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SCIENTIFIC REQUIREMENTS FOR SYNCHROTRON RADIATION IN THE UK

Report of a Panel to review synchrotron radiation science in the United Kingdom

Recommendations p. 39.

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CONTENTS

Appendices

Figures

Tables

I. INTRODUCTION

1. The inauguration of the Synchrotron Radiation Source (SRS) at the Daresbury Laboratory by the SERC in 1980 provided a dedicated source of light in a broad spectrum from hard X-rays through the vacuum ultraviolet to the infrared. It has generated scientific activity in a wide range of imaging, spectroscopic and diffraction studies in biology, chemistry, materials science and physics. The development of beam lines and specialised instrumentation has now reached a stage when it is appropriate to review the strengths and weaknesses of synchrotron radiation science funded by the SERC. Such a review is also made timely by the proposal to construct a European Synchrotron Radiation Facility (ESRF) and for the need to consider the future of the SRS in the light of such developments. As the ESRF would provide a state of the art source for hard X-rays, it is necessary to consider a separate future provision of a complementary brilliant source in the soft X-ray and vacuum ultraviolet regions for UK synchrotron scientists.

2. Accordingly, in October 1985 the Science Board of the SERC agreed on the establishment of a Synchrotron Science Review Panel (SSRP) with the following terms of reference:

(i) **To review the UK community's requirement for synchrotron radiation facilities in the foreseeable future in the light of achievements made so far using the SRS at the Daresbury Laboratory and sources elsewhere.**

- The Panel interpreted the future to refer to the next fifteen years, ie to the end of the century. It was also agreed that "sources elsewhere" should be taken to include the potential impact of laser facilities on the needs and provision of synchrotron sources.

(ii) **In particular, to consider the complementarity of the SRS and the planned ESRF, the long term plans for the SRS, proposals for a VUV ring, and an appropriate level for any UK involvement in construction and operation phases of the ESRF.**

- The Panel agreed that this should include consideration of the SRS/University interface, ie which experiments or development work should be carried out at the Daresbury Laboratory and which in Universities. There was a need to consider what could be achieved on the ESRF that could not be done on the SRS. There was consequently a need to consider technical options for the future provision of synchrotron facilities at the Daresbury Laboratory, including construction of a new VUV ring.

(iii) **In achieving these objectives, to take evidence from the Chemistry, Biological Sciences and Physics Committees, and the Synchrotron Radiation Facility Committee.**

- It was agreed that this term of reference should be broadened to include the taking of evidence from the Laser Facility Committee, the Materials Committee of the Engineering Board, and to consult industry.

3. The Review Panel met four times. In addition, it heard a two day presentation on the scientific achievements using the SRS at the Daresbury Laboratory, and on possible future developments using synchrotron radiation, presented by the SERC Synchrotron Radiation Facility Committee and leading UK researchers. It commissioned and received several papers on the scientific and engineering possibilities for development of the SRS both in the short term and in the long term (up to the year 2000).

4. The Review Panel conducted a survey of views of both the broader academic community as well as present users of the SRS in the UK. There was also a survey of industrial companies including those who had used the synchrotron radiation source through direct arrangements or indirectly through CASE projects or other collaborative awards.

5. Members of the Review Panel visited and reported on progress and future plans of all major synchrotron sources in the United States, Japan and Europe. The Directors of these sources were directly consulted on their plans for the future and their opinions on the strengths and weaknesses of the UK SRS programme. In the event, it proved exceedingly difficult to extract the critical review sought.

6. The Biology, Physics and Chemistry Subject Committees and the Synchrotron Radiation Facility Committee and Laser Facility Committee of the Science Board and the Materials Committee of the Engineering Board were consulted for their views on both the scientific achievements at the Synchrotron Radiation Source at the Daresbury Laboratory and the scientific opportunities created by the proposed construction of a European Synchrotron Radiation Facility.

7. The views of the Agricultural and Food Research Council, Medical Research Council and Natural Environment Research Council were also sought.

8. The Panel was asked to present its report for preliminary discussion at the Science Board meeting on 25 June 1986.

II. SYNCHROTRON RADIATION SCIENCE AND THE SERC SYNCHROTRON RADIATION SOURCE (SRS)

9. Synchrotron radiation is generated when relativistic electrons or positrons are restricted by magnets to follow a curved path. The radiation is white, of high brilliance and good collimation and it is polarised.

10. The SRS facility at present comprises the source (a 2GeV electron storage ring injected by a linear accelerator followed by a booster synchrotron) with a superconducting wiggler magnet(1) and a permanent magnet undulator(2), and eleven beam line front ends which split into a greater number of individual beam lines and feed 31 experimental stations or instruments including those still under construction. These include five test stations not fitted with permanent instruments. In four cases alternative instruments share one beam line. Table 1 lists the 31 stations.

Footnotes:

(1) A superconducting wiggler magnet is an array of 3 (or more) high field dipoles which produce white radiation with a spectral cut-off shifted to shorter wavelengths.

(2) A permanent magnet undulator is an array of many alternating low field dipoles. Interference occurs between radiation from successive dipoles and a strongly peaked spectrum is produced.

History of the development of the SRS

11. Construction of the source and three beamlines was approved in May 1975 and first circulating beam was achieved in June 1980. By then the superconducting wiggler was also under construction, but the funding profile had been such that no beamlines had been completed. Scheduled operation commenced with 1.8 GeV beams in May 1981 and full power became available on a regular basis (2 GeV high current) from April 1982.

12. By May 1981 the commissioning of two beamlines and three stations had begun. Since then the rate of beamline and instrument construction has been resource-limited and total operation time was, for the first few years, compromised by the need to have shut-downs to install beamline front ends as these were funded, and by the fact that access to the experimental areas was only possible during stable stored beam time (or shut-downs) but not during filling or accelerator studies periods. The shielding has now been improved so that this no longer applies.

13. The wiggler started regular operation, with stations connected, late in 1983/84 and is now scheduled throughout user beam time. A soft X-ray broad-band undulator has been installed and tested and will be brought into use when the beamline and monochromator are connected, during 1986.

14. After a year of very successful operation from April 1982 to March 1983, a cavity window vacuum leak precipitated a series of window problems which culminated in the SRS being out of action from mid-September 1983 to mid-January 1984 and operating at reduced energy (1.8 GeV) until June 1984. Since then the problems have been completely under control though the windows are still tested every morning.

15. The source statistics are shown in Table 2. This clearly shows how operating efficiency has increased steadily since the machine was commissioned; how the operating hours per year have increased as the need for shut-downs has diminished, and how 1983/84 suffered from the window problem. The loss of useful time was greater than implied by the Table as it does not distinguish reduced energy operation. With a total beam time of over 6000 hours per annum the SRS is operating for 2-3 times longer per year than any other source. It is now working very reliably and well up to its specification. Between 1981/82 and 1985/86 the number of stations taking

.ABLE 1 EXPERIMENTAL STATIONS AT THE SRS

Magnet	Stations	Technique
1	1.1	Surface science: under construction. Low energy toroidal grating monochromator
	1.2	Surface science: under construction. High energy spherical grating monochromator
2	2.1	Time-resolved small angle scattering and fibre diffraction (TRXSD): under construction
	2.2	Ultra-small angle scattering and TEST: under construction
3	3.1	Photo-ionisation spectroscopy (atomic and molecular): Seya monochromator
	3.2	High resolution spectroscopy (atomic and molecular): 5m McPherson monochromator
	3.3	Photoelectron spectroscopy (gas phase): Toroidal grating monochromator
	3.4	Soft X-ray EXAFS (SOXAFS) and contact microscopy/lithography
5 (Undulator Magnet)	5U	Focussing soft X-ray microscopy using undulator magnet: under construction
6	6.1	Angle dispersed photoelectron spectroscopy (solids): Grazing incidence monochromator
	6.2	Angle dispersed photoelectron spectroscopy (solids): Toroidal grating monochromator
	6.3	Surface EXAFS (SEXAFS)
7	7.1	EXAFS (with or without pre-mirror)
	7.2)*	Protein crystallography (PX) high angle fibre diffraction (HAPD)
	7.3)	Small angle scattering and fibre diffraction (SAS/FD)
	7.4	Transmission EXAFS; Energy dispersive EXAFS (under construction); TEST
	7.5)*	Topography (TOP): double crystal
	7.6)	Topography: white radiation

Magnet	Stations	Technique
8	8.1	EXAFS
	8.2	Small angle diffraction (SAD)
	8.3	TEST
9 (Wiggler magnet-hard radiation)	9.1	Powder diffraction (PD)
	9.2	EXAFS (hard X-ray)
	9.4a*)	Topography : double crystal or white radiation
	9.4b)	Surface diffraction: under construction
	9.6	Protein crystallography. FAST TV detector High angle fibre diffraction (HAFD)
	9.7	TEST. Laue diffraction energy dispersive diffraction : under construction
10	10.1	Test chamber : initially for optical components
12	12.1	Fluorescence lifetimes and time resolved spectroscopy
13	13.1)*	Infra-red spectroscopy
	13.2)	General purpose spectroscopy : to be re-built post HBL. FT IR spectroscopy development under consideration by SRFC

(EXAFS-Extended X-ray absorption fine structure)

* signifies dual purpose or separate stations which are not independently operable

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TABLE 2 SRS YEARLY OPERATING STATISTICS 8/6/81 to 31/3/86
(based on data from 1 April to 31 March each year)

	MULTIBUNCH BEAM		81/82	82/83	83/84	84/85	85/86
1.	Scheduled Multibunch	(Hrs) :	2195	3179	2232	4392	5400
2.	Achieved Multibunch	(Hrs) :	1391	2132	1597	3293	4157
3.	Allowance for filling and inspection	(Hrs) :	244	353	248	488	600
	Multibunch efficiency (2/(1-3))	:	71.3	75.4	80.5	84.3	86.6
	SINGLE BUNCH BEAM						
.	Scheduled Single bunch	(Hrs) :	--	694	312	978	1144
5.	Achieved Single bunch	(Hrs) :	--	360	157	561	789
6.	Allowance for filling and inspection	(Hrs) :	--	77	35	109	127
	Single bunch efficiency (5/(4-6))	:	--	58.3	56.7	64.5	77.6
	WIGGLER BEAM						
7.	Total Wiggler Beam	(Hrs) :	--	--	292(*)	2922	3933
	Wiggler efficiency (7/(2+5))	:	--	--	--	75.8	79.5

(*) Wiggler not scheduled for all this period

	TOTAL BEAM					
Total Scheduled Beam	(Hrs) :	2195	3873	2544	5370	6544
Total Possible Beam	(Hrs) :	1951	3443	2261	4773	5817
Total Achieved Beam	(Hrs) :	1391	2492	1754	3854	4946

NOTE: Beams of less than 2 hours duration are not counted in the "Achieved Beam"

beam for commissioning or for experiments has grown from 3 to 21 (counting alternates as one) so that the number of station-hours per year has increased 25 times, with a large part of the increase effectively occurring since June 1984.

16. Under an Agreement established in March 1982 the programme of biological research at the SRS is jointly funded by SERC and the Medical Research Council (MRC), who also contribute to the cost of relevant capital developments at the SRS such as the High Brightness Lattice. In addition, the two Councils jointly fund the Biological Support Laboratory which provides the on-site facilities necessary for the preparation and characterisation of biological samples. The Laboratory provides a scientific environment that enables the biological community at large to undertake research and development related to synchrotron radiation at Daresbury, and the staff carry out an approved in-house research programme.

17. At the end of 1981 SERC reached an Agreement with a consortium of industrial firms for use of the SRS. The Industrial Consortium includes the British Petroleum Company Ltd, Imperial Chemical Industries plc and Shell Research Ltd. The Agreement covers the period January 1982 to March 1987 and involves the provision of the order of 400 service shifts. The Consortium receives the usual back-up services provided by the Daresbury Laboratory, although additional payments are required for data processing and access to other facilities beyond those of a "standard" nature. The Agreement allows the Consortium members to carry out proprietary research at the SRS without the need to go through the SERC peer-review system. The majority of the work carried out by the Consortium members involves the use of the EXAFS stations together with a small amount of time on the small-angle scattering and powder diffraction stations.

18. On 2 December 1982 an agreement was reached between the SERC and the Nederlandse Organisatie voor Zuiver Wetenschappelijk Onderzoek (ZWO) concerning the use of the SRS by experimenters from The Netherlands, and the provision by ZWO of a beamline and two stations on Port 8 of the SRS and an operational scientist. The stations for Small Angle Diffraction studies and the station for Extended X-ray Absorption Fine Structure (EXAFS) studies have been installed and commissioning is well advanced, and several Dutch scientists have already used existing experimental stations at the SRS. The Agreement expires on 1 December 1987 and a review will be undertaken during 1986, when extension of the Agreement beyond 1987 shall be considered.

19. Since November 1981 the Swedish Naturvetenskapliga forskningsrådet (NFR) has purchased station-shifts at the SRS to enable Swedish scientists to submit experiment applications through the SERC's peer review procedures either independently or in collabortion with UK researchers. So far Swedish scientists have used of the order of 200 shifts.

Scientific Achievements at the SRS

20 The major scientific achievements at the SRS are described in detail in Appendix 1. These descriptions are based on the presentations made at the science review meeting on 7 February 1986 by members of the Synchrotron Radiation Facility Committee and leading UK researchers, with views of members of the Review Panel. Here we summarise the main research areas and achievements at the SRS and introduce some more subjective commentary. The topics are set out in a series of headings based on synchrotron techniques and subject areas of science arranged in an order designed to reflect the spectral range of synchrotron radiation moving from hard X-rays through soft X-rays, ultraviolet and the infrared region.

21. X-ray topography is an imaging technique which maps localised lattice strains in nearly perfect crystals and is used to produce photographic images of defects such as dislocations and stacking faults. It has been used to great effect at the SRS for dynamic studies of changes in defect structure during physical and chemical processing, for statistical examination of crystal growth and for experiments exploiting unique features of synchrotron radiation such as diffuse scattering of white radiation in the identification of "voidites" in diamond. The community is active, it is carrying out experiments which would otherwise be impossible and is working at the forefront of international science.

22. Protein crystallography has exploited synchrotron X-ray radiation in several different ways. The most promising work concerns time-resolved studies of enzymes undergoing reactions. This has already been achieved at the SRS using conventional techniques but exploiting the high brilliance of the source. Laue techniques are being developed to use the even higher flux of white radiation from the storage ring. Exposure times of a few seconds on small crystals yield thousands of Bragg spots which will be used to solve structures. Protein structure solving has been achieved on many crystals at higher resolution because of the unique X-ray optical properties of

synchrotron radiation. Extremely small crystals have also been shown to be usable. Elsewhere anomalous dispersion techniques using several X-ray wavelengths have been used to solve the phase problem by working near the absorption edge of natural metal ions or ions added to the crystals. This is a major opportunity which the UK community will be well placed to exploit now that the FAST area detector is starting to operate satisfactorily. The protein crystallography community in the UK is well organised, has been well served by the SRS and enjoys a high international reputation. In the future, improved conventional sources coupled with the new generation of area detectors may supplant the SRS for routine rapid data collection. The time released will be rapidly absorbed, however, by other novel experiments which demand the characteristics of the SRS.

23. After initial problems, X-ray diffraction of powders and amorphous solids has become a flourishing and productive area of synchrotron science in the past twelve months. The spectral continuum is being exploited to determine partial correlation factors using anomalous dispersion, and energy dispersive techniques are being used for rapid data collection under changing pressure and temperature. The collimation of the beam gives excellent resolution in a technique that depends on separation of diffraction peaks and determination of their shapes while the high intensity allows rapid data collection. Zeolite structures are being determined, binary metallic glasses examined and induced phases in inorganic compounds studied. The science at the SRS is clearly now expanding quickly and is internationally competitive.

24. Synchrotron radiation has revolutionised X-ray absorption spectroscopy. Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy exploits the tuneability of the radiation and is used in the vicinity of the absorption edge of a metal to determine the distance to the surrounding atoms. A related technique - X-ray Absorption Near-Edge Spectroscopy (XANES) - refers to the spectrum closer (50eV) to the absorption edge and requires a more complex multiple scattering theory but gives angular information as well as distances. The methods have been powerful tools in the study of metal ions in a variety of metalloproteins and some important successes have been obtained at the SRS. The methods are equally powerful in the study of metals in glasses, in catalysts and in metal complexes in solutions. Surface-sensitive EXAFS have extended the use of the technique in the areas of surface chemistry and catalysis.

25. X-ray fluorescence (XRF) for trace element analysis at the SRS has demonstrated sensitivities for metal ions of an order of magnitude greater than those obtainable when using conventional laboratory-based sources. The trace element analysis demonstration experiment was a joint UK/Dutch venture on the topography station which has already demonstrated 0.05ppm for copper in glass, analysed arsenic in silicon, and correlated impurities in precursor germanium with poor device performance. The method has applications in biological systems of agricultural and medical interest.

26. Small angle scattering using X-rays of ~1Å wavelength gives important structural information on viruses, biological fibres and synthetic polymers especially when supported by electron microscopy, neutron scattering and modelling. The major advantage of synchrotron radiation is the intensity which allows studies of weakly diffracting specimens and time resolved studies which are impossible with rotating anode X-ray generators. Several of the UK groups working in the area of muscle still have their major achievements at Hamburg. Although work at the SRS has been slow due to lack of station time and of resources to provide state-of-the-art detectors, there are notable achievements in polymers, liquid crystals and several biological systems including collagen and some exciting time resolved studies on DNA transformations.

27. A range of photoelectron spectroscopic, and lately diffraction, techniques exploiting the brightness, tuneability and polarisation of synchrotron radiation over the entire energy range - UV, VUV and soft and hard X-ray ranges - are being applied to surface science. There have been significant advances in photoemission studies of metals in semiconductors, on the electronic structure of random substitutional alloys, on low dimensional metal/metal systems, on growth mechanisms of semiconductors on semiconductors and in the technique of surface EXAFS. The international standing of the work is high but the investment is low compared to that of Germany and the United States.

28. Soft X-ray microscopy using synchrotron radiation offers considerable promise for the biologist in producing images of living systems in an aqueous environment without fixing, staining or freezing. The method will exploit the window between 23Å and 43Å where proteins absorb more strongly

than water and should ultimately give a resolution of ~100 Å, although specimen damage may restrict exposure times. Contact imaging using a photosensitive resist has been actively pursued at the SRS. A scanning microscope using a zone plate is being developed and will soon be used on the undulator line at the SRS. UK groups currently lead the world in technical achievements in this area.

29. Synchrotron radiation makes available exciting possibilities for the study of atoms, molecules and clusters using soft X-rays and VUV radiation in spectroscopy, collision physics and molecular dynamics. The experiments are not only of fundamental importance but also provide services to astrophysics, plasma physics, the study of low dimensional solids, photochemistry and surface science. Highlights have included the study of photoionisation of charged ions, and the determination of decay modes of molecular ions. Future use of the "threshold electron" technique will lead to insights into long range electron-electron correlations.

30. The Theory Group at Daresbury provides strong support for certain areas of research in the SRS programme. For instance, it has developed theoretical and computational methods for calculating photoemission, EXAFS and XANES spectra, and also absorption spectra of atoms, ions and molecules, which have been crucial for the extraction of information about atomic and electronic structure of atoms, molecules, solids and surfaces. Magnetic and alloy systems are examples of solid-state materials now under investigation; new surface methods are also being developed which will contribute to the interpretation of surface-sensitive probes.

31. There has been very little activity in far infrared spectroscopy, where preliminary experiments have demonstrated a high background to noise ratio probably due to the design of the extraction optics. The optics are now being re-designed for installation when funding permits: potential applications are in infrared active lattice modes and dielectric properties of a range of materials.

32. The portfolio of experiments at the SRS has notable gaps; for example work elsewhere includes digital subtraction angiography (described in paragraph 33), circular dichroism, magnetic X-ray scattering, inelastic scattering, standing wave analysis and a fluorescent Mössbauer demonstration experiment. Some undoubtedly represent lost opportunities of importance but

it would be unrealistic to expect the UK community to be equally active in all areas of synchrotron radiation science.

33. Angiography - the non-invasive imaging of blood vessels - can exploit the tuneability of synchrotron X-ray radiation by subtracting images just above and below the absorption edge of the iodine in the contrast medium. It may prove to be useful in identifying incipient blockage before occlusions occur in coronary arteries. This is an area where the initiative must come from the medical community. It is the subject of considerable activity in Stanford, at DORIS in Hamburg and at the Photon Factory in Japan. However, the cost per patient may rule out the use of the technique on a routine basis. Little interest has been shown so far by the UK medical community and no work in this area has proceeded at SRS. It would be wise to maintain close contact with the groups at other sources so that prospects can be re-evaluated.

34. The experiments described in paragraphs 21 to 33 all depend on multi-bunch mode operation - 160 bunches of electrons circulating in the ring - which generally produces the maximum output. In single bunch mode the SRS delivers 210ps wide pulses every 320ns. The teething problems in developing reliable single bunch operation at the Daresbury Laboratory were considerable and it was not until 1985 that single bunch mode was 70% reliable at a ring current of 20mA; 15% of SRS running time is now allocated to this mode. In the last year progress has been very encouraging in fluorescent lifetimes and time-resolved studies on fluorescent depolarisation anisotropy. These have given information about the structure and dynamics of biological systems such as phospholipid bilayer membranes and proteins, as well as inorganic systems such as novel reactions in gaseous ion-pair states. This latter experiment being uniquely possible on a synchroton source.

Views of the Subject Committees and Other Research Councils

35. The SERC Subject Committees and other Research Councils were represented at the review of synchrotron radiation science held by the Panel on 7/8 February 1986 and subsequently produced reports which are included in Appendices 2 and 3. Committees noted with regret the lack of discussion of costs and the consequent difficulties in making statements concerning "value for money".

36. The Biological Sciences Committee was impressed by the scientific achievements, especially in protein crystallography, in small angle scattering of fibres and in EXAFS of metalloproteins. It found a "modest potential" for wet X-ray microscopy but felt this was some years away from being achieved. Some useful achievements using the single photon counting instrument for fluorescence anisotropy were also identified.

37. The Chemistry Committee felt that the most widely used application for synchrotron radiation to chemical science was in structure determination in its broadest sense, including X-ray diffraction, X-ray absorption spectroscopy, X-ray topography and photoelectron spectroscopy. It noted the applications of relevance to the Committee's forthcoming initiative on catalysis and interfaces. The Committee took the view that, although lasers are more convenient in the visible and near ultraviolet regions, the synchrotron is the only practical source of tuneable radiation for spectroscopy at wavelengths shorter than 250nm. The Chemistry Committee noted that at very long wavelengths the flux and brightness of the synchrotron radiation source become superior to those of tuneable laboratory sources, making vibrational and microwave spectroscopy attractive.

38. The major areas of interest to the Physics Committee were X-ray topography, the study of surfaces and interfaces of relevance to low dimensional structures (LDS) and catalysis initiatives, and VUV and soft X-ray studies of atoms where there was considerable potential in limited areas. The Physics Committee was not enthusiastic about the achievements in physics at the SRS. It noted the contributions of physicists in the development of areas such as EXAFS, X-ray microscopy and far infrared spectroscopy but saw little applicability to physics either in these areas or in small angle scattering, in trace element analysis or in single bunch mode experiments. The Committee recognised the interest to biophysicists and medical physicists of protein crystallography and angiography. In general the Committee considered that the physics at the SRS was not outstanding and that there was a history of technical problems which required the SSRP to consider the management and reliability of the facility. The Physics Committee noted that expenditure on physics research at the SRS was probably about 67% of that of mainstream grants and exceeded that allocated to low dimensional structures.

39. The Laser Facility Committee noted that research of impressive quantity and quality had been carried out in the past year of sustained operation, but that VUV and single pulse operation had not been as productive as main stream X-ray work. The Laser Facility Committee considered lasers to be the most appropriate sources for wavelengths above 120nm because of low cost, flexibility and extremes of accessible characteristics such as short pulses, high spectral brightness and narrow bandwidth. From the comments of the Laser Facility Committee and discussions at the February Review Meeting the Review Panel noted that although undulators clearly will provide VUV and soft X-ray radiation brighter than the SRS, this is a region of the spectrum also available in the radiation from intense plasmas generated from excimer lasers. For certain time-resolved experiments where high peak power and short pulse duration are required, laser sources will be invaluable. For other work the plasma source remains to be developed and its competitiveness in terms of average brightness (average flux per solid angle), cleanliness (perhaps requiring elaborate differential vacuum pumping), and cost remains to be assessed. Moreover the low duty cycle may create difficulties for some types of detector.

40. The Synchrotron Radiation Facility Committee (SRFC) was enthusiastic about the research achievements at the SRS and felt that the resumé included in Appendix 1 was useful, but noted that the description of activity in protein crystallography underplayed the unique contribution of the SRS. It also noted that the resumé referred mainly to work carried out in the past year and hoped that this would not be taken to indicate that little had been achieved previously. It requested that the attention of the Review Panel and other Committees be drawn to the summaries and list of publications presented in previous Daresbury Laboratory Annual Reports. The SRFC was critical of omissions in the reports of the Subject Committees. For example, the SRFC placed greater emphasis on the time-resolved experiments than was contained in the report from the Biological Sciences Committee. The SRFC was particularly concerned about the report from the Physics Committee, which it considered to be open to misinterpretation. It felt that the slow progress at SRS in atomic and molecular science was associated with difficulties in the development of suitable monochromators. Nevertheless, of the seven items listed by the SRFC as highlights in the 1985/86 programme, three came from atomic and molecular beam workstations.

41. The Materials Committee, of the Engineering Board, considered that more members of the Materials community were becoming aware of the capabilities of the SRS. Given the excellent state of working order which the Committee understood that the SRS had now attained, and in view of the spectacular advances in the understanding of materials which current instrumentation trends were making possible, the Committee foresaw the SRS playing a gradually increasing part in its work. It was of the essence, however, that the facilities and data interpretation be provided as a service on a reliable 'production' basis, with strong user control. The major areas of interest to the Materials community were held to be surface science, topography, small angle scattering with liquid cell facilities, rocking curve analysis of thin epitaxial films, EXAFS (atomic sites or clusters in solids) and lithography using a dedicated VUV source. Longer term interest would include surface EXAFS (semiconductors, metals and ceramics), small probe (1 μm) microanalysis and X-ray microscopy (polymers). The Committee would be keen to see more substantial Engineering Board involvement in the SRS. It recommends, however, that this be conditional on achieving a consensus that the SRS is a 'production' machine and that any modifications requiring a significant down time should be subject to a vigorous cost benefit analysis involving all users.

42. The Agricultural and Food Research Council (AFRC) supports a limited number of projects, both in its Institutes and at universities, in which use is made of synchrotron radiation. There does, however, appear to be an increasing requirement for the use of SRS techniques in the research programme which would confirm that the limited experience to date values the use of these facilities in the achievement of agricultural and food research objectives. This increased use is expected to continue in the future as the benefits from the use of SRS techniques are established. One specific area that is reporting an increased requirement for the SRS facilities is the food research programme. The long term plan for the SRS would appear to offer the kind of facility that would be appropriate to support the AFRC's proposed research programme, and there is no indication at this time that the planned ESRF would offer particular benefit for the AFRC programme over that to be provided by present and projected SRS facilities.

43. The Medical Research Council (MRC) commented that bearing in mind developments at the SRS now in the pipeline to which it has agreed to make a

capital contribution (the high brightness lattice and the time resolved X-ray diffraction facility), the Council foresees that there will continue to be biomedically important and timely projects for which access to a synchrotron source will be esssential. Projects which meet these criteria at present include in particular time-resolved studies, for example of enzyme kinetics in crystals and of muscle contraction. Adequate beam-time from an appropriate source needs to be allocated to these advanced projects, if necessary at the expense of less advanced projects, and they should be properly supported with the required instrumentation.

44. The Natural Environment Research Council (NERC) commented that there is currently very little active participation in the SRS programme by research workers in the NERC field. Work by researchers at Manchester University, involving use of EXAFS on glasses as a means of modelling melt structures, however, is highly regarded by the NERC. Looking to the future, the research interest is likely to grow and the ability to detect very low level trace elements (in comparison with conventional techniques) is potentially of such great interest, for example in geochemistry, that NERC involvement may grow rapidly. One area of fruitful NERC/SERC collaboration could be joint projects, utilising the facilities and expertise of NERC-supported high pressure and high temperature experimental facilities, with SERC materials scientists.

Comments of the Review Panel

45. The Synchrotron Science Review Panel is enthusiastic about the quality of the research now being achieved at the SRS. It notes that problems with the RF cavity windows and other machine faults denied the scientific community reliable access for considerable periods in 1983 and 1984, and that it took several years to build and commission a reasonably comprehensive set of instruments and stations. The period since mid-1984, however, has witnessed a spectacular growth in high quality research over a broad area as the source consistently performed up to its specification. In 1985 over 6000 hours of beam time were provided - an extremely high figure for a storage ring. The availability of a good beam and the implementation of new beam lines and experimental stations has revolutionised the research: this is particularly true of surface studies using photoemission and SEXAFS, and generally in X-ray spectroscopy and X-ray diffraction applied to the study of molecular structure.

46. The Review Panel is concerned about the "sluggishness" in funding and implementing decisions concerning equipment and new ideas at new experimental stations particularly in the surface science area.

47. The Review Panel notes the lack of high quality and reliable detectors. The FAST area detector will radically change protein crystallography in the future, and a reliable wire chamber has now been achieved; but investment is urgently required in a wider-ranging development of detectors for most beam lines. This is a world-wide problem. Effort in this area, as in other aspects of instrumentation such as monochromators and mirrors, over the next few years, would pay substantial dividends. This is particularly so for those which might have multilayer optical coatings similar to the multilayer systems which are part of the current Science and Engineering Boards initiatives in growing such structures. The work is challenging and could, at least in part, be appropriate to University research departments, providing valuable training and possible spin-off to other (non-synchrotron radiation) applications.

48. The Review Panel is concerned about the almost total lack of activity in synchrotron studies of materials by the Engineering Board research community and lack of enthusiasm and imagination amongst physicists for synchrotron research in many areas of solid state physics. This is in direct contrast to activity at other synchrotron sources which concentrate on solid state physics and materials science. The Review Panel noted, however, the Materials Committee's views that the interest of the UK Materials community is now expected to grow.

49. The Review Panel wishes to underline the importance of diffraction and spectroscopic studies in the chemical sciences.

50. The Review Panel welcomes the new structure of user support now being set in train at the SRS. The appointment of Professor M Hart as Science Programme Coordinator has had a stimulating effect on activity, and the organisation of support staff into teams responsible for experimental stations is welcomed.

III. THE ACADEMIC USER COMMUNITY

51. The survey of the academic community included SRS users and Heads of Departments of Biological Sciences, Chemistry, Physics, Materials Science and Electrical Engineering in Universities and Polytechnics. The findings of the survey underlined the widespread depth of interest in the use of synchrotron radiation. Research groups in some 49 Universities and University Colleges and 9 Polytechnics were identified who expected either to continue or to develop research programmes involving the use of synchrotron radiation. Within these centres the survey confirmed that the spread of interest pervaded many branches of science; research groups were located in some 37 Biology Departments, 42 Chemistry Departments, 33 Physics Departments and 11 Departments of Engineering (including Materials/ Metallurgy Departments). The summary of the energy ranges of interest to the academic community identified from the survey is given in Figure 1.

52. The activity and interest of the Biological Sciences community was reflected in replies from 37 different departments which were mainly biochemical or biophysical in orientation. The main areas of interest were in cell or molecular biology or medical biophysics and covered a range of techniques including X-ray diffraction (15), small angle scattering (17), time-resolved fluorescence spectroscopy (16), X-ray microscopy (7) and EXAFS (17). There was also limited interest in angiography, circular dichroism and mutagenesis studies (over a range of wavelengths) which are not currently planned for the SRS. There is a general interest in time-resolved studies reflecting the importance of the dynamics of biological systems. The community expressed concern that proper beam line support personnel, good detectors and a broader range of support facilities such as cold rooms are made available (though two cold rooms are now available at the SRS).

53. Some 42 Chemistry Departments expressed an interest in synchrotron radiation science and the potential user community appears to be larger than that in biology. The areas of interest mentioned covered materials science (20), general chemistry (34), surface science (24), atomic and molecular physics (6), condensed matter physics (7) and molecular and cell biology (8). Instrumentation was of special interest to eight groups. The major techniques were EXAFS (38), X-ray diffraction (18), small angle scattering (10), fluorescent studies (16), photoelectron spectroscopy (19) and

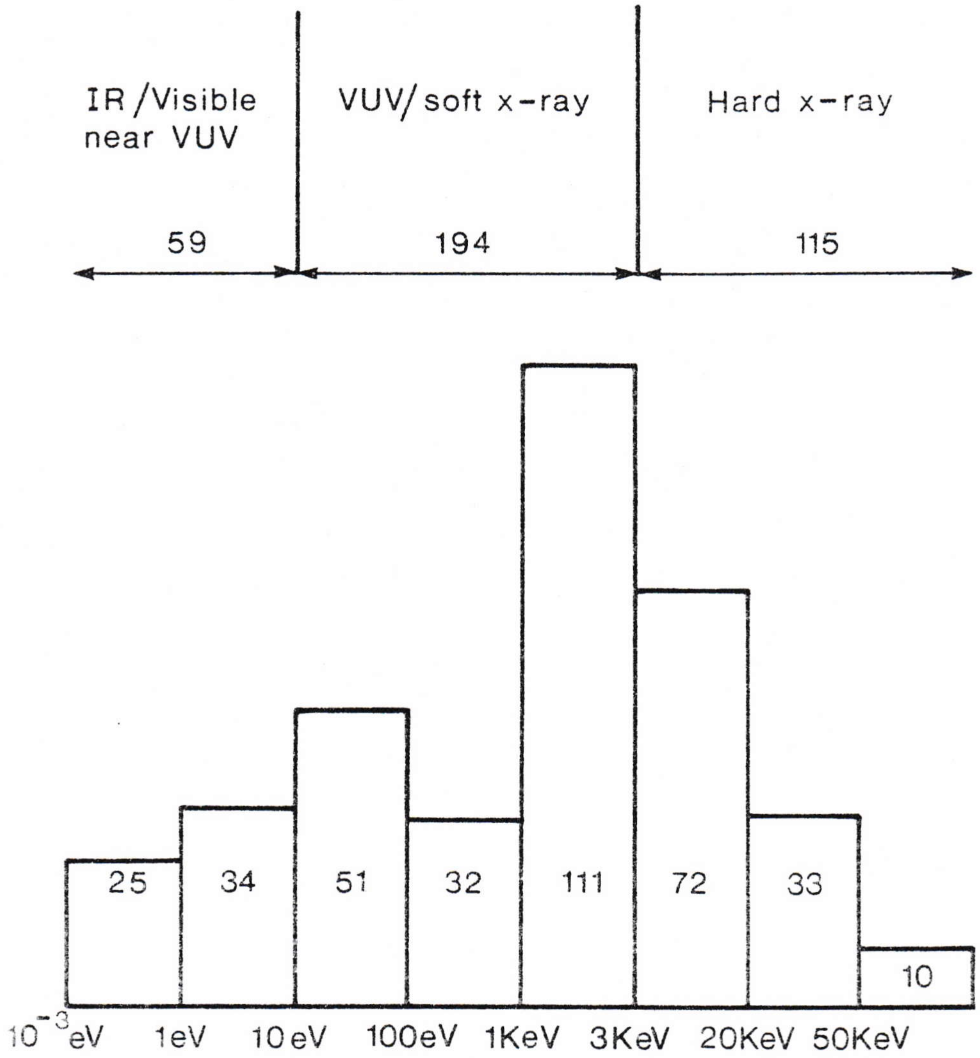


FIGURE 1: SUMMARY OF ENERGY RANGES OF INTEREST TO ACADEMIC USERS (NUMBER OF RESEARCH GROUPS SHOWN IN FIGURES) - AS DERIVED FROM THE SURVEY OF ACADEMIC USERS

topography (3). The community appeared to be generally happy about SRS facilities although shortage of experimental stations and personnel are of concern.

54. A total of 33 Physics Departments responded to the survey and demonstrated the existence of a large community with a wide range of interests which included atomic and molecular physics (9), condensed matter physics (22), materials science (21), surface science (14) and some biology (5). The techniques included EXAFS (16), X-ray diffraction (15), photoelectron spectroscopy (12), microscopy (3) and topography (3). There were many comments that the SRS satisfied the needs of present users although many commented on the desirability of improving instrumentation and in particular detectors. There appeared to be widespread support for more intense ultraviolet facilities.

55. There was very limited interest in synchrotron science expressed by Electronic and Electrical Engineering, Materials and Metallurgy Departments. Only eleven departments replied to the questionnaire. The main interests were in absorption spectroscopy (11), photoelectron spectroscopy (3), fluorescence spectroscopy (2), X-ray diffraction (6) and topography (3). The Review Panel is concerned about the lack of achievements by engineering departments in synchrotron radiation science.

56. The Review Panel notes the steady growth of the user community, as shown in Figure 2. Taking into account the undoubted influence of the window problems in 1983/84, on the demand for time, the subsequent rise in demand for beam time is broadly in line with the predictions of the SRFC in 1983 of a 20% growth in activity per annum between 1980 and the early 1990's.

57. The Review Panel is concerned that the interest shown in the physics community is not reflected in the SERC Physics Committee's comments. This disparity requires further investigation.

IV. INDUSTRIAL INTEREST IN SYNCHROTRON RADIATION SCIENCE

58. The survey of industrial interest in synchrotron radiation has involved (i) companies that have already been involved in the SRS programme,

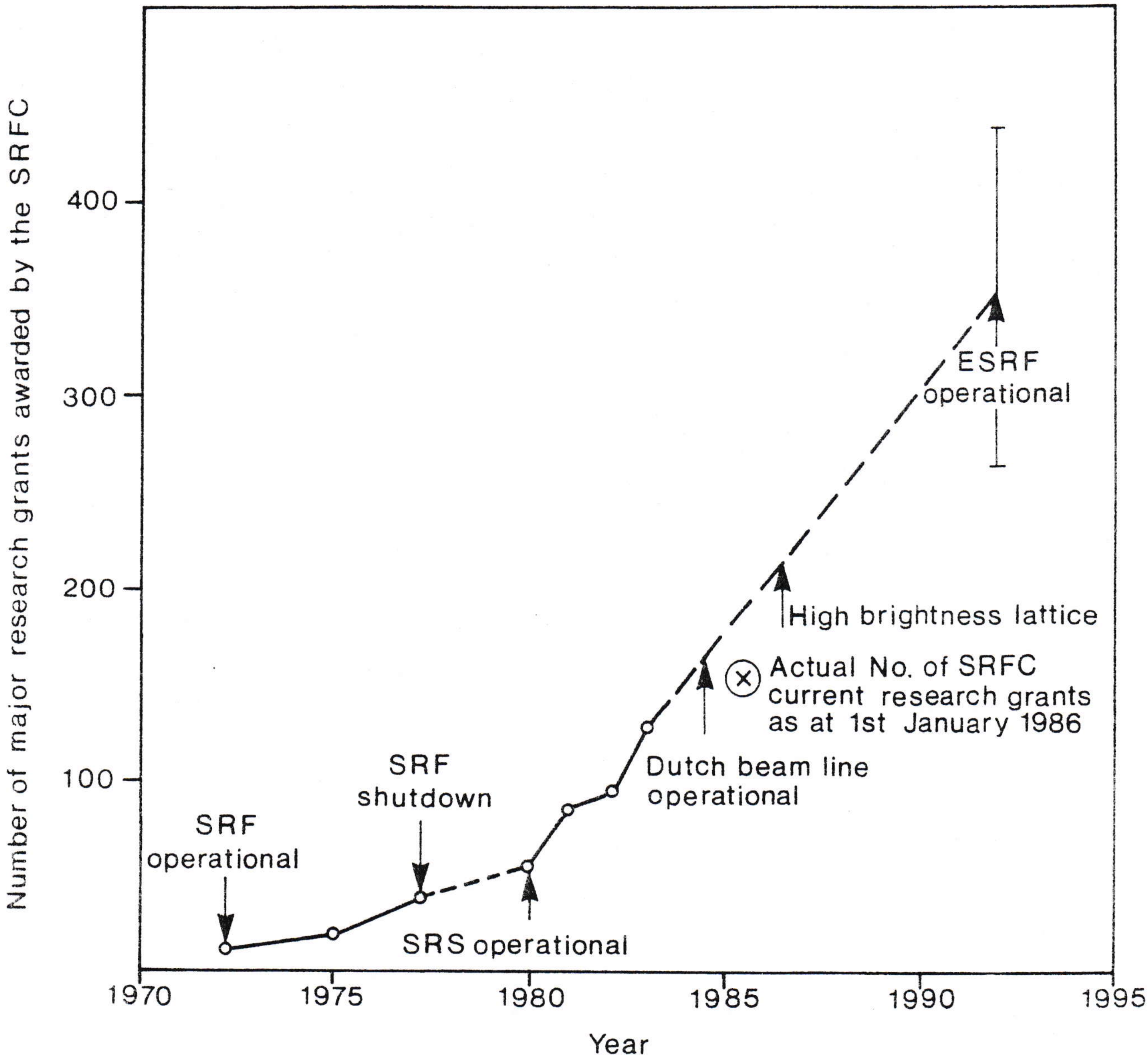


FIGURE 2: GROWTH OF THE UK SYNCHROTRON RADIATION USER COMMUNITY AS PROJECTED BY THE SYNCHROTRON RADIATION FACILITY COMMITTEE (SRFC) IN 1983

either independently (eg industrial consortium members) or in collaboration with academic researchers and (ii) companies that have not so far been involved in the SRS programme.

59. In the first category some 22 companies, involving more than 40 research groups, were approached. Each company was asked to record the expected future development of their requirements for synchrotron radiation and to comment on any barriers to progress in their use of synchrotron radiation sources, including the use of facilities overseas. Details of the SRS and ESRF parameters were provided, together with brief extracts from the October 1984 European Synchrotron Research Project (ESRP) Report. 11 companies replied to the survey.

60. In the second category 54 companies were approached. They were chosen from the chemical, optical, semiconductor and mechanical engineering industries with an R and D expenditure greater than £1M per annum. Details of the SRS and ESRF parameters and a copy of the Report of the ESRP Study Group on "Industrial Uses of Synchrotron Radiation" were provided. Each company was invited to comment on the nature of their potential interest in future SR research and on any barriers to progress in their future use of SR facilities, including those overseas. 16 companies replied to the survey.

61. Extracts from 15 of the most detailed of the 27 replies are included in Appendix 4 which also contains a list of the 12 other companies who replied to the survey.

62. Very little interest was shown in lithography for below 0.5 μm soft X-ray replication of sub-micron devices and circuits. Only one major UK company indicated a programme in this area. Industrial preference was for stand alone X-ray systems where precision laser interferometric wafer stages and general layer to layer alignment can be optimised. This cautious approach contrasts with interest in Germany, United States and Japan. The electronics industry expressed interest in topography for semiconductors and surface EXAFS for dispenser cathodes.

63. Several companies with activities in the development of catalysts have current work at the SRS in absorption spectroscopy (EXAFS), X-ray powder diffraction, single crystal analysis and trace element analysis. Similar techniques have been used by companies involved with amorphous

structures such as metallic alloys or random aggregates such as cements. These techniques offer opportunities for expansion in the industrial area.

64. Biological and organic polymers have been studied by the food and synthetic materials industry using small angle scattering and EXAFS. As the food industry becomes more research oriented there should be opportunities for future industrial activity in this area also.

65. Industrial respondents to the synchrotron survey were much more critical of the service provided by the Daresbury Laboratory than their academic counterparts. Comments included:

- We would welcome a more reliable and better organised service with easier access so that we could schedule our work in advance.

- In addition to problems such as non-reliability, poor technical guidance/access to computing facilities/program documentation, overcrowded experimental areas and inadequate supporting laboratory facilities, certain techniques do seem to be oversold. It is important ..... to give instruction to set up experiments to give good, reliable data, rather than illustrations of what might be achieved by the techniques at their limits.

- The principal requirement for "industrial" use of the SRS is the reliability of the source itself and here the experience has not been very happy. It is necessary to obtain access on a fairly short time scale, say six weeks: many industrial problems have a tendency to appear to go away if a short term solution is not found!

- We may point out that in the past we have encountered difficulties with the EXAFS equipment not being ready for use for our work.

66. The uniformity of these complaints from industrial users partly reflects the difficulties with the source and the experimental stations in the past, much of which has been rectified prior to the past eighteen months. It also highlights the need for a proper service if industry is to be attracted to the SRS. University users have probably had no better service but they are more prepared to carry out experiments themselves,

given the basic facility. The Review Panel welcomes the establishment of a service in EXAFS which should be helpful and a similar pattern may be useful elsewhere. Certainly a special industrial liaison responsibility needs to be organised at the Daresbury Laboratory.

67. A second major area of criticism by industrial users concerned costs. Most felt the existing cost per hour excessive and some argued that given the payment of taxes by industry access ought to be on the same basis as that of academia, ie peer review but no charge, unless secrecy and no publications were required. Others favoured the use of CASE student awards and found this mode of interaction very useful. (Some 23 UK companies have been involved in 41 CASE projects making significant use of the SRS, see Appendix 4). Medium and small size companies found the alternative concept of building a beam line and making 25% available to academic users "particularly unattractive, demanding high manning levels and long term commitments to untried technology." In spite of these criticisms the industrial consortium has had a successful collaborative contract with SERC to use the SRS (this expires in 1987) for catalysis, polymers and surface coatings. This has allowed substantial technical progress in EXAFS, small angle scattering and topography and its use is seen as an important part of the companies' research activities in the future. It is hoped to extend the range of techniques to include fibre, film and liquid crystal diffraction, trace element analysis and 2D X-ray diffraction techniques for interfaces and surfaces.

68. Industrial respondents seem to be happy with the potential facilities at the Daresbury Laboratory and saw little prospect for use of a European Synchrotron Radiation Facility unless it were more economic.

69. The Review Panel notes the varying modes of interaction with the SRS required by the electronics, catalyst, materials and food industries. Where the technology is new and untried, exploratory agreements at no charge need to be used more flexibly, perhaps at the discretion of the Chairman of the SRFC or the Director of the Daresbury Laboratory. Equally there are opportunities for CASE projects and Co-operative Research Grant programmes through University/Industry collaborations. It is unlikely that UK companies have reached the critical size where building of beam lines becomes attractive as with the "big four" in Japan, (NTT, Hitachi, NEC and Fujitsu), and alternative collaborative arrangements along the lines of the

ICI, BP, Shell consortium need to be investigated. Such arrangements might include the use of an external agency acting on behalf of the SERC to both co-ordinate and develop industrial interest in use of the SRS. In addition, the Department of Trade and Industry should be encouraged to take into account the potential for industrial access to the SRS in its support of industrial research and development.

V. WORLDWIDE SYNCHROTRON RADIATION FACILITIES

70. The Review Panel undertook a detailed review of synchrotron radiation facilities on a worldwide basis. Appendix 5 contains a brief summary of their conclusions which have been based on direct visits. Appendix 6 contains reference data on synchrotron radiation laboratories worldwide.

71. The Review Panel notes the tremendous activity in storage ring construction and development in all major industrial countries of the world. Broadly the activity can be summarised in four categories:

(i) Synchrotron radiation sources comparable to the SRS (often not purpose-built as light sources but adopted later to provide synchrotron radiation) exist in the USA (eg SPEAR, CHESS), in Germany (DORIS), France (DCI and ACO), the Soviet Union (at Novosibirsk), Italy (ADONE) and Japan (Photon Factory). Most have been operational for several years and have a range of experimental stations comparable to those of the SRS, producing hard and soft X-rays, vacuum ultraviolet and ultraviolet radiation.

(ii) Later, purpose-built rings have been designed specifically for X-rays (NSLS II at Brookhaven) or for the VUV (BESSY in Berlin, Super ACO in Paris, NSLS I, Alladin at Wisconsin). BESSY was built especially for industrial soft X-ray lithography, and small industrial rings are now being developed in West Germany (Berlin), in Japan (eg by NTT), and in the UK (Oxford Instruments) for this purpose.

(iii) For advanced X-ray work, 5-6 GeV rings are proposed in the USA, in Japan, and in Europe (ESRF). At Stanford, PEP (a large high energy physics machine) may become a dedicated 8 GeV synchrotron source in 1987 (equivalent in specification to a purpose-built 6 GeV ring). In Japan, several "Technopolises" (industrial centres) propose to incorporate synchrotron radiation sources up to 6 GeV in energy.

(iv) For the increasingly important spectral region between 10 and 3000 eV, there are proposals for 1.5 GeV all-undulator rings at Trieste (CARS), Berkeley (ALS) and Berlin (BESSY II) which will be optimised to produce intense radiation in the soft X-ray and vacuum ultraviolet regions.

72. Few storage rings are presently operational three shifts per day throughout the year. For example, DCI Paris operates for 1300 hours per year compared with 6000 hours for the SRS at the Daresbury Laboratory. In Tsukuba, the Photon Factory runs for only four months of the year: this is a matter of policy and/or finance to allow developments to instrumentation to take place in between the periods of experimental studies. DORIS Hamburg is currently operating 6500 hours per year, but only 2200 in dedicated mode for synchrotron radiation.

73. The manpower at other synchrotron radiation sources is difficult to compare with that of the SRS. Many synchrotron radiation sources appear to have fewer personnel on their staff (particularly on computing) and fewer administrators. For example, HASYLAB has nine scientists and ten engineers and technicians: the Photon Factory in Japan has a staff complement of far fewer than 100 scientists, engineers, technicians and administrators. However, many sources operate for fewer hours and some give less support to users - in instrument construction and operation, data handling, data analysis and so on. BESSY, for instance, provides no facilities downstream of the monochromators. HASYLAB has a large number of postgraduate students who commit over half their time to station and user support. At Brookhaven, the membership of the Participating Research Teams numbers several hundred. Other differences include: differences in access to workshops and in industrial staff numbers; differences in handling administration and computing; support for the source and for the provision of insertion devices, beam steering etc; the use of private engineering companies and contract staff; the number of long-term visitors. Nevertheless, it is unlikely that the SRS is staffed in a perfectly efficient manner. The Review Panel believes that more manpower is necessary to provide

satisfactory user support but that this could probably come from within the presently foreseen complement. However, in order to make a proper assessment, a much more thorough study is required.

74. Most synchrotron radiation sources have a greater industrial activity than the SRS. Beam lines are being constructed by private companies at the Photon Factory and the Brookhaven National Synchrotron Light Source. Costs per hour appear to be comparable to those at the SRS when the facilities provided are taken into account.

75. Most synchrotron radiation sources have a considerably greater activity in materials science and solid state physics than in biological sciences, in contrast to the position at the SRS. For example, at the Stanford Synchrotron Radiation Laboratory X-ray physics and materials science are represented by:

> Structure of crystalline and amorphous materials; coordination of impurities and alloying species; structures of and phase transitions in surfaces and thin surface layers; kinetics of structural changes in materials; phase transitions at high pressure; electronic structure of materials; fundamental X-ray scattering and absorption physics; atomic physics.

In addition there is activity for the production of Very Large Scale Integrated (VLSI) semiconductor devices and other microstructures.

VI. THE POTENTIAL FOR DEVELOPMENT OF THE SRS

76. The Review Panel considers the maintenance and continued updating of machine and experimental facilities, to at least the year 2000, to be the most important objective for the future development of the SRS. This objective is both scientifically essential and straightforward in engineering terms.

77. The Panel's review has underlined the importance of the planned installation of the High Brightness Lattice (HBL), towards the end of 1986. This involves substantial changes to the arrangement of focussing magnets around the ring (known as the lattice). This major upgrade of the SRS

performance will match the increasing world-wide trend towards exploiting the very high radiation brightness possible in advanced storage rings, and bring the SRS close to state-of-the-art.

78. The Review Panel considers the implementation of a second superconducting wiggler magnet at the SRS to be an immediate and pressing priority because of the length of time that will necessarily be involved in the planning, construction and commissioning phases of the project. A start to the assembly of a second wiggler magnet in 1988 would allow its beam lines and 5 experimental stations to come on line from 1990-1991 (see Table 3, pages 42 and 43).

79. The present wiggler magnet is used for powder diffraction (9.1), EXAFS of elements with atoms of atomic number $\geqslant 30$ (9.2), topography for transmission work with atoms of atomic number $\geqslant 15$, (9.4) protein crystallography, fibre diffraction and small angle scattering (9.6) and interferometry, Laue diffraction, energy dispersive and exploratory work (9.7). A conflict already exists for station 9.4 with a 4-circle diffractometer for surface science. This would be resolved by a second wiggler magnet which would also have beam lines for energy dispersive powder diffraction, where there is an explosion of demand, anomalous dispersion studies of liquids and amorphous materials, duplication of station 9.6 to allow protein crystallography and small angle scattering to operate as dedicated experimental stations and a further EXAFS station with special optics.

80. The Review Panel is concerned that major programmes for the provision of access by UK researchers to new synchrotron radiation facilities should not interfere with current plans for the installation of a complement of around 30 experimental stations at the SRS. Continued development of instrumentation and detectors at the SRS should be a priority.

81. The Review Panel sees the ESRF, the SRS and an all-undulator VUV/soft X-ray ring essentially as complementary facilities. Unlike accelerators for high energy physics, synchrotron radiation sources do not become obsolete because higher photon energies become necessary. Exciting science will be achieved on all three sources because of the special characteristics of each. By the time that the ESRF and VUV/soft X-ray rings are fully operational (early 1990's) the UK synchrotron radiation community is likely

to have doubled in size. Thus, the existence of the other sources will not result in a decrease in either the quality or quantity of demand for the SRS.

82. The Review Panel sees opportunities for wider international collaboration in the SRS, along lines similar to those involved in the collaborations with Sweden and with the Netherlands. The provision of capital costs (and the associated operating costs) in this way would allow the exploitation of the SRS to be considerably increased. It would be possible under this scenario, to increase the number of experimental stations to about 40, which is the maximum number defined by the layout of the SRS.

VII. EUROPEAN SYNCHROTRON RADIATION FACILITY (ESRF)

83. In its operation to date, the Daresbury SRS has allowed the development of a strong, well consolidated effort in the broad use of synchrotron radiation for scientific research. The proposed upgrading of the source by the installation of the High Brightness Lattice (HBL) will enable UK scientists to maintain this position into the near future. As new national sources, currently being inaugurated and developed, come into full operation it will become more difficult to hold this position. Whereas excellent science can still be produced, the diminished characteristics of the SRS relative to the potential of other sources will limit the horizons of UK workers.

84. The inauguration of the ESRF and continued UK participation in the operation and development of the facility will provide the necessary expansion in horizons for X-rays. The enhanced source will bring significant advantages in source brilliance and extended energy range (Figure 3). These improvements will greatly extend the range of operation of experiments. They will allow increased spatial resolution and operation on a shorter time scale and with smaller samples. The potential capability of time resolution is at the sub-millisecond level. In total, it will open a new range of operation to the user both in the extension of existing studies and for novel experiments.

CONTENTS

Appendices

Figures

Tables

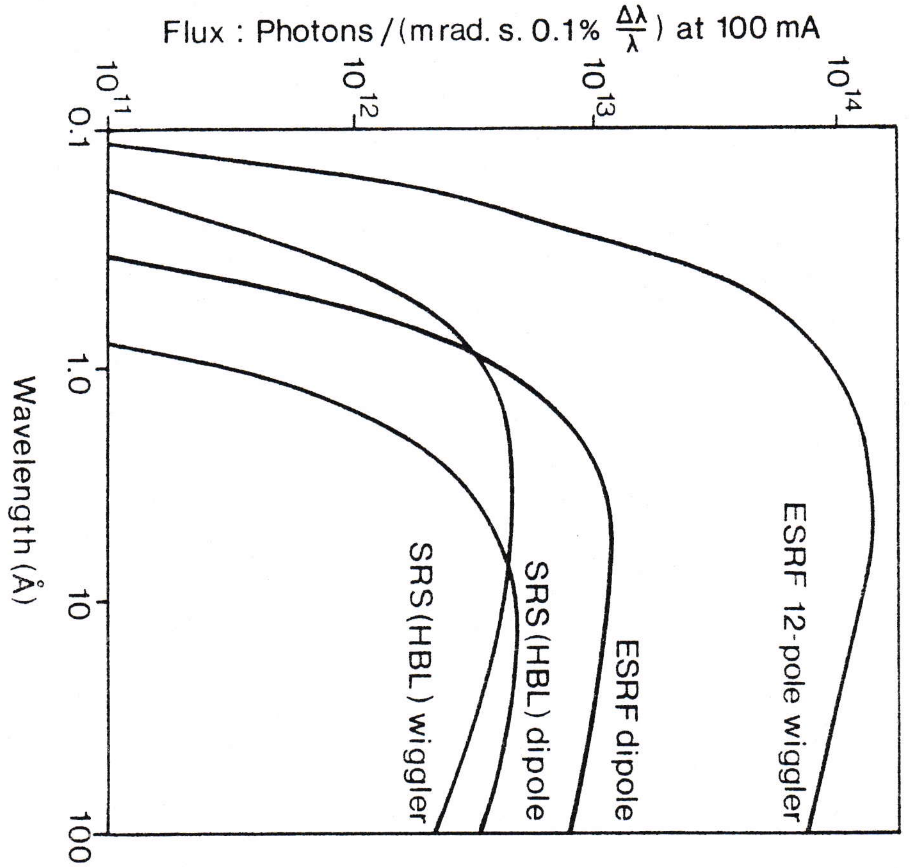
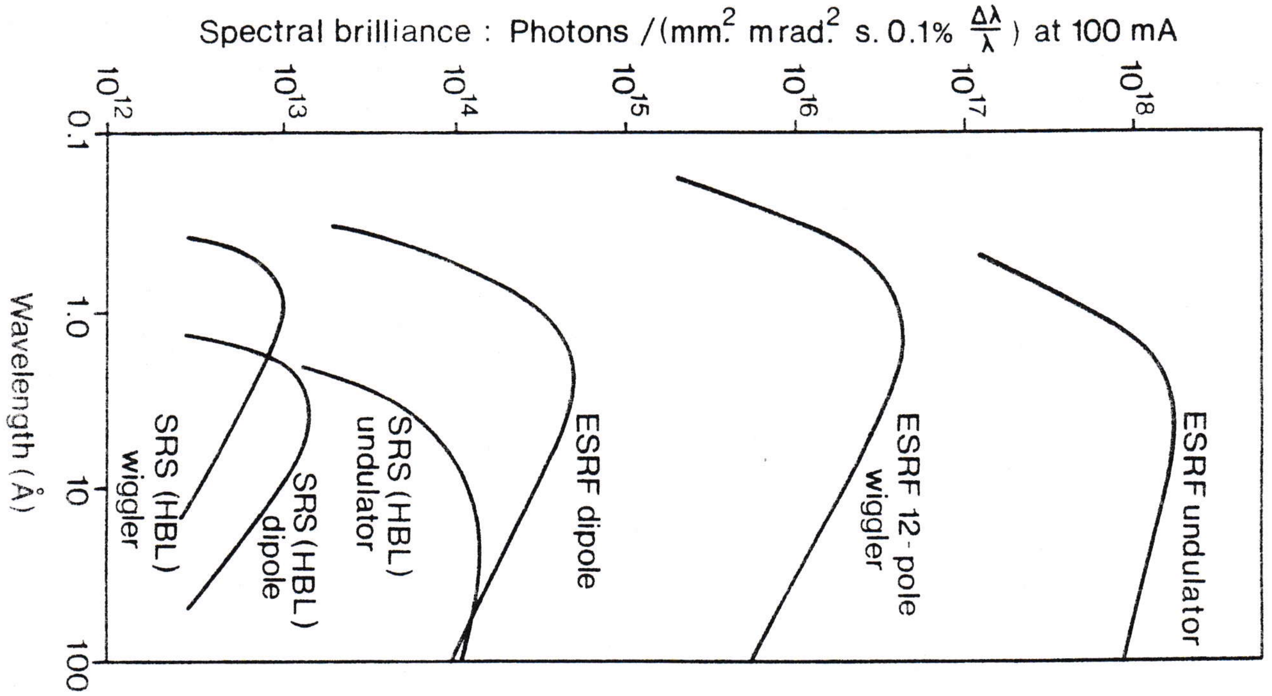


FIGURE 3:

A COMPARISON OF SOURCE PARAMETERS FOR THE SRS AND THE PLANNED ESRF



85. The potential scientific impact of the source has been well-described in two major reviews:-

- the Final Report of the SRFC Working Group on the ESRF
- the Report on the European Synchrotron Radiation Project (Buras and Tazarri, October 1984).

Both of these reports are available to Board members. They describe the improved potential of the ESRF over other sources and define a range of potential new experiments which could be carried out using the source. Many of these experiments will be impossible even on the improved (post HBL) SRS or other present generation sources eg Photon Factory, Tsukuba and the National Synchrotron Light Source, Brookhaven. A short summary of the experiments which was included in the SRFC's Working Group Report on the ESRF is set out in Appendix 7 to this report.

86. If research in the UK involving the use of hard X-ray synchrotron radiation is to flourish into and beyond the next decade, it is essential that UK participation in the ESRF is pursued. The ESRF will allow experiments to be carried out which are impossible or extremely difficult on conventional sources. For example, the high energy resolution of the order of 1meV will make phonon studies possible. High temporal resolution will allow microsecond time-resolved studies of biological systems such as enzymes, membranes and muscle and of phases changes in inorganic materials under extreme conditions of pressure, temperature, electrical and magnetic fields requiring pulsed conditions and direct timing rather than stroboscopy. A combination of high spatial, temporal and energy resolution will be advantageous in spectroscopy, diffraction, scattering in X-ray radiography materials science, solid state chemistry and biology. The ESRF will also make possible fluorescent Mössbauer resonant absorption experiments, circular dichroism, gamma-ray diffraction and studies of magnetic scattering having a broad range of applications in physics, chemistry and biology.

87. Based on the currently proposed involvement, the UK share of the ESRF will be equivalent to a few stations. This would be inadequate to maintain the total forecast UK hard X-ray effort. Most work would still have to be accommodated on the SRS with the ESRF used for those experiments for which its characteristics are essential and which would be impossible at Daresbury.

VIII. VACUUM ULTRAVIOLET (VUV)/SOFT X-RAY SOURCE

88. The energy range covered by the vacuum ultraviolet/and soft X-ray regions is 5eV (ca.2000Å) to 3000eV (ca.4Å). This range not only covers the valence levels of all atoms, molecules and solids, but also takes in the K levels of the elements up to chlorine. The experience at Daresbury and elsewhere has shown that the success of experiments in this spectral region is compromised at high energy storage rings because of the hard X-ray component.

89. The scientific communities which have the greatest need for an intense, polarised light source within this energy range (as would be provided by a suitably designed all-undulator ring) may be grouped under the following headings: (i) solid state physics and chemistry and surface science; (ii) gas phase physics and chemistry; (iii) biology. To date, the solid state physics and chemistry and the surface science group has made the most use of this energy range, though more recently the gas phase group has begun to make some major advances.

90. The spectral range from 200 to 1000 eV is particularly important because it covers the edge regions of carbon, nitrogen and oxygen, where there are important applications in chemistry and surface science and possibly also in biology. At the present time this is a spectral area which, on a worldwide basis, is rather underdeveloped, and this is particularly true at the SRS. The reason is that plane grating monochromators do not survive the high intensity of hard X-rays from the source, an example of the degree of incompatibility between hard X-ray and VUV demands on a single ring.

91. Solid state physics and chemistry and surface science. The substantial advances achieved to date at the SRS in this area are summarised elsewhere in this report. Here the following points may be noted:

(i) Angle resolved photoelectron spectroscopy is the single most powerful tool for studying band structures of solids, interfaces and surfaces, and the electronic structure of adsorbates. These experimental studies therefore underpin a very large and important area of solid state physics and chemistry, surface science and catalysis.

(ii) The techniques of EXAFS and its surface version SEXAFS have been widely exploited in these studies, covering a remarkably wide range of chemistry, physics and biology. The availability of a monochromator to cover the energy range 200 to 2000 eV would very greatly expand this area of work, bringing in the elements C, N and O, and also the related technique XANES.

(iii) An arsenal of powerful surface science techniques, not included above, has been developed which covers the VUV energy range, including: photon stimulated ion desorption; photoelectron diffraction; and high resolution core level shift spectroscopies.

(iv) More intensity would allow these studies to move into the very important time-dependent domain.

92. Gas Phase Physics and Chemistry. This is the most demanding area in terms of photon flux; the signal is derived from 10^9 to 10^{10} atoms. This community would benefit enormously from an all-undulator VUV/soft X-ray ring. Energy resolution (~10 meV) is also the most demanding. In its most powerful mode, these studies are made using supersonic molecular/atomic beams to provide gaseous species with well-defined rotational, vibrational and translational motions; crossed with the polarised photon source, a range of experiments can be performed, from molecular fragmentation to small metal cluster formation. These studies also strongly exploit the time structure of synchrotron radiation.

93. Biology. This community has yet to benefit significantly from radiation in the VUV region, but, particularly when the energy range 200 to 2000 eV can be exploited, there will be a very wide range of important applications. In addition to EXAFS and XANES, these include soft X-ray microscopy, for which the energy range 100 to 1000 eV is ideal, photoelectron microscopy, and holography, providing the opportunity to examine samples under wet conditions. These imaging techniques have a major advantage over the analogous electron-based techniques: incident probe damage is significantly reduced. Finally, the investigation of chemical sensors and biological layers associated with electronics would stand to benefit very substantially from a high-intensity dedicated VUV/soft X-ray source.

94. To provide access to more beamlines to meet the needs of an intensive programme of research in the VUV/soft X-ray region, bearing in mind the technical problems and extra cost of using X-rays and lower energy radiation from the same source, the best option would be to build a new source for lower energy radiation and use the SRS mainly for X-radiation. The level of present and anticipated demand requires a dedicated UK source, as does the nature of VUV/soft X-ray experiments, which demand extended periods of interactive experimentation and sample preparation. The option of collaboration in the proposed and existing European facilities is rejected on the grounds that it would be wholly inadequate to satisfy these needs.

95. The SRS could be completely rebuilt to provide very high brightness beams, including soft X-ray and VUV undulators, but this would involve a shut-down of at least 2 years and X-radiation would still emerge from all beamlines. The circumference would increase from 96 m to about 200 m and the extra cost of new experimental areas would be £4M. The cost of rebuilding the ring would be of the same order as the cost of the small ring mentioned below, but by using existing components a state-of-the-art performance would not be achieved. For these reasons the Review Panel does not support this option.

96. The lowest-cost option is to build a new ring constrained to fit (more or less) existing buildings. This would be similar to SUPERACO (800 MeV, low emittance) but with only four straight sections (3 undulators, for VUV radiation only, at most). The cost of the ring would be £5M with perhaps £1M for building work. This option is not supported by the Review Panel, as a major centre of scientific interest is in the soft X-ray region of the spectrum and moreover there is a requirement for a larger number of ultra-high brilliance beamlines.

97. A state-of-the-art VUV/soft X-ray undulator source with at least 8 undulators would cost £9-10M and need a new building costing £4-5M. This could be accommodated at Daresbury, using the existing injector. It would be fully competitive with sources being proposed elsewhere and is viewed by the Review Panel as the best option.

98. Similar to the multipole wiggler an undulator is a periodic electromagnetic structure which causes the electron beam to oscillate transversally. The angular deflection is, however, kept below the emission

angle of the synchrotron radiation, $1/\gamma$, so that there is coherent addition of radiation intensity from the different tangential points. Depending on angle of observation and wavelength, constructive interference occurs, giving rise to pseudo-monochromatic radiation. In comparison to synchrotron radiation emitted from dipole magnets, undulators offer the following advantages:

(i) Intensity: The achievable photon fluxes can be increased by one or two orders of magnitude;

(ii) Brilliance: The increase in brilliance of the order of 10^4 can in principle be transformed into high resolution without any significant loss of intensity.

(iii) Flexibility: Different undulators can be optimised for different experiments and used independently of each other on the same storage ring.

99. The realisation that the next generation of dedicated VUV/soft X-ray storage rings would be largely undulator-based came with the proposal in 1983 to build a so-called advanced light source (ALS) at the Lawrence Berkeley Laboratory. The construction of a 1.3 - 1.9 GeV storage ring with 12 straight sections was planned. Preliminary proposals for similar machines in Berlin, Trieste and Tsukuba have since appeared. The electron energy of this type of storage ring is particularly significant: at 1.3 GeV it is possible to cover the spectral range up to 400 eV photon energy with the fundamental of the undulator(s) and up to 1500 eV with the fifth harmonic. At 1.9 GeV the fundamental extends up to 1 keV. (These values are based on a magnet gap of 40 mm.)

100. The Free Electron Laser (FEL) shows promise in the longer term of even more intense radiation in the infrared through to the VUV, perhaps down to 1000Å. Although the Review Panel did not look in detail at the FEL a watching brief should be kept on developments. Any new VUV/soft X-ray ring should be designed to allow the possibility, perhaps using a "bypass", of a FEL development. Appendix 8 to this report sets out the current status and prospects for the future development of Free Electron Lasers.

IX. CONCLUSIONS

101. Access to synchrotron radiation is now vital to many areas of science and engineering (extending widely through biology, chemistry, physics, materials science and metallurgy), while in other areas its application is an important contribution to a portfolio of applied techniques. The UK synchrotron radiation research community has continued to grow apace as the SRFC predicted in the early 1980's. Interest in the application of synchrotron radiation is extensive among academic researchers, with research groups being found in some 58 universities and polytechnics in the UK. Interest is also growing slowly among industrial researchers and the initial early successes in attracting industry to the SRS, via the industrial consortium, need to be built upon. In the course of the Panel's review, scientists supported by other Research Councils have expressed keen interest in developing their use of the SRS. Again the success of existing collaborations, in this case involving the Medical Research Council, needs to be built upon.

102. Scientific pressure for access to state-of-the-art synchrotron radiation sources remains high in the UK and overseas. The successful operation of the SRS, particularly in the past 18 months, has emphasised this. The scientific pressure extends across the spectrum of synchrotron radiation from hard X-rays through to soft X-rays, the VUV and the IR regions.

103. Some important areas of science, and techniques in the application of synchrotron radiation, are not currently being tackled by UK scientists. These represent potential areas for growth, although it is equally recognised that the UK cannot be expected to be active in all areas. Examination of the international scene, however, does lead the Panel to conclude that a greater involvement of solid state physicists and materials scientists in the SRS programme could be expected.

104. The SRS is an important synchrotron radiation source, of international class, that is capable of being maintained and developed as a highly competitive state-of-the-art facility until at least the year 2000. The review has underlined the importance of the planned installation of the High Brightness Lattice, which will bring the SRS close to state-of-the-art.

105. If the UK is to maintain a competitive edge in the application of synchrotron radiation within a range of fields spanning chemistry, physics and biology, access to a new dedicated VUV/soft X-ray ring with undulators (giving much higher brightness than presently available) is essential. A single storage ring covering the entire energy range from hard X-ray to IR is no longer a viable, state-of-the-art proposition. By allowing the current SRS to be dedicated to hard X-ray users, that user community would be much better served; a new low energy ring, to be built at the Daresbury Laboratory, would be a cost-effective means of providing the UK VUV/soft X-ray community with access to an instrument which would allow them to compete at the forefront of their research fields. Industrial interest in the low energy ring, already demonstrated in Japan, would undoubtedly follow, particularly from the semiconductor and catalysis industries. The level of present and anticipated demand requires a dedicated UK source, as does the nature of VUV/soft X-ray experiments, which demand extended periods of interactive experimentation and sample preparation. The option of collaboration in other European facilities has been considered and rejected as a long term solution, on the grounds that it would be wholly inadequate to satisfy these needs.

106. The participation of the UK in the ESRF will provide an expansion in horizons for many areas of science exploiting hard X-ray synchrotron radiation. This enhanced source will bring significant new advantages in terms of source brilliance and extended energy range - it will open a new range of operation to the user, both in the extension of existing studies and for novel experiments. Participation in the construction phase of the ESRF will be important for the UK. Early involvement of UK scientists in the definition of experimental stations will help ensure the machine is optimised for the science that the UK users will want to do. The construction phase of the ESRF can be expected to draw heavily on the expertise of UK scientists and engineers; this could prove something of a disadvantage for the SRS if key UK staff were to be attracted to ESRF appointments.

107. The Review Panel has identified the need for a restructuring of user support at the SRS. It is important to achieve the appropriate balance in manpower required both to maintain a state-of-the-art facility and to provide the necessary level of user support (particularly for industrial

users or users requiring a service facility) and this will require careful judgement of the resources to be devoted to each. The Panel considers that there is a need to establish strong direction in the scientific programme for the SRS and that this should influence the appointment of key research staff at the Laboratory. The Panel further concludes that the development of a high quality in-house research programme, under strong scientific direction, would play an important role both in the full exploitation of the scientific opportunities offered by the SRS and in the development of user support. These actions would further complement and build upon the organisational arrangements recently set in train by the Daresbury Laboratory.

RECOMMENDATIONS

UK Synchrotron Sources

108. The adequate resourcing and continued updating of machine and experimental facilities at the SRS is the most important objective in any scheme for the provision of UK synchrotron radiation sources for an increasing body of scientists. The Review Panel considers the funding of a second superconducting wiggler magnet at the SRS to be an immediate priority, in order that its beam lines and five experimental stations come on line from 1990/91 (see Table 3).

109. Access by UK researchers to a new dedicated high-brilliance VUV/soft X-ray source is essential if research in the academically and commercially important VUV/soft X-ray area is to remain substantially competitive in the UK. This is the second priority determined by the Review Panel. The Panel therefore recommends an immediate start to the planning of a VUV/soft X-ray ring (in addition to fully resourcing the SRS as in Recommendation 1 above) in order that the beam lines and experimental facilities begin to come on line in 1991/92. An alternative, albeit less desirable (delaying the availability of the VUV/soft X-ray ring and its experimental facilities until 1996), would be to operate the SRS on a "reduced" duty cycle once the ESRF is in operation, and to use the resulting manpower and operating-cost savings to part-fund a VUV/soft X-ray ring at the Daresbury Laboratory (see Table 3).

European Synchrotron Radiation Facility

110. For UK science exploiting hard X-ray synchrotron radiation to flourish beyond the next decade, UK participation in the ESRF is essential. The Review Panel has not considered the question of funding UK participation in the ESRF, recognising that this is linked to international negotiations on large facilities for condensed matter research. Nevertheless, it believes that the UK's needs would require a level of involvement of the order of 15%.

Other Recommendations

111. The Daresbury Laboratory, together with the Synchrotron Radiation Facility Committee, should give further urgent consideration to the most cost effective development of user support at the SRS. The Laboratory's current plans for the introduction of Project Support Teams, which presently only involve a few percent of the total complement, and the identification of individual scientists and technical staff with responsibility for user support at each of the operating stations should be firmly established, widely publicised, and developed in the light of experience.

112. The Review Panel recommends the appointment of a Director of Scientific Research for the SRS, either on a full-time basis or as a joint University - Daresbury Laboratory appointment. It considers that the scientific programmes exploiting the synchrotron radiation facilities would be considerably enhanced if such an appointment were to be made.

113. The Review Panel further recommends that the Synchrotron Radiation Facility Committee, together with the Director of the Daresbury Laboratory and the present Research Coordinator/future Director of Scientific Research for the SRS, should consider the development of a programme of in-house research activity to be strictly assessed by the normal standards of peer review. The demands of such a programme of research will identify future needs for the appointment of key scientists, well-established in their field, who would be expected to contribute to the overall scientific direction of the SRS programme.

114. Consideration should be given to the important need to increase exploitation of the SRS by industry and research workers beyond the remit of

the Science Board (eg the materials community of the Engineering Board) and indeed of SERC (eg for research sponsored by AFRC, MRC and NERC).

115. The Science Board should investigate the extent to which further international participation in the SRS could be achieved, building upon the success of the existing collaboration with the Netherlands and with Sweden. The capacity for increased use of the SRS, by the development of new beamlines, exists and the possibility of access to a state-of-the-art facility may well prove attractive to other countries and their involvement would clearly benefit the UK programme - not least through the potential for shared costs.

TABLE 3: FORWARD LOOK: A FINANCIAL SUMMARY OF THE RECOMMENDATIONS OF THE REVIEW PANEL

	Forward Look (cash planning levels) (£M)				
	87/88	88/89	89/90	90/91	91/92
1. Present Forward Look for the SRS:	8.75	9.00	9.25	9.25	9.25
2. Proposed Central Guideline for a fully resourced SRS:	8.75	9.50	9.75	9.75	9.75
3. Plus Second Wiggler and five instruments:*	-	1.10	1.10	1.10	0.65
Total: up to	8.75	10.60	10.85	10.85	10.40

*Experimental facilities on the second wiggler would come on line from 1990/91

4. VUV/Soft X-ray ring:

(i) IMMEDIATE START

- on this basis the scientific requirements and the basic scheme for the new ring would be worked out during the HBL shut-down, with engineering design starting once the HBL work was over. The VUV/soft X-ray ring project would then proceed in parallel with, and in addition to, a full SRS programme.

The capital cost has been estimated at £9.3M for the machine and £4.2M for the building. The manpower would be about 250 man-years costing about £6M, including some intra-mural expenditure. The design fees for the building would add 20% to its cost. This total expenditure of just over £20M would be mainly incurred over a five year period. Experimental facilities would begin to come on line from late 1992.

	88/89	89/90	90/91	91/92	92/93	93/94
Building (incl design)	1.0	2.0	2.0	-	-	-
Machine capital	0.3	0.5	3.0	5.0	0.5	-
Machine manpower and design	0.5	1.5	1.5	1.5	0.7	0.3
Beam Lines and Insertion devices (incl manpower)	-	-	2.0	2.0	2.0	2.0
Total	1.8	4.0	8.5	8.5	3.2	2.3

TABLE 3: continued

(ii) NEW RING STARTED IN 1992

- on this basis the five years from mid-1987 to mid-1992 when ESRF would be starting commisioning, and the second wiggler on the SRS would be operating into five stations, would be used to slowly create much of the design of the new ring.

During 1992, construction work on the SRS beam lines would stop, and the ring would be scheduled in such a way as to release the maximum engineering and machine manpower. Scientific manpower would start designing beam lines and instruments and insertion devices for the new ring.

To build the new ring the same total manpower would be used. Construction would take four years. Experimental facilities would begin to come on line from 1996/97. The total capital spend required would be:

	£M	
Machine	9.3	
Building	4.2	
Building design	0.8	
Spend on insertion devices and beam lines in this period	3.0	
	17.3	(ie £4.325M pa on average)

If the non-staff costs on the SRS are halved by reducing operating time and suspending development/improvements, this will release £2.5M pa. So the extra cost to create the new ring, under these circumstances, would be £1.825M pa (average) for four years ie £7.3M in total. This would bring the total annual budget for synchrotron radiation at the Daresbury Laboratory up to £12.125M in 1992/93, compared with a budget of £10.3M, for the same year, for a programme not including the new VUV/soft X-ray ring but with the second wiggler project completed.

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Professor A Bradshaw	Fritz Haber Institute, Berlin
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The following also attended one or more (as shown in brackets) of the Panel's meetings:

Professor J Bordas (1)	Daresbury Laboratory
Dr D H Clark (3)	Central Office, SERC
Professor P Duke (1)	Daresbury Laboratory
Professor L L Green (3)	Daresbury Laboratory
Professor M Hart (4)	Daresbury Laboratory/ University of Manchester
Professor I H Munro (1)	Daresbury Laboratory
Dr A Parsons (1)	Daresbury Laboratory
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7. Daresbury Laboratory Annual Report 1984/85 (and preceding years, as appropriate)

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1. Final Report of the Synchrotron Radiation Facility Committee ESRF Working Group, December 1983

2. 1985 Review of the MRC/SERC Agreement over use of the SRS: Report to the Cell Board, Medical Research Council, December 1985

3. Future Plans for Provision of Synchrotron Radiation for the UK Community - General Introduction, D J Thompson, Daresbury Laboratory, February 1986

4. A Forward Look at Synchrotron Radiation Research in the UK, I H Munro, Daresbury Laboratory, February 1986

5. Use of the SRS on a Repayment Basis, P J Duke, Daresbury Laboratory, February 1986

6. Computing at Daresbury Laboratory in Relation to the Needs of the Synchrotron Radiation Research Programme, M Hart, Daresbury Laboratory, February 1986

7. Free Electron Lasers - Current Status and Future Developments, M W Poole, Daresbury Laboratory, April 1986