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Synchrotron Radiation in the UK— The Challenges and Opportunities

Ian H. MUNRO

Institute for Molecular Science (IMS), and
*University of Manchester Institute of Science and Technology (UMIST)**

By the year 2000, the SRS at Daresbury Laboratory will have been in almost continuous operation for 20 years. During that time it will have evolved to become the largest single science facility in the UK and will have had a major impact on UK science. This article comments on some of the strengths of the science and technology associated with the SRS and considers the opportunities and challenges which lie ahead in terms of source development and new scientific initiatives.

1. Introduction

During the late 1990's, the sheer scale of synchrotron radiation activity world wide became quite apparent. Accelerators and the associated facilities which have been set up to undertake world class synchrotron radiation research are now, in many cases, extremely large and very expensive and are located in major research institutes. In the case of the UK which only has a single synchrotron radiation source (although it also buys access to 14% of the beam time at the ESRF in Grenoble) the total operating costs for SR related activities are between 1% and 2% and the capital cost of constructing even a relatively modest replacement for the SRS would considerably exceed 10%, of the entire UK annual science budget. These percentages are presumably higher in those countries which support several synchrotron radiation sources.

Nevertheless, the published scientific and technological output is considerable, has a substantial international impact and continues to grow rapidly in key areas of basic and applied science. At present there are probably around four to five thousand publications world-wide produced annually on synchrotron radiation and related topics (about six or seven hundred from the UK) and the first Nobel prize for work dependent primarily on the use of synchrotron radiation has already been announced. At the 6th International Conference on Synchrotron Radiation Instrumentation held in Himeji, Japan in August 1997[1], the maturity of the field was clearly apparent in terms of the variety and the extent of the development of electron storage rings and of the multiple pole magnetic insertion devices (mainly undulators) intended to provide radiation with qualities required by their particular scientific application. This move toward application specific storage ring and insertion device design will no doubt continue and become extended throughout the next decade. Much less apparent was the vision of what should be—for want of a better description—the 4th (or at least a new) generation of synchrotron radiation sources.

The identification of the likely scientific and technological benefits which might be generated by the construction of new sources in the future is exercising the minds of scientists and others, particularly in those countries who either do not have convenient access to one or who feel that a new source will be vital to remain internationally competitive in the future-which is the case in the "single source" UK. This article presents a personal view of some of the challenges together with some of the achievements and opportunities which influence synchrotron radiation research in the UK and elsewhere.

2. Evolution in source design

Users demands for improved flux and brilliance have not changed since the first synchrotron radiation measurements were made fifty years ago and it is unlikely that their needs will be met in full even by the new, high energy and high brilliance sources of the 1990's (built in Europe, the USA and Japan.)[2-4].

A summary giving a guide to the substantial improvements in source characteristics over the past thirty years is given in **Table 1**. It is to be noted that the size and cost of the sources constructed in the 1990's are both substantial although the number of beam lines and stations has not sig-

* Department of Physics, University of Manchester Institute of Science and Technology (UMIST)
PO Box 88 Manchester M60 1QD UK
TEL (+44)0161-200-8880 FAX (+44)0161-200-8881 e-mail Ian.H.Munro@umist.ac.uk

nificantly increased from that of the sources of the 1980's and in some cases the number is less (since the number of long insertion devices in each ring is limited by the high cost of rings with very large circumference.) This "cost per station" could become even greater for ultra high brilliance sources and become the limiting factor. Also to be noted is a steady reduction in the minimum (vertical) source dimension of from ~few 100 microns in the 1980's to ~few 10's of microns in the 1990's. Although not specifically referred to, electron beam stability and control inside each storage ring with respect to the photon beam lines (with a target of about 10% of the electron beam dimensions) may also become a technical limiting factor[5].

Table 1. A summary of the primary characteristics of electron storage rings used as synchrotron radiation sources

ERA	BRILLIANCE Photons s^{-1} $mm^{-2}.mrad^{-2}$ .1% bw^{-1}	FLUX Photons $s^{-1}.mr^{-1}$ .1% bw^{-1}	BEAM SIZE microns^2	COSTS ~M$
~1960's ~1970's Parasitic, synchrotron and storage rings				
"1st generation"	10^{*12}	$\sim 10^{*10}$	$>10^{*6}$ i.e.>1 mm^{*2}	"Free"
~1980's Purpose built Storage rings mainly dipole radiation	$\sim 10^{14}$	10^{12}—10^{14}	10^{6}—10^{5}	5—100
"2nd generation"				
~1990's Low emittance Mainly insertion device High photon brilliance Storage rings	10^{17}—10^{22}	10^{14}—10^{15}	10^{5}—10^{4}	~100 to ~>1000
"3rd generation"				
>2000 Ultra high brilliance rings?? "4thgeneration"	$>10^{20}$	~10^{15}?	10^{4}—10^{3}?	~~1000??
or small specialist rings??	~10^{33} maxm.			

3. Optimised synchrotron radiation facilities and the pursuit of brilliance

It was already clear in the 1970's and 1980's that the pursuit of ever increasingly brilliant light sources was only one aspect of a much greater challenge to obtain the highest flux possible at the specimen and to be able to extract the maximum amount of information from the experiment. It is not possible to cover all the aspects of this problem which are given in summary form in **Table 2** and have been discussed elsewhere[6]. Simply designing storage rings with higher brilliance may be the ongoing choice for many accelerator physicists for obvious reasons-but it can be misleading.

A quantitative study of the requirements of any experiment must be driven by matching the source, the beam line optics and the detectors to derive the maximum flux into the phase space volume of the specimen[7].

This fact took many years to be absorbed and acted by the synchrotron radiation user community. Its recognition and importance are now evidenced by the fact that the integrated capital costs for all the beam lines and equipment around each storage ring is likely to be at least as great as the capital cost of the storage ring itself. This information is understandably unpalatable at a time when scarce resources are being sought for the construction or approval of a new storage ring source, as is the case now in the UK. When ignored it can only lead to a situation in which the basic characteristics of the source cannot be exploited in full.

It was disappointing that during the 1980's, even after twenty or more years of experience in using SXR/VUV, the measured output from VUV and SXR beam lines and mono-

Table 2. A list of the areas in which optimisation must be sought in order to derive the maximum advantage from synchrotron radiation sources and facilities

1. SOURCE	Machine parameters vs. Capital cost Machine parameters vs. Operating cost Machine efficiency/reliability/durability
2. BEAMLINE INSTRUMENTATION	Beam position monitors Controls and safety Ownership and responsibility
3. PHOTON TRANSPORT	Reflecting elements Dispersing elements Compensation and controls
4. EXPERIMENTAL CHAMBER AND SAMPLE CONTROL	Sample preparation/management/integrity Experiment control
5. SIGNAL DETECTION	Detectors Speed/area-time-energy-resolution/ Reliability/cost
6. DATA ANALYSIS	Speed/storage capacity Specialised software for analysis Networking
7. OFF-LINE SUPPORT LABORATORIES	Sample preparation/ support Off-line experiments

chromators frequently remained in the region from 1% to 0.1% of the accessible input flux and gave resolving powers typically around 10^3. In the 1990's, optical surfaces with small slope errors (from 0.1 arc sec or greater) with good surface figure became commercially available leading to attainable resolving powers of $\sim 10^4$ and giving perhaps $\sim 10^{12}$ photons per sec or more at the sample (in 3rd generation rings): but there is still room for improvement[1,8-11].

In the hard x-ray range, imaginative efforts are being made to preserve the large increases in brilliance which derive from low electron beam emittance and from the spatial and energy selectivity of undulators through the use of cooled, controllable mirror surfaces[1,12-16].

Recently a beam line has been set up for x-ray diffraction and x-ray fluorescence "microprobe" studies which delivers a beam at the sample of 10^{10} photons per micron^2 at 13 keV and with a bandwidth of 10^{-4} [17].

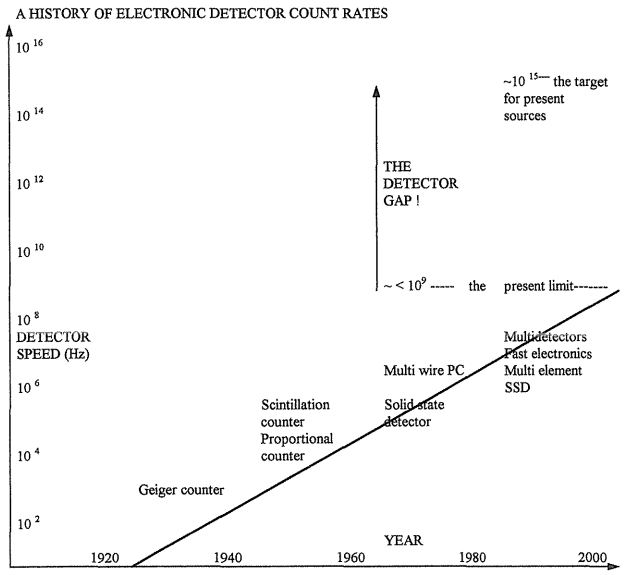

Figure 1. A plot of the count rate of detectors as a function of time to year 2000.

4. Detectors for synchrotron radiation

It has already been noted[6] that the dramatic increases in x-ray photon brilliance and flux had not always been matched by corresponding gains in those other technologies essential to exploit this advantage-except for that of computing power and speed where the rate of progress has been large, predictable and continuous (from 10^5 to around 10^6 mflops.). In the area of synchrotron radiation detectors, integrating area detectors have shown some small progress and although there have been striking improvements in the history of electronic detectors neither have kept pace with the needs of the synchrotron radiation community in terms of speed, energy or spatial resolution, dynamic range or speed of readout. **Figure 1** illustrates that in terms of count rate at least, present day detectors are not even able to match the needs of some of the experiments that were being attempted using synchrotron sources of twenty five years ago! The gap between what is accessible in terms of detectors and what is available in terms of synchrotron radiation remains extremely large.

Many differing user communities have identified detectors to be the most significant limiting factor for their experiments. What is surprising is how few resources have been set aside for synchrotron radiation detector research—a complete contrast with the very closely related field of elementary particle physics where around 20% of the total project budget may be used for detectors, data acquisition and processing[18]. At the SRS at Daresbury Laboratory, specific efforts are being made in selected areas to improve the quality of the science through the encouragement of detector

Table 3. A survey of the objectives and the corresponding benefits accessible through a programme of detector development using the SRS

TECHNIQUE	IMPROVEMENT	EFFECT
Macromolecular and small molecular Crystallography	Faster readout detectors (faster image plates, MWPC's, CCD's)	Higher throughput on stations
	Lower noise devices (parallax free MWPC's, slow scan CCD's)	Extends range of samples Good data from small crystals before radiation damage. High accuracy data for anomalous dispersion
Non crystalline diffraction and scattering	Higher count rate detectors (MWPC's)	No attenuators therefore gives more efficient beam use Higher time resolution-to msec domain for liquid crystals and muscle. Real reaction kinetics can be followed
	Curved MWPC detector	Allows time resolved SAXS/WAXS on polymers, membranes etc
Powder diffraction	Curved proportional counter	Decreases collection time by ~1000 so increases throughput. Allows time resolved high resolution diffraction for real reaction kinetics on syntheses etc
	Higher count rate scintillators	Decrease collection time by 10 times so increase throughput
EXAFS	Higher count rate electronics	Gives increase in throughput or more dilute samples possible
	Improved photodiode array system	Gives higher time resolution so real chemical reaction kinetics can be studied No longer diffusion limited
Surface and Molecular Science	Multi channel electron detectors	More efficient use of beam. Can easily be 1000 times faster

research, albeit with very limited resources.

Some outstanding results which have already been achieved allow "molecular mapping" in the investigation of molecules by using a two dimensional scanning technique which arose directly as a result of the development of an electron image sensing chip "multi-detector"[19]. Results have been described in the areas of resonance Auger decay processes (Krypton) and in a study of vibrational selectivity in autoionising decays in N_2O.

Table 3 lists some of the potential benefits identified for the SRS which would result from a wholly attainable detector improvement programme extending over two or three years (and whose costs were roughly estimated to be about 4 M$.) Of course, the rate at which these critical developments become accessible to SRS users will depend entirely on the priority and funding given to detector research and development[20,21].

Within the UK an ambitious programme to generate innovative microelectronic pixellated sensors and advanced CCD technology (IMPACT!) has been funded with participation from industry, universities and representatives of the particle physics, space science and synchrotron radiation communities.

Synchrotron radiation facilities have generated few mature detector groups partly because the need for detectors often arises from many individual techniques or beamlines at once-leading to some very difficult choices!. Industry is poorly placed to offer any "solutions" and the solutions which are offered are either (usually inadequately) modified devices from other applications or else they need complex, long term commitments which will compete with the resources focused on the immediate day-to-day science programmes. This could become the most important development area needed to ensure the long term success of synchrotron radiation research programmes.

5. The Synchrotron Radiation Source at Daresbury Laboratory

A summary of the current operating parameters and a drawing of the SRS facility are given in **Table 4** and in **Fig. 2**. The SRS is a medium energy (2 GeV), medium emittance ($\sim 10^{-7}$ m.rad.) electron storage ring with a relatively small number of insertion devices (2 wavelength shifters, 2 multipole wigglers and 1 undulator) and a rather short straight section length (1.2 m). It is not possible to add more insertion devices within the existing structure. From the beginning, the UK user community have required that-given the characteristics of the machine-the SRS should provide the absolute maximum amount of usable beam time and provide minimum interference to the running of experiments. Users are not required to become radiation workers and all beam line user areas are accessible at all times. The SRS has a unique operating record. Normally running for ~7000 hours per year it has now "clocked up" about 90000 hours of beam time since the first user experiments in 1981. The SRS operates continuously (i.e. 24 hours and 7 days with one major shutdown per year) with one injection per day. Start currents are in the range 250 to 300 mA and the stored beam lifetime is greater than 20 hours. The >90% efficiency of storage ring operation is aided by an excellent system of fault monitoring on the beam lines and on the storage ring which allows important weaknesses to be systematically and quantitatively identified—and hopefully rectified as a matter of priority[24].

Approximately 10% of the total operating time is allocated to accelerator physics to improve SRS performance at injection, in single bunch mode, to minimise the dynamic aperture (e.g. for the purpose of installing the new multipole wigglers), and to improve beam position control and stability. **Figure 3a** shows recent results which have lead to a substantial reduction in the beam cross section as a consequence of operating the SRS in "gapped beam" mode[22] (i.e. with the

Table 4. The normal Operating Parameters of the SRS

Storage ring energy	2 GeV	Horizontal emittance	~1.1 10^{-7} m rad
Ring circumference	96 m	Beam Size	~2200.600 micron (at 2.5% coupling)
Lattice type	FoDo	Beam Current at Injection	~300 mA
Pre injector (Lineac) energy	12 MeV	Beam Lifetime	~30 hours
Injector (booster synchrotron) energy	600 MeV	Ring Period	320 ns, 160 bunches
Radio frequency	500 MHz	Single bunch operation	<50 mA, fwhm ~180 ps
Operations	~5000 hours multi bunch: ~ 600 hours single bunch ~1000 hours other Total ~7000 hours pre year		
Beamlines	9 Dipole lines	@ 3.2 keV	
	1 5T three pole wiggler	@13.3 keV	
	1 6T three pole wiggler	@16.0 keV	
	1 10 pole (1 m) undulator	76–1240 eV	
	2 9 pole 2T wigglers	@~6 keV	
Stations	~40 for ~~3000 registered users		

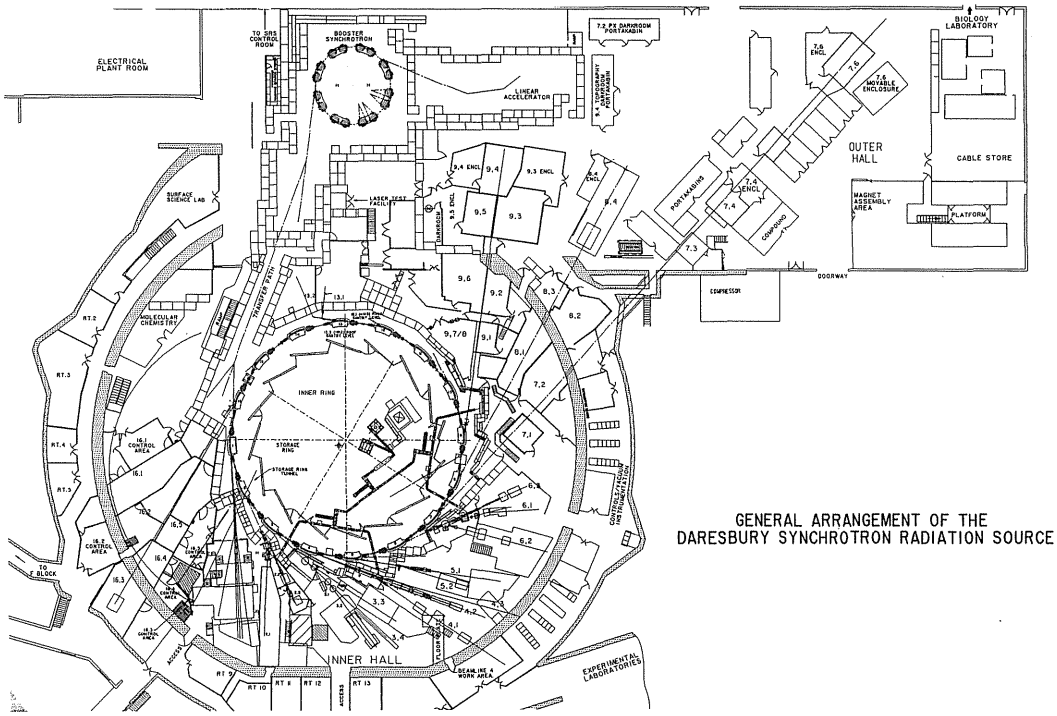

Figure 2. General arrangement of the Daresbury Laboratory Synchrotron Radiation Source (the SRS).

SRS only partially filled.) **Figure 3b** shows the great improvement in beam orbit control and in vertical beam position using a simultaneous global feedback system from individual beam line photon monitors[23].

6. The SRS Upgrade

In 1995, a strategy for synchrotron radiation science and technology in the UK was produced[21] which proposed among other things that the existing SRS machine should be fully developed and exploited (called the SRS "Upgrade") even before replacement of the SRS beyond 2000 with an accelerator having substantially higher brilliance (and cost).

This is being achieved by installing two 9 pole, 2 Tesla multipole wigglers to give over one order of magnitude improvement in flux in the soft and medium x-ray regions. These devices are relatively cheap and are located in the last two straight sections (straights 6 and 14) accessible in the SRS. The output spectra shown in **Fig. 4** will move the SRS closer in output, at least in flux terms, to the new large "3rd generation" machines.[24] Three of potentially four new Upgrade beamlines will become operational in 1999 and will be used to support substantial collaborative programmes in macromolecular crystallography, soft x-ray spectroscopy and the area of nanoscience.

7. Materials Science using synchrotron radiation

About two thirds of the science activity at the SRS is supported and funded by the respective Chemistry, Materials and Physics programmes within EPSRC (the Engineering and Physical Sciences Research Council) and also by NERC (the Natural Environment Research Council) together with lesser levels of support from the E.U. and elsewhere. The programme covers a wide range of scientific endeavour and exploits all the various technologies linked to synchrotron radiation-from hard x-rays to millimetre wavelength far infra red. This work is described in detail in CCLRC Daresbury Laboratory Annual Report Annexes[24] and an overview of the scope of the work undertaken during 1996–1997 is presented in **Table 5**. The programme will be illustrated below with examples drawn from areas in which SRS instrument development has significantly added to the quality of the science produced.

8. High pressure studies

A good example of the importance of detector technology at the SRS can be seen in the first introduction of image plates for high pressure powder diffraction studies. High pressure cells are a "simple" way in which interatomic distances may be modified by amounts that lead to dramatic changes in structure and properties. This information is ideal to test and advance calculations in which density is a variable which, in turn, will allow major progress in our ability to calculate structural bonding and stability, electronic energy levels and solid state properties e.g. associated with high T_c materials, planetary physics etc. The small sample volume especially in very high pressure cells results in very low signal levels from, often, very weakly scattering materials. The early use of an image plate to allow complete powder rings to be recorded was followed by integration around the rings to give excellent powder averaging and a data quali-

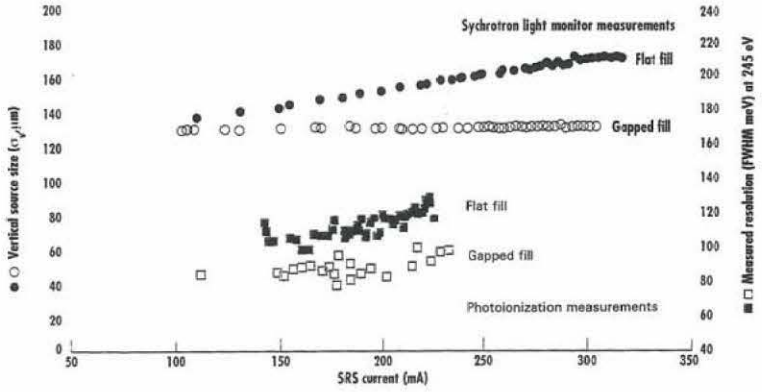

Figure 3(a). Operation of the SRS using Gapped Beam.

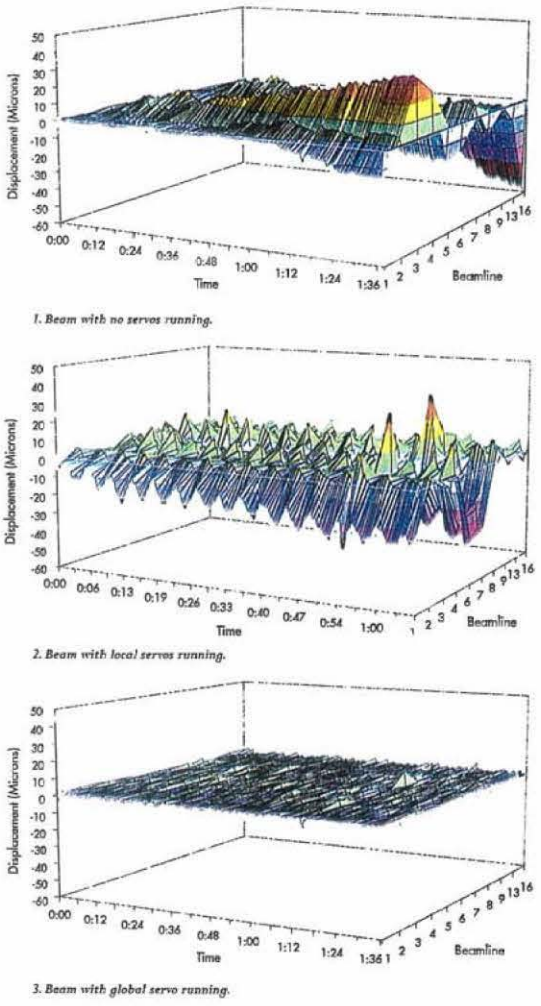

Figure 3(b). Operation of the SRS using Global feedback from photon beam position (tungsten vane) monitors on beam lines.

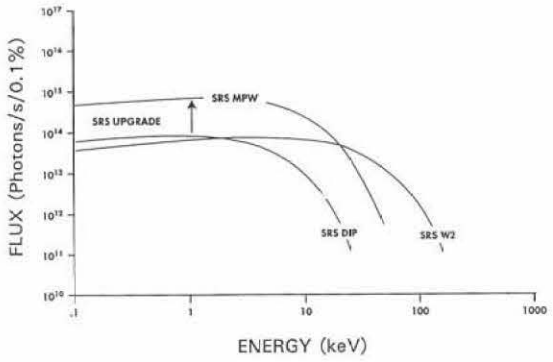

Figure 4. Spectra for the two 9 Pole, 2 Tesla multipole wigglers currently being installed at the SRS.

Table 5. The scientific programme at the SRS—a 1996–97 summary based on experimental reports

Materials/Chemistry/Physics	Biological Sciences
Ab initio powder diffraction	Biological spectroscopy
Alloys	Fibre diffraction
Catalysts	Food science
Inorganic complexes	Membrane and lipid systems
Liquid crystals	**Protein crystallography**
Magnetic materials	Solution scattering
Ceramics and glasses	Time resolved spectroscopy
Geology and minerology	
Metal oxide and nitrides	
Molecular spectroscopy	
Nonlinear optical materials	Experimental Techniques
Polymers and polymer electrolytes	
Porous and meso porous materials	
Semiconductors	
Sols, gels and emulsions	
Superconductors and sensors	
Surface spectroscopy and diffraction	
Thin films and multilayers	
X-ray spectroscopy	

SRS science activity on the basis of number of science reports in 1996/7. Bold type indicates a major activity (around 10% or more). Biological science represents about one third of the overall total.

Table 6(a). Structural systematics of group IV, III–V and II–VI semiconductors from all other work, prior to 1995. Structures shown as shaded have all been amended in SRS studies. Phases shown in italics have one or more variable atomic coordinates

IV	Si	Diamond	β-tin	SH	*Int. (mono)*	hcp	fcc	
	Ge	Diamond	β-tin	SH	dhcp			
III–V	AlN	Wurtz	NaCl					
	AlP	ZB	FCC					
	AlAs	ZB	NiAs					
	AlSb	ZB	β-tin					
	GaN	Wurtz	NaCl					
	GaP	ZB	β-tin					
	GaAs	ZB	*Pmm2*	*Imm2*				
	GaSb	ZB	β-tin	SH				
	InN	Wurtz	NaCl					
	InP	ZB	NaCl	β-tin				
	InAs	ZB	NaCl	β-tin				
	InSb	ZB	β-tin/*Pmm2*	unknown	hex/*orth.*	SH	bcc	
II–VI	CdO	NaCl	CsCl					
	CdS	ZB/Wurtz	NaCl	*Pmmn*				
	CdSe	Wurtz	NaCl					
	CdTe	ZB	NaCl	β-tin	*Pmm2*			
	ZnO	Wurtz	NaCl					
	ZnS	ZB	NaCl					
	ZnSe	ZB	NaCl	SH				
	ZnTe	ZB	mono	mono				
	HgO	*orth./Cinn.*	NaCl					
	HgS	*Cinn.*	NaCl					
	HgSe	ZB	*Cinn.*	NaCl	β-tin			
	HgTe	ZB	*Cinn.*	NaCl	β-tin	distorted bcc		

Table 6(b). Phases studied at SRS, 1992–97. New results and amendments to previous identifications are shaded

IV	Si	Diamond	β-tin	*Imma*	SH	*Int (mono.)*	hcp	
	Ge	Diamond	β-tin	*Imma*	SH			
III–V	AlSb	ZB	*Cmcm*					
	GaP	ZB	*Cmcm*					
	GaAs	ZB	*SC16*	*Cmcm*	unknown			
	GaSb	ZB	*Imma*	bcc				
	InP	ZB	NaCl	*Cmcm*				
	InAs	ZB	NaCl	(*Cmcm*)				
	InSb	ZB	Immm	*Super-Cmcm*	*Imma*	Immm	bcc	
II–VI	CdS	ZB/Wurtz	NaCl	(*Cmcm*)				
	CdSe	Wurtz.	NaCl	*Cmcm*	unknown			
	CdTe	ZB	*Cinn*	NaCl	*Cmcm*	uunknown		
	ZnS	ZB	NaCl	*dist-NaCl*				
	ZnSe	ZB	NaCl	*Cmcm*	*dist-Cmcm*			
	ZnTe	ZB	*Cinn.*	*Cmcm*	unknown			
	HgO	*orth./Cinn.*	tetrag.	NaCl				
	HgS	Cinn.	NaCl	*dist-NaCl*				
	HgSe	ZB	*	*Cinn.*	NaCl	*Cmcm*		
	HgTe	ZB	*	*Cinn.*	NaCl	*Cmcm*	bcc	

*Also a 'hidden' transition from ZB to a C2221 phase (Cmcm) denotes that the previous identification of the structure can be shown to be incorrect, and that the true structure is very probably, but not yet certainly, Cmcm. The prefix 'dist' denotes 'distorted'.

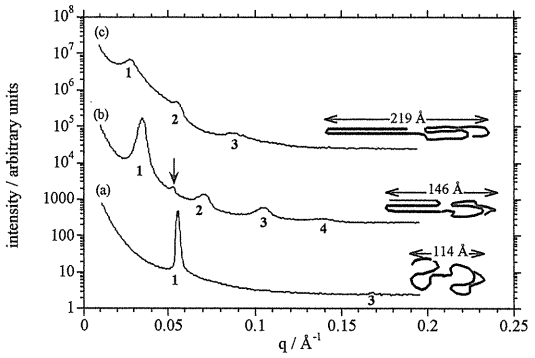

Figure 5. SAXS patterns for copolymer $E_{74}B_{37}$ showing the ordered melt structure (T=90°C), the metastable structure (T_c= 42°C) and the equilibrium, once-folded structure grown at 50°C by a self-seeding process. Roman numerals indicate the positions of the reflections from the stacked lamellae and the arrow indicates the position of the peak arising from the coexisting ordered melt. The insets show calculated repeat lengths for possible conformations. See 29, 30).

ty unrivalled by any other technique[25,26].

An illustration is given in **Tables 6a** and **6b** of dramatic scale of the activity in deriving new phases or obtained from a repeat of previous work on semiconductor materials at the SRS during the past five years. The work reveals a revised picture of the systematics and a higher level of structural complexity and inter relationship as a consequence of this development which is now being extended to extremely high pressure and temperature studies.

9. Synthetic polymer research

During the 1980's a substantial programme of research and development became essential in order to carry out effective measurements on ordered, but non crystalline biological material such as muscle and collagen. This required a substantial investment in fast reliable detectors suitable for small and wide angle x-ray diffraction and scattering and capable of yielding time resolved information (e.g. from active muscle) on a time scale of around 1 ms. This type of equipment is of course also ideal for the study of synthetic polymer materials and, in particular, to observe structure development in polymer processing[27].

A major activity has resulted at the SRS which is concerned with the fundamental aspects of the thermodynamics of order-disorder transitions e.g. in block copolymers and also with applied aspects such as the crystallisation of films. **Figure 5** shows data from an extensive study of structure using SAXS, WAXS, low frequency Raman spectroscopy and Differential Scanning Calorimetry on a series of linear and cyclic homopolyethers and block polyethers. Block copolymers that have disordered or lamellar melt phases show an increase in length scale on crystallisation of the oxyethylene (E) unit which implies stretching of the amorphous oxybutylene (B) unit above that experienced in the melt. Higher mass copolymers had folded stems whose length was determined by a balance between the free energy

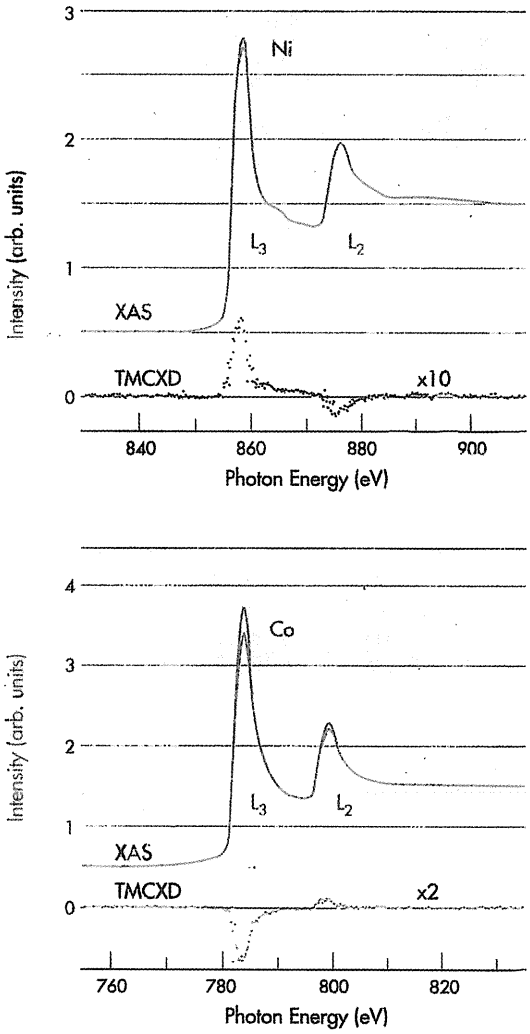

Figure 6. TMXCD applied to films of Ni (the upper plot) and to Co-Ni (the lower plot). Because the magneto crystalline anisotropy effect partially rotates the orbital magnetisation towards the preferred magnetic direction, this novel technique is able to measure the orbital magnetisation along the x-ray beam direction which is orthogonal to the applied external field. See 32).

of E-chain folding, B-chain stretching and crystallisation kinetics. The most interesting part of this work has been the study of the evolution of morphology actually during processing. As a consequence, it should be feasible to relate processing and morphology to the mechanical properties and the actual function of the design material. This is an opportunity which has resulted in substantial industrial collaboration and cooperation in a programme ultimately designed to observe polymer extrusion on-line under pilot plant conditions on an x-ray beamline[28-30].

10. Magnetic materials

Recently there has been a great upsurge in interest in the spectroscopy of magnetic materials. This is due in part to the development of magnetic multilayer science and technology but also to the introduction of sum rules which make it possi-

ble to directly measure the spin and orbital magnetic moments of a material using the technique of magnetic circular dichroism[31]. Magnetic circular dichroism is an element specific technique which determines the magnetisation along the direction of an applied external magnetic field and in which the difference in absorption for left and right circularly polarised light (usually in the SXR range of L edge absorption—e.g. for iron at ~710 eV.) can be used to separate the spin and orbital components. It arises because for example in Ni which has empty 3d spin down states in the presence of a field, only 2p states with spin down can be excited into the vacant 3d states. When the orbital motion of the 2p states is in the same direction as that of the circularly polarised light the transition probability is larger while when the motions are in the opposite direction the probability is smaller yielding the MCD difference spectrum.

A recent development has been to try to establish how the orbital magnetisation of two different types of atoms interact and couple to the surface using a new technique called Transverse Magnetic Circular X-Ray Dichroism (TMCXD)[32]. TMCXD has been applied to films of Ni and Co-Ni and has been able to measure the orbital magnetisation along the x-ray beam direction (orthogonal to the applied field) by exploiting an effect known as magneto crystalline anisotropy. **Figure 6** shows results from TMXCD applied to films of Ni and Co-Ni. This work has helped understand how by adding a film of magnetic cobalt as thin as three atomic layers to a nickel layer (33 atoms thick) the nickel magnetic moments, usually normal to the surface, are induced to align with the cobalt magnetisation direction in the surface plane. In this circumstance, it requires a relatively strong external field to restore the perpendicular magnetism which will vanish again once the field is removed[33,34]. Spin polarised photoemission experiments offer yet another "window" on surface electronic structure and magnetism by which the net spin density of valence electrons can give an important insight into the magnetic properties especially of transition metal systems in which any magnetism due to the orbital moments is largely quenched. Two spin polarimeters are in use at the SRS, both of which achieve spin resolution by Mott scattering from a foil of heavy atoms such as gold. Measurements are made on "primary" valence electrons and on secondary electrons in studies of amorphous alloys, in surface and interface effects in composites and in multilayers[35].

11. Nanoparticles and nanostructures

The early promise of the use of synchrotron radiation as a revolutionary tool for the development of the smallest feasible feature size in surface (semiconductor) lithography and also as a unique source to provide mass produced micron size devices (or smaller) using the methods of deep lithography have yet to come to fruition. No doubt this is primarily a function of cost effectiveness rather than technical feasibility. However, another related subject has taken over which should possibly become a new main focus for

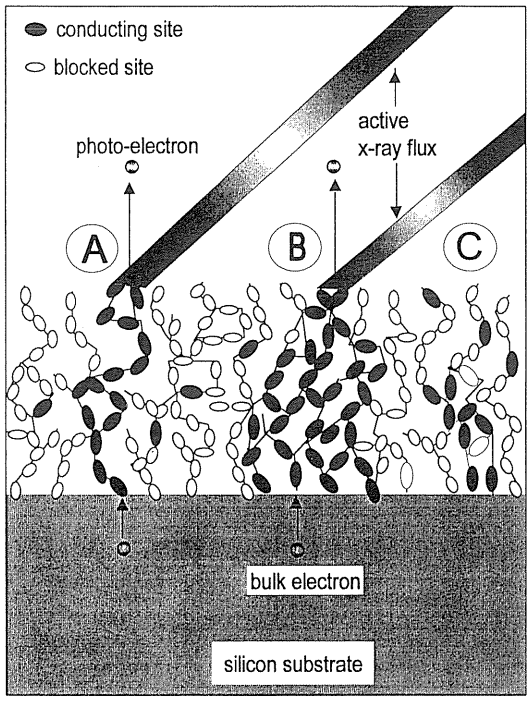

Figure 7. A schematic drawing of a film of porous Si clusters. When illuminated with x-rays, only the flux intersecting the surfaces of percolating clusters contribute to the electron yield. Cluster A with a small number of sites will present a high resistance and cluster B a low resistance while C is non percolating and does not contribute to current flow. A and B have been given the same surface area—showing that photoelectron emission based measurements are more sensitive than contact based techniques. See 36, 37).

research. The ability to create gas clusters in the 1970's led to measurements on supported and unsupported clusters in the 1980's and to the evolution of the science of carbon based nanostructures (following the discovery of C_{60} and carbon nanotubes). There are quite new and fundamental issues in understanding the scientific and technological problems associated with nanostructures. The technological importance of reducing electronic circuits to atomic sizes is immense. It raises challenges such as the need to introduce new measuring methods to give information on the chemistry, electronic structure and behaviour of such small "solids". Applications will include dispersions and coatings, high surface area materials (e.g. catalysts), sensors, quantum dot laser sources, electronic quantum devices of all kinds and the ability to synthesise new organic materials. The changes in behaviour occur at sizes typically less than 5 nm. Clusters containing from a few to a few tens of atoms must be understood and described theoretically. The boundaries between surface and bulk properties become blurred in this region and electronic behaviour is defined by shape, size and surface chemistry in addition to the internal atomic arrangement. Synchrotron radiation will surely play a very important part in probing such systems by x-ray scattering, SXR/VUV spectroscopies, FTIR spectroscopy between 50 and 500 cm^{-1}, photo assisted etching, surface chemical reactions and the in-situ observation of surfaces using scanning

probe and other microscopies.

Recent work at the SRS has provided a new way to visualise the x-ray absorption processes associated with Si nanoparticles[36]. In this work, the x-ray excited optical luminescence (XEOL) provides a connection between the chemical and structural information from XANES and EXAFS and the electronic properties which determine the luminescence. Data taken around the Si L edge has shown that for porous Si there is a progressive blocking of conducting sites with decreasing temperature shown in **Fig. 7** leading to a loss of fully percolating clusters[37]. Results of this kind relate to our understanding of how electrons can propagate through a system which is perfect at the nanoparticle level but may have variable connectivity between the particles.

"Molecular microscience" a name suggested for that science needed to provide the underpinning for electronic and communication devices for the next century, covers Si ULSI and mesoscopic single electron devices, nanoparticle based lasers, display materials and nanofabricated catalysts all of which will be ideal candidates for study in the range 10 eV to ~10 keV using high flux, high resolution synchrotron radiation beamlines.

12. Summary

The rapid expansion and evolution of single techniques has now given way to the simultaneous application of as many methodologies as are affordable, feasible and useful during the period of exposure of samples to the x-ray beam. "Combined techniques" which have been applied extensively to the study of amorphous material and glasses in the 1980's are also being used to reveal the structure and function changes in catalysts during fabrication and application[38]. The wide ranging studies on atomic and molecular adsorbates (associated with surface orientation study using XANES) will gradually move toward research in process and surface engineering with a particular focus on buried interfaces and disordered systems with specific industrial applications in mind. High resolution powder diffraction is an extremely effective method for the study of complex systems (e.g. cements[39]). and for monitoring initial growth and ordering on metals. Magnetism and magnetic structures will be resolved using x-ray spectroscopy and (observed for the first time at the SRS) magnetic diffraction[40]. New states of matter associated not only with high pressure but also with new molecular chemistry and new nanostructures will be identified using a combination of high resolution diffraction, EXAFS, x-ray photoelectron and luminescence spectroscopies. In the UK, x-ray microscience, microfocus imaging and combined imaging methods will probably become fully effective only following construction of the replacement for the SRS.

The major scientific challenges will become increasingly associated with "real" materials. This means that samples may be "dirty", very hot or very cold, at very high or very low pressure, very large (~metres) or very small (e.g. quantum devices) and of course much biological material will be very wet. These needs can all be met but probably such experiments will become more expensive.

"Problem-driven" science needs the maximum possible amount of information from each sample. This in turn implies the simultaneous application of several techniques whenever it is feasible since synchrotron radiation is ideal as a tool to derive short and long range atomic order and at the same time to yield chemical (molecular) information on sub micron dimensions and with a time resolution which can be of the order of nanosecond or less.

13. Synchrotron Radiation and the Biological Sciences

The potential advantage of synchrotron radiation over other sources of radiation for the measurement of biological structures was recognised from the late 1960's to be in its extreme brilliance in the x-ray region. The first really challenging application was to attempt to use radiation mainly from synchrotrons to derive time resolved (~milli-sec), low angle (~1 milli radian) diffraction information from poorly ordered, weakly diffracting (and highly hydrated) samples of insect muscle[41].

This early initiative, closely paralleled by x-ray small angle and crystallographic studies in the UK[42] and somewhat later by the use of the SPEAR storage ring for protein crystallography[43] were of the very greatest importance. This was not primarily for the new science they produced but because it showed so clearly that neither the available technology for beamline optics (mirrors in particular) nor the fast readout linear x-ray area detectors with good spatial resolution available at that time could properly exploit the x-ray brilliance produced by those synchrotron sources of the 1960s.

The seminal decision to use synchrotron radiation as a major tool for research in the UK bio sciences was taken around 1980 when the Medical Research Council, jointly with the S.R.C. (the UK Science Research Council), decided to provide support for the construction of an entirely new Biology Support Laboratory (the B.S.L.) alongside the SRS[44].

The B.S.L. was planned to provide those skills in biology and biochemistry not normally available at such large facilities and which are essential for the preparation, assessment and preservation of biological material. The B.S.L was also to create a research base from which some of the world leading programmes in protein crystallography might be supported late in the decade.

Figure 8 illustrates a selection from the many crystal structures which have been obtained at the SRS partly as a consequence of this early initiative.

14. SR opportunities for biological structure studies

There have been many strategic reviews to consider which areas of research would derive the maximum benefit from the use of synchrotron radiation. In each case, the advantage to structural biology has been identified and has grown in scale as a consequence. In 1996, the BBSRC (the UK

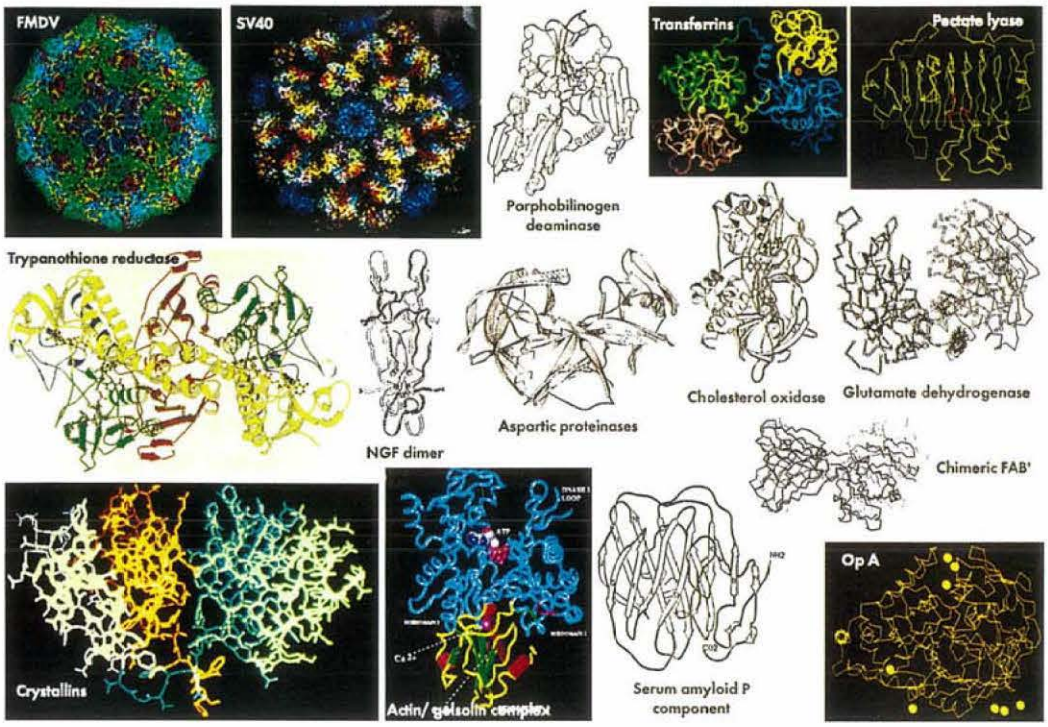

Figure 8. A collage of typical macromolecular structures, viruses, proteins and enzymes determined during the last few years using data derived from the SRS.

Biotechnology and Biological Sciences Research Council) produced an extremely important (from the point of view of the UK synchrotron radiation community) report which specifically attributed the leading position of the UK in structural biology to the SRS at Daresbury Laboratory[45].

Within the UK, research in structural biology is rather highly concentrated in a small number of institutions and university departments. The principal source of funds for this work (i.e. about 80%) is derived about equally from the BBSRC and the MRC. Although there is a small, but significant level of usage of synchrotron radiation at the ESRF and at other facilities outside the UK and although there is an increasing use of other techniques, it is envisaged that x-ray crystallography using synchrotron radiation will dominate large molecular structure determination for the foreseeable future.

Indeed, this prediction proved to be a prophetic one since in October 1997 a Nobel prize was shared by Dr J. E. Walker of MRC Laboratory of Molecular Biology in Cambridge for work undertaken, almost wholly using the Daresbury SRS, to establish the structure of F1-ATPase (which corresponds to the spherical head component of the ATP synthase complex.) This very important molecule plays a crucial role within cells by exploiting the flow of protons through the mitochondrial membrane to generate ATP from its component parts, inorganic phosphate and ADP. The molecule is roughly "lollipop" shaped having a spherical head of ~10 nm diameter and and a "stalk" of about 4 nm which is normally embedded in the inner mitochondrial membrane At the time, this was the largest asymmetric structure ever determined using x-ray diffraction methods[46].

15. Macromolecular crystallographic "structure factories"

The BBSRC review of 1996 also drew attention to the very high value placed by the pharmaceutical industry on structure determination and on access to the SRS. Pharmaceutical companies are among the primary wealth creators in the UK and for the purposes of new drug design they place at a premium the ability to rapidly establish new structures. There are very many steps involved in such a development, including crystal growing, the derivation of the diffraction pattern, its analysis and associated computing and theoretical modelling together with biochemical intervention to achieve any necessary molecular modification. Therefore mechanisms for ensuring rapid and optimal access to the SRS are of greater importance to this community than ever before. Because of the strong competition for beam time, it is the actual access to SRS beam time that has become the limiting factor. The BBSRC report[45] strongly recommended that sufficient beam time must be available for routine crystallography, that state-of-the-art stations must be available for high resolution studies and that at all times the development of new techniques and of new detectors must be supported. These arguments would of course be echoed also by all those other research communities who wish to effectively exploit synchrotron radiation.

Without a synchrotron radiation source in the UK there

would certainly be inadequate beam time available at other (non-UK) facilities and control over such resources and their scientific and technical priorities would be difficult. For these reasons, the biological science community have been the main driving force behind the recent Upgrade to the SRS to give two additional high flux protein crystallography stations which will become operational by 1999. This community are also strongly committed to supporting the replacement of the SRS with a new, all insertion device storage ring (DIAMOND) within the next five years without losing access to synchrotron radiation in the UK at any time (i.e. without any intervening "dead time"). Wherever it is difficult to obtain crystals, for example for membrane proteins and other particles, it is anticipated that many of the new probe and other microscopies and especially NMR will play an important role. Even in these cases however, synchrotron radiation will be used to contribute to studies of complex biological particles including carbohydrates and other "difficult" materials using wide and small angle x-ray scattering methods.

16. Biological Spectroscopy

The primary use of the SRS within the Biosciences has largely been for crystalline structure research and for measurements on relatively ordered fibrous material. Nevertheless there has always been a significant use in biology across a rather wider range of endeavour best described as "biological spectroscopy."[47]

The methods used include EXAFS, radiation damage measurements, VUV circular dichroism, time resolved fluorescence techniques and a variety of imaging techniques which include soft x-ray microscopy and confocal imaging. These methods are ideal for "real" (i.e. wet) samples and are particularly important when they can be combined with crystallography or x-ray scattering.

17. Biological EXAFS

An example of the power of EXAFS has been in its application to a study of plants which are able to hyper-accumulate levels of toxic material (in this case of metals) that would kill other plants. The plant Alyssum Lesbiacum absorbs nickel very effectively from the soil and moves the metal upwards into the plant tissues. Since there are around 400 different hyper-accumulator species known at present, each of which is tolerant to one or two metals, an ability to identify the metal binding sites is of the greatest importance. In work on Alyssum lesbiacum at the SRS[48] fresh material from the plant (xylem sap) was used without any prior treatment for the EXAFS experiments. This work has given direct evidence that Ni binds to the amino acid histidine in leaves, roots and sap. The Ni is specifically bound to one of the N atoms within histidine and therefore tightly bound inside the histidine molecular cage. Experiments of this kind could help derive a wholly novel method for the decontamination of soil by selectively trapping them in removable plant systems.

Of course, there are very many other examples of EXAFS in biology[49] where the potential of the method has been clearly established and it will continue to expand, in conjunction with x-ray scattering an diffraction methods, in the future.

18. Circular Dichroism for macromolecular structure studies

Circular dichroism spectroscopy measures the relative transmission of left- and right-circularly polarised light in a region where the biological material is already absorbing (perhaps very strongly.) The amplitude of a CD signal is only a very small fraction (from 10^{-4} to 10^{-6}) of the absorption signal and it usually lies in the UV and LiF VUV region where all biological structures such as polypeptides, polysaccharides, membrane structures and aromatic fragments absorb. The CD signal derives from the interaction of circularly polarised light with these asymmetric molecules and specific features such as alpha-helix and beta-sheet and many others can be characterised and "assayed" by their unique CD spectra. Indeed, the CD spectrum of any large biomolecule can be quantitatively "decomposed" into the range of major substructures from which it is built up. The value of the analysis depends not simply on the quality (S/N) of the CD data but very importantly on the spectral range over which the comparison can be made (i.e. on the total amount of information). Since commercially available instruments become rather ineffective below 200 nm and since most structures of importance display the majority of their absorption around or below 200 nm, the evolution of synchrotron radiation based CD for biology should be of great importance and potential. The opportunity has not yet been fully realised because of the rather low fluxes available at the sample in the VUV region, largely due to inefficient instrumentation. Early work in the field at Wisconsin, NSLS Brookhaven[50] and at Daresbury[47,51] has used linearly polarised light to obtain right/left switchable circularly polarised light via a photoelastic modulator. Despite the inefficiency of such methods using dipole radiation the advantages of the principles have nevertheless been demonstrated. **Figure 9** presents results from a study at the SRS using rapid acquisition times to investigate beta-sheet formation of amyloid fibrin of prions and Alzheimers disease beta-protein in solution where circular dichroism was used to investigate the spontaneous "in vitro" formation of amyloid like filaments from synthetic peptides. The results showed the spontaneous formation of a beta-sheet structure from a disordered one, by comparing the CD spectra with a data base of spectra from known structures. The results also showed that it was possible to control whether amyloidosis occurred or not by replacing individual amino acids in the peptide[51]. These are examples of experiments that are not possible with x-ray crystallography or NMR.

With an efficient and optimised high flux, medium resolution beam line for spectroscopy in the VUV (still something of a rarity), perhaps using a helical undulator for circular

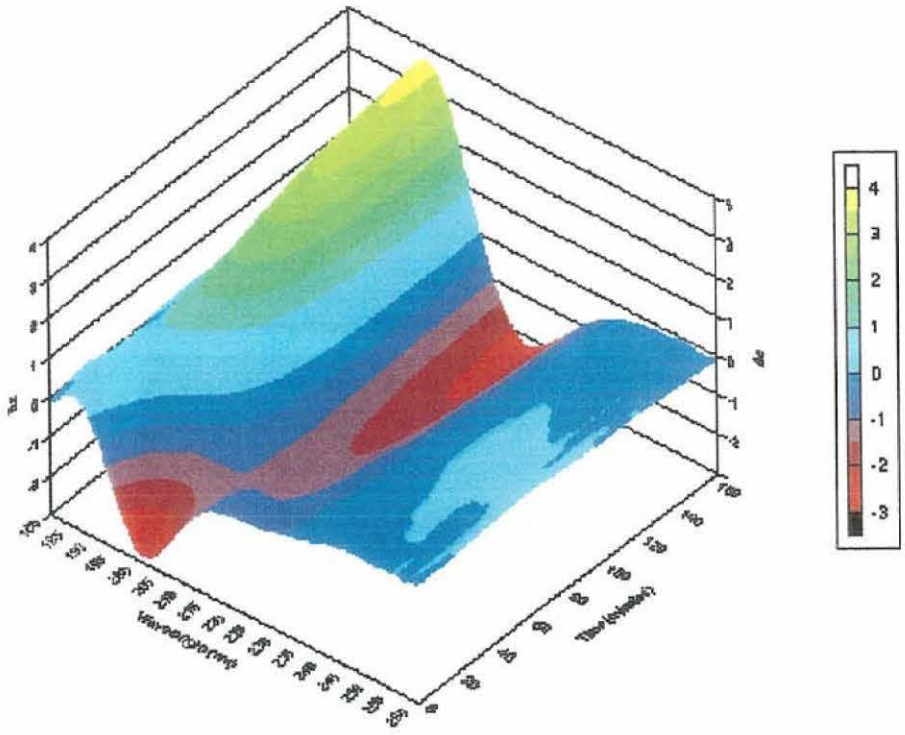

Figure 9. A CD spectrum measured at the SRS between 180 nm and 280 nm observed over 160 minutes, to identify the spontaneous formation in vitro of amyloid-like fragments from synthetic peptides. The data reveal the spontaneous formation of a beta-sheet although it was found by replacing individual amino acids in the peptide possible to control whether amyloidosis occurred or not. See 51).

polarised light generation although the slow switching time of the undulator may preclude fast time studies, the prime measurements for the future would be protein alpha- and beta-structures below 200 nm; peptide aggregates below 170 nm; to stimulate ab initio theoretical analysis of peptide links and aromatic fragments; to observe primary and secondary structures in DNA below 180 nm to measure the effects of solvents and chromophores on nucleic acid structures down to ~130 nm and to study membrane bilayers to ~140 nm. Finally, given the availability of reliable fast mixing (stopped flow) methods, perhaps even in conjunction with laser pulsed methods, it would be straightforward to extend wet CD structure studies to at least around 1 ms and perhaps make some significant contribution to the identification of intermediate states during protein assembly[48].

19. Biological Imaging

Apart from whole body (e.g. heart and brain imaging) and therapy for which very high energy and high brilliance sources are essential in order to achieve the necessary penetration, synchrotron radiation has been seen since the very earliest days to offer the chance for high spatial (at least lateral) resolution imaging using wet (and perhaps living) samples. The logic behind these developments has been that the use of shorter wavelengths (~nm) should give greatly improved spatial resolution over conventional microscopy and that at around the C K edge the so-called "water window" would permit thick (~few microns) and wet samples to be used. The realisation of these objectives has been dependent on the development first of the Fresnel zone plate and second on the ability to fabricate mirror surfaces with the necessary surface figure and surface texture to focus such very short wavelength radiation. The technological limit of resolution (lateral) is about 10 nm and a feasible target would be to achieve around 10^{11} photons s^{-1} in ~50 nm spot size at ~300 eV. The evolution of the technology and the attempts to achieve holograms of biological objects can be followed through the proceedings of the series of International Conferences on Synchrotron Radiation Instrumentation[52,1]. One difficulty is the rather low numerical aperture of such systems leading to large (greater than 1 micron) axial resolution, another is the amount of radiation damage sustained by the sample. The field continues to be very active, but from the point of view of the bioscientist, it has not yet "taken off".

A wholly different approach has been developed at the SRS where a wide variety of contrast modes can be combined with a lateral resolution approaching, and an axial resolution exceeding that obtained using a soft x-ray device while delivering very much lower dose to the specimen. This microscope uses the principle of confocal imaging combined with synchrotron radiation[53] for the first time.

The use of two circular (pinhole) apertures yields a lateral resolution of approximately wavelength/3. The axial resolution (that is, the depth of focus) is approximately equal to the wavelength used. The minimum diffraction limited

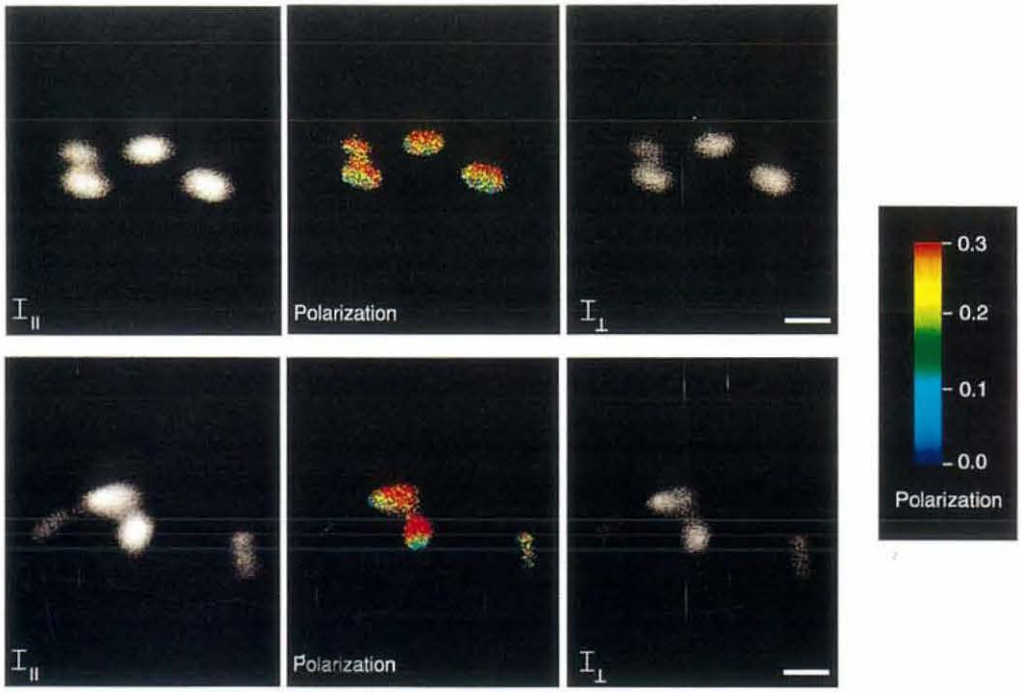

Figure 10. Images of dormant spores of Bacillus Subtilis from the confocal microscope at the SRS viewed in fluorescence polarisation contrast. The images arise from the fluorescence of the intrinsic probe tryptophan excited at 266 nm in polarised light. Images of opposite polarisation are collected and the polarisation map shown is calculated to indicated the regions of high probe mobility (or fluidity) within the highly dense spore state prior to its change into an active bacterium. Bar=1.1 microns. See 53).

volume achievable by the SRS confocal system is therefore about 70 nm × 70 nm × 200 nm when operating close to 200 nm. Of course, this resolution advantage over a conventional microscope is gained at the expense of field of view and therefore a scanning system is incorporated in order to gain a complete image of the sample. This spatial selection also results in very high contrast in the image since information is taken solely from the small volume of the sample illuminated thus giving greatly reduced scatter. The system is immensely versatile used with intact and wet biological specimens, it can be operated to give reflected light contrast or fluorescence (probe) contrast and the input wavelength can be quickly scanned across the range from 200 nm to ~700 nm. The provision of LiF, MgF or synthetic silica objective lenses or of a good quality reflecting objective should enable the microscope to operate effectively at much shorter wavelengths down to ~160 nm and perhaps even lower. The microscope has been used to provide three dimensional images by "optical slicing" in which a succession of images each with very small depth of focus (~>200 nm) are obtained by moving the plane of focus progressively through the sample. Sample contrast can easily obtained using fluorescence polarisation imaging giving information about molecular (probe) orientation and probe mobility within the sample and an example is given in **Fig. 10**. The system has also been used in a non-scanning mode, when a near diffraction limited volume of interest is selected within the sample in order to carry out "microvolume spectroscopy" in which specific internal structures within a single cell (such as the cell wall, cytoplasm or nucleus) are studied using fluorescence lifetime, polarisation, intensity or spectrum over any period of time to interrogate cell behaviour.

20. Radiation Damage Studies

It is only a few years since the subject of radiation damage seemed uppermost in the minds of the new community of biologists whom were contemplating the use of synchrotron radiation for research[54].

Those early concerns now appear to be of less importance to the large numbers of scientists who use protein crystallography, small angle scattering and imaging for their research. However, an understanding of radiation damage and a proper description of the mechanisms by which ionising radiation loses energy in biological material leading to molecular (genetic) changes and to biological lesions remains as a problem of the greatest importance. Although synchrotron radiation is an ideal source for this type of research, sound experiments are difficult to conduct and the high fluxes needed are not easily attainable from dipole sources. Work has been carried out at the SRS on the action spectra, (that is, fragment yield versus excitation wavelength) for single- and double-strand break induction in plasmid DNA. The data suggest that in the (dry) DNA system 8 to ~25 eV photons induce single strand (ssb) and double strand (dsb) breaks via a common precursor species which has a 12 to 20 fold higher probability of generating a

ssb than a dsb. A weak threshold at around 8 eV also indicates a common mechanism-with differing efficiencies-for the formation of ssb and dsb[55,56].

A great deal more work using synchrotron radiation is needed in this whole area of research covering excitation energies from ~eV to ~>keV.

21. Synchrotron radiation in Medicine

The application of synchrotron radiation based techniques to medical research and to clinical medicine is not particularly new. In fact one of the reasons for the development of cyclotron accelerators in the 1940's was linked to their potential use as a generator for x-rays! In the UK, discussions held during the 1980's failed to generate any major interest in body imaging (of the head or heart) or-in the 1990's-to continue with any significant investment into the applications of soft x-ray microscopy. In part, this was a consequence of the somewhat low brilliance and low (2 GeV) energy of the SRS. The use of high energy accelerators (e.g. at Hamburg and Stanford) and of large, "3rd generation" synchrotron radiation facilities has enabled steady progress to be made in the field of angiography and this is recorded regularly at International meetings on Synchrotron Radiation Instrumentation.

Table 7. Synchrotron Radiation in Medicine in the UK

BONE
Pathology of bone
Measuring bone density
Quantitative mapping of calcium and protein in normal and osteoporitic bone
Bone prostheses
CARDIOLOGY AND VASCULAR STUDIES
Mechanisms of calcification of bioprosthetic heart valves
Vascular structures
Synchrotron radiation coronary angiography*
MAMMOGRAPHY
Correlation of calcifications with in situ carcinoma
Diffraction studies of calcifications
Mammography using SR
SR analysis of breast tissue samples
NEUROLOGY
Parkinsons disease (iron storage)
Myelin pathologies
Photodynamic therapy
Amyloid studies
Microtomography of bee brain
Microbeam therapy of brain*
SOFT TISSUE
Muscle research
Study of collagen and cartilage
Eye research, x-ray test for Macular Corneal Dysatrophy
Structures in soft and mineralised tissues, diffraction from urinary stones
Hair damage following chemical treatment
Transdermal drug administration (skin structure study)
Tendon studies
RADIOLOGY
Atomic environment of metals in human tissue.
Monitoring hormone uptake (fluorescence)
Radiation damage studies

(*work not undertaken inside UK)

At the SRS, a largely new field of application of synchrotron radiation has now emerged in which small and wide angle x-ray diffraction and scattering, EXAFS, powder diffraction, fluorescence probe methods and imaging methods (confocal imaging, tomography) have been successfully applied to understand and study the biological structures which correlate with "medical" problems. **Table 7** summarises some of the work undertaken in this field inside the UK. A striking feature is the amount of fresh information which is revealed when x-ray diffraction is used to give detailed information about protein structure, e.g. of amyloid proteins and then circular dichroism used to observe dynamic behaviour including the spontaneous formation of amyloid like fragments[57]. This kind of study may help to inhibit the growth or to dissemble the extremely stable amyloid fibrils which resist clearance by proteolytic enzymes and accumulate in vital organs causing a variety of pathological problems. X-ray diffraction has been successfully used to study corneal collagen packing in healthy eyes and in eye displaying Macular Corneal Dystrophy-a condition characterised by the synthesis of abnormally large proteoglycans which tend to aggregate[58].

Similarly, in low angle diffraction from nerve myelin sheath and using core cut samples from normal, benign and malignant breast tissues, a clear delineation is often given between normal and damaged tissue. Synchrotron radiation data may indicate a more complex crystallisation pathway for breast calcium deposits than previously assumed. In the case of urinary stone disease x-ray powder diffraction data allows the stone mineral phase, crystallite size and internal organisation of the stone to be interrogated and this is contributing to the design of synthetic simulant systems.

For the future, there must be a very rapid expansion in using synchrotron radiation for the determination of all biological macromolecules which can be produced in crystal form—however small. In medicine, there should be a continuing role for synchrotron radiation to play in terms of angiography and brain imaging[59,60]—although the extent to which it will become anything like a routine clinical procedure is far from clear and will likely be dependent on the cost and accessibility of synchrotron radiation sources. For medical pathology however, where samples are weakly diffracting, poorly ordered and often wet and small it would appear that the use of synchrotron radiation x-ray diffrac-

tion at low and high angles could, often for the first time, reveal structures at the molecular level to correlate with a medical condition. Surely this must be an area for future growth.

Biotechnology, pharmaceuticals and medicine continue to be huge wealth creators. Synchrotron radiation offers the best and most rapid access to high quality structural information in all fields of biology using crystallography, small and wide angle x-ray scattering and some imaging. Although access to synchrotron radiation will be crucial to maintaining and enhancing a competitive advantage, it is at present the case that the achievements of synchrotron radiation in biological structure studies far outpaces investment from the Life Science community. It is certain that fresh demands for synchrotron radiation will come from a largely hidden (at present) community of non-specialists in synchrotron radiation who wish to undertake bio-structure studies rapidly and conveniently.

To summarise, synchrotron radiation is a tool which is indispensable to UK science and which already has a well defined role to role to play for the foreseeable future in the determination of the atomic structures of a huge range of natural materials.

22. The Cost of Synchrotron radiation

The 1990's synchrotron radiation research environment at facilities around the world has gradually changed from the obvious individualism of the early years which were often associated with long periods of access to the beam. Synchrotron radiation is now no longer really "small science" despite the fact that at the SRS for example, about 50% of the beam time awarded in 1996 was for less than 2 days and about 95% for less than one week.

In scientific papers it is normally unfashionable to consider cost. However, the greater the cost, the greater the attention which will be paid to the value of the synchrotron radiation research output. In 1996, the "Round Table" of European Synchrotron Radiation Facilities assembled information from France, Germany, Italy, Sweden and the UK (twelve rings in all). An abbreviated summary (not including the ESRF)[61] shows that: total operating budgets are ~180 m$ per year: total user capacity is ~40000 station days per year (when each facility operates for from 200 to 250 days per year; total number of stations is ~200 (1996) and this should rise to ~250 by year 2000; there are around 15000 users-perhaps as many as 20000, and around 80% of them use photon energies above 100 eV. Across Europe, beam time charges are made to non nationals (but paid for via the E.U.) which range from 2000$ to 6500$ per day The ESRF costs are about three times greater and are met by payments from participating countries who receive beam time access primarily according to their contributions. Within the UK itself, all beam time is charged to the appropriate funding agency (e.g. Medical, Natural Environment, Engineering and Physical Sciences, Biotechnology and Biological Sciences Research Councils) or to whichever other private Institution or industry make use of it. This system is intended to support only the most important and urgent programmes needing synchrotron radiation and to ensure that there is strong "tensioning" between all UK facilities (e.g. neutrons, lasers) and between research carried out at UK home laboratories and UK facilities. World wide, the level of usage of synchrotron radiation beam time was predicted to rise by a factor of two over ten years to about 100000 station days in year 2000[62]; the final total may be higher still given the pressure to increase station numbers and also ring operating periods even on existing rings.

If only because of "value for money" reasons, it is therefore a serious matter that sources, existing and planned, offer more brilliance and flux than beam line instrumentation can usually deliver to the sample. It also matters that when high signal levels are available from the sample they often cannot (in the case of x-ray scattering and diffraction at least) be fully exploited because of the inadequate speed of most present day detectors.

Given the immense national investments in the big new facilities of the 1990's (~1000 m$ for each of ESRF, APS, SPring8) perhaps some fresh ideas are required to maximise the efficiency in terms of the ways in which the users work with them! A striking innovation in this area is the remote operation of a beam line (by the University of Wisconsin-Milwaukee) in the Spectromicroscopy Laboratory at the ALS[63]. This "Collaboratory" is planned to give remote access to three analytical tools to provide spatially resolved chemical information down to the atomic scale.

For many years there have been Participating Research Teams who may be wholly responsible for the costs and operation of their beam line as at NSLS and most facilities make a charge to "industrial" users who are then provided with scientific support and beam time (at the SRS at least) but are not required to publish the results of their investigations.

An alternative approach is provided at the SRS where a new service called DARTS (Daresbury Analytical Research and Technology Service) was set up in response to requests from industrial (also academic users) to provide a data collection service for powder and single crystal diffraction, EXAFS and small angle scattering, in order to buy access to SRS staff skills and experience as well as beam time. Whatever model emerges, it is clearly nonsense for all those who wish to use synchrotron radiation (from fresh graduates to professorial staff) to have learn about the details of storage rings or beam lines or even to spend time to learn how to use such highly complex systems-this will become the role of trained and highly skilled station scientists.

23. The value of synchrotron radiation

The reviews of the science programmes which have been based on the use of synchrotron radiation in the UK[64] have always strongly supported the level of activity in the UK and recommended expanded programmes for the longer term to include not only a replacement for the SRS as a world class source of x-rays but also to develop a source optimised for high brilliance in the soft x-ray and VUV region. For tactical, if not for financial reasons a purpose built VUV/SXR

Table 8(a). DIAMOND—the principal parameters

Stored beam energy	3 GeV	Ring Circumference	345.6 m
Injection energy	3 GeV	Lattice Type	16 cells DBA with 2 super straights
Beam Current	~300 mA	Maximum I.D. lengths	
Radiated Power	650 kW	Bunch Length	~33 ps
Emittance (h, v)	14.3, 0.14 nm-rad	Beam Lifetime	~20 hours
Source Size (fwhm)			
Low Beta Straight	260, 50 micron		
High Beta Straight	1070, 35 micron		
Super Straight	890, 90 micron		

Table 8(b). Parameters of "Generic" Insertion Devices for DIAMOND

I.D. Name	Period (mm)	B max Tesla	K max	Gap (mm)	N periods	Length (m)
U21	21	0.424	0.83	10	214	4.5
U31	31	0.687	1.99	10	145	4.5
U48	48	0.512	2.30	20	93	4.5
U80	80	0.864	6.46	20	56	4.5
U120	120	0.625	7.0	20	37	4.5
MPW	136	1.6	20.3	20	33	4.5

source remains as an option of lesser priority but still presents clear and important new opportunities in photophysics, chemistry and biology.

In November 1997 the USA, Department of Energy (DOE), produced the first major review of synchrotron radiation sources and science, since a "Seitz-Eastman Report" carried out by the National Research Council-National Academy of Sciences called "Major Facilities for Materials Research and Related Disciplines" was completed in 1984-some fifteen years earlier!

This new review-the BESAC report[18]-identified the great importance of synchrotron radiation sources and confirmed the good quality of science coming from them.

Of special note was the fact that synchrotron radiation was able to generate advances in all basic and applied sciences including for example, geological and environmental research. At the time of the Report, synchrotron radiation related activities were responsible for about 25% of the total Basic Energy Sciences budget in the USA. In addition, the report noted that synchrotron radiation sources had attracted a great deal of industrial interest (and funding) across a very wide range including microanalysis, catalyst studies, thin films, polymer processing, drug design, surface and deep lithographies etc. and continues to diversify. The recommendations (including a budget increase of ~11%!) were directed primarily toward strengthening existing programmes on well established facilities to seek yet higher quality and a higher quantity of research. The report writers were very impressed by the programmes at the "second generation" sources. The need for all three hard x-ray sources in the USA to extend their work on atomic and magnetic structure studies on all kinds of biological and non biological materials was clear, together with the maintenance of a robust programme on electronic structure and interaction studies including for example bonding in solids. The smaller community concerned with fundamental studies of atoms, molecules and surfaces were seen to have made their major contribution during the 1980's and early 1990's.

24. The strategic plan for synchrotron radiation in the UK

Synchrotron radiation has played and will continue to play a crucial role in the overall UK science programme. The SRS Upgrade will be completed in 1999 and will develope the SRS to capacity by the addition of two multipole wigglers to feed at least three stations. Some additional resources to help maintain the UK lead in crystallography and selected detector technology are being provided. After the Upgrade it will be pointless to modify the ~25 year old SRS any further. It should then be replaced with an "all insertion device" facility (DIAMOND) to retain UK world class competitiveness well beyond 2000. The DIAMOND design[64] has flexibility, very high flux, small source size and is optimised for operation at ~10 keV. The parameters for DIAMOND are given in **Tables 8(a)** and **8(b)** and an artists view of the facility is shown in **Fig. 11(a)** and **(b)** together with a general arrangement drawing of the "racetrack" layout. Gains in flux of up to 500 times more than the SRS wiggler and in brilliance of up to 10^4 times the wiggler are expected. Continuity of access to synchrotron radiation by the SR community is essential i.e. the "seamless" transfer of users from the SRS to DIAMOND is planned together with the transfer of the new Upgrade stations and the latest detector technology. It is known that many UK companies, and institutions are anxious to play a role and at least one non-government organisation has announced advanced support for the project. At the time of writing, it seems reasonably probable that an announcement to declare formal approval of the DIAMOND project will be made during the summer of 1998. If, and when such approval is given, it will represent a tremendous "vote of confidence" by the UK

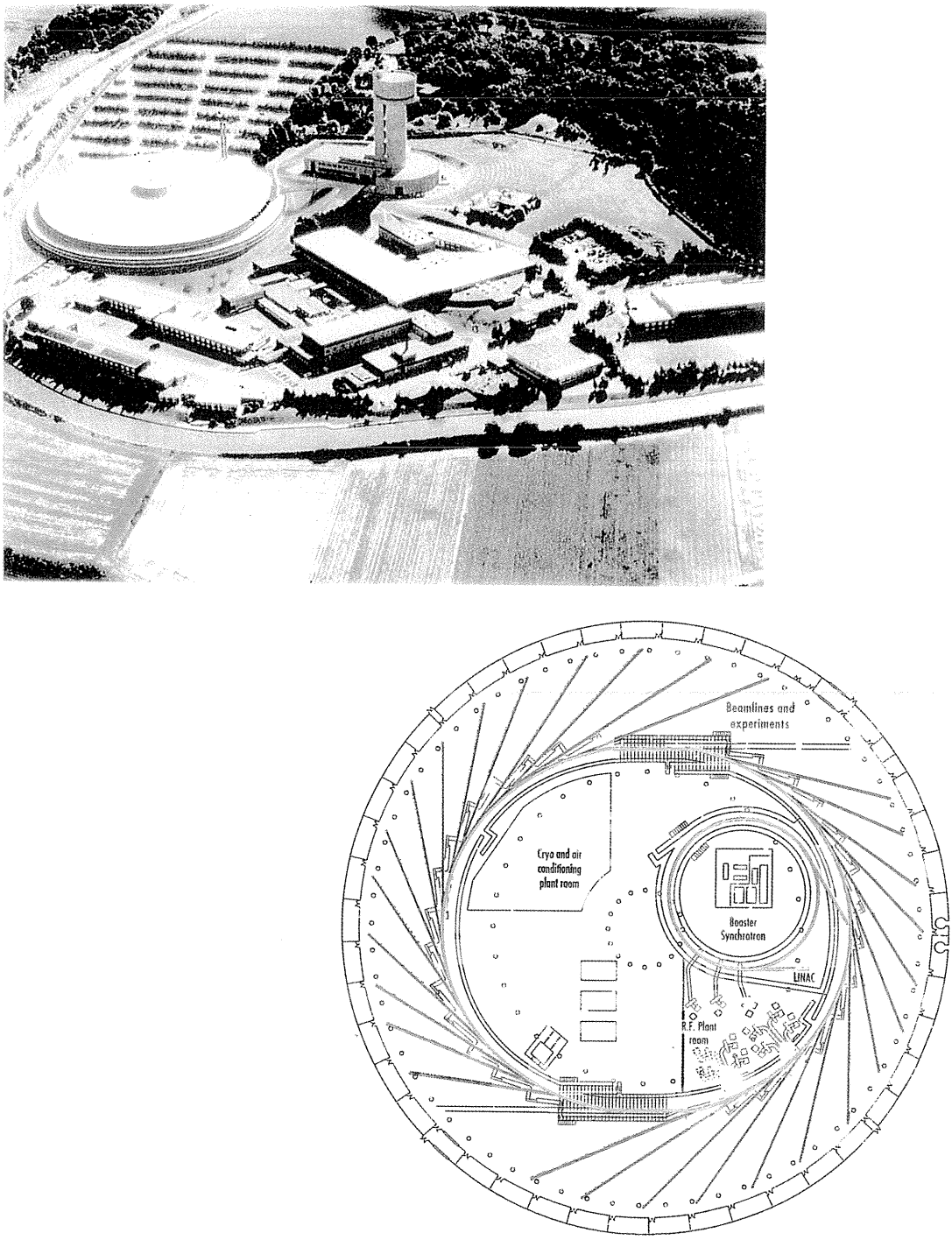

Figure 11. The upper picture presents an artists view of the DIAMOND source which may be built at Daresbury Laboratory. The lower picture gives the general arrangement proposed for the "race-track" lattice of DIAMOND[64].

community for the promise of new science to emerge from the long term future use of synchrotron radiation.

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