue. There is an extensive range of testing machines which can be used to provide model validation. Other work focuses on residual stress at the micro- and macro-scale and on how this affects fatigue performance. More fundamental work is carried out to investigate crack tip deformation processes using digital image correlation and X-ray tomography to validate analytical and numerical modelling. This will feed into improved methods of fatigue life prediction, particularly under non-uniform loading.

Cracks in material lead to structural failure, but these originated microscopically and developed to larger pronounced, detrimental features upon increasing load. The understanding of their damage and their failure modes is important. The challenge is that the damage and failure are complicated due to the complex structure of designed materials. For instance, crack initiation and growth in fibre-enforced materials is very different from traditional materials, in that an impact will cause damage to the stiffer fibres inside the bulk first via shock wave, before a crack becomes visible at the surface, although the material is weaker at the surface in the traditional sense due to the lack of binding forces. Similar failure processes occur under shock peened surfaces. *In situ* experiments to study the formation of microcracks are now possible as demonstrated by the work on Ag-Cu based multi-metal matrix composites analysed using high energy X-ray tomography and diffraction, and 3D crack quantification in a quasi-brittle material. The propagation of cracks in bio-materials, such as bone, is directly related to its toughness and thus techniques such as tomography can assist in the assessment of the quality of these materials. Further research and development in this field could lead to better understanding of bone pathology and treatment.

Improvement in the integrity of these materials will lead to high reliability and effectiveness of components ranging from small scale electronic devices to large civil structures which will directly benefit our quality of life. Due to high societal demand, these issues will be subjects of intense investigations and research activities will continue for the next 10 years, in conjunction with sensitive modelling techniques.

Microstructure and Defects: Analytical advancements and investigations of microstructural features and imperfections in crystal structures are important to improve our understanding of their effects to material performance and behaviour. These features are crystalline domain size, shape and their distribution and the nature and density of defects (microstrain) such as dislocation, twinning, stacking faults and lattice misfits. While traditional approaches are used to adequately analyse simple cases (good uniformity particle size, isotropic strain), innovative methods are emerging for complex systems, e.g. heavily deformed metals, composites with anisotropic strains and nano-materials. The manufacturing of materials with specifically designed microstructure is just one aspect of the understanding of modern materials.

Stress and Strain
Applied: X-ray diffraction is commonly used for non-destructive measurements, but the development of fast and high resolution 3-D diffraction and imaging together with modelling will be advancing to such a state that that these will be used routinely for *in situ* loading studies of complex dynamic systems. The feasibility study of *in situ* stress analysis inside a running internal combustion engine using high energy synchrotron X-ray beams (75 – 150 keV) is a good example to inspire future work.

Residual stresses and Eigenstrain: *The good* – compressive residual stresses, e.g. introduced into a metal's surface by mechanical or laser peening, can improve its materials properties; strain hardening, crack and scratch resistance. *The bad* - unintended tensile residual stresses in components or mechanical pieces can cause premature failures. Traditional X-ray diffraction methods for residual strain measurements will continue to be used to study a wide range of materials, in particular mechanical and electrical components. *The beautiful* - using high energy micro-focussed beam for deep penetration and high spatial resolution studies, precise quantitative determination of internal strain distributions in materials are now possible. In recent years, diffraction strain tomography has also been developed for high precision evaluation of internal structure in materials offering submicron resolution 3D imaging.

Texture analyses: Many mechanical components and processed materials including geological rocks are textured; crystallites within have preferred orientations. Materials properties such as strength, deformation (fracture and crack) and resistance (mechanical, chemical and radiation) can be highly dependent on the crystallites' alignment. The development of unfavourable textures in materials during fabrication can create weaknesses which affect their operational lifetime and even exacerbate failures. As textures are global features, *ex situ* studies using synchrotron methods are often not required. However, *in situ* studies during fabrication or processing using the latest or next generation of fast area detectors would be more useful for the understanding of the underlying mechanism of texture development. This has been recently demonstrated with the *in situ* X-ray diffraction experiment of the oxide growth in thin film Zr alloys during aqueous corrosion. The alloys are used as uranium fuel road cladding in light water nuclear reactors. In order to understand corrosion and the hydrogen pick up mechanisms of the metallic materials in the harsh environment, it is important to understand the crystallographic texture of the thin oxide films that form during service. This information can be crucial to engineers and metallurgists for the production of alloys with improved radiation resistance strength. Future *in situ* studies could lead to tailored textured materials fit for specific tasks and the prevention of the development of unfavourable textured materials.

Gas and liquids in soil: Carbon Capture Storage - steady increase in global greenhouse gas concentrations has the potential to lead to considerable changes in climate worldwide. Carbon Capture and Storage (CCS) offers an extremely helpful addition to the energy landscape, allowing us to maintain traditional infrastructure (and a certain reliance on fossil fuels) while reducing their environmental impact. One of the principal difficulties with CCS is the ability to demonstrate the safety of underground storage at times of the order of a thousand years. The complex behaviour at elevated pressures and temperatures is key for the underlying physics governing dynamic multi-phase flow and reactive transport processes. Fracking - in sight of the increasing issue of covering the global energy needs all available resources have to be exploited including the access to them. In the recent past the option of fracking providing huge additional oil reserves has led to a controversial discussion. Similar to the challenges and opportunities related to carbon storage (see above), the extraction with the new method requires a much deeper understanding of the mechanism involved. Again multi-phase studies in three dimensions under high pressure and temperatures, the temporal evolution etc. will be at the core of studies in the future.

Alloys, Superalloys and Composites: With an exceptional combination of high temperature strength, toughness and corrosion resistance, Ni-base superalloys are widely used in aircraft and power generation turbines. Continued improvements in their properties are possible using the information obtained from high energy X-ray tomography and high-resolution diffraction to further our understandings of the deformation due to the development of micro-features. There is limited scope for improving the temperature-cycle efficiency of these alloys so there is a clear need for the development of new alloy systems to replace Ni-base superalloys. Alloys with excellent mechanical properties such as Al-Si-Cu have potential applications in many automotive applications (engine blocks and cylinder heads). The challenge ahead is to better understand and to resolve the issue of “Fe-pick up” during recycling processing which produces undesirable brittle alloys. With the advent of composite materials, the possibility for local modifications of microstructure and new manufacturing techniques such as 3D-printing, engineering materials are being designed and manufactured with desirable mechanical or thermal response for specific applications in mind. For example, metal matrix composites such as Ti-based with continuous SiC fibre reinforcement for aerospace applications offer high strength and stiffness in defined directions at reduced weight. Diamond facilities will play an important role in future research on these emerging advanced alloys and composites, and also the developments of their production process using diffraction and spectroscopic techniques and increasingly X-ray imaging.

Processing and treatments: Diamond will continue to be crucial in the advancement of thermal metallurgical processing, surface and indentation treatments to produce improved engineering materials. For instance, shock peening can vary the strain state in a controlled way and the effectiveness of treatment is quantifiable using imaging or diffraction methods, e.g. laser-shock peened surfaces prevent crack initiation locally at vulnerable parts of the component, such as the root area of a jet engine’s fan blade. Synchrotron techniques could be used to further develop other processes such as controlled thermal quenching, raid plastic deformation to achieve preferred microstructure orientation. Also *in situ* synchrotron studies of traditional homogeneous and isotropic materials which are under continuous development by the invention of novel alloys or processing routes could be benefitted, including mitigations of damage which is known to occur during processing of modern materials, e.g. in casting of semi-solid alloys.

Materials

(i) Energy materials

Nuclear power: It is a top priority in many national strategies for nuclear energy to meet the challenges of our huge unprecedented energy demands in the future, because it is low-carbon emission, relatively cheap, and based on fuels that could last for thousands of years. Synchrotron X-rays will provide a deeper knowledge of materials for the nuclear industry such as radiation-resistant solids, corrosion resistant fuel cladding and next generation of reactor fuels. Oxide dispersion strengthened steels are promising materials to resist radiation damage which is important for developing next-generation nuclear reactors. The distribution, chemistry and shape of nanoparticles in these microstructures, and their influence on the matrix chemistry and irradiation response, play a crucial role in predicting how effective materials will be during service. Zr-alloys used as fuel cladding in pressurised water reactors are known to suffer from aqueous corrosion and the effective burn-up of the uranium fuel. As premature cladding failures are very costly and reduce operating lifetime, understanding the corrosion kinetics is thus of great importance for undertaking more accurate lifetime predictions and improving cladding tubes. The γ-phase U-alloys undergo structural changes when exposed to different environmental conditions in a nuclear reactor. Thus, future study of phase transformations in thin film alloys that are thermally cycled over months to years will properly assess their potential and viability as new sources of fission fuel.

Batteries: Li-ion battery (LIB) and next generation of battery materials

With distinct advantages (re-chargeable, high energy density and slow losses), LIBs have attracted intense research focusing on improvements in energy density, durability, low cost, safety and environmental friendly. This essentially involves the search for novel materials with enhanced electrochemical properties to be used for the battery cathode, anode and electrolyte. New materials can be studied using a range of synchrotron techniques including scattering, imaging, spectroscopy and diffraction at Diamond to probe a large range of length scales (10^{-10} m – a few mm). *In situ* synchrotron techniques have been successfully applied to probe structural changes that occur in LIB materials [e.g. $LiFePO_4$, $Li(Fe_{1-x}Mn_x)SO_4F$] while undergoing electrochemical cycling and to discover new materials ($LiFeSO_4F$, Li-spinels and Na compounds) for the next generation of devices. Long duration experiments (LDE) to study effect of many cycles of power charge/discharge to the electrochemistry will be interesting. Future research in LIB materials will continue and additional attentions will be in the next generation of high power density materials (Li-air, Li-S).

Photovoltaics: Our ability to convert solar radiation, which delivers a vast amount of power to the earth's surface, is not efficient. One drawback of current solar cells is that they do not withstand long-term exposure to solar radiation. Future research using silicon nanoparticles in solar cells may provide one solution to increasing the viability of solar energy. Other photovoltaic materials such as dye sensitised solar cells (DSCs) are a promising low-cost photovoltaic technology based on a porous layer of titanium dioxide nanoparticles coated in a molecular dye, which absorbs sunlight in a similar way to the chlorophyll in green leaves. Polymer solar cells have also attracted considerable research interest due to their potential of being environmentally safe, lightweight, flexible and efficient. More research is clearly needed to improve their efficiency by maximising transfer of electrons from absorbed sunlight to the nanoparticles and by harvesting light from all parts of the solar spectrum. More investment is required to scale up these lab processes to commercial plants to realise the full potentials of these solar cell materials. Diamond will certainly play a key role in this area of research and development.

Phase-Change Materials (PCMs): These materials undergo a phase transition (such as dissolution or melting) when they absorb heat and then undergo a reverse transition (crystallisation or freezing) when they cool. Salt hydrates display many desirable properties but their performance degrades over time. It is therefore vital that researchers develop a fundamental understanding of the crystallisation, melting and dissolution processes to engineer new PCMs with longer lifetimes. Using Diamond could help to develop a compact heat store that could replace domestic boilers, hot water tanks and air-conditioning units. By incorporating PCMs into advanced engineering systems, the technology has the potential to make a significant impact on global energy use. The challenge is to ensure that the performance of devices is reproducible over thousands of thermal cycles, which requires advanced materials research.

SOFC (solid oxide fuel cell) materials are finding important applications as emergency back-up power supplies and in electric powered vehicles. However the high temperature operating conditions currently required can lead to limited lifetimes of the SOFCs due to corrosion and breakdown of cell components, while the long start up times limit their use in mobile applications. There is thus a drive to find novel fuel cell materials than can operate efficiently at lower temperatures. As more materials with the right properties for SOFC applications are emerging, *in situ* experiments at operational conditions (high temperatures and electrochemical) have been recently performed at Diamond. *In situ* work to study the phase stability of lanthanum nickelate with a ceria-based electrolyte and strain distribution in nickel-yttria stabilised zirconia interface have been carried out at Diamond to understand the thermal behaviour of and mechanical properties of SOFC materials. In addition, uncovering the fundamental principles that govern electrochemical reactivity is key to designing new materials for fuel cells, electrolysers and alternative energy technologies. The knowledge gained will certainly improve future fuel cell designs and the materials used for the electrodes/electrolytes (mechanical reliability, lower operating temperature and cost).

Biofuels: With favourable net CO_2 emissions, biofuels have gained considerable political attention as they are feedstocks from sustainable resources such as soy, rapeseed and palm dates. Unlike fossil fuels, the problems of wax formation or crystallisation in these "green" products occur at winter temperatures (<10°C), causing blockages in the fuel delivery system. These problems have not been well studied. The crystallisation processes in fossil fuels can be desirably disrupted using additives, however the phase behaviour (structural and morphological changes as function of T-P) of bio-products is far more complex due to the lack of understanding of their varied molecular structures. This fundamental understanding needs to be obtained on this present generation before the picture is complicated by the introduction of the next generation of biofuels. Their long-term stability and slow chemical degradation need to be investigated. Future studies of bio-fuels (intrinsic structure, morphology, fuel production and combustion processes) using multiple Diamond techniques such as small angle scattering, imaging and diffraction are anticipated.

(ii) Functional and Applied Materials

Multiferroics: These are materials that exhibit at least two of the three characteristics of ferroelectricity, ferromagnetism or ferroelasticity. They have many potential applications such as for new materials with improved magnetoelectric coupling strength for future information storage devices. As the ferroelectric and ferromagnetic ordering phenomena are often intrinsically mutually exclusive, these materials are rare, e.g. $Ga_{2-x}Fe_xO_3$ and $K_{3-x}Fe_5F_{15}$. Understanding these materials will require systematic studies of the crystal structures and their relationships to the two physical properties at non-ambient conditions. The recent success of observing domains at the surface of a $BiFeO_3$ single crystal using magnetic diffraction will pave the way to understand domain formation in these materials which is crucial to the development of multiferroic technology.

Ceramics, glasses and novel amorphous materials

With desirable electrical properties, lead zirconium titanate (PZT) ceramics are used widely in electrical and electronic devices. As PZT contains up to 60% wt. of lead, there is considerable international effort to find viable lead-free alternatives to mitigate the health and environmental concerns. As stoichiometry and property are strongly correlated, both compositional and structural engineering approaches will be required to "tune" potential candidates to possess dielectric and piezoelectric properties that match or surpass PZTs. Families of promising ceramics such as alkaline niobates (K-Nb-O, Na-Nb-O) and their solid solutions and titanate perovskites (Ba-Ti-O, Bi-Na-Ti-O) and bismuth perovskite solid solutions will generate intense research at Diamond. The understanding of structural evolution and dynamic of new lead-free thermoelectric ceramics (e.g. Ca-Co-O and Bi-Sr-Co-O) will be important as well as these are potentially useful to convert “waste” heat to clean electricity.

Digital storage media applied in DVD-RAM technology exploit the rapid kinetics of reversible optical switching between crystalline and amorphous forms of chalcogenide compounds. The timescales involved hint at the importance of “crystal-like” domains that persist in the amorphous state. Very recently, a number of phase change chalcogenides have also been shown to produce very strong nonlinear optic effects. This behaviour implies the persistence of local noncentrosymmetry across the crystal-to-amorphous transition. The structure of novel glasses (chalcogenide) which are important for optoelectronic devices will be increasing in the future. Other areas where engineered glasses are making important contributions include biomedical applications such as prosthetics and bone integration materials.

Clay minerals have important applications in geological waste containment, water storage and heavy metal sequestration. The important science of poorly crystalline clays centres around their physical properties on the atomic scale; e.g. the structure of the interlayer water and host/guest interactions with adsorbed species. Natural hazards such as earthquakes and volcanoes are determined by the structural and mechanical properties of solid and fluid silicates. These materials typically contain networks of linked SiO_4 and AlO_4 tetrahedra, and local structure probes are essential because there is considerable flexibility of these networks that gives rise to dynamic disorder.

Ionic liquids are a broad family of structurally mobile salt phases with a number of key energy related applications: in carbon dioxide capture, nuclear fuel reprocessing, solar energy and battery electrolytes. To understand local structure/property relationships in this family is key to the continued development and commercial exploitation of functional ionic liquids. The problem faced by the relevant community is that the structural variations that occur during solvation and flow extend over the 10-50 Å length scale, which is inaccessible using spectroscopic technique. To date there has been a heavy reliance on simulation data, but by characterising local structure correlations using XPDF, we could provide valuable experimental constraints on the development of these models.

Energetic materials: Fast reacting and explosive materials are now routinely used in many life-saving safety systems where both rapid reaction and deployment is essential (e.g. airbags, seatbelt tensioners and explosive bolts). The requirements for such materials are: (a) non-activation in normal use and handling; (b) rapid reaction when triggered; (c) long-term stability against decay and or degradation in performance

Nanomaterials: Nano materials are characterised by the influence of the particle size on its physical and chemical properties. This area covers a wide range of interesting research and potential applications. Nanoparticles research will continue to increase in the next decade. For examples, gold nanoparticles (GNP) in cancer research as these can carry drugs directly to tumours without damaging healthy tissue and have potential uses for imaging and radiotherapy which will improve diagnosis and treatment. Although medicine is not within the current remit of E&M (see the ‘Biomaterials and Medicine’ section,A1.7) , it has to be pointed out that many new routes in treatment of diseases (e.g. cancer) can be exploited based on this technology as the example given above. Nano particles are important for emulsions and paint since the particle size impacts on the colours produced. The industrial impact of any new development in this area is huge, e.g. biochemists are discovering that although gold is usually chemically inert, GNP can be an extremely effective catalyst.

Nanosheets or single-layer nanomaterials (e.g. graphene, BN, Zn_2Al–borate) give rise to a range of enhanced properties for the potential development of advanced functional materials. The enhanced electrical/electronic properties of nanowire or single-atom device architectures will also be intensively investigated. A number of “nanostructured” materials assume important environmental roles; examples include nanomaterials generated as fine-scale dust in volcanoes (“volcanic ash”), the role of nanomaterials in the atmosphere to nucleate water droplets, and key mineral phases such as ferrihydrite, which is also used in biological systems as a natural store of iron.

High T_c superconductors: The fundamental behaviour of this class of materials is covered in Condensed Matter Physics (see A1.1). E&M beamlines at Diamond will continue to play an important role in the material development. For example, superconducting materials of tri-layered thin films, known as Josephson junctions; these are the basis of technologically important devices such as SQUID magnetometers, already commercially available, and potentially useful for quantum computers.

Technical Innovations to Meet the Scientific Challenges

Future E&M research and developments to meet the challenges discussed above will be tackled using primarily diffraction, imaging and scattering techniques at Diamond. In order to facilitate these activities, the technical requirements are identified and grouped as follows: machine and new beamlines; X-ray sources; endstations and upgrades; sample environments; detectors; software and.

The Machine and New Beamlines

A machine with a lower emittance to improve the brilliance is important for coherent imaging (I13-coherent branch) and the provision of 2-3 orders of improvement in photon beam brightness will improve the data quality in imaging, diffraction (I13, I12, I11 and I15) and scattering (I12, I15-1) experiments.

Multiple DBA lattice upgrade to increase the number of IDs for new beamlines

- XPDF – ideally the existing branch line should be sourced by an independent MPW for wavelength tuneability (E=30–100 keV) as resonance XPDF experiments can be conducted to study composites with low electron contrasts. High-energy brightness beam allows fast time-resolved (ms) and high spatial resolution (a few μm) experiments.
- Long duration experiments (LDE) facility – to be sourced by an independent ID replacing the existing I11 facility (EH2) as it is expected to be heavily oversubscribed.
- High-energy high-brightness beamline (40-60 keV) – to be sourced by a superconductor undulator to generate high energy X-rays (E=40-60 keV) for combined techniques of high contrast imaging, high resolution powder diffraction and engineering SAX (25 m long experimental hutch).

Sources

- I13-imaging branch: cryo-cooled or superconductor undulator (CCU or SCU) to generate high energy X-rays (E=30 keV or above) for material science applications rather than just bio-material research.
- I15-1 XPDF: a high B-field MPW to improve the flux at high energies (E=65 and 76 keV) for fast time-resolved (ms) and high spatial resolution (few μm) experiments.
- I11: SCU upgrade (already planned) for the generation of high energy X-rays (E=30-40 keV) to penetrate sample environments and high absorption samples, particularly useful for LDE.

Endstations and Upgrades

In general, the major components such as the optics (monochromator, mirrors) and diffraction apparatus of the existing beamlines will be old in 5-10 years and will lose their effectiveness to perform experiments for new science. Therefore, optical components need to be replaced with higher specifications and endstations should be upgraded or re-built. There are also specific developments for different beamlines as described below.

- X-ray Dark-Field Imaging (I12): In analogy to the much used EM technique of dark-field imaging, high energy X-rays can be used to produce microscopically resolved images to study in detail the micro-features in matter. The number of material and engineering applications is tremendous. The advantage of X-rays technique is that no sample preparation is needed, in contrast to TEM. This makes *in situ* experiments feasible on realistically sized samples. In addition, true 3D representations can be done via the well-established X-ray computed tomography process.
- Simultaneous SAX and Powder Diffraction Facility (I12): The combined technique will add extra capability to increase the scope of E&M research.
- Combined Angular and Energy Dispersive Facility (I15, EH2): This method can provide very fast and high quality data to study phase diagrams in a wide temperature and pressure range (1200 K < T < 2000 K; P < 20 GPa) the using the Paris Edinburgh large-volume press.

Sample environments

In situ studies at operational or non-ambient conditions are decisive for the scientific outcome. To have dedicated technical teams (engineers and technicians) and additional lab space to develop non-ambient cells and centralised support are common to all the beamlines. Support groups to cover high T-P devices, low T cryogenic systems, high P-T gas cells, high power laser and others are essential in the future.

The specific requirements for each beamline are listed below.

- Easy to load DACs and high throughput study of high-pressure (HP) samples for non-specialists (I15, I15-1 and I11)
- High magnetic field (B_{max}=18 T) combined with He-cryostat (300mK) (I15)
- Specialised material processing (fast machining and processing, T > 2000 °C, mechanical loading at high temperatures) inside a ring that is suitable for *in situ* tomography and diffraction. (I12)
- High temperature (HT) gas flow cells (1200°C) with remote control capability and integrated mass spectrometer for low-hazardous and hazardous gases (flammable, corrosive and toxic) (I11, I12, I15-1)
- Large sample volumes at intermediate pressures up to 10 kbar (below DAC) for diffraction and tomography (I11, I12)
- High P-T crystallisation cells with laser heating/shocking and online Raman or IR spectrometer. (I11, I12, I15)
- Small sample cells and integrated data acquisition with large temperature (< 4 to 7000 K, laser heating) and pressure range (< 350 GPa) with online analysis: UV, IR and Raman for *in situ* measurements to probe the structural, chemical and electronic features. (I15 and I15-1)
- HT vacuum furnace to operate between 500 – 2000°C, particularly for *in situ* wide and small angle scattering. (I12)
- Low temperature HP cell (±50°C and P_{max}=30 MPa) to study the growth “trigger” mechanisms in biofuel crystallisation and the effect of additives as a function of T-P. (I11)
- Portable HT-P devices could also be used for complementary experiments at other beamlines (e.g. spectroscopic and single crystal diffraction).

Detectors

As our existing 2D flat panel detectors (e.g. Pixium and PerkinElmer) with minutes to sub-seconds/pattern and pixel size ~ 150–200 μm, the next generation of high speed and high spatial resolution (μm- nm) area devices are needed. This is common requirement for all our imaging, diffraction and scattering beamlines to capture fast processes such as plastic deformation, impact phenomena, condensation, electrochemical reactions and crystallisation, etc. Again, dedicated staff and resources are needed to develop and support these detectors.

The key specifications: fast frame rate (kHz - MHz), high-energy efficient (high Z scintillation materials), increased active area to increase angular range (A3 → A2 or tiled 2D detectors), high signal-noise ratio (10^6–10^7), operate between E=30-150 keV, good energy discrimination and reduced pixel size (≤100 μm for diffraction, ≤10 μm for imaging) or optimised pixel sizes. At the same time, the detector electronics must be link to the storage ring for synchronised or accurate gating data acquisition by taking full advantage of the short bunch (ns) structure of the electron beam.

Software

In general, all beamlines request improved resource; dedicated software scientists and supporting staff.

Imaging and Tomography - Improve data storage & reduction capability (speed and capacity) with specific software development, e.g. in Dawn

Powder diffraction (angular and energy dispersive) – to develop data analysis and refinement software (batch mode) to handle large data volume, high quality (publishable) 2D and 3D displays are useful.

Wider Views on the Future of Diamond

Temporal, spatial and coherent resolutions are limited by the brilliance of Diamond's existing DBA lattice. We will certainly lose out to our international competitors who have or will have new diffraction limited storage rings (DLSR) or upgraded SR sources using designs based on multi-bend achromatic (MBA) lattice, e.g. MAX-IV, APS, SPring-8 and ESRF. ADiamond lattice upgrade is therefore essential as it should then provide 2-3 orders of magnitude higher brightness and better coherence than the existing ring. The development and co-location of a UK FEL will bring technological and scientific synergy, like SPring-8 and SACLA.

If extra resources are available, Diamond should widen its scope beyond the "bright light" facility. Perhaps it could be expanded with new "satellite" research laboratories to serve the additional needs of different science areas. The vision should include a Centre of Material Research (CMR) in strong partnership with universities. The user facility will be equipped with a range of bench-top analytical apparatus for the characterisation of optical, electrical, magnetic and thermal properties, and with mechanical rigs to test engineering materials. It should have spectroscopic instruments such as Raman, Brillouin, IR and UV spectrometers. Lab space could be assigned for the development of sample environments as those mentioned above. Any material data obtained would be helpful to the interpretation of results obtained at beamlines. The development of scientific expertise using these instruments and data interpretation would enhance our capability and reputation.

In addition, internal restructuring to form Science Colleges to represent various research areas should be considered as a part of our preparation to deliver world-class science. The formation of colleges such as Energy, Functional Materials, Nanostructures and others should be considered. To develop on-site expertise with dedicated engineers or technician for nano-mechanics would be helpful. As the existing beamline staffing level does not have sufficient resource to engage long-term research activities due to demanding user support, additional research scientists (and students) should be appointed to these colleges. The college staff will be working in collaboration with beamline staff from as many beamlines and support groups as possible. Support groups such as engineering, detector, data acquisition, IMF and others may have to be reorganised to maximise their resources and streamline their services as the needs for the challenges ahead would be quite different.

A 2.6 Condensed Matter Physics (Science Champion: Jörg Zegenhagen)

Introduction

Condensed matter physics (CMP) aims at unravelling the intrinsic collective and correlated properties of solids and liquids and their phases (superconductors, ferromagnets, superfluid…). The properties studied are tomic structure, electronic/magnetic structure, single particle, collective and correlated excitations (phonons, excitons, plasmons, magnons …) as well as derived properties (dielectric constants, elasticity and permeability, …) of increasingly complex materials, of surfaces and interfaces, of materials at reduced dimension (dots, wires, sheets) in the ground or the excited state under influence of temperature, pressure and magnetic field. Experimental CMP has a close relationship with fundamental theory. CMP is partly oriented towards pure science as an investment in the future and partly application driven, such as the intensive semiconductor research that has been pursued over the last 60 years for information, laser, solar technology. Over the last 30 years or so, the experimental tools offered by SR have played a major role in the advancement of knowledge in CMP.

Presently at Diamond, roughly half of the beamlines are dealing with CMP issues within the above mentioned frame (and note too that some aspects of CMP overlap strongly with what is presented in some other areas of science in this report- for example 'Engineering and Materials'): Structure using X-ray or electron diffraction, scattering and imaging are (or will be) covered by I07, I09, I11, I14, I15, I16, I18, B18, I20; electronic or/and magnetic properties are (or will be) covered by I05, I06, I08, I09, I10, B18, I20, I21, B22. Some of these beamlines address (atomic or mesoscopic) structure and spectroscopy, such as I06, I09, I10, B18, I18, I20. Already today, practically all techniques are applicable (almost) on the µm scale (and below).

Scientific Challenges

2.1 Fundamental Aspects of CMP

2.1.1 Structure, Symmetry, Topology and Dimensionality

Identifying and investigating the 2D (and 3D) electronic/band structure and spin polarised current of topological insulators (e.g. $BiSe_2$, $BiTe_2$) requires sensitive spectroscopic tools such as ARPES, XMD, (R)IXS, which are surface and bulk selective as well as *in situ* surface preparation facilities. Heterogeneous interfaces between wide band-gap insulators such as $SrTiO_3/LaAlO_3$ exhibit a high mobility, conducting 2D electron gas exhibiting magnetic as well as superconducting properties. Understanding its formation requires further development of penetrating, high resolution chemically sensitive structural (e.g. GIXRD, HAXPED, XSW) and spectroscopic tools (such as HAXPES, HARPES, (R)IXS , XANES) which need to provide specific information about the nm wide interfacial region. Similar probes with high count-rate capability and excellent signal to noise ratio are needed for other dilute systems such as doped semiconductors and insulators. For 0D (e.g. magnetic and quantum dots), 1D (such as carbon nano-tubes or III/V semiconductor nano-wires), 2D (e.g. [chiral]surfaces and sheets such as graphene, silicine, MoS_2, WS_2, or magnetic multilayer and exchange bias systems) and inhomogeneous systems, the structure, electronic and magnetic properties are confined and the corresponding analysis techniques require a small beam (micro- and nano-focusing) and spatially resolving (X-ray scanning microscopy or imaging) probes such as SXM, (HAX)PEEM, SP-PEEM. The study of field doping at solid electrolyte interfaces also requires penetrating structural and spectroscopic probes as well as specific sample environments.

2.1.2 Complex Solids and bulk properties

High temperature superconductors (HTS, e.g. $YBa_2Cu_3O_{7-\delta}$), CMR materials (e.g. $La_xSr_{1-x}Mn_{3-\delta}$), multiferroics ($BiFeO_3$) are (mostly) perovskite derived, complex, highly correlated (mostly d-band) materials with a rich phase diagram. Such complex materials are the materials of the future and their analysis requires bulk sensitive and high resolution structural and spectroscopic probes. Minute changes in doping levels change their properties giving rise to charge, spin, and structural order or sub-phases on small length scale, requiring high spatial (~nm) resolution. In particular the interplay between superconductivity and magnetism in HTS needs to be finally understood and iron pnictides (e.g. LaFeAsO) are here of particular interest. All these materials need to be studied over a wide range of doping or chemical composition, down to lowest temperatures (and at high magnetic fields). They display large unit cells and obtaining true bulk structural, phononic, electronic, and magnetic properties requires penetrating probes either "photon out" such as IRS, XRD, XANES, (R)IXS or "electron out" with high kinetic energy such as HAXPES, HARPES, HAXPED and with an energy resolution which is at present not available.

2.1.3 Time Dependencies and Excitations

The field of opto-stimulation and manipulation of superconductivity and magnetism promises precise control of the relevant degrees of freedom allowing the interplay of competing orders to be disentangled. The transient response of the electronic and magnetic system and phonons of CM can then be studied on ultrafast timescales. For example, magnetic excitations in nanostructures are key to understanding reversal dynamics and X-ray probes allow element and site-selective monitoring of femtosecond magnetisation reversal following impulsive excitation using transient magnetic fields. Fermionic-Bosonic coupling in high-Tc superconductors can be unravelled using time-resolved ARPES and time-resolved RSXD on the ultrafast timescale, important for fluctuating and static charge density waves. The use of femtosecond X-rays to study the microscopic texture of hidden non-equilibrium phases, by optically creating transient crystal structures with new and unexpected functionalities, would then allow materials to be designed with specific properties at equilibrium.

2.1.4 Quasi- and Highly Disordered Crystals, Amorphous and Inhomogeneous Condensed Matter

Investigations of short and long range structure, defects (e.g. phasons), symmetry (whether centrosymmetric or not) and electronic bandstructure of quasicrystals, such as Al-Pd-Mn or Al-Cu-Fe, need penetrating probes (tender or hard X-rays) to reveal the true bulk structure (because of modified interface regions). The same holds for disordered crystals, amorphous and inhomogeneous CM such as alloys (e.g. magnetic permalloys), glasses (also metallic) and quenched melts. They all need penetrating, high spatial resolution structural and spectroscopic probes for local chemistry, structure, vibronic, electronic and magnetic properties.

2.1.5 Quantum Phenomena and Quasiparticles

Quasiparticles as a result of correlation and correlated excitations are a characteristic feature of all condensed matter. Coupled Fermion systems with Boson character as a result of correlations (Cooper pairs, superfluid ^{3}He) are particular exciting and more of these appear to be emerging as well as new exotic magnetic structures such as Skyrmions. Most of these effects of correlations, as many other quantum phenomena, are only observable at low temperature. Two fascinating states of matter that remain elusive are toroidal moments and magnetic monopoles. The detection of local as well as non-local manifestations of toroidal and magnetic-monopole moments is currently a key aim of condensed matter. RIXS with even further increased energy resolution (< 10 meV) is well suited for the study of these collective phenomena.

2.2 Applied CMP

2.2.1 Information Technology

Quantum dots, nanowires, and quantum wells for laser applications need structural and spectroscopic probes with high spatial resolution; the same holds for multilayer nanometer-scale magnetic structures in current magnetic devices; semiconductor/oxide interfaces for high-k applications and semiconductor/soft matter interfaces for low-k applications need penetrating structural and electronic probes; electronic and magnetic spectroscopic probes are needed for present research on spintronics (dilute magnetic semiconductors such as GaMnAs, spin valves, spin transistors)

2.2.2 Energy Materials

Band structure engineering used long time for semiconductors is now used for light harvesting CM (such as hybrid organic–inorganic lead halide perovskites $APbX_3$); super-capacitors using the electrochemical charge separation in the Helmholtz layer feature different interfaces such as metal/electrolyte, oxide electrolyte, carbon/electrolyte; ion conductors are important for fuel cells; bulk sensitive structural and electronic (e.g. identifying oxidation states) probes are required. The analysis of all these systems, in particular *in situ*, requires bulk sensitive structural and spectroscopic tools

Technical Developments

3.1.1 Source: Storage Ring and Electron Beam

All of the spectroscopic techniques employed for CMP are very photon hungry and benefit from every increase in brilliance in particular for further increasing the energy resolution. The smaller emittance and higher brilliance associated with the envisaged multi-bend-achromat lattice will thus benefit strongly experimental techniques such as RIXS, ARPES, HAXPES. The smaller horizontal beam size is of advantage for a grazing incidence techniques such as grazing incidence HAXPES, GIXRD and imaging techniques such as (HAX)PEEM and will benefits also further the energy resolution for RIXS by decreasing the beamspot on the sample. The smaller beam size will allow obtaining nm focusing (with higher flux) more easily.

3.1.2 Source: Insertion Devices

Enhancing the photon flux, especially at higher energies, for more penetrating bulk probes, is desired as provided by CPMUs.

3.2 Optics

Beamline optics needs to be capable of conserving the emittance, transmit maximum flux, tailor the beam size (mm to sub-μm to nm) and bandpass (pink to 10^{-2} to 10^{-4} to 10^{-6} and below) and deliver stable beam position. Monochromator crystals are needed with better thermal response (e.g. highly heat conducting [perfect] diamond or isotopic pure silicon); multilayer monochromator with variable band-pass (about 10^{-2} to 10^{-3}) high reflectivity (> 80%); mirrors with smallest slope error; self-cleaning environments for mirrors; ultra-stable monochromator mechanics; efficient and fast switchable variable polarisation in the X-ray regime

3.3 Beam Properties

There is a limit to how much flux samples can take, but increased brilliance can be immediately converted into a quality factor e.g. increasing energy resolution for spectroscopy or coherence for imaging. High brilliance is of particular advantage for low investigating dimensional systems (0D, 1D, 2D). Snapshot measurements are necessary if the flux on the sample exceeds the damage threshold,

3.4 Beam Diagnostics

Beam size and position monitors (sub-μm resolution); beam intensity monitors (< 1% absolute and < 10^{-2}% relative); accurate and reliable energy calibration;

3.5 Beam Stability (on Sample)

Higher beam stability of < 0.1μm on the sample over short and long time scale (hour) needs improvement of the storage ring (see section 3) and most of the present optical elements

3.6 New Techniques

The use of X-ray or generally photon interference techniques is becoming increasingly interesting with increasing coherence of the source. Employed since long time by the X-ray standing wave technique (using the photo effect), it allows spatially resolved spectroscopy. This principle can be extended to other spectroscopic techniques such as (R)IXS (see below); using different means for producing the XSW using beam splitters, length scales from sub nm to µm can be covered. This is especially useful for complex, inhomogeneous samples discussed under 2.12 and 2.14. A more coherent source would be very beneficial also for employing related Fourier imaging techniques with atomic resolution such as holography for structure, electronic and magnetic properties. ARPES is meanwhile extended to the soft (SARPES) and hard (HARPES) X-ray range provided increased bulk sensitivity which is required for the study of the chemical and electronic structure of buried interfaces such as the $SrTiO_3/LaAlO_3$ 2D electron gas. With higher resolution HAXPES, the phonon (recoil) effect, visible as energy shift in spectra, can be further explored . PEEM can be extended into the hard X-ray regime (HAXPEEM) to render the probe more sensitive for bulk and buried interfaces. With wide angle lenses for HAXPES analysers, covering angles larger than ±30 degrees, chemical composition can be studied with sub-nm depth resolution to a depth of beyond 20nm (ARXPS). Polarisation dependencies should be routinely employed in PES to "switch off" certain electronic states.

3.7 (Re)New(ed) Beamlines

B22 could increasingly be used for condensed matter physics studying low level electronic, vibronic, and possibly magnetic excitations advantageously (in previously discussed correlated systems) employing the µm spot size for small crystals or inhomogeneous systems. A hard X-ray (about 6 to 15 keV) IXS beamline would allow energy resolution down to 5 meV and large flexibility in the sample environment, e.g. for studying effects such as field doping at solid electrolyte interfaces or excitations under high pressure. Furthermore, RIXS could be combined with structural techniques such as XRD and XSW. It is conceivable to obtain the necessary energy resolution by the beamline optics; ways to obtain the best energy resolution at the analyser/detector need to be discussed. A low-temperature aberration corrected PEEM would provide better spatial resolution as well as improved transmission for faster data collection.

3.8 Detectors

Photoelectron detectors with higher throughput and count rate capabilities and larger acceptance angle for HAXPES with better energy and angular resolution and efficient spin filter/detection for ARPES and HARPES; possibly other electron detector types such as TOF, for time resolved measurements or completely new concepts need to be discussed; large area 2D photon detector with small pixel size (≈5 µm), low (zero) dark counts and high count rate for (R)IXS; large area 2D energy resolving X-ray pixel detector for XRFS, XANES, (S)EXAFS.

3.9 Experiment Control and Data Analysis

Better and automatic experiment control will relieve the beamline staff and enhance the rate of success. Some experiments in the field of condensed matter change from experiment to measurement and can be automated to large extent (e.g. grazing incidence X-ray diffraction, powder diffraction, electron spectroscopy). In conjunction with sample robotics this will allow studying series of samples, where the individual sample is of little interest compared to result on the series (e.g. doping dependence in superconductors or CMR materials). Because of the flood of data, reduction needs to be performed on-line yielding immediate information about the success of the measurements. The user should leave at least with preliminary results regarding chemical composition, structure, electronic structure, etc.

3.10 Experimental Conduct and Sample Environment

Snapshot experiments (measuring before the beam changes the sample): Spectroscopy at ultra-low temperatures (<< 4K) e.g. of magnetic or superconducting phases; structure of metastable phases such as undercooled water. Special cells will be needed to study solid/liquid and solid/electrolyte interfaces in particular with spectroscopic tools such as (HAX)PES. Measurements need to be extended to higher and particular lower temperature and to higher magnetic fields. High pressure phase transitions being another issue.

3.11 Diamond as a Laboratory: From Experiment Preparation to Publication

Diamond has to engage more in the preparation of the experiments and the digestion of the results of the beamtime. Growth of sensitive samples (e.g. clean surfaces) and pre-characterisation, to assure the sample quality, is crucial for the success of many experiments. This requires various sample preparation (e.g. MBE, PLD, electrochemical cells,...) and off-line characterisation (XPS, LEED, Raman and IR spectroscopy, ellipsometry, MOKE, STM/STS, ...) facilities. Diamond also needs to engage strongly in the data analysis, in transforming the result of experiments/ measurements into publication which will require considerable computing (hardware, software, personnel) resources.

3.12 Beyond Diamond

An XFEL source for fs time resolved and pump/probe experiments for electronic, vibronic excitations and the coupling between these will be invaluable for CMP (e.g. the Heisenberg RIXS instrument proposed for the XFEL in Hamburg).

A 2.7 Environment, Earth Sciences and Cultural Heritage (Science Champion: Fred Mosselmans)

Potential opportunities in the Environmental, Earth and Heritage Science fields

The ability of synchrotron radiation to determine the chemistry, speciation, structure, morphology of the most complex materials, making it the best technique for examining the natural environment. SR will be deployed to address the great challenges of:

- the safe disposal of radioactive wastes
- the cycling and remediation toxic elements
- the protection and sustainable exploitation of our soils
- the search for new mineral resources
- determining the origin of the solar system and planetary evolution
- understanding mechanisms operating at the Earth’s interior, and magmatism at the surface.
- the indicators and responses of Earth materials to climate change
- understanding the evolution of life from the fossil record

Safe and economic disposal of radioactive waste

The safe disposal of our radioactive waste is one of the most challenging and urgent issues facing the UK, and other nuclear nations worldwide. Mineral, geochemistry and geological science is at the centre of the UK search for a Geological Disposal Facility (GDF), and the building of a robust safety case.

It is critical to understand the interaction of the large range of short and long lived radionuclides with the clays and cementitious materials of the engineered GDF, and with the complex components of the geosphere as the GDF evolves and decays over 1M yr.

There is a need to understand the chemistry and structural environment of radionuclides present in potential stable wasteforms (for instance glasses) in order to better manage and engineer their safe disposal.

It is important to understand how the wasteforms, containers, engineered components and host rocks will modify under the cumulative radiation dose they receive from contained and escaping wastes.

- X-ray spectroscopy (XAS) is the only technique that provides the key chemical speciation in these complex systems, providing information on mobility, immobilisation**,** sorption and complexation needed for modelling GDF performance
- For transuranic elements and other radionuclides, analysis at the 10ppm level is essential for relevance to ‘realistic’ conditions and it also reduces experimental risk.
- As oxidation states are often the key to solubility, and thus transport properties, defining them is essential for planning responses to potential radionuclide releases into the environment. HR-XANES using emission spectroscopy has the potential to greatly improve our ability to define oxidation states.
- X-ray tomography and diffraction play an important role in understanding the mechanisms of corrosion and break-down of the original waste containment and subsequent corrosion of the contents which leads to radionuclide release into the environment.
- In addition to the GDF context, XAS is the only technique to determine the properties of radionuclides in contaminated environments, leading to remediation strategies.

The cycling of elements in the near surface

Understanding the fate of pollutants in the environment is vital to developing strategies for remediation of contaminated land. For low level pollutants it is vital to probe the chemistry of samples at environmental concentrations and conditions, using XAS. Similarly, soils are one of the Earth's resources under major threat and we require blueprints for sustainable use – the cycling and depletion of nutrients is a crucial component of this process.

- Regulatory levels for many toxic elements in aqueous systems are often very low; ultra-dilute XAS is crucial to understanding their speciation and hence behaviour.
- STXM is an essential technique to study the critical role that microbes play in elemental cycling in the subsurface. Microbial interactions with toxic metals lead directly to their bio-availability. Determining the interactions in bacteria-mineral-solution systems provides a holistic insight into bacterially-mediated redox processes. This requires sub-µm beams with chemical analysis & imaging, for instance to see intra-cellular activity.
- There is increasing concern (and ignorance) about the behaviour of nanoparticles in the environment and their inorganic and organic interactions. Imaging cellular interactions with X-ray beams allows the chemical interrogation of the nanoparticles and their bio-consequences.
- Identification of the location of toxicants in organisms, and their speciation, via high resolution tomography of whole organisms (soft and hard tissue) will provide an understanding of their cycling and bioavailability.
- Understanding the soils system to protect and sustain it, involving the cycling of carbon and major (K, Mg, Ca) and minor (e.g. Se, Mo) nutrients, requires spatially resolved analysis of the mineral, microbial, rhizosphere, and plant system using microfocus XAS, XRD and chemical tomography.
- The structure and chemistry of atmospheric particulates reveals their natural or anthropogenic sources, and examining their interaction with living organisms defines their ecological effects.

Climate related studies

The consequences of climate change on the microscale, and identifying, validating and interpreting physical climate change indicators, is critical to this fertile debate.

- Determining the crystal chemistry of trace element-based paleothermometers is essential to understanding the thermodynamic models that underpin such behaviour. Measuring and speciating trace elements which may accumulate in diurnal cycles requires high resolution, high accuracy XAS.
- Understanding the important processes in biomineralisation will influence planning for Carbon Capture and Storage using in situ SAXS and XRD.
- Interrogating the chemistry of ancient dust can help understand the pattern of global air circulation and its influence on climate using XRF and XAS
- Understanding slow, near equilibrium processes in rocks, minerals and manmade structures elucidates atmospheric weathering reactions, aqueous alteration and leaching, amorphisation and ageing in natural glasses. Much mineral weathering is mediated by biofilms; SXM can be used to study the bacterial interactions with mineral surfaces that are important to understanding these processes and the influence of future climate conditions on them.
- *In situ* laboratory studies of sea ice mineralisation pathways under varying environmental conditions using in situ XRD will help understanding of their role in altering the Earth's albedo has consequences for our global radiation budget.
- The behaviour of aerosols affects cloud formation and rainfall. Thus, the earth's energy budget. Time-resolved SAXS reveals the nucleation processes involved.

Earth resources

The Earth's mineral resources are continually depleted and the identification of new and strategically safe resources to support the UK's manufacturing base is essential.

- Bio-processing methods offer new and improved processing of critical elements, such as the heavy lanthanides. This technology has the potential to reduce the energy input required and waste produced for many types of ore extraction. Understanding the interaction between bacteria and metal ions here is crucial to developing and optimising such methods, using XAS and imaging technologies.
- An understanding the local chemistry of elements (XAAS, XRD, 3D tomography) in minerals will identify new sources and resources and enables the design of smarter extraction technology, with the aim of minimising energy input, waste produced and environmental damage.
- X-ray tomographic imaging can be used to look at bulk structural changes in materials subjected to chemical or bio-processing methods of mineral recovery. The same methods can aid the understanding the physical porosity of bio-leaching feedstocks on larger length scales - SAXS/XRD may be used for sub-micron length scales.
- Understanding nutrient cycling coeval with the determination of the chemical state of elements as they are bio-processed requires chemical interrogation of metals/non-metals as they are processed by cells.
- SR has a key role to play in the search for untapped and ever more complex sources of oil and gas, providing information on their formation and character to ensure maximum energy recovery. To achieve this high resolution, rapid imaging at the micro and nano-scale is needed to examine the nano-porous rock systems; this will enable characterisation of the reservoirs and plan extraction. 4D studies of flow, reactions, fractures, in porous rocks through porous rocks and experimental cells (oil/gas/water/CO2) are also required to optimise recovery techniques. (I13?).
- High resolution, sub-micron chemical imaging and characterisation of organic/fluid or organic/chemical interactions of examine petroleum source rocks, and organics in shale reservoirs, will allow determine the nature of petroleum generation (STXM/I13?). Bulk and microfocus XAS of dilute, redox and environmentally sensitive proxies (Mo, Re, U, Os) can provide novel information on petroleum forming processes. Understanding organic -S and metal-S speciation is important in many oil-bearing systems and provides information on oil sources and potential separation of this deleterious element.

The Earth system

Understanding how our planet works requires determination of the processes involved at the surface and the deep earth processes at relevant P and T conditions.

Near surface processes

- Using *in situ* diffraction /imaging to examine materials under extreme conditions will allow us to understand and predict the behaviour (e.g. phase transformation) of natural materials under exotic, non-equilibrium and/or short-lifetime conditions (shockwave, transient thermal events, "tipping point" transitions etc.) within natural environments, e.g. impact events, volcanism, transient hydration, destabilisation events on terrestrial and other planetary surfaces.
- Identifying mineralisation pathways in differing ice compositions representative of various environments (e.g. Earth, Europa, Enceladus) both past and present will provide an insight into our glacial periods, and these cold worlds.
- Understanding the flow patterns of elements in volcanic fluids will reveal the dynamics of melt flow processes.

- To fully understand mineral formation/alteration (biogenic or chemical) and Earth surface processes, it is essential to be able to undertake XAS of the most abundant elements such as Mg, Al and Si that form 30% of the crust; this can't currently be done at Diamond.

Deep Earth science

To understand the structure and composition of the Earth's mantle and core in the critical zone, there is a need to study geological materials at very high temperatures and pressures.

- High-pressure high-temperature experiments of deep Earth materials in their solid form have been successfully performed for a few decades but measuring weak total X-ray scattering from possible deep Earth liquids is a challenge; this is important for our understanding of the core-mantle-boundary layer, the inner-outer core region (geodynamo that sustains the Earth's magnetic field), the structure of subduction zones where material is recycled back into the deep Earth (volcanism, earthquakes), and also for our understanding the historic 'Hadean' magma ocean.
- Partitioning of metals such as Fe in high pressure melts is hard to study experimentally; XRF with a sub-micron beam on HTP DAC systems could address this. Laser heating is essential for this work.
- Rheological and elastic properties in these deep earth systems at extreme conditions provides an experimentally based understanding of their properties of these to be examined; access to a large volume, HPT press would enable these investigations.
- To look at processes such as phase transitions, e.g. olivine to perovskite and fluid flow require dynamic studies on short timescales.

Planetary and Extra-terrestrial science

SR is an excellent tool for the study of planetary systems because of the ability to examine materials under exotic conditions, *in situ,* and the ability to examine the tiny, fragmentary nature of extra-terrestrial materials using nano and micro X-ray beams

- Experimental high-pressure and high-temperature studies of molecular solids (e.g., mixtures of rare-gases with hydrogen and CO_2) and planetary ices (e.g., H_2O-H_2, NH_3, CH_4) will provide input for models of formation and structure of planets. Experiments can determine e.g. if models such as "helium rain on Jupiter" or "methane rain on Titan" are realistic possibilities.
- Studies of cosmic dusts and cosmic dust analogues will provide an understanding of the life cycle of particulate matter as it cycles between circumstellar, interstellar, proto-planetary nebulae and planetary environments, including comets: e.g. amorphous to crystalline transformations and mineral phase evolution via thermal processing; amorphisation of crystalline dust phases via ion implantation and other disruptive processes.
- Cryo-mineralogical alteration and processing of within and by multi-component ice mantles on dust grains by temporally short thermal excitation mechanisms (e.g. shocks, UV spikes, energetic ions)
- *In situ* hydration/dehydration studies, combining structural measurements with spectroscopic measurements of mineral systems (e.g. sulphates), found on planetary surfaces.
- *In situ* gas-solid interactions between minerals, ices and atmospheric gases – alteration of existing and formation of new mineral phases via gas interaction at high temperatures (eg silicate carbonation, clathrate hydrate formation in ices at low temperature), atmospheric scrubbing (eg noble gas depletion on Titan); stability field measurements.
- Interrogation of the microphases present in meteorites and material from space retrieval missions to gain an insight into early solar system conditions and planetary evolution.

Evolution of life

SR is providing new insights in to the evolution of life on our planet by adapting techniques to examine examples from our fossil record.

- In the field of palaeontology, imaging fossils in 2 and 3D, in particular larger (50cms-2m) specimens, and their chemical and morphological interrogation is demonstrating the ability to gain new insights to our knowledge of animal/plant evolution through geological time. The mapping of large area objects requires special stages, fast scan times and high speed data processing.
- Prebiotic macromolecular-mineral interactions in primitive environments and materials can be achieved by morphology templating and structure modification, phase stabilisation, surface adsorption, effects of mineral chirality and biomineralisation products and their environmental stability.

Heritage Science Research

The multifarious synchrotron radiation techniques provide wide opportunities to examine cultural assets and contribute to art historical, archaeological and conservation research in the field of heritage science. This research is highly interdisciplinary; therefore a dialogue needs to be enabled with the sector. At present there are issues inhibiting development:

- Cultural heritage practitioners and researchers may find it difficult to undertake a synchrotron experiment on their own. They often need to rely either on collaboration with academic or facility staff to apply and perform experiments, as well as to extract meaningful data and knowledge. Hence, to expand Diamond engagement with this field, there is a need for a dedicated science support team to liaise with practitioners as well as non-science researchers (curators, historians, conservators) to work with them to build interdisciplinary synchrotron science research.
- Many cultural heritage institutions have relatively undeveloped scientific infrastructure, thus in some projects, access to our well-equipped labs may be equally valuable. Hence publicising the availability and supplying guidance in their use, effectively some sort of one-stop-shop for using Diamond for cultural heritage institutions, might substantially increase our interaction with this sector.
- Building partnerships with a major heritage science research body in a similar manner to way the ESRF/Soleil have done is a potential way to provide an avenue to improve Diamond's impact in the sector. The Centre for Doctoral Training in Science and Engineering in Arts, Heritage and Archaeology at UCL, University of Oxford and University of Brighton[24] could represent such a body.
- Secure storage and safe operational conditions, particularly for valuable and delicate objects, are required. Hence controlled environmental temperature and humidity control on beamlines will be required for some objects. Additionally, for valuable objects, museum-level security is required.

Analysis of artefacts from paintings to jewellery will provide information on the techniques used to fabricate them, address issues of their historical context, provenance or date of creation, and identify mechanisms of their degradation. In relation to the characterisation of such samples and objects:

- Most users would require access to several techniques at the same time (if objects are given the permission to travel, then it is preferable if all relevant analyses are carried out during one visit).

[24] The CDT represents a partnership of more than 50 institutions, including major museums, galleries, libraries and archives in the UK, and thus an excellent opportunity for Diamond to engage with heritage science more strongly and develop impact.

- Many cultural heritage objects are comparatively large, e.g. Roman tablets and paintings - a large XRF imaging facility would enable research into such objects, although it would require tight environmental control and security.
- Studies of “hidden objects” at high speed, e.g. scrolls that cannot be unwrapped, objects where the ink is overwritten or faded, or unopened archaeological vessels, could be carried out using synchrotron tomography.
- Understanding the degradation of materials is often best achieved with a multi-technique approach – therefore combined IR and X-rays platform grants would facilitate investigations. Often the surface species causing degradation are dilute, so micro and high flux beamlines are needed, while ensuring that analyses remain non-destructive.
- Preservation of buildings, including those from the 20^{th} century with listed status, requires understanding of the mechanisms of environmental degradation and proposed conservation techniques. For building stone, concrete, cladding materials (e.g. marble tiles) tomographic imaging and X-ray diffraction can help understand how materials respond to water uptake, freeze-thaw action and solar thermal cycling.
- Of increasing interest are contemporary and modern materials. Studies of degradation of these requires IR and X-ray imaging, and often diffraction, due to the non-homogeneous distribution of degradation phenomena across a cross-section. Similar applications include understanding the distribution of pigments or binder in paint layers.

Often, these application of synchrotron techniques on art and heritage objects has a very a high impact. To liaise with the user community better, and to interpret the results of analyses in the context of a historical or conservation research questions, it would again be beneficial to have a dedicated cultural heritage liaison person.

Summary of Main Technical Requirements:

- For many environmental studies ultra-dilute XAS is essential and needs pushing towards and beyond 1 ppm. Thus the main branch of I20 needs to deliver reliably, and detector development needs to continue to higher total count rates. This would cover a large UK community which is currently unable to plan experiments at environmental relevant concentrations.
- For the radioactive materials research, it is important to have on-site laboratories for experiments and sample manipulation near to the ring, and to have the capabilities for “routine containment” allowing measurements of radioactive materials on a range of high-end beamlines. Thus, a properly equipped, active samples handling lab is require, handling protocols and cells developed and new beamline designations. Hopefully the NIRO/NIRAB bid will further this.
- High resolution XANES at the actinide L_3 edges (especially for dilute samples) requires a large area secondary spectrometer in the 10-15 keV range on a reliable high intensity EXAFS beamline. With high count rate low noise thick silicon detectors with fast digital read-out systems e.g. XSPRESS3, EXAFS on metals at environmental concentrations can be approached.
- The ability for actinide N-edge spectroscopy will allow long lived radionuclide – microbial interactions to be undertaken; this may require developments on I08.
- A new lattice giving much smaller horizontal emission would provide more flux in a small focussed beams, potentially an order of magnitude more flux on I14 and I08; this would benefit/enable the nano studies proposed above; on I18 microfocus EXAFS with a smaller beam and the microfocus I15 high

pressure dynamic work in the deep earth section will also become more ‘realistic’. The latter also needs integrated laser heating.

- Cryo-undulators on scattering beamlines e.g. I11, I22 may substantially increase the flux at higher energy 15-30 keV, thus enabling X-ray scattering studies in more substantial “cells” than is possible at lower energies. It would also enable even more flux at the high end of I18 – relevant to imaging actinides.
- For the faster and larger object tomography expts: better imaging detectors on I12, more efficient high energy imaging and diffraction detectors; a hexitec detector will provide spectroscopic imaging higher dynamic range, lower noise, and quicker readout time. This will require faster data storage and processing of data. Fast readout low noise high dynamic range area detectors are also needed for the diffraction and potentially SAXS dynamic studies, though these will operate at lower energy.
- For looking at the XANES/ EXAFS of light elements, a B07 non-UHV endstation with a fluorescence detector for XAS covering energies up to 2 keV to include the Si K-edge. This would specialise in the important geo-elements, where nano-focusing is not required.
- For bulk XRF, a beamline with a large mapping stage, some pink beam and a <100 micron sized beam would enable ultra-dilute XRF imaging of large objects, useful for both Heritage Science and Palaeontology objects.
- A large volume press on I15 would enable bigger volumes to be studied than in a DAC enabling stress and strain studies under extreme conditions.
- Laser heating combined with sub-micron focusing on I18 would enable fluorescence studies of partitioning experiments.
- For handling large cultural heritage objects an atmospherically controlled large store (adapting the I15 store) and atmospherically (humidity) controlled environments on beamlines.
- Video microscopes on beamlines to identify the correct part of a heritage science sample to be examined without having to expose other parts of the sample to the beam.
- Environmental science is inherently multidisciplinary and often requires more than one technique; the ability to handle proposals using different beamlines needs to be developed to avoid the current double jeopardy and the likelihood one allocation panel does not have the expertise to appreciate the main thrust of the science.

Resource

- A Diamond scientist responsible for liaising with Heritage Science practitioners, who helps them through the entire Synchrotron experiment process.
- For many of the above process experiments, new sample environments are required. A dedicated team that oversees Diamond environmental “cell” and experimental platform development to ensure that cross-beamline transferability is facile which will ensure integrity to multi-beamline experiments.

Other

- Access to expert referees for heritage science applications, either on the panel or via external advice.

Appendix 3 - Enabling Technology

A 3.1 Developing a strategy for Detectors at Diamond

A long-term detector strategy has been developed for Diamond to try to meet the aspirations of scientists who require increasingly faster detector rates, increasing sensitivity or spatial resolution, perhaps also with energy discrimination, and higher performance for softer or harder X-rays. The Detector Group within Diamond has particularly strong expertise in aspects of spectroscopy and small pixel areas detectors and therefore the plan envisages much of the development to be carried out in collaboration with other laboratories and institutes - and in particular with STFC Technology Laboratories on the Harwell Campus and at the Daresbury Laboratory - as well as purchasing detectors from companies such as Dectris. Our 'wish list' for new detector technology will be shared with many other synchrotron facilities so we envisage establishing collaborations, particularly with those based in Europe, probably with support from H2020 funding.

Detectors for time resolved experiments

Detectors with sub-microsecond time resolution and possibly down to the nanosecond range will open the way to new experiments across material science (I11 and I12), in small angle scattering (I22), in IR (B22), and in X-ray photon correlation spectroscopy (I13).

Area detectors with high frame rate are used in time resolved experiments with millisecond or sub-millisecond resolution. The Eiger or Medipix families of detectors can run with frame rates higher than 1 kHz; up to tens of kHz with reduced registers

Microsecond time resolution may be achieved with hybrid technology area detectors by triggering, or pump-probe methods, but the duty cycle tends to be very low. The situation for point detectors is more varied than area detectors and experiment dependent but generally time resolution of microsecond or sub-microsecond are achieved with appropriate gating and triggering.

Higher performance area detectors

Current detectors are not capable of counting all of the photons produced in the time required and therefore area detectors are needed that are better performing in terms of detection efficiency, maximum count rate and frame rate.

The new MX beam lines will produce very high photon flux at the detector: to use it generates a detector must cope with high photon flux and also deliver high frame rate (say around 1 kHz). SAXS and small molecule crystallography share this need. The second major need is for better detection for photon energy greater than 20 keV. Beamlines include materials science I11, I12, I15, I19, and life sciences: VMXm.

Detectors with better counting rate already exist. These hybrid detectors stemming from Cornell University, manufactured by ADSC operate in integrating mode provide single photon sensitivity with a saturation input counting rate of 10^8 12 keV photons per second per pixel at 300 frames per second. Competition at the PSI is developing the Jungfrau detector for the Swiss XFEL. Dectris and the Medipix consortium have both produced detectors with high-Z sensors to give better performance above 20 keV. CMOS sensors can run to a faster frame rate than CCDs. A detector of this type has been developed at Diamond for I12 and a detector system built along the same guide lines will be developed at ESRF as part of their upgrade.

Area detectors with different functionalities and geometry

There is a distinct need for area detectors with different functionality. I19 requires energy windowed area detectors and smaller pixel size (with respect to the Pilatus standard 172 μm) is a goal for many beamlines. Some such as I13 could exploit detectors with very small pixel size, of the order of 15 μm. In future detectors with novel geometries would benefit SAXS/WAXS beamlines and powder diffraction on I11 and I15-xpdf. Pixel sizes of ca 50μm are available in detectors from Dectris and Medipix and some energy discrimination is available for Medipix3 chips and on the 25μm pixel detector Monch under development by Dectris.

Better performing spectroscopy detectors

Beam lines devoted to spectroscopy mostly use germanium and silicon drift detectors both for XRF and XAFS experiments and the detector is often the single factor that limits performance. In order to improve sensitivity and the throughput of the beamline the strong need is to improve the count rate and effective energy resolution of these detectors.

Germanium monolithic multi-element detectors have the highest throughput of their category, The Xspress2 processor with these detectors offers 300-400 kHz input counting rate with the energy resolution required for XAFS: equivalent to a global counting rate of 19-26 MHz for the 64 elements detector at Diamond. Silicon drift detectors can run with the Xspress3 pulse processor to an input counting rate in excess of 1 MHz per channel. The 384 channel Maia XRF detector developed by Brookhaven for the Australian light source is highly competitive but not available to other facilities.

Although the detectors for the EDE branch of I20 are not strictly spectroscopy grade detectors they are mentioned here since the lack of availability of I0 monitors has been a barrier known for more than two decades.

Area detectors for soft X-rays

Improved soft X-ray area detectors would bring enormous benefits both for diffraction, imaging and spectroscopy. CCD cameras are generally limited in size and frame rate. I06, I10, I08, B24 are examples of such beam lines. The area detector used on the inelastic X-ray scattering beamline will provide one of the major barriers to performance. I08 requires a detector with limited area but very fast. A frame rate of the order of 1 kHz has been mentioned. Diamond participates in the Percival collaboration, led by DESY, that is trying to develop such a CMOS sensor suitable for soft X-rays (energy range 250 eV – 3 keV) with 27 μm pixel size and large area (10 cm x 10 cm) and high frame rate (120 Hz).

Other detectors

Beam monitors are not completely satisfactory. More-compact beam stop monitors would be very valuable for small angle scattering beam lines. Other beam lines would be benefit from **more accurate beam position monitors** able to withstand the beam power and also those with very little interaction with the beam when used permanently (i.e. **thin devices**). In future MX beam lines require beam position monitors for the use in feedback loops. An **APD capable of working in the soft X-ray regime** have been required by I08. Finally **Bolometers** could be improved for B22, as IR detectors, and by I16, as very high energy resolution X-ray detectors. Summary of the Diamond Detector Landscape

Detector type	Desired performance	Available performance	Other remarks
Area detector for time resolved experiments	Sub-microsecond or nanosecond time resolution.	**Medipix3** running at 30 kHz frame rate (1 bit counter) or **Eiger** running at 24 kHz frame rate (this frame rate is not available in the commercial version). **Rapid** can achieve 10 us or better. **Timepix3** can achieve a time resolution of time or arrival of events at nanosecond level.	Rapid is based on an obsolete technology. Timepix3 requires engineering. The counting rate per pixel cannot exceed 2 MHz and there are limitations in the global counting rate still to be assessed.
High detection efficiency area detectors	Detection efficiency very close to 100% in the entire range of operation of the beam line.	Detection efficiency close to 100% for most of the beam lines of Diamond (with the only exception of I12) can be achieved with **CdTe hybrid detectors**. Other detectors that can be used are **hybrid germanium detectors.** **Flat panel detectors and scintillators coupled to CCDs** have detection efficiency depending on the thickness of the phosphor.	Engineering of systems using CdTe is required. Gaps between chip are a drawback. Commercial Pilatus detectors use CdTe but they are very expensive. Hybrid germanium detectors are under development at DESY. They may become available through DESY's spin-off company.
Area detectors with high counting rate capabilities	Tens of MHz per pixel or more.	100 MHz per pixel **ADSC detector**, 25 MHz **Jungfrau.**	Jungfrau is at prototyping stage. The noise, linearity and mismatch between nominal and actual performance of these detectors have not been assessed yet.
High throughput spectroscopy detectors	For XAFS global counting rate in excess of 100 MHz (or a few hundreds MHz) in the same area of the detectors presently installed (4cm x 4 cm at I20) For XRF is required a larger solid angle coverage that entails larger arrays with custom geometry.	The global counting rate achieved at I20 is around 25 MHz. Detectors used for XRF are mainly silicon drift detectors that are available in limited arrays and with packaging that is difficult to use very close to the sample.	An important parameter that is not discussed here is the peak to valley ratio. This parameter can limit the sensitivity of the detector and has to be taken into account properly.
Area detectors with small pixel size	The pixel size that is generally mentioned is 50 μm.	Medipix3 has 55 μm pixel size and Eiger 75 μm.	I13 is an exception as they would like a pixel size still smaller. Around 15 μm.

Appendix 4 – Prioritisation Process

5.1 Strategic options

The process for developing a 10-year Vision and a 5-year Strategy for Diamond was presented in the Introduction (**section 1.2**). This has involved a high level of external engagement and input from Diamond's key stakeholders to shape the 10-year Vision described above. It has also involved a comprehensive process of scrutiny and challenge internally, led by Diamond's Executive Team, to further shape the 10-year Vision, and also to evaluate **strategic options** for a preferred 5-year Strategy and Programme to meet the scientific and societal challenges outlined in the Vision. This has included assessing individual submissions from the scientific areas and technical groups within Diamond at various stages in the process against screening criteria for Suitability, Feasibility and Acceptability:

Suitability:

- Does it fit with Diamond's core purpose?
- Does a strong user community exist for this or could it be developed?
- Does it exploit Diamond's existing strengths (i.e. expertise, capabilities etc.)
- Does it exploit opportunities and Diamond's potential?
- Does it protect our current position as a leading facility (world leader and/or world-class) compared with other leading facilities

Feasibility:

- Will the technology be available?
- Is Diamond capable of becoming a world leader or world-class in this area?
- Can our ambition (i.e. the contribution we would like to make) be funded?
- Can we ensure that the calibre and capacity of resources can be supplied?
- Can we ensure the physical infrastructure can be supplied?
- Can we deliver the development in the timeframe (as set out in the road map for implementation)?
- Could all the necessary collaborations be secured?
- Can competition from other leading Synchrotron (and other relevant light sources) facilities be coped with?

Acceptability:

- Will the proposed development be acceptable to Diamond's stakeholders (e.g. shareholders, research councils, users/industry etc.)
- Will the proposed development deliver an acceptable level of economic and societal impact?
- Will the proposed development be appropriate to the general expectations within Diamond?
- Will Diamond's relationship with outside stakeholders need to change?
- Will it expose Diamond to either new or unacceptable levels of risk?
- Are the assumptions underpinning the proposed development/contribution by Diamond sufficiently robust?

Management within the scientific areas and technical groups, in consultation with their teams, were also required to prioritise their submissions into three distinct categories: **must do**; **highly desirable**; and **desirable**, setting out a clear rationale for:

- the contribution and level to which each priority would support the achievement of Diamond's 10-year Vision

- the contribution that each priority would make toward the achievement of the UK's national scientific priorities (as defined by BIS); and
- the expected benefit in the context of developments within the worldwide synchrotron community.

They were also required to identify both the capital and any increased operational costs associated with each priority, covering the 5-year period 2014/5 - 2019/20. These submissions were again scrutinised and challenged by the Executive team.

This process has enabled the financial resources required to be modelled for the period 2014/5 - 2019/20- covering all of the above categories - to support the delivery of the Diamond 10-year Vision. These are grouped primarily into 'must have' projects – option1 – and 'highly desirable' projects – option 2. Projects assessed as 'desirable' were not considered any further, and any projects associated with the 'Diamond II' lattice upgrade were also considered separately as the case for such an upgrade has yet to be made, requiring and detailed technical assessment linked to the scientific opportunities the different technical options would provide. This will be the subject of a separate process.

Appendix 5 - Participants at the Diamond 'Vision' Meeting – September 30th – October 1st 2014

First Name	Surname		Organisation	Science Area (Working Group)
Andy	Akerman		Diamond Light Source	
Lise	Arleth	Working Group Chair	University of Copenhagen	Biomaterials & Medicine
Peter	Ash		Johnson Matthey	Chemistry & Catalysis
Alun	Ashton		Diamond Light Source	
Adam	Babbs		Medical Research Council	
Asa	Barber		Queen Mary University of London	Soft Condensed Matter
John	Barker		Evotec	Integrated Structural Biology
Andrew	Barrow		Rolls-Royce	Engineering & Materials
Riccardo	Bartolini		Diamond Light Source	
Isabelle	Boscaro-Clarke		Diamond Light Source	
Gérard	Bricogne		Global Phasing Ltd.	Integrated Structural Biology
Oliver	Bunk		Paul Scherrer Institut	Biomaterials & Medicine
Chris	Christou		Diamond Light Source	
Gianfelice	Cinque	Science Champion	Diamond Light Source	Biomaterials & Medicine
Ralph	Claessen		Universitat Wurzburg	Condensed Matter Physics
Paul	Collier		Johnson Matthey, RC@H	Chemistry & Catalysis
Jo	Collingwood		University of Warwick	Biomaterials & Medicine
Tom	Collins		Wellcome Trust	
Lucy	Collinson		Cancer Research UK London Research Institute	Integrated Structural Biology
Rob	Cooke		Heptares Therapeutics	Integrated Structural Biology
Susan	Daenke		University of Oxford (Instruct)	Integrated Structural Biology
Andy	Dent		Diamond Light Source	
Sofia	Diaz-Moreno	Science Champion	Diamond Light Source	Chemistry & Catalysis
Robert	Docherty		Pfizer	Biomaterials & Medicine
Karen	Edler	Working Group Chair	University of Bath	Soft Condensed Matter
Gwyndaf	Evans		Diamond Light Source	Integrated Structural Biology
John	Evans	Working Group Chair	University of Southampton & Diamond Light Source	Chemistry & Catalysis
Chuck	Fadley		University of California, Davis & Lawrence Berkeley National Laboratory	Condensed Matter Physics

Adrian	Finch		University of St Andrews	Environment, Earth Sciences & Cultural Heritage
Paul	Freemont	Working Group Chair	Imperial College London	Integrated Structural Biology
Paul	Fuoss		Argonne National Laboratory	Engineering & Materials
Giacomo	Ghiringhelli		Politecnico di Milano	Condensed Matter Physics
Clare	Grey		University of Cambridge	Engineering & Materials
Gerhard	Grübel		DESY Hamburg	Engineering & Materials
Dave	Hall		Diamond Light Source	Integrated Structural Biology
Andrew	Harrison		Diamond Light Source	
Georg	Held	Science Champion	University of Reading	Chemistry & Catalysis
Mark	Heron		Diamond Light Source	
Madeleine	Humphreys		Durham University	Environment, Earth Sciences & Cultural Heritage
Jonathan	Hyde		National Nuclear Laboratory	Environment, Earth Sciences & Cultural Heritage
Chris	Jacobsen		Argonne National Laboratory	Biomaterials & Medicine
Anne	Kavanagh		AstraZeneca	Biomaterials & Medicine
Jim	Kay		Diamond Light Source	
Alexander	Korsunsky		University of Oxford	Engineering & Materials
Peter	Lee		University of Manchester	Engineering & Materials
Ken	Lewtas		Lewtas Science & Technology	Soft Condensed Matter
Malcolm	McMahon		University of Edinburgh	Environment, Earth Sciences & Cultural Heritage
Des	McMorrow		London Centre for Nanotechnology, UCL	Condensed Matter Physics
Colin	Miles		BBSRC	
Dino	Moras		Institut de génétique et de biologie moléculaire et cellulaire (IGBMC)	Integrated Structural Biology
Susan	Morrell		EPSRC	
Fred	Mosselmans	Science Champion	Diamond Light Source	Environment, Earth Sciences & Cultural Heritage
Bob	Newport	Working Group Chair	University of Kent	Engineering & Materials
Andy	Parsons		NERC	Environment, Earth Sciences & Cultural Heritage

First Name	Surname		Organisation	Science Area (Working Group)
Richard	Pattrick	Working Group Chair	University of Manchester	Environment, Earth Sciences & Cultural Heritage
Simon	Phillips		Research Complex at Harwell	
Trinitat	Pradell		Universitat Politechnica de Catalunya	Environment, Earth Sciences & Cultural Heritage
Neil	Pratt		STFC	
Bill	Pulford		Diamond Light Source	
Paolo	Radaelli	Working Group Chair	University of Oxford	Condensed Matter Physics
Robert	Rambo		Diamond Light Source	Integrated Structural Biology
Christoph	Rau	Science Champion	Diamond Light Source	Biomaterials & Medicine
Trevor	Rayment		Diamond Light Source	
Nick	Rees		Diamond Light Source	
Guenther	Rehm		Diamond Light Source	
Nathan	Richardson		MRC	
Stephan	Roth		DESY	Soft Condensed Matter
Helen	Saibil		Birkbeck College	Integrated Structural Biology
Cecilia	Sanchez Hanke		Diamond Light Source	Condensed Matter Physics
Kawal	Sawhney		Diamond Light Source	
Jos	Schouten		Diamond Light Source	
Sven	Schroeder		University of Manchester	Chemistry & Catalysis
Tom	Scott		University of Bristol	Engineering & Materials
Dominic	Semple		Diamond Light Source	
Elizabeth	Shotton		Diamond Light Source	
Ian	Sinclair		University of Southampton	Engineering & Materials
Stephen	Skinner		Imperial College London	Engineering & Materials
Steve	Smerdon		MRC National Institute for Medical Research (NIMR)	Integrated Structural Biology
Dhruvananda	Sockalingum		University of Reims Champagne-Ardenne	Biomaterials & Medicine
Stuart	Stock		Northwestern University	Biomaterials & Medicine
Matija	Strlic		UCL, Bartlett	Environment, Earth Sciences & Cultural Heritage
Dave	Stuart		Diamond Light Source	
Chiu	Tang	Science Champion	Diamond Light Source	Engineering & Materials
Nicola	Tartoni		Diamond Light Source	
Nicholas	Terrill	Science Champion	Diamond Light Source	Soft Condensed Matter
Geoff	Thornton		University College London	Chemistry & Catalysis
George	Tranter		Chiralabs Limited	Biomaterials & Medicine
Richard	Walker		Diamond Light Source	

Mike	Walter		University of Bristol	Environment, Earth Sciences & Cultural Heritage
Martin	Walsh	Science Champion	Diamond Light Source	Integrated Structural Biology
Silvana	Westbury		Diamond Light Source	
Rudolf	Winter		Aberystwyth University	Soft Condensed Matter
Philip	Withers		University of Manchester	Engineering & Materials
Hartmut	Zabel		Ruhr-Universität Bochum - JGU Mainz	Condensed Matter Physics
Jorg	Zegenhagen	Science Champion	Diamond Light Source	Condensed Matter Physics

Appendix 5 - Glossary

ARPES	Angular resolved photoelectron spectroscopy
ARXPS	(Take-off) Angle resolved X-ray photoelectron spectroscopy
BBSRC	Biotechnology and Biological Sciences Research Council
CD	Circular Dichroism
CCS	Carbon Capture and Storage
CLF	(STFC) Central Laser Facility
CMR	Colossal magneto resistance
CPMU	Cryogenic Permanent Magnet Undulator
DBA	Double-Bend Achromat
DISCo	Diamond Industrial Science Committee
DDBA	Double-Double Bend Achromat
EM	Electron Microscopy
EMF	Electron Microscopy Facility
EPSRC	Engineering and Physical Sciences Research Council
EXAFS	Extended X-ray Absorption Fine Structure
GIXRD	Grazing incidence X-ray diffraction
HAXPED	Hard X-ray photoelectron diffraction
HAXPEEM	Hard X-ray photoelectron microscopy
HAXPES	Hard X-ray photoelectron spectroscopy
HARPES	Hard X-ray angular resolved photoelectron spectroscopy
hRIXS	RIXS in the Heisenberg limit ($\Delta E \Delta t \approx h$)
HTS	High temperature superconductivity
IXS	Inelastic X–ray scattering
ID	Insertion Device
IR	Infrared
IRS	IR spectroscopy

LLRF	Low Level RF
MBE	Molecular beam epitaxy
MOF	Metal Organic Framework
MOKE	Magneto optical Kerr effect
MPL	Membrane Protein Laboratory
MRC	Medical Research Council
MTBF	Mean Time Between failures
MX	Macromolecular Crystallography
NERC	Natural Environment Research Council
PDB	International Protein DataBank
PEEM	Photoelectron emission microscope
PES	Photoelectron spectroscopy
PLD	Pulsed laser deposition
RAL	Rutherford Appleton Laboratory
RCaH	Research Complex at Harwell
RF	Radio Frequency
(R)IXS	(Resonant) inelastic X-ray scattering
SAC	Scientific Advisory Committee
SARPES	Soft X-ray angular resolved photoelectron spectroscopy
SAXS	Small Angle X-ray Scattering
SC	Superconductor
SCU	Superconducting undulators
SEM	Scanning Electron Microscopy
(S)EXAFS	(Surface) extended X-ray absorption fine structure
SP-PEEM	Spin polarised PEEM
STM/STS	Scanning tunnelling microscopy/spectroscopy
STFC	Science and Technology Facilities Research Council
TEM	Transmission Electron Microscope

TOF	Time of flight
UHV	Ultra-High Vacuum
UV	Ultraviolet
WAXS	Wide Angle X-ray Scattering
XANES	X-ray absorption near edge structure
XM(C,L)D	X-ray magnetic (circular, linear) dichroism
XRFS	X-ray fluorescence spectroscopy
XSM	X-ray scanning microscopy
XSW	X-ray standing waves