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SCIENCE RESEARCH COUNCIL

SCIENCE BOARD

POLICY AND PROGRAMME STATEMENT OF THE SCIENCE BOARD 1974

Note by the Deputy Head of Division

The Board will recall that at their last meeting they considered a first version of the document which is to be put to Council as an account of the Board's present activities and future intentions.

The document has now been revised in the light of the comments expressed by members of the Board.

The Board is invited to AGREE to the transmission of the document to Council, subject to any amendments that they wish to see made to it.

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SCIENCE RESEARCH COUNCIL

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POLICY AND PROGRAMME STATEMENT OF THE SCIENCE BOARD, 1974

Memorandum by the Deputy Head of Division

1. Summary
2. Introduction
3. Current Board policies on the support of research in Universities and Polytechnics
4. Expenditure on grants to departments
5. Central facilities
6. Research associated with central facilities

1. SUMMARY

This report draws attention to the changing pattern of Science Board support of research in Universities and Polytechnics. The Board attaches prime importance to the direct support of research in academic departments, and recognises that in view of the increasingly severe restrictions on University funds it will need to adopt an increasingly flexible policy to ensure that research that it wishes to see done is made possible. The Board considers it vital to maintain in this way the momentum of academic research in its areas of interest, and in particular the activities of leading young workers for whom permanent academic appointments are not likely to be available in the near future. This may involve the support of workers more senior than those customarily maintained through research grants or the support of these and others over longer periods than has been common in the past. A second major influence on the Board's policies is the increasing sophistication and cost of research equipment which is reflected both in the cost of apparatus installed in departments (towards which little contribution may be expected in the future from host departments), and in the increasing part played by major central facilities. Whereas such facilities were previously required mostly in relatively specialised disciplines such as high-energy physics, they are now becoming necessary for large communities of users in a wide range of disciplines within the 'little sciences'. Neutron beam research is an example

in which the Board is already active, and within which substantial expansion is expected: and in the past year Board and Council have approved the establishment of two other major facilities - a new source of high-intensity synchrotron radiation and a high-powered laser laboratory.

The report gives a summary account of the research activities of the Board, emphasising the increasing interaction between major scientific disciplines and stressing the importance that the Board attaches to stimulating a flow of trained workers into areas of research which it wishes to prosecute.

## 2. INTRODUCTION

The responsibilities of the Science Board extend over the whole range of the natural sciences except for high-energy physics and most of nuclear physics, covering a range from sub-atomic and atomic systems, through simple and complex molecules to macromolecules, both synthetic and natural, and thence to the study of biological systems at the subcellular and cellular levels and finally at the level of the whole organism. These interests cover a large part of all the scientific activities in UK universities and other academic institutions.

There are two main methods by which the Board provides funds for University research. The first is by making grants 'for a stated period to initiate and develop a specific investigation of timeliness and promise in which the applicant is personally engaged, or to enter promising or modified fields of research, or to take advantage of developments in apparatus offering improved techniques in promising lines of research already established'. Such awards are intended to meet the cost of the resources, both of personnel and materials, necessary for a specific research programme to be carried out, beyond what a well-established department might be expected to provide from University funds. A second mechanism, becoming increasingly important in the Board's activities, is the provision of central facilities to which University workers may have access. This is a reflection of the increasing sophistication of the equipment necessary for research, which means that more and more areas of science need equipment too complex and costly to be given to every worker or every department needing to use it. In the case of equipment still on a comparatively small scale (as, for instance, advanced nuclear magnetic resonance spectrometers) the needs of Universities have been met by providing selected departments with instruments on condition that they devote a specified proportion of instrument time to meeting the requirements of other departments. Increasingly, however a demand is arising for major facilities that can only be provided on a central site, to meet the requirements of large communities of workers drawn from many departments. These now play an important part in the Board's activities,

and, as is discussed below, are likely to become more prominent in the future.

The Board also makes a substantial, if indirect, contribution to the support of research in University departments through the provision of studentships for training recent graduates in the methods of research. Most of these studentships are awarded through the allocation of quotas to departments recognised as giving good training to young research students, which are often also recipients of substantial research grants from the Board; the work of research students, therefore, augments the direct support of research areas which the Board has considered to deserve support. The Council is at present reappraising its overall policy in the award of studentships, and it is possible that in the future a closer relationship may be established between the provision of research grants and of training awards. In 1974, 1900 studentships were awarded in the Science Board area, corresponding to a total expenditure (on the maintenance of students and on research training support grants to departments) of £2.5M.

There is a fundamental difference between the funding of a dedicated central facility and providing funds to University departments, which must be recognised before any comparison is made of the Board's activities within them. In the former case the Council has to meet the global costs, both direct and indirect, of the operation. By contrast, Council funding of a department is supported at two levels from University funds: first, as mentioned above, by the resources expected to be found in the department, and second by a proportion of the general overhead that goes to maintaining and operating the University. While it is difficult to provide a quantitative estimate of what this support is, it can be said that for every pound provided by the Council a further sum of at least two pounds must be found from public money to underpin it. This means that the expenditure of £6.75M on Science Board research grants in 1975/76 represents a total of something more like £20M: this is to be compared with the estimated expenditure on central facilities of £8.9M.

This duality of support has important implications in the present restrictive financial climate: not only (as has hitherto been the case) may the Board have insufficient funds at its disposal to fund all the research that it would wish to see carried out, but the support which would have been expected to be provided by the University when funds were more readily available may not be forthcoming. The immediate effect of such restrictions is that the departmental contribution to the cost of a research project may be greatly diminished or even non-existent; even more importantly, Universities are finding it increasingly

difficult to assimilate a research project initiated by the Council into their general departmental activities by the process of 'take-over' after research projects initiated by the Council have become established. The momentum being gained by these developments in recent months is clear from the major awards made by the Board at its meeting in December 1974. In several instances the Board recognised that it would be unrealistic to insist on the take-over by the University of on-going projects as had been the intention when the previous awards were made, and agreed to extend the current awards. Such considerations arose in the case of the provision of services by University departments (such as the NMR services mentioned above): the Board saw the need for extending the initial support but recognised that long-term commitments to arrangements of this kind will represent an increasing drain on its resources. Problems over the long-term support of personnel, whose broader implications are discussed later, are already arising. A recent example arose when the Board received a request for the permanent support of a key worker associated with one of its major projects. He had previously been supported on the understanding that the University would assimilate him into its permanent staff, but this has proved impossible, even though his University attaches high priority to his take-over. Situations of this kind are expected to become increasingly common and to lead to increasingly heavy demands on the funds of the Board. Against this, however, we must recognise the real possibility not only that the hoped-for increase in Science Board research grants may not be forthcoming, but that the restrictions on funds made available to academic institutions by direct Government subvention will mean that the number of academic staff will not grow (and may even fall). Beyond that, an increasing emphasis on undergraduate teaching would mean that individual staff have little time for planning or supervising research.

The Board is considering the possibility of consolidating its support of some research groups over longer periods than is generally the practice, recognising that this may prove essential if a vigorous programme is to be pursued, and Committees are now examining their activities to see if and where such consolidation might be valuable. Within this context it has also discussed the possibility of the long-term support of workers more senior than those usually associated with research grants, which would give them security of tenure over periods of ten years or even more, during which time they would establish their own research groups generating their own research applications. Practices of this kind would, in fact, be no more than a ratification and extension of existing activities of the Science Board. The Enzyme Chemistry and Technology Committee has recently recommended support for a

further five years (making ten in all) of the Oxford Enzyme Group for basic services (of measurements and of materials preparation) against which proposals for specific research projects are expected to come forward, and the Biological Sciences Committee expects applications in the next year for further substantial funds for the continuation of major research programmes which have already been supported from 1966. The Chemistry Committee, also, is likely to be asked to extend its support of work at the Royal Institution which dates back also to 1966. To pay the salaries of senior workers over long periods would, however, be a more radical departure. Support is already given to individuals at professorial salaries on research grants but in every case on the explicit undertaking that after the termination of the grant their support will be provided by the University.

Any contraction in the commitment of the academic community to research will influence the activities of the Science Board's central facilities as well as University work as such. The concentration of effort on a central facility creates a kind of 'special area' to which a minimum commitment is implicitly made for the foreseeable future and if that commitment is to be properly met it is essential that research schools training able young workers should continue to flourish in Universities. In this connection, however, the case has also been made that the existence of sophisticated facilities will of itself attract young workers, who will gain expertise essential both for the future of academic research and for any technological developments which may arise from these fields of research.

Overall, the Board recognises the need to maintain a flexible position within its own activities which will take into account the changing pattern of the support of research from University funds, and in particular to ensure that there are no major discontinuities in the level of activity in Universities in research which it wishes to see carried out. It recognises that this policy will require continuing dialogues and close collaboration with other Research Councils and with the University Grants Committee.

### 3. CURRENT BOARD POLICIES ON THE SUPPORT OF RESEARCH IN UNIVERSITIES AND POLYTECHNICS

Recent years have seen a development from the position of a few years ago, when specific funds were held in a Board reserve to be devoted to special areas of research which had been identified and assessed by Committees as suitable for preferential funding, to one in which no special funds are reserved for fields which have received special assessment, but in which it is hoped that the

publicity given to particular areas will of itself attract proposals sufficiently meritorious to contend for funds with all other proposals put to the Board. This is a result of the consensus view that the funding of special areas met with limited success. There is no doubt that many applications of high quality have resulted from the invitations, either explicit or implicit, made to the academic community to come forward with research proposals - the subject of surface science, in particular, is considered to have benefited considerably from the Board's initiative - but nevertheless the proportion of high-quality applications stimulated in this way which were supported was considerably lower than those generated spontaneously, suggesting that most first-class workers were already receiving support. The most thorough assessments of 'special areas' so far have been made by the Chemistry Committee: its conclusion in the case of photochemistry was that 'few big names had been attracted into the field, and, although the exercise on the whole had been fairly successful, the big disappointment had been that it had failed almost completely to promote collaboration between physical chemists - and inorganic chemists and biologists'. The current view of the Committee is that research in selected areas is best encouraged by holding meetings to bring together workers, particularly from different disciplines, into selected areas, and it cited the field of colloid science to which it has recently given special attention, as one where workers from various disciplines are being brought together. The Committee has recently suggested that the complementary interests of physicists and chemists in areas of spectroscopy might similarly be encouraged. A similar view has been taken by the Biological Sciences Committee which sets up panels to assess the two major areas of developmental biology (reporting in 1971) and neurobiology (where its activities culminated in a joint SRC/MRC report produced this year). The opinion of the developmental biology panel that 'it was very difficult to identify the profitable areas of research and that it was undesirable to set aside special funds for particular fields of endeavour since this often led to a lowering of academic standards' was reflected in the neurobiologists' conclusion that no priorities are discernible in the field that could be justified purely on scientific grounds, and their opinions are reflected more generally by the Committee.

A disappointment frequently arising in the assessment of special areas has been the failure to stimulate high-quality work of applied, and more particularly industrial, connotation. This criticism has arisen in fields as widely diverse as photochemistry, magnetism (in which a recent Panel activity of the Physics Committee succeeded in stimulating a major programme of high quality applied research in only one case), and in industrial biology, where a sustained effort

was made over six years by two successive working parties, but was terminated in 1972 after having failed to identify any important area that was not adequately catered for by other funding bodies. The Mathematics Committee has been particularly active in its attempts to stimulate the interactions appropriate to its emphasis on applicable mathematics, having set up a study group under the aegis of its engineering mathematics panel at which industrialists present problems (largely concerned with the field of differential equations) in engineering to which it appears that mathematicians might be able to contribute; and in the field of operational research it is considering the establishment of a National Centre for Simulation Studies which would be particularly concerned with the problems of industry and other institutions concerned with applied problems. Preliminary assessment is now being given to a major proposal. The Enzyme Chemistry and Technology Committee is also taking steps to encourage programmes relevant to industrial interests. It already gives major support to a University group concerned with the fundamental technology required for the production of enzymes in relatively large quantities, and has recently set up a working group whose intention is to stimulate suggestions from industry of topics of fundamental research relevant to industrial needs.

There is, however, a consensus among Committees of the Board that the immediate deficiencies in the way of the support of particular areas lie among trained personnel rather than financial resources. Particular emphasis is paid in the field of mathematics to the need for intercourse between workers at the highest level. Thus the Board contributes £40K annually to the Institut des Hautes Etudes Scientifiques, an advanced study institute providing permanent facilities for mathematicians to meet. Mathematicians of a comparable level of seniority were involved in a year long symposium recently held at the University of Warwick, at which workers in a wide range of disciplines had the opportunity of identifying and discussing problems of mutual interest. The Committee has also agreed to support four symposia on specific fields of mathematical research at the University of Durham in association with the London Mathematical Society. The need for the exposure of students to more than one scientific discipline has arisen in the case of developmental biology, where in 1974 a 'research workshop' was funded at which relatively senior workers, at postdoctoral level and beyond, with expertise in the fields of developmental biology and neurobiology spent a fortnight giving and receiving instruction in each others' techniques and disciplines. A tangible outcome of the activities of the Industrial Biology Working Party has been that the Council, acting through the Biological Sciences Committee, now advises the Leverhulme Trustees on the award of Leverhulme Fellowships in Industrial Biology, which were set up to enable industrial workers to spend short periods in Universities, primarily to acquaint University workers

with industrial problems by supervising a project and by giving lectures and seminars. The Biological Sciences Committee has recently noted, with regret, that the fellowships so far awarded have been few and the activities stimulated have, generally, not been of a high quality. The scope of the scheme is now being extended in the hope of attracting better proposals. Awards of this kind complement, at a more senior level, the 'cooperative awards in science and engineering' through which students at the postgraduate level carry out research projects in association with both an academic and an industrial supervisor. Additional emphasis is to be placed on CASE awards in the future, and Committees of the Board propose to examine the operation of the scheme within their own fields.

More generally Committees have identified a need for a visiting fellowship scheme open to university workers less senior than those for whom the existing senior visiting fellowship scheme is designed. The activities of the Engineering Mathematics Panel are again relevant here: one of its earliest activities has been to set up a special scheme to cater for students at the immediate postgraduate level, by which a number of research studentships and advanced course studentships are reserved for mathematicians undertaking studies in departments of engineering and technology. A recent joint meeting of the Science and Engineering Boards has agreed that this scheme should continue to be encouraged. The Board hopes that stimuli of this kind will establish the cadres of workers who will produce the first-class applications of future years in these preferred areas.

#### 4. EXPENDITURE ON GRANTS TO DEPARTMENTS

This paper has already mentioned the increasing demands on expenditure for equipment that will arise as apparatus becomes more sophisticated and new techniques emerge and develop which lead to increased applications for major items of hardware. An extreme consequence of this trend is the demand for new major facilities, discussed below, but it will also be reflected in future requests for conventional research grants. For example, in the field of surface studies, which has been identified by both the Physics and the Chemistry Committees as likely to grow in the future, a major grant was made last year for the on-line computer control of a group of experimental programmes, and similar applications may be expected in the future. An ion scattering spectrometer, which at present costs well over £100,000, has been developed, and is likely to play an important part in a substantial range of surface studies. Substantial demands are likely to arise for the operation and maintenance of major facilities installed in Universities with Board funds. For instance we are likely to receive a request for upwards of £50K for the upgrading of the Dynamitron accelerator at Birmingham (for which £300K has already been provided) to achieve nanosecond pulsing, and a

substantial addition to its ancillary computing equipment has been identified by a special panel as a sensible development that the Board may well be invited to fund in the future. The ion implantation panel of the Physics Committee has recommended an injection of funds in the near future to build up the facilities centred on accelerators at the Universities of Salford, Surrey and Sussex.

A common feature of the development and application of instruments is that new techniques often originate in discoveries in experimental physics and then find applications as research tools in other areas such as physics and biology. This is well illustrated by the Board's support of nuclear magnetic resonance spectroscopy. Continuous wave NMR at relatively low fields is now a standard technique in chemistry laboratories and the emphasis of the Board's support is now on more advanced instrumentation involving  $^{13}\text{C}$  and other nuclei using Fourier transform techniques. This has proved an important complement to proton resonance in many areas of organic and inorganic chemistry, for instance the study of highly saturated systems with few functional groups. Such instruments have hitherto been sufficiently costly to justify their being allocated among departments on a regional basis, but recently they have become commercially available at prices within the scope of individual departments. More costly instruments, useful within specific areas of application, are now becoming available, and the future pattern of funding of NMR machines is now seen as involving the provision of a small number of these advanced instruments on a service basis, with smaller machines being provided by departments. Other developments are expected in the construction of very high field instruments, of particular value in the study of large molecules in low concentrations. In this connection, a proposal is expected from the Oxford Enzyme Group for an instrument operating at about 450 MHz to follow up recent important innovatory work on the determination of the structure of large molecules in solution using techniques based on spin and relaxation effects. Such field strengths have been made possible by recent developments in the technology of superconducting wire. At the same time the Physics Committee is supporting investigations of multiple phase and double resonance techniques and their application to the study of solids; and of diffraction NMR techniques which in principle allow the resolution of magnetic resonance effects in a solid lattice with a spacing of  $8\text{\AA}$ . A related experiment allows the spin-density distribution of liquid-like objects to be mapped, and it has been suggested that this could provide a route to imaging biological structures in vivo that would complement electron microscopic methods in being sensitive to hydrogen atoms and in avoiding the specimen damage that results from exposure to an electron beam. While this must be regarded as a remote possibility it provides an instance of how basic physics

research could open the way to a new and important technique, which would give rise to a new range of instruments.

A similar picture arises in the Board's support of electron beam techniques and its provision of electron microscopes. The use of the electron microscope for morphological studies is primarily in the field of the biologist. The Biological Sciences Committee has adopted a policy similar to that of the Chemistry Committee in the provision of standard instruments, insisting that the use of any instrument shall be dominated by programmes of research of a quality acceptable to it. Demands of this kind are likely to become more pressing as the restrictions on University funding for equipment become more severe. An important development in the application of electron beam techniques to biology is in the use of microprobe analysis. This technique, already well established in the physical sciences and particularly in metallurgy, depends on adequate specimen preparation and handling for success in biological work, and a major programme supported by the Biological Sciences Committee emphasises these aspects. This type of investigation may be expected to grow in the future, though first-class applications have so far been few. The development of novel electron microscopes as such lies outside the Board's field of interest (the Engineering Board supports a major programme for the development of an instrument with ultra-high resolution) but support has been given to a University group concerned primarily with the study of surface phenomena requiring an instrument of novel design which is being developed jointly by the applicant and the manufacturer - an example of how research and instrument development are often closely related. Electron microscopy has so far played a comparatively small role in chemistry, but a recent report has identified areas, particularly within solid state chemistry, which could benefit from it. The report refers to areas of development of common interest to physicists and biologists, and makes the suggestion that electron optics centres might be established in which the overlapping interests of different disciplines were jointly pursued.

Mass spectrometry is another area which is attracting the interest of several committees, especially in view of its development as a tool for the accurate analysis of relatively complex molecules, including proteins. Combined gas-liquid chromatography-mass spectrometric techniques are well established in organic chemistry and biochemistry and the Committees of the Board may expect substantial requests in this field in the future, particularly in view of the fact that this area of investigation does not readily lend itself to service operation. Furthermore, these techniques have now reached a stage of development at which data processing systems are likely to be requested for use with them. Awards have also been made for the construction and use of the recently

developed ion kinetic spectrometer for use in protein sequencing. Here, again, there is close collaboration between user and manufacturer in the development of novel instrumentation which is being monitored by the appropriate Committees.

Similar developments in other areas may be expected to affect the Board's expenditures in University departments in the future. Laser-Raman spectroscopy is an example where the chemist has already benefited from developments in a field in which the Physics Committee is actively concerned, and the suggestion has been made that closer relationships should be established between chemists and physicists to explore new areas of potential interaction.

The Science Board's interest in the life sciences merits special mention because the methods and techniques of biology often differ in important respects from those of the physical sciences. An important administrative distinction also exists. Whereas most of the applications of the physical sciences are to be found in the field of engineering - as is evidenced, for instance, in the close interaction between the solid state interests of the Physics Committee and the activities of the Electrical and Systems Engineering Committee of the Engineering Board - most of the interactions of the Biological Sciences Committee are with other Research Councils which are responsible, in the broadest sense, for the applications of biology, and for the strategic research that goes to support them. Thus the joint SRC/MRC panel on neurobiology has identified most of the important areas of future development in that field as being directed towards clinical applications which lie outside SRC's province. A common theme in SRC's interests in biology is the increasing emphasis on quantitative methods. Several examples have arisen in the discussion above, and to them should be added the major support given to investigations by X-ray crystallographic techniques of molecules of biological significance. The suggestion has recently been made that closer relations should be established between the Council's interests in the study of synthetic macromolecules (part of which falls within the responsibility of the Engineering Board) and of natural macromolecules. Quantitative methods have had a profound effect on recent whole organism studies, a particularly striking example being the investigation of the biochemical basis of memory and learning. Computer techniques have revolutionised the approach to neurophysiology and psychology. In this connection the Board is at present considering, in association with the Engineering Board, its future policy with regard to cognitive science, which has been defined as the attempt to understand the processes which underlie perception, memory, reasoning, language and other forms of cognitive activity in computational or other equally precise terms, and thus involves the application of the methods of quantitative science to the study of the most complex organism known. It

is a field likely to make considerable demands on the capacity of large computers, and the Board's participation in this field (which has affinities with the subject of artificial intelligence to which the Engineering Board gives considerable support) could represent a substantial component of the Board's future demands on central computers.

It is impossible within the scope of this report to give an account of all the research being carried out through minor grants, but a brief survey is now given of trends underlying the areas of research supported by the Board. A characteristic of much contemporary work in physics and physical chemistry is that as equipment and techniques become more refined, more accurate experimental tests of theory are made possible, which in turn stimulate the development of more sophisticated theories. Thus a subsequent section of this report refers to the way in which a priori computation in physics and chemistry have reached a stage of refinement at which they can uncover experimental inaccuracies, and the mutual reinforcement of theory and practice is evident in the substantial support given to the Physics Committee for theoretical and experimental studies in fields such as the collision interaction between simple atoms and molecules and of excitation and ionisation processes in atoms and molecules. In the field of solid state physics a comparable theme underlies contemporary developments: whereas earlier theoretical developments were able to give an idealised description of the characteristics of substances, current developments are moving towards the description and calculation of properties such as lattice vibration behaviour, superconductivity, semiconductivity, and magnetic properties, of real materials. Understandings of this kind contribute to our knowledge of the relation of macroscopic properties of solids to sub-atomic phenomena, which will bridge the gap between the interests of the metallurgist and the physicist in, for instance, establishing direct relationships between dislocation theory and the electronic structure of metals. The interests of the physics committee in surface studies and in amorphous materials can be considered as further examples of the study of more complex models. Early solid state studies using a perfect crystal lattice as a model are now being developed by the introduction of a surface or of randomness in the three-dimensional structure. Hence the close relation between theoretical studies on, for instance, the radiation-matter interaction involved in low energy electron diffraction and in Auger spectrometry and accurate experimental methods (which have themselves only been made feasible by the advent of ultra-high vacuum techniques). In the study of amorphous

materials an important advance in recent years has been the discovery of the ways in which a metal-insulator transition can occur. Techniques of materials preparation have contributed to the study of materials of limited dimensionality which are attracting interest in a number of connections, including transport behaviour and superconductivity. Mention should also be made of the interaction of theoretical and experimental studies of the incidence of superfluidity at extremely low temperatures in helium III, which is a unique system for our understanding of the ground states of condensed matter.

There are clear affinities between contemporary developments in physics and in physical chemistry. The Chemistry Committee, in a recent appraisal of the work that it has supported over the past three years, has commented favourably on researches into the physics and chemistry of surfaces, and in particular to the application of photoelectron spectroscopy and low energy electron diffraction to studies of simple crystal surfaces and the chemisorption of simple organic molecules on them. This work has affinities with certain aspects of organometallic chemistry by leading to the establishment of parallel concepts in the homogeneous catalytic activity of metal complexes and the heterogeneous catalysis of reactions by surfaces, and has considerable implications for the evolution of a general theory of catalysis. The Committee has been impressed by work carried out with its support on kinetic spectroscopy, and particularly with recent advances in the identification of free radicals by mass spectrometry and with those innovations in flash photolysis techniques which are providing details of the mechanisms of radiative and radiationless transition in electronically excited polyatomic molecules. In physical inorganic chemistry, electron microscopy has contributed to our understanding of inorganic solids, such as simple transition metal oxides, through the observation of crystallographic shear, microheterogeneity and superstructure ordering, and the Committee wishes to develop further work directed towards the relationship of ultramicrostructure with the phenomena of electron and atom transport in inorganic solids.

Synthetic chemistry owes much to the development of spectroscopic and crystallographic techniques which can provide rapid and unequivocal determinations of molecular structure. The current emphasis in organic chemistry is towards the development of new synthetic methods. New approaches in this direction reflect the interaction between useful synthons (molecules or fragments having general potential as synthetic 'building bricks') and the recognition of new reactive small molecules and intermediates. In both organic and organometallic chemistry 'hot atom' techniques are leading to the production of molecules thermodynamically stable but kinetically labile which could have considerable potential in chemical

synthesis. Multi-stage synthesis of larger specific target molecules is also an important field and the Chemistry Committee expects that synthetic studies of biomacromolecules, based both on solid and soluble polymer supports, will be a growing area of research in the future.

The special role of the life sciences among the Board's interests has already been mentioned. A common factor among many current developments is the increasing application of the quantitative methods of the physical sciences to the study of complex living systems, and it is significant that biological research plays an important and increasing part in the use of major facilities such as neutron beam and synchrotron radiation sources, and the central role of nuclear magnetic resonance spectroscopy in the Oxford Enzyme Group has already been mentioned. A few examples may be cited here. At the molecular level, the stereochemistry of many biosynthetic steps in primary metabolism is becoming established and extended to studies of natural product biosynthesis, and nuclear magnetic resonance techniques are applied to the study of biosynthesis in natural plants and fungi. NMR techniques are now sufficiently sensitive to be used with the very small quantities involved in enzyme preparation studies. At a higher level of complexity the cell membrane, whose understanding will play a key role in our knowledge of the adjustment of a cell to its environment, is being studied through several approaches. High-voltage electron microscopy gives information on the three-dimensional organisation of membrane systems. A range of biophysical techniques is being used in an attack on the difficult problem of the relation of the molecular organisation of the cell to its biological function. This is an area where the interests of the biologist and the chemist interact closely. Since the complexity of membrane structures makes few systems amenable to sophisticated analysis a substantial amount of work has been carried out using artificial or semi-artificial membranes. At a still higher level of complexity of investigation the disciplines of developmental biology and molecular biology are converging in work seeking an answer to the central question of how gene function is controlled so that it leads to different gene expression in different parts of a multicellular organism: this is an area in which the interaction of biochemists, biophysicists and geneticists will play an increasingly important role. Finally, at the highest level of organisational complexity, two examples of the interaction of biochemistry with neurobiological studies may be mentioned: evidence has been adduced for the occurrence of biochemical changes in the brain during the learning process, and the highly specific substances responsible for pituitary control identified. Another aspect of the quantitative nature of modern biology is the role that contemporary techniques of classification theory play in numerical taxonomy and in population and biometrical genetics; and computational and mathematical model building plays a part in contemporary developmental biology and neurobiology. Biologists have been prominent in the interdisciplinary rencontres supported in recent years by the Mathematics Committee.

## 5. CENTRAL FACILITIES

The introduction to this paper pointed out the increasingly important role played by central facilities in the activities of the Board. Those which so far concern it are of two classes:- (i) for the study of the interaction of radiation with matter; and (ii) for the provision of computing resources beyond the scope of individual institutions.<sup>1</sup> Several current developments within these areas will affect the Board's future requirements for funds and a brief account is given of them here.

(1) Interaction of radiation with matter. As investigations become more refined and the necessary sophisticated instrumentation becomes available, the need arises for successively more powerful probes for the study of the structure of matter. A crudely historical approach would first refer to techniques using electromagnetic radiation, with the development of optical techniques, both in microscopy and spectroscopy, being followed by the use of X-ray methods and then by the use of radiofrequency sources, for instance in the study of dielectrics and in nuclear magnetic resonance techniques. In parallel with these is the exploitation of the wave nature of massive elementary particles - electrons and neutrons - in the study of matter.

An important example is the case of neutron radiation. In some respects it differs from the other examples given here, since to obtain fluxes of neutrons sufficiently intense to be useful in a wide range of investigations of the study of matter, a nuclear reactor is necessary, and since reactors first became established neutron fluxes have been extracted from them as probes for the study of condensed matter. The Board, through its Neutron Beam Research Committee, has access to beam sources at AERE Harwell and AWRE Aldermaston and to a slow neutron cell on the linear electron accelerator at Harwell. Beyond this, however, the need arose for fluxes of higher intensity from a reactor dedicated to the production of neutron beams for experimental purposes, and the UK, through the Science Board, has acquired a one-third share of the high thermal flux reactor at the Institut Laue-Langevin at Grenoble. Use of these facilities was reported for the first time in the NBRC's annual report earlier this year. The estimated expenditure on the ILL facility in 1975/76 is £3.7M, and expenditures rising to £3.9M in 1980/81 are contemplated in the forward look. It is an indication of the rapidly increasing demands of research using neutron

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<sup>1</sup> Strictly speaking this is a Council responsibility, as the Atlas Computer Laboratory, whose funds are found from the Science Board budget, has responsibilities to University workers other than those within the Science Board's field of interest.

techniques that the need for still higher fluxes has already been mooted, and a study programme has been outlined which will consider the merits of various possible sources. Particular attention will be paid to the production of pulses of neutrons in a target bombarded by accelerated particles: the programme on the linear accelerator at Harwell supports experiments complementary to those mounted on the reactors at Harwell and at ILL and provides some practical experience of pulsed neutron sources. The Board's forward look includes a total provision of £2.8M for work on the next generation source, with expenditures of £80K, £200K, £1000K and £1000K in successive years from 1976/77.

The Neutron Beam Research Committee has recently determined that its policy shall be the provision in the UK of instruments complementary to those at the ILL, of specialised facilities unavailable elsewhere, and of instruments suitable for preparatory work to ensure that the ILL facilities are used effectively. Its present recommendations involve the construction of four new instruments (and the commissioning of a new cold source for one of the Harwell reactors). Capital schemes of this kind are included in the payment to AEA and MOD for the facilities mentioned above: with the LINAC development programme, a total expenditure of £1.4M, falling to £1.2M in 1980/81, is included in the current forward look. Expenditure on neutron beam research also includes the support given by the Neutron Beam Research Unit at the Rutherford Laboratory for on-going programmes and for developing new instruments and techniques. Annual expenditure over the next five years is expected to be about £0.7M.

Until recently neutron beams were the only radiation source that would be economically provided on a central facility, but the position has changed in two important respects, both of which have a direct bearing on the policies of the Board.

(i) The first major development is in the provision of synchrotron radiation facilities. Since 1970 the Board has provided funds (currently at a level of about £300K per annum) to enable workers to make parasitic use of the high-intensity electromagnetic radiation generated in the NINA electron accelerator at Daresbury. The intensity and characteristics of this radiation make it valuable in a wide range of investigations many of which are inaccessible with conventional laboratory sources. Recent developments have followed trends similar to the recent history of neutron beam experimentation, experience with the existing source showing the need for still higher fluxes of radiation provided by a dedicated source with no commitment to high-energy physics. Preliminary work has already begun (with the additional stimulus of the impending closure of the NINA accelerator) on the design and construction of a

dedicated storage ring which will be as advanced a source of radiation as any in the world. The ultimate cost of maintaining and operating the fully established facility is estimated as between £1½M and £1½M per annum, and present estimates of the expenditure incident in 1975/76 for design studies on the new development, as well as operating the existing facility, are £0.94M. Following Board and Council's approval of the project, authority is now being sought from DES.

(ii) Detailed proposals are now being set out for a cooperative research programme involving the interaction of high-powered laser pulses with matter. The work of several UK university groups now active in this field has reached a stage at which further substantial development requires a flux so intense that it could only be provided on a central facility. The principal scientific objectives of the programme would be the study of non-linear interactions of very intense optical and infra-red radiation with matter and the creation and study of superdense plasma by laser compression. A facility of this kind would also make possible basic research relevant to the highly important problem of the production of energy by controlled thermonuclear fusion. Developments in this direction are outside the remit of the Council, but are of great interest to the Atomic Energy Authority, and plans are at present being worked out with the Atomic Energy Authority for the joint funding of a high-powered laser centre. At present only tentative costings of the development are possible, though it is expected that the Council's (and hence the Science Board's) contribution to the project will be about £1M per year over the years 1975/76 to 1977/78, and £1½M per year thereafter. This project, too, awaits authorisation by DES following its approval from Board and Council.

(2) Central computing facilities. Current estimates allow for an expenditure of £1.8M on the Atlas Computer Laboratory. The current policy of the Laboratory is to provide major allocations of computing time to workers whose computational programmes have been approved by subject committees of the Council. The computing resources available are the Laboratory's own ICL 1906A machine, and 20% of the time of the IBM 370/195 machine installed at the Rutherford Laboratory primarily to meet the needs of nuclear physicists. The value of the service function of the Atlas Laboratory at the present day, when - in contrast to the position in its early years - it represents only a small proportion of the computing resources available to Universities, is that it is capable of reserving large blocks of time to individual users in a way that is not possible at regional centres or on University computers, and this important need is expected to continue for several years at least. The demands of computational physics and chemistry for computing time are discussed briefly below with the suggestion that progress in certain important directions will be chiefly limited by the

availability of computing power; this may equally apply in areas such as fluid dynamics of primary interest to the Engineering Board. The Council is, therefore, currently considering the policy to be adopted when the next generation of major computers becomes available, which is expected to be in about five years. The future structure of the Council's computing effort is, however, at present sub judice, and no allowance for a future major computer is at present included in the Board's forward look.

A second role of the Atlas Laboratory has been the development of suites of software and programmes in, for example, X-ray crystallography and quantum chemistry and statistics. X-ray crystallographers represent a major proportion of the users of the 1906A computer, and it has recently been estimated that 80% of all current UK publications in the field that involve the use of computational methods acknowledge the role played by the Atlas Laboratory. It has recently been decided that the role of the Laboratory in applications of software development should be extended by further encouraging collaboration between University workers and the Laboratory staff in the development of theoretical models and associated computer programmes. This 'Meeting House' concept is already being developed, with the specific topic within theoretical chemistry of electronic correlation in molecular wave functions being selected for study. Another possible field of interest, mentioned again below, is the development of the complex programs involved in the fields of cognitive science and artificial intelligence which are currently attracting the interest of Science and Engineering Boards.

The Physico-Chemical Measurements Unit, operated by the Atomic Energy Authority, is another central facility funded by the Board, on which an expenditure of £150K in 1975/76 is envisaged. This provides a service to University departments of use of physico-chemical instrumentation for nuclear magnetic resonance, mass spectrometric, infra-red and Mössbauer spectrometric techniques: in contrast to the major facilities described above, the PCMU as has now evolved is seen as fulfilling two major roles; (i) allowing departments access to costly instrumentation such as Fourier transform NMR while establishing a case for provision of equipment to their own laboratories; (ii) providing instrument (and to some extent interpretation) services to departments or institutions too small to be able to make a good case for their own instrument. The Board considers that these functions justify provision for continued expenditure on the PCMU at about the current level. In future the PCMU will be a responsibility of the Chemistry Committee.

A discussion of central facilities must include the suggestion made in 1973 by a Panel which reported on 'materials science and the Science Board'. It

identified the lack of suitable materials as often being a fundamental problem in the way of research in this area, and suggested that groups should be set up capable of meeting these needs. Since the requirement for particular materials is often transitory, the Panel considered that these groups should be capable of moving to different topics after a period of, say, five to seven years. It suggested that SRC establishments were suitable sites for groups of this kind. The need for supplies of special materials has been echoed by the Physics Committee with particular reference to the preparation (and characterisation) of alloys relevant to research in magnetism. The Physics Committee already supports groups at Oxford and Birmingham involved in materials preparation. A group of French and British scientists which met to discuss the field of liquid crystals research identified a need for the preparation of deuterated compounds, and the Neutron Beam Research Committee has also recognised the need for the production of special materials, also identifying (among other things) the need for deuterated materials. An important demand for the development and production of new optical materials is expected to arise from the demands of non-linear optics: the proposed developments mentioned above in the field of high-powered lasers underline this need. Recent discussions between the Science and Engineering Boards have identified engineering interests in this area, particularly in the field of interest of the Electrical and Systems Engineering Committee, where economic pressures can often make the demand urgent. The Committee has determined on the establishment of three or four centres, each with its own expertise. The Boards here agreed that the provision of materials is urgent and that an attempt should be made to accommodate their requirements under one administrative arrangement.

## 6. RESEARCH ASSOCIATED WITH CENTRAL FACILITIES

### Computation

Present and future users of computational methods have recently been assessed by specialist panels. Major demands for computational facilities fall into two broad classes. The first, in which computation plays sufficiently important a role in the interpretation of experimental data as to justify the substantial costs involved, is typified, within the area of interest of the Science Board, by its use in X-ray and neutron beam crystallography. The second major area of application, now of increasing importance, is the use of computational techniques as a predictive tool complementary to, or even competitive with, the experimental approach. Thus in the field of computational chemistry, calculations of the electronic energy levels of the ground states of molecules are now being succeeded by the study of excited and unstable systems, and of

systems existing only in laboratory and astrophysical plasmas, that are not amenable to direct experimental observation. The calculation of ground states has now reached a level of accuracy at which theory and experiment play complementary roles. In the case of simple molecules calculation has been able to demonstrate the existence of experimental inaccuracies, though our present state of knowledge of the electronic structure of more complex systems means that we still depend heavily on experimental comparison. Dynamic calculations are now being developed at the microscopic level to determine the potential energy surfaces involved in chemical reactions, and the solution of the time-dependent equations of quantum mechanics for systems of interacting atoms and molecules is leading to a greater measure of understanding of the nature of chemical reactions: an area of considerable importance in view of the wide use given to the somewhat crude models of chemical reaction at present available. Dynamic calculations at the macroscopic level involve the simulation using a comparatively small number of units of the  $10^{23}$  atoms or molecules encountered in macroscopic assemblies, and are related to the investigation of thermodynamic and transport phenomena. The large-scale computer simulation of assemblies of interacting molecules is expected to contribute to many areas of work, including (among those to which the Atlas Computer Laboratory is already contributing) the study of the gaseous, liquid and solid state of small polar and non-polar molecules, liquid and solid ionic states and their mixtures, and networks simulating amorphous bodies and their vibrational spectra. Thus, for instance, current attempts at the direct numerical solution of Newton's equations for large ensembles of interacting particles have led to an improved understanding of the nature of the fluid state which may culminate in the quantitative prediction of the physical properties of particular fluids under conditions of temperature and pressure that are difficult to attain experimentally. Computational methods are also expected to play an increasing role in the study of the physics of condensed matter - e.g. the calculation of bond structures and electronic properties of solids and of defects in solids, and in plasma physics and magnetohydrodynamics. In this last field computer studies have already played an important role in the study of radiation-plasma interactions, and it is expected that further demands on computing resources will arise from the high-powered laser programme mentioned above.

The use of computational techniques as a predictive tool requires computer machinery of great versatility and power, for only then is the computational scientist able to devise models sufficiently close to reality, and to solve the resulting equations to the necessary degree of accuracy. There is often a sharp increase from the scale of operation appropriate to a project designed to produce a rough simulation of an experimental situation and one which aims at quantitative information of direct relevance to the experimentalist. As

predictive methods become more widespread and more accomplished we may expect a correspondingly sharp increase in the demand for major computing equipment.

#### Research related to the use of synchrotron radiation

The high-intensity electromagnetic radiation available over a wide continuous range of wavelengths from a synchrotron source extends the range of experiments accessible with conventional radiation sources of lower intensity and limited frequency range: and beyond that, its characteristics of 100% polarisation and time-modulation throughout the spectral range make possible experiments inaccessible using conventional sources. Many types of experiment to be carried out with synchrotron sources are, therefore, of a kind already extensively supported, particularly by the Physics Committee, in University departments. Two broad classes of research may be identified:-

- (i) the determination of electronic states and levels by observing absorption, reflection and fluorescence data, and photoelectron yield;
- (ii) obtaining information, both structural and electronic, about the material under observation from measurements of the energy, momentum and angular distribution of the scattered photons, usually in the X-ray region.

Studies of free atoms and molecules are of importance in complementing theoretical studies of the quantum structure of complex atoms and molecules and in providing basic data relating to studies of chemical reactions, radiation processes in plasmas and to the interpretation of astrophysical data. The intensity and continuous nature of synchrotron radiation makes it appropriate for the determination of photoionisation and photoexcitation cross-sections, and for photoelectron spectroscopic experiments involving the measurement of the energy distribution of the electrons ejected by the incident photons - a class of experiment related to the technique of electron spectroscopy for chemical analysis (ESCA) which is already a familiar analytical and investigational tool in the Laboratory. Additional information on the coupling of the optical electrons can be obtained from the study of the angular distribution of emitted electrons, for which a polarised source is necessary, and the time-modulated nature of synchrotron radiation makes possible measurement of the time-dependence of the radiative decay of excited systems. Data times obtained will be required for the development of vacuum ultra violet and X-ray lasers involving spectral transitions in these regions, at present only accessible by less direct or less accurate means.

The second broad area of interest in synchrotron radiation studies is in the investigation of condensed phases. Absorption, reflectivity and fluorescence studies in the extreme ultra violet will permit the more accurate determination of the optical constants of materials, and measurements of absorption and

reflectivity at high resolutions provide accurate information on the electronic band structures of solids. The photoelectron spectroscopy of solids with synchrotron radiation, making use of observations using radiation over a wide spectral range, offers the possibility of separating bulk and surface effects, for instance by allowing a distinction to be drawn between Auger electron emission peaks and photoelectronic peaks in complex spectra: developments of this kind open the way, for instance, to the investigation of chemisorption on metal surfaces and surface reactions. The advantages of high intensity and the ability to select a given wavelength from a continuous flux open up new approaches for structural studies for X-ray diffraction: for instance making accessible observation of radiation scattered through small angles and thus corresponding to the large lattice spacings of interest in the study of, for instance, polymers and amorphous materials, since there would be scope for operating at the highest wavelengths not absorbed by the material under investigation and mitigating the difficulties of working at very small angles of scattering. Biological systems, with their large distances between repeating units, are similarly appropriate for study with synchrotron radiation, which is also necessary for other reasons: firstly because biological systems are largely composed of elements of low atomic number and hence are of low scattering power (cf. the discussion below of neutron diffraction in the study of biological systems) and because the phenomena involved, for instance in the study of striated muscle, are often transient and the time available for recording a diffraction pattern is short. (Because of the speed with which a diffraction pattern can be obtained with high intensity source it has been suggested that central sources of synchrotron radiation may largely replace conventional laboratory sources for routine X-ray structural investigations.) Finally, the characteristics of synchrotron radiation make possible the determination of atomic distribution functions in amorphous materials.

Since the Board's recommendation has been that a source should be built that achieves radiation intensities about two orders of magnitude higher than that available with the existing source, it is appropriate to consider what classes of experiment will be feasible that are not accessible with the existing accelerator. In general terms these correspond to those in which the incident beam is reduced in intensity before final measurement by a succession of severe attenuations, or in which the requirements of time-resolution effectively reduce the signal received by the measuring instrument. This means that the new source can alone make accessible time-resolved measurements with polarised light, time-resolved X-ray diffraction studies, and lifetime measurements on atoms and molecules, and also X-ray optical techniques, polarised light spectroscopy, X-ray fluorescence studies and fluorescence emission spectroscopy, and Compton and X-ray Raman scattering techniques. It will also facilitate the measurements of photoionisation cross-

sections of atoms and molecules, high resolution spectroscopy of atomic and molecular species and of condensed phases, and photoemission studies which are accessible with difficulty, if at all, with the existing machine.

#### Research using high-powered lasers

Two broad classes of research would be made possible by a high-powered laser facility: (i) the study of non-linear interactions of very intense optical and infra-red radiation with matter; (ii) the creation and study of superdense plasmas similar to those occurring in stellar interiors.

The phenomena of absorption and reflection of radiation by plasmas, whose study would, generally, be accessible with single-channel lasers, are a field of scientific importance in their own right, and also provide the essential basis for other important areas of experimental physics. Thus the availability of ~~multi-~~terrawatt laser pulses of duration in the range  $10^{-10}$  to  $5 \times 10^{-12}$  seconds would open the way to the exploration of various approaches to the generation of high-powered lasers in the vacuum ultra-violet and X-ray spectral regions. Experiment and theory have already shown that laser plasmas can act as exceptionally powerful and efficient flash X-ray sources; efficiencies of about 20% have been reported in the conversion of laser power to X-ray power. The production of X-ray sources has implications for several areas of physics: the study of the source itself; the ionisation, recombination and excitation of inner and outer orbital electrons; the generation of ionic spectra not otherwise produced in the laboratory; the use of the X-ray source for subnanosecond resolution absorption spectroscopy and X-ray transmission photography, and the study of photoionisation processes. These applications relate to incoherent sources: a still more important goal is the development of tunable lasers in the X-ray and ultra-violet regions which would have many applications in plasma diagnosis, laboratory astrophysics and spectroscopy. There is particular interest in intense tunable ultra-violet sources for photoemission studies at wavelengths down to the soft X-ray region, a need which can also be met by synchrotron radiation. Several feasible schemes for producing X-ray lasers have been proposed. There are grounds to suggest that for heavier elements an X-ray laser could be pumped by picosecond laser pulses, which could be a practicable proposition; other approaches make use of  $n=3$  to  $n=2$  transitions in hydrogen-type atoms of high atomic number and of  $np \rightarrow ns$  transitions in isoelectronic neon-type ions.

The production of superdense plasmas by multichannel laser compression is also of interest in its own right as well as opening the way to new areas of experimental physics - as well as involving important basic research relevant to the production of energy to thermonuclear fusion, as has been mentioned in section 5 above. The basic problem in the production of a superdense plasma is to specify the form of the laser pulse in terms of energy, duration, wavelength, coherence and symmetry, that is required to compress a pellet of material in a way that produces at its centre a small volume of highly compressed high temperature plasma. Computational methods play an important part in this field since laser compression, which presents formidable experimental difficulties, is especially suitable for computer simulation studies. Basic physical investigations that would be made possible with a multichannel laser facility include: (i) Nuclear interactions. In a nuclear fission reaction the neutron free path prior to multiplication is inversely proportioned to the density of the nuclei. An increase in nuclear density by laser compression could, therefore, increase the utilisation of the fission neutrons and decrease both the critical dimension and the critical mass. Pulsed microcritical masses might be used to produce high intensity fluxes of neutrons and neutrinos. (ii) Laboratory astrophysics. The superdense plasma produced by laser compression would be comparable with those in stellar interiors, and with the possibility of the controlled introduction of impurities would enable studies of models of stellar interiors to be undertaken in the Laboratory. (iii) High magnetic fields. Flux compression is a well-known way of producing very high magnetic fields from an initial low cost-produced flux density, and explosive compression has been considered and investigated experimentally. Laser compression carries such possibilities a stage further, though the application of magnetic fields thus produced would be largely limited to spectroscopic studies.

#### Research using neutron beams

Neutron beam experiments for the study of condensed matter may be divided into two groups - those involving elastic scattering (e.g. diffraction) in which only changes in momentum are important, and inelastic scattering where, although changes in momentum are monitored, it is the change in the energy of the neutron which is of particular interest. Different kinds of information are derived from the two classes of experiment: elastic scattering experiments give information about the positions of atoms, whereas inelastic scattering experiments provide a direct means of studying the vibration of atoms in crystal lattices and of spin waves in magnetic materials. The dynamical behaviour of liquids and polymers can be explored by inelastic

scattering experiments, complementing infra-red and Raman spectroscopic studies. It is a measure of the way in which an area of science can evolve that when the use of the domestic facilities, and even of the ILL reactor, was first conceived, the emphasis was on elastic scattering, the focus of interest has now moved to inelastic scattering; and though neutron beams in the UK and at the ILL were used first by physicists, they are now being increasingly used by chemists and biologists.

#### Specific areas of research

Neutron and magnetic crystallography: Since the nuclear scattering cross-sections for neutrons fluctuate irregularly with atomic number the elastic scattering of neutrons by condensed phases can provide information complementary to that from X-ray techniques. In particular it can locate hydrogen atoms that are not detectable by X-ray crystallographic methods. Moreover, the neutron is unique among available forms of radiation in possessing a magnetic moment but no charge, so that most of our knowledge of magnetic interactions at the atomic level is derived from neutron scattering experiments. Diffraction experiments may be carried out on single crystals or powders. The number of conventional single crystal investigations has not increased drastically in recent years, in part because of the difficulty of obtaining sufficiently large crystals and in part because of the time involved in a complete investigation. Nevertheless many structural problems remain to be solved by single crystal methods. The most challenging involve the complete determination of biological structures, including those of proteins. For these, the use of neutrons of both long and short wavelengths is envisaged, together with the use of anomalous dispersion techniques for phase determination. A recent development, which is still at a very early stage, involves the use of dynamically polarised neutrons. It holds out the possibility of the selective investigation of chemically interesting sites in systems of this kind.

Much early work using neutrons was concerned with the determination of magnetic structures, but more recently our understanding of magnetic materials has been greatly extended by the use of polarised neutrons. Detailed magnetisation density distributions may be determined and related to the nature of covalent bonding in transition metal, rare earth and actinide compounds. The use of polarised neutrons is not restricted to magnetic crystallography. Recent developments have opened the way to distinguishing between spin-incoherent and other forms of nuclear scattering, between paramagnetic and other incoherent scattering and magnon and phonon scattering in ferromagnets and antiferromagnets. Polarised neutron scattering is thus also expected to contribute to knowledge of the structure and dynamics of liquids and of the magnetic behaviour of binary alloys.

An unexpected development has been the rapid upsurge in structural investigations of polycrystalline samples. There are several advantages in the use of powders. More rapid collection of data is possible and measurements over a range of temperature and pressure are facilitated: moreover powder methods do not require the use of single crystals which are sometimes difficult or impossible to obtain. It is, however, the realisation that the large number of heavily overlapping reflections obtained from a powder need not preclude a detailed structural analysis which makes feasible the study of a very large number of structures, including those of low symmetry. Powder studies on a range of molecular crystals are now leading to insight into the nature of hydrogen bonding in hydrogen halides and into intermolecular forces in hydrocarbons. In the field of solid state inorganic chemistry, new light has been thrown on the electronic influences affecting structure through the determination of the local environment of ions of their distribution in a wide range of compounds. Recent investigations include crystallographic studies of shear and block structures such as perovskites and tungsten bronzes. Since many non-stoichiometric compounds contain large proportions of light atoms information can be gained which illuminates the clustering and short-range ordering of defects, and has stimulated theoretical work on ionic crystals. Powder diffraction techniques have been used in the study of ferroelectrics and antiferroelectrics and in the investigation of magnetic ordering effects. Determinations of magnetic moments in a range of simple inorganic compounds have allowed the quantitative estimation of d-orbital covalency which can be compared with recent theoretical calculations, and the determination of magnetic structures of more chemically complex systems is to be expected, as already exemplified by the recent investigations of optically transparent ferromagnets as a first step in the examination of exciton-magnon transitions.

Liquids and amorphous solids: The whole field of the structure and dynamics of simple liquids, solutions and glasses is one to which neutron beam techniques will make an important contribution. Structure factors have been determined for monoatomic liquids (metals and rare gases) and for binary liquids. Techniques of isotopic enrichment have thrown further light on the structure of water and have enabled the quasi-lattice distributions of dissolved ions in concentrated solutions to be determined for the first time. Experiments on  $^3\text{He}$ , a quantum Fermi liquid, have already shown some unexpected features. Studies on simple liquids again provide an example of the complementing by experimental observation of contemporary theoretical investigations, and in the studies of binary liquids little has so far been done on molten salts and molecular liquids. Though increased attention is being paid to conventional glasses there is as yet little work on amorphous materials; and studies which have given information on the partial structure factors in isotopically

substituted glasses may in the future be extended to magnetic glasses.

The dynamical behaviour of solids: Inelastic scattering of neutrons plays a basic part in the study of lattice dynamics. The use of thermal neutron beams in the study of ferroelectrics, semiconductors, superconductors and Jahn-Teller systems aim at determining the influence of lattice dynamics on other physical properties. Such investigations have recently been extended to structurally and chemically more complex systems such as layer compounds and molecular crystals including plastic and liquid crystals and polymers, and may be expected in the future to detail information on intermolecular forces which may match the insights gained into interatomic forces. Chemists may also be expected to become increasingly interested in cooperative magnetic phenomena, hitherto very largely the province of the physicist. Magnon dispersion curves provide the only direct determination of exchange interactions. The line widths and shifts of phonon and magnon lines provide unique information on the interactions between elementary excitations.

Chemistry and materials science: Neutron spectroscopic studies of molecules complement the investigation of vibrational modes by infra-red and Raman methods where transitions are forbidden or are too weak to be observed optically. Such investigations extend to matrix isolated systems and to the study of adsorbed molecules whose properties may be altered by interaction with the surface. The recent development of instruments with very high energy resolution holds out the promise that rate processes down to  $10^7$  or perhaps  $10^6$  per second can be observed. The separation of rotational and translational fluids is made possible, as well as the study of a range of rapid chemical reactions. At very high energy resolutions it is in principle possible to observe the nuclear quadrupole splitting of a range of nuclei: hyperfine splitting in cobalt has already been observed.

Polymer studies have benefited in particular from the combination in the neutron scattering process of a short time-scale of interaction and the long wavelength of low-energy neutrons. As well as providing further information on polymer configuration neutron studies have detected the motion of side-groups and thrown light on the effect of fillers such as carbon black in rubbers. Future work is expected to provide information on the collective excitation of the polymer chain. In the fields of metallurgy current investigations of the aluminium-zinc system have illustrated the potential of long-wavelength neutrons in the study of pre-precipitation phenomena in alloys. The observation of fluctuations in magnetisation in magnetic alloys lead directly to information on the electronic structure.

Biology: The application of neutron beam techniques to the study of biological systems is an important growth area. The earliest example of elastic scattering studies on a single crystal was the determination of the structure of vitamin B12, and work is at present in progress on insulin (complementary to the structural studies at Oxford in which the Atlas Laboratory is involved). Small-angle scattering is used in the study of the structure of biological macromolecules in solution - for instance in the determination of the quaternary structure of ribosomes and small-angle diffraction techniques in structural studies of biological membranes and liquid bilayers, fibrous proteins, chromatin and viruses. Quasi-elastic and inelastic scattering methods are used to investigate the dynamical properties of water in a number of biological structures, and it has been suggested that neutron scattering experiments might throw light on, for instance, the vibrations propagated along the fibre axes of muscle and collagen, information relevant to an understanding of the structural organisation of these materials.