Free-Electron Laser (FEL) Strategic Review

Science & Technology Facilities Council

Contents

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1. Foreword by Professor John Womersley, STFC Chief Executive

STFC's vision is to maintain the UK as the best place in the world to do research, to innovate and to grow business. We strive to ensure the UK science which we support remains globally leading and continues to deliver great benefit for society and the economy. Realising this vision means identifying, understanding and seizing new opportunities. This is vitally important in emerging areas that can open new avenues of discovery.

The rapidly advancing science of Free-Electron Lasers (FELs) is such an area. Recognising its importance for the UK science community, STFC commissioned a strategic review of the science and facility access. As part of the strategic review, we have developed a UK strategic approach for FELs. Its purpose is to guide STFC's planning over the next five years, give clear guidance on the importance of FELs, on how the user community should grow and the need for a timely decision on the UK building a FEL.

FEL science has already demonstrated enormous potential in helping tackle global challenges in areas such as energy, security, transport and drug development. This review concludes that the unique capabilities of FELs can offer new and remarkable insights across a diverse range of fields, from life sciences through to advanced materials.

As this strategic approach notes, creating a UK capability in FELs would give us a leading international role at the heart of new scientific collaborations. It would allow us to forge strong bonds with organisations across the established and successful UK innovation landscape and it would assist in delivering competitive advantage for UK industry in support of growth, jobs and, most importantly, societal benefits.

STFC will work with the UK Research Councils to support the growth of the UK FEL user community. We will work with Government to endeavour to secure investment for a new large facility in the UK, ensuring we are in a position to make a decision on the development of a FEL facility in 2020.

The UK and STFC already have strong foundations on which to build a world class FEL facility. With our scientific and technological expertise, we have an enviable track record of delivering large scientific facilities, and we have the international standing to grow and sustain a global research and innovation communities around them.

STFC already hosts the UK's leading optical laser facility. The co-location of a FEL facility with high-powered and high-energy lasers would allow us to offer a unique capability unmatched by any equivalent facility in the foreseeable future.

The ambition and potential for the UK is clear. This strategic review provides the blueprint for how it can be realised.

As with all STFC's underpinning research and innovation strategies, the FEL strategic review provides input to STFC's strategic goals of world class research, innovation and skills.

2. Executive Summary

From physical, material and life sciences to ground-breaking investigations into soft condensed matter, Free-Electron Lasers (FELs) provide a range of opportunities to achieve significant advances that extend the boundaries of our knowledge. Thanks to their three defining characteristics – short pulse length, high brightness and spatial coherence – FELs have unique capabilities that enable them to address key scientific challenges in a way that no other type of facility can match.

Crucially, FELs have the potential to open up new areas of science where the UK can become a world leader and where UK businesses can generate competitive advantage, for example in pharmaceuticals, energy security and other strategically important fields.

As well as recognising that a UK FEL facility will be needed to meet our future research needs, it is clear that the UK should increase its engagement with XFEL.EU (the European X-ray Free-Electron Laser), currently the world's leading machine and a facility that could meet our capacity and capability requirements in the short term. In order to meet our future capacity requirements, the UK should also explore how best to facilitate access to other machines around the world; these include LCLS-II (the Linac Coherent Light Source at Stanford University, USA), SwissFEL (at the Paul Scherrer Institute, Switzerland), SACLA (the SPring-8 Angstrom Compact Free-Electron Laser in Japan) and PAL-XFEL (the Pohang Accelerator Laboratory X-ray Free-Electron Laser in South Korea). Access to LCLS-II is particularly important to fields of science such as time-resolved and angle-resolved photoemission spectroscopy (trARPES), resonant inelastic scattering (RIXS) and the characterisation of non-equilibrium processes (e.g. combustion), where high average X-ray power is critically important and there is a need for a high-repetition-rate constant stream of pulses (see 'A Cleaner Atmosphere', p.23).

To ensure the UK is better equipped to exploit FELs, the FEL user community among UK scientists needs to be developed further. Coordinated measures to boost and strengthen the UK's scientific community in XFEL science are essential and should engage Research Councils UK, international photon facilities and UK Higher Education Institutions, while capability in key areas of underpinning technology should also be further developed to complement scientific endeavour and enable the UK to build a FEL facility in the future.

Based on the annual increase in proposals submitted to LCLS, even if the UK maximises its opportunities for access to existing and near-future XFEL facilities, it is anticipated that our demand will exceed this level within 10 years. In the long term, the UK's capacity requirements will be best served by constructing a UK FEL facility with a specification designed to meet our needs. Building such a facility would advance UK science, aid the growth and retention of the UK industrial base and assist the development of key technology and skills that would benefit other large UK science facilities as well as our high-tech industry sector. Experience at LCLS shows that demand increases rapidly once a facility opens.

In order to address the majority of the key science challenges, the ideal UK facility would deliver hard X-rays and would also have a high repetition rate. However, there are questions over the current affordability of such a facility; a best compromise specification will need to be defined to fit UK science. Options for this include a SwissFEL-like facility, which would provide a significant enhancement to meet the growing capability and capacity requirement for UK scientists and industry. It would also complement XFEL.EU and LCLS-II, which will remain essential for a small number of applications that demand a high repetition rate and which include combustion diagnostics, multi-dimensional spectroscopy, time-resolved RIXS and ARPES.

The UK has a unique opportunity to co-locate an XFEL with the state-of-the-art suite of ultrafast, high-energy, high-powered laser sources currently in place at STFC's Central Laser Facility (CLF) on the Harwell Campus. No similar co-location of optical and X-ray lasers is envisaged anywhere else in the world. Such a step would therefore provide the UK with world-leading facilities for creating and probing matter at extreme conditions, unmatched for the foreseeable future and therefore highly attractive to international users. By 2020, STFC should ensure that the UK is in a position to take the final decision on whether to build an XFEL in this country and on what kind of machine to construct. It is clear that outline design work and significant prototyping work will be required.

Internationally, FEL science is advancing rapidly and offers enormous promise in terms of tackling a whole range of pivotal scientific challenges. The UK should not simply stand by and watch this happen. We are currently in a competitive position thanks to our use of facilities across the globe. The next task must be to invest in this field so that opportunities can be exploited and the UK can assume a key role in the international community active in this exciting sphere of science.

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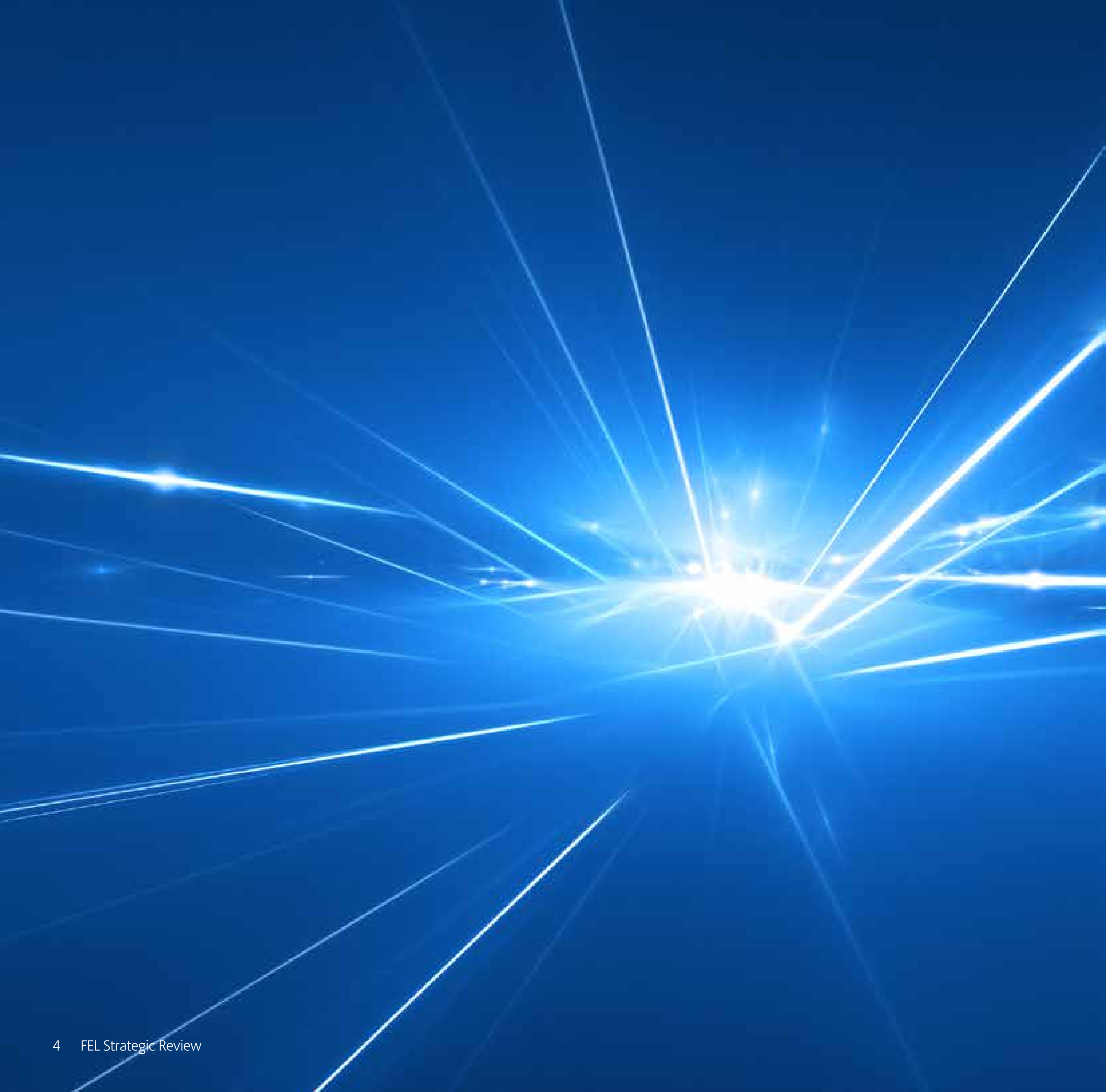


3. Introduction

3.1. About the FEL Strategic Review

Carried out by an expert panel drawn from across the physical and life sciences, this review was commissioned by STFC's Executive Board in recognition of the UK's and STFC's need to develop a strategic approach for the provision of FEL facilities. (See Annex C FEL Review Terms of Reference.

The panel:

- identified key scientific challenges that would benefit from access to a FEL facility;
- considered the ability of existing and near-future FEL facilities to address these.

The resulting strategic review incorporates feedback from STFC's Science Board, Physical Sciences and Engineering Advisory Panel, Life Sciences and Soft Materials Advisory Panel and Accelerator Strategy Board.

3.2. What is a FEL?

Free Electron Lasers produce 'light' that has properties similar to those of optical laser light but at frequencies ranging anywhere from X-rays to microwaves. A key feature is that FELs produce extremely bright, ultra-short pulses of light that allow atomic-level measurements of structure and function with unprecedented time resolution. In fact, the light is so bright and the pulse is so short that measurements are unaffected by atomic motion and can be made before the radiation has damaged the matter being investigated.

Thanks to such capabilities, FELs will open up areas of research that were previously inaccessible. For example, researchers can harness these facilities to map the internal details of viruses, decipher the molecular composition of cells, make 'movies' of chemical reactions and probe extreme states of matter that might only exist for a nanosecond. FELs can also help scientists to study the physical and chemical processes of combustion taking place inside engines, investigatethe formation and motion of twins and dislocations in highly-stressed advanced alloys and determine the structure of molecular materials that can only be crystallisedas nanocrystals.

Although a number of important areas of science require infrared/terahertz FEL facilities, the majority of the key scientific challenges identified as part of this Strategic Review need access to XFELs. Infrared and terahertz frequencies are considered in the case for ARTFUL (Advanced Infrared/Terahertz Facilities for Users of Lasers), a statement of need submitted to the Engineering and Physical Sciences Research Council (EPSRC) and focusing on mid-range facility provision at ALICE (Accelerators and Lasers in Combined Experiments) at Daresbury Laboratory and at FELIX (Free-Electron Laser for Infrared Experiments) in the Netherlands. The strategy set out in this document therefore focuses solely on XFELs.

3.3. Why Do We Need FELs?

The way that FELs produce X-ray radiation gives very different characteristics from radiation produced by synchrotronX-ray sources:

- The pulse length only lasts tens of femtoseconds (i.e. around 10^{-14} seconds) – more than three orders of magnitude shorter than X-ray pulses from a synchrotron and shorter than the atomic vibration periods in molecules. This means data collected from a single FEL pulse is unaffected by the motion of atoms, which can cause 'smearing'.
- The peak brightness of an XFEL is a billion times greater than that of a synchrotron, so a complete dataset can be collected in an exceptionally short length of time (i.e. in $\sim 10^{-14}$ seconds from a single X-ray pulse). This means data is unaffected by any radiation damage caused by the X-rays.
- The radiation from FELs exhibits unprecedented spatial coherence, allowing new X-ray imaging techniques.

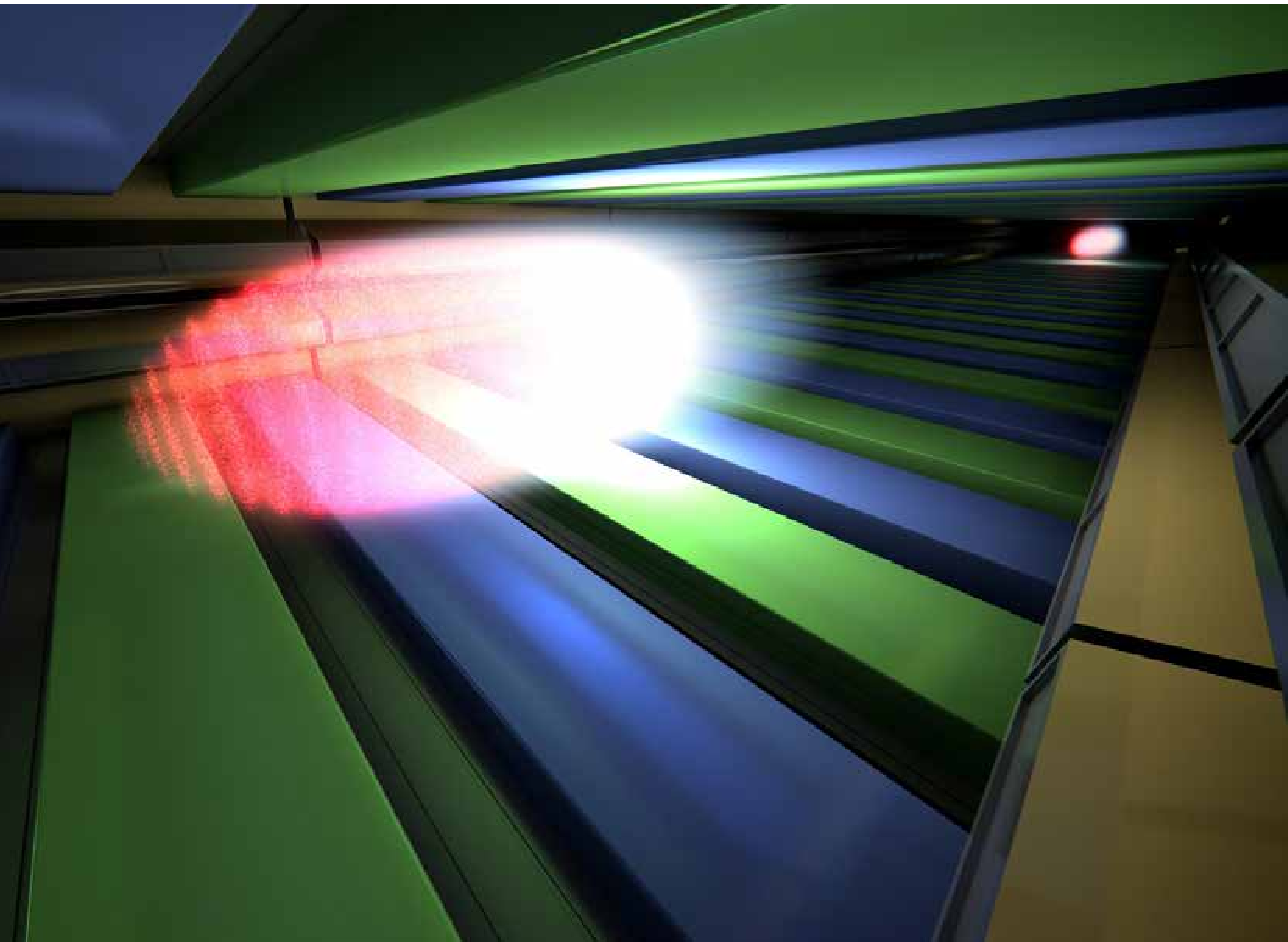
These three defining characteristics – short pulse length, high brightness and spatial coherence – give FELs their unique capabilities and open the door to studies of the ultra-small and the ultra-fast that were previously impossible to undertake. Quite simply, FELs can address scientific challenges in a way that no other type of facility can replicate, providing the opportunity to deliver significant advances in knowledge through the study of a wide range of systems and spanning everything from physical, material and life sciences to investigations of soft condensed matter.

Furthermore, the time-structure of the X-ray beam produced by a FEL makes it ideally suited to 'pump-probe' experiments (see Section 4.1). Such experiments require access to a wide range of world-class ultrafast, high-energy, high-powered auxiliary laser sources – all of which can be found at the CLF on the Harwell Campus. Co-locating a FEL with the CLF's unparalleled range of state-of-the-art laser technology would provide the UK with a FEL facility unmatched for the foreseeable future. Highly attractive to international users, these world-leading facilities could, for instance, create and probe solids and plasmas at extreme conditions.

While FELs are uniquely suited to pump-probe experiments, other experiments currently limited by radiation damage would also benefit greatly from using an XFEL. They include experiments on biological matter or those requiring element-specific and surface/interface-sensitive probes of monolayers or heterostructures,

Collectively, all of these factors mean there is a strong case for investing in a UK XFEL. A facility of this kind would allow the UK's capacity requirements to be met and would offer capabilities tailored to specific UK needs; it would also lead to the advancement of UK science, the growth of UK industry and the development of key technology and skills. The community of XFEL users in this country is growing and it is anticipated that, by the time specific recommendations are made on the characteristics of such a facility, the UK will have around 50 active user groups, averaging one for every research-intensive university. Growth to this level would indicate that FEL use has become a significant priority for this country's research communities; it would also help in defining the specifications of a UK XFEL facility.

Generation of X-ray laser flashes in an undulator © European XFEL (Design: Marc Hermann, tricklabor)



4. FEL Science

As noted above, FELs' unique capabilities enable them to address important scientific challenges beyond the scope of other types of X-ray or laser facility. Some of these challenges are explored further in the following subsections. More detailed information on each of these examples, including how FELs will solve the challenges and why these cannot be addressed by other techniques, is provided in Annex A: FEL Science (p.22).

4.1. High Temporal and Spatial Resolution

When combined with optical lasers, FELs offer the possibility of conducting time-resolved pump-probe experiments with atomic spatial resolution and femtosecond time resolution. An optical laser is first used to 'pump' the sample under investigation and initiate a process or reaction that results in the sample assuming a short-lived state or configuration. After a delay that can range from nanoseconds to 10 seconds, the sample is then 'probed' by the FEL beam to capture an image of it. By making repeated measurements at different delay times, a 'movie' can be compiled from the individual images.

Key challenges requiring the time and spatial resolution delivered by FELs include:

- Bond making/breaking – understanding the intermediate steps in a chemical reaction.
- Understanding the dynamics of structural changes in membrane proteins and soluble proteins.
- Understanding photocatalytic water-splitting (see below).
- Catalysis – understanding catalytic processes by following reaction pathways.
- Chemistry at the nanoparticle scale – obtaining scattering and spectroscopy data from individual particles.
- Light-matter interactions in semiconductors and 2D materials – understanding how charge, spin, orbital and lattice degrees of freedom interact to produce emergent phenomena and exotic states of matter.
- Matter at extreme conditions – understanding mechanisms of deformation, melt, recrystallisation and polymorphic phase transitions.
- Properties of warm dense matter (WDM) – understanding fundamental WDM and hot plasma properties and dynamics.

Photocatalytic Water-Splitting

Achieving a detailed understanding of how biological systems harness energy to split water into oxygen and hydrogen would open up the possibility of using solar power to produce hydrogen (and possibly hydrocarbons). The 'oxygen-evolving complex' (OEC) in cyanobacteria, green plants and other biological systems uses photons from the sun to drive a cycle in which two water molecules are split into an oxygen molecule plus four protons and four electrons. FEL science can play a key role in understanding this process of photocatalytic water-splitting and the three crucial stages of excitation, charge separation and redox reaction.

The OEC has five redox states, known as 'S' states (S_0 to S_4). Synchrotron studies of the process are difficult to conduct because X-rays damage the manganese centre of photosystem II crystals and induce redox changes, scrambling the 'S' states. FELs avoid this problem because they can capture images before radiation damage occurs. After using a laser flash to set the 'S' state, an XFEL can be used to determine the structure of that state before going round the other four states to 'see' the real catalytic process.

The further development of water-splitting systems also depends crucially on improving detailed understanding of excitation and charge transfer processes – a level of understanding which FEL-based science is ideally suited to provide.

Time Resolution in Macromolecular Crystallography (MX)

Change in atomic structure during protein function occurs on a nanosecond to femtosecond timescale too short for conventional methods of structure analysis. Prior to the development of XFEL radiation, two different approaches were adopted for use with synchrotrons:

- 'Slow' reactions engineered to allow frozen snapshots to be collected conventionally from different crystals at different time-points throughout the reaction process. While this approach has generated profound insights, its time resolution is limited to microsecond diffusion times and it often involves taking averages over a range of different states (losing the definition of a particular molecular state).
- 'Pump-probe' (see above) where a reaction is triggered by a light pulse and a complete dataset is then recorded from a series of still images, using Laue diffraction. Although this approach has generated profound insights, it is limited by time resolution. Furthermore, white-beam Laue radiation is unsuitable for large unit cells or highly mosaic crystals. In addition, triggering the reaction uniformly across the crystal is almost impossible and this means taking an average of different states (making it necessary to deconvolute multiple structures to obtain single species).

Very recent pioneering work at LCLS has used XFEL radiation to study the very short-lived states of photoactive yellow protein, harnessing the pump-probe technique. FEL methods had particular advantages, with the efficiency of triggering the reaction using a nanosecond laser proving to be a factor of four higher than achieved at a synchrotron, due to the small crystals that could be used for the experiment. As the 'probe' pulse (and thus the data collection) was completed in femtoseconds, time regimes as short as 10 nanoseconds after the 'pump' pulse could be explored. The quality of the resulting data allowed detailed structure determination of previously unseen states.

If achievable, single-molecule imaging with atomic resolution would also have a huge impact. The likelihood that XFELs will be able to do this in the foreseeable future is, however, very low. As the number of photons per pulse is likely to have to increase by two or three orders of magnitude, significant technical developments in both sources and detectors would be required.

4.2. Diffraction Before Destruction (Out-running Radiation Damage)

FELs' ability to obtain diffraction or imaging data from a sample before radiation damage harms or destroys it – an ability demonstrated in the case of photocatalytic water-splitting (see above) – is especially vital in the analysis of soft and biological material. In the past, the use of X-rays has been limited by the radiation damage these can cause. When using an XFEL, however, the exposure time is relatively short and this allows imaging to be completed before the effects of radiation damage become apparent. Potential applications include:

- Nanocrystallography – structure determination of protein crystals that are sensitive to radiation damage.

Devising New Medicines: Integral Membrane Proteins (IMPs))

FELs' unique ability to outrun radiation damage means that one of their key areas of application is in devising new medicines, a field of research where the UK is a recognised world leader.

IMPs are the target of many drugs. For example, 40% of human medicines that are currently prescribed target G-protein coupled receptors (GPCRs), a single class of IMPs. The genome sequencing revolution has identified thousands of membrane proteins, many of which have not yet been exploited but are known to be central to pain, cancer, learning, memory, nerve transmission and homeostasis of vital nutrients. (The disruption of blood glucose homeostasis, for example, results in diabetes.) Work in both industry and academia is studying these newly discovered proteins and (as evident from the utilisation of GPCR structural information derived using synchrotrons) is leading to the design of entirely new medicines. We can be certain that structural information has the potential to result in new therapies directed at pain receptors, neurological signals and novel cancer targets, for instance.

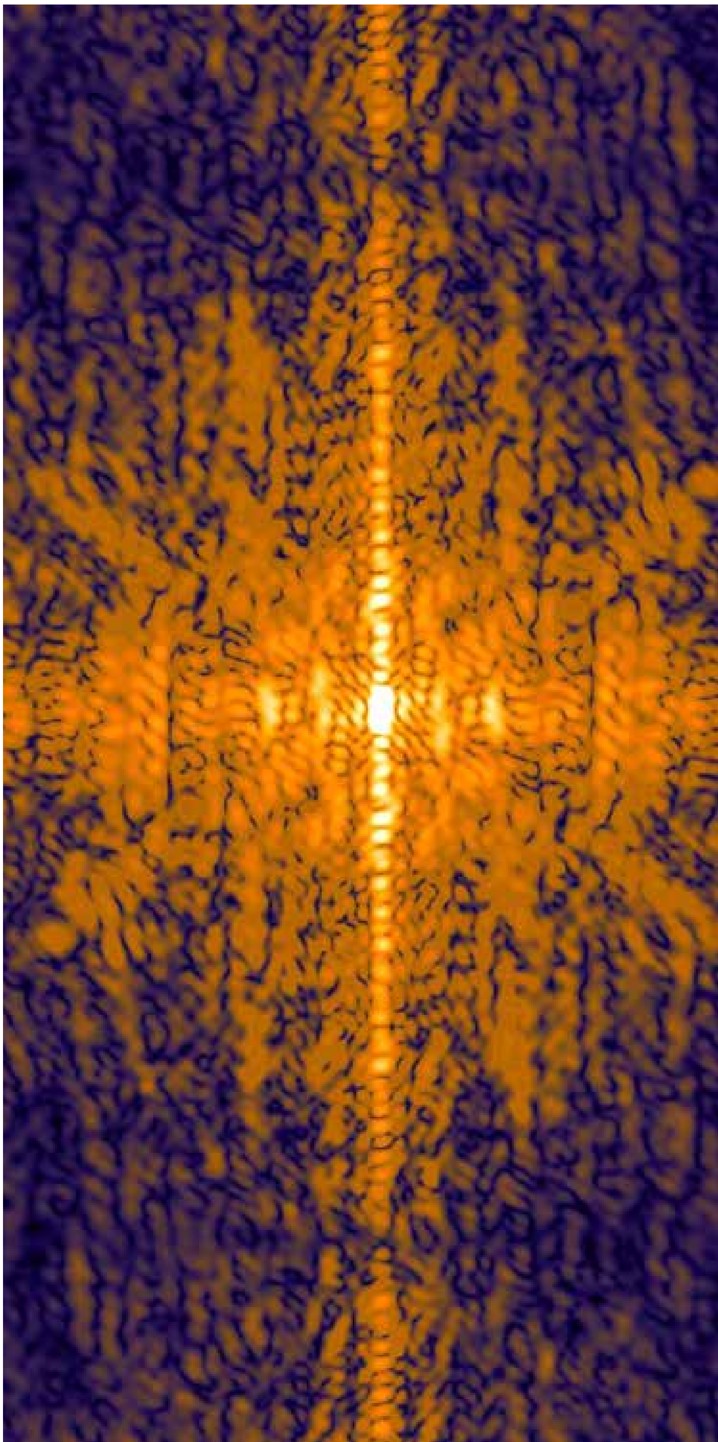
IMP crystals are often very small (i.e. less than 10 microns), making it impractical to image them using electron microscopy (EM). They also tend to be poorly ordered, limiting the ability to describe the protein in atomic detail using current methodologies on account of the radiation damage these would cause. Both of these problems can be overcome by harnessing a FEL to obtain high-quality diffraction data.

4.3. High-Coherence Imaging

The unprecedented coherence of FEL radiation opens the door to high-coherence X-ray imaging techniques, including:

- The study of nucleation – understanding polymorphic outcomes arising from nucleation.
- 3D imaging of biological systems – high-resolution imaging of biological samples between 30 and 300 nanometres in size.

Simulated diffraction pattern. Credit: European XFEL



5. Industrial Impact

FELs offer a whole variety of new scientific opportunities across a wide range of industries, from physical sciences and engineering to pharmaceuticals. Rolls-Royce has already performed experiments at LCLS (see 'Advanced Materials for the Future', p.11) and pharma companies are investigating the use of FELs to study systems only obtainable as nanocrystals. Meanwhile, SwissFEL has been successful in attracting users through industry information days.

Industrial use of new techniques generally follows a pathway where industry collaborates with academic groups and with facilities scientists to develop techniques and methods to the point where paying for beam-time becomes cost-effective. This is the pathway followed by Rolls-Royce at LCLS and it is also exemplified by the development of MX, where there is now extensive use of synchrotron radiation by pharmaceutical companies. Feedback from the Protein Structure Determination in Industry (PSDI) group, however, suggests that these companies currently consider buying beam-time at an XFEL too expensive. Nevertheless, following the example of synchrotrons, sample preparation and delivery techniques at FELs will improve and it is likely that the purchase of beam-time will become cost-effective for particular types of problem.

Fields of industrial research ideally suited to FELs are summarised below.

5.1. Pharmaceuticals

Companies working on drug discovery are very interested in the potential for FELs to determine the structure of molecular materials that can only be crystallised as nanocrystals. This is relevant both to new materials and to new ligands bound to previously solved structures, with FELs' time resolution and special resolution making them ideal for studying samples of this size.

5.2. Chemicals

There is industrial interest in generating direct insights into reaction mechanisms through the use of very rapid pump-probe experiments to observe intermediates. This capability is uniquely available at FELs and has potential for application with both molecular and solid-state systems, mostly in the field of catalysis. In tandem with the high-powered lasers available at the CLF, a UK FEL facility could develop a world-leading position in this sphere.

According to Johnson Matthey, a British multinational speciality chemicals and sustainable chemicals company:

"The ability of FEL technologies to probe the structure of materials over very short timescales and study basic aspects of catalytic mechanisms would be of great value to UK industry. By understanding the fundamental factors controlling catalytic processes, we will be able to improve the performance of industrial catalysts used in a number of areas such as emissions control technologies (e.g. particulate destruction and NO_x removal)."

5.3. Particulates and Pollution

Air pollution by particulates is acknowledged as a serious environmental and health concern. In London, the target of an hourly limit of 200 micrograms of NO_2[1] is breached several days each year. Our knowledge of the chemistry of these particulates is limited, however, with almost all studies based on averages of many particles. Relying on global averages, though, may not help in fully understanding the risk profile of pollution. Evidence suggests that the smaller the particle, the more penetrating and therefore the more disproportionately hazardous it is. Single-particle studies of surface reactions in particulate matter smaller than 2.5 micrometres – and therefore capable of passing into the lungs' alveoli – would provide essential new chemical insights.

The extreme brilliance of XFELs enables scattering and spectroscopy data to be obtained from individual nanoparticles – data that cannot be obtained using synchrotrons. In addition, XFELs make it possible, for particulate systems, to look at representative average properties and the distribution away from the average. This would greatly improve the study of aerosols and air pollution.

5.4. Engineering

There is also industrial interest in using FELs to follow very fast reactions and phase changes in molecules such as those used as fuel additives. This would enable the development of materials that could withstand much more extreme operating conditions in terms of pressure and temperature. Similarly, interest exists in understanding deformation and phase transformation at very short timescales in advanced engineering materials operating at extremes of temperature and mechanical stress. The time resolution of pump-probe FEL techniques makes them ideal for studying such materials.

1 http://uk-air.defra.gov.uk/assets/documents/National_air_quality_objectives.pdf

Advanced Materials for the Future: Rolls-Royce at the LCLS

Titanium and its alloys are widely used in aero-engine manufacture due to their strength and lightness. Zirconium alloys, meanwhile, are used in nuclear reactors as a result of their low neutron-scattering cross-section and their resistance to corrosion. Understanding how such alloys behave when pushed to extremes not only drives innovation in material design and engineering – ultimately, it also delivers the improved materials of tomorrow.

In March 2014, researchers from Rolls-Royce, working with researchers from Imperial College London and the University of Cambridge, were the first industrial users of the LCLS XFEL. They used the Coherent X-ray Imaging (CXI) beamline to study pressure-induced phase transformations, twinning and high-velocity dislocation motion in thin-foil samples of titanium and zirconium and their alloys. Twinning can strengthen alloys and the researchers hoped to secure direct observations of twins forming in samples shocked by an optical laser, with the aim of determining the rate at which they formed and building some understanding of the role of the material chemistry in the twinning process. They also wanted to follow the motion of dislocations and how these multiplied. Previous attempts to obtain this information at synchrotrons had been unsuccessful due to inadequate intensity and temporal resolution.

The intensity of the LCLS X-ray pulses, coupled with the experiment's pump-probe nature, enabled diffraction data to be obtained with exceptional temporal resolution (50 femtoseconds); the micro-focusing abilities of the facility meant that data was obtained from a single grain in the sample. Twin formation was clearly observed, along with pressure-induced phase transitions to the metastable ω-phase.

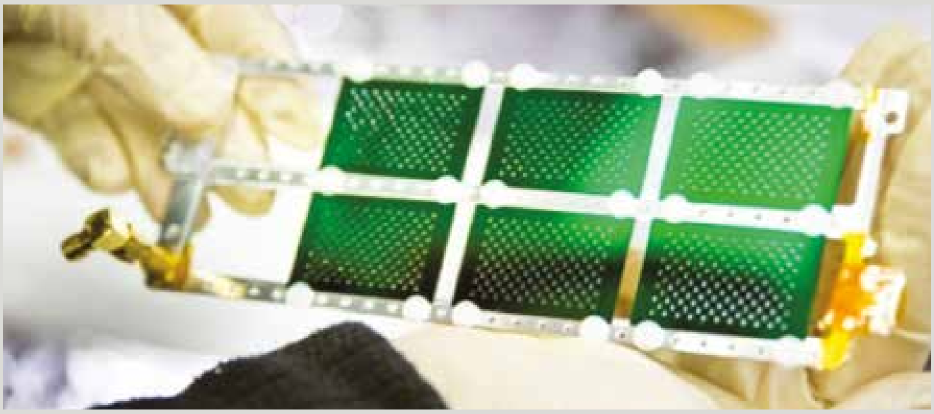


Figure 1: Titanium alloy samples prepared for study on the LCLS. The experiment was designed to produce new insights into the materials' laser-shocked state. (Fabricio Sousa/SLAC)

Not only was it impossible to use a synchrotron to gather data of this kind; the information obtained during the experiment was unique and, coupled with computer modelling over multiple length-scales, will lead to improved predictive capability regarding how such materials work and how they could be improved. Further studies are planned, particularly on the multiplication of dislocations.

6. FELs as a Complementary Tool

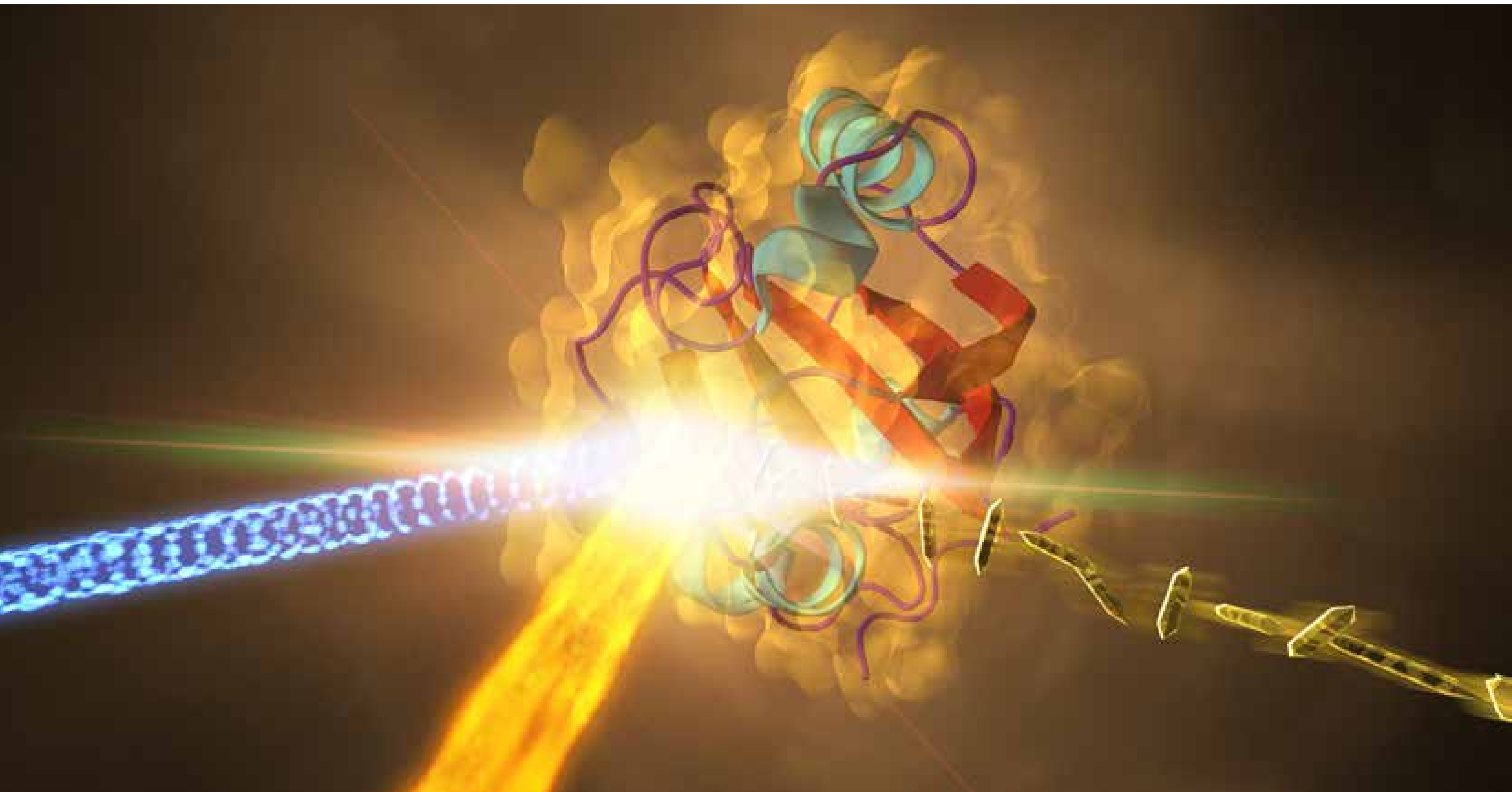
Without doubt, FELs offer unique capabilities that are a wonderful addition to the scientific armoury and complement existing techniques. The ability to disentangle the processes taking place in chemical reactions by 'watching' bond-breaking and bond-making, or to make detailed studies of transient states that may only exist for a nanosecond or less, depends on the extreme brightness that FELs deliver.

But such extreme brightness is not required for studies where data can be obtained over seconds, minutes or hours using synchrotron radiation, neutrons or cryogenic electron microscopy (cryo-EM). FELs, then, complement existing large facilities and will certainly not replace them. Demand in UK science and industry for synchrotron X-rays and neutrons will remain high – for example, in the fields of structural biology and biomedical science. In particular, the presence of 'big pharma' in this country relies on iteration between structural biology and medicinal chemistry to optimise drug discovery, design and manufacture.

Crystallisation of individual proteins followed by X-ray structure determination will continue to facilitate molecular-level insights into mechanisms of action, as well as the utilisation of structural information in drug design. Existing synchrotrons will cater for this need and the vast majority of structural studies will be carried out at synchrotrons for the foreseeable future. This is due to: the ready availability of synchrotrons compared with XFELs; the routine automation they offer for static, crystallised samples (XFEL technology is currently not matched to the necessary throughput rate for the majority of structural studies); and the fact that, for structural studies, synchrotron use is much cheaper and has a faster set-up time.

Turning to EM, protein crystallography – currently the primary method of deriving molecular insights into larger assemblies (>200 kilodaltons) – is being superseded as cryo-EM rapidly develops. The emergence of direct electron detectors has revolutionised the use of EM in the last 2 years; moreover, with no crystals needed and the phasing of structures being more straightforward, cryo-EM will compete with XFELs in this area. Anticipated advances in detector technology indicate that EM is yet to realise its full potential and pharma companies are currently beginning to invest in EM rather than XFEL facilities.

In structural biology, then, XFELs will be used in situations where their capabilities provide a distinct advantage over other techniques – especially where studies require a high level of time resolution, where samples require the ability to outrun radiation damage and for non-homogeneous samples. The wider justification for an XFEL as a resource for structural biology and biomedical science lies in its unique capabilities and this will need to be balanced against developments in the use of EM.



7. A strategic approach for the UK

This strategic approach for developing a UK FEL focuses on two key objectives:

- meeting the UK's immediate XFEL needs using existing and near-future facilities (Section 7.2);
- preparing to meet the UK's long-term needs by constructing an XFEL facility in this country (Section 7.3).

The first step towards realising the UK's potential in the field of FEL science, however, is to grow its XFEL community (Section 7.1).

If the UK wants to maintain its world-leading position in the areas of science described in this document and reap the industrial benefits stemming from this, 'do nothing' is simply not an option. FEL science is advancing fast and, while the UK currently has a competitive position based on its use of facilities in other countries, we must invest in this area to remain at the forefront of this exciting, rapidly evolving field. This will generate many benefits, not just to UK science but also to the wider UK economy. As noted in Section 5, high-tech manufacturing industry (e.g. automotive, aerospace and pharma) is already using FELs to gain competitive advantage and the presence of a UK FEL with unique capabilities would foster such usage. In addition, developing a FEL in the UK may help industries associated with building accelerators, detectors and big-data IT to develop their expertise and capability.

7.1. Strategy for Growing the UK's XFEL Community

The UK currently has a community of 20 research groups using XFELs, comprising around 80 researchers based at 12 different institutions. They have been using LCLS, SACLA, FLASH (Free-Electron Laser in Hamburg) and FERMI (Free-Electron Laser Radiation for Multidisciplinary Investigations) to carry out research into:

- protein structural dynamics;
- nanocrystal protein structures;
- matter at extreme conditions;
- fast modifications to metals;
- time resolution of prototypical photo-chemical reactions (isomerisation and the role of conical intersections);
- ultrafast electron dynamics in molecules.

Interest in the advantages of using FELs is growing and needs to be encouraged. A fundamental aspect of the strategy outlined here is the highlighting of the immediate action needed to support further development of the UK XFEL community. This could be achieved by:

- further investing in current and near-future facilities internationally to support access for users from the UK;
- attracting new researchers by funding training opportunities such as studentships, travel grants, targeted fellowships/calls and a cross-Research Council Centre for Doctoral Training (CDT);
- targeted project funding from the relevant Research Councils;
- re-engaging communities associated with previous proposals for UK FEL facilities.

Such measures would enable the community to grow so that, in 5 years' time, there would be at least 50 active groups of FEL users in the UK and one in every research-intensive university. Currently, all of these universities are likely to have users of other facilities (e.g. synchrotrons and neutron sources) but not necessarily FEL users. As noted in Section 3.3, community growth to the levels envisaged would signal that FEL use had become a significant priority for UK research communities. Having a larger, better established XFEL user community would also make it easier to define more accurately, and secure evidence regarding, the UK's research and innovation requirements. This would allow a well-informed debate covering key issues such as: future priorities; how best to support UK researchers; and future decisions on optimum design specifications for a UK XFEL.

7.2. Strategy for Meeting the UK's Immediate Needs

The UK plans to contribute approximately £30 million in capital funding to the construction of XFEL.EU (i.e. 2.5-3% of total construction costs). In addition, the UK is part of two consortia:

- The Helmholtz International Beamline for Extreme Fields (HIBEF) consortium: the UK's contribution is DiPOLE (Diode Pumped Optical Laser for Experiments), whose construction has been funded by STFC and EPSRC at around £4 million each, with operating costs yet to be confirmed.
- The Serial Femtosecond Crystallography (SFX) beamline consortium: the UK is to contribute £5.65 million to this beamline through BBSRC (the Biotechnology and Biological Sciences Research Council), MRC (the Medical Research Council) and the Wellcome Trust. To guarantee access for UK users, the UK will have to contribute to the €100 million per year running costs; the level of this contribution would determine the level of UK access.

Once XFEL.EU becomes operational in 2017, it will have the capability to address the majority of key scientific challenges that would benefit from FEL access, due to its ability to provide both hard and soft X-rays at a high repetition rate (see Table 1, p.16). This high-repetition-rate hard X-ray capability will provide a significant advantage over other facilities (including LCLS-II) for applications such as hard X-ray spectroscopy and crystallographic structural imaging (see Annex A: Section 9.1, p.22, and Section 9.2, p.26). Although XFEL.EU will have the capacity to support initial UK needs, it will not however have the capacity to support a growing UK community of FEL users.

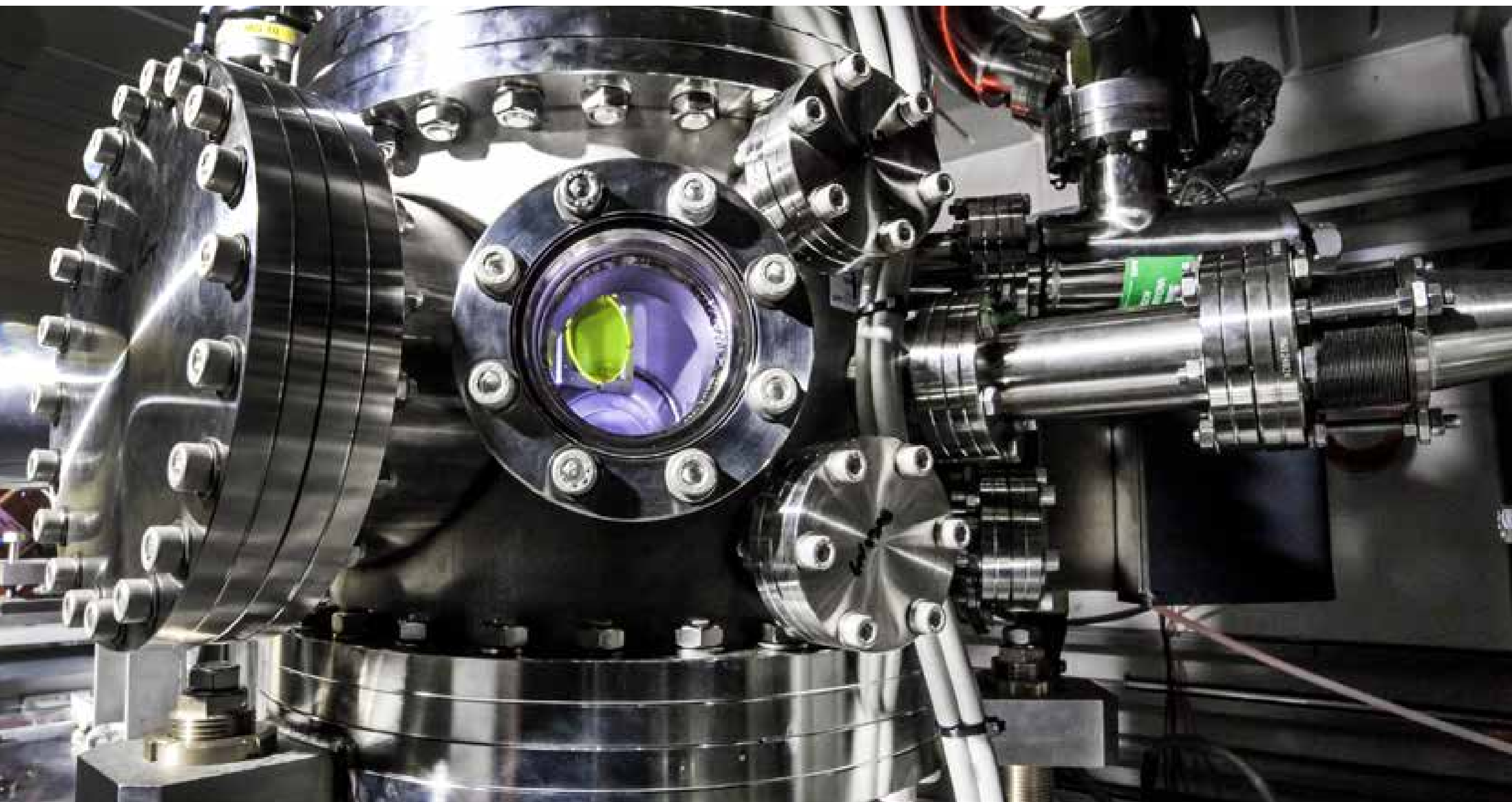
In 2014, the UK had around 30 user visits to XFELs. (A user visit is defined as one individual or member of a research team working at an XFEL for the duration of an experiment.) The majority of these were at LCLS, where 2.6% of the user visits were from the UK. Looking ahead, with regard to XFEL.EU:

- Once operational, XFEL.EU will have 200 days of user operation per year, with 6 teams each working a 12 hour shift every day (through careful scheduling of experiments).
- A typical team could have 10 members and a typical experiment could use 5 days of beam-time.
- This means there could be a total of 2400 user visits at XFEL.EU each year (6 x 200 x 10 / 5).

The level of access available to UK researchers will ultimately be related to the level of funding from the UK:

- For planning purposes, it is likely that a level of access one to two times that of the UK's contribution to XFEL. EU's capital costs (2.5-3%) could be secured, which would give the UK between 2.5% and 6% of XFEL.EU beam-time.
- Assuming the middle value of this range (4.25%) gives approximately 100 user visits a year (i.e. 4.25% of 2400). Added to the current level of 30 user visits to LCLS, this would give the UK a total of around 130 user visits to XFELs per year.

As highlighted earlier, experience with similar facilities shows that demand increases rapidly once a facility opens. Figure 2 below shows that, at LCLS, the percentage of proposals scheduled (indicated by the red line) fell by half between October 2009 and March 2014. By contrast, Figure 3 shows that, after its first year, the percentage of proposals scheduled at the Diamond Light Source (again indicated by the red line) remained between 50% and 60%. This is thought to be because XFELs are a relatively new type of facility; as more science is demonstrated on them, more researchers become aware of the potential benefits and want to apply for access. When Diamond started operating, on the other hand, most researchers would already have been aware of the benefits of using it.



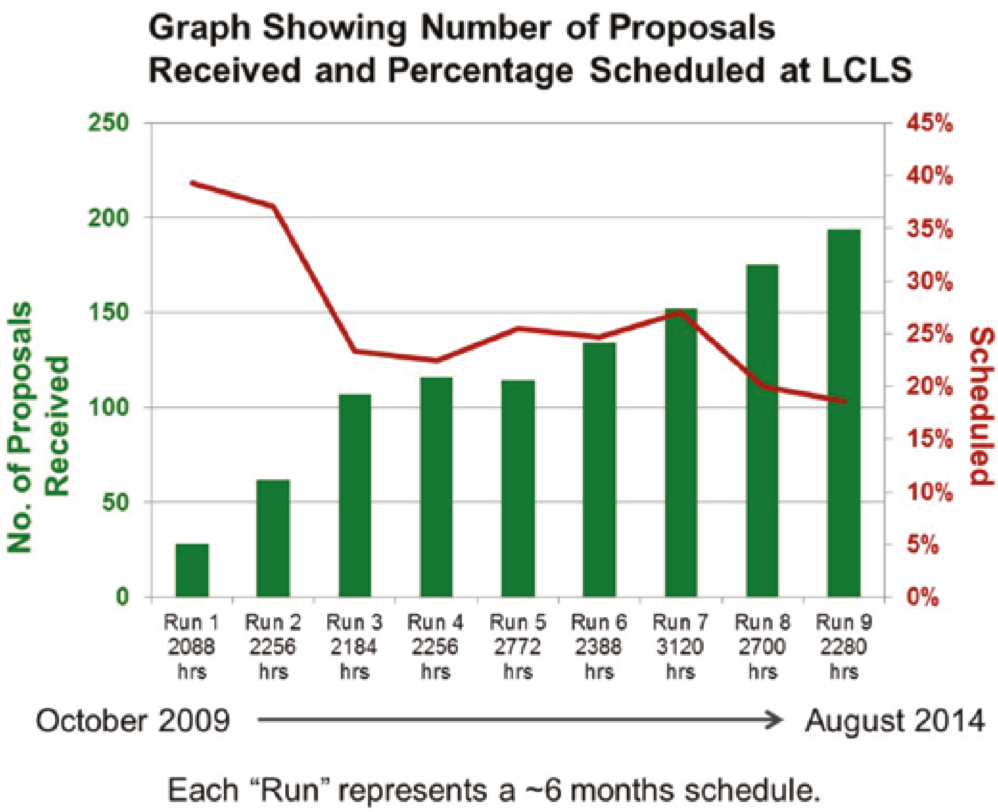


Figure 2: Proposals received and scheduled at LCLS

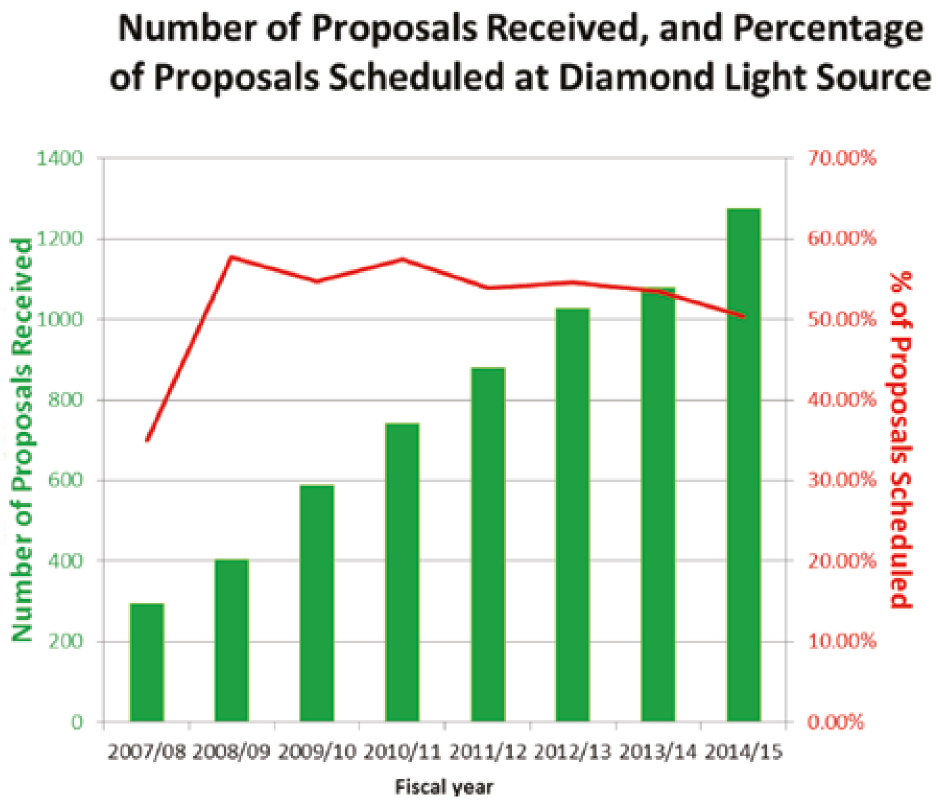


Figure 3: Proposals received and scheduled at the Diamond Light Source

The ukfel.org response[2] to the 2014 UK government consultation on proposals for long-term capital investment in science and research[3] was supported by 400 signatories. This reinforces the thesis that the group of potential XFEL users in the UK is much larger than the current community of users. Figure 2 shows that the number of proposals received annually at LCLS increased from 28 to 194 over a period of four and a half years. If UK demand for access to XFEL facilities grew at roughly the same rate, then, even starting from the 2014 level of 30 user visits a year, it would only take until 2020 for the UK's capacity requirements to exceed the 130 user visits available at LCLS and XFEL.EU (i.e. 3.2 years at an annual increase rate of 54%). Similarly, if UK community grew to the 50 UK groups mentioned in section 7.1, each demanding 2 experiments of 5 days per year, with 4 people per group, the UK would require 2000 user visits. This significantly exceeds the available user visits.

To meet the intermediate requirements of its growing XFEL community, the UK would need to invest further in XFEL.EU and other existing and near-future facilities (as shown in Figure 4, p.17), with the ambition of building on its influence and its participation in science and instruments at LCLS, PAL-XFEL, SACLA and SwissFEL. A limitation on FEL beam-time access in the short term would be a major challenge to the growth of the UK FEL community. These steps could therefore allow the UK to increase its level of access, although determining by how much would require negotiations with the FEL facilities.

As well as seeking to increase available *capacity*, it will be necessary to ensure that the UK has access to the *capabilities* it needs. While XFEL.EU can provide bursts of radiation at a repetition rate of 27 kilohertz, there is a gap of around 0.1 seconds between each burst. The design of LCLS-II allows elimination of these gaps. This means that, for areas of science where a high-repetition-rate constant stream of pulses is needed (e.g. trARPES, RIXS and combustion diagnostics), LCLS-II will be the best facility.

The exact specifications of a UK facility will be developed over the next four years based on the emerging community need. While the ideal source would produce high energy X-rays (up to 10keV) at a high repetition rate (>100 kHz), with current technology this is only deliverable using superconducting RF and at relatively high capital and operations cost. In developing the specifications for a UK FEL the tradeoffs between cost and performance will need to be considered. It will make sense to consider a number of options; one of these options is likely to be a SwissFEL-like design, but with beamlines tailored to UK requirements. This would be a normal conducting X-ray FEL, operating at energies up to 10keV, with a repetition rate of around 100Hz.

Any UK financial involvement with LCLS should focus on providing support to UK researchers using it; as the facility is funded by the US Department of Energy, the UK cannot become a shareholder. This places a limitation on UK access, which means LCLS can only provide part of the solution to the capability and capacity needs of a growing UK community of FEL users.

Key parameters of major existing and near-future XFEL facilities are summarised in Table 1.

Facility	Energy (keV)	Repetition Rate (Hz)	Minimum Pulse Length (fs)	Time Synchronisation to Optical Laser (fs)	Operational from Year
XFEL.EU	0.23-29	27,000	<10	10	2017
LCLS-II	1-25				
1-5	120				
1,000,000	1	1	2020		
LCLS	0.25-11.3	120	<5	50	2009
SwissFEL	0.18-12.4	100	11	<10	2016
SACLA	4-20	60	30	<10	2011
PAL-XFEL	0.27-20.6	60	60	<10	2016

Table 1: Comparison of key parameters at existing and near-future XFEL facilities worldwide

1 http://ukfel.org/wordpress/wp-content/uploads/2014/06/UKX3.pdf

2 https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/321522/bis-14-757 -consultation-on-proposals-for-long-term-capital-investment-in-science-and-research-v2.pdf

XFEL.EU

- The best facility for the majority of the UK user community's needs.
- The UK plans to contribute around £30M (2.5-3% of total construction costs), with a further £13.5M through consortia.
- More funding is required to increase UK access.

Meeting the UK's immediate needs

LCLS-II

- This upgrade to the XFEL at Stanford University will improve wavelength range, repetition rate and pulse length.
- The best facility for science requiring high average X-ray power and a high-repetition-rate constant stream of pulses.
- Funded by the US Department of Energy – becoming a shareholder is not possible, so we will consider how best to support UK researchers. there.

SwissFEL / SACLA / PAL-XFEL

- These are XFELs in Switzerland, Japan and South Korea.
- Investment to secure access to these facilities may be beneficial if the UK's capacity requirements are not met by XFEL.EU and LCLS-II.

Figure 4: Meeting the UK's immediate needs using existing and near-future XFEL facilities

7.3. Strategy for Long-Term Access to FEL Facilities

As outlined in Section 7.2, maximising the UK's opportunities for access to existing and near-future XFEL facilities may allow about 130 user visits per year; but the UK's required level of access is likely to exceed this level by 2020 and expand to exceed 2000 user visits. This growth will take place against a backdrop of increasing worldwide demand for FEL access, but with limited plans – and currently only in Sweden and China – to build FELs in the future. The obvious conclusion is that opportunities for the UK to secure access for its growing FEL user community will reduce as worldwide demand competes for diminishing time on existing and new facilities.

In the long term, then, the UK's capacity requirements would be best served – and may perhaps only be possible to meet – by the construction of a UK FEL. Such a facility would also benefit the UK's research and innovation communities by fine-tuning capabilities and technologies to deliver advantage for highest-priority science areas: for example, ensuring that better optical lasers are available to improve the ability to deliver pump-probe experiments, investing in better spectrometers or detectors, putting polarisation control in place, or introducing improved timing capabilities. Aside from any capability advantages, constructing and operating a UK FEL facility would also provide a significant opportunity to develop important skills and technology within UK academia and industry in areas such as big data and instrumentation (see Annex B: Underpinning Technologies p.29).

As with the development of any new facility, the technology needs of a UK FEL far outstrip current capabilities. So the decision to design, construct and develop such a facility would provide a tremendous boost to the development of skills and technology that would inevitably benefit the construction and operation of other large science facilities in the UK – for example, delivering improvements in high-performance X-ray imaging that would benefit the Diamond Light Source – as well as boosting the commercial application of emerging technologies in UK industry.

Why Should the UK Build a Dedicated FEL Facility?

- There is a significant opportunity for areas of UK science to develop and maintain a world-leading position and for strategically important sectors such as pharma, transport and energy to generate competitive advantage.
- Current and near-future international facilities do not have the capacity to support the growing UK user community – user visits are expected to exceed the available 130 user visits per year by 2020.
- Facility specification could be tailored to match the specific capability needs and strengths of the UK's research communities and UK industry in a way that would be impossible through collaboration with other countries.
- The UK could realise a unique capability through the co-location of a FEL with high-powered and high-energy laser facilities, unmatched by any equivalent facility in the foreseeable future.
- Such a facility would provide maximum opportunities for developing the UK's capabilities in the following underpinning technology areas: accelerators, detectors, lasers, simulation, control, data acquisition, data analysis, data storage, theory, target design and manufacture, and diagnostics.
- Significant industrial opportunities exist in all of these areas.
- Building a dedicated FEL facility would improve the UK's ability to construct and operate other large science facilities

The time taken from fully committing to the construction of a UK FEL facility to it becoming operational is likely to be at least 6 years. The final decision on whether to build an XFEL in the UK (and to what specification) is unlikely to be taken before 2020, following further assessment of the user community size, the science case and a business plan.

To prepare for this decision, the following actions are recommended in parallel with the development of the user community (also see Figure 5, p.20):

1. Initiate a programme to define the required specification and prepare preliminary costings.
2. Develop a fully coordinated FEL R&D programme, building on existing expertise in the following areas:

a. accelerators;

b. detectors;

c. lasers and auxiliary light sources;

d. diagnostics;

e. sample environment and target delivery;

f. simulation, control, data acquisition, data analysis and data storage.

3. Strategically plan the development of the skills base required to deliver the necessary technologies.

The CLARA (Compact Linear Accelerator for Research and Applications) test facility at Daresbury Laboratory is being developed as a FEL test facility. It should be used for developing aspects of the accelerator technology that would underpin a UK FEL such as radio frequency (RF) structures, single-shot diagnostics, timing and synchronisation. The developments required in each area of underpinning technology are covered in greater detail in Annex B: Underpinning Technologies (p.29).

The exact specifications of a UK facility will be developed over the next 4 years based on the emerging needs of the user community. The ideal source would produce high-energy X-rays at a high repetition rate, taking into account the latest technologies. In developing the specifications for a UK FEL, the overall cost – including construction and running costs – and a number of options for source specifications will be considered.

One of the options is likely to be a SwissFEL-like design, though with beamlines tailored to UK requirements. This would be a normal conducting XFEL operating at energies up to 10 kiloelectronvolts, with a repetition rate of around 100 hertz. Capable of addressing the majority of the key scientific challenges relevant to FELs, such a facility would complement other international facilities. The small number of 'signal-hungry' applications (e.g. RIXS and non-linear X-ray spectroscopy) would continue to be delivered via UK access to XFEL.EU (through our subscription) or LCLS-II.

The costs of constructing and commissioning an enhanced SwissFEL-like facility are estimated to be around £500 million, with annual running costs of £25-50 million for two to three beamlines. SwissFEL will operate with two beamlines and XFEL.EU will initially operate with three beamlines, with an upgrade to five proposed for 2018-20. As accelerating gradients are gradually increasing, for the same cost a facility built in 5 years' time could have a higher energy than current facilities.

Co-location with Lasers

Much of the chemical and condensed phase science envisioned at an XFEL (including plasma and extreme conditions – see p.24) requires state-of-the-art ultrafast, high-powered, high-energy auxiliary laser sources well synchronised to the X-ray pulses.

While such lasers are available in a number of central laboratories worldwide that specialise in high-power laser development, none of these laboratories are co-located with any existing (or planned) FELs. The UK has a world-leading capability in high-power laser science, pioneered over decades at the CLF and the Atomic Weapons Establishment (AWE). In particular, the CLF's development of high-repetition-rate kilojoule-class lasers will provide the UK with a unique capability to study laser plasma physics. An XFEL co-located with the CLF's petawatt and high-energy laser facilities on the Harwell Campus would provide the UK with unique, world-leading facilities for creating and probing matter at extreme conditions – and unmatched by any equivalent facility anywhere in the world for the foreseeable future.

The technologies associated with the design and construction of FEL facilities are developing rapidly and there is an opportunity to learn from the construction and commissioning of near-future facilities. This means the UK could build an XFEL whose performance is significantly superior to that of the current generation of machines. As discussed above, it would also be possible to incorporate a capability advantage by focusing on the UK's particular needs.

Once an ecosystem of national facilities is in place across several countries, it may be desirable to arrange formal partnerships and collaborations. International researchers can already apply for access to UK facilities and a reciprocal arrangement exists for facilities in other countries. Consideration of international partnerships and the potential for the UK to host an international facility will be undertaken at an early stage.

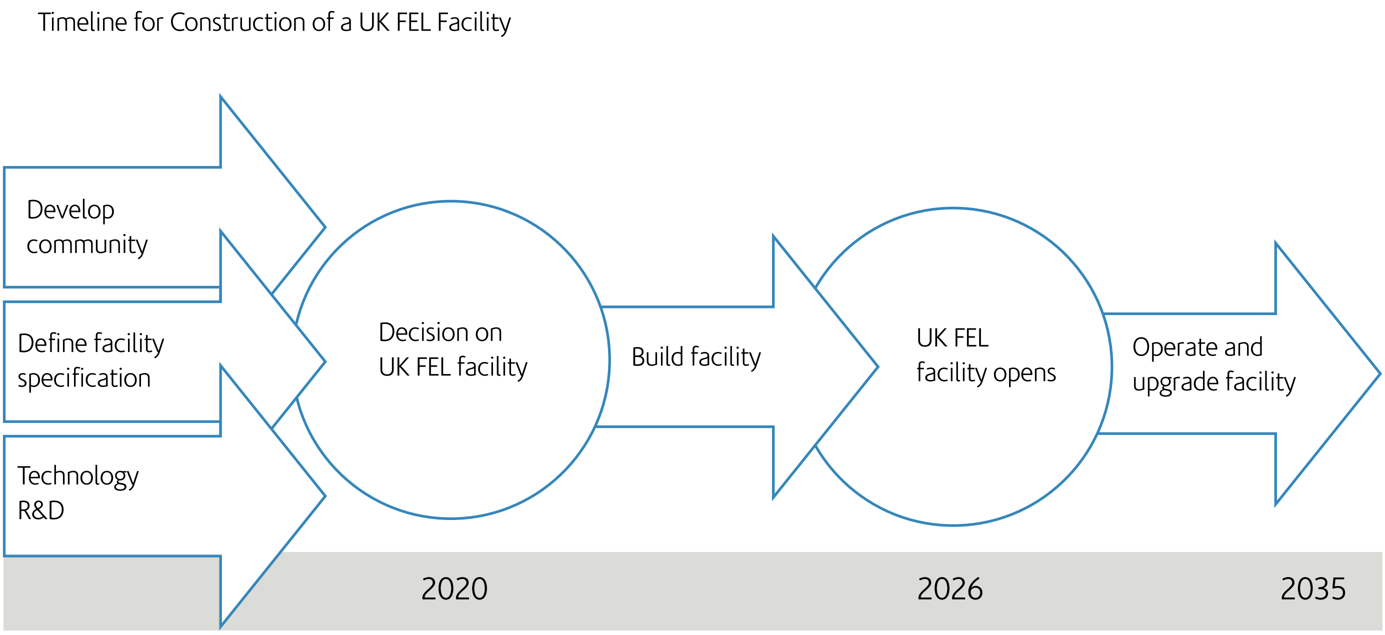
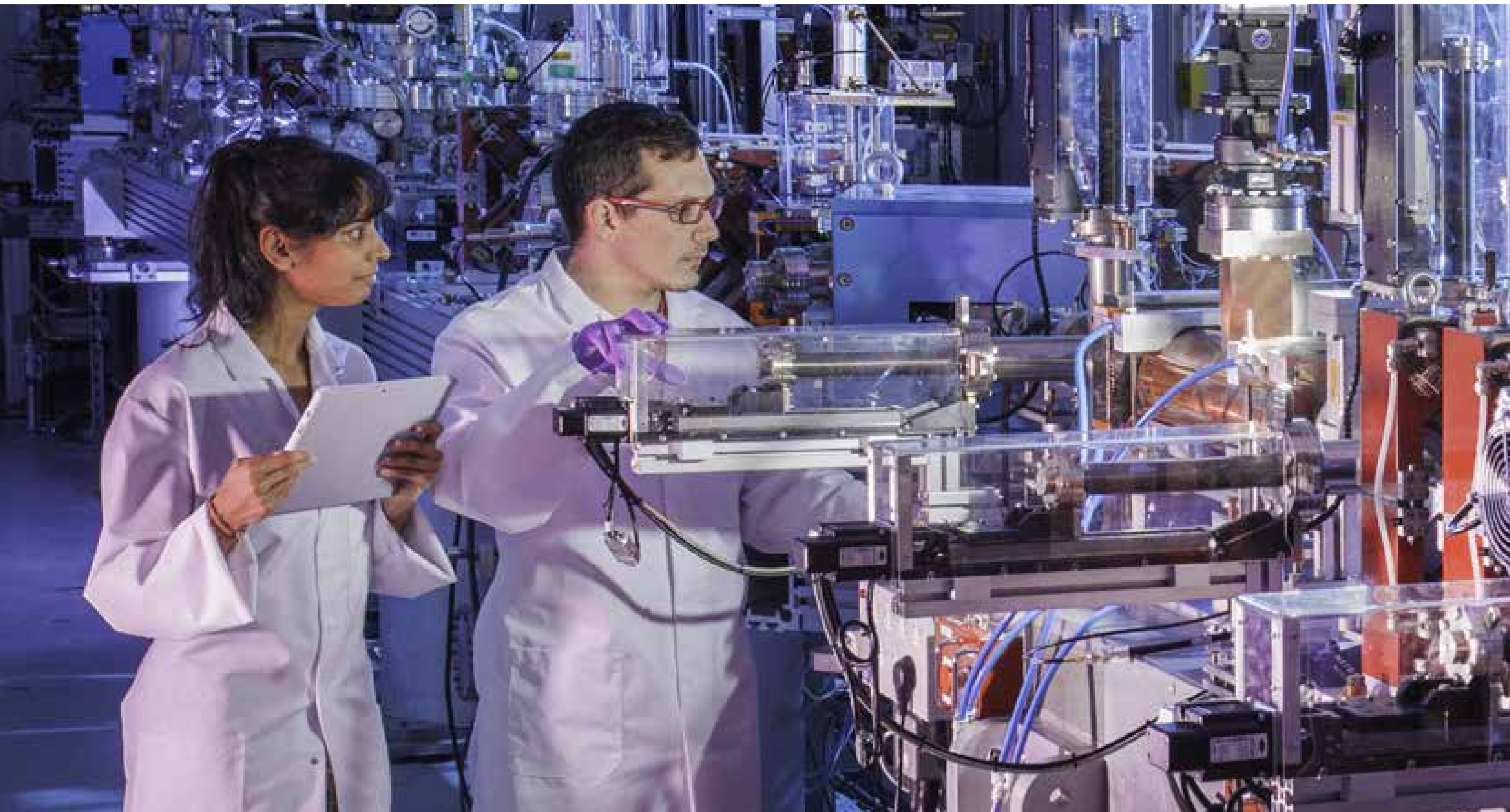


Figure 5: Timeline for construction of a UK FEL facility



8. Conclusions

FELs offer very bright, ultra-short pulses of light which allow atomic-level measurements of structure and function with unprecedented time resolution. Such facilities are already allowing UK frontier science to develop and maintain a world lead, while strategically important sectors such as pharma, transport and energy are using FELs to generate competitive advantage. The strategic approach set out in this document recommends routes to better equip the UK user community to exploit current FEL capacity worldwide.

We will benefit from our commitment to XFEL.EU and should look to increase our engagement with this facility, although we should recognise that it will be insufficient to meet the UK's medium-term or long-term capacity requirements. The UK should also explore how best to facilitate access to LCLS-II (USA), SwissFEL (Switzerland), SACLA (Japan) and PAL-XFEL (South Korea).

Building a UK facility would lead to the advancement of UK science, the development of competitive advantage for the UK's industrial base and the development of key technology and skills of benefit to the high-tech industrial sector and other large science facilities in the UK.

In the long term, the UK's capacity requirements could be best served by constructing a UK FEL facility. Its specification should be designed according to the capabilities that the UK needs, taking advantage of the unique opportunity to co-locate an XFEL with the state-of-the-art ultrafast auxiliary laser sources currently located on the Harwell Campus. This would equip the UK with leading-edge facilities for creating and probing matter at extreme conditions, unmatched for the foreseeable future by any equivalent facility anywhere around the world.

In 2020, following completion of the outline design work and the significant prototyping work required, STFC and the UK would be well placed to take a decision on whether to build an XFEL in this country and what kind of machine to construct.

To restate a key message: 'do nothing' is not an option. FEL science is advancing rapidly, the UK already has a competitive position based on its use of FEL facilities elsewhere – and we must invest in this area in order to remain competitive on the global stage.

9. Annex A: FEL Science

Some of the key science challenges that exploit each of the unique capabilities of FELs are discussed below.

9.1. High Time and Spatial Resolution

When combined with optical lasers, FELs offer the possibility of making time-resolved pump-probe experiments with atomic spatial resolution and femtosecond temporal resolution. Once the optical laser has initiated a process/reaction, or created the desired state of matter, the FEL beam can be brought in after a delay that can vary from 10s of femtoseconds to nanoseconds, capturing a snap-shot of the sample at that time. By making repeated measurements at different delay times, a "movie" can be made from the individual snap shots.

Key examples of science challenges that require the time and spatial resolution that FELs provide are:

- Bond Making and Bond Breaking. Understanding the intermediate steps in a chemical reaction is hugely important in a range of disciplines from catalytic chemistry to life sciences and pharmacology. This could lead to the development of novel catalysts, the design of new drugs mimicking transition states of biological catalytic processes, and could potentially open up new synthetic capabilities in organic and inorganic chemistry. At the core of any chemical reaction are the changes of geometric and electronic structure, occurring on timescales from picoseconds (for larger-scale geometric changes) down to attoseconds (for electronic dynamics). X-ray FELs give pulses of X-rays that are as short as 1 fs (or less) and so can access all the relevant timescales.

  The Challenge: to develop a firmer conceptual understanding and more accurate theory of the key events in chemical reactions and molecular interactions as a function of time. The associated knowledge and techniques will then be applied to the more technologically oriented challenges highlighted below.

  How FELs Will Solve it: the few-femtosecond (fs) X-ray pulses from FELs allow a "movie" of a chemical reaction to be created with few or even sub-femtosecond snapshots (using time resolved pump-probe experiments). While X-rays (in general) allow structure determination to the sub-Angstrom scale (via diffraction and X-ray spectroscopy) and the local electronic state in the vicinity of a given atom (by X-ray spectroscopy), no existing (non-FEL) X-ray source can give us the time-resolution and peak brightness to permit the pump-probe measurements needed to resolve chemical dynamics on all time scales. Synchrotron X-ray pulses are too long (by a factor of 10,000 or more) to resolve the few fs timescale pulses of the electronic and fast nuclear component of bond making/breaking. Laser based X-ray sources are still at an early stage of development: HHG sources give excellent temporal capability (few 100 attoseconds) but are not bright enough for most pump-probe applications and in any event only offer low photon energies (< 0.3 keV). Other laser based sources (Compton and betatron) rely on high intensity laser sources and these currently lack the high repetition rate and high average power to compete with FELs (they are many of orders of magnitude away from what is already available at X-ray FELs with as yet not clear technological path to catch up let alone compete with the next generation like XFEL.EU and LCLS II).

  There is a large and energetic UK community of around 20-30 groups in this area of research, with a lot of activity in laser based experiments and some in X-rays (including the chemical dynamics activity in the Research Complex at Diamond).

- Understanding the Dynamics of Structural Changes in Membrane and Soluble Proteins. FELs can be used to capture the structural dynamics of biological systems in real time, allowing correlation between the reaction chemistry and protein structural changes. Success in this area will enormously improve our understanding of how key proteins work and how to manipulate their activities for clinical and commercial benefit. For example: making designer enzymes, better understanding drug-target interactions, and making nano-machines and motors.

  The Challenge: Understanding and treating human, animal, and crop diseases and infections is a well-recognised challenge. Often both understanding the cause of the problem and devising treatments depend upon determining the three dimensional structures of key membrane and soluble proteins, and understanding dynamic changes within their structures.

  How FELs Will Solve it: The unique time resolution of FELs means they can be used to capture the structural dynamics of biological systems in real time. They are the only type of facility that gives access to all of the interesting time-window between 50-100 fs and a few ps, allowing correlation between the reaction chemistry and protein structural changes.

The UK is currently strong in this area. There are groups that focus on systems biology and dynamical studies at the University of Manchester, the University of Bristol, UCL, and the University of Kent. Many of these are involved in BBSRC Networks in Industrial Biotechnology and Bioengineering (NIBB), including Biocatnet, BioProNET, and Metals in Biology. There are also a number of structural biology groups that do dynamics studies on their system in particular. The UK's Centre for Process Innovation and several start-up companies are involved in this type of work.

A Cleaner Atmosphere

Combustion is likely to remain our primary source of energy for electrical power generation and transportation for many decades. Research has shown that it is a complex process, involving chemistry and turbulent flow dynamics (see Figure 5). The ability to capture a "3D movie" of the chemistry and particulate formation going on in real combustors is urgently needed to optimise their design for the reduction of emissions of CO_2, NO_X, and other harmful gases and particulates.

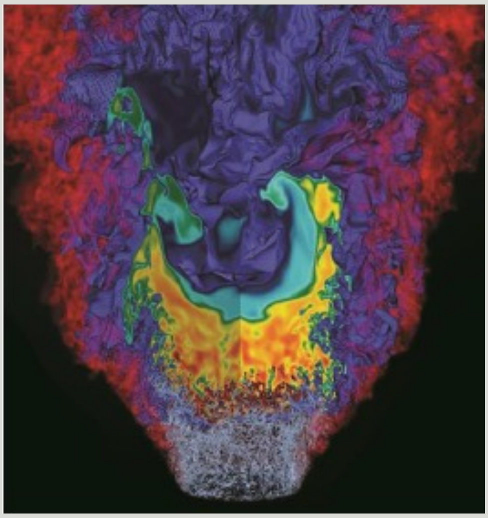


Figure 6 - A computer simulation of the spatial distribution of N_2O, NO and OH species in a hydrogen flame.

A high repetition rate X-ray FEL would permit the processes of combustion to be stroboscopically imaged with high spatial resolution and chemical specificity using X-ray techniques such as resonant inelastic scattering (RIXS) and X-ray coherent anti-Stokes Raman scattering (XCARS). These snapshot techniques require high photon flux for a "single frame", i.e. $>10^{10}$ photons in a single pulse in a narrow spectral interval. High repetition X-ray FELs (such as the planned LCLS II) uniquely offer the single shot brightness along with the 0.1 to 1 MHz repetition rate for stroboscopic imaging demanded by this science.

Chemical and physical processes at individual aerosol and nano-particles (e.g. soot) are believed to play crucial roles in atmospheric chemistry. Soot particles in the environment can pass through the lungs and the blood to tissue, leading to serious health problems. Very little is known about these aerosols and particles because they are so hard to study in detail with current technology, and their properties cannot be simply scaled from larger well studied assemblies. Recently, however, small angle X-ray scattering (SAX) at LCLS has been used to image individual nanometre-sized particles of soot whilst in flight. These structural methods can simultaneously be applied with the time resolved chemical probes of RIXS and XCARS to uncover for the first time the details of the chemistry and physics of individual aerosol and soot particles in the atmosphere. This will give powerful new insights into the chemical and physical processes at the interfaces of the atmosphere e.g. with the oceans.

- **Warm Dense Matter (WDM)**. WDM is of central importance in fusion science, laser plasma science, laboratory astrophysics, and in modelling the cores of large planets and exoplanets. It lies between the liquid and plasma states. WDM is too dense to be described by weakly-coupled plasma physics, yet too hot to be described by condensed matter physics.

  The Challenge: to create WDM states in a wide range of materials within a laboratory environment and study its formation and properties.

  How FELs Will Solve it: WDM can be created on short timescales using either high power (short pulse length) optical lasers or soft X-rays from a FEL. Using soft X-rays from a FEL to do the heating creates a much more uniform heated state as the X-rays have much greater penetration into the sample than optical light, due to the absorption length of optical light being so short. Once WDM is created it expands and cools very rapidly, so can only be studied with an extremely rapid experiment. The pulses of 10s of femtoseconds from an X-ray FEL make this possible: they can be used to perform ultra-fast X-ray spectroscopy and scattering to probe the local structure, density and other physics properties. They can also be used to study the structural dynamics of the solid-to-plasma phase transition.

  The UK community in this area is strong, with key groups based at University of Oxford, Imperial College, and Queen's University Belfast.

Plasmas and Extreme Conditions

Plasmas are often referred to as the 4th phase of matter – in addition to solids, liquids, and gases. They exist over a very wide range of pressures and temperatures, and are the most abundant form of ordinary matter in the Universe. High-powered lasers can compress and heat materials to the extreme pressures and temperatures found otherwise only in the cores of planets, or within inertial fusion fuel targets. Dense plasmas (those as dense as solids) are particularly difficult to study, but can be created for a few nano seconds using high-powered lasers.

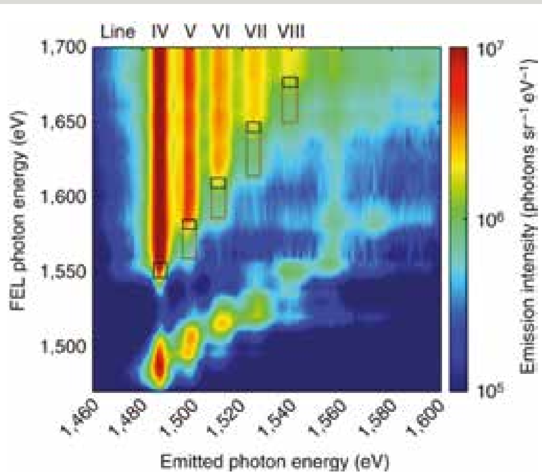


Figure 7 - Experimentally measured Kα intensities from a solid-density Al plasma as a function of the spectrally resolved emission (horizontal axis) and XFEL X-ray pump photon energy (vertical axis). Emission from Al charge states 4+ to 8+ are marked.

Techniques such as X-ray scattering, spectroscopy, diffraction, Thompson scattering, X-ray emission (see Figure 6) and absorption spectroscopy, and phase contrast imaging allow the structure, density, atomic coordination, and electronic structure of dense solid and dense plasma states to be determined in situ. To do this on states that exist for only a few nanoseconds (and to study transitions between the solid, liquid and plasma states) requires short pulses of ultra-bright X-rays, well synchronised to the powerful optical lasers that create the states of interest.

Research at the LCLS has provided wholly new insights into the mechanisms and timescales of structural phase transitions, on melting and recrystallization in solids, on the strength of materials under dynamic loading, and on the transition to the dense plasma state. These studies have utilised the unprecedented brightness of the LCLS, and its ability to synchronise the X-ray and optical lasers to make "movies" of the transitions on nanosecond and sub-nanosecond timescales. The techniques being developed have applications in the development of more durable materials (e.g. for shielding to protect satellites from high-speed space debris), and stewardship of nuclear stockpiles.

Studies of material response to shock compression are in their infancy at the LCLS, but the quality and clarity of the results means that it will already forming a key scientific programme at XFEL.EU from 2017. UK researchers will play a central role in such science, with the UK providing the high-energy high-repetition rate optical laser that will be used to create a wide range of extreme states of matter.

- **Light-matter Interactions in Semiconductors and 2D Materials**. Time resolved X-ray measurements of strained semiconductor nanostructures using FELs will help to understand atomic motion and migration during and after switching events.

  The Challenge: further improving the science underpinning current data processing and transmission paradigms and obtaining a microscopic description of what occurs in devices for quantum state manipulation. For example, more rapid aging of all types of devices is an increasing concern as devices shrink and have higher switched energy densities.

  How FELs Will Solve it: pump-probe time-resolved X-ray spectroscopy using the femtosecond pulses from X-ray FELs will permit atomic level understanding of the electronic states in the material. The timescales of the atomic motion and migration are too short to allow synchrotrons to be used for this, and it is extremely challenging using laser based sources due to the limited photon energy range and low photon flux.

Microporous Catalysts used in Petrochemical Catalysis, Selective Oxidation and Environmental Catalysis

These have been the subject of several decades of investigation due to their industrial importance, and because their crystallinity has allowed detailed information to be obtained on active site structures in several cases. Our knowledge of mechanisms is very limited and to a large extent based on computational modelling. Examples of such catalysts include:

- the copper based de-NOx zeolitic systems used in auto-exhaust catalysis, where we know that the extra-framework Cu ions provide the active site but have no definitive knowledge of the de-NOx mechanism;
- the titanium substituted zeolites (e.g. the industrial TS-1) used in oxidation catalysis where the intermediate created by the coordination of peroxide species to the titanium has been determined (as shown in Figure 8), but there is no experimental understanding of how the activated oxygen in this species effects oxidation of (e.g.) alkenes to epoxides.

Catalysis is a key area of contemporary chemistry and chemical engineering which poses major fundamental scientific problems, and is a growing area of research in EPSRC's portfolio. It also underpins a large component of manufacturing industry with a potential economic impact of multi-billion pounds. To design new processes and develop new catalysts we need to improve our understanding of the molecular basis of catalytic processes. A scientific consensus about the molecular origin of catalytic activity remains elusive for many technologically important classes of catalyst materials.

For example: The industrial Cu/ZnO catalyst is used worldwide in the conversion of syngas to methanol. Despite intensive study using both computational and experimental methods, there is no detailed understanding of the mechanism of this key reaction.

The time resolution of FELs relative to other types of facility means that they are uniquely able to capture a "movie" of catalytic reactions. This will lead to a significant improvement in our understanding of the molecular transformations that determine catalytic action, starting with light driven reactions and then progressing to more general catalytic processes.

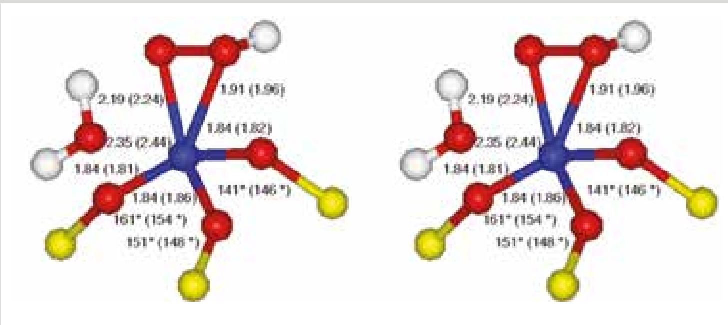


Figure 8 - Peroxide coordinated active site in Ti substituted micro/meso-porous catalyst. Calculated and experimentally determined configurations are compared.

- **Understanding and Controlling Interactions in Correlated Quantum Systems.** In future devices for fast high-capacity data processing, the underpinning processes in both storage media and transducers will operate on a sub-nanometre spatial scale and a femtosecond time scale.

  The Challenge: a greater understanding of the physical principles underlying the operation of these devices is required.

  How FELs will solve it: an X-ray FEL can be used to understand ultra-fast magnetisation dynamics, and mechanisms for optically excited super conductivity in correlated materials at room temperature.

  Time resolved X-ray spectroscopy allows a unique insight into the coupled electronic, spin and geometric changes going on as the material undergoes a laser induced phase change. No other X-ray source can provide the temporal structure and flux required.

  There is a new generation of experiments in which the functionality of solids is controlled by light. Unveiling these physical principles may lead to a new generation of optoelectronic devices and exploring unknown regions of the free energy landscape of solids. The use of X-rays to study the microscopic texture of these hidden phases, for example by reconstructing optically induced unstable crystal structures with unexpected functionalities, may provide new inspiration for materials design and recreate these properties at equilibrium.

- **FEL Photonics**. Photonics is the science and technology of generating, controlling, and detecting photons. Most photonic applications are currently in the range of visible and near-infrared light, but FEL research will enable the range of photonics to be extended from visible light into the X-ray realm. There is potential in this area for the development of new organic photosensitive materials for transistors, computers, lasers, and other light sources using the insights provided by ultrafast X-rays. Then there is a new area of research into non-linear effects at very short wavelengths. In this latter area are prospects for the development of X-ray multi-dimensional spectroscopy that can uncover the full information on the atomically localized electronic excitation and transient quantum coherence in materials/molecules undergoing physical or chemical change. There is already significant theoretical progress that demonstrates the potential of such a technique and first experiments on stimulated X-ray Raman scattering have already succeeded at LCLS.

- **The Challenge**: to develop the field of X-ray photonics thereby enabling the imaging of ultrafast physical, chemical and biological processes.

- **How FELs Will Solve it**: they provide the ultra-short, coherent light and high brightness X-ray pulses required. No other X-ray source has the brightness, temporal duration or coherence to enable this: they are short by a factor of a billion on brightness.

  There are a few key groups working in this area in the UK including at Imperial College, the University of Southampton, the University of Strathclyde, and the University of Warwick. Photonic materials is a growing area of EPSRC's research portfolio.

9.2. Diffraction Before Destruction (Out-running Radiation Damage)

The analysis of soft and biological material by X-rays has always been known to be limited by radiation damage. Currently the technological solution to this problem is to flash-cool the sample to slow the effect of damage. There is evidence that such cooling and subsequent X-ray irradiation can introduce subtle and potentially confounding structural changes. (This issue also affects cryo-EM.)

Due to the inherently short exposure time compared with the intrinsic kinetics of damage, the use of X-ray FELs allows imaging to be completed before the effects of radiation damage become apparent. For example:

- **Nanocrystallography**. For protein crystals the useful dose limit is thought to be less than 500 kGy for a room temperature sample, which can be absorbed in under a second in an unattenuated synchrotron beam. This has imposed a severe limit on our ability to examine crystals, since the strength of the diffracted beams (reflections) is proportional to the flux density of the incident beam.

  The Challenge: to capture images of protein crystals that are sensitive to radiation damage.

  How FELs Will Solve it: the ability to out-run radiation with X-ray FELs means they can be used to examine protein crystals in a way that would be severely limited by radiation damage if a synchrotron was used.

  This will require new sources and new technologies for sample preparation and sample delivery. The UK is a leader in these areas with a strong commercial sector working with the academic centres. These new technologies can be expected to spin off beyond structural study. GPCRs and other IMPs have been the focus of many of the successful X-ray FEL protein structural experiments to date.

X-ray FELs – Avoiding X-ray Damage

Photosystem II (PSII) is the first protein complex in the light-dependent reactions of oxygenic photosynthesis that occur in plants, algae, and cyanobacteria. As well as its profound scientific importance in understanding the evolution of life on earth, it is a key focus in the drive to split water with sunlight for the production of clean energy. PSII is easily damaged by X-rays, and so cannot be studied on a synchrotron. The effects of X-ray damage can be avoided (or at least very significantly reduced) by using FEL radiation, since the experiment is over within the femtosecond pulse duration, before the atoms can move (although electrons may have been displaced).

The Mn_4CaO_5 cluster at the heart of PSII has been visualised at LCLS at around 5 Å resolution using a "pump and probe" method, leading to crucial insights into its mechanism. The data revealed that the cluster re-arranges during reduction, with one manganese atom moving out from the cubane shaped structure of the cluster.

The ability to visualise such fragile and reactive metal co-factors (non-protein chemical compounds) in their true state is very important for many of the most chemically important biological processes (oxygen evolution and nitrogen fixation).

The UK currently has groups working in this area at the University of Oxford (viruses), the University of Saint Andrews (membrane proteins), and Imperial College. Additionally, groups that work with metalloproteins will benefit from access to X-ray FEL facilities, as metal centres damage extremely fast in an X-ray beam. There is technical expertise at the Diamond Light Source in sample mounting for the XFEL.EU.

Understanding the Mechanisms of Radiation Damage in Biology, Medicine and Engineering Materials

The high intensity X-ray pulses from a FEL offer a unique way to emulate the sudden electronic damage caused by exposure to ionizing radiation.

This information is key to the following areas:

- understanding the damage mechanism in protein crystallography;
- diffraction studies in structural biology (with X-rays or electrons);
- understanding dose and damage in radiobiology and radiotherapy;
- the study of radiation damage pathways in materials used in the nuclear industry;
- safe storage strategies for existing radioactive waste.

This is a topic of current scientific importance. Parts of the relevant communities (e.g. structural biology and nuclear engineering) are very strong in the UK.

9.3. High Coherence Imaging

The unprecedented coherence of FEL radiation opens the door to coherence X-ray imaging techniques. For example, to study:

- **3D Imaging of Biological Systems**.

  The potential of FELS for 3D imaging of biological systems has not yet fully been realised, but progress has been made recently in this area. For instance, 2D FEL images have already been obtained from a number of different irreproducible (i.e. non-identical) samples such as live cells, organelles, and viruses.

  The Challenge: to generate 3D visualisations of biological systems.

  How FELs Will Solve it. 3D imaging is possible with EM but is difficult because electrons do not penetrate the sample very far, so very thin samples are required (and the chemistry of the sample cannot be determined using electrons). Some 3D imaging of biological systems can be done at synchrotrons, but the lower coherence limits the amount of information that can be captured. The high brightness and coherence of the pulses from X-ray FELs mean they are the most suitable type of facility for this. A 3D reconstruction of the giant mimi-virus particle (450 nm diameter) at a resolution of 125 nm has been successfully extracted from X-ray FEL diffraction patterns.

  Obstacles to improving the resolution are currently low hit rates and the need for improved detectors and retrieval algorithms as well as higher X-ray FEL flux. These are all feasible future developments, opening up the possibility of 3-D imaging of biological samples between 30-300 nm.

Liquids and Nucleation

X-ray FELs can be expected to provide novel and potentially game-changing insights into the physics of the liquid state, and liquid-liquid and liquid-solid transformations.

With a time resolution of around 10 fs, FELs offer the unprecedented possibility to take a snapshot of a liquid at time scale orders of magnitude less than the molecules' relaxation times (rotational and positional relaxation etc. are greater than 1 ps). These "instantaneous" coherent diffraction images can be unique tools to investigate basic questions, such as whether it is possible for liquids (such as water, liquid chalcogenides, and even liquid Si) to consist of two co-existing fractions with different structure and density. The destruction and re-forming of these fractions should occur on ps time scales, allowing them to be imaged with a "single particle" coherent diffraction imaging experiment on a FEL, where the single particle is a liquid drop. Liquid physics is an area of science in which the UK is well established.

The femtosecond pulses from FELs may also provide unique insights into nucleation: as each FEL pulse contains in the order of 1011 photons, there are enough photons to produce an image of a crystal nuclei as small as 12 nm before the sample is damaged due to radiation. This area is important in fundamental science (e.g. in understanding liquid solid transitions, and solidification processes in crystal growth), and in industry. In the pharmaceutical industry, polymorphism (the occurrence of several crystalline forms of the same compound) can be hugely problematic as regulatory procedures require the specification of a specific polymorph, which may sometimes not crystallise during production. It is known that nucleation processes can exert a crucial influence over the polymorphic outcome of crystallisation, and the ability to probe the early states using FELs could make a key contribution.

10. Annex B: Underpinning Technologies

There are a number of key areas of technology which would underpin the development of a UK FEL facility, and capability in each of these needs to be further developed within the UK in order to enable UK science to take full advantage of FELs in pursuing frontier science. Even if a UK FEL is not constructed, the technical capability could be redeployed on other accelerator projects in the UK, or internationally thorough collaborations. Many of the skills and technologies and skills developed in these areas will also be applicable to the construction and operation of other large facilities.

10.1. Accelerators and Free-Electron Lasers

Developments in accelerators could lead to better FEL performance (intensity, stability, coherence, shorter pulses, and two colour output) and/or lower cost (e.g. higher quality factor (Q) superconducting cavities, lower beam energy, shorter facility length, and designs optimised for mass production).

Ongoing Activities in the UK

The UK has experience in most of the areas of accelerator science required for development of a world class FEL, particularly those related to electron beam technology through work at ASTeC / the Cockcroft Institute (CI), Diamond Light Source (DLS), and the John Adams Institute (JAI). The CLARA test facility at Daresbury Laboratory will address many of these areas directly (guns, RF structures, laser issues, single shot diagnostics, timing and synchronisation). The CLARA low emittance gun and first accelerating section was installed in 2015 and will be commissioned in 2016. The VELA gun is already operational and giving valuable opportunity to study and develop laser and RF stability, single shot diagnostics, deflecting cavities, etc. and CLARA will extend these opportunities much further. It is very difficult to develop state of the art accelerator technologies in isolation. It is only through bringing them together in a facility such as CLARA that they can be properly tested and proven.

Next Steps Towards the Construction of a UK FEL:

- Develop a fully coordinated FEL R&D programme, encompassing the accelerator, FEL, beamline, detectors, lasers, and end stations.
- Promote an integrated approach between machine designers, operators, and users.
- Finish the completion of CLARA as an R&D facility in support of a future UK FEL.
- Strengthen engagement of the accelerator institutes in FEL modelling and technology developments.
- Collaborate internationally with FEL facilities where appropriate.
- Offer PhD studentships, post docs, and training in the critical technology areas relevant to a UK FEL listed in the first section above (as discussed in "Strategy for Growing the UK's XFEL Community" on page 13).

Potential for UK Industrial Growth and Skills Development

The overall increase in the skill base in accelerator technology would ultimately allow improvements in performance and cost savings for other accelerator projects, and these benefits would also be experienced in industries which use accelerator technology.

Novel Acceleration Techniques

Wakefield accelerators driven by lasers or particle beams can produce accelerating gradients three to four orders of magnitude greater than conventional accelerating structures. They therefore hold promise as drivers for future high energy physics machines and free-electron lasers as well as compact radiation sources. Moreover, they offer a route to the production of electron beams with properties that cannot be produced conventionally that are of relevance to FELs – in particular simultaneously high energy (GeVs), very high bunch charge (10s nC) and ultra-short short duration (10s of fs). Considerable R&D is going-on worldwide on both laser (LWFA) and beam driven (PWFA) plasma wakefield accelerators, in Universities and in large accelerator labs (DESY, LBNL, RAL, SLAC). Progress has been rapid in recent years, and the UK has developed considerable experience, particularly in LWFA (e.g. at Imperial College, the University of Oxford, RAL, and the University of Strathclyde). While improvements continue to be made with both techniques, technical difficulties (poor stability, limited repetition rate, low wall-plug efficiency, difficulty of multi-staging etc.) need to be overcome before they can be considered mature enough to use them as the basis of any large-scale user facility. Over the next 5 years or so LWFA experiments are likely to develop significantly, and the UK should certainly continue R&D in this direction, however these are essentially experiments in their own right. Smaller-scale LWFA-based soft X-ray FEL facilities could in principle also be developed, but with limited parameters (photon energy, pulse energy, repetition rate). It is not believed that wakefield accelerators will play a significant part in the strategic approach for provision of an X-ray FEL user facility in the foreseeable future.

10.2. Detectors

In this rapidly evolving field, the timescales of instrument development and manufacture mean that prototype systems must be demonstrated well in advance of any UK beamlines coming on stream. In existing FEL facilities, a number of specific development programmes were undertaken to ensure that every beamline had appropriate technologies available for it to use and to build its image and data processing. In each case early development was necessary to enable timely system construction and installation.

Ongoing Activities in the UK

- Soft X-ray imager: "PERCIVAL" (RAL, DESY, Elettra, Diamond, PAL). Designed at the Rutherford Appleton Laboratory (RAL) and funded internationally, this will deliver high-performance X-ray imaging for a range of experiments at FEL and synchrotron sources.
- Hard X-ray imager: "Large Pixel Detector LPD" (RAL, Glasgow, and European XFEL): A novel high dynamic range multi-gain pixel detector for the FXE beamline at the European XFEL.
- DAQ processor: "TrainBuilder" (RAL, Imperial College, European XFEL). Developed by STFC for European XFEL, the TrainBuilder will provide readout for all of the large 2D Mega-pixel detectors at European XFEL.
- Not directly related to FELs, the high performance DAQ and signal processing for SKA, the LHC, and the ESS and high frame rate imagers for synchrotrons such as the Diamond "Excalibur" are all relevant systems recently developed in the UK.

Ongoing Activities Globally

- CSPAD and ePix at SLAC, AGIPD at DESY and PSI, Jungfrau at PSI, and DSSC at European XFEL are other key detector systems being developed globally. Only the CSPAD has actually seen any significant continuous beamline use and manufactured on any scale, so significant learning and refinement of the other systems will inevitably follow.

Next Steps Towards the Construction of a UK FEL:

- Establish a UK development programme to drive new instrument developments matched to our requirements.
- Further develop existing strong links between STFC-RAL

and the Stanford Group (SLAC-LCLS), and between the UK and the European XFEL-DESY teams.

- Engage in the testing and evaluation of detector systems used in current FEL facilities and those in development in order to apply those technologies to our needs and understand their performance limits.
- Ensure there will be sufficient capacity across the National Laboratories and academia to develop the necessary technology areas of ASIC design, microelectronics assembly and bonding, DAQ firmware and software development, image handling and processing.
- Continue to work with industry wherever possible for manufacturing electronics.

Potential for UK Industrial Growth and Skills Development

STFC holds patents for Charge Coupled Devices (CCDs) in CMOS technology. UK companies are keen to exploit this technology to develop extremely high frame rate infra-red cameras which are not currently commercially available. This means there is high potential for UK spin-outs and support for UK industry. STFC has a strong track record in this area having developed many commercial systems (e.g. high frame rate visible cameras and image sensors in transmission electron microscopes).

Investing in the development of instrumentation, electronics, and image processing will also lead to many training opportunities for students to engage in the processing and management of image data.

10.3. Lasers and Auxiliary Light Sources

All current FEL facilities have ultrafast lasers as an integral part of their end stations. The majority of experiments at FLASH and LCLS involve a laser as part of a pump-probe scheme, to prepare a sample or diagnose what is happening. It is likely that the demands for more advanced laser systems will grow as the science matures. Future schemes to control the coherence of the X-rays will require laser conditioning of the electron beam. This means that lasers will become a vital part of the light source technology. In the future there are possibilities of laser based electron acceleration either by adding auxiliary light/beam sources to FEL experiments, or perhaps (for softer X-rays) using lasers in primary electron acceleration for a FEL.

Ongoing Activities in the UK

Across several UK university labs and the Central Laser Facility (CLF) a great deal of effort is being devoted to various aspects of the laser technology which would be required for a UK FEL facility. Mostly this research is part of other programmes. CLF is especially strong at high average power systems, high peak power, and some aspects of ultrafast and non-linear optics (NLO). CLF and the University of Oxford built the DiPOLE laser, which will be used as the “pump” for pump-probe experiments in the HIBEF beamline at XFEL.EU.

Ongoing Activities Globally

DESY and European XFEL have invested heavily in high rep-rate lasers for the needs of the unique pulse structure of the European XFEL and FLASH. SwissFEL has invested in NLO based THz sources. FLASH (at DESY) has developed electron beam based THz sources. Laser based time stamping techniques have been developed at SLAC (Stanford). New laser dressing schemes for coherent FELs are being developed at FERMI (Trieste, Italy) and SLAC. Much of the technology developed for the Extreme Light Infrastructure could also be of use.

Next Steps for the Construction of a UK FEL:

- develop a coordinated national approach to deliver the laser R&D required to set up an advanced FEL facility;
- work closely with international and commercial partners to exploit the R&D already developed or in the pipeline;
- determine the importance of co-locating a UK FEL with a high powered laser, and the logistics of achieving this.

Either a warm or a superconducting machine would require high end laser systems for extreme intensity (100 TW up to PW+ class lasers) and high energy (kJ/ns). These are vital for leading work on matter in extreme conditions (MEC). Ideally the highest possible repetition rate should be aimed at which will require significant R&D if the FEL is to be fully exploited.

Potential for UK Industrial Growth and Skills Development

UK based companies could play a key role in developing the newer laser technologies. Similar circumstances have strengthened the scientific laser industries elsewhere (notably in France) in recent years.

UK academic science is strong in laser applications, but less so in developing new laser technology. The construction of a UK FEL facility would provide a strong impetus for adventurous new R&D across a range of laser technologies in both the academic and industrial sectors.

10.4. Simulation, Control, Data Acquisition, Data Analysis, and Storage

The high data rates and volumes generated by FELs are a fundamental part of the technology. European XFEL gives estimated data rates of 10-40GB per second per instrument, and a total stored data volume of 10-50PB per annum. This is in similar ranges to the CERN LHC and the Square Kilometre Array projects. As detectors improve this data rate may go up, possibly by one or two orders of magnitude.

The high data rate means that the signal to noise ratio is low and early filtering and selection of useful data is vital for the effective generation of meaningful results. The data volumes involved require a high data-throughput compute resource near the facility so that processing can be undertaken without requiring large data transfers. Comparison with models and simulations need to be undertaken to focus the experiments, reduce the chance of low quality experiments and to provide meaningful interpretations of results. Tailored algorithms must be developed so that computations are completed in a tractable length of time.

Ongoing activities in the UK

- Data and computational infrastructure are provided by STFC and by Diamond Light Source to support the work of the ISIS and Diamond facilities. ISIS and Diamond provide data acquisition and filtering expertise together with in–experiment analysis capability. Diamond is also the UK Hub for the European XFEL.
- STFC's Scientific Computing Department (SCD) provides data archiving and scientific modelling capability; increased use of SCD's capability for post-experimental analysis is under current development, and is expected to significantly increase over the next few years. SCD also provides code development and other support to EPSRC and BBSRC Collaborative Computational Projects (CCPs), providing modelling and analysis codes of relevance to potential FEL science areas; for example, the CCP4 Dials project is developing software for serial crystallography on European XFEL
- SCD operates machine rooms at both Rutherford Appleton Laboratory and Daresbury Laboratory. Other activities hosted by SCD that are of relevance include the GridPP Tier1 centre, currently managing some 15PB of data, and the JASMIN high data-throughput resource for the climate science community, and the Hartree HPC centre concentrating on technology transfer to industry.
- Additional capability in the UK in high-performance computing includes DIRAC, EPCC, and EBI. Such national infrastructure may be more interoperable under a UK-Tier 0 initiative.
- Other current activities of a similar data scale include astronomy experiments, in particular the Square Kilometre Array (SKA) currently under construction.

Ongoing Activities Globally

- European XFEL and LCLS are developing a range of techniques and tools, especially in data acquisition. These could be of particular importance.
- Lawrence Berkeley Laboratories and Oak Ridge National Laboratories in the USA are both developing tools and processes which effectively utilise an HPC centre in conjunction with experimental facilities.
- Other large scale science projects are developing data selection and management techniques at scale including the SKA and CERN-LHC.

Next Steps for the Construction of a UK FEL

Technological innovation in the compute resource is required in the following areas:

- system of distributing and coordinating data through the community;
- mass integrated domain metadata at systems level;
- cloud access to HPC (transparent through virtualisation);
- novel hierarchical data storage and object data storage techniques;
- parallelisation techniques on codes to new HPC architectures;
- effective middle ware development and utilisation for effective workflow and visualisation;
- energy efficient user of computing as power consumption becomes a major limiting factor;
- machine learning for computing assists on image filtering and selection and analysis;
- development in intelligent and high-performance algorithms.

Co-location of data storage and compute is desirable to overcome network capacity issues, and proximity to the FEL is desirable to overcome data movement overhead.

Potential for UK Industrial Growth and Skills Development

HPC and big data are significant areas for technology advancement and big data is one of the UK's eight great technologies. UK industry benefits directly from the development of HPC capacity.

The support of the computing needs of a FEL facility would provide opportunities for the development of expertise in computing technology and computational science.

10.5. Sample Environment and Delivery Target Assemblies

For a FEL to be of any scientific or practical value the final beam will need to irradiate a sample and this sample needs to be delivered in the form of a target for the beam. The sample material(s) and geometry determine the experiment. Under most operational conditions the sample will be destroyed on every shot. The focal spot will usually be very small and, therefore, every sample aliquot that constitutes the target for a beam shot needs to be made, characterised, and positioned to ultra-high precision.

Ongoing Activities in the UK

- The most similar current activity is that of the Target Fabrication group in the Central Laser Facility at RAL and the group's spin out company Scitech Precision. The group is in an internationally leading position in establishing microtargetry solutions for high repetition rate high power lasers.
- There is also an advanced Target Fabrication group at AWE but their specialisation is in very complex targets.

Ongoing Activities Globally

- There is some activity at DESY, particularly on the HIBEF station, but the technologies have not yet been demonstrated.
- The ELI pillars have plans to develop capabilities which might be of interest but will probably not be applicable for many years.

Next Steps for the Construction of a UK FEL

- The throughput of current wafer-based microtarget fabrication needs to be increased.
- Faster progress is required to develop robust, high accuracy positioning systems potentially by extending current technologies.

Potential for UK Industrial Growth and Skills Development

There could be commercial opportunity for the supply of positioning systems and target batches.

The skills developed by scientists and technicians would support future activity in the field and would be transferable across a wide range of microtechnology sectors. Techniques developed for targetry would also probably have application in many other microtechnology sectors.

10.6. Diagnostics

Diagnostics are essential for controlling the accelerators used in FELs and for understanding the experiments being carried out. In-situ beam diagnostics are essential for X-ray FELs, as their output is much more variable than that of modern synchrotrons operating in top-up mode. Photon diagnostics are needed for pulse-to-pulse normalization of experimental signals, which is essential because the actual beam position, profile, pulse arrival, and intensity vary over the course of measurement. The main goal of photon diagnostics is to create tools that can characterize, store (as data) and display various properties of light (pulse length, spectrum, intensity, polarization, wave front) without interfering with its propagation from the photon source to the user.

Ongoing Activities in the UK

The UK is not playing a major role in this area at present.

Ongoing Activities Globally

- Notable developments are occurring in countries that are already constructing and/or operating FELs (Japan, US, Germany, Italy, Switzerland, Korea). This includes all aspects of electron and photon detection. These developments are absolutely essential for incorporation into the design and construction process for a UK facility.
- There is worldwide collaboration for rapid development of electron and photon diagnostics. The diagnostics are constantly improving experiments at SACLA and LCLS, implying that by the time that a potential UK FEL facility would be constructed, off-the shelf solutions in the femtosecond domain for SASE will be available.

Next Steps for the Construction of a UK FEL

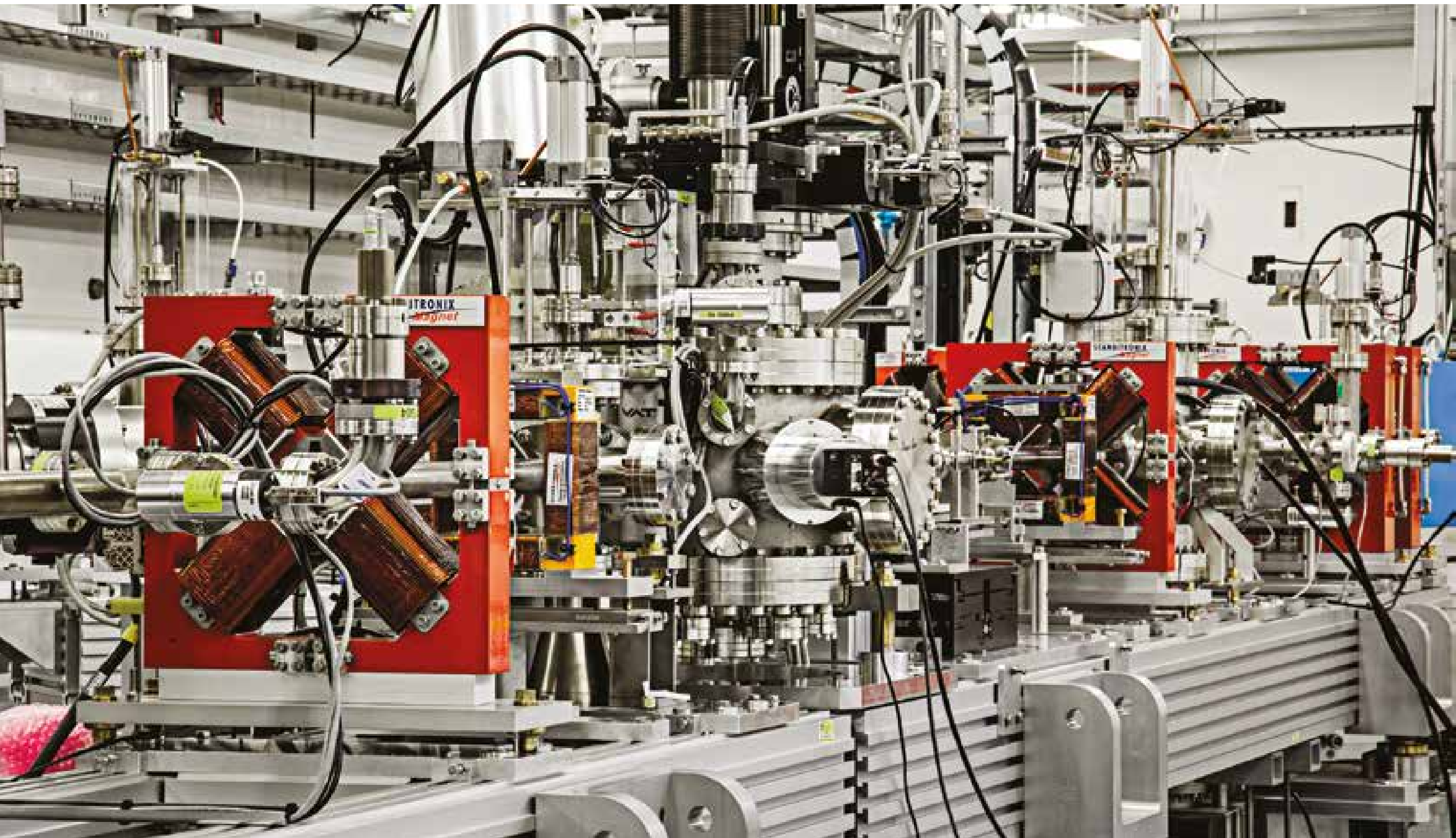
- Further developments in photon diagnostics which characterise entire beam profiles as to both their phase and amplitude, and also are rapid enough for inclusion into rapid feedback schemes for accelerator/laser control, would strongly inform the design of a leading edge UK facility.

- There is the opportunity for original R&D into the technologies required for the subfemtosecond ("attosecond") regime.
- Another area for development of next generation facilities is photon diagnostics sufficiently rapid for incorporation in active feedback loops for accelerator/ laser control. This would enhance FEL performance (in the case of both self- and external seeding).

Potential for UK Industrial Growth and Skills Development

High-performance electron and photon diagnostics have many potential applications from biomedicine to defence, and their design, construction and use represent an opportunity for companies and investors in all associated sectors.

FEL diagnostics are at the cutting edge of ultra-high speed detection and data processing for data collection, decision making and control, and thus represent an excellent training ground for high technology workers in the UK economy.



11. Annex C: FEL Review Terms of Reference

1. Introduction

1.1. As part of the Programmatic Review, STFC's Science Board considered the future of large facility provision for the UK and made the following statement and recommendation.

"The national and international context for large facility provision and future planning is evolving rapidly, and a coherent strategy for the future development of UK large facility provision must be developed.

We recommend that Science Board lead reviews in the areas of neutron and photon provision and develop a coherent strategy for UK large facility provision."

1.2. STFC Executive Board has previously considered how to implement this recommendation and it is recognised that free-electron lasers (FELs) is a key area where the UK / STFC needs to develop a strategy for facility provision. STFC Executive Board has agreed the following Terms of Reference and process for the development of FEL strategy.

1.3. This strategy will:

- identify the key science challenges that require FEL access;
- identify the requirements for FEL access in terms of both capability and capacity;
- identify opportunities for meeting these access requirements;
- provide a roadmap for user community development;
- identify the requirements for any underpinning technology or skills / capability needs noting where such development may also be important for other types of facility.

2. Towards a UK FEL strategy

2.1. The purpose of this review is to produce a strategic document that includes:

- a 15 – 20 year vision for UK FEL access;
- a 7 year strategy for FEL access, UK FEL facility provision, community development, and underpinning technology/skills.

2.2. This document will provide a basis for shaping future support for FEL science, FEL facility provision, and any long term technology developments in areas such as accelerators and instrumentation.

2.3. To achieve this, an expert group be convened; terms of reference for which are provided in Paragraph 3. This group will ensure that all key stakeholders (including the other Research Councils, Wellcome Trust, relevant facility directors, technical experts, and academic and industrial user communities) are fully engaged in the process.

3. Terms of Reference

3.1. Building on the outcome of the 2013 Programmatic Review and the direction already established within STFC of participation in XFEL and CLARA, examine the long term key science challenges that require FEL access based on inputs from the UK Research Councils, the UK science community via relevant STFC advisory panels and user groups, industrial stakeholders, and relevant facility directors. This includes:

- exploring the scientific and industrial opportunities arising from FEL science that will benefit the UK;
- exploring any competing experimental methods;
- identifying any potential impacts on other facility provision.

3.2. Identify the requirements to address the key FEL science challenges. This includes:

- identifying FEL access requirements in terms of both capability and capacity;
- exploring the best approach to develop the UK FEL community.

3.3. Identify means for meeting the UK's FEL access requirements. This includes:

- examining the current international landscape for FEL facilities based on currently available strategies and roadmaps;
- identifying potential future facility opportunities in the UK and abroad (including developments of existing facilities), evaluating their advantages and disadvantages based on fit to UK need, technological feasibility, and barriers to

access, and identifying how they could be delivered;

- identifying any technologies that need to be developed in areas such as accelerators, detectors or instrumentation or skills that need to be maintained in the UK in order to underpin future UK FEL science.

3.4. Identify potential capital and operating costs, and potential technology and instrumentation R&D costs.

4. Expert panel

4.1. The review will be conducted by an expert panel comprising:

Tony Ryan Chair – University of Sheffield

Gabriel Aeppli – Paul Scherrer Institute

Massimo Altarelli – European XFEL

David Brown – University of Kent / Charles River

Richard Catlow – University College London

Elspeth Garman – University of Oxford

Peter Henderson – University of Leeds

Malcolm McMahon – University of Edinburgh

Jon Marangos – Imperial College

Jim Naismith – University of St Andrews

Richard Walker – Diamond Light Source

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UK Astronomy Technology Centre, Edinburgh; Chilbolton Observatory, Hampshire;
Boulby Underground Science Facility Boulby Mine, Cleveland.

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