

Report from the review of U.K. Light Sources

Submitted by

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Executive Summary

The committee was briefed by representatives of the existing and future UK user communities for light sources, the directors of existing facilities, and the proponents of new facilities or major upgrades. All the major European light sources where UK users are significant participants were included. The committee also had access to other documents, and called upon additional expertise in the review. The committee feels comfortable that it received adequate input to gain an appropriate perspective from which to advise STFC as it plans to expand scientific opportunities for UK light source users.

In general, the committee was very impressed by the standard and leadership of UK light source science. The SRS has played an important historical role in the growth of synchrotron radiation science. The UK has been a major player in the outstanding success of the European Synchrotron Radiation Facility. The Diamond light source is an exemplar of the possibilities for new 3rd generation sources, and the UK community is poised to benefit from this well-built new source.

We heard about two major new proposals for light sources. The 4GLS and Sapphire are two very different ideas for fourth generation sources which cover a wide range of wavelengths, and access ultra-fast timescales. In the committee's opinion, however, neither proposal is yet appropriate for approval.

The committee feels that the community in the UK most involved in 4GLS, with an interest in the spectral region from THz radiation to soft x-rays, needs to come together and start fresh to identify the optimum UK facility which would serve their needs. In this "reinvention" process, we strongly recommend that likely developments in optical laser technology in the next five to ten years be incorporated from the "ground up". Through strong collaborations with, and investment in, the Central Laser Facility, we believe that an innovative and integrated suite of accelerator and optically based light sources could emerge which would better serve UK science. Such a modified "4GLS" could adequately address the longer wavelength range and ultrafast pump-probe regime not served in the UK today, and could propel the UK community into a leadership role in Europe and beyond.

Diamond is an outstanding new facility for the UK, and the Diamond team under Prof. Materlik's leadership are to be applauded for their success so far. They will remain busy for the next few years ensuring that the machine operates reliably and at the state-of-the-art, and delivers the scientific impact anticipated. During this time they should continue to explore with their users options for providing UK scientists with access to ultra-fast x-ray sources, including long-term possibilities for new sources.

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Recommendations

INNOVATIVE ACCELERATOR RESEARCH AND DEVELOPMENT

1) The activity to develop an energy-recovery LINAC prototype (ERLP) at Daresbury should be encouraged as an innovative contribution to the international arena of accelerator science. We endorse the positive efforts to develop a center of excellence for accelerator science and technology at Daresbury. Modest proposals to expand the ERLP facility to focus on accelerator developments, and possible extensions as a user facility should be pursued.

PROPOSED NEW FACILITIES

2) The scientific activity behind the proposal to build the 4GLS facility has been productive and should be encouraged. There is a diverse user community engaged in the effort, and many innovative accelerator ideas in the design. In addition, it is clear that the UK community interested in the IR, VUV and soft-x-ray spectral regions is strong yet not well-satisfied by existing UK facilities. However, the committee feels that the 4GLS proposal, as it has been developed so far, is not convincingly the best step for the UK to provide the highest scientific impact to this community. The facility is technically ambitious - there are many capabilities embodied in one facility, from THz to soft x-rays. A key to the proposal is the simultaneous use of more than one color of light for pump and probe, yet it is not always clear, even to the potential users, how these might be used together. While the scientific case contains some really good ideas, it is not clearly matched to the facility plan. The committee believes that there is good science in this arena, but it needs to be more clearly articulated in the context of any proposed facility.

More significantly, the committee feels that possible role of “conventional” (i.e. non free-electron) lasers to provide better capabilities for several of the wavelength ranges in the 4GLS suite has not been sufficiently explored. When one considers the time scale and magnitude of the proposed investment for 4GLS, it seems that investments in laser developments could pay off handsomely. The Central Laser Facility (CLF) is a great resource for this sort of development, and with their experience in user facilities they could combine the appropriate amount of risk and predictability. One can anticipate, for instance, that the versatility of high-harmonic generation sources from gases and surfaces will improve substantially in the foreseeable future, especially with regard to average power, spectral range and tunability. In general, the portfolio of innovative laser-based sources is presently expanding with unprecedented vigor towards either side of the visible spectrum, opening new perspectives for user facilities. We recommend that the user community around the UK be brought together for one or more workshops on frontier science in the ultrafast and long wavelength regions, and this community be closely

engaged in designing an innovative new proposal for a 4GLS which makes more extensive use of laser developments and has a more focused scientific case. Any developments should be evaluated in the European context, since there are several related VUV and soft x-ray facilities under construction or proposed in Europe. However, we expect that the UK could take a leadership role in Europe and beyond.

3) The Diamond facility presented a proposal for Sapphire, an ultra-fast source for hard x-rays. This facility has been discussed with the Diamond scientific advisory committee, but has not yet had extensive discussion with the potential user community. The committee saw the possibilities in the proposed single pulse facility, which would provide short brilliant pulses but without lasing. However, the committee was concerned that the proposal, as shown, was simple but not highly innovative, and would likely be superseded by new laser-based technologies before it was finished construction. In addition the machine group at Diamond will be busy in the next few years making sure that the existing Diamond machine delivers on its promise during operations, with improved reliability and enhanced performance. The committee therefore felt that it is premature to go ahead with a formal proposal to build Sapphire in the next few years. Nevertheless, the committee encourages Diamond to involve its users in planning for the future of ultra-fast hard x-ray facilities in the UK and elsewhere, and to couple with the effort recommended above in the softer x-ray region.

4) The involvement of the United Kingdom in the XFEL facility is very important for the future of x-ray science. Specific examples from the science presentations in the areas of atomic physics and high energy density physics showed that the UK has groups amongst the best in the world. It is suggested that a concerted effort be made to increase the science user community for XFEL through the funding of a research institute, like PULSE at Stanford, or the Center for Free Electron Laser Science at DESY. The proposed Institute should encourage research at existing FEL facilities, at FLASH or the LCLS, in preparation for the opening of the XFEL. In general, the STFC can perform an important role as a portal to other facilities in Europe and worldwide, as they have done by supporting the ESRF and the XFEL. The role of the UK in developing detectors for XFEL is an important one, and should be broadened to include other FEL sources such as FLASH and LCLS. The CLF can play a similar role in the development of laser systems for these sources.

EXISTING FACILITIES AND PROPOSED UPGRADES

5) The committee was impressed by the success to date of Diamond. A compelling story for the need of continued investment in Diamond beamlines was made. The facility did not yet have any major scientific results to show, but this is not unexpected considering that Diamond has not been running long. The committee is concerned that not all the beamlines at Diamond be “tied up” too soon. In particular, the committee felt that it is too

early to commit to the construction of specific Phase III beamlines. The committee also recommends that the plans for construction of Phase II beamlines be opened for further discussion amongst the community as late as possible. It is also clear that a close cooperation with the Soleil source in France would be mutually beneficial, and could provide better support for the soft x-ray community in the UK. The committee was concerned about the apparent lack of instrumentation development at Diamond, and the perception that many beamlines have been purchased using “off-the-shelf” technology. The committee recommends that after Diamond has operated for three years, an independent international review committee be brought in to evaluate the success so far, and in particular the plans for the future, prior to firm plans for Phase III commitments.

6) ESRF and its proposed Upgrade: The committee was impressed by the success of ESRF and the important role it plays for British scientists. It appears that the UK “gets its money’s worth” from ESRF, in that British scientists are very competitive with the community elsewhere in Europe. The proposed upgrade of ESRF will improve many beamlines for imaging and nanoscience, and the UK should provide support for this, while being intimately involved in ESRF user discussions on prioritization of upgrade projects.

7) Central Laser Facility: It appears to the committee that the Central Laser Facility could play a larger role in the development of UK light sources. While they were coordinated to some extent in the proposals for 4GLS and Sapphire which were presented to the committee, it appears that the possibility of major developments in laser technology in concert with accelerator sources has not been fully considered. For example, the development costs aimed at the accelerator sources seem to be one to two orders of magnitude above those considered for new laser projects. The committee encourages the CLF to “think big” in its proposal for new light sources. One gets the impression that their ideas are tailored to fit into modest (one or two million pound) funding profiles, yet one can ask what they could do with ten times that number to revolutionize accelerator-based light sources which typically cost one hundred times more? In a European comparison CLF already has a unique record as “the” UK national facility in the laser sector, with an unusually large user community utilizing the breadth and high quality of the equipment and services being offered. Moreover, with their HiPER project CLF is pioneering the first truly international civilian laser project on a Giga-Euro scale. Hence, they are in a position, and should be strongly encouraged, to pursue plans for novel user-oriented light sources at a substantially larger funding profile than presently planned. Only then does a comparison between laser- and accelerator-based light sources appear meaningful.

We feel that with the strong user facility success of CLF, the opportunity exists for the UK to take a leadership role for laser-based light sources in the future. An essential step

will be the identification of user needs through the workshops proposed in recommendation 2).

8) Detectors: The committee applauds the UK involvement in detector development, with examples such as the new detectors planned for the XFEL, but recommends that the funding level for detector development be substantially increased. UK scientists should also expand their participation in international detector development projects.

Background Material

The committee was convened by the CCLRC, later to become the STFC, to provide a perspective on current UK Light Sources, their plans for the future and new proposals. We began with a meeting at the Hilton Hotel, Heathrow Airport on March 29th, 2007. There the committee met to discuss with Robert Donovan, Henry Hutchison and Andrew Taylor, the terms of reference and execution of the review. The primary data gathering for the review occurred at a three day meeting held at the London Marriott, County Hall from Monday 16th through Wednesday 18th July. Participants in the review were invited by STFC. The committee invited additional expert review input from Prof. Ingolf Lindau (Lund University), Prof. S. Chattopadhyay (Cockcroft Institute), Prof. Friso Van der Veen (Swiss Light Source), and Prof K Ueda (Tohoku University).

The review agenda is found in Appendix 4. As well as the committee and advisers, present at the review were Professor Robert Donovan, Prof. John Womersley and Dr. Andrew Taylor from the STFC. The first day of the review consisted of a series of presentations from expert users with an interest in current and future facilities. The second and third days focused on detailed presentations of existing UK facilities, future proposed facilities, and international facilities with a strong UK interest, specifically the European Synchrotron Radiation Facility and the European XFEL in Hamburg.

An executive summary and recommendations were forwarded to STFC in October 2007. Those form the first sections of this document. The remainder of this document provides further background information from the review. Since public release of the recommendations we have received some feedback from facilities which has been considered in completing the background section.

Expert User input

Most of our user input came from oral presentations listed in Appendix 4, but in addition we received a few letters from users who were unable to be present at the review. What follows, does not represent an exhaustive summary of the talks, but rather a few examples that were viewed as key to the terms of reference of the review.

Prof. Dave Stuart from Oxford University presented a comprehensive overview of the current and future prospects for protein structure determination in the United Kingdom. UK scientists have solved with synchrotron radiation many important biological structures over the last ten 10 years. Prof. Stuart himself has a made important contributions to the structures of very large viruses at SRS and at the ESRF. He emphasized that for complicated systems (big viruses, membranes) the bottleneck is the screening of a very large number of samples. Thus the increased capacity offered by Diamond and other European sources is of great importance to this community. While the

talk focused on x-ray diffraction, Prof. Stuart considered the possibility of using high pressure or soft X-Rays for specific applications. In addition, he briefly discussed the possibility of small angle scattering experiments, time resolved experiments, exploitation of the coherence, FEL possibilities and IR experiments which could take advantage of next generation sources.

Prof Ian Robinson recently returned from the USA to join University College, London, and is thus an important addition to the UK light source user community. He has strong links with Diamond. During the last few years, Ian has been exploiting the coherent properties of SR for “lensless” X-Ray microscopy. Last year he reported on some interesting work, performed at APS, measuring and inverting diffraction patterns from Pb nanocrystals. He is planning to continue in the same direction but integrating the “ptychography” recently introduced by Rodenburg et al., (Phys.Rev.Lett, **98**, 034801, 2007). His work will couple strongly to the XFEL. He emphasized the necessity for the development of FEL detectors and the importance of having a university involvement in the development of UK facilities.

Prof. T. Rayment (U. Birmingham) represented users interested in engineering problems and in environmental and earth science. As an engineering example, he presented an in situ tomographic imaging study of corrosion to identify the existence and the role of ductile bridges during inter-granular cracking and the subsequent inhibition of the growth of the crack. For environmental and earth sciences he gave various examples (pollution of soils and water by arsenic, metal speciation in earthworms etc.). He emphasized that various methods were needed to tackle these problems: XRD, SAXS/WAXS, XAS, EXAFS, MXCD, XPEEM, STXM and IR spectromicroscopy. To this end, scientists have been using various facilities: including SRS, ESRF, and BESSY. For the future he stated his community’s interest in the Phase III beamlines at Diamond, coordinated investment in detectors and the 4GLS. He also emphasized the need for collaboration between facilities.

Prof. J. Evans (Southampton) gave a talk on sustainability and catalysis. There are two main challenges:

To view steps in catalytic reactions in real time. Specifically, the measurement of dynamics on a time scale less than the molecular vibration time, and to observe kinetics of primary steps and transients on a longer time scale (upwards of 1 ps).

To move from a molecule to processes.

He presented some interesting experiments done at the ESRF and showed preliminary results on a Ge microstrip detector able to reach a resolution of 1 μ s.

This research makes the following demands on future SR requirements:

Dedicated chemical processing beamline

QEXAFS + XRD + IR, Raman, uv-visible etc.

Chemical speciated XAFS & RIXS

Adsorption sites and oxidation state

Time resolved studies

μ s mixing

ps uv-visible or medium-far IR excitation, X-ray probes

Imaging: Atomic through mesopores to microchannel reactors.

Non storage ring requirements;

Kinetics: (500 fs – 10 ps)

XANES and EXAFS – electronic & atomic structure

Dynamics (10 fs)

XANES and EXAFS – electronic & atomic structure

State selective excitation

Pump with polarised IR (~ 100 fs)

Prof. C. Latimer spoke as a representative of the atomic and molecular science community. They mainly perform gas phase experiments to investigate the electronic and chemical properties of atoms and molecules. They work typically in the range 5-40 eV.

This community has been quite active in the past: there are currently seven groups working in the field (Manchester, Queen's Belfast, Nottingham, Birmingham, STFC, Southampton and Open University).

Present situation: of the four beamlines existing at SRS, only one remains until the end of 2008. The various groups have been trying to obtain beam time at Elettra, Bessy, Astrid, ALS and SLS.

Short term future: one possible solution could be to share or to have a fully dedicated beamline at SOLEIL.

Long term future: 4 GLS would be a unique opportunity.

Prof. J. Underwood (UCL) gave a very interesting talk. High-order harmonic generation (HHG) in atomic gases by high intensity laser fields has proven to be a powerful tool to produce coherent light in the extreme ultraviolet and attosecond pulses. The ionization and electron recombination steps of HHG are dependent on the particular symmetry of the highest occupied molecular orbital and its orientation with respect to the laser field. This enables a unique time resolved probe of the electronic orbital structure (Phys. Rev. Lett., **98**, 20307, 2007). Experiments are performed at RAL with the ASTRA laser and support the planned upgrade (ARTEMIS).

Prof. M. George (Nottingham) made a presentation on the UK National facility, installed at RAL, for the use of ps IR light (PIRATE). It is a pluri-disciplinary laboratory. It seems to be very successful and oversubscribed. A new titanium sapphire laser (10 KHz, 2x10W) to deliver fs and ps pulses is under commissioning.

Prof. J. Wark (Oxford) began his talk by pointing out that the Oxford Group (including Wark, Cavalleri, Hooker and others) was the most active in their field in the UK with more than 20 publications in Nature, Science and Phys. Rev. Lett. in the last five years. His group is mostly involved with plasmas created by high power lasers, X-ray lasers and time resolved X-ray diffraction. The work is mostly done outside of his laboratory (RAL, Los Alamos, LLNL, SPPS...). He gave a brief report on some recent work: the direct observation of the bcc to hcp transition in shock-compressed Fe via nanosecond X-Ray diffraction (Phys. Rev. Lett., **95**, 075502, 2005), the non thermal melting of indium (Phys. Rev. Lett., **95**, 125701, 2005), the shock deformation of face-centered-cubic metals on sub-nanosecond timescales (Nature Materials **5**, 805, 2006).

He made the following recommendations:

- maintain UK at forefront of High Power laser science
- support the FELs at DESY and Stanford
- buy a station at LCLS (£2-3M)
- support SAPPHIRE
- transform ERLP into a user facility

Profs. R. Catlow (UCL) and G.Thornton (UCL) described future work which could benefit from 4GLS, in catalysis and other areas. They emphasized the need for 4GLS, where they could do pump-probe experiments using a THz laser for the pump. However, it appears that they would need hard x-rays for the probe, at least for some experiments, and these would not be provided by 4GLS.

Prof. A. Cavalleri has been working in the last few years, first in Berkeley and now at Oxford, on pump-probe experiments. He is focusing mostly on strongly correlated electron systems. During his presentation, he reported on a nice experiment done on a manganite, $\text{Pr}_{1-x}\text{Ca}_x\text{MnO}_3$. By using 200 fs laser pulses centered at 71 meV (17 THz), Cavalleri et al., report (Nature, 2007) a prompt, five- order of magnitude drop in resistivity. $\text{Pr}_{1-x}\text{Ca}_x\text{MnO}_3$ has three dominant phonon modes at 5.5, 10 and 17 THz. The 17 THz mode corresponds to Mn-O stretching. They show that the vibrationally-driven band gap collapse observed is not related to hot carrier injection and is uniquely attributed to a large amplitude Mn-O distortion. For the moment, due to the lack of a broad band laser, they can't cover the three phonon modes. In the future, it is clear that this kind of experiments could be very important to understand the role of the electron-phonon interaction in the high Tc superconductors

Prof. G. Aeppli, head of the London Center for Nanotechnology (LCN) particularly emphasized the need in his field for very rapid access to Diamond. This is done, in some cases, in protein crystallography, so it should be possible in other fields.

Prof. T. Wess (Cardiff) said that there were about 60 groups (300 people) in the UK doing small angle scattering experiments, using either neutrons (ILL, ISIS) or X-Ray (ESRF, SRS and in the future Diamond). He showed some recent results obtained on fibrilin. He emphasized the synergy of neutrons and X-Rays and on the necessary detector development.

Facility Presentations (existing and future)

4GLS

4 GLS is a proposed low energy photon facility from THz to VUV/soft x-rays, primarily below 1000 eV, at the Daresbury Laboratory. The user community it addresses is based on both traditional synchrotron radiation and laser facility users as well as a new user community that may arise from the synergy of combining a set of accelerator based coherent and spontaneous sources. The scientific case was presented in an extensive document in 2001 (passed Gateway 0 in 2002) that pointed to a potential user community of more than 900 scientists. Over the last few years the scientific case has evolved and gained focus. An updated version of the scientific case, "4GLS Science Landscapes", was

presented to the Panel July 18, 2007. At the core of the proposed science are the so-called “Flagship Programmes”:

- Electron dynamics of the chemical bond
- Quantum chemical control
- Origins: A programme of laboratory chemistry and physics in support of astronomy and astrophysics
- Probing the low-energy photoresponse of atomic nuclei
- Reactive pathways in catalytic chemical processes
- RESRAD: Reaction dynamics of excited states and free radicals in chemistry and biology
- Biocatalysis, photosynthesis and membrane proteins
- The relationship between protein structure, protein dynamics and protein function
- Molecular assemblies in the extracellular matrix and cell signaling
- Cell imaging and spectroscopy
- Spin@4GLS
- Atom scale correlation of chemical and electronic structure in solids
- Many-body properties of solids studied by time-of-flight angle-resolved photoemission
- Spectroscopy

The 4GLS facility is based on three inter-related accelerator systems. At the heart is a 600 MeV, 1.3 GHz energy recovery linac (ERL). It supports five undulators for spontaneous emission in the VUV/soft x-ray region with 100 fs to a few ps time-structure and one VUV free-electron laser in the region 3-10 eV (operated at 4.3 MHz). A second mode of operation at 750-900 MeV with a separate photoinjector, 1 kHz, supports an XUV free-electron laser for the spectral region 8-100 eV. Finally there is a stand-alone IR free-electron laser operating at 13 MHz and covering the spectral region 2.5 to 200 micron. An elaborate matrix has been worked out where the radiation from these different sources

can be combined for classes of pump-probe experiments. The underlying philosophy is a combination of sources that provides unique capabilities to address the kind of scientific problems discussed in the flagship programs. A conceptual design report was published in 2006 addressing the technical aspects of the injector systems, the superconducting linear accelerators, electron beam transport systems, free-electron laser systems (including seeding schemes), photon transport systems, timing and synchronization, cryogenic systems and civil construction. A detailed technical design report, TDR, is planned for March 2008. It will include details of beam-lines, end-stations, detector developments, costs and schedules.

4GLS is being developed in close collaboration with both national and international partners. The Central Laser Facility at Rutherford Appleton is involved providing its laser expertise. Development programs in both science and technology are in place with Jefferson Laboratory, Cornell ERL project, SLAC, LBNL, FERMI@ELETTRA, MAX-lab in Lund, CLIO in Orsay and ISP in Novosibirsk. 4GLS is a partner in EUROFEL and is on the ESFRI (European Strategic Forum for Research Infrastructures) roadmap for free-electron lasers together with FLASH, FERMI, BESSY FEL and MAX-IV FEL.

4GLS has established an Industrial Advisory Board. The latest conference with interested industrial partners earlier this year attracted more than 100 participants.

A preliminary cost estimate was given at £240 million (includes £60 million for buildings). In a phased approach the first phase is estimated to £180 million (includes £60 million for buildings). With an approval in 2008 4GLS is anticipated to be ready for users in 2013/14. There are upgrade options for 4GLS: in the short term to enter the attosecond regime and increase the repetition rate (now 1 kHz) for the XUV FEL), in the long term to add recirculating arcs to extend the wavelength region to 1 or a few keV.

In 2003 the ERLP (Energy Recovery Linac Prototype) project was funded to address the R&D issues for 4GLS and to build-up the necessary knowledge base for 4GLS (4GLS is the only actively proposed ERL project in Europe). ERLP is in collaboration with both national and international laboratories, in particular Jefferson lab, and has received much interest from the outside community. ERLP is presently being commissioned: all the basic hardware has been installed, first light has been extracted from the photoinjector, the cryogenic systems have reached the specified 2K/4K levels and the superconducting rf cavities are under testing. Energy recovery is planned to be achieved by the end of this year. ERLP was originally funded at a level of about 14 million pounds. More recently, November 2005, additional funding (about 3 million pounds) has been received to initiate science program on ERLP. These include x-rays from Thomson scattering, THz spectroscopy of live tissues and pump-probe experiments on the carrier dynamics in nanoparticles and thin films.

We were happy to see the growth of the Cockcroft institute, and recommend that the ERLP facility should be further developed as a test facility for accelerator concepts, and possibly for user applications.

While the committee was impressed by the 4GLS proposal and community, we had some serious reservations which are expressed in the recommendations section. These reservations come from the observation that more synergy between lasers and accelerators for such multi-color pump probe facilities should be more deeply explored. Additionally, the committee formed the impression that the proposal was attempting to incorporate too many capabilities and lacked scientific focus. There is a strong UK community with an interest in this kind of science, and the Daresbury group should be applauded for engaging with them. So while the committee believes that 4GLS as presented is not the optimal proposal for the UK, we strongly believe that the communities should be encouraged to work at developing a single UK proposal which incorporates the state-of-the-art in laser developments.

Diamond

Diamond is a 3 GeV storage ring, injected by a linac+booster. The first electrons were injected in May 2006. Since then, most of the expected performances have been achieved (as seen in table I) although not in routine user operations.

	Target	Achieved
Energy	3 GeV	3 GeV
Beam current (mA)	300	220
Horizontal emittance (nm rad)	2.7	2.9
Vertical emittance (nm rad)	27	avr-50
Lifetime (hours)	>10	20 at 125mA

Table I: Diamond target and achieved parameters as of the time of the review

The maximum current (300 mA) has not been achieved for the moment because the 2nd cavity is under commissioning but 220 mA have been injected. For user operation, the current is of the order of 130 mA due to outgassing of the vacuum chamber. A horizontal emittance of 2.9 nm has been achieved, with a very good coupling (0.15-2 %). The beam

optics seems to be well understood. Slow orbit feedback keeps the orbit stability at the BPMs to $\sim 1 \mu\text{m}$, The fast orbit feedback is ready for operation

The six in-vacuum undulators, the Apple II undulator and the 3.5 T superconducting multipole wiggler are working as expected, the users having control of the gap. Various modes to exploit the time structure have been tested. Finally, the top-up mode should be operational for the users in January 2008. During the first 1524 hours of user's mode, the dead time for failures and injection was 9 %. It is likely that this number will decrease quickly.

Phase I Beamlines (October 2002/January 2007)

Seven beamlines were planned and built during this period: they have been open to users since the beginning of 2007. They include three beamlines devoted to protein crystallography working in the range of (0.5-2.5 Å) but optimised for 0.98 Å. They are fully automated with cryocooling and ADSC CCD detectors. Preliminary electron density maps obtained by various groups were presented and seem to be of very good quality. Knowing the strength of the UK community in this field, these beamlines should be very successful.

The fourth beamline is a nanoscience beamline: it is the only one of the phase I in the soft x-ray domain. It is an important area because both spectroscopy and diffraction of nano-objects can be done with soft x-rays. Some nice preliminary results were presented, such as PEEM images and a demonstration of resolving power of 10,000 for the monochromator. The committee noted that soft x-ray beamlines are amongst the most demanded at many facilities (Spring 8, ALS, ESRF.....) and the present resolving power and resolution of the PEEM is not at the world's best. The committee encourages Diamond to aim at the state-of-the-art.

The fifth beamline (Materials and Magnetism) is a high intensity, high resolution X-ray scattering and diffraction facility. It uses an in-vacuum undulator and covers the energy range 3.5-25 keV, with focusing between 3.5-15 keV. Data from the two first user groups were presented on magnetic tunnel junctions and high resolution diffraction from a phase contrast KTP ferroelectric grating showing the possibilities of the experiment but also some radiation damage.

The sixth beamline (Extreme Conditions) is a high energy beamline for single crystal and powder diffraction experiments under high pressures and temperatures. Using a superconducting wiggler (3.5 T), it covers the range 20-80 KeV with up to 3 in-line stations. The first experiment was used to obtain the total scattering Pair Distribution Function analysis of cation locations of zeolites. Some user groups are planning to have

an international collaboration for high throughput combinatorial chemistry (mainly aimed at solid state hydrogen storage).

The last beamline of phase I is a microfocus spectroscopy beamline: the vertical focusing is for the moment 15 μm , the target being 1 μm . Preliminary results on a sample of the Santa Caterina meteorite were shown.

Phase II and III Beamlines

We did not have any detailed presentation on the expected performances of the phase II beamlines. Fifteen beamlines are under construction and will be installed by the end of 2011.

Phase III has a budget of £76.7M for 13 beamlines. A large fraction is still under discussion at the SAC. The construction of the first beamlines would start in 2008 and the last one will be installed by 2015.

During the presentation, the challenges for the Science Division were presented:

- finish beamline commissioning and optimisation of phase I
- assure stability and get all components/methods working
- shift from construction project to user operation

The committee feels that the management should be ambitious in its choices for Phase II beamlines, and should leave as much time as possible for user community input to ensure that beamlines are at the state of the art when they come on line. The budget per beamline is generous, but there do not appear to be many instruments with world leading performance. We understand the challenges of working with the user community to satisfy their demands for flexibility, and the need to develop world-leading capability. We encourage Diamond management to strive for more world leading instruments in the Phase II and III. In addition, it was felt that it was time for Diamond to develop a stronger instrument development R&D program. In the recommendations the committee noted its concern with the lack of this R&D effort and commented that the strategy that Diamond chose for the first beamlines appeared to be based on “off the shelf” technology. While this may have been the right strategy to get the facility up-and-running with state-of-the-art beamlines, we feel that the UK’s pre-eminent facility should grow to provide “bleeding-edge” as well as “leading-edge” capabilities for top UK users.

Finally we note that while we are very impressed with Diamond’s performance and plans, we were not in a position to give a fair and detailed review to the facility, e.g. on the phase II beamline plans. Such a review could provide good input to Diamond and the

STFC. We recommend that after two to three years of operation, an independent review committee be convened to look in detail at Diamond and provide more substantive recommendations for the future.

Sapphire

At the end of the Diamond presentation, we learned about a proposal to build a 3 GeV linac, next to the storage ring. The main purpose is to produce pulses shorter than 100 fs in the hard X-ray. The first estimation of the cost is £80M.

The committee applauds the innovative thinking, but feels that Sapphire is not yet mature enough to be considered as a viable proposal for the following reasons:

- This will divert a fraction of the machine group and there are still important developments to be done on Diamond.
- 10^7 - 10^8 ph/sec for an investment of 80 M£ is questionable.
- One has the impression that this is a first step for a FEL and we are not convinced that this is the right strategy.
- Has the option for an ERL upgrade of Diamond been considered seriously?
- Have the tradeoffs between warm and cold technology for the LINAC been evaluated?

We encourage further dialogue with the UK user community on ultra-fast sources for the future. We see XFEL as meeting the hard x-ray communities needs, and particularly encourage discussions in the longer wavelength region as discussed under the 4GLS proposal section.

European Synchrotron Radiation Facility (ESRF)

The ESRF is a very successful 6 GeV third-generation synchrotron facility which is heavily used by the United Kingdom scientific user community. It appears that the UK community is competitive in obtaining beam time by peer review, and their work is of very high calibre judged by the publication output in regular and high impact journals.

The ESRF has developed a plan for a major upgrade designed to keep it at the forefront as new facilities come on line. The key components of the upgrade, beyond modest accelerator improvements, are major beamline improvements.

SRS

The SRS facility is based on a 2 GeV storage ring. It started operation in 1980 and was the first dedicated user facility built especially for production of synchrotron radiation. It was covering the spectrum from IR to Hard X-rays.

In 2000, 39 experimental stations were distributed around the storage ring. With currents in the range of 150/250 mA, the facility was delivering about 4,500 hours per year of beam time, the number of users per year being of the order of 1400. Since 2006, a managed programme of station reductions has been implemented as part of the “sunsetting” of the facility towards closure in December 2008.

It is obvious that with the construction of Diamond, the scientific production has slowed down in 2006 and 2007. However, very good work has continued in the field of protein crystallography which was, for many years, the strongest field of SRS (being the best facility in Europe until the completion of the ESRF beamlines). For many years, McMahon, Nelmes et. al., have produced remarkable results in the field of materials under high pressure, pointing out clearly that the source is not the most important parameter, except if you are trying to reach extremely high pressure.

Other areas can also be cited like the work of Ungar et. al., on liquid crystals or the magnetic studies of nano-objects by van der Laan et al., (although many experiments were not done at SRS).

One should also point out that SRS has been paying much more attention to detectors than any other facility in Europe (they have developed very good multi-element solid state detectors and large multi-wire proportional chambers used in various facilities).

With the closure of SRS at the end of 2008, the scientific UK community may face some problems because the soft X-ray domain will not be very well covered at Diamond (one beamline in phase I, one in phase II and one in phase III). Knowing the development of nanosciences and nanotechnology and the fact that the spectroscopy and diffraction of nano-objects is often done in the soft X-ray region, that could be a serious problem. This is addressed in our recommendations re 4GLS and Diamond.

XFEL – the European X-ray Free Electron Laser

The concepts for next generation accelerator based photon sources are based on the use of linear accelerators. The two concepts, free electron lasers (FELs) and energy recovery linacs (ERLs), have different goals. FELs aimed at peak brilliance achieved with large photon number per pulse, extremely short duration and diffraction limited emittance while ERLs aim at maximizing average brilliance. On the world FEL scene there are three projects in various phases of construction aimed at the 1 Ångström regime: the Linac Coherent Light Source (LCLS) being built at the Stanford Linear Accelerator Center in Menlo Park California due to begin user operations in summer of 2009, the SPring-8 Compact SASE Source (SCSS) being constructed in Harima, Japan and due to begin operations April 2011 and the European XFEL in Hamburg, Germany which will begin operations on the 2013-2014 time scale. The FLASH FEL is already operational in Hamburg as a national facility accessing the wavelength range from 30 nm to 6 nm in the near term. They have demonstrated that there is sufficient intensity in the 3rd and 5th harmonics for experiments so that when the European XFEL becomes operational there will be FEL radiation in the Hamburg area extending from 30 nm to 0.1 nm. The UK is a partner in the European XFEL.

The scientific case and the technical details for the entire European XFEL are described in the Technical Design Report, http://xfel.desy.de/tdr/tdr/index_eng.html. The project was launched on June 5, 2007. The initial agreement for the XFEL provides enough funding for 17.5 GeV electron energy and three of the 5 radiators described in the TDR.

There are world class researchers in the UK that can utilize both FLASH and when available, the European XFEL. In particular there are groups in atomic physics and high energy density science that are already engaged in FLASH experiments. The commitment of the UK to the initial phase of the European x-ray facility is strongly supported and further they should look closely at joining in full funding of the facility so that it reaches its design goals as soon as possible.

The high energy density researchers loosely organized by Prof. Justin Wark could gain early access to facilities at LCLS with a modest (£2-3 M) investment. This permits this community access to FEL research capability ~ 4 years earlier than will be available in Hamburg. Thus they would be in a unique position to fully exploit the European XFEL in its early operational phase with a 'second generation' instrument based on experience gained at LCLS.

The UK should utilize the unique aspects of the RAL campus for 'in kind' contributions to both the XFEL with detector development and potentially the LCLS HEDS effort with laser development.

Central Laser Facility - CLF

It appears to the committee that the Central Laser Facility could play a larger role in the development of UK light sources. While they were coordinated to some extent in the proposals for 4GLS and Sapphire which were presented to the committee, it appears that the possibility of major developments in laser technology in concert with accelerator based sources has not been fully considered. For example, the development costs aimed at the accelerator sources seem to be one to two orders of magnitude above those considered for new laser projects. The committee encourages the CLF to “think big” in its proposal for new light sources. The committee has the impression that their ideas are tailored to fit into modest (one or two million pound) funding profiles, yet one can ask what could they do with ten times that number to revolutionize accelerator-based light sources which typically cost one hundred times more? In a European comparison CLF already has a unique record as "the" UK national facility in the laser sector, with an unusually large user community utilizing the breadth and high quality of the equipment and services being offered. Moreover, with their HiPER project CLF is pioneering the first truly international civilian laser project on a Giga-Euro scale. Hence, they are in a position, and should be strongly encouraged, to pursue plans for novel user-oriented light sources at a substantially larger funding profile than presently planned. Only then can a comparison between laser- and accelerator-based light sources be meaningful.

Present status of CLF:

According to the management's own statement “the CLF philosophy is to provide world leading laser facilities to the international research community, to be the preeminent laser user facility within Europe, and to be fully competitive with all other international laser laboratories A principal tenet of this strategy is to ensure the CLF staff provide sufficient leadership, guidance and enabling capability to allow the UK community to capitalise on their current strong position in this field.”

The committee feels that CLF has an excellent record in fulfilling this mission. CLF has, in recent years, operated the world's only working Petawatt laser (VULCAN, presently being upgraded to 10 PW), together with a multi-purpose, high-power short-pulse laser system (ASTRA, presently being upgraded to include a 2x500 TW station GEMINI), and an inter-disciplinary *Lasers For Science Facility*, focusing mainly, but not exclusively on ultra-fast spectroscopy of molecular and biological species. In addition, CLF has developed and refined leading edge laser sources and concepts (e.g. Optical Parametric Chirped Pulse Amplification OPCPA) and a multitude of diagnostic, spectroscopic and target technologies.

In a European comparison CLF is one of the largest national laser laboratories, offering one of the broadest ranges of research facilities and laser sources. It is unique in combining fusion-oriented high-power and high intensity lasers (VULCAN and ASTRA,

respectively) on the one hand, and ultra-short high repetition rate spectroscopic lasers (Lasers for Science) on the other. This poses considerable challenges on the management of operations, user selection, user services and on the broad expertise of in-house researchers, which all appear to be well met.

CLF exhibits another unique characteristics in a direct comparison between the “large four” European countries (the UK, France, Germany and Italy) that operate major national laser laboratories or “Laser Research Infrastructures” (using the EU terminology). France and Germany each have several national science organisations such as CEA and CNRS, or MPG, WGL, FhG and HGF, respectively. They operate at least one, sometimes more than one laser laboratory each. Italy's INFN is only beginning to establish a major national laser facility (the existing, spectroscopy-oriented LENS laboratory has a multiple-source funding structure). The French and German laboratories cover, as a whole, a similar or even wider breadth of facilities and research, but are individually more specialised than CLF. Most notably, however, none of them appears to have a comparable national importance as “the” inter-disciplinary national user facility in the laser sector. Germany, for comparison, has chosen to installed large numbers of femtosecond laser systems at universities through the DFG science foundation, resulting in a much larger autonomy of the user community when it comes to laser spectroscopy research.

It is outside the scope of this report to judge on the relative effectiveness of these national policies. Given the size and the international standing of the present national laser community the UK approach appears to work well within its own environment, and CLF appears to fulfill its broad and unique service mission much to the satisfaction of the national researchers.

Future plans for CLF:

CLF has restricted its presentation in front of this committee to the *Lasers for Science* facility, deliberately omitting the high-power activities which were thought to be outside the scope of this light source review (though they amount to more than 60% of CLF's overall activities). In the present context, however, it is worth noting that CLF is underpinning its role as a world-leading laser facility through a recent proposal to the European Strategy Forum on Research Infrastructures ESFRI. If realized this project, HiPER (a 800 M€ proposal believed to exceed national resources) will be the world's first multi-national laser facility together with ELI, a French proposal for a 200 M€ ultra-high intensity laser for basic research. The challenges in the HiPER project lie, among others, in the development and demonstration of the fusion mechanism, and in the pioneering task of gathering a laser community with yet little experience in supra-national activities behind this project.

On the other hand, CLF is well aware and at the forefront of the current rapid developments in the laser sector which open up completely new research and application opportunities, especially when it comes to new wavelength generation, high average powers, attosecond pulses and ultra-high intensities opening the way to new physics of light-matter interactions. For more than 40 years lasers have made enormous progress in power, intensity, pulse duration etc. but not in spectral coverage, especially (but not only) towards the UV and x-ray region. This is even more painful in view of the fact that UV- and x-ray light is the light of the micro- and nanotechnologies (both for diagnostics and manufacturing), and of biological structural and dynamics research. Coherent sources in this spectral domain are indispensable for future research and technological progress. There is currently an unprecedented wealth of complementary approaches to generate coherent light in these spectral regions, frequently based on relatively compact and affordable laser sources.

CLF plans to engage in the highly competitive race for new laser facilities through the following projects:

- **ULTRA**, a facility for both time-resolved and steady state IR and Raman spectroscopy to address key chemical and biological questions (£1.8 M),
- **ASTRA-Artemis**, bringing together the cutting edge optical technology used to generate few-femtosecond UV and XUV pulses with the x-ray diagnostics that are typically only found at synchrotron facilities (£2M project, together with Diamond).
- **Laser Nanoprobe facility**: nanoscale imaging and force measurements for proteomic, cell, and DNA-protein interaction studies.
- **Facility for Attosecond Science and Technology (FAST)**: to exploit attosecond pulses across the broad range of disciplines through building a *national attosecond facility*, believed to become a worldwide unique facility complementary to the next generation of accelerator based light sources e.g. 4GLS, X-FEL and Diamond-Sapphire, with which collaborations are planned.
- **DIPOLE – Diode Pumped Optical Laser for Experiments**: novel high-power lasers with shot repetition rates measured in Hertz rather than minutes or hours (as is present state-of-the-art) experiments” into a new generation of statistical, advanced data gathering modes. Coupling to proposed facilities such as DIAMOND-SAPPHIRE, and/or the XUV arm of 4GLS is believed to provide a “truly spectacular source capability”.

- **Advanced Imaging for studying biological function:** in partnership with Daresbury Laboratory, it is proposed to develop a portfolio of advanced nano-scale technologies (label and label-free NSOMs) for user programme building on the current expertise at CLF. There are also plans to expand programmes to use synchronised pump-probe UV-THz using the ERLP and time-resolved UV-resonance Raman for protein structure and dynamics.
- **Combining lasers with next-generation accelerator sources:** According to CLF it is quite clear that “conventional” laser technology will play a significant role in the emerging suite of next-generation light sources. Apparently, the UK user community has already identified a number of specific areas where lasers should be incorporated. In certain spectral windows lasers would dominate the light source of choice (eg UV, visible and in some cases the mid IR). Many experiments were considered that would benefit from combining accelerator sources (hard x-ray, XUV, VUV and THz) with existing laser technology in a variety of pump/probe combinations.

Assessment of CLF

CLF is a comparably large, world-leading laser research facility with an unusual interdisciplinary breadth, ranging from high-power fusion-oriented research to molecular and biological spectroscopy. In the national context it plays a unique role as service-oriented user facility, providing almost exclusively the instrumental basis (lasers plus diagnostics) and scientific expertise for a comparably large fraction of the national user community. In a European comparison CLF was so far highly successful with this strategy, complementing the inventory of European laser laboratories and offering a certain fraction of its services to the European user community through EC-funded activities such as LASERLAB-Europe, the European network of national Research Infrastructures .

Like all laser facilities CLF is facing challenges through unprecedented rapid developments in the laser sector, especially with regard to new wavelength generation, high average power, attosecond pulses and ultra-high intensities. CLF is preparing to tackle these challenges through a number of competitive projects at the level of few million pounds each. Given the proven expertise of the CLF staff there is no doubt that the laboratory has excellent chances to succeed in all these projects, especially given the fact that it pursues strong collaborations (in many cases in leading roles) with the above mentioned European network and with global partners.

Some of these projects bear direct relation to accelerator based light sources and applications such as pursued by 4GLS and Diamond-Sapphire. The committee

appreciates the fact that contacts between the laser and the accelerator communities have already been established, but it feels that there could be a much closer collaboration and synergy between research efforts from either side.

While many of the world-wide pursued laser-based concepts for novel light sources are still in an experimental (sometimes even pre-experimental) stage, they appear, as a whole, worth the effort to undertake studies for their up-scaling towards specifications which match or exceed present or near-future accelerator-based sources. Such studies may already exist, but they have not been presented in the context of the present review. The committee notes, however, that the proposed Pan-European ELI facility (in which CLF participates) provides a basis for various aspects of such up-scaling.

In its main research field, laser fusion, CLF has already demonstrated the willingness to move towards new dimensions by proposing one of the first multi-national laser facilities, HiPER, a project on a Giga-Euro scale. The committee believes that CLF, given sufficient resources, is in a position, and should be strongly encouraged, to pursue plans for novel user-oriented light sources at a substantially larger funding profile than presently planned. Only then a comparison between laser- and accelerator-based light sources appears meaningful.

Appendix 1: Committee Roster

UK Light Source Review Committee

Dr Murray Gibson - Argonne National Laboratory (Chairman)

Dr Jerome Hastings - Stanford Linear accelerator Center

Professor Yves Petroff - Former Director, European Synchrotron Radiation Facility

Professor Wolfgang Sandner - Max-Born Institute Berlin

Advisers

Professor Swapan Chattopadhyay (Cockcroft Institute)

Professor Ingolf Lindau (Stanford)

Professor Friso van der Veen (PSI)

Professor Kiyoshi Ueda (Tohoku University)

Appendix 2: Terms of Reference

REVIEW OF LIGHT SOURCE PROVISION FOR UK

Terms of Reference

- To consider the scientific capabilities and opportunities provided by the current light sources in the UK;
- To consider opportunities for collaboration with other countries in the provision of access for UK scientists;
- To consider the complementarity of existing and new sources in underpinning scientific programmes;
- To ascertain the size and nature of the Light Source community and advise on which potential facilities would best serve their needs;
- To make recommendations on criteria and an overall strategy which should inform decisions on the operation and development of current sources and the construction of new facilities.

Appendix 3: Announcements

UK Light Source Review

A review of the UK's Light Source strategy is now underway. An independent, international Panel of experts has been formed to consider the scientific capabilities and opportunities currently available to UK researchers, and to make recommendations on an overall strategy which will inform decisions on the development of current and new facilities.

The Panel members are:

Dr Murray Gibson - Argonne National Laboratory (Chairman)

Dr Jerome Hastings - Stanford Linear Accelerator Center

Professor Yves Petroff - Former Director, European Synchrotron Radiation Facility

Professor Wolfgang Sandner - Max-Born Institute, Berlin

Professor **Robert Donovan** has been appointed by STFC as the Review Co-ordinator, assisted by Dr Andrew Taylor and Prof John Womersley.

The full **Terms of Reference** for the Review can be viewed at the link.

<http://www.scitech.ac.uk/About/Strat/Council/AdCom/UKLSR/UKLSRev.aspx>

The first (preparatory) meeting of the Panel was held in London on 29 March 2007. The Panel will next meet in London on 16 July 2007 with invited expert users, and on 17, 18 July 2007 with key Facility Directors. The Report will be finalised by the end of September, 2007.

Further updates on the progress of the Review will be added on a regular basis.

Announcement sent to users and light source directors:

Dear Colleagues,

UK Light Source Review

This is just to update you on progress with the Light Source Review. First the venue is now confirmed and we will meet in the London Marriott County Hall, close to Westminster Bridge, at 9:30 a.m. on Monday 16th July. The meeting should be finished by about 3:30 p.m. and we hope that as many Users as possible will stay for the entire meeting.

The Panel has not requested any written input from the Users but if you feel strongly about a particular issue you should feel free to make a written contribution (not more than two sides of A4; it would be helpful if this could be delivered to us electronically).

A website for the Light Source Review has now been established and you can access this at

<http://www.scitech.ac.uk/Home.aspx>

Should you have any questions please feel free to contact me.

I look forward to seeing you on the 16th of July.

Yours sincerely

Robert Donovan

Appendix 4: Agenda for Review Sessions in July

UK LIGHT SOURCE REVIEW

London Marriott County Hall

Monday 16th July, 2007

(BY INVITATION ONLY)

Dr Murray Gibson - *Chairman*

Dr Jerry Hastings

Professor Yves Petroff

Professor Wolfgang Sandner

Professor Robert Donovan (*in attendance*)

Assisted by: Professor John Womersley

And Dr Andrew Taylor

Agenda for Expert User Session

09.00: Introduction from Robert Donovan (STFC / Edinburgh)

09.10: Prof Dave Stuart (Oxford)

09.35: Prof Simon Phillips (Leeds)

09.55: Prof Nigel Scrutton (Manchester)

10.15: Dr Nicholas Stone (Glos. Royal Hospital)

10.35: Prof Ian Robinson (UCL)

10.55 - 11.15 Break & Contingency

11.15: Prof Trevor Rayment (Birmingham / Cambridge)

11.35: Prof John Evans (Southampton)

11.55: Prof Colin Latimer (Queen's, Belfast)

12.15: Dr Jonathan Underwood (UCL / OU)

12.35: Prof Mike George (Nottingham)

12.55: Prof Roy Newell (UCL)

13.15 – 13.45 Lunch & Contingency

13.45: Prof Justin Wark (Oxford)

14.05: Prof Richard Catlow (RI / UCL)

14.25: Prof Geoff Thornton (UCL)

14.45: Prof Andrea Cavalleri (Oxford)

15.05: Prof Gabriel Aeppli (UCL)

15.25: Prof Bruce Hamilton (Manchester)

15.45: Prof Tim Wess (Cardiff)

16.05: Closed Session With panel, Prof Lindau , Prof Chattopadhyay ,Prof van der veen and Prof Ueda.

UK LIGHT SOURCE REVIEW

London Marriott County Hall

Tuesday 17th July, 2007

(CLOSED SESSIONS)

Programme:

9.00 am Refreshments

9.30: Diamond – presentation by Professor Gerd Materlik and Dr Richard Walker

11.30: Central Laser Facility – presentation by Professor Mike Dunne and Professor Tony Parker

13.00: Lunch

14.00: XFEL/FLASH – presentation by Doctor Massimo Altarelli

16.00: ESRF – presentation Professor Bill Stirling and Professor Francesco Sette

UK LIGHT SOURCE REVIEW

London Marriott County Hall

Wednesday 18th July, 2007

(CLOSED SESSIONS)

Programme:

9.00 am Refreshments

9.30: 4GLS/ERLP – presentation by Professor Elaine Seddon and Professor Mike Poole

11.30: SRS – presentation by Dr Tracy Turner and Dr Paul Quinn

12.30: Lunch

13.30: Panel Discussion, summing up and Outline/Draft Report.

17.00: Close