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Synchrotron Radiation Research in the UK

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The origins, development and growth of synchrotron radiation science and technology in the UK, and an account of the expansion of the synchrotron radiation research programme, its highlights, current activities and the prospects for the future expansion of synchrotron radiation activities within the UK, are presented.

Keywords: UK synchrotron science; UK synchrotron radiation technology.

1. Introduction

The observation of radiation from electrons in a synchrotron in April 1947 (Elder, Gurewitsch, Langmuir & Pollock, 1947) gave us a brilliant source of white light and X-rays with the now rather inappropriate appellation 'synchrotron radiation'. It immediately helped to promote the generation of a definitive classical theory for the calculation of the radiation pattern polarization and spectrum generated by accelerated electrons (Schwinger, 1949). Within ten years the first experimental study of the angular, spectral and polarization properties had been undertaken and contrasted favourably with all the predictions made in the classical radiation theory of accelerated electrons (Tomboulian & Hartman, 1956). This work included the first synchrotron radiation spectroscopic study (of metallic Be and Al) and the prediction that synchrotron radiation should be an ideal source as a UV/VUV standard for the purpose of calibrating detectors. Subsequently, this led to seminal work by R. P. Madden, K. Codling and others at the National Bureau of Standards in the USA on inner-shell electron excitations and the discovery of autoionizing states in rare gases – an early and excellent revelation of the potential value of synchrotron radiation in scientific investigation (Codling, 1994).

Within the UK, Dr G. V. Marr at Reading University prepared an application in 1964 for funds to use accelerators at Glasgow University to exploit synchrotron radiation as a source of UV and VUV. By 1966 a small grant (£2000) was awarded to fund a feasibility study which led to the recommendation that the Glasgow Linac be used as the electron source and a superconducting magnet system used to impose radial acceleration to yield synchrotron radiation. This would have been, of course, the world's first 'superconducting dipole wavelength shifter'! Unfortunately, the funds were not actually allocated until 1967, and by 1968 it was clear that neither the superconducting magnet technology needed for the project nor the long periods of time needed on the linac could be achieved. Instead, the funds were diverted to the exploitation of the 300 MeV (3 Hz) electron synchrotron in the Physics Department at Glasgow University. For the following few years this small facility supported a significant programme of VUV spectroscopy and detector calibration led by scientists from Reading and Glasgow universities and the Culham and NPL laboratories, until the Glasgow facility was closed in 1972. By that time the new 'SRF' (Synchrotron Radiation Facility) had already become operational at Daresbury Nuclear Physics Laboratory.

2. The Synchrotron Radiation Facility (SRF) – the early years

Quite independently and unknown to the Reading University group, the Molecular Photophysics group from Manchester University had been undertaking a preliminary survey and measurements at the newly operational Daresbury Laboratory 4 GeV electron synchrotron (called NINA). I. H. Munro obtained permission in 1966 from the then Daresbury Nuclear Physics Laboratory (DNPL) Director (A. Merrison) to construct and operate a UV beamline 'parasitically' on NINA (Fig. 1). First measurements commenced in April 1967. By January 1969, as a direct outcome of this early work, a comprehensive scientific proposal to establish a user facility to exploit the synchrotron radiation from NINA had been submitted to the SRC (UK Science Research Council), incorporating the results from the preliminary survey (Hamilton & Munro, 1969). Subsequently, from about 1970, the operating energy of NINA was increased to 5 GeV.

It is greatly to the credit of the council of the SRC, and to the special panel set up by the physics committee in particular, that the potential merits of synchrotron radiation were recognized so clearly. As a consequence, by the end of 1969 decisions had been taken to close the Glasgow Linac, to transfer all the existing Glasgow effort to the NINA synchrotron and to fund the construction and operation of a national synchrotron radiation facility (the SRF) at Daresbury with an initial five-year grant of £360 000 – a very large sum for those days! The recommendation of the physics panel was actually that a larger facility than had been originally suggested should be built! The SRF finally would house two beamlines (north and south) providing beam to six experimental stations and two preparation laboratories. Since the operation was to be wholly 'parasitic', no charge was to be made by the SRC Nuclear Physics Board to the SRC Science Board for the use of NINA for its synchrotron radiation research programme!

The science programme initially approved in 1970 included (i) VUV molecular spectroscopy of organic solids in the region 100–200 nm (Manchester University; S. S. Hasnain, T. D. S. Hamilton, I. H. Munro, E. Pantos); (ii) absorption spectra of atoms and molecules from 0.1 to 100 nm, and instrument design (Reading University; K. Codling, G. V. Marr, J. B. West); (iii) absorption and reflection spectra of thin films and metal single crystals, 2–200 nm (Oxford University; W. Hayes, J. Beaumont); (iv) optical properties of solids, 50–200 nm (Cambridge University; A. Joffe, Y. Liang, J. Bordas); and (v) synchrotron radiation as a spectral standard, 90–400 nm (National Physical Laboratory; P. Key). By 1972 these initial user groups had begun to establish their experimental programmes and very soon additional bids were received in the areas of photoelectron spectroscopy, X-ray reflectivity studies, applications in biology including small-angle diffraction and scattering and soft X-ray microscopy.

At this time the world annual output of scientific papers on synchrotron radiation was increasing extremely rapidly (Marr & Munro, 1971; Marr, Munro & Sharpe, 1972). The eventual massive growth of interest and activity in high-brilliance X-ray science research that characterizes so much of the exploitation of synchrotron radiation today worldwide had just begun (Fig. 2). In 1971, at the Third International Conference on VUV Radiation Physics in Tokyo, Japan, several papers identified the potential benefits of synchrotron radiation and offered novel instrument design for the VUV and SXR regions. This conference led to the world's first International Symposium for Synchrotron Radiation Users at Daresbury Laboratory in January 1973 (Marr & Munro, 1973). It was held during one of the foggiest periods of weather in northwest England ever recorded! The international advisory committee included, among others, Y. Cauchois, U. Fano, R. Haensel, R. P. Madden, T. Sasaki and W. E. Spicer. There were, among the 36 presented papers, descriptions of the early programmes of work from Daresbury, Bonn, Hamburg, Orsay, Tokyo, Washington, Glasgow and Wisconsin. At that time, one advantage of working within a major high-energy physics facility was the access to early world-class computer facilities. As early as 1968, the first proposal had been made to design and operate a monochromator by computer at Daresbury Laboratory and this was operational by 1972. Since that time, the always limited amounts of beam time available to users, combined with their high cost and the high level of demand, have

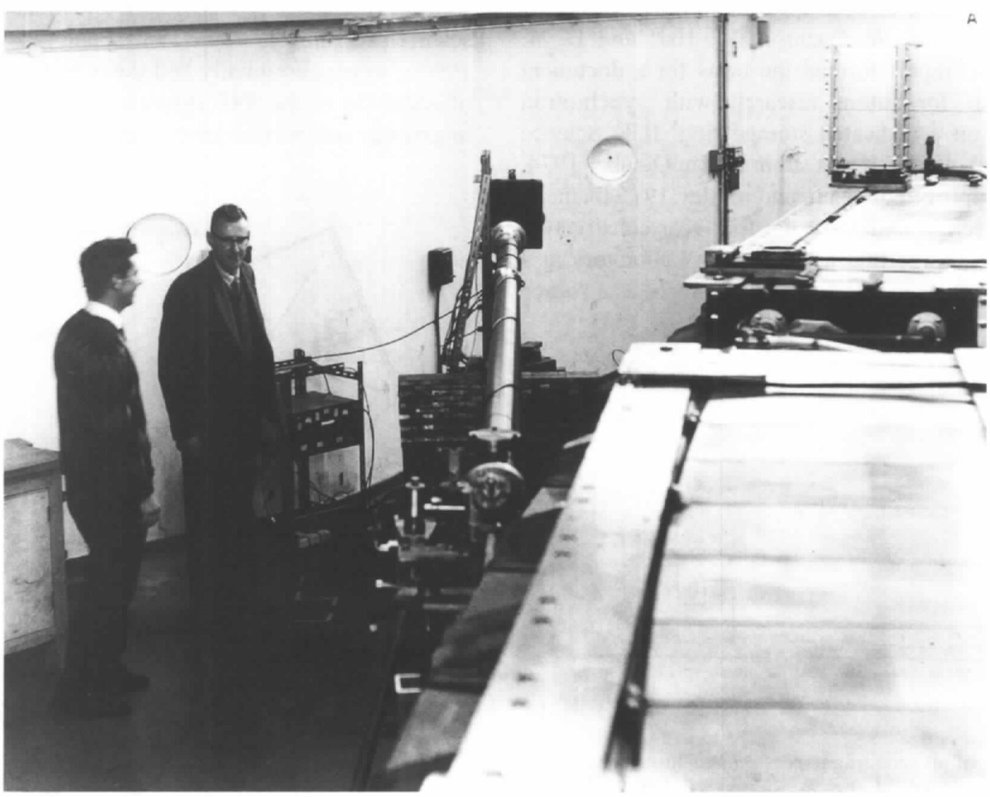


Figure 1
The first synchrotron radiation beamline on NINA constructed in 1966/1967 by Manchester University (Department of Physics) (I. H. Munro and T. D. S. Hamilton).

resulted in equipment at synchrotron radiation facilities becoming probably more intensively used than any other apparatus in pure research. In order to achieve this, computer control is almost mandatory for most aspects of the experiment, including the operations of the beamlines and of the accelerator itself.

3. The end of the beginning!

Already, by 1972, the UK Science Research Council (SRC) had conducted a review of the UK commitment to research into high-energy and elementary particle physics and had come to the conclusion that the UK could probably not continue to afford to maintain a large internationally competitive national high-energy particle accelerator. As a consequence of this, NINA, and with it its parasitic SRF, were proposed for cessation of operations before the end of 1977. All this within one year of start-up of the SRF and only six years after first operation of NINA! By 1973 the closure of NINA (at the end of 1977) became inevitable. The very rapidly growing, and vociferous, young synchrotron radiation user community of some 40 researchers from 12 universities insisted that the SRC should either adapt NINA as a full-time source of synchrotron radiation or should build a replacement synchrotron radiation source, perhaps using NINA components and buildings.

A science panel (chaired by P. McWhirter) had already been established to address this problem under the aegis of the physics committee by late 1972 with a membership of K. Codling, W. Hayes, H. E. Huxley, I. H. Munro, G. Saxon and co-opted members W. Cochron, M. Hart and D. W. Turner. The panel report formed the basis for a document entitled 'A plan for future research with synchrotron radiation based on a dedicated storage ring' (UK Science Research Council, 1973). It was submitted in October 1974, when the SRC approved the plan, and in May 1975 financial approval was given to undertake the four-year construction of a 2 GeV 1 A storage ring at Daresbury Laboratory at a capital cost of £3 million, purpose-built to serve as a source of synchrotron radiation (Daresbury Laboratory Report, 1973, 1976). It was, by todays criteria, a decision of considerable scientific and financial consequence which was taken extremely speedily. The approval of this purpose-built dedicated source of X-rays in the UK led the way into a new era of dedicated synchrotron radiation sources around the globe including NSLS, ALADIN, the Photon Factory and many others.

The SRF (see Fig. 3) finally closed down with the switch-off of NINA at 1100 on 1 April 1977. The full history of the SRF represented a remarkably successful venture, since at comparatively modest cost, from 1972 to 1977, it met the needs of the rapidly growing community of UK users with such widely differing interests. The level of intellectual exchange between the physicists, chemists and latterly biologists working together on the beamlines enabled many scientific problems to be resolved in a manner which often ignored the traditional departmental 'intellectual boundaries' prevailing at that time in the university sector. The best surface science research or the study by X-ray diffraction of biological material might well simultaneously require input from trained physicists, chemists and biologists and there is no doubt that, during the 1970's and the early 1980's, the SRF and the SRS provided excellent working models of multidisciplinary science centres – a feature that the university sector reluctantly recognized and ultimately had to emulate.

The five-year research output from the NINA SRF appeared as some 190 articles, approximately 96 of which were in refereed journals. The foundations of many of the science programmes of the 1980's, and in some cases of the 1990's, were substantially laid down in those first few years of operation of the SRF (Munro, 1979). Radiation damage to gratings and mirrors gave an early indication of the X-ray

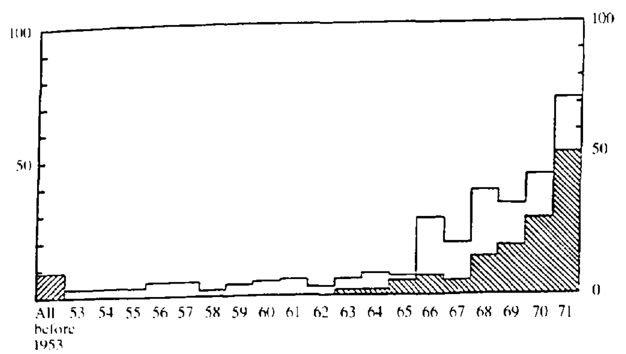


Figure 2
The annual output of all scientific papers on synchrotron radiation research based on Marr, Munro & Sharpe (1972). Papers on astrophysical synchrotron radiation are excluded. Upper line: all publications. Lower (hatched) area: papers in X-ray diffraction, solid-state physics and atomic and molecular physics.

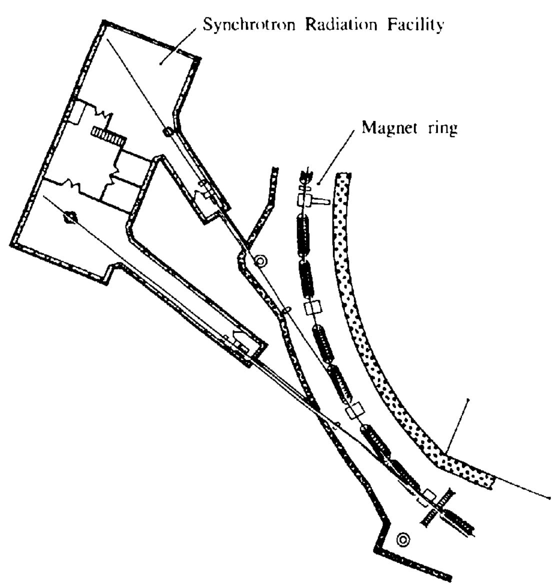


Figure 3
A plan of the Daresbury Synchrotron Radiation Facility on NINA, operational from 1972–1977.

power associated even with a low current synchrotron radiation source. A theory of electron scattering was published by J. Pendry in 1975 (Lee & Pendry, 1975) leading to immense benefit to the users of the EXAFS and XANES techniques and ultimately to the first international EXAFS conference in 1981 held at Daresbury (Garner & Hasnain, 1981). The first ever synchrotron radiation experiment using energy-dispersive X-ray scattering was published (Bordas, Glazer & Munro, 1976). M. Hart (Beaumont & Hart, 1974; Hart, 1975) established X-ray topography at Daresbury and undertook work which led to the design of X-ray instrumentation (monochromators, interferometers) now used worldwide. G. V. Marr and J. B. West (West & Marr, 1976) made many absolute photoionization cross-section measurements on rare gases which still stand today, and the work of R. H. Williams (Coleraine), C. Norris (Leicester), R. J. Pettifer and P. Woodruff (Warwick), B. Tanner (Durham), T. D. S. Hamilton (Manchester) and D. J. Fabian (Strathclyde) broke fresh ground in a variety of new areas of research. J. Beaumont, J. Haselgrove, H. E. Huxley, J. T. Randall, J. Bordas and others helped establish the UK programme to study biological materials using small-angle X-ray diffraction and scattering methods – one of the principal activities at the SRS during the 1980's and 1990's.

4. The SRS – the first purpose-built storage ring dedicated to X-ray research

In April 1974 a large and very lively meeting was held at Reading University, organized by the Institute of Physics, to discuss 'synchrotron radiation and its applications to the analysis of problems in scientific investigation'. It was already clear (because, of course, of the peak flux and brilliance in the X-ray region) that the most likely growth areas for synchrotron radiation should be those of X-ray (including soft X-ray) science and technology in general and of studies of condensed matter systems (biological and non-biological) in particular. The debate naturally included discussions on the most appropriate geographical location for such a centre including an (unsuccessful) attempt to identify the academic 'centre' of the UK! The fortunate selection of Daresbury Laboratory as the site for the new source was largely a pragmatic one and it certainly helped (together with the construction of the Nuclear Structure Facility) to assure a scientific life for Daresbury Laboratory long after the cessation of high-energy physics research.

The selection of the parameters for the SRS was less straightforward. The restricted total sum of money likely to be made available necessitated the re-use of many of the buildings and much of the equipment associated with NINA (the magnet power supplies, for example). With hindsight, perhaps too optimistic a view was taken about the target circulating current (1 A, subsequently dropped to 500 mA), although the SRS is at present probably the most reliable and heavily used storage ring in the world and routinely achieves 300 mA. The selection of a conventional 600 MeV booster synchrotron as injector, combined with a ramp and store facility for the storage ring, was seen to offer routine operation economically at any energy from 1 GeV up to a maximum of 2 GeV. Most importantly, it would fit easily within the old NINA buildings and, with straight sections of around 1.2 m, would leave sufficient space for the installation of superconducting high-field bending magnets (*i.e.* for 'wigglers' or 'wavelength shifters') (Daresbury Laboratory Report, 1976).

A serious consequence of the decision to close down the only source of synchrotron radiation in the UK (the NINA SRF) long before the SRS had been constructed was the creation of a 'gap' – a period without any access to synchrotron radiation for users within the UK. The SRS was being assembled and constructed during the period from about 1976 to 1979 and began operation in 1980. In this intervening ('gap') period the previously outstandingly active research programme associated with the SRF effectively vanished. A major exodus took place, from 1977, of many of the leading UK synchrotron radiation scientists – a process which unquestionably benefited other facilities then operational in Europe, the USA and elsewhere. The 'gap' presented serious difficulties to students and academic staff alike for whom continuity in research is vital. Although the SRC were generous in their support for users to work at facilities outside the UK, it was to be several years before a coherent science voice was heard again from the synchrotron radiation community.

In the 1970's the users were, in the main, wholly committed to working at the SRF. On the other hand, the user community of the 1980's were drawn, in general, from outside academic and other institutions for whom access to synchrotron radiation was important or even essential but for whom it would normally represent only one component part of a larger research portfolio. This attitude led to the operational philosophy for the SRS. New users would submit a scientific application which, once approved, would result in the provision by SERC and Daresbury Laboratory of all the necessary equipment, beam time and SRS staff support necessary for a successful outcome. By the end of the 1980's this would result in the pre-eminent position of the SRS in terms of its operation as a *user* facility in which provision was made for scientific and technical support at most stations for most experiments, even perhaps leading in some cases to help to users with analysis and interpretation of results!

The formal inauguration of the SRS took place in November 1980 in the presence of the Secretary of State for Education and Science and the Chairman of the SRC (G. Allen). Within two years of start-up, 12 stations were in operation and by 1983 the first insertion device – a 5 T three-pole superconducting wiggler wavelength shifter – was successfully installed to meet the rapidly growing needs of the X-ray diffraction community for radiation at $\sim$12 keV. The completion of the source by 1980 reflected well on the accelerator staff at Daresbury, although the somewhat conservative design chosen for the SRS was perhaps one penalty paid for the very short time between the initiation of the project in 1972 and its approval. The primary emphasis of the UK user community was on maximum flux, an electron energy of 2 GeV, short bunch length (< 1 ns) and the smallest affordable electron beam cross section in the vertical direction. It was a pity that neither the user community nor the source designers were able to fully recognize the feasibility of and opportunities with insertion devices and the need for long straight sections. The project cost rose to £4 million by 1976, finally to about £5.5 million at completion (including about £0.7 million for stations on two beamlines). A serious omission at the time was not to recognize the full costs for instrumentation of beamlines on the facility. This initial underestimation led to difficulties for many years in attempting to obtain full and proper costs for subsequent new equipment. The initial design of the SRS was such as to enable it to operate routinely at either 1 GeV for VUV/SXR users and up to 2.0 GeV for X-ray users. In fact, this facility was never exploited and the SRS was always operated at its maximum energy to meet the primarily X-ray needs of the user community.

The most significant early 'vote of confidence' in synchrotron radiation at the SRS was provided by the UK MRC (UK Medical Research Council) who, through an agreement with the SRC in 1982, gave support to establish an entirely new Biology Support Laboratory (the 'BSL') alongside the SRS. The BSL was to provide the base from which the world-leading programmes in protein crystallography would be supported later in the decade. Extensive facilities for the preparation of biological and biochemical materials and for the assessment of their viability were provided since, wisely, these were seen to be essential to the future success and the excellence of the future life sciences programme. In a 50:50 agreement with the SRC, the MRC also provided part funding for some beamlines and for the first (5 T) wiggler. In 1983 J. Bordas was appointed to the position of Head of the BSL and set in motion a programme to undertake biological small-angle X-ray diffraction and scattering and to stimulate research in life sciences in general using the SRS. This early initiative undoubtedly anticipated and helped to stimulate and generate the now rapid growth in the biological and medical applications of synchrotron radiation in the UK and elsewhere.

5. The SRS in the 1980's

The early 1980s was a period of rapid change and of considerable optimism in terms of the potential opportunities in research and technological gains to be made using synchrotron radiation. New sources in the USA, Japan and Europe were being constructed or planned. Countries without direct access to synchrotron radiation established connections with those who had. By 1984 the SRS had joined in a formal agreement with the Netherlands Research Council ZWO (later NWO); an agreement which was to survive with great success until 1994. Through this highly fruitful science collaboration, a new UK/Dutch beamline was constructed on port 8 incorporating a unique EXAFS

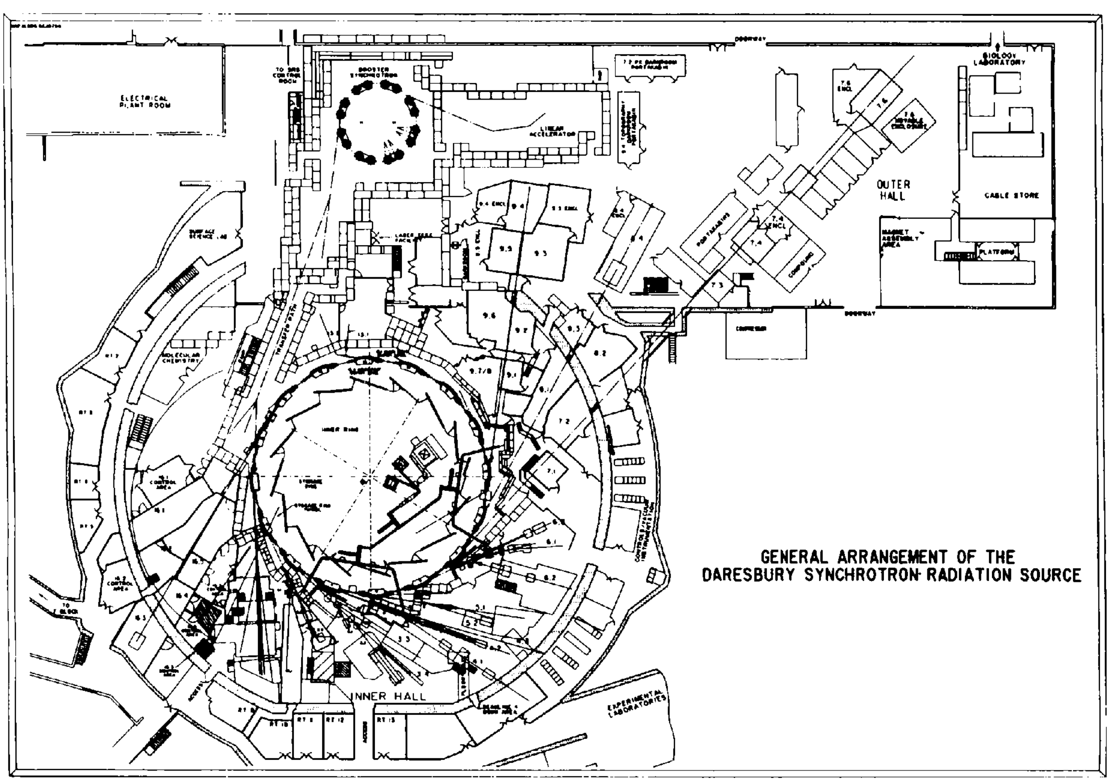


Figure 4
A plan view of the SRS and its beamlines.

station design and also a station for small-angle X-ray diffraction (Van der Hoek *et al.*, 1986). In fact, the world's first directly cooled X-ray monochromator emerged from this effort in 1985 (Bijeleveld *et al.*, 1986) setting the scene for direct cooling of X-ray crystal monochromators by drilling water channels in the Si crystal. Later, the agreement with NWO would lead to the construction of a station for surface X-ray diffraction, for UV confocal imaging and a substantial contribution to general instrument development on the SRS.

Agreement was also established with the Swedish Research Council (NFR) covering work in crystallography and in atomic and molecular physics. At about the same time the SRS became host to a consortium of major UK companies (Shell, BP, ICI), who for more than a decade purchased access to beamlines on the SRS. This group was named 'the Industrial Consortium' and helped to generate an early awareness of the manner in which industrial users would wish to exploit synchrotron radiation.

During the early 1980's various synchrotron radiation facilities being commissioned around the world frequently encountered 'teething troubles'. The SRS was no exception (suffering mainly from r.f. window problems) and it was not until 1984 that machine operation became acceptably routine to the users. During this 'learning' period the user facility had expanded to about 20 stations on seven dipole magnet ports around the SRS. The initial groups of stations for atomic and molecular spectroscopy on port 3, for surface and bulk studies on port 6, and for EXAFS, crystallography, interferometry and topography on port 7, were to become eclipsed by the rush by a new generation of X-ray users for access to the 5 T wiggler (port 9) where the substantially

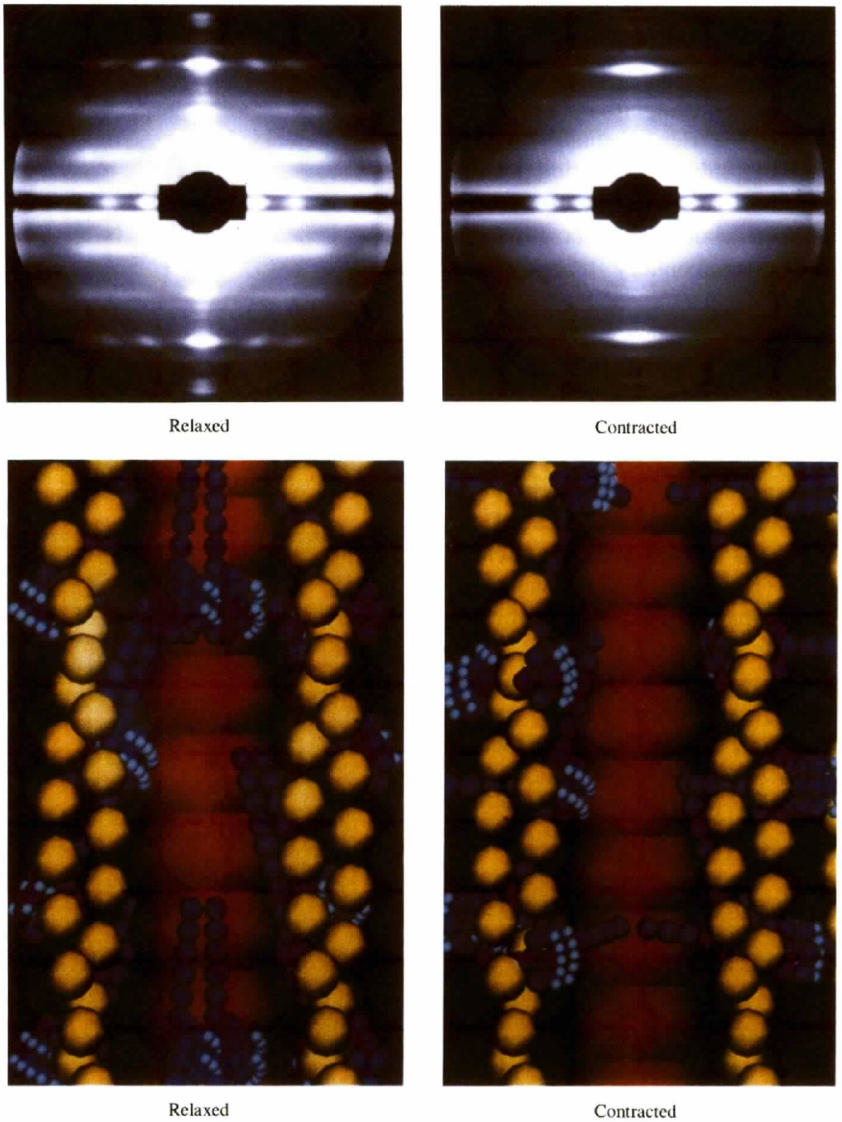


Figure 5
A high-resolution difference X-ray diffraction pattern (between resting and contracted muscle) illustrating the changes undergone by the filament structures when muscle tissues undergo isometric contraction. Model structures showing the interaction between the thick and thin filaments in muscle at rest and during contraction are shown below.

higher X-ray flux at ~12 keV was to be exploited for powder diffraction, EXAFS, surface diffraction and protein crystallography (to be used finally by a total of eight independent stations).

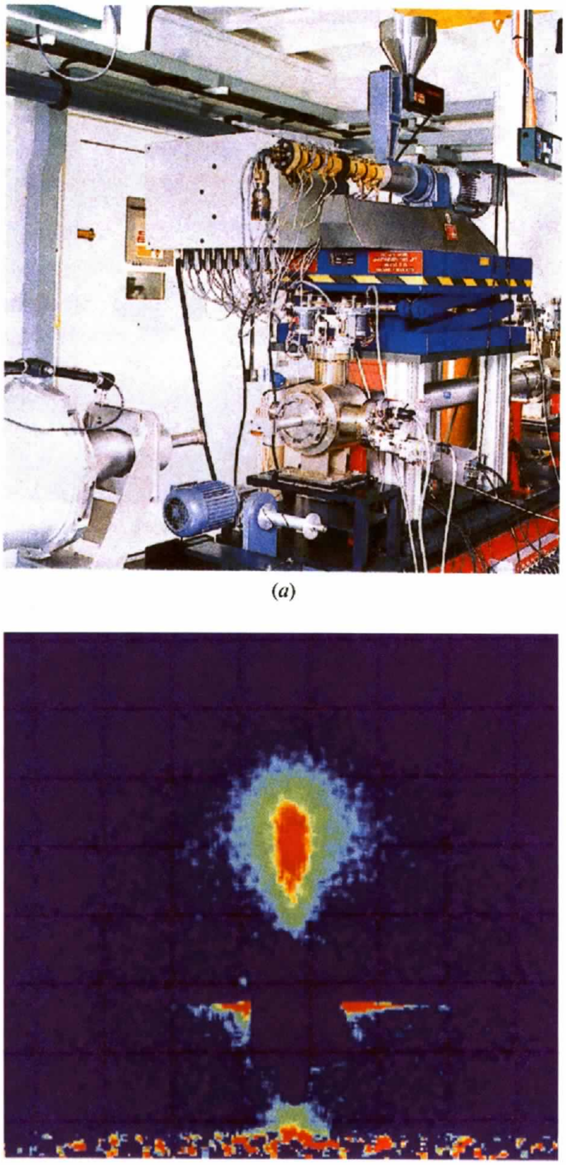
6. The SRS High-Brightness Lattice

Once again in the 1980's, almost mimicking events of the 1970's, the demand for an improvement (to parameters and characteristics of the source) emerged almost before the science programme had yielded really hard evidence of its merit. As early as 1980, V. Suller had outlined an advantageous modification to the lattice of the SRS. By doubling the number of quadrupoles it would be possible to reduce the electron-beam emittance to just above 10^{-7} m rad, a figure of merit reasonably close to that of the NSLS and the Photon Factory and which would keep the SRS 'in touch' even with the new sources planned for construction in the 1990's. More importantly, the full benefit from the first wiggler and from the installation of the (planned) second high-field (6 T) wiggler would be realised only after this modification. Following approval in 1983 and after considerable agonizing by the user community over the scientific 'cost' of yet another substantial period without synchrotron radiation, the High Brightness Lattice (HBL) was incorporated to time and budget (rather less than £1 million) by 1987 (Daresbury Laboratory Report, 1980).

Prior to the HBL installation, the scientific policies and guidance provided by the SRFC (Synchrotron Radiation Facility Committee) under a succession of able academic chairmen helped compensate for the fact that the SRS never had a director of scientific research – a serious omission. The science priorities of the day set by the SRFC were to hold the SRS in good stead up to the 1990's. For example, in the mid-1980's priorities were the enhancement of the reliability of the accelerator and stations and user friendliness; the development of facilities for biological time-resolved X-ray diffraction (mainly muscle and fibrous tissue); X-ray microscopy for biology (to use the newly installed 1 m undulator); surface X-ray diffraction (joint programme with the Netherlands); new surface science facilities (including a station for spin-polarized photoemission); and new facilities for below-red interferometry, and the development of dispersive EXAFS, which were all agreed prior to the HBL installation and were mostly fully operational shortly thereafter.

Also during the 1980's the UK government instigated a wide-ranging series of efficiency reviews at all levels associated with work in the public sector. As a direct consequence, Daresbury Laboratory (now within SERC: the UK Science and Engineering Research Council) was reviewed from financial, managerial and scientific points of view. Science reviews were also undertaken regularly by MRC, ZWO (Netherlands), NFR (Sweden) and finally by the SERC itself, the latter review being conducted by a panel under the Chairmanship of T. Blundell in 1986. The outcome of the subsequent 1987 'Blundell Report' (UK Science and Engineering Research Council, 1986) (endorsed and later partly implemented by the SERC) was to provide a vote of confidence in the quality of the science being generated by the SRS; to recommend the immediate installation of the second (6 T) superconducting wiggler; to support the participation of the UK community in the ESRF programme for high-energy and high-brilliance X-ray studies; to investigate the feasibility of a UK VUV/SXR ring; and to improve the level of organization of user support at the SRS, and to appoint a Director of Scientific Research.

Towards the end of the 1980's, and following the rapid and extremely successful rehabilitation of the SRS after its



(*b*)

Figure 6
(*a*) Experimental set-up for studying small-angle diffraction from a polymer during extrusion. Distance down the line is directly proportional to time. (*b*) An example of the changes in diffraction intensity is shown.

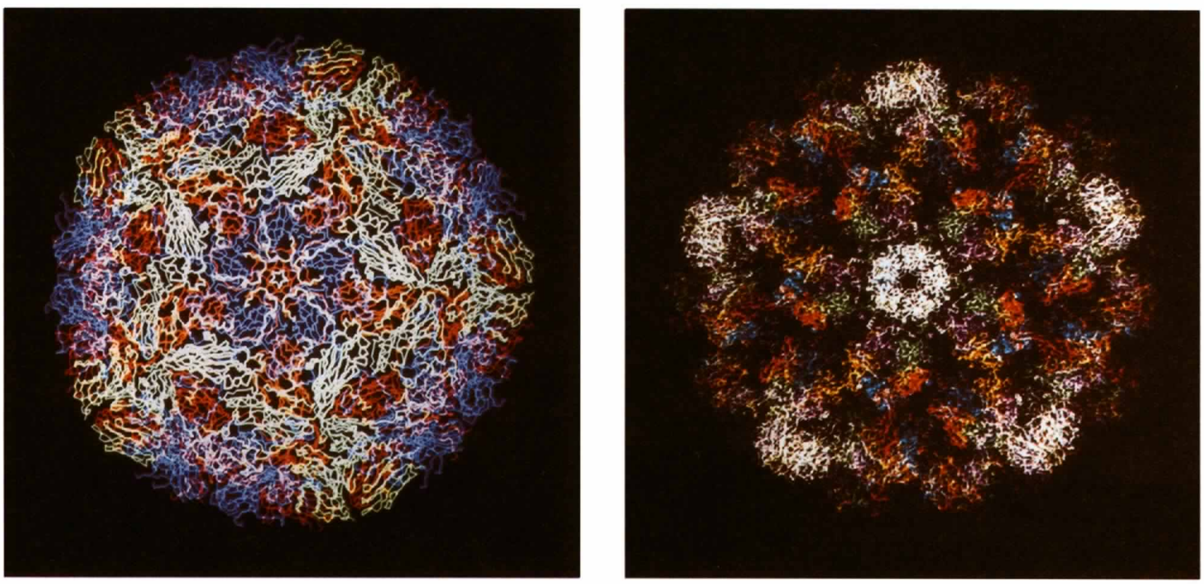
HBL modification, a succession of changes occurred largely as a result of the influence of national politics. Financial cuts were applied (again) supposedly to be neutralized through efficiency gains; the Materials Science Laboratory and materials science station 9.3 became active; and an Industrial Liaison Unit was established at the laboratory (later to become Daresbury Research Services, DRS) and the first PRT (participating research team) at the SRS was established. Two stations were built and 'owned' for surface science research by the Liverpool University IRC (Interdisciplinary Research Centre, for surface science).

7. A move from basic to strategic and applied science – the 1990's

The growth of activity at the SRS at Daresbury Laboratory is strikingly illustrated in Fig. 4. By 1990 over 30 stations were scheduled and in routine use, and the user community numbered approximately 1500. There was a high level of usage supported *via* the European Commission programme on Human Capital and Mobility. The SRS programme was managed jointly by a Head of Science (J. Bordas) and a Head of Accelerator activities (D. J. Thompson). The second (6 T) wiggler and five stations for small-angle scattering, process engineering, powder diffraction and ultra-dilute X-ray spectroscopy were under construction and largely completed and in scheduled operation by 1995/1996.

In 1993 the UK government introduced a White Paper on UK policy on Science and Technology. The recommendations contained within it would set in motion the greatest changes in UK science management and scientific priorities for at least a quarter of a century. From the very beginnings in 1970 the pre-eminence of physics at the SRS had been challenged, firstly by the chemistry community making use of the SRS for various surface and bulk studies, and subsequently in the exploitation of EXAFS. An EXAFS 'service' had already been established by chemists at the SRS by 1984! By the mid-1980's the expansion of interest by the life science community in synchrotron radiation was becoming clear from the growth in protein crystallography (using single wavelength and multiple wavelengths with anomalous dispersion), which was taking place at the same time as the world-class studies on muscle, collagen and other ordered biological material (observed using small-angle X-ray scattering and diffraction), and by biological spectroscopic studies (radiation damage, imaging, time-resolved fluorescence studies) in the UV and VUV regions.

By the early 1990s the new strengths in the UK synchrotron radiation research programme resulted in the priorities for targeted equipment investment becoming structural molecular and cell biology, then materials science, surface science and finally atomic and molecular spectroscopy and X-ray physics. The 1993 White Paper forced 'public accountability' firmly onto the shoulders of the scientific community. It gave considerable emphasis to the importance of the transfer of state-of-the-art technologies from the public to the private sector and ensured that, for the rest of the 1990's at least, support should be primarily for programmes on applied and strategic science rather than pure science. This policy change led to the view that the most basic 'value for money' objective was to operate the SRS for as many days per year as was feasible with the



(*a*) (*b*)

Figure 7

Two of the world-leading macromolecular structures solved using protein crystallography data from the SRS. (*a*) Foot-and-mouth disease virus, FMDV (Oxford group; Acharya *et al.*, 1989) and (*b*) SV40 virus (Harvard group; Liddington *et al.*, 1991), projects which both utilized the intense short-wavelength (0.9 Å) beam capability of the SRS wiggler station 9.6 (Helliwell *et al.*, 1986), a unique facility at that time in the world.

highest possible (and measured) efficiency of operation of source, beamlines and stations. The greatest area for fresh concern of course became instrumentation – always an afterthought in the history of synchrotron radiation facility planning! The very high cost of using a station at the SRS (approximately £1000 per 8 h shift even in 1992) meant, in funding terms and hence desirability, that short experiments might have an advantage over long ones. X-ray diffraction, scattering and spectroscopy experiments usually use less beam time (typically a day or a few days) compared with surface science and gas-phase experiments (typically a few weeks, even months). All the above led to the obvious conclusion that whenever and wherever possible, multi-angle/wavelength or energy or multi-dimensional experiments and detectors must be devised. As many measurements as are feasible should be carried out simultaneously on every sample while they are being illuminated by the very costly synchrotron radiation photons in order to enhance the effectiveness of source exploitation. A new strategic plan for all detectors on all SRS stations therefore had to be devised.

8. Some scientific achievements and applications from the SRS

8.1. *Life sciences*

The early involvement of the Medical Research Council helped ensure that the SRS was close to the forefront of the development of new synchrotron radiation applications in biology.

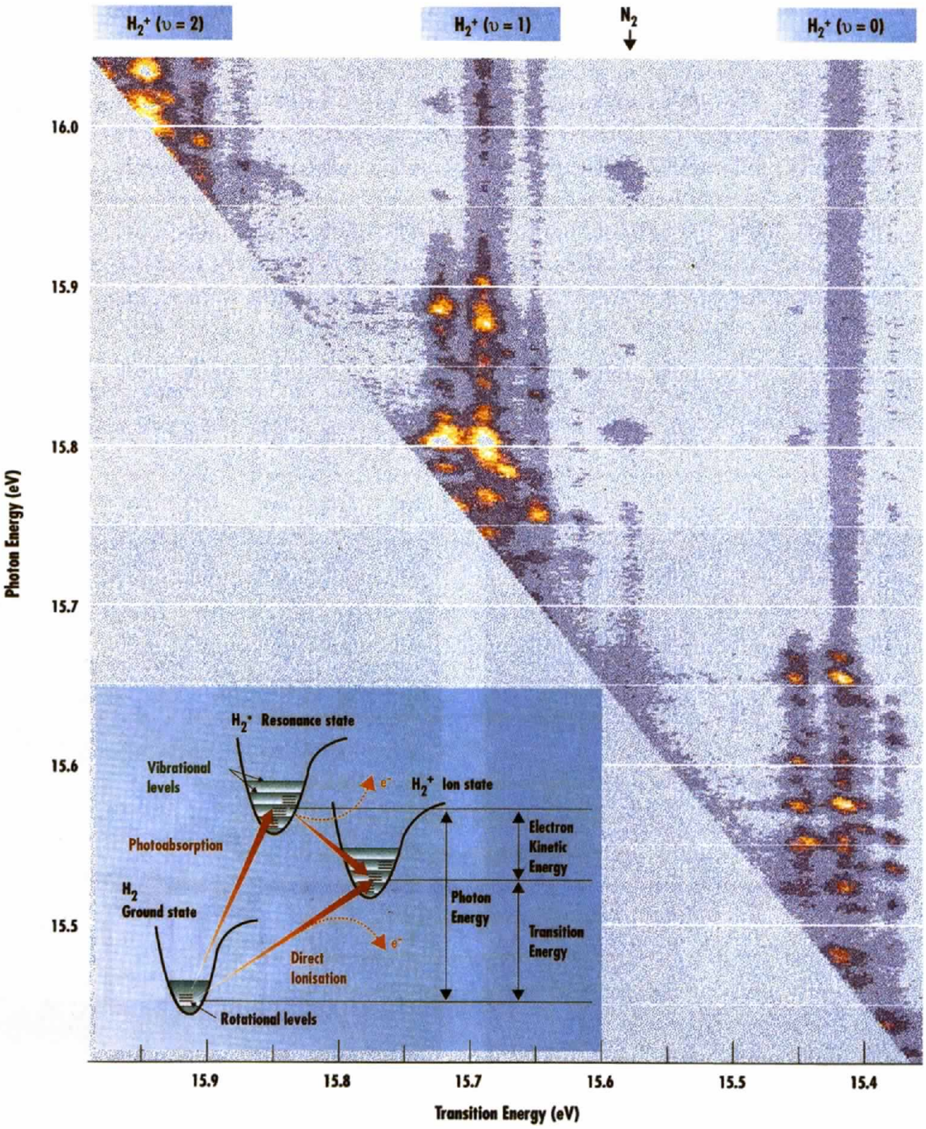


Figure 8
A two-dimensional photoelectron spectrum of molecular hydrogen, obtained using a novel two-dimensional scanning technique. The inset is a schematic representation of the processes that give rise to the electrons detected in the experiment. Direct photoionization produces the bands parallel to the photon energy axis. The three groups of bands correspond to the three lowest vibrational levels of the ground state of H_2^+, and the substructure is due to rotational transitions.

The construction of beamlines for small-angle X-ray diffraction and scattering (SAXS) from non-crystalline material has helped give direct information on, for example, human cornea, muscle, DNA fibres, the self-assembly of cell organelles and many others. In 1986 an experiment on DNA fibres showed for the first time that the D form, like the B form, must be right handed (Fuller, Mahendrasingam & Forsyth, 1988). By the early 1990's, results from a large muscle studies programme prompted a review of the then views of muscle construction (Bordas, Mant, Diakun & Nave, 1987) (see Fig. 5).

The power of the SAXS method has more recently been combined with wide-angle X-ray scattering (SAXS/WAXS) (Bras *et al.*, 1995). Together, for the first time, both long- and short-range order could be observed in biological and non-biological polymers. Using the combined method, pioneering work has been undertaken on the evolution of structural features within synthetic polymers during their fabrication processes, perhaps offering the opportunity to develop improved manufacturing procedures for these immensely important materials (see Fig. 6).

The desire to correlate biological structures with their function helped create an extremely successful UK programme in the area of protein crystallography at the SRS led, initially, largely by the work of J. Helliwell (Helliwell, 1979, 1992). Since then, a world-class research activity has emerged yielding the solutions of the structures of a wide variety of important molecules including the foot-and-mouth disease virus, SV40 virus (around 50 nm in diameter – the largest structure ever tackled in 1991), HIV-1 proteinase, light harvesting compound and many others (see Fig. 7). In addition to X-ray studies, novel applications were developed at lower photon energies to study biological

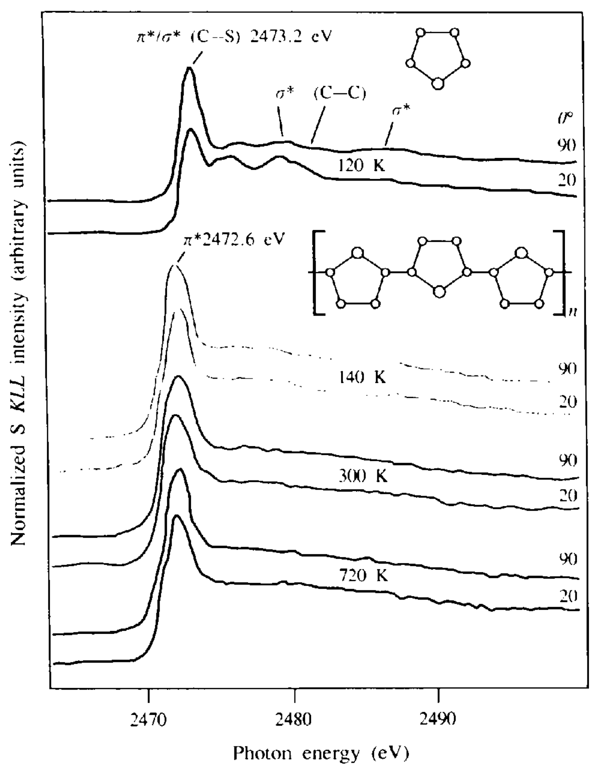


Figure 9
A study of substrate-catalyzed polymerization of thiophene on haematite *via* sulfur *K*-edge NEXAFS to characterize as a function of temperature the polymerization of thiophene vapour on a single-crystal haematite surface.

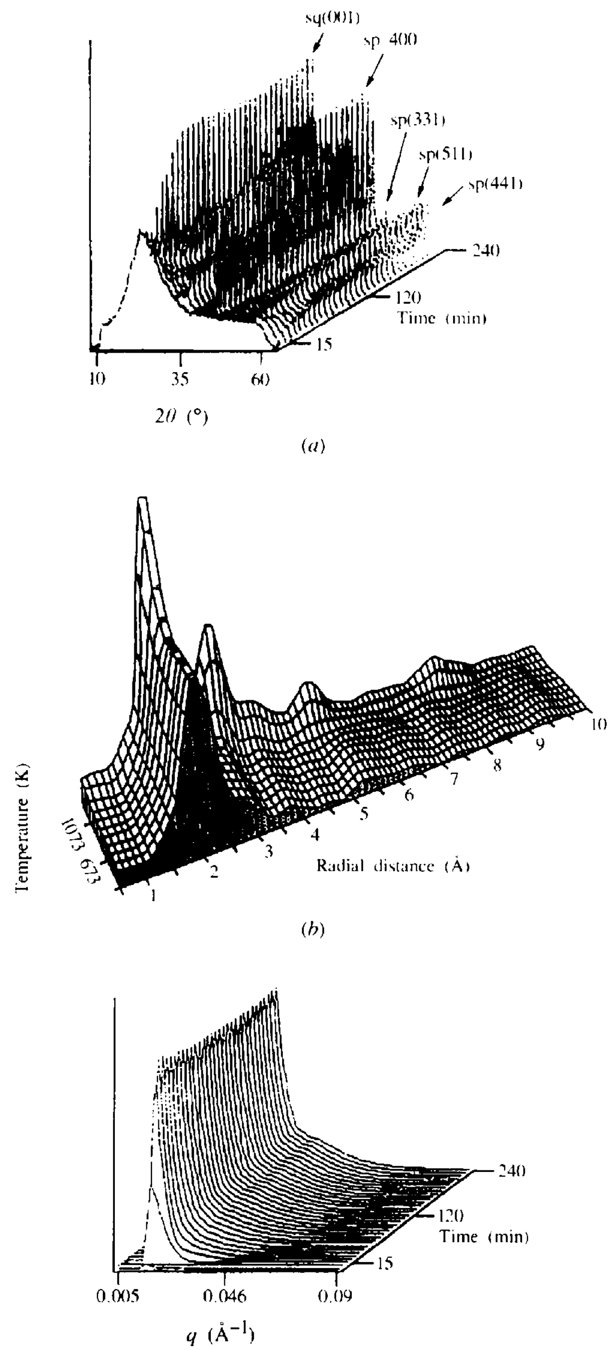


Figure 10
The synthesis of the catalyst cordierite studied using XRD SAXS and XAFS at 2273 K. (*a*) Bulk crystallinity (WAXS), (*b*) nucleating dopant environment (XAFS) and (*c*) microstructure (SAXS).

systems including VUV circular dichroism combined with stopped-flow methods, UV near VUV confocal imaging and a wide range of studies on membranes using fluorescent probes.

8.2. *Physical sciences*

In the physical sciences (which at present occupies some 70% of the total programme) the SRS has been used to identify and measure the various mechanisms available for electronic decay and energy transfer in a range of systems of atmospheric, photochemical and photophysical importance. New methods, which were used to study the vibrational and electronic states of doubly ionized atoms and merged beams of photons with ions, have revealed substantial discrepancies with the theoretical predictions for cross sections. Fluorescent methods have been used to observe for the first time the decay of molecular excited states, ions and photofragments (Cafola, Reddish & Comer, 1989). As an example, Fig. 8 presents an entirely novel method for 'molecular mapping', which in this case is a two-dimensional photoelectron spectrum of molecular hydrogen obtained using a unique photoelectron spectrometer design.

The SRS has helped evolve many methods to interrogate and help understand the structure of surfaces and surface states. Photoemission, surface photoelectron diffraction, EXAFS and glancing-angle X-ray diffraction have been used. Noteworthy areas of study have been in noble metal/semiconductor interface formation, the initial stages of molecular beam epitaxic growth of semiconductors (germanium/gold in particular) and the study of adsorbates such as Ni on Pd(110). Another example of such work is the study of catalysis using sulfur *K*-edge NEXAFS (see Fig. 9). The polymerization of thiophene vapour on a single crystal of haematite has been characterized as a function of temperature. The work was partly funded by British Nuclear Fuels plc and is important for the corrosion protection of engineering steels using sulfur ligand chemistry.

Most striking has been the expansion of materials structure studies leading to the creation of X-ray diffraction methods for the study of powders and the observations of microcrystalline growth. The evolution of structures within cement and various other complex materials have illustrated the power of synchrotron radiation methods (Barnes, 1995). Of special note has been the work by R. Nelmes and his group (Nelmes & McMahon, 1994). In the period from 1991 to 1995 they created a powerful new technique which uses an integrating image-plate detector to considerably enhance the signal-to-noise ratio of weak features and to simultaneously identify preferred orientations from small samples. Their work at high pressure on semiconductor structures has resulted in the reassignment and discovery of more crystalline parameters in a period of about four years than had been achieved worldwide in the previous 30 years!

From the very early 1980's, amorphous structures (mainly glasses) and catalytic systems have been studied at the SRS by N. Greaves and others. This work has relied on the combination of X-ray diffraction and X-ray absorption (EXAFS) measurements being carried out simultaneously on materials *in situ* (a situation unique to synchrotron radiation). The use of environmental chambers (see Fig. 10) at up to 2273 K has led to the study of zeolites during dehydration and reduction to form metal clusters and also, for example, to the study of the conversion of aurichalcite to a copper catalyst. Glancing-angle measurements in the observation of the progressive oxidation of steel and the electrode position of protective zinc phosphate coatings and the use of anomalous-dispersion effects combined with resonant X-ray diffraction to study metal structures in borates, phosphates and garnets have been among many research projects at the SRS between 1985 and the present.

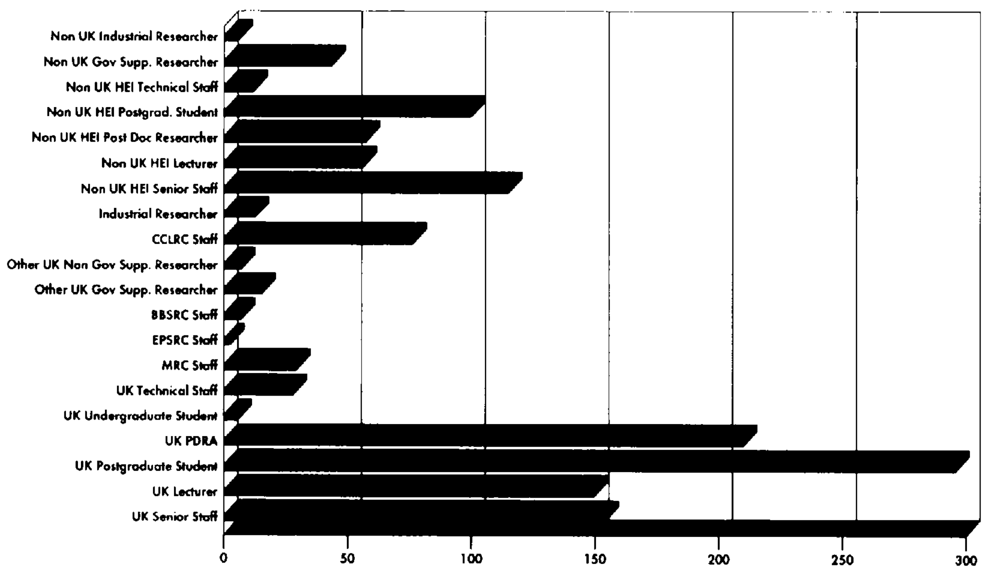


Figure 11
SRS users defined by user category in 1995.

Table 1
The construction portfolio of new stations in 1995.

Function/technique	Goals
EUV/VUV spectroscopy	Electronic spectroscopy of atoms and molecules (including gases, solids, clusters)
Chemical crystallography	Structural studies by X-ray diffraction from crystalline small-molecule materials
Solid and liquid interface X-ray diffraction	To study structure at interfaces, particularly involving liquids
High-resolution single-crystal diffraction	Materials science and magnetic scattering phenomena
Energy-dispersive diffraction (extreme conditions)	X-ray diffraction from samples at high pressures and temperatures (to 250 kBar, to 2273 K)
Ultra-dilute EXAFS spectroscopy	State-of-the-art EXAFS studies on ultra-dilute samples

Table 2
The final parameter list for the SRS, 1997.

Storage ring energy	2 GeV
Ring circumference	96 m
Ring lattice	FoDo
Pre-injection energy (Linac)	12 MeV
Injection (booster) synchrotron energy	600 MeV
Radio frequency	500 MHz
Ring period	320 ns, 160 bunches
Single-bunch operation	Up to 50 mA with FWHM pulse of ~180 ps
Horizontal emittance	1.1×10^{-7} m rad
Beam dimensions	~2200 × 600 µm (at 2.5% coupling)
Beam current after injection	~ 300 mA
Beam lifetime	~30 h
Operations	~600 h per year scheduled for users
	~5000 h multibunch ~600 h single bunch
Experimental lines	
Nine dipole lines	3.2 keV
5 T three-pole superconducting wiggler	13.3 keV
6 T three-pole superconducting wiggler	16.0 keV
Ten-pole (1 m) undulator	76–1240 eV
About 40 stations operational for ~4000 registered users	
Two beamlines for two 2 T nine-pole multipole wigglers (under construction)	

9. The status of the SRS as a 'mature' facility

The Blundell review of 1986/1987 gave considerable recognition to the merits of the UK synchrotron radiation science programme which helped it survive through the financial constraints of the early 1990's. The Blundell Review recommendations were that the installation of the second wiggler should be followed by the construction of a 'third-generation' VUV/SXR ring (latterly called DAPS – the Daresbury Advanced Photon Source), although this particular project came to naught only after a great deal of energy had been expended on the science case and technical design.

In fact, by 1991, it had already been decided by SERC that a second full review of synchrotron radiation science was required. This – the Woolfson Review (EPSRC, 1994) – finally reported its findings in 1993 and their recommendations have effectively defined the course to be followed by the UK synchrotron radiation community up to the end of the decade. The review established that the real costs of using a station were equivalent to over £3000 per day with 24 h operation of the SRS. Once again, the area of instrument development (environmental chambers, detectors *etc.*) was seen to be crucial in order to extract full benefit from the source. Further investment in the ESRF was seen to be a parallel valuable activity *but the primary recommendation was that synchrotron radiation X-rays were now vital to the scientific health of a large number of academic and other UK research communities spanning the boundaries of biology, chemistry and physics.* The SRS user community were asked to plan for an all-insertion device, high-flux and

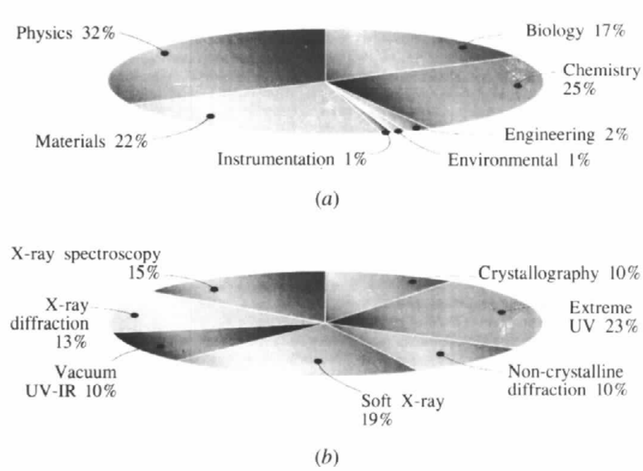


Figure 12
Usage of the SRS by (*a*) science area and (*b*) technique.

medium-energy X-ray storage ring to meet the growing needs and increasing technical demands of the UK by 2000 and beyond in order to ensure that the UK programme would be competitive in world terms. VUV/SXR activity was confirmed to be important but of a lesser significance such that construction of a 'third-generation' VUV ring should only follow the completion of the X-ray ring.

The implementation of this strategy was then immediately overtaken by events! The implementation of the 1993 White Paper led to the immediate dissolution of the SERC and to the creation of new smaller research councils and to the merger of Daresbury and Rutherford Appleton Laboratories to become (in 1994) a totally new 'Central Laboratory of the Research Councils'. The official title of the organization is

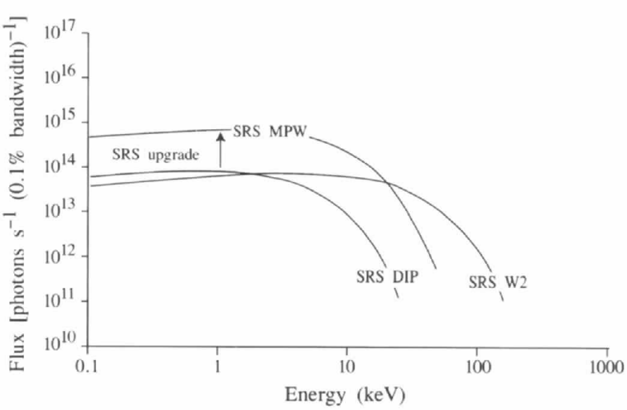


Figure 13
The spectral output from the upgrade (two nine-pole 1 m 2 T multipole wigglers with 20 mm operating gap).

The Council for the Central Laboratory of the Research Councils (CCLRC). By that time, the SRS was operating for approximately 7000 h per year with an efficiency of $\geq$90% with a typical start-up circulating current of <300 mA catering to the needs of some 3500 users and covering a whole span of user types (see Fig. 11). The scientific output from the SRS had reached approximately 600 refereed publications per annum by 1994/1995 and the number of stations scheduled for regular use was still growing.

The strength and growth of the research programme in terms of applied and strategic objectives as well as in basic science is well illustrated by the portfolio of stations under construction in 1994/1995 and their specific objectives (see Table 1), and the current parameters of the SRS are presented in Table 2. Fig. 12(*a*) shows the mid-1990's SRS usage in terms of science activity (number of proposals) and in terms of effective cost or investment (proportion of beam time) (Fig. 12*b*) given to the various areas of scientific endeavour. During the past decade there has been a steady growth in condensed phase research in materials science and life science studies. The level of activity in basic science has declined. Some activities (for example, in the area of gas-phase or surface studies in the VUV/SXR ranges) need long periods of beam time and are relatively speaking 'expensive' branches of synchrotron radiation research. In part, this has been due to the perpetual and lamentably low level of investment in instrumentation. In many areas of VUV and SXR research multi-energy (or wavelength) detection of photons or of electrons should immediately reduce data-gathering times by two or more orders of magnitude and also the high real cost of beam time should make sample

Figure 14
The new 3 GeV source, DIAMOND, proposed for Daresbury Laboratory.

preparation on line (in surface science studies, for example) a luxury which is difficult to justify.

10. Future prospects for synchrotron radiation in the UK

It is now almost exactly 30 years since the first small and insignificant synchrotron radiation experiments in the UK took place using NINA in April 1967. The level of activity has now grown to become the largest national science facility in Britain with the widest range of science activity and the largest facility user community, supported by around 250 full-time staff.

The requirement for high-flux and high-brilliance X-rays in order to characterize biological and non-biological materials alike is widely recognized to be essential in the pursuit of basic, strategic and applied science objectives. The Director General of Research Councils in the UK Office of Science and Technology has stated that 'the SRS plays an important role in the transfer of technology from the science base to users – something that the government is keen to foster'.

The concluding phase in the life of the SRS has been the recognition that the flux in the region up to ~10 keV could be enhanced by around one order of magnitude following the installation of two multipole wigglers in the SRS. This final development phase has been driven and strongly supported by the life sciences community seeking further opportunities for protein crystallography. The development – called the SRS Upgrade (Munro, 1995) – will introduce two nine-pole 2 T multipole wigglers with 20 mm gap into the SRS lattice (see Fig. 13). Following completion of the upgrade in 1999, it will be unlikely that the SRS could or should be developed any further. By that time this 'second-generation' symmetrical all-dipole SRS, with 1.2 m straight sections, will have evolved significantly towards the next (third) generation of sources. By 1999 it will include five added insertion devices (two nine-pole 2 T multipole wigglers, one ten-pole undulator, one 5 T three-pole and one 6 T three-pole wavelength-shifting superconducting multipole wigglers).

The current 'acid test' of the value of synchrotron radiation to the UK research community has been to assess the full cost of beam time for every individual research programme proposal. This cost, combined with all additional costs for equipment and staff, is considered alongside the (usually smaller) costs of non-synchrotron radiation research proposals. With a charge for beam time in 1997 of £4000 per 24 h day, the total cost of beam time alone for some science programmes can amount to a substantial fraction of one million pounds over a three-year period. Therefore, it is obviously now the overwhelming scientific merit of the programme at the SRS which maintains its strength and growth within the UK scientific community.

For the future (beyond 2000) the level of access to the ESRF, the present world-leading facility in which the UK has a 14% share, is seen to be wholly inadequate (in volume terms) to meet the needs of the future UK community. Along with Switzerland, France, Spain and others, the UK has proposed the construction of a new national source to give the quality and quantity of X-ray beams needed to maintain competitive national programmes in the characterization of condensed matter for the foreseeable future (20 years or more).

The recent provision of funds to provide for the 'upgrade' of the SRS and to build three (probably four) new associated stations is seen to be a vital step towards obtaining the full support from the community of UK research councils (Biotechnology and Biological Science, Engineering and Physical Sciences, Natural Environment, Particle Physics and Astronomy, and the CLRC itself) for the construction of a totally new source to replace the SRS early next century. The new source, called DIAMOND (Fig. 14), will be a high-flux $\geq$3 GeV storage ring with the potential for development of unique 20 m insertion devices to meet any needs which can currently be perceived from the existing and from the potential user communities.

Thirty years on from 1967, the 'parasite' on the NINA electron synchrotron has actually devoured its host and become 'big science' in its own right, resulting in the creation of the largest single-facility user community ever to exist in the UK.

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