The scientific case for the ESS project

Study report

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Foreword

The concept of the European Spallation Source – a next generation neutron source for European science and technology – arose out of a panel set up by the European Commission in 1990 to examine the provision of neutrons in Europe. This panel drew attention to the serious problem that was likely to arise after the turn of the century as many of the smaller neutron sources reached the end of their economically and technically viable life [1]. Unless action was taken soon, they predicted a serious drought of neutrons with all its consequences for European science and its exploitation.

Consequent upon the panel's report, an initiative of the Forschungszentrum Jülich in Germany and the Rutherford Appleton Laboratory in the UK resulted in a series of workshops that examined the technical feasibility and the instrumentation needs of a next generation pulsed spallation source [2]. Subsequently, in 1994, the CEC approved a proposal from a consortium of laboratories in several European countries to examine the technical feasibility and likely cost of a 5 MW sharp pulse spallation source. As part of this study, the Scientific Case for such a source would be developed, an operation which was supported with funding by the European Science Foundation.

This study report, together with the appendices, is that Scientific Case.

In parallel with the European Spallation Source study, the European Science Foundation also decided to assess the general scientific case for neutrons. As part of this process, a workshop held in Autrans, France, in January 1996, brought together some 80 scientists from a broad range of scientific fields. In addition to a number of 'expert' neutron scatterers, this workshop also involved leading scientists for whom neutrons were not their major experimental technique. Their expertise in other powerful techniques such as synchrotron radiation and nuclear magnetic resonance was essential to ensure that neutrons could be assessed in context.

This workshop, published as a report by the European Science Foundation[3], clearly established not only the power of neutrons, but the potential of neutron techniques in the future scientific and technological development of Europe.

With the case for neutrons so established, this document builds upon the Autrans report in asserting an exciting, vibrant, and powerful case for a next generation pulsed neutron spallation source. The Scientific Case was developed by a large number of the condensed matter community in Europe, from universities, industry, and large national and international research laboratories. For practical reasons, ten scientific themes were selected, and the scientific case for each one explored by a team of leading scientists under the guidance of a Theme Co-ordinator. The subject areas chosen and the mix of scientists within each theme, underline the interdisciplinary nature of much neutron research. Similar teams were set up to examine the instrumentation that would be needed to deliver the science.

Although neutron sources, like synchrotron sources, are large machines, requiring large institutions to run them, the science performed on them is what is often called 'small' science. This is in contrast to 'big' science – experiments that may last several months or even years, each one performed by large teams at international research institutes. In the neutron and synchrotron cases, typically teams of a few scientists will use one instrument at the facility for a short period (as little as one day to perhaps as much as two weeks) to perform a specific experiment which is often part of a wider research programme that may also use a variety of other – often complementary – techniques. The breadth and diversity of the neutron community is documented in a recent report, which also underlines the importance of neutron techniques

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[1] Report of the EC Large Scale Facilities Neutron Study Panel (1990)

[2] Expert Meeting on Accelerators, Simonskall (1991), Expert Meeting on Target Technologies, Villigen (1992) and Expert Meeting on Instrumentation and Techniques, Abingdon (1992)

[3] ESF Framework Studies into Large Research Facilities : Scientific Prospects for Neutron Scattering with Present and Future Sources, Autrans (1996)

as an essential element in wider investigations [4]. This bringing together, at a central facility, of many scientists for short periods of time has resulted in much cross-fertilisation of ideas, and consequent enhanced international collaboration that has been to the good of European science. Thus, ESS will, in addition to delivering frontier science, build on our experience of existing central facilities to act as a positive force in the further development of European coherence.

It is also clear from the following pages that the purely scientific case for the ESS is exceptionally strong. However, a case for an expensive facility must be made to significant degree on its potential to increase the exploitation of science for wealth creation and enhancing the quality of life in Europe. Hence, the case presented here focuses on the tremendous potential – some would say necessity – of a next generation source for the exploitation of the exciting advances that have been made in condensed matter science in the past twenty years, and will continue to be made in the near future.

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[4] Published in Neutron News Vol.7/ 3, p. 35 (1996)

Neutron science

Neutron scattering provides basic microscopic information on the structure and dynamics of materials which underpins our understanding of condensed matter in fields as diverse as materials science, chemistry, biology, the earth sciences and physics. It has made outstanding contributions to our detailed understanding on a microscopic level of technically important materials such as plastics, proteins, polymers, fibres, liquid crystals, ceramics, hard magnets and superconductors as well as to our understanding of fundamental phenomena such as phase transitions, quantum fluids and spontaneous ordering. The 1994 award of the Nobel Prize for Physics to Brockhouse and Shull for their pioneering efforts in the 1950s was a public acknowledgement of the importance of neutron scattering to the scientific community.

The neutron is, in many ways, the ideal probe for the study of condensed matter, having significant advantages over other forms of radiation in the study of microscopic structure and dynamics. Neutrons interact with matter through all four forces, the strong, weak, electromagnetic and gravitational interactions, but it is the interaction via the strong force which makes neutrons a unique probe in condensed matter. A list of the most important properties of the neutron is given in the box opposite.

Europe is pre-eminent in neutron science. The scientific achievements of reactor-based steady state neutron sources such as the Institut Laue Langevin in Grenoble or the newer accelerator-based pulsed neutron sources such as ISIS in the UK are extensively documented in the scientific literature, in reviews (see for example the recent ESF/ENSA Autrans Report *Scientific Prospects for Neutron Scattering with Present and Future Sources*), and in the annual reports of the facilities themselves. The present proposal for the European Spallation Source, a next generation neutron source, will ensure that neutron beams of the highest quality are available early next century to a broad spectrum of users from academia and industry.

The development of third generation synchrotron radiation sources and other new techniques, such as scanning tunnelling microscopy, is also making an impact in condensed matter science,

The main advantages of neutrons

The main properties of the neutron that are exploited in scattering studies can be summarised as follows.

- The *energies* of thermal neutrons are similar to the energies of atomic motions. A wide *range of energy scales* may be probed, from the neV energies associated with polymer reptation, through molecular vibrations and lattice modes, to eV transitions within the electronic structures of materials.
- The *wavelengths* of thermal neutrons are similar to atomic spacings, providing structural information over nine orders of magnitude in length scale (10^{-5} to 10^{4} Å). Measurements are thus possible over distance scales ranging from that of the wavefunction of the hydrogen atom to those of macromolecules.
- Neutrons see *nucle*i, rather than the diffuse electron cloud seen by X-rays. This has major advantages, such as allowing us to see clearly light atoms such as hydrogen in the presence of heavier ones, and to distinguish neighbouring elements more easily. The fact that the scattering cross-section of an atom generally varies between isotopes of the same element allows us to exploit *isotopic substitution* methods to yield structural and dynamical information in even greater detail. It also facilitates the use of *contrast variatio*n, which enables us to contrast out parts of a complex system, for example the nucleic acid or the protein component of a virus.
- The neutron's *magnetic moment* is ideally suited to the study of the microscopic magnetic structures and magnetic fluctuations that underpin magnetic phenomena in materials.
- Neutrons only *perturb* the experimental system *weakly*. This greatly facilitates interpretation and often means that neutron scattering provides the most reliable scientific results in areas as diverse as the structure of water or the strain mismatch in superalloys used in turbine blades.
- Neutrons are *non-destructiv*e, even to complex, delicate biological materials.
- Neutrons are *highly penetratin*g, allowing the *non-destructive* investigation of the interior of materials. This makes them a genuine microscopic *bulk prob*e, makes routine the use of complex environments such as furnaces, cryostats, and pressure cells, and enables the study of *bulk processes under realistic condition*s.

but in a complementary way which only strengthens the case for an enhancement of Europe's neutron capability. The development of a third generation neutron source is timely and widely recognised as a priority for European science and technology.

The need for a next generation neutron source

Neutron scattering is still very much an intensity limited technique. As sources have developed in strength, the sophistication of experiments has increased tremendously. Measurements of total cross-sections in the 1930s and 1940s gave way to differential scattering in the 1940s and 1950s which allowed structure to be explored. The high flux reactors of the 1960s and 1970s allowed dynamics to be studied and cold sources exploited; the 1980s saw the first tentative use of polarisation analysis and the exploration of high energy and wide dynamic range studies on pulsed sources. The 1990s have seen problems of increasing complexity being tackled, many of them of relevance to the wealth-creating industries through e.g. the development of neutron reflectometry. All of these developments required an increase in source strength as well as investment in instrumentation and techniques.

Originally it was the physics-based community which pioneered and developed neutron scattering techniques. The expansion in the use of neutrons in recent years has come from chemists, biologists and material scientists realising the potential of these techniques [5]. Future user communities will be interested in increasingly more complex and advanced materials and systems and will seek to answer increasingly more complex questions about them. The emphasis in future measurements will be on higher precision and better resolution rather than simply increasing the throughput of experiments. Time dependent processes and kinetic studies will become routinely possible, with data being processed in real time. Parametric studies – observing changes with pressure, temperature or concentration – will enable us to obtain a 'whole picture' view of a problem rather than merely the tantalising glimpse of only a few pieces of a jigsaw puzzle.

The specific scientific case for a next generation neutron spallation source is developed in detail in Chapter 2.

Neutron sources

Neutrons have traditionally been produced by fission in nuclear reactors optimised for high neutron brightness. The neutrons from such steady state sources are produced continuously and, after thermalising the high energy (MeV) neutrons in the surrounding moderator, beams are emitted with a broad band of wavelengths. Wavelength selection is generally achieved by Bragg scattering from a crystal monochromator or by velocity selection through a mechanical chopper. In this way, high quality, high flux neutron beams are made available for neutron scattering experiments. Steady state fission reactors dedicated to the production of neutrons for condensed matter research produce many tens of MW of heat within the reactor core. For every available neutron generated in the fission process, 190 MeV of energy is released. In the most advanced reactors using highly enriched fuel, heat dissipation in the core approaches the limits set by current materials technology.

A more recent development are accelerator-based pulsed sources which produce neutrons in a totally different manner. In this *spallation* process, neutrons are released by bombarding a heavy metal target with high energy particles from a powerful accelerator. Typically, 30 MeV

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[5] See Neutron News Vol. 7/3, p 35, (1996)

of energy is dissipated for every neutron generated. This low heat dissipation combined with the low duty factor of pulsed accelerators means that high neutron brightness exceeding that of the most advanced steady state sources can be achieved with the release of only a modest amount of heat generated in the target.

Although there have been significant advances in instrumentation at steady state reactors in the past 30 years, the sources themselves have shown only modest gains in flux. In contrast, accelerators have advanced tremendously in this period through the development of linear accelerators, strong focusing synchrotrons, charge exchange injection, radio-frequency quadrupole (RFQ) technology, sophisticated beam dynamics, computer control and particle tracking codes. This has meant that accelerator based neutron scattering sources have grown in strength by five orders of magnitude from a mere curiosity in the 1970s to a position where they compete with the best reactor sources today. In recent years, neutron scattering instruments using advanced time-of-flight instrumentation have been developed which can utilise fully the high intrinsic brightness of these sources. As a result, neutron beams produced by present day 100 kW beam power accelerators now rival those of the best reactors in the world. The potential exists to increase beam power further by more than an order of magnitude.

The most advanced sources in Europe – ISIS and ILL – form a complementary pair: they both have unique features, but there is significant overlap in their capabilities. The development of either of these technologies might have been be an acceptable route to a third generation neutron source. The US embarked on a 'super-ILL' study – the Advanced Neutron Source project at Oak Ridge National Laboratory. A project team working for more than a decade produced a fully costed engineering design for a sophisticated 350 MW reactor (ILL is a 57 MW reactor) which may be taken as the reference case for a third generation reactor-based neutron source. The project has since been terminated on cost grounds.

The emergence of accelerator based sources as a viable contender and possibly the only feasible route to a next generation neutron source is more recent. ISIS, at 160 kW, is more than an order of magnitude more intense than, for example, the IPNS pulsed neutron source (Argonne, USA) built a decade earlier, and is even more effective due to developments in neutron instrumentation. Rapid advances in accelerator technology in the 1980s suggest that progression to a 5 MW pulsed spallation source is possible. The evaluation of the feasibility and costing of such a source is the purpose of this present European Spallation Source Study.

The detailed report of the European Spallation Source Technical Study is published separately.

ESS source specification

The source specification for the European Spallation Source is based on an accelerator producing:

- an average proton beam power of 5 MW at a repetition rate of 50 Hz;
- a proton pulse length on the target of 1 µs or less;
- a 50 Hz target station, accepting up to 5 MW of beam power;
- a 10 Hz target station, accepting up to 1 MW of beam power.

In order to provide the instrument suite appropriate to the science that can be performed on the ESS, the two target stations will be optimised differently. One will operate at 10 Hz/1 MW, optimising the performance of instruments using mainly long wavelength neutrons, while the

Figure 1: ESS Campus

second will operate at 50 Hz/4MW for high intensity/high resolution applications. Both target stations will operate by horizontal injection into a liquid mercury target. Compact liquid water and liquid hydrogen moderators, appropriately optimised neutronically, will feed eighteen independent beam ports, some of which will be equipped with multiple guide bunches, on each target station. The neutronic performance anticipated from this specification will make the European Spallation Source some 30 times brighter than ISIS, presently the world's most powerful source of this type. With appropriate development in neutron instrumentation, advances in data rates of up to three orders of magnitude may be anticipated in some fields.

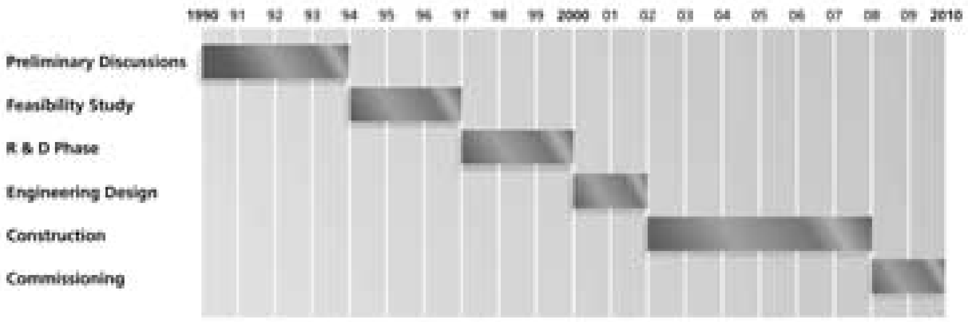
The reference suite of 44 instruments is described in chapter 3.

The 5 MW beam power is developed in a 1.334 GeV H^- linear accelerator with a duty cycle of 6% at 50 Hz. Two 60 mA H^- ion sources feed two independent 175 MHz radio-frequency quadrupoles. These two beam lines are funnelled at 5 MeV into a 350 MHz drift tube linac for acceleration to 70 MeV. Further acceleration to 1.334 GeV is achieved in a 700 MHz coupled cavity linac. A 180° achromatic bending region in the transfer line between the linac and rings is used to achieve momentum and transverse beam collimation. This is an essential feature to control the beam halo prior to injection. High efficiency charge-exchange H^- injection of 1000 turns into each of two accumulator rings is achieved using an elegant painting scheme in the longitudinal and both transverse planes. Containment in 400 ns bunches is followed by sequential extraction giving the desired 1 µs proton pulse to either of two targets.

Full details of the ESS feasibility study can be found inVolume III. An artist's impression of the ESS campus is shown in figure 1.

Time scales for the ESS

The anticipated time scale for realising a project of this magnitude is long. The technical feasibility study was concluded at the end of 1996. The ESS R&D phase will start in 1997 and extend over a period of 3 years. Detailed engineering work could start in the year 2000 with the ESS fully available for science in the year 2010:



The European Spallation Source Technical Study (published in 1997) has demonstrated that an accelerator with 5 MW beam power is feasible, and has provided a reference design. Based on the anticipated performance, several hundred members of the existing and potential scientific user community have considered, through extensive consultations, discussions and workshops, what might be achieved in condensed matter science were the ESS available today. Ten teams, each under the guidance of a Theme Co-ordinator, considered the scientific opportunities of the ESS in a number of scientific themes ranging from physics to biology. Although it is not possible to reliably predict the future, their extrapolation of present day scientific quests has revealed the potential impact that the ESS will make, both on our fundamental scientific knowledge and on the exploitation of this underpinning science for increased wealth creation and enhancement of the quality of life. In addition, new scientific questions will undoubtedly appear – no-one foresaw the Nobel Prize winning high temperature superconductors or fullerenes a decade ago. Some of the scientific problems identified might remain challenges, but the history of neutron scattering over the past 50 years leaves us in no doubt that an advanced neutron source of the ESS specification will make a real impact on basic, strategic and applied research in Europe.

The reports from the scientific theme groups form the foundation for the ESS science case presented in this chapter. The reports themselves are available as ESS Internal Reports [6].

Four additional expert groups, in consultation with the theme groups, identified the instrumentation required to deliver the scientific programme. They also identified areas where an R&D programme is needed to fulfil the promises of the ESS. The reference instrumentation suite is presented in the next chapter. The reports from the Instrument Working Groups are also available as ESS Internal Reports [6].

New opportunities created by the ESS

The ESS will deliver a raw neutron intensity of up to 30 times that of ISIS, presently the world's most powerful pulsed spallation source. Based on the experience with pulsed sources over the past ten years, further effective intensity increases will be available from optimised moderator design, neutron optical elements such as neutron guides and capillary focusing devices, as well as instrumentation optimisation. The instrumentation parts of the ESS study have indicated that, depending on the particular kind of experiment being performed, effective intensity gains from one to three orders of magnitude over ISIS will be available.

This effective neutron intensity gain will be used in a variety of ways, with trade-offs possible between intensity, resolution, sample size and time. We can perhaps indicate as follows, ways in which these global 'technical opportunities' will be exploited in the expected scientific programme of the ESS.

"We will be able to make measurements to higher resolution in both space and time."

Trading increased intensity for higher resolution will enable accurate and precise structure refinements on the increasingly complex systems that are central to modern materials science. Excitation spectra of these more complex systems will also be measurable accurately. Dynamics

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[6] Details of these reports will be available on www.risoe.dk/ESS

of quasicrystals will be accessible as will the tunnel splittings of the upper excited states that give high quality information on the precise shapes of potential functions. Spectral studies of the binding of molecules such as chromophores and therapeutic biomolecules will be possible, as will studies of the solution environment of excited state distortions of dissolved molecules.

" We will be able to measure weaker signals."

The promise of full polarisation analysis will be realisable for the first time, with major implications over a wide range of studies from the separation of coherent and incoherent contributions to the signal measured – e.g. in soft solids work – to the use of full spherical polarisation analysis methods in magnetism. The power of neutrons will be available to study details of the *subtle effects* and *small changes* that are seen to be increasingly important in controlling the behaviour of new materials (e.g. high temperature superconductors). In isotope substitution studies – which exploit one of the most powerful of neutron methods – *smaller differences* will be measurable accurately, enabling the use of the technique with an increased number of elements. Of particular potential here is the extension of the technique to carbon, with all its implications for studies relevant to molecular biology, biotechnology, and pharmaceuticals.

"We will be able to make measurements over shorter times."

This will allow us to measure structure and dynamics over a much *wider parameter space* than presently possible. Following variations with pressure, temperature, magnetic or electric field, concentration, etc. will allow us to *solve real problems*, rather than do single experiments that show us only a small fraction of the picture. Since structure-property relationships are usually of key importance, experiments designed to solve materials related problems or to understand an important process almost never involve a single sample or a single set of experimental conditions. Tens, or even hundreds of data sets may be required to obtain the information needed. An example of major importance in chemistry and biology is a full understanding of through-solvent interactions, in particular the hydrophobic effect. This requires isotopic substitution measurements of solutions over a wide range of concentrations, temperatures, pH, ionic strength, and pressure that just cannot be covered with existing sources.

Shorter time measurements will allow real-time neutron studies of chemical reactions, for example, real time structural and dynamic measurements of catalysis. Kinetic processes and materials behaviour under non-equilibrium conditions can be followed. There will be a dramatic reduction in the unit cost of certain neutron measurements, opening up the technique to routine industrial exploitation. An example here is the measurement of residual stress in engineering studies. The ESS Engineering Centre (see p. 87) will carry out such measurements at a unit cost which is an order of magnitude less than at present. Measurements over shorter times will also enable neutrons to be used regularly in industrial process optimisation. Furthermore, the nucleation growth problems that pervade much of materials research – so-called TTT (time-temperature-transformation) process – will be opened up fully to the unique power of neutron techniques. Shorter times will naturally increase experimental throughput, allowing much more of the high quality science presently not possible because of the scarcity of neutron beam time.

"We will be able to make high quality measurements on smaller systems"

Some samples are *inherently small*, such as a crack tip: the strain distribution around this could be probed using the ESS. Other samples are small because *only small amounts of material are available* – often the case in the development of new materials. Isotopically enriched samples needed to exploit isotope substitution techniques often come in only small quantities. The ESS will enable us to probe *spatial variations* – of a whole range of important properties – in real space with a resolution of 50 µm. *Structures and dynamics of surfaces and interfaces* will become accessible routinely to neutrons for the first time and experiments on thin layers – e.g. giant magnetoresistance materials – will yield higher quality data. Solution studies will be possible at *lower concentrations* than is presently possible, opening up concentration regimes that are particularly important for understanding the processes controlling biomolecular interactions.

"We will be able to use more extreme sample environments."

Experiments under extreme sample environment conditions offer the prospect of new and exciting science. Extreme environments generally restrict experimental conditions significantly: only very small sample volumes are possible (e.g. at very high pressures of 25 GPa and beyond), or experiments have to be conducted in short times because the environment cannot be maintained for an extended period (e.g. extreme low temperatures – nK and even pK) or the duty cycle of the equipment is low (e.g. magnetic fields beyond 15 Tesla can be obtained only in a pulsed mode with duty cycles at present limited to 0.5 to 1 Hz). Examples include studies of hydrogen bonding under extreme pressures to probe the detailed nature of this important interaction (e.g. ammonia above 25 GPa), and elucidating the phase diagram and magnetic structure of nuclear spins in elemental copper below 6.10-8 K.

The scientific impact of ESS in specific areas

The brightness of the ESS will open up a host of opportunities for new and cost-effective science and technology developments in Europe. We cannot hope to predict reliably what these specific developments in the early years of the next millennium will be – in the early 1980s, no-one would have predicted high temperature superconductivity in perovskite structures. We can, however, extrapolate from the present and foresee where, **were ESS available today**, major advances would be possible. Working at the limits of present sources, demonstration experiments are giving us glimpses of the future possibilities that ESS would enable us to realise routinely. The advent of this next generation source will take us over a major threshold to the solution of whole ranges of scientific and technological problems that are relevant to today's societal needs, and to the fundamental science that will underpin tomorrow's technological developments.

This section summarises some of the basic, strategic, and applied science that ESS would make possible were it available today. All the examples given capitalise on one or several of the technical opportunities opened up by the ESS that were discussed in the previous section (high resolution, short times, inherently small samples etc.). There is clearly much overlap between the chosen themes. Increasingly, frontier science is interdisciplinary, and it is increasingly difficult to place sensible boundaries between areas. Some scientific areas have a long history of using neutron scattering and have consequently achieved a great deal using the technique. Others represent new frontiers that are just beginning to see the possibilities of neutron techniques. In the following summary of the Scientific Case, we have chosen to represent all areas equally, in order not only to highlight scientific disciplines in which neutron methods are already well established but also to reflect the growth potential of new areas.

Further details are given in the ESS Internal Reports, which present the full documents of the working groups of European scientists that have, for the past two years, been considering the scientific and technological impact of ESS in the various fields.

Polymers and soft matter

Soft matter encompasses a wide range of molecular materials such as polymers, surfactants, and colloids. The physics and chemistry of these systems is of increasing technological importance, the area often being driven by the commercial significance of products that are a highly complex mixture of components and structures.

All these materials share the same basic properties: weak interaction between the structural units, large thermal fluctuations, large numbers of internal degrees of freedom and a macroscopic softness indicative of a weak modulus of elasticity. The range of distance and time scales relevant to performance (e.g. vehicle tyres) can be remarkable. These common features make them susceptible to a variety of experimental approaches, of which synchrotron radiation, electron and light scattering, and neutron scattering play important roles. The specific advantages of neutrons make them particularly powerful in this area and, despite the relative weaknesses of presently available intensities, the unique information that neutrons can give have led to many scientific 'breakthroughs' in the field (see box). Soft condensed matter studies using neutrons have therefore grown explosively over the past decade. The problems being addressed impinge significantly on the commercial world.

The future trend in soft solids is towards the understanding, and ultimate control of, ever more realistic complex materials. The ESS performance characteristics are superbly matched to advancing this understanding and hence to enabling optimal design and effective exploitation of these complex materials. Being a pulsed source, its instruments can deliver simultaneously the wide dynamic length and time range in one measurement that this complexity demands. The flux increase over present sources will allow experiments to be performed on smaller samples with better resolution in shorter times, on more dilute samples, and with changes in environments such as temperature, pressure, external force fields, that are relevant to conditions faced in various processing functions (e.g. electrochemistry, rheology). Real opportunities will be presented to study off-specular scattering, grazing incidence diffraction, and surface inelastic scattering. More systematic studies of transient states will yield better insights into dynamic behaviour than available at present, with time-slicing possible over much shorter time intervals (seconds rather than minutes). Studies of time-dependent processes will open up the unexplored fields of the dynamics and kinetics of surfaces and thin films, while full polarisation analysis will have a major impact on the field through the reduction of background noise.

Major advances would be made in (static and dynamic) small angle studies of anisotropic and isotropic systems of polymeric and surfactant origin, including rheological properties of technically important systems, as well as in improving our understanding of the structures of adsorbed organic molecules and polymers at air-liquid, liquid-liquid, and liquid-solid interfaces. The important long time - short length scale dynamics regime, critical in the study of soft solids, will begin to be accessible. Much-needed insight will be gained into technologically important materials such as detergents, paints, inks, coatings, composite materials such as polymers and alloys, areas of food stability such as emulsion stability, foams, gels, as well as lubricants and fuel additives.

The following broad areas of soft solids studies will gain major benefits from the ESS.

Bulk dynamics and processing of soft solids

Many industrial processes involve extensional flow, ranging from simple pipe flow to deliberate alignment by extrusion. As the volumes of uniform flow for investigations such as diffraction

Achievements in soft solids using neutrons

In polymer structure:

- dimensions of the Gaussian coil structure of a single chain in the melt, and the affirmation of the screened excluded volume model;
- single chain behaviour in blends;
- verification of scaling laws on polymer solutions and microemulsion systems;
- structure of diblock copolymers;
- relationship between microscopic and macroscopic deformations for rubber elasticity;
- structure of, and density profile normal to, a polymer layer at an air/water interface.

In polymer dynamics:

- new light on viscoelasticity of polymer melts;
- direct information on polymer reptation and particle fluctuations, fundamental to understanding rheology of complex systems;
- single chain dynamics (α and β relaxations) in a bulk system;
- cross-links in networks for rubber and triblock copolymers;
- deformation and relaxation of elongated polymer melts under shear;
- interdiffusion of mixed polymer films;
- surface ordering of a block copolymer film;
- the influence of heterogeneity of polymer glasses on their thermodynamics.

In liquid crystals:

- correlations in the smectic B phase;
- conformation of liquid crystal polymers using contrast variation;
- the structure of water in lyotropic and microemulsion phases.

In surfactant structure:

- the measurement of simple micellar shape, size, and effective structure;
- determination of the interaction profile in a concentrated micellar system;
- location of species in mixed surfactant micelles and their relationship to curvature;
- curvature, structure, and form measurements of simple microemulsion systems in
- equilibrium, at inversion points and at extreme pressures and temperatures;
- structural measurements in non-liquid media such as microemulsions in plastic;
- crystalline phases, in near-critical and supercritical fluids and in gels;
- structure of adsorbed surfactant layers at an air/liquid interface;
- mixture composition at the air/water and air/solid interface.

In surfactant dynamics:

- interfacial fluctuations and the relationship to elasticity for droplets and vesicles;
- phase behaviour of spread monolayers of insoluble surfactants such as fatty acids;
- shear alignment of surfactants self-assembled into anisotropic species;
- correlated undulations in lamellar phases.

In particulate colloids:

- stabilisation of colloids using polymer adsorbates (polymer brush dynamics);
- effects of intensive properties on the stabilisation of surfactant coated colloids;
- the structuring of colloids at an interface;
- studies of the coalescence of colloids as precursors to film forming.

methods for alignment studies are often small, the ESS flux will aid development of such methods. The required constitutive equations spanning the dimension range from macroscopic to molecular will be derivable from the molecular level information obtained as a function of extrusion conditions combined with stress and velocity field measurements. The ESS intensity will allow the avoidance of wall effects and the use of viable values for extrusion pressures. In short, it will be possible to follow, under realistic conditions, the mechanisms controlling these processes, and hence provide the information needed to optimise them.

The microscopic deformation undergone by many materials – e.g. polymer melts – under flow can be studied, for example emulsion structure flow and polymers under extrusion processes. Quasi-elastic and inelastic neutron measurements on polymer melts in extrusion will lead to a more complete description of the energy spectrum in polymers as they are extruded. Important questions such as the possible existence of correlations between internal (Rouse or reptation) modes with the velocity imparted by the extrusion process can be addressed.

The ESS intensity will allow small scattering cross-section events to be followed under flow. The properties of tailored peptide-based polymers that may be used as 'smart' complex fluid and rheological modifiers at low concentrations can be studied. Measurement under flow of polymer melts, with selective labelling of parts of molecules, will be the key technique in the developing science of structure/rheology relationships for polymer processing, allowing questions such as the roles of molecular branching and polydispersity to be addressed. Similar partial labelling methods could be exploited in important studies of the flow behaviour of multicomponent systems where phase behaviour is often considerably modified by a stress field. Examples include multi-component micellar dispersions, polymers with particles, and mixtures of different particles. The changes in phase behaviour of surfactants with water and/or oil under shear will also be accessible.

Structures and dynamics of microemulsions at high temperature, pressure, and ionic strength

These systems are of interest in many varied fields, from encapsulation in pharmaceutical delivery systems to oil recovery. Present neutron studies of self-assembly systems are intensity limited to relatively high surfactant volume fractions. ESS will remove this severe restriction, opening up the detailed study of micelles in the region of the critical micelle concentration, and of associated dynamic phenomena such as micelle breakdown, and micelle-vesicle spontaneous transitions and structural phase changes.

For microemulsions, ESS will allow a range of important studies such as the investigation of the size redistribution mechanism on mixing large and small droplets (a process occurring on a time scale of ~1 s), and the use of microemulsions as steric templates for the *in-situ* synthesis of surfactant-stabilised nano-particle spheres, rods and discs (e.g. the photocatalyst CdS). It will also be possible to study effectively small structures in the presence of larger ones, for example water nano-droplets in a water-in- oil-in-water dispersion that are of relevance to the food industry. Another example would be to probe specifically the structure of enzyme-water-surfactant microreactor clusters in the presence of water-in-oil microemulsions, systems that are used for novel and selective organic synthesis. Surfactant systems will be accessible to study at the lower concentrations where system behaviour is closer to ideal, for example in reverse vesicle systems and flexible rods. For the latter system, the energy required to break the rods can be determined.

The ESS will also result in new scientific achievements in the following areas of soft solids and polymer science and technology

- Improved understanding of the thermodynamics, dynamics, and transport properties of complex fluids in porous media. Questions that can be addressed include how the interfacial surface area of the hydrocarbon changes with time during oil recovery or soil remediation, how the flow of water or surfactant changes hydrocarbon distribution within the soil or rock, and the mechanism of hydrocarbon dissolution;
- phase dynamics of diblock copolymers, for example charged or polyelectrolyte systems applied to processing;
- understanding fluid transport in gel systems, important in the food, pharmaceutical and agrochemical industries. The diffusion of molecules in porous media can be addressed, as can the dynamics of gels and cross-linked networks and the optimal design of polymers to give desired release profiles;
- multicomponent transport through membranes. Relevant questions relating to drug delivery systems include: how does the polymer transport during release and what is the release mechanism, as well as the structure and dynamics of the polymer, both in the bulk of the polymer membrane, and at the internal (with the active agent) and external (outside world) interfaces?
- the conformations of polymers in complex media, where they often impart the material functionality (e.g. fibres, films, foods). The effects of additives which change properties can be explored, for example the structural effects of changes in rubbers on addition of e.g. silica, graphite, and their relationship to wear and other functionalities;
- the ageing of polymeric glasses can be studied through secondary relaxations. These relaxation processes are of utmost importance, as they determine the mechanical properties of glassy polymers such as engineering thermoplastics, for example the ductility of polycarbonate;
- protein-lipid organisation, including the structure of proteins in membranes and of other molecular constituents. Questions that can be addressed include the global shape of membrane proteins, the arrangements of various elements of the structure, the location of individual amino acids and the association of membrane proteins with other molecules within and near the membrane;
- detailed studies of the interfacial behaviour of block copolymers will improve our ability to tailor the interfacial structures to deliver particular interfacial properties. Examples of relevance include thin film polymer forms such as resistors and device packaging and the optimisation of practical coating processes from solutions and latices;
- studies of composition and structure of surfactant mixtures at interfaces will improve our ability to quantitatively model surfactant adsorption (with clear applications to detergency and anti-corrosion) and to predict the composition of complex surfactant mixtures at interfaces;
- improved understanding of polymer adhesion, including the advantageous or deleterious effects of additives or chemical action. In composite materials, knowing the chain arrangement close to the interface between a polymer and non-polymer will help us understand many of the most important properties of such composites;
- reflection and off-specular studies of flowing surfaces and boundaries of sheared surfactant/polymer systems. Such work will lead to improved understanding in important areas of engineering practice such as hydrodynamic lubrication and the behaviour of boundary lubricants at interfaces;
- the structural arrangements of liquid crystals at substrate surfaces. These have a significant bearing on the understanding of display devices. For example, simple specular reflection at the solid/alignment layer/liquid interface will determine the penetration of liquid into the alignment layer and glancing angle diffraction will observe the smectic layers as they are truncated by the surface;
- through the use of labelled compounds and appropriate time-slicing, new information will be obtained on the hydrodynamics of film drainage in thin foam films in air, or between liquid phases;
- the interfacial organisation of copolymers that are used at liquid-liquid interfaces for emulsion stabilisation, liquid-liquid extraction, and liquid homogenisation.

Interfacial properties of surfactants and polymers

This is a vast and rapidly-growing field, in which all aspects of disordered and semi-ordered interfaces have been opened up to study by specular and off-specular reflection. Langmuir-Blodgett films have been studied for many years. However, future work will be directed at unravelling the surface behaviour of complex molecules such as polyelectrolytes, biomolecules, liquid crystal polymers and molecules with specific functions such as chromophores.

The high flux of the ESS will enable the study of more complex systems through contrast variation methods. Furthermore, the fact that measurements will be possible in a few seconds will allow data to be taken as a function of surface pressure at realistic compression rates, rather than the present necessity to hold a certain pressure for times during which relaxation and dissolution processes can make the interpretation of results unclear or erroneous.

Off-specular scattering, with the advantages of isotope labelling, is likely to become the method of choice for determining the long and short range in-plane structure. For example, the intermolecular distances and the segregation of species into patches in a mixed monolayer could be measured. The degree of scrambling of the layers in non centro-symmetric organic multilayers as a function of distance from the substrate surface may enable the improvement of electro-optic or ferroelectric properties of the systems.

Improving the performance of biosensors requires an understanding of the adsorption/penetration of a solute at a deposited mono- or multilayer, which may contain an immobilised protein. The degree of penetration of the solvent and solute will be measurable, as will the distribution of any immobilised guest molecules in the film. The use of small samples will make a major impact, removing the sometimes insurmountable problem of preparing large uniform samples. Complementary experiments with synchrotron radiation, in spectroscopy, and by electrochemical methods will thus become more informative.

The use of small samples will make a major impact, as difficulties associated with preparing large uniform samples can present sometimes an insurmountable problem. Complementary experiments with synchrotron radiation, spectroscopy, and electrochemical experiments will thus become more informative.

Spread monolayers can act as templates for solute adsorption at an interface, a technologically very important area for which neutron reflection and off-specular scattering can provide the ideal investigative tools. Areas of immediate interest include gaining an insight into the early stages of biomineralisation, probing the early stages of surface fouling in developing biocompatible surfaces, and the building up of self-assembling multilayers as an alternative to Langmuir-Blodgett deposition. Studies will be possible on the spread lipid monolayers used to mimic a cell membrane and its interactions with surrounding proteins and nucleic acids. Off-specular scattering allied to contrast variation will clarify the in-plane organisation of the different components. Transverse and in-plane fluctuations in lipids and proteins in membranes – central to a large part of the biological function of these materials – will also become accessible.

Electrochemistry and electrode processes

In situ studies of electrochemical processes and the electrode surface will yield important structural information relating to transport and reactivity parameters on the short time scales appropriate to these processes. These measurements are presently possible only on long time scales. Lateral inhomogeneity measurements will give insight into the nature of homogeneous deposits and rough surfaces, as found in 'real' electrochemical applications. The ESS will be able to provide the dynamic structural information which will throw light on the poorly-understood time variation of electrode activity, giving information that will be both vital and unique, and complementary to that from spectroscopic probes. In situ polymerisation at electrode surfaces, and the structure and dynamics of in situ polymer layers at an electrochemical interface, will also be accessible.

Disordered materials

Disordered materials, which include liquids, glasses, and disordered crystalline matter, play a central part in our daily life. Water covers two thirds of the Earth's surface and is a major component of our bodies and the food we eat. Glasses are in our windows, in optical fibres for communications, used for stable coatings on medicines, and even eaten as candy. Ionic conductors are in batteries in cars (electric cars in the future), mobile telephones and computers. Most of materials science is concerned with the control of materials' properties through defects or disorder of various kinds, yet our understanding of disorder is still inadequate.

The study of disordered materials often requires techniques that are optimised differently from those for well-ordered crystalline materials, and the specific advantages of neutron scattering have made it one of the most important of the available methods. As neutron sources and instrumentation have developed, studies have moved from simple 'model' systems towards more complex 'real' systems, especially those with technological applications. A central aim is to improve our understanding of how the structure and dynamics of disordered materials, and their relationship to the fundamental interatomic interactions, control properties relevant to an application. As we increasingly tackle the more complex systems of modern materials science, we need to obtain structural and dynamic information over a wide range of parameters such as temperature, pressure, electric, or magnetic field, and with more element specific information. Moreover, for disorder studies to be useful requires accurate and precise measurements of weak, diffuse scattering, which becomes an increasing challenge as system complexity increases. The ESS will provide the neutron resources these requirements demand if the particularly powerful neutron techniques are to be fully exploited together with the relevant complementary techniques such as NMR, third generation synchrotron sources, and computer modelling.

Achievements in disordered materials using neutrons

- Neutrons have provided much of our basic understanding of both single particle motions and collective modes in simple liquids, neither of which could be explained by theory developed for crystals.
- Our knowledge of the detailed structures of binary liquid metals and molten salts has come from exploiting isotope substitution. This has led to, for example, an understanding of charge ordering in ionic liquids.
- Isotope difference work on ionic solutions has quantified solvation geometries directly, showing that tables of solvation numbers in text books were often totally wrong.
- Almost all our knowledge of structures of metallic alloy glasses comes from neutron isotope substitution work, which has led to important ideas on the role of concentration fluctuations in structural ordering.
- Neutron measurements on network glasses have confirmed Zacharaisen's random network model.
- Neutron scattering has been the most important technique in studies of the glass transition, particularly in testing the predictions of mode coupling theory.
- Techniques developed for simple liquid work have been extended to routine use in polymer studies and in biophysics.
- The simplicity of the neutron-nucleus interaction has led to neutron measurements having a major influence on theoretical developments. Examples include the development of memory function formalism. The development of mode coupling theory has spawned a whole new area of research into the glass transition, of major applied as well as fundamental importance.
- Neutrons have similarly played a central role in the development of computer simulation techniques now used widely from fundamental physics and chemistry to biology. The potentials used in simulations are almost always validated by comparison with neutron scattering data.

In disorder studies, the ESS offers major advances in, amongst others, the following key areas.

Interactions in solution: 'liquid state crystallography'

Through the exploitation of the isotope substitution difference technique, neutrons are unique in enabling us to essentially characterise fully the structures of solutions, by giving us access to the three structural correlations (solute-solute, solute-solvent, and solvent-solvent). Moreover, in appropriately chosen systems, we can perform important measurements in solutions of arbitrary complexity. Building on the pioneering work on ionic aqueous solutions, (which revolutionised our understanding of electrolytes), we can now look at more subtle effects in solutions of polar, charged, and apolar molecules that are of fundamental importance in much of chemistry, biology, and biotechnology. Present experiments, however, despite the useful information we have obtained, are really only demonstrations: to solve the underlying problems – e.g. the nature of the hydrophobic interaction, the physical basis of the Hofmeister series, the effect of protein stabilisers or denaturants on solvation shells of particular chemical groups on the protein, or even the basic phenomenon of solubility which is still poorly understood - we need to study liquid structures as functions of temperature, pressure, concentration and solvent variation (e.g. added ions), and work at lower concentrations. Only with ESS do we have this capability. In addition to its fundamental importance in chemistry and biology, this work has major potential to influence developments in biotechnology and food science. A whole new area of interactions in non-aqueous solutions can be opened up. A particularly exciting possibility is the knowledge-based design of aqueous solvents to replace non-aqueous ones used in existing processes, with clear advantages to energy-use efficiency and environmental pollution minimisation.

Disorder in crystals

Disorder can be crucial in determining the properties of technologically important materials, for example high temperature superconductors. Stimulated by instrumentation developments allied to the parallel development of appropriate computer modelling techniques, neutron studies in crystalline powders are beginning to make a strong impact. However, the experimental requirements are severe, as the diffuse scattering contribution that is the focus of the studies may be very small, so high absolute accuracy is essential. To extend the approach beyond the few demonstration experiments that have recently been performed, a source with the power of ESS is essential.

The examples are legion. (a) Accurate disorder studies will be possible of those real (as opposed to simple model) crystalline fast ion conductors that are candidates for applications such as fuel cell electrodes and sensors. For example, $La(Sr)MnO_3$ is an oxide conductor at high temperatures, of interest in fuel cells. It is also a giant magnetoresistant material at low temperatures, where it is of interest for magnetic recording devices. The complexity of such materials requires their study as functions of composition, different dopants etc., and under specific conditions (e.g. high temperature, applied voltage). Crystallographic information will need to be correlated with local structure and diffuse scattering information for multi-phase samples. The high penetration of neutrons will enable these studies under operating conditions. (b) High quality disorder studies will become possible on new ceramic materials, most of which contain both crystalline (sometimes more than one) and 'amorphous' phases, and for which the material strength can depend not only on controlling the amount of amorphous component, but also on the preparative technique used to effect this control. ESS will make it possible to probe these important structure-property relationships, particularly under operating conditions, for example Si_3N_4 ceramics for coatings in future car engines. (c) The ability to study much smaller samples than is presently possible will facilitate major advances in our understanding of melting and freezing, through diffuse scattering studies of short range order/ disorder. Combined neutron diffraction/EXAFS studies will be potentially important in studies such as local melting around impurities in bulk materials.

Neutron Brillouin scattering

The whole area of neutron Brillouin scattering will be opened up, resulting in major improvements in our understanding of the dynamics of liquids, glasses, and polymers in the region intermediate between the microscopic and the macroscopic. It will allow us to probe time dependent systems that are too fast for real time small angle neutron scattering and spin echo spectroscopy. Examples range from fundamental systems such as the dispersion of collective modes in liquids with a high sound velocity (e.g. Li), to those of applied importance such as the slow dynamics of phase separation, polymeric and large molecule liquid dynamics and combustion processes in the transition regime between hydrodynamics and microscopic dynamics. The recent entry into this area of third generation synchrotron sources is already demonstrating the power of the complementarity of neutron and X-ray techniques by their jointly giving information on second order correlations of the conduction electrons that seems inaccessible in any other way.

Interfacial studies of liquids and amorphous materials

Wide Q range reflectivity studies of liquids and amorphous materials at interfaces will be opened up. Ordering at liquid metal surfaces will be accessible, where neutrons have advantages in studying surface segregation in liquid metal alloys. Complementary – perhaps even simultaneous – studies with X-rays could be very powerful. Molecular orientation and the local density profile at the liquid/vapour interface for molecular systems could be studied, as could diffusion or ion conduction at interfaces, e.g. between an electrode and electrolyte in a battery or fuel cell. Detailed studies of fluids near a solid substrate will be possible, for example surface critical phenomena (among which are wetting and pre-wetting transitions) and surface layering – an example being the study of wetting in binary fluid mixtures such as fluid alkali metal/alkali halide systems.

The ESS will also result in new scientific achievements in the following areas of science and technology relevant to liquids, glasses, and disordered materials

- High energy resolution, wide energy range studies of the liquid-glass transition of 'strong' glass formers, where the time scales of the two main relaxation processes are not similar, will become possible as a function of temperature. Isotopic substitution studies should help to clarify the origin of the 'boson' peaks in the density of states. Discrimination between different models for the relaxation processes will be possible by decoupling temperature and density effects through pressure variation studies.
- Studies of the strong effects of network modifiers on network glass properties will be extendable to more realistic complex systems using smaller isotopic differences (hence extending the modifiers whose influences can be studied), and working at smaller modifier concentrations. Studies of (four or five component) glasses with increasing technological applications will be opened up (often in conjunction with other complementary techniques), including doped glasses for optical fibres, pressure or magnetic sensors.
- *In situ* studies of glass formation using sol-gel techniques, sometimes as thin films, offer possibilities for preparing glasses with tailor-made properties by control of the fabrication process.
- Detailed structural studies of glasses whose electrical properties change on doping (e.g. doped chalcogenide glasses such as Ag in GeS_2) will improve our ability to develop the electronic application of such materials as photosensors.
- New types of amorphous thin films, e.g. 'diamond-like' hydrogenated carbon, have very favourable physical properties such as hardness and chemical inertness. Through the ability to work with smaller samples and isotopic differences, an improved microscopic-level understanding of these properties will be obtained.
- Real progress will be possible in our ability to distinguish the different vibrational modes in network glasses. Isotopic substitutions will enable the selective identification of modes.
- Glasses prepared over a wide range of porosities can have specific commercial applications. The *in situ* studies that are needed, if we are to control the porosity and tailor it for specific applications, will be possible.
- In metallic glasses, sufficiently accurate structural data will be accessible to probe how preparation or subsequent treatment affects variation in properties, e.g. anisotropy, which can have major effects on e.g. magnetic properties. We will also be able to perform rapid characterisation of the wider range of glasses that can be produced by new methods such as ball milling and solid state amorphisation.
- Polarisation analysis, the combination of neutron and X-ray methods, and computer modelling, will properly open up magnetism in glasses for the first time, including small samples such as thin films where the technological emphasis is likely to be. For example, the cross-over between short-range and domain ordering which may be crucial for macroscopic properties can be studied.
- Structural and dynamical measurements over the complex phase diagram of ion-conducting glasses such as $(AgI)(Ag_2O)(B_2O_3)$ will become feasible. These systems offer the prospect of high ionic conductivity with improved magnetic properties, for use in e.g. batteries or fuel cells.

- Ion-conducting polymers – of considerable future importance for e.g. lightweight batteries, electric cars, smart windows – tend to be complex polymers with additives. Structurally, they involve length scales from 1 to 1000Å, while dynamically there are relevant motions over times scales from 10^{-12} to 1 s. The information required over these wide ranges and at suitable accuracy is not available on present sources in reasonable times.

- Structural and dynamical studies across phase diagrams of simple liquids, including the low density regions, will be accessible. No simple liquid has been studied in such detail, yet there are fundamental phenomena we do not fully understand, such as those close to the critical point – for example, why is there a metal-insulator transition in liquid metals close to T c ?

- Accurate scattering measurements in the low Q region (0.05-0.5$Å^{-1}$) that will be possible for the first time will give directly the long-range terms in the two-body interaction potentials, while the constant-temperature pressure derivative of the scattering will yield the three-body terms.

- High accuracy measurements as functions of pressure and temperature will enable us to unravel the complex bonding behaviour in liquids such as S, P, Se, Te, and As.

- The determination of electron distributions in disordered systems will be possible by combining precise neutron and X-ray data from ESS and ESRF, with major applications both in materials and fundamental studies (e.g. the nature of the Mott transition).

- Structural studies of three and four component molten salts will be relevant in chemical processing (e.g. electrolytic production of aluminium; radioactive waste treatment) or for future accelerator-driven sub-critical power reactors. Related structural work on e.g. oxides and sulphides requiring higher temperatures and *in situ* studies of molten salt electrochemistry will be facilitated.

- Pressure and temperature variation studies of those – often complex – liquid systems showing behaviour intermediate between metals (electronic conductors) and salts (ionic conductors) are needed to relate the microscopic structure and dynamics with the macroscopic electronic/ionic conductivity.

- Through measuring partial dynamical structure factors, the collective dynamics of multicomponent liquids can be tackled and suitable potentials derived in conjunction with molecular dynamics calculations.

- Progress in understanding the dynamics of molecular liquids (water being an important example) will be made through high resolution dynamical structure factor measurements over a wide energy range.

- Two particular areas of work on liquid crystals will become accessible, namely (i) molecular flexibility and its role in the formation of thermotropic liquid crystals and liquid crystal polymers, and (ii) the distribution of molecular orientations and the correlation of the orientations of neighbouring molecules. There will also be significant benefit to studies of aligned liquid crystals samples.

- Structural and dynamical measurements will become possible on complex proton conductors (for e.g. batteries, fuel cells) and hydrogen storage materials which have low hydrogen concentrations.

- We will be able to exploit the recoil atom in the deep inelastic neutron scattering method as a probe of the local environment. The technique could study fundamental problems such as the level of quantum effects in simple monatomic fluids, and quantum effects in simple molecular liquids (e.g. ortho- and para-hydrogen). Hydrogen sites and hydrogen content could be identified in metals (hydrogen storage), as could hydrogen-bonding in semiconductors (e.g. silicon for solar cells, carbon for ultra-hard coatings).

Structural materials chemistry

In modern society, new functional and structural materials and the objects and devices made from them, play an increasingly important role. Obvious examples include ceramics and composites, magnetic and electro-optical materials, catalysts and chips. New materials for health include pharmaceuticals and bio-compatible materials for implants, while for energy storage, improved batteries are being developed. In addition to synthesis and property tailoring, understanding of behaviour under life-conditions and degradation is increasingly required for safety, recycling, and pollution control. Today, we need to understand the behaviour of a material, not from *cradle* to grave, but to the *cradle* of its next incarnation.

The understanding of the exploited properties of new materials requires a knowledge of their structures, together with the mechanisms of possible interaction with their operating environment. Neutron scattering has played a principal role in developing this understanding in almost every area of the modern structural chemistry which is central to new materials development and characterisation (see box). Topics ranging from catalysis to magnetism[7] and from battery materials to superconductivity have been profoundly advanced as a result of detailed structural insights gained from neutron diffraction.

Achievements in structural materials chemistry using neutrons

- Underpinning the global research effort in high temperature superconductivity by initial structure determinations and subsequent detailed structural investigations. Of particular importance has been the demonstration of the charge transfer concept of hole doping with oxidation, and that the superconducting temperature was related to the evolution of structural order.
- Providing through the Rietveld technique the most accurate, reliable, and complete refined structures from powder diffraction data.
- Time resolved studies of formation (e.g. of high temperature superconductors under hot zoning conditions), ageing (e.g. Mg-stabilised zirconia ceramics), and operation (e.g. *in situ* discharge of alkaline batteries) of functional materials.
- Structural studies of bulk samples under extreme conditions (e.g. high temperature, high pressure, in catalytic reactors).
- Together with X-rays, characterisation of host-guest interactions in e.g. zeolites.
- Nearly all that is known about magnetic structure is based on neutron diffraction data, for example demonstration of the NÈel model, the wide variety of incommensurate structures that include spirals, fans, and cycloids, and asymmetric magnetisation.
- In combination with X-rays, determination of charge distributions that are essential for understanding some of the most profound details of a crystal structure, for example the effects of charge transfer, magnetostriction, and the onset of superconductivity.
- In molecular compounds, the most definitive answers to structural problems, especially (i) accurate positional parameters of all atoms; (ii) accurate determination of thermal motion; (iii) structures in which hydrogen bonding plays a major role (e.g. ferroelectrics, hydrides, and hydrates, including the role of water in biomolecular systems).
- Structure, disorder, and phase transitions in fullerenes and their derivatives.

At the frontier of synthetic chemistry and materials science is the creation of new materials by rational design. As evidenced by the drive to higher temperature superconductors, these new materials are becoming increasingly complex, and are – at least in the initial development stage where structural characterisation is essential – usually produced in only small quantities. Required behaviour also increasingly depends on subtle effects in these materials. Furthermore, the increasing need to follow changes in structures under extreme conditions (e.g. pressure, temperature) and over the short times of chemical or phase transformations, requires high quality structural data on small, complex systems over short times. The increasingly severe demands placed on experimental techniques by these trends can be met by ESS instruments, which will provide the core means for understanding in detail the birth, life, and rebirth of the many new materials that are being developed to meet present and future materials performance challenges. The advantages of neutrons in accurate crystallographic studies (see pages 102-106) will be essential to meeting these challenges effectively.

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[7] Magnetic structures in crystalline materials are considered in more detail on page 88.

The following key areas show some of the major advances that will be possible with the ESS that make specific use of the advantages of neutron techniques.

In situ and rapid real-time measurements of structural changes

Time resolved experiments are necessary if we are to follow chemical kinetics, solid state reactions, phase transitions, and chemical reactions in general. An example of importance is charge/discharge processes in batteries. However, with the trend towards more complex materials, combined with the synthesis of smaller samples, we are reaching the limits of what is currently possible. ESS will take us over this threshold. It will enable us to parametrise subtle structural distortions with temperature or pressure, and obtain detailed microstructural information as external conditions are changed. ESS instruments will be able to deal with milligram quantities of synthesised material and systems in which the component of interest may be present in only dilute amounts.

Rapid real time structural measurements – sometimes in conjunction (possibly simultaneously) with complementary techniques – will follow in real time the kinetics of phase transitions, chemical reactions, and relaxational phenomena, with time slices as small as seconds or less. Examples include high resolution characterisation of structural changes under gases that are important for optimising chemical processes (with applications to catalysis, conducting materials, and sensors), chemical kinetic processes during solid state synthesis and the bulk response of complex composite materials to changes in physical or chemical environment.

The ESS will also result in new scientific achievements in the following areas in structural materials chemistry

- The precise determination of tiny structural changes under variable temperatures, pressures, and applied fields or accompanying e.g. electronic transitions, and the precise determination of subtle magnetic changes that accompany structural distortions. Examples range from colossal magnetoresistance materials and spin-Peierls systems to metal-organic molecular conductors
- Structures of fundamental systems such as quasicrystals and incommensurate structures from smaller and hence more homogeneous samples, including the temperature dependence of the modulation wave vectors.
- Precise line shapes studies of changes in secondary order parameters (e.g. microstrains) accompanying phase transitions, and critical scattering.
- Structural studies of *intrinsically* small systems, for example of a surface, or of a grain boundary, or where intrinsic sample inhomogeneity requires characterisation of sub-millimeter compositional variations in a superconductor or concentration gradients in a chemical cell. Studies on very small magnetic single domain crystals (well below 0.01 mm^3), will yield unambiguous magnetic structures, for example in magnetoelectric single domain crystals.
- Structural studies of samples available only in very small quantities, e.g. due to exotic or difficult synthesis conditions. Examples of the latter include determining the cation distribution in diluted magnetic semiconductors and small crystal co-ordination chemistry studies on, for example, the nature of the metal-hydrogen interaction, work which is important in mapping the reaction path in catalytic hydrogenation and in exploiting weak metal-hydrogen interactions in molecular engineering.
- Measurement under higher pressures (up to 100 GPa) than presently accessible, often on smaller samples, will open new frontiers in solid state high pressure research. For example, in studies of the important metal-insulator transition, the possibility that the magnetic transitions observed in nickelates at 30 and 55 GPa might be the sign of the progressive closing of a charge transfer gap could be tested.

Not only will *in situ* structure determination over multidimensional phase diagrams be possible (e.g. as a function of temperature, pressure or atmosphere), but these can be performed simultaneously with measurements of electrical, thermal or magnetic performance. The application to product synthesis, operation and processing is clear. In situ structural studies of reactions on surfaces – possibly combined with neutron spectroscopic studies – will throw detailed light on existing and novel catalytic processes. Rapid ordering of, for example, oxygen vacancies in response to pulsed electric or magnetic fields, can be followed.

Structural studies of complex materials

The high resolution capability of ESS instruments will take powder neutron studies into a new regime of complexity, giving us a major tool for the accurate structure refinement of the complex new materials that are continually being developed at the frontier of materials science. Examples include subtle solid solutions created to give oxide ceramics optimised properties, self assembling structures with sophisticated topologies and heterogeneous nanoscale structures with attractive technological properties. Subtle structural distortions can be parametrised as a function of temperature and pressure, differences between local and average structures characterised and detailed microstructural information obtained in conjunction with average crystal structure.

Chemical reactivity and molecular motions

Vibrational spectroscopy is a frequently-used technique in both fundamental and applied research. It has already achieved important results across *chemistry* (e.g. organic, mineral, metals, surfaces, hydrides, organometallic, polymers, materials, conductors, catalysts...), *physics* (e.g. vibrational density of states, phase transitions, superconductors, bulk and cluster magnetism, mechanical properties of solids) and *biology* (hydrogen bonds, dynamics in small molecules, water, polypeptides, DNA bases, drugs).

The neutron technique is complementary to optical (infrared and Raman) techniques, providing new results that allow a better understanding, and consequently more effective use of, infrared and Raman. Vibrational frequencies depend on chemical bonds linking atoms, and on interactions between molecules, while intensities depend on interactions between the incident radiation (optical) or particles (neutrons) and the sample. For optical spectroscopy, reliable use of the intensities is problematic, as they are related to quantities that are uncertain (derivatives of dipole moment or components of the polarisability tensor). In contrast, the simplicity of the neutron-nucleus interaction means intensities derived from neutron vibrational spectroscopy can be fully and effectively exploited. Moreover, measurement of spectra over a broad range of energy and momentum transfer also gives important spatial information on the vibrational wave functions. Exploiting these advantages, major achievements have been made by the technique that are of both fundamental and applied interest (see box p.73).

Neutron spectroscopy to date has been limited, because of beam intensities, by the size of sample required to obtain an adequate spectrum, and by the resolution achievable being lower than the optical techniques. ESS offers large flux and significant resolution improvements that will compensate these limitations, and thus allow major development of the field and its application. For example, data collection time reductions from several hours to 1-2 minutes will dramatically widen the availability and applicability of the technique, with major results for both fundamental science and applied areas such as in situ catalysis studies. Many outstanding fundamental problems will become tractable and new fields of investigation opened. More complicated spectra will be resolvable and larger molecules such as fullerenes, and the binding of therapeutic biomolecules, will be more effectively analysed. Band-shape analysis at higher momentum and energy transfers will allow us to investigate the dynamics of molecules in their excited states. Weak features of non-hydrogen atoms, internal vibrations of matrix-isolated species, samples under very high pressure in anvil cells, and new protonic species will become observable. Spectra of weak coherent scatterers will provide further information on vibrational dynamics that has been little exploited so far.

The following key areas of vibrational spectroscopy are among those that will benefit particularly from the ESS.

Fundamentals of atomic and molecular interactions

Major advances will be made in our understanding of the fundamental forces that hold atoms and molecules together. It is these force fields that control the behaviour of molecules, yet they are still far from being understood. We will be able to measure data of sufficient quality on simple systems to obtain force-fields by refinement of the data against a model in a way similar to Rietveld refinement of crystal structures. Such a development would result in a revolution in vibrational spectroscopy of the same order as that brought about in powder crystallography by Rietveld methods. A particularly attractive prospect is the possibility of being able to obtain specific information on electron dynamics from *photon minus neutron maps*, in a way similar to the static electron densities we can now derive from *X-ray minus neutron maps*.

We will be able to begin to address problems on larger, more complex, less symmetrical systems. In the biomedical field, this would include studies of e.g. anti-tumour and other drugs whose binding is believed to be mediated through hydrogen motions. Industrial interest would be found in the consequent ability to study surface interactions of real feedstock molecules rather than the model systems that are the present focus of study. ESS will liberate neutron vibrational spectroscopy from being limited to high cross-section studies, e.g. hydrogen. This consequent ability to tackle non-hydrogenous systems will open up a whole vast, relevant area of inorganic chemistry and its applications, including carbide and oxide systems. In network glasses, it may be possible to see the weak features which will enable us to understand, for the first time, the complex dynamics of these commercially important systems.

Achievements of neutron chemical spectroscopy

- The state of the majority of adsorbed hydrogen on the hydrodesulphurisation catalyst MoS_2 was determined to be molecular, not atomic.
- The local organisation of the reactive molecular species of benzene on a nickel surface was determined. The benzene remains some 85% associated, lying parallel to and about 2.5Å away from the surface.
- The local diffusion of molecules through solids, such as zeolites, can be followed by neutrons where other methods either fail or are inappropriate.
- The simultaneous determination of structure and dynamics of a chemical species in preparation enables unstable reaction trajectories to be characterised in great detail.
- Neutron spectroscopy has assisted crystallography in locating hydrogens away from the points of high symmetry where crystallography had previously placed them.
- The observation of solitons in solids and the demonstration of all the expected, but previously not observed, properties.
- Determination of densities of vibrational states across the whole fundamental vibrational range has demonstrated the importance of low frequency modes in easing bulk displacements in motions in polymers (reptation), and in the diffusion of bulky molecules in zeolites.

Vibrational dynamics on surfaces: catalysis

As inelastic incoherent scattering sees hydrogen most clearly, neutron spectroscopy has, to date, tended to concentrate on hydrogen-containing systems. The adsorbed species can be identified and their geometry and strength of bonding at the surface ascertained, without many of the background, absorption, decomposition or fluorescence problems that limit IR or Raman studies. Thus, new information has been obtained on catalysis studies involving hydrogen, for example in determining unambiguously the form of hydrogen (molecular or atomic) active during catalysis. ESS will extend this powerful approach to important non-hydrogen systems, for example to follow the vibrational dynamics of CO, an important reagent and good optical probe on surfaces, during a chemical process. Other chemically and environmentally-important surface processes would also be accessible, such as those involving N_2, O_2, NO, SO_2, and CO_2, including NO_x emissions handling and more efficient desulphurisation techniques.

The ESS intensity can also be exploited by studying the behaviour of new catalysts where the concentrations of hydrogen on the surfaces are small, for example low hydrogen loadings on oxide supported metal catalysts down to sub-monolayer coverage. The origin – and hence the minimisation – of contamination from 'spill-over' of reagents from the active part of the catalyst to the support can be tackled; a problem which is difficult for optical spectroscopy. Real-time kinetics of existing and new catalytic reactions can be studied for optimisation of these processes. This work has particular applications in, for example, post-combustion automotive and fuel cell catalysts.

Chemical reactions at general interfaces

The ESS intensity will mean that chemical reactions in samples as thin as 3 µm will be accessible. We will thus be able to follow processes in buried interfaces such as a glue attached to its binding surface and curing, for example carbon-fibre/resin composite surfaces. The penetrating power of neutrons will also make neutron techniques superior to optical ones in optically opaque systems: understanding the complex changes that occur when a paint dries is an industrially and environmentally important example. ESS will also open up the new filed of inelastic/quasielastic neutron scattering, in which the dynamics of a molecule excited into a specific state can be followed as a probe of the molecule-environment interaction. Thus the way in which specific vibrational distortions change the rotational dynamics, for example of a solute in solution, can be determined. This process is perhaps akin to working under an external pressure perturbation, the difference being that the perturbation here is anisotropic and the 'pressure' is generated internally and at the specific site of interest. Combining this technique with isotope substitution offers a vast range of possibilities.

Rotational tunnelling spectroscopy

ESS will facilitate major advances in both the understanding and specific exploitation of rotational tunnelling spectroscopy. More dilute samples and weaker scatterers can be studied, more fine structure will be resolvable for the tunnelling bands and lower frequency tunnelling transitions will be observable. Present conflicts between dynamical models relating to coupling of rotors are likely to be resolved and insight into the quantum to classical transition gained. This is a major interest by quantum theorists. The tunnel splitting of excited modes should also be measurable, particularly when used in conjunction with the recently developed single crystal techniques. Again, the observation of tunnelling in deuterated compounds – just observable in ideal cases presently – should become routine with the improved signal to noise of ESS instruments. In addition to the importance of this work in fundamental studies, significant advances to applications will be possible, for example in understanding the rotational dynamics of hydrogen molecules in organometallic complexes with its potential impact on our understanding of homogeneous catalysis. Simultaneous studies of structure and dynamics of complex samples, and their transformations under changed external conditions (e.g. in intercalates and clathrates) are just possible now; the intensity of ESS will be needed to exploit the power of the approach, for example, in studies relevant to waste management.

The ESS will also result in new scientific achievements in the following areas in chemical spectroscopy

- Fast data collection immediately opens up the power of neutron vibrational spectroscopy to the growing materials science area. Although critical information such as local chemical bonding in amorphous systems is easily available from the technique, beam time limitations simply prevent this powerful tool's exploitation in materials development.

- 'Localised chemistry' will become a viable field of study. For example, we will be able to study corrosion at the head of cracks.

- Chemical processes and force field studies will be possible up to 200 kbar, and under applied electric field. Neutrons are the most sensitive technique for determining often large off-diagonal terms in the dynamical matrix, and pressure gives us much needed additional flexibility in such studies, e.g. in work on plastics.

- The dynamics of quasicrystals will become accessible. The high resolution of ESS will enable the exploration of the larger number of critical points expected to result from the higher dimensionality of the vibrational force field.

- Reaction kinetics will be followed with characteristic times of seconds. Examples include adsorption into/onto metals and electrochemically active oxides.

- Study of local environments of a specific chemical group via perturbation of the vibrational spectrum will become possible, with obvious applications in catalysis. At low Q values, we will be able to follow changes in rotational and translational dynamics of a chosen group (e.g. methyl) as it moves. Furthermore, as the change in band width at higher Q will be related to states of agglomeration, we will be able to use the technique to follow changes such as the build-up of a monolayer on a surface, or changes in intermolecular couplings.

- A major improvement will be possible in our understanding of proton transfer, including proton tunnelling, of central importance in much of chemistry, physics, and biology. ESS will enable the experimental work that is needed to reconcile the conflict between recent observations of tunnelling transitions and conventional models. The very small tunnel splittings of upper excited states – very informative of the shape of a potential – will be accessible on ESS.

- Determination of concentrations and kinetic energies of hydrogen at very low concentrations using neutron Compton scattering. This has major materials applications in protonic conductors, metal hydrides, and catalysis. Extension to other impurities such as boron, nitrogen and oxygen has materials relevance, e.g. in metal embrittlement.

- Protonic species – some of them new – have been found in protonic conductors, such as $(H^+)_4$ near Mn^{4+} vacancies in γ-MnO_2 , and H_3O^+ in hydrated β-alumina. ESS will enable the characterisation of these, and other yet-to-be-identified, low-concentration mobile charge-carrying entities.

- Measurements of coherent scattering, presently marginal, will become a major area of study. This work will tell us the phase relationships an atom has with its neighbours, and give direct access to off-diagonal terms in the dynamical matrix. This work has very high potential in glassy systems.

Biology and biotechnology

The exploitation of neutrons in biological problems has been severely limited by the inadequate flux of even the most powerful existing sources. Nevertheless, neutron scattering has played a significant role over the past 20 years in our understanding of the structure and dynamics, and hence the functioning, of biological macromolecules (see box). Work has aimed at understanding both *general principles* of the physical chemistry of macromolecules, for example the general characteristics of internal motions in macromolecules and macromolecular assemblies such as model membranes, and *specific biological systems* such as the light-driven proton pump bacteriorhodopsin, or the mode of interaction of the chaperonin GroEl with its substrate partially-folded proteins.

Achievements of neutrons in biological science and technology

- The positioning of all the 21 proteins in the 30S subunit of the ribosome of *E. coli*, as well as the general arrangement of protein relative to RNA. Structural information has also been obtained on the HIV-1 reverse transcriptase sub-unit arrangement, and the spatial arrangement of *E. coli* RNA polymerase bound to DNA with and without transcription factors.

- Determination of function-critical hydrogen positions in enzymes, for example that in the catalytic triad of trypsin. Accessibility of labile hydrogens in different parts of lysozyme and other proteins. Orientations of ring systems and methyl rotors.

- Determination of solvent organisation in proteins and other biomolecular systems at room and low temperatures. This work has rationalised, for the first time, the factors apparently controlling water orientations at biomolecular interfaces.

- Determination of protein-DNA distribution in the nucleosome and of the RNA, protein, and lipid distribution in spherical viruses.

- Unique information has been obtained on solvent interactions in tRNA and halophilic proteins, and on detergent interactions with membrane proteins.

- Determination of water levels in different parts of starch granules, leading to a deeper understanding of the gelatinisation process.

- Characterisation of the large amplitude internal motions in small proteins, and of a dynamical transition that is correlated with function in bacteriorhodopsin.

- Determination of phospholipid multilayer structure by selective deuteration. Studies of motional processes in the bilayer have provided the basis for our present view of the bilayer as a dynamically rough and extremely soft surface.

- Characterisation of adsorbed protein single and multilayers at the air/water and oil/water interface.

- Determination of the protein-detergent distribution in membrane protein crystals, and the localisation of lipid in a lipoprotein.

- Structural information on the purple membrane, including hydration properties, localisation of the retinal chromophore in bacteriorhodopsin, the positions of specific (-helices and the structure of trapped intermediates in the bacteriorhodopsin photocycle.

Molecular biology requires systematic studies over a large range of similar molecules and of different conditions. For much of biology, it is the small differences between closely-related systems which are of importance. The large increase in flux of ESS will make such systematic studies possible for the first time, enabling molecular biology and biotechnology to begin to take a fuller advantage of the power of the neutron probe. For example, molecular cell biology will be a major growth area in the coming decades, and one that is of high relevance to both wealth creation though biotechnology and the quality of life through health engineering. A battery of methods, including neutron scattering, will be required to understand the functioning of the cell at the molecular level. This understanding is vital in our ability to control disease, improve materials and preserve our natural environment for future generations.

Key areas where the ESS will result in significant progress include the following.

Macromolecular complexes: protein-nucleic acid interactions

Cellular processes depend on interaction between large numbers of macromolecules. Such assemblies range from simple pairs (e.g. transcription factor-DNA) to large complexes with many components (e.g. signal recognition particle, transcription complexes). We need to determine the structures of such complexes, and their assembly, if we are to understand how they work. Solving such problems will require a wide spectrum of structural methods, of which neutron methods will be particularly important. For example, small angle neutron scattering (SANS) will be able to detect conformational changes upon complexation, explore stoichiometry under different solvent conditions and study kinetics. Low resolution structural information using contrast variation could provide the information needed to put together high resolution structural information gained from NMR or X-rays into a model for the complete complex. A variety of molecular complexes, often quite labile, are continually being discovered – for example the signal recognition particle. These will require a high neutron flux to provide important structural information.

Low resolution neutron techniques have already been used successfully in the analysis of, inter alia, the internal *E. Coli* ribosome structure, the HIV-1 reverse transcriptase sub-unit arrangement and the spatial arrangement of *E. Coli* RNA polymerase bound to DNA with and without transcription factors. The number of components participating in such a process as transcription in eukaryotes is, however, much larger than in the above bacterial (prokaryotic) systems. ESS will enable us to apply these methods to large eukaryotic complexes such as the regulated transcription complex in eukaryotic cells. Furthermore, analysis of large protein-nucleic acid complexes will be possible, yielding results which will be important for understanding the mechanism of gene regulation, and processes such as cell development, and differentiation and de-differentiation in malignant cells.

ESS will allow us to move beyond static structure and to make kinetic measurements of proteins as they move along the DNA during RNA synthesis. An example is the translocation of DNA dependent RNA polymerase (which catalyses the transcription of the genetic information of DNA into RNA) along the DNA during RNA synthesis in real time. Static distance measurements have been successfully performed; kinetic distance measurements will be possible with the much higher neutron intensities of ESS.

The dynamics of macromolecular systems

Although we can learn much about how systems such as enzymes may operate from a knowledge of their structures, we need information on their motional properties if we are to understand fully their operation as the molecular machines they are. As well as understanding the principles that lead from sequence to structure ('the protein folding problem'), we need to understand also those that lead from structure to dynamics and function. The wide range of timescales over which this information is needed requires the use of an arsenal of physical techniques, of which neutron scattering is a central one.

As in other frontier areas of neutron scattering, the limitations of available sources have meant that the few exploratory measurements of protein dynamics have been made have been largely confined to determining general characteristics of dynamics. The next step is to examine a wider range of proteins and other macromolecules in order to determine if a diversity in internal motions might accompany the diversity of biological structures, for example by examining the dynamics of thermophilic or halophilic proteins, mutant proteins, partially folded proteins or proteins with substrates or inhibitors bound.

ESS will enable such dynamical measurements as functions of, for example, solvent, bound substrate and pressure, and will also open up the technique to a much wider range of systems. The study of the dynamics of different parts of the macromolecule through appropriate partial deuteration will allow us to focus on the active site or binding regions, or on the co-operative zippering or breathing motions of a part of a protein at transition temperatures. Complementarity with other techniques will also be exploitable more effectively. For example, X-ray diffuse scattering from protein crystals gives information on correlated displacements in and between protein molecules. Neutrons will be able to energy analyse the coherent diffuse scattering, and thus give information on the time and length scales of correlated motions between different unit cells and within proteins. The nanosecond timescale motions of different parts of macromolecules in solution will be accessible from coherent inelastic scattering using the spin echo technique that has been so successful in revolutionising our understanding of polymer dynamics.

Membrane function and biomembrane processes are closely related to lipid bilayer dynamics. Despite this, our knowledge here is still rudimentary, and sometimes contradictory. The dynamics is complex, being determined by a hierarchy of motional processes. ESS will give us access to the wide range of timescales involved. For example, the motion of parts of the lipid molecules (e.g. the head groups) may be filtered out, and motional processes at different time scales will be distinguishable (e.g. the chain dynamics from the lateral diffusion). Collective and molecular motional processes may be evaluated by simultaneous measurements with backscattering and/ or time-of-flight spectrometers and neutron spin echo instruments. In-plane and out-of-plane motional processes may be separated by variation of the scattering angle. Quasielastic measurements of highly oriented bilayer stacks at different hydrations could shed light on the question of why such stacks do not swell indefinitely under maximum hydration, and thus provide clues to the basic intermolecular forces acting between membranes. A particularly novel and attractive direction is the opening up of the slow time scale (~10^{-7}s) regime through the use of ultracold neutrons.

Food science and technology

These approaches are also applicable to the very large variety of industrially relevant problems in soft matter that involve lipid problems, for example in food science. Many potentially important experiments in food science and technology this field are currently flux-limited. With the high neutron flux of the ESS, many kinetic questions will be soluble for the first time. These include the kinetics of adsorption of proteins – an issue at the heart of food colloidal stability as well as relating to protein fouling during processing – and competitive interplay between small molecules and protein adsorption. Kinetics are at the heart of many food processing operations. Small angle neutron scattering will permit study of water redistribution within complex assemblies during unit operations. Additionally, high resolution structural studies will allow partial structure factors to be obtained with good accuracy for complex systems including glassy foods, for which the processing path may be significant. It should be noted that many of the biotechnology-related issues which can be addressed by ESS are generic across other areas of biology, polymers, and soft matter, as described elsewhere in this section.

The ESS will also result in new scientific achievements in the following biologically-relevant fields

- Studies of the processes that control aggregation in food science-related gels and emulsions. Examples include whey protein, gelatin, starch, polysaccharides, casein, soy proteins and mixtures of various of these.
- The structure of proteins at surfaces under expanded or compressed conditions, a property that is related to the formation and stability of emulsions and foams. Pressure is often used as a means of inactivating bacteria and other agents harmful to conservation.
- Kinetic studies of chaperone-mediated protein folding. The chaperones' ability to suppress protein aggregation assists in ensuring correct protein folding and in renaturing proteins after heat-induced denaturation. They are potentially of high technological significance if they could be understood sufficiently to be used in the activation of recombinant proteins.
- Low resolution neutron crystallography studies of the organisation of virus particles where the availability of only small crystals prevents effective work on existing sources. Such work will exploit complementarity with X-rays and electron microscopy. In cases where good crystals cannot be obtained (presently the case for enveloped viruses), small angle neutron scattering with contrast variation, allied with electron microscopy, will be a very powerful tool for determining the overall organisation of the particle.
- Although the ribosome sub-particles have been crystallised, and are being studied by high resolution X-ray crystallography, there exists as yet no way to determine the phases of the X-ray structure factors. Low resolution neutron crystallography will be of help in defining a particle envelope or inter-subunit boundary.
- Crystallographic measurements on protein crystals with unit cells up to 10^6 $Å^3$. These will allow the specific location of critical hydrogen atoms and hydrogen-bonding interactions, and hydrogen exchange studies to determine the protection levels of the amide hydrogens in the protein main chain. The positions and orientations of functionally-important water and other solvent molecules will be determined. Incoherent background can be dramatically reduced by cloning and expression of perdeuterated material. A particular possibility here is crystallographic studies of membrane protein-detergent crystals.
- Neutron contrast variation studies of glycoproteins, where the role of sugars in modulating function is poorly understood and present studies are limited by the low contrast between sugar and protein.
- Reflectivity studies of membrane-protein systems. These will give information on the penetration of small parts (e.g. hydrophobic loops) of protein into the membrane. Experiments in which only low protein coverage is available will become feasible.
- Grazing incidence or normal diffraction studies of in-plane organisation of membranes. Such work will increase understanding of functional mechanisms where protein-protein signalling within the membrane is of importance. Neutron specular reflection in conjunction with isotopic labelling of the component membrane lipids will be able to determine the detailed molecular architecture of synthetic erythrocyte membranes.

Earth and environmental sciences

The exploitation of neutron scattering in the Earth and Environmental Sciences is at an early stage. Many of the problems have, until recently, simply been too complicated for neutron sources and instrumentation. An example is the accurate study of crystal structures of minerals as a function of temperature, work which is now possible on the highest resolution powder diffractometers. It is, however, very clear that the potential of neutron techniques in these fields is enormous. Many of the specific advantages of neutrons are particularly relevant to the study of natural materials that are fundamental to many problems in the Earth and Environmental Sciences. Examples include structural changes under pressure and high temperature, and location of light elements in complex structures. The fact that hydrogen is central to so many problems in geology and the environment means there are countless potential applications of neutron techniques to hydrous and other light-element containing minerals.

Although much work can be done on existing sources, in many important areas of potential application, present sources and instrumentation are inadequate. The flux of the ESS will remove these restrictions, and enable the community to tackle many crucial problems related to geological and environmental processes. Sample environments will allow in situ studies of the constituent materials of the Earth under the temperature and pressure conditions of the deep Earth, while the probing of structure and motions of relatively complicated minerals will give new insight into the complex interactions that govern the behaviour of Earth materials in their natural environment. Underpinning information will be accessible that will enable the modelling of fundamental processes ranging from deep-focus earthquakes and volcanic eruptions to the transport of pollutants in the Earth's crust.

ESS will allow major advances to be made in, among others, the following key areas.

Equations of state of complex minerals

In order to better understand Earth processes, it is essential to know the response of the crystal structures of complex minerals – the constituents of the Earth – to changes of temperature and pressure of geological relevance. In addition to studying natural rock forming minerals, the facts that they have complicated chemical compositions and have experienced complicated and unknown geological histories means we also must study compositionally simpler, laboratory synthesised phases whose pressure and thermal histories are known.

With present sources, it is possible to study the temperature evolution of relatively complicated minerals, and the pressure evolution of relatively simple minerals. What is actually needed is an understanding of the evolution of complex minerals – for these are the constituents of the Earth – *with temperature and pressure together*. ESS will overcome two (related) restrictions imposed by existing sources. First, the small volumes required for combined high pressure and high temperature work presently require long counting times and yield inadequate signal to noise ratios. Secondly, existing sources are insufficiently powerful to allow measurements at many pressure/temperature points in a single experiment, as data acquisition times are presently too long. Both these restrictions will be overcome by ESS, which will thus facilitate, for the first time, structural measurements of complex Earth-forming minerals over the pressure-temperature space that is of geological relevance. For the synthetic mineral studies, neutrons have the additional advantage of being able to see through the synthesised material still within its container, without the need to break up the material.

The ESS will also result in new scientific achievements in the following areas of earth and environmental sciences

- Minor components such as water can have dramatic effects on the viscosity of silicate melts, and it is the viscosity of a magma that controls, to a large degree, the explosive nature of most eruptions. Structural and dynamical studies on these melts under geological conditions will examine questions such as how protons depolymerise silicic melts, as well as other fundamental studies necessary to lead to an understanding of volcanic eruptions.
- Basic information such as the density, bulk modulus and its pressure derivatives, of silicate melts and the mantle phases. This is needed for the interpretation of measured seismic velocity profiles.
- Total scattering measurements of the orientational disorder in silicate minerals at high temperatures and pressures.
- Equilibrium and kinetic measurements of order/disorder processes under geological conditions, and studies of kinetics of reconstructive phase transitions and *in situ* equilibrium phase diagrams.
- The pressure and temperature dependencies of phonon dispersion curves of complex silicates. These data are essential if we are to model effectively – and hence understand – the properties of the inner Earth.
- Phonon density of states measurements of hydrogen-containing minerals during changes in crystal structure (e.g. through a phase transition or during dehydration).
- Texture information on natural geological materials. This can be correlated to macro- and micro-strain analysis to establish strain ellipsoids of critical crustal areas. Valuable information will result relating to new resources and to danger estimation of earthquakes.
- Structures of mineral surfaces, including of adsorbed molecules, or in contact with a fluid. Such work has major applied implications. For example, understanding the adsorption of e.g. PCBs and heavy metal ions is important in pollution management, while other studies could relate to the prevention of crystal growth in scaling problems.
- Magnetic transitions at very high pressures, for example the $S=2 \rightarrow 0$ high to low spin transition for Fe at very high pressures. By reducing the volume of octahedrally co-ordinated Fe^{2+} by 10- 25%, it can have a profound influence on the equations of state of the majority of minerals in the mantle and at the mantle-core boundary.
- Electronic transitions in minerals at high pressures and temperatures. Because of their influence on crystal field stabilisation energies, these transitions can govern the inter and intracrystalline cation partitioning of 3d elements in minerals.
- Studies of slow motions of hydrogen (including water) in minerals. Such work is important for our understanding of chemical processes in the Earth relevant for both fundamental and environmental control/protection reasons. In nominally anhydrous minerals, trace quantities of hydrogen can significantly alter the properties of a mineral. Proton diffusion, can be measured directly, including *in situ*.
- Characterisation of the structures associated with important trace elements in water under geological conditions. Almost nothing is known about fluid water under mantle conditions, beyond the fact that it is essentially a molten salt $HO\text{-}H_3O^+$, and is presumably highly corrosive and chemically active.
- Structural studies under high pressures and temperatures to describe the chemical properties and stability domains of certain light molecular compounds important for fundamental physical chemistry and planetology (e.g. $Ar(H_2)_2$, $(CH_4)_n$ $(H_2O)_m$, and H_2 itself). These have relatively complicated structures and we need to work with very small volumes.

Hydrous and nominally anhydrous minerals at high temperature and pressure

An understanding of hydrous minerals is essential if we are to understand the circulation of water through the Earth's crust and into the deep interior of the Earth, and their effects on potentially catastrophic Earth processes. At present, we do not know what happens to water in minerals as they are taken to the conditions found in the Earth; the neutron's ability to see hydrogen makes this a natural study for the technique. Some of the hydrous minerals that may be found deep inside the Earth can only be produced in quantities that are too small for present-day sources: they will be studied effectively with the ESS.

Hydroxyl groups have been detected in many natural high pressure minerals that were previously thought to be water free. The amounts are small, but when integrated over the whole mantle, not only do we see that global quantities of water can be stored in this form, but also these influence all properties of the mantle such as the elastic and rheological properties (earthquakes, subduction, convection), thermodynamic properties (melting, phase transitions), and also geochemical processes through the (under these conditions) aggressive properties of water. The flux of ESS will for the first time enable us to locate the OH, and begin to understand the effect of pressure and temperature on the stability or the equilibrium amounts of water incorporated in these phases.

High resolution tomographic studies of in situ deformation in rocks

Observations of the geometry and organisation of crack networks in artificially deformed rocks show that the strain associated with brittle deformation is not homogeneously distributed, but becomes progressively localised in narrow zones of intense deformation. The fundamental process of crack linkage and strain localisation that precedes brittle fracture remains poorly understood, primarily because of the difficulty of measuring heterogeneous strain distributions and strain localisation in rock samples during deformation. Existing techniques can measure only the *average* strain across the length of the strain gauges or displacement transducers used. What is required is to measure the strain distribution within the interior of the sample volume, specifically away from the free surfaces. The enhanced intensity of the ESS would enable such high resolution studies of in situ deformation to be studied for the first time.

Engineering

Neutron scattering offers unique insights into the performance of industrial components and industrial processes, insights that will be ever more necessary if European industry is to compete successfully in increasingly competitive global markets. Often the systems examined are complex, such as oils, welds, engines, and complex components, and these often experience harsh chemical, mechanical, thermal, and processing environments. Under such conditions neutrons are well suited to perform *in situ* measurements. Their high penetrating power makes neutrons also particularly well suited to non-destructive testing of real materials and components in their as-fabricated or in-service condition.

Neutron diffraction provides a unique means of establishing the state of stress deep within complex components. As such, it is a powerful tool for refining finite element models which are crucial for the more intelligent component development which is driven both by (a) improved performance demands from less conservative materials utilisation and design, and (b) industries such as aerospace and nuclear power where component failure is simply unacceptable. Neutrons are central to optimising processing technologies and for highlighting stress-related problems when they arise. In many cases – for example during the deep drawing of beverage cans, or the optimisation of the superconducting properties of high T_c superconducting ceramics – preferential orientation of grains, or *texture*, is of crucial importance. Here neutrons have major advantages, including the ability to follow the evolution of texture during recrystallisation at elevated temperature. Few engineering materials are truly homogeneous, and neutrons can provide a range of information on *microstructure* over spatial ranges from 1 nm to 1 µm that is important to materials designers as well as process engineers. Relevant systems include precipitates in metallic alloys, defects in semiconductors and particle size dispersity in colloids and aerosols. Neutron reflectometry is beginning to be exploited for the study of protective *layers and coatings*, and other surface-related engineering applications.

Neutron *radiology* covers a range of imaging and inspecting techniques. These methods are beginning to be used in 'real time' application to follow changes as they develop, and finding application in diverse fields, including tribology and lubrication, studies of fast chemical processes (e.g. in pyrotechnics and aerospace), two-phase flow, transport of water and hydrogenous liquids in ceramics, building materials, soil and rocks, as well as solidification and segregation processes such as casting in materials science and metallurgy. *Neutron depth profiling* quantifies distributions of important light elements (e.g. boron) in optical, polymer, metal alloy and especially microelectronic materials, while of several neutron analysis techniques, prompt gamma activation analysis is particularly useful in the determination of non-metals (H, N, C, Si, P, S) or trace elements with high neutron capture cross-sections (B, Cd, Gd) that are not readily determinable by other techniques.

Presently, engineering use of neutrons is dominated by large aeroengine, aerospace, and power generation companies with major safety-critical problems. Currently, available beam intensities mean many experiments take over a week to complete, and are thus simply too expensive for regular and more widespread use. It is important to remember that engineers are interested in actual components and processes rather than small specimens. In contrast to basic research, it is not possible to scale the problem to fit the constraints imposed by a standard spectrometer. The placing of an *Engineering Research Development & Test Centre* at ESS will establish a more flexible environment, better able to meet the demands made by industrial engineering applications. As such, the Centre will greatly increase the range of experiments available to the engineering community. It will also make them economically feasible, taking engineering use of neutrons over the cost threshold that is presently preventing the full exploitation of the technique. Thus ESS will enable engineers to exploit effectively, to the advantage of European technology, the powerful neutron methods that have been developed at the frontiers of neutron scattering and neutron physics over the past 20 years.

An Engineering Research, Development and Test Centre for Europe

The realisation of the ESS will give Europe the opportunity of establishing the World's first Engineering Research, Development, and Test Centre for the cost-effective utilisation of neutron beams. This flagship Centre will house the engineering and neutron facilities as well as provide the technical expertise for Europe's engineers and material developers to measure stresses, observe microstructures and monitor behaviour during process or in-service. The Centre will revolutionise engineering measurements, bringing cost-effective neutron measurements to a much wider range of industries for the first time.

In addition to the cost reduction, ESS will open up new opportunities in engineering applications. Areas in which very significant advances may be expected include:

- ***in situ* studies**
e.g. fatigue behaviour, thermal cycling stresses, stresses in rotating machinery (such as aeroengine components), oxidation of surfaces – experiments which often require complex environments and fast data acquisition times;
- **real time studies**
e.g. dynamics of aggregation and coalescence of aerosols, suspensions, paints and petrochemicals, ageing of alloys, and the design of stress relief procedures – currently data acquisition times are too slow;
- **process monitoring**
e.g. powder processing, sintering, welding, cutting, wear, hardening, carburising – the current difficulty of simulating process conditions will be overcome by the available flux and instrument design;
- **three-dimensional maps of stresses and textures**
within engineering components – currently such experiments take too long;
- **neutron tomography**
to produce three-dimensional images of, for example, the behaviour of lubricants inside working engines, isotope specific radiography. In this area, ESS will give neutrons the ability to parallel in the engineering world the revolutionary developments that have been made possible in medical diagnostics through magnetic resonance imaging.

The Centre will allow the mounting of large engineering components on instruments, and their in-service observation. Expertise will be provided which will advise companies on the potential of the techniques available, design experiments or trials, and assist in carrying out and analysing experiments. Cost effectiveness will be attained by a combination of factors. These include the greater efficiency in cost per neutron from a European facility the size of the ESS over existing central facilities, a dramatic increase in the rate of data collection consequent on the higher flux, greater neutron collection efficiency and instrument optimisation. As an example, the cost for a single *non-destructive* neutron residual stress measurement will be of the same order of magnitude as a conventional shallow hole drilling measurement which will give less, and less reliable, information. The technique would thus be opened up to a very much wider engineering community for the first time.

Instruments within the Centre will provide a variety of measurement opportunities. *Strain measurements* will be possible to 0.1 mm linear resolution with an accuracy of 50 µstrain, with performance monitorable under in-service conditions, together with simultaneous basic texture information. *Textures* will be measurable quickly and accurately, including in dynamic studies. Texture maps can be produced within forged or other deformation-processed components. *Microstructural and chemical* information will be available for complex materials and processes providing 0.1% phase sensitivity under extreme pressures (~100 kbar) and temperatures (~2000 K) with collection times of a few minutes, while state-of-the-art *reflectometry* will be available for e.g. *in situ* monitoring of the growth of oxidative and corrosive films. For *radiology*, instrumentation will be provided that will exploit stroboscopic neutron imaging to allow very fast time-dependent examination of fast phenomena, together with high resolution computed (element and temperature specific) neutron tomography and scanning methods of chemical analysis (gamma activation, neutron capture, and neutron activation).

A major part of the work of the Centre will be in *residual stress* measurements. Smaller gauge volumes than used presently will be accessible, and dynamical work will be opened up. A wide range of engineering problems will be soluble, many of them related to expensive failures, especially in fatigue or stress corrosion environments.

The Engineering Research, Development and Test Centre will facilitate the following broad range of neutron-related measurements

- Time-resolved experiments to both monitor and develop *processing performance and technology* will lead to new processing strategies in areas such as powder metallurgy, mechanical alloying, molecular beam epitaxy, sputtering, recrystallisation and heat treatment and rapid solidification. Monitoring the extent of sintering of metals and ceramics as a function of heat treatment temperature will provide information about the number, size and shape of the voids. Time resolved small angle scattering will be especially useful for the development of nano- and microparticle ceramics.
- Spatial *variations of textures* caused by deformation processing can be mapped non-destructively to yield texture maps throughout components, both before and after various treatments and processes. Valuable information will thus be provided to designers, especially in the aeroengine industry where expensive trials and microstructure studies are required to optimise component microstructure. Kinetic measurements may also be possible to observe recrystallisation or grain growth on a local scale, possibly during deformation in real time.
- Real time small angle scattering studies will quantify *in-service ageing* as a means to assess remnant life of components, as well as their performance characteristics with temperature. Studies of creep cavitation cracking will allow quantification of voiding as a function of component thermal and mechanical history.
- In *chemical engineering*, exploration of the very wide parameter space that controls colloid stability (e.g. pressure, temperature, pH value, relative concentration, polymer structure and polymerisation degree, particle size, surfactants and stabilisers) will result in improved colloid performance with respect to e.g. process control, stabilisation. This will have impact on enhanced oil recovery, better control of aerosol dispersions, paints and inks. Dynamical studies of coagulation, aggregation, and sedimentation will be possible. Information about in-cycle fluctuations will advance our understanding of lubrication in reciprocating engines.
- Commercial *neutron radiological work* will be facilitated, for example, in corrosion and moisture detection in aluminium aircraft structures, in inspection of adhesively-bonded metal/composite parts and of precision cast parts such as turbine blades for the remnants of core materials. Neutron radiography will also be exploited in inspections of pyrotechnical devices in the aerospace industry, in the production of explosives and in the quality control of car airbag gas initiators. A major expansion will be possible in the use of the technique in examining paintings, objects of art, archaeological objects and in forensics. The use of neutron-nuclear methods developed by the fundamental physics community will make neutron autoradiography element-sensitive by exploiting element-specific γ-rays.
- *Real time radiological techniques* will open up new possibilities for inspecting moving objects or studying fast time-dependent phenomena. The distribution and transport of oil in running engines, and the lubrication of bearings can be followed, as can solidification and segregation processes in metallurgy and materials science. Studies of evaporation processes and transport of coolants will have extensive applications for example in R&D of cooling technology, improvement in operation of pumps, valves, visco-clutches, carburettors and of whole engines in the auto and aircraft industries, in the petrochemical industry and in improving coffee machines and fire extinguishers.
- *Neutron tomography* with high (200 µm) spatial resolution and under quasi-real time conditions will extend the applicability of three-dimensional neutron imaging and can be used for e.g. destructionless investigation of small engines and devices, and in *in situ* investigations of chemical processes. Other industrial and materials applications include examining objects with complicated internal structures, reciprocating engines and monitoring the performance of lubricants. Furthermore, by exploiting neutron resonances, three-dimensional tomographic images can be obtained of *temperature distributions, which are specific for each element.* The temperature distributions of technically-important alloy components (e.g. Mo, W, Sn, Ta, Nb) can thus be monitored under operating conditions.
- Neutron analytical methods will enable fast *non-destructive chemical analysis* for a series of elements, for example hydrogen concentrations in titanium alloy jet engine turbine blades at concentrations of about 100 µg/g Ti. Gamma activation analysis will become practical as an analysis technique in studying natural and man-made atmospheric aerosols.
- In *nuclear engineering*, investigation of irradiation generated degradation will lead to a better understanding of structural integrity and better life-time predictions. The potential of ESS in determining stresses deep within the weld has already been mentioned. The Centre will have a major capability in radiation damage studies, for example the behaviour of cladding and its interaction with the fuel is an important issue in fission systems. The effects of radiation induced hardening and embrittlement also remain challenges, as well as cracking effects caused by stress corrosion hastened by radiation damage. Dynamic studies of the cooling of nuclear fuel rods in nuclear safety studies will be possible.
- In addition to its exploitation for engineering-related measurement, the presence of the Centre at a source of the power of the ESS will act as a catalyst for the *development and technology transfer* of new techniques for engineering exploitation that are based both on neutron scattering and neutron-nuclear methods.

The definition of effective *stress relief treatments* can be made on the basis of direct measurement; the ability to study the evolution of stress non-destructively and in real time will lead to gains in our understanding of the relative relaxation rates of the hydrostatic and deviatoric stresses. High temperature behaviour can be studied effectively where the decay of residual stresses is important, such as in pressure vessel steels. Residual stress distributions and phase contents in case hardening and carburising will be quantified, as will their effect on fatigue crack growth under surface stresses. The retention of life-extending residual stressing treatments such as peening, prestretching, etc. during service can be monitored. By exploiting the pulsed nature of the beam, it will be possible to study stress changes during fatigue cycling (<10 Hz) and to map how they evolve with component life. High spatial resolution will enable stress problems through interfaces to be followed; examples include thermal barrier coatings used to protect turbine blades. The evaluation of the effect of thermal stresses between dissimilar materials in assemblies under conditions of varying temperature or applied stress will lead to improved designs, minimising thermal distortion or stress.

Stress measurements will have a major impact on the improvement of *health and safety* standards. Neutron diffraction is the only means of measuring non-destructively the stress field deep within welds, of critical importance in the aerospace and nuclear plant industries. Through giving quick, accurate, and inexpensive information about the state of stress, especially at welded joints and other sites of high stress and low reliability, optimised fabrication procedures can be developed with lower levels of non-conformance rejection. Reliable measurements of residual stresses within well-characterised welds will facilitate the reduction of the level of residual stress by intelligent weld process design, or by subsequent thermal or mechanical treatments, and the development of finite element weld models. Other benefits of wider exploitation of residual stress quantification include reducing life cycle costs and improving safety management of critical components.

Condensed matter and materials physics

Modern condensed matter physics is guided by the Nobel Prize winner Phil Anderson's maxim that ***"many is different***", i.e. when we put 10^{23} atoms together, they produce behaviour, such as superconductivity or magnetic order, never anticipated on the basis of even the most detailed knowledge of the individual atoms. Example of questions in this field include: what constitutes a metal? Are all metals eventually superconductors? How does electrical dissipation arise in superconductors? Do liquids always freeze at zero temperature? In addition to being of fundamental importance, the answers to such questions are the basis of materials science and engineering.

The impact of neutron scattering on core activities in condensed matter physics – which include magnetism, superconductivity, quantum systems, lattice dynamics and phase transitions – has been of outstanding importance. When important new materials, such as the heavy fermion systems or the high temperature superconductors, are discovered, neutron scattering is the choice of probes to investigate the fundamental physical microscopic properties. These range from the basic atomic and magnetic structures to the dynamics of the atoms and magnetic moments, and are often concerned with the solution of simply posed problems in quantum mechanics and statistical mechanics.

Neutron scattering is the only method for the determination of *magnetic structures* and *magnetic excitations*. This is simply because the generalised magnetic susceptibility, which describes all that can be known about the microscopic spatial and temporal correlations of the magnetic moments in a material, is directly proportional to the neutron cross-section. The use of sophisticated techniques like polarised neutron beams and three dimensional polarisation analysis have further enhanced the capabilities of magnetic structure analysis with neutrons, for example, the determination of the absolute spin configuration in magnetoelectric crystals such as Cr_2O_3 . Neutron scattering has also been an essential experimental tool in *phase transition studies* and related *critical phenomena*, and has played a seminal role in the rapid growth of our knowledge of the microscopic origin. The discontinuities of structure, dynamics and physical properties at structural phase transitions, the associated critical phenomena and lattice dynamics, the role and properties of defects etc., constitute a rich field of enquiry which informs our whole understanding of the physics of pure and applied condensed matter.

An area of increasing importance concerns the properties of thin films, multilayered structures, surfaces and buried interfaces. Neutron scattering has already demonstrated that it can contribute unique information in this field, providing detailed information about structure on a nanometer scale.

Many important technical developments that now pervade our way of life derive from condensed matter physics and owe much to the knowledge gained of neutron techniques.

As in other scientific areas, a major, indeed a qualitative step forward, will be realised in condensed matter physics with the availability of a next generation spallation source. Areas that will particularly benefit include experiments on thin films of magnetic, semiconducting and superconducting materials, and studies of kinetic and non-equilibrium phenomena. Intrinsically smaller and more complex systems will become accessible, as will the measurement of smaller cross-sections over larger ranges of space and time. The high flux of the ESS should allow us to use neutrons as probes to investigate *local* variations in the time and space correlation functions in inhomogeneous samples. Condensed matter physics will also be a major beneficiary of the increased ability to work under even more extreme conditions, for example high pulsed magnetic fields (30 Tesla and beyond), very high pressure (500 kbar and more), and very low temperatures indeed (picoK). These experiments will be at the cutting edge of science. In addition to their fundamental interest to condensed matter research, they also carry with them the potential for technological innovation.

In the following sections we describe the potential advances that the ESS would bring to some key areas in condensed matter physics.

Strongly correlated electron systems

Strongly correlated electron behaviour is the source of many of the most dramatic discoveries in condensed matter physics in recent years, including high temperature superconductivity, superfluidity in ^3He, heavy fermion behaviour, and the quantum Hall effect. In these systems the electrons cannot adequately be described by either localised atomic models or by one-electron band theory and the central problem is to develop an understanding of the microscopic mechanism. The required neutron measurements of the generalised susceptibility over a wide dynamical range present a number of serious technical challenges. The signal may well be weak (typical for actinide compounds), the magnetic response may be strongly broadened by hybridisation of the 5f-electrons, or (in transition metals) measurements of the excitation spectrum are needed at very high energies where the spin waves interact with single-particle interactions, the 'Stoner'-excitations, which extend over most of the Brillouin zone.

Although a start has been made on these measurements using today's most intense sources, the information is still very limited. ESS would make these measurements, including parametric studies, straightforward, allowing for substantial progress to be made in understanding the electronic structure in these materials. The consequent increase in our understanding of related phenomena such as that of high temperature superconductivity is likely to be dramatic.

Achievements of neutrons in condensed matter and materials physics

- Almost everything we know about magnetic structure – from the early demonstration by Shull of antiferromagnetism in simple systems, to the complex magnetic structures being developed as hard magnets – has come from experiments with neutrons.

- Inelastic neutron scattering has provided unique information on the interaction and anisotropy energies which determine the Hamiltonian operator. Extensive measurements on magnons and crystal field excitations over a wide range of frequency and momentum space have revealed e.g. the interaction of the spin waves with the single particle excitations (Stoner continuum) in iron. Similarly, measurements of phonons and their density of states have improved our understanding for example of the role of phonons in the martensitic phase transition in the IVb metals.

- Neutrons have provided the definitive crystal structures in *high temperature superconductors*, which have served as the basis of all considerations of the superconducting mechanism and have led to production of better quality samples. Neutrons have precisely located the positions of the oxygen atoms, where the charge carrying holes reside. Neutron spectroscopy has provided unique information on the nature of magnetism in high temperature superconductors, on the interplay between magnetic fluctuations and superconductivity and on the role of the lattice dynamics.

- Neutron diffraction provided the first microscopic evidence for flux line lattices in conventional superconductors and played a major role, especially at higher magnetic fields where no other technique can image flux lines, in accounting for the large dissipation in the high-T_c materials.

- Outstanding results from space and time-dependent studies of *correlated electron systems* include proof of the importance of correlations for the spin dynamics and the antiferromagnetic character of the spin correlations.

- Major contributions to our understanding of *model systems for statistical physics* in one, two and three dimensions, include the verification of the Haldane conjecture, determining the properties of the Haldane gap, and the discovery of solitons, as the characteristic elementary excitation of strongly non-linear magnetic systems.

- Polarised neutron reflectometry of surface and interface *magnetism in thin films and multilayers* is providing technologically relevant information. Important examples include the observations that the magnetic order can propagate through non-magnetic layers and that giant magnetoresistance is not necessarily associated with antiferromagnetic coupling.

- One of the most fundamental questions in condensed matter physics concerns the liquid and solid phases of ^{3}He and ^{4}He. Experiments with neutrons have provided unique and important information on, for example, the Fermi liquid parameters of ^{3}He, the Bose condensation of liquid ^{4}He and the magnetic structure of solid ^{3}He. The importance of understanding these quantum systems was highlighted by the award of the 1996 Nobel prize in physics for the discovery of superfluidity in ^{3}He by Lee, Osheroff and Richardson.

- Pioneering experiments have been made on *nuclear spin* ordering in Cu and Ag, which are antiferromagnets below 70 nK and 600 pK respectively. These observations of one of the weakest interactions in a solid is a significant step towards defining the ultimate ground state of electronically non-magnetic materials.

Flux lattice studies in superconductors

The motion of the flux line lattice in type II superconductors is inhibited by pinning to material defects, such as precipitates or dislocations. When the electrical current exceeds a critical value, the superconductivity is destroyed as the flux lattice breaks free and starts to flow. A proper understanding of the microscopic nature of this process would have major implications for developing more effective high temperature superconductors.

With existing neutron sources we are just about able to study the static properties of the flux lines. Even so, experiments have been restricted to a small corner of the phase diagram in magnetic field, electrical current and temperature, where a well ordered flux-line lattice exists. With a source like the ESS it will be possible to extend this work to examine regions where the flux lines have decomposed into 'pancake' vortices, which are effectively decoupled from layer to layer, and the region above the 'irreversibility' line where it is believed that a liquid of flux lines or pancakes exists. Also experiments on the dynamics of the magnetic flux lattice in such superconductors would become feasible, allowing the examination of the motion of the flux line lattice against an applied current. Changes of the viscosity of the flux liquid due to the presence of extended pins could be studied, together with their role in the growth of short range order. Such experiments are of particular interest for technical applications since they will help to optimise the current densities in exploitable superconducting materials.

Neutrons and thin films

Surface neutron scattering under glancing angles is a technique in its infancy. The flux of ESS will enable us to realise its full potential in thin film and interface studies. The optimisation of devices for the thin film industry (magnetic storage media, recording devices, spin valves, giant magneto-resistance materials, erasable recording systems with extremely high storage capacities) will rely heavily on detailed knowledge of the microscopic properties. Many of these are only accessible through neutron scattering techniques, e.g. determination of the total magnetic moment, moment formation, interface polarisation, exchange coupling, spin density distribution, vector magnetisation profile, properties of buried interfaces. Also real time studies e.g. of the effect of laser annealing on magnetisation will become possible. With a source such as the ESS it may even become possible to study phonons and magnons at interfaces. Although these play an important role in the performance of semiconductor devices, we at present have little direct information concerning them.

Studies under extreme environmental conditions

The pulsed nature of the neutron beam makes it particularly attractive to combine it with pulsed sample environments that can produce the extreme conditions where the frontiers in physics are often found. Pulsed electric and magnetic fields come immediately to mind. In the case of pulsed magnetic fields, studies under significantly higher magnetic fields (30 Tesla and more) than can currently be achieved with superconducting technology will become feasible. The low duty cycle of these magnets requires the flux of the ESS, in particular where dynamical properties are to be probed. Examples include metamagnetic transitions in heavy fermion systems that arise from quenching of the Kondo effect by the large magnetic field, and field-induced transitions in magnetic systems.

A very exciting prospect is the possibility of examining with neutrons non-linear optical materials when illuminated by pulsed lasers. This would provide unique and novel information at the microscopic level on the effects of a high intensity electromagnetic wave on the structural and dynamic properties of these materials, and also reveal details of the relaxation processes.

The ESS will also result in new scientific achievements in many other areas in condensed matter physics, including the following

- The full potential of complete polarisation analysis will be realised for the first time. The consequent ability to separate magnetic and nuclear scattering routinely, as well as the separation of coherent and incoherent scattering arising from nuclear spins, will open up a wide range of new science. Examples include measurements of spin-dependent cross-sections in ^{3}He and ^{3}He-^{4}He mixtures to test the fundamental Fermi liquid theory (which is essential to the theories of high temperature superconductivity), and the unambiguous separation of phonons and magnetic excitations in magnets, especially above their ordering temperatures. The recent development of polarising ^{3}He filters will open up the field of polarisation analysis to a wide range of white beam applications.

- Ultrahigh resolution and increased overall sensitivity will reveal the full complexity of the spin structure in complex and technologically relevant magnetic materials.

- The magnetic structure of molecular materials – presently difficult as they have large unit cells, contain light atoms and have magnetic moments delocalised in organic ligands or in free radicals – will become more accessible.

- Measurements of magnetisation distributions (using polarised neutrons) in systems which are more complex, which have larger unit cells and/or are very weakly magnetic, will become possible.

- The ability to measure weak cross-sections will enable the expansion of studies on systems which carry very small magnetic moments (e.g. molecular magnets, all of the known ‘magnetic’ heavy fermion systems). Up to now only exploratory experiments have been possible.

- *In studies* where dilute quantities of paramagnetic ions are used to provide a weakly interacting probe of the host lattice magnetism, the ability to work with very dilute quantities of the probe ions will minimise the interactions between the paramagnetic ions which would otherwise lead to exchange broadening.

- The most detailed structural, dynamic and magnetic information on materials is obtained from single crystal studies. This is because there can be marked anisotropies in the physical properties varying with crystallographic directions. The weak interaction of neutrons with matter requires relatively large single crystals on present neutron sources. The recent history of new materials (e.g. high temperature superconductors, heavy fermion systems) which exhibit unusual ground states, has shown that neutron investigations of these new compounds are vital, even before large crystals have become available.

- We will be able to use the neutron as a *local probe* of structure and dynamics of materials. Direct spatial imaging should be possible with a resolution of 50 x 50 μm^2. Combined with a scanning device, we would be able to entertain the possibility of a near field neutron microscope as a bulk probe. This new tool could be used for the local imaging of magnetic (domain) structures, and could have a significant impact on a wide range of metallurgical problems (e.g. the observation of *in situ* crystal growth).

- In nanocrystalline materials, whose properties can be markedly influenced by the high interface/volume ratio (for example, ceramics tend to become ductile, while fcc metals can be significantly harder and stronger), it should become possible to determine, for example, the local magnetisation and nanoscale magnetic correlations in relation to the microstructure and the interface. Such information is highly relevant in assisting the technological demand for smaller devices.

- Lineshape studies of collective excitations, presently limited by the trade-off between flux and resolution, will be made routine. For example, in superconductors, phonon linewidth changes on passing through T_c provide a direct measure of the electron-phonon interaction and shed light on the role of electron-phonon interaction in 'normal' and 'unusual' superconductors. The improved resolution combined with high flux would also fuel the search for the marginal Bose liquid with an unusual scaling of the phonon lifetime, analogous to the non-Fermi liquid behaviour observed in some heavy fermion systems.

- The high resolution will facilitate the accurate measurements of the excitation spectra of much more complex systems that are being synthesised and in commercial use. For example, such experiments on hard magnetic materials (a present-day example being $Nd_2Fe_{14}B$) are needed if we are to understand the magnetic properties on a microscopic scale in order to guide the development of improved magnets. Polarisation analysis is needed here to separate magnons and phonons.

- Very low temperature (picoK) work will be possible on problems such as the superfluidity transition in ^3He, the ground state of metallic systems and nuclear ordering.

- In high pressure studies, not only will higher static pressures be accessible with smaller samples, but 'single shot' experiments that probe behaviour under explosive compression will become feasible.

- Major expansion will occur in a wide variety of time resolved studies, e.g. in non-equilibrium processes. These will include both 'real-time' and stroboscopic techniques. Reflectometry studies *in situ* and in real time will be able to follow e.g. surface oxidation and magnetic domain relaxation. Critical scattering in real time (as a sample is being cooled or heated through a transition) will be accessible. Stroboscopic measurements that are already possible for studying structural changes through a phase transition will be extendable to measurements of diffuse and inelastic scattering;

- Parametric studies, – following changes with temperature, pressure, magnetic or electric field, alloy composition, etc. – will become routine. The ability we will have to explore this multidimensional space more fully will lead to a qualitative improvement in our understanding of real solid state problems. For example the canonical heavy fermion system UPt_3 exhibits an unusual and fascinating (B,T,p) phase diagram established by bulk measurements. Although there is strong evidence for unconventional superconducting behaviour, only very sparse microscopic information as has presently been obtained by inelastic neutron scattering is available to help with the understanding.

Fundamental neutron physics

Although the major use of neutrons is in studying structure and dynamics of matter and materials, the neutron is also a powerful probe for fundamental physics. The European Spallation Source is therefore of intense interest for neutron physics research, both for fundamental studies and the exploitation and further development of neutron nuclear methods for applied R & D.

During the past 25 years, our world view of physics has changed dramatically in several areas. Neutron physics has made major – and in some cases decisive – contributions to this process. On the grand scale, cosmology has evolved into an exact science, and neutron physics has played a significant part in this. For example, at the end of the 1980s, free neutron decay data were able to contribute to fixing the number of particle families at three. At the opposite scale, experimental measurements have been made of many of the neutron interaction parameters required if we are to answer important particle physics questions. Furthermore, recent years have seen the emergence of a number of universal rules which govern the behaviour of complex systems, and here again, neutron physics has played a significant role in establishing the rules which govern the sudden changes of state of matter during a phase transition.

Many crucial questions remain to be answered and the increased flux of neutrons from ESS will enable major progress to be made in a range of areas. For example, a number of unique experiments can be performed which will help (a) to determine the basic structure of the elementary interactions of nature; (b) to elucidate the history of the Universe, and (c) to study various questions from the field of quantum and measurement theory. Finally, a number of important new nuclear physics applications in industrial science and engineering will become feasible.

The following three 'flagship' experiments will be possible on the ESS.

The question of the handedness of nature

In the late 1950s, it was recognised that the weak interaction – one of the four known forces – is exclusively left-handed. Most Grand Unified Theories, however, start with a left-right symmetric universe, and explain the evident left-handedness of nature through a spontaneous symmetry breaking at a critical energy, a scenario which, if true, would mean that the neutrino today should carry a small right-handed component. Although limits on this right-handed component have been derived from free neutron and muon decay experiments, what is really needed is a clear-cut 'yes' or 'no' experiment. Such an experiment is the beta-decay of unpolarised neutrons into hydrogen.

What is so interesting about this decay is that one of the four hydrogen hyperfine states cannot be populated at all if the neutrino is completely left-handed. A non-zero population of this substate would therefore be a direct measure of the right-handed component of the weak current. This experiment has severe background suppression requirements for which the pulsed structure of ESS, allied to its intensity, is well suited. Thus, with ESS it may be possible to prove for the first time that, first, nature does not possess an intrinsic handedness, and secondly, that there is exciting new physics beyond today's Standard Model.

The question of isotopic-spin invariance

It is believed that the strong nuclear force is essentially the same for protons and neutrons, or, more generally, for up quarks and down quarks. This assumption leads to the concept of isotopic spin as a conserved quantity.

Isotopic-spin invariance can be tested by measuring the proton-proton, proton-neutron, and neutron-neutron nuclear singlet scattering lengths at low energies. However, as the scattering process is dominated by the Coulomb interaction, our knowledge of the proton-proton scattering length is doubtful, while the neutron-neutron scattering length is even more uncertain. The best way to check whether the measurements we have on these scattering lengths really signal a breakdown of isotopic-spin invariance is a direct measurement of the neutron-neutron scattering length via the scattering between free neutrons.

As the interaction rate for this process scales with the square of the momentary neutron flux density, the high peak pulse intensity of ESS has huge advantages. The planned ESS experiments also makes use of the time structure by allowing the ‘fast’ neutrons of one pulse to hit the ‘slow’ neutrons of a preceding pulse. Calculations show that such an experiment should be entirely feasible, with even better signal/background ratios possible using polarised neutrons. It will make a significant contribution to the understanding of one of the four known forces of nature.

The question of the baryon asymmetry of the universe

In the big bang, equal amounts of matter and antimatter were produced. As subsequently matter and antimatter could annihilate each other, only a few heavy particles (‘baryons’), and a roughly equal amount of antiparticles should have escaped from this early period. Our mere existence contradicts this expectation: about 108 times more baryons remain than predicted, and almost no antibaryons have survived. So far, the only viable solution to this problem – proposed by Sakharov – is the violation of charge-parity (CP) symmetry, which, in all reasonable contexts, is equivalent to a violation of time (T) symmetry, a symmetry which describes the invariance of all basic interactions of nature under a reversal of ‘the arrow of time’.

Although violations of CP-symmetry have been observed in the decay of kaons, this one positive result is not sufficient to verify Sakharov’s conjecture, nor to identify the origin of CP- or T-violation. Both Grand Unified Theories and Sakharov’s conjecture require T-violating amplitudes that are orders of magnitude larger than can be accommodated in the present Standard Model. Another generation of experiments is therefore needed to obtain a decisive answer. An appropriate method is to search for both P- and T-violating amplitudes in certain neutron-nuclear resonances at which the weak P- (and we believe also T-) violating amplitudes are enhanced by several orders of magnitude. The high peak intensity epithermal beam, a widely tuneable energy, and sharp timing offered by ESS will increase the present sensitivity for T-violating amplitudes by orders of magnitude. Consequently, there is a good prospect that both the question of matter-antimatter symmetry of the Universe, and the question of grand unification, can get decisive answers.

The ESS will also result in new scientific achievements in several other areas of fundamental physics

- A high intensity polarised cold neutron beam can be used for measurements of some dozen observables relating to free neutron decay. These data can be used to answer different physics questions ranging from cosmology and astrophysics to the present standard model of particle physics and beyond.
- The same beam can be used to measure the weak interaction between nucleons, which can be isolated by its unique property of complete left-handedness. A major challenge is to see a measurable non-zero polarisation on samples of hydrogen or helium.
- An ESS ultra-cold neutron (UCN) source will host two long-term projects: the search for an electric dipole moment of the neutron, and free neutron decay. In addition, ultra-cold and very-cold neutrons ($1\ \mu eV < E < 100\ \mu eV$) will be used for investigating a wide variety of problems in general physics, including phase topography, anomalous Larmor precession, Berry phases, Coriolis and tidal forces, ultra-cold neutron microscopy and inertial versus gravitational mass. Potential uses of ultra-cold neutrons in condensed matter physics will be explored, such as UCN reflectometry, elastic, and inelastic scattering. For example, in surface reflection, energy changes less than 10^{-11}eV can be resolved, while in superfluid ^{4}He, the liquid helium excitation spectrum can be measured.
- An undermoderated high resolution beam will enable many experiments currently out of range on existing sources. Interesting questions can be posed such as what happens when one pulls on a quark inside the neutron, the answer to which gives unique information on the slope of the quark-quark potential and relates to quark confinement.
- Experiments on an ESS fast neutron beam can move us towards an understanding of one of the most difficult theoretical problems in physics, namely the description of a mesoscopic quantum system with an intermediate number of strongly interacting particles. Relevant questions that can be tackled in this area include the following.
  - What is the signature of a mesoscopic quantum system whose classical counterpart is chaotic?
  - In what way does the transition from a mesoscopic regular quantum system proceed to a chaotic quantum system?
  - How does a mesoscopic strongly-interacting quantum system reach equilibrium?
  - Was there an inflationary period in the early phase of the big bang?
  - How are the heavier elements produced in stellar processes?

Exploitation of other particle sources at ESS

Besides neutrons with a range in energy covering 16 orders of magnitude, the proposed ESS will also provide high intensity sources of γ–rays, electrons, positrons, four kinds of neutrinos (separated in time), two kinds of muons (polarised), three kinds of pions and of fission products covering a large part of the table of isotopes. Although the case for ESS is centred on the use of neutrons in applied and fundamental condensed matter and materials studies, several non-neutron uses, which are totally consistent with the primary use, also have great potential. These are summarised below.

Muon spectroscopy for condensed matter science

The exploitation of the muon in condensed matter has, with the advent of both continuous and pulsed spallation sources at e.g. the Paul Scherrer Institute in Switzerland and at ISIS in the UK, established itself as a promising field of study which is experiencing strong growth as the technique's potential becomes increasingly realised by the appropriate communities.

Muons provide a powerful probe of condensed matter. They can be implanted into virtually any material, to give, through monitoring of its spin polarisation, information about local structure and dynamics. The muon can serve as a microscopic magnetometer, giving a direct measurement of local magnetic or hyperfine fields, including the spatial distribution of these fields as in high temperature superconductors, and their temporal fluctuations as in magnetic phase transitions. The muon's defect interactions are essentially those of the proton, and hence it can report on hydrogen defect centres such as those important in semiconductors, or illuminate studies of hydrogen in metals. Its mass, being one ninth of that of the proton, favours the observation of quantum effects, such as the influence of zero point energy on chemical bonds and quantum tunnelling.

The intense source of muons that can be provided by the ESS would be exploited by the growing community in several ways. First, with up to seven stations on the pulsed muon facility, the increasing needs for muon spectroscopy can be met over a broad range of studies that include metals and alloys, defect states in semiconductors, magnetic and superconductivity, diffusion in liquids and solids, chemical reactions, and the study of short-lived intermediates and free radicals. Present sources cannot satisfy this demand.

Secondly, the ESS intensity will open up new muon-based science. For example, the small spot size of a possible quasi-continuous beam would enable muon studies on materials which are available in only small quantities, such as biological samples, single crystals of new magnetic or superconducting materials, or samples requiring expensive isotope enrichment to get the right nuclear spin. Furthermore, level crossing resonance experiments that measure quadrupole splittings and involve only nuclear spins will become feasible. This would open up the enormous amount of this spectroscopy waiting to be done on questions such as local electronic structure and screening in semiconductors and metals.

A slow muon facility for surface and interface studies

The ESS intensity will make possible an ultra-slow muon beam, opening up to muons the increasingly important areas of surfaces and thin layers. This source will exploit the sensitivity and selectivity of muon methods, coupled with the importance of hydrogen in connection with surface states and surface restructuring, in studies of surface, multilayer, and interfacial systems. Examples of key problems that will be open to attack include:

- flux line lattice of two-dimensional Josephson junction arrays;
- de Haas-van Alphen states in nearly two-dimensional metallic systems;
- vortex lattices in superconducting films and multilayers;
- spin polarisation in non-magnetic layers between magnetic layers;
- spin dynamics in nearly two-dimensional metallic systems;
- diffusion on surfaces;
- spin structure in magnetically ordered systems.

Other possible developments include depth profiling of nanophase materials such as the one-dimensionally modulated multilayers of enormous technological potential. This use of slow muons is exploitable further as an important tool in assisting the development of engineered multilayered materials with nanometre or mesoscopic scale modulations.

Muon particle physics

ESS will be particularly useful in exploring topics in muon particle physics. These include: (a) precise tests of the standard model, and (b) the accurate determination of fundamental constants. Both involve high precision experiments with good counting statistics. Hence new sources with high muon fluxes such as ESS are indispensable for further progress.

Precision measurements on the free muon will provide very accurate tests of quantum electrodynamics and of the weak interaction, while the Fermi coupling constant of the weak interaction can be obtained from the precision measurement of the muon lifetime. Right-handed contributions to the left-handed muon decay amplitudes can be searched for. Experiments on muonic systems (e.g. μ^+e^-) can provide precise tests of bound state quantum electrodynamics. Information on the electric and magnetic form factors of the proton can be obtained, data that are important for empirical corrections necessary in hydrogen spectroscopy. Polarised muonic ^{3}He could be used to search for T-invariance violations in nuclear muon-capture.

Neutrino studies

The ESS offers unique possibilities for the most advanced experiments in intermediate energy neutrino physics. From the decay of pions from the spallation target, and the subsequent decay of muons, neutrinos of different flavours will emerge with energies up to 53 MeV. The resulting neutrino intensities of 3.5×10^{15} will exceed those of the ISIS facility by more than a factor of 60. This unprecedented high flux of 'beam stop' neutrinos will open up a new area of neutrino physics, with strong impacts on particle physics, astrophysics, and cosmology.

The physics motivation for the studies that would be undertaken at an ESS neutrino source arises from the following fundamental yet unsolved problems

Neutrino mass:

- are neutrinos *massive* particles?
- if they are, do they obey mass mixing giving rise to *neutrino oscillations*?
- do neutrino masses obey a generation hierarchy as implied by the see-saw *mechanism*?
- do massive neutrinos contribute to the *hot dark matter* in the Universe?

Neutrino identity:

- *Majorana-* or *Dirac-neutrinos*: are neutrinos identical with their antiparticles?
- do sterile, *right handed neutrinos* exist in nature?

Neutrino structure:

- does an inner structure of the neutrino give rise to a non-vanishing magnetic moment and a finite charge radius?

Other topics:

- is the total or flavour *lepton number* violated in processes with neutrino emission?
- do scalar or tensor type Lorentz structure interactions contribute in neutrino production interactions (*deviations from V-A*)?
- do pions or muons obey new and *exotic decay modes*?
- does coherent scattering of low energy neutrinos off nuclei exist?
- is neutrino *coherent scattering* the dominant mechanism of energy transfer in supernova explosions?
- to what extent is neutrino-electron scattering affected by *destructive neutral current/charge current interference* of W- and Z-gauge boson exchange (as predicted by the Standard Model)?

In addition, a 'decay-in-flight' neutrino beam line, producing muon neutrinos with energies in the 60-200 MeV range could be used to measure (a) ν_μ-proton elastic scattering at low momentum transfer, and (b) charge current ν_μ-induced reactions on nuclei. The former would provide quantitative information on the problem of any heavy quark content of the nucleon and its spin structure, data which would be independent and complementary to the ongoing programme of polarised charges lepton-nucleon scattering at CERN and SLAC. The latter would provide needed nuclear structure information and/or Standard Model tests, as well as additional information on the strangeness content of the nucleon.

All these experiments would be feasible. The sensitivity to neutrino oscillations would greatly exceed all existing limits of accelerator-based oscillation experiments, while ESS-based measurements on all other topics above will improve our current knowledge on these fundamental questions by at least an order of magnitude. The ESS would be the most intensive neutrino source for the coming decades, through which most of the unanswered questions in the field of neutrino physics could be resolved within a few years.

Radioactive nuclear beams

One of the main frontiers of nuclear physics is the study of nuclear reaction induced by beams of unstable, radioactive nuclei. Such radioactive nuclear beams (RNBs) also have a wide range of potential applications in studies of condensed matter, chemistry, atomic physics, medicine, and biology. The dominant view in the field is that the ideal production method is to impinge a ~100 µA beam of ~1 GeV protons on a heavy metal target. Thus, a RNB taking the 100 µA beam of neutral hydrogen, created in the injection process, would provide a benchmark facility to enable major progress to be made in this field and its possible applications.

In *nuclear structure*, even the simplest ideas concerning the radius of the nucleus, and the relative locations in the nucleus of the protons and the neutrons, have been overturned by early experiments with beams of neutron rich light elements such as ^{11}Li. As we continue to add an excess of neutrons or protons to stable nuclei, we can expect a feast of new results and new phenomena which are almost certain to alter our view of nuclear structure. We have little idea of the *properties of nuclei* as the neutron/proton ratio is varied. Such studies will be feasible on ESS.

A knowledge of the properties of unstable nuclei is one of the keys to *nuclear astrophysics*. The observed elemental abundancies result from a complex competition between successive reactions along pathways far from the stable nuclei. If we are to reproduce the observed elemental and isotopic abundancies – the clues to the environment at the sites of heavy element nucleosynthesis – we need to determine the properties of the unstable nuclei lying along the paths of the network of reactions in which they are created. Such experiments would be possible on an ESS RNB source. This source could also be exploited to solve outstanding problems in nuclear chemistry, including the chemistry of the heaviest elements ($Z \geq 105$).

In addition to such fundamental studies, the ESS RNB could be used in *materials science* work. Ion beams of stable isotopes are widely used both to modify materials and for surface processing, ion implantation being of vital interest to semiconductor microelectronics, the manufacture of specialised tools and advanced metallurgy. Radioactive ions *of the same chemical species* implanted into a host sample will report back on their local microscopic environment via modification to their radioactive decay pattern. Although a whole battery of such techniques has been developed, their exploitation is largely limited to the ISOLDE facility at CERN, which is limited, not only by intensity (~2 µA), but also in energy which restricts implantation close to the surface. The ESS facility would enable implantation at much greater controlled depth, vastly expanding this whole field of study into many areas of increasing importance such as multilayer semiconductor devices.

Medical applications are also possible, including radiotherapy of tumours, where energetic heavy ions enable lethal doses to be localised at the tumour site.

The ESS RNB facility could provide the nuclear data needed for *nuclear waste transmutation*. In order to assess the usefulness of the many possible routes for transmuting long-lived and toxic fission products, we need a knowledge not only of the spallation reaction cross-sections of the isotopes of interest, but also of the spallation product distribution, to ensure we are not just replacing one problem with another.

Irradiation for fusion materials research and development

Present research and development of plasma interactive and structural materials for fusion reactors relies completely on simulations. This is unsatisfactory, as the transfer of simulation data to fusion conditions entails much uncertainty. Consideration has therefore been given to the possible use of neutron sources in fusion materials development.

A serious candidate for the needed source of high energy neutrons is a spallation source. Such a source in the MW power range has advantages, including a well-matched recoil spectrum, the ability to match required helium and hydrogen production rates and a more homogeneous flux distribution than a d-Li stripping source, the main other contender. On the negative side, the sharp time structure of ESS is unhelpful, as it would lead to high instantaneous damage rates and H/He production rates, making transfer of results under these conditions to the fusion case uncertain. Secondly, the large irradiation volume required for fusion materials work is likely to degrade the source performance for its primary neutron use.

The above assessment relates to magnetic confinement fusion. However, parallel efforts to develop inertial confinement fusion have different requirements. In particular, the pulse lengths, power densities, and repetition frequencies are appropriate to those of ESS. It is possible therefore that the high fluxes of fast neutrons delivered by ESS would make it an ideal test bed for materials development for inertial confinement fusion. A *prima facie* case therefore exists that warrants a more detailed assessment.

Isotope production

Two isotopes that have been identified for possible production on ESS because of their high commercial value in medical applications are Tc-99m and Sr-89. The latter is marketed as a pharmaceutical (used as a palliative for secondary prostate cancer) at approximately 1 \$M/kg, while the former is the basis of most gamma-camera medical imaging.

Appropriate routes exist for producing both these isotopes on a source with the characteristics of ESS, with a specially designed partial moderator to attain the required intermediate neutron spectrum. Although further detailed design calculations for the neutronics and yield are required, together with analysis of the required chemistry, again there is a *prima facie* case for considering commercial isotope manufacture on ESS for the two isotopes Tc-99m and Sr-89.

Complementarity of the ESS with other techniques

The range of techniques available to the condensed matter scientist

Our understanding of the behaviour of materials depends ultimately on an understanding of structure and dynamics, not only on the atomic-level but also – especially when we are concerned with in-service performance of increasingly complex systems – at the higher mesoscopic level of aggregation. Our knowledge at both levels is based on the exploitation of a wide range of sophisticated experimental techniques. Some of the most important are X-ray and neutron scattering and spectroscopy, nuclear magnetic resonance, infrared, Raman and Brillouin spectroscopy, electron spin resonance and Mössbauer techniques, and light scattering. Direct space techniques such as electron and field ion microscopy have been joined recently by scanning tunnelling microscopy and related scanning probe techniques. The power of all these techniques is enhanced by theory and computer modelling.

In general, each of these techniques is optimised to see different aspects of structure and dynamics. X-rays see electrons, while neutrons see (in the main) nuclei. X-ray spectroscopic techniques such as EXAFS see local atomic environments through the 'eyes' of the electron, while nuclear magnetic resonance sees local environment through effects on nuclear spins. Each also sees a particular range of spatial dimensions, which may range from the atomic level to the mesoscopic scale, and/or a range of time scales which may range from those of the fundamental molecular vibrations to periods of hours or longer. Of the direct techniques, electron microscopy again 'sees' electrons, while the scanning probe techniques respond to a variety of tip-sample interactions whose 'imaging' is only just beginning to be understood.

There is much complementarity between many of these techniques, depending on the problem being tackled. Each technique has its particular strengths. It is the effective and efficient exploitation of these strengths that makes the use of complementary techniques particularly powerful. Thus the *array* of appropriate experimental methods available can often be crucial in solving materials-related problems. As complexity increases, the need to exploit the specific advantages of complementary techniques also tends to increase. It has been said, even of an apparently simple problem like understanding the structure and dynamics of water, that it is not a problem that we can solve by hitting it on the head. We need to back it into a corner. We can only do that by making effective ('complementary') use of all the available appropriate experimental and interpretational techniques.

Moreover, many of the available techniques are 'indirect', in that the data they give require interpretation in terms of a conceptual, interpretive model. In these cases, the conclusions drawn will depend upon the validity of the assumed model, and increasingly, computer simulation techniques are used to assist in these cases. Other methods measure directly the information we need. Of these, neutron scattering is arguably the most powerful set of techniques, the use of which is pivotal to our understanding of the atomic and mesoscopic level structures and dynamics in molecules and materials. Neutron techniques can give us unambiguous information simultaneously on *both* structure and dynamics, over a wide range of spatial and temporal scales. One of their central attributes is that they 'see' atomic nuclei directly. This not only makes available to the scientist a whole range of sophisticated techniques, but also means that interpretation of the results is often extremely simple and model-free.

In setting out some of the scientific opportunities that the ESS would open up, the use of complementary techniques in solving problems is often specifically stated. We summarise here some examples in which complementarity is particularly important. This also underlines further the need for a next generation neutron source in order to enable us to make full complementary use of advances in other techniques, for example the advent of third generation synchrotron X-ray sources, biomolecular engineering, and computer modelling.

Examples of complementarity

Neutrons scatter from the atomic nucleus; thus, in contrast to X-rays, neutron-derived details about atomic position and movement are uncomplicated by the convoluted structure of the electron distribution. Thus, *single crystal neutron diffraction* provides in general the most precise and reliable structural information that may be obtained. Not only is this particularly true for location of hydrogen atoms, but the *combination of x-ray and neutron diffraction data* gives the most precise experimental information on electron distributions, and hence information on bonding in chemical systems. Thus, both x-ray and neutron methods are necessary if we are to understand some of the most subtle but profound details, such as the effects of charge transfer, magnetostriction and the onset of superconductivity, and will be of increasing use in the derivation of electrostatic parameters for the ab initio study of molecular and supermolecular materials.

Neutron powder diffraction provides the most accurate and reliable results that are largely free from systematic errors, despite the advent of third generation synchrotron sources. Increasingly, and even more so with the advent of the ESS, the complementary strengths of both X-rays and neutrons will be exploited in powder studies. As a few heavy atoms may dominate the diffraction pattern, X-rays are usually the method of choice for structure solution; neutrons are preferred for structure refinement, as all atoms are roughly equally visible, and generally larger samples result in smaller systematic errors. The host/guest configurations in the framework structures of zeolites provide an example of this powerful complementarity in a complex structure of technological importance. X-rays provide the initial framework details. Neutrons then give direct location of the active acid sites (i.e. the hydrogen position), the location, ordering, condensation processes and dynamics of the sorbate molecules inside the channels and cavities, and the topology of e.g. Al/Si segregation of the tetrahedral atoms which are the reactive centres in the zeolite framework.

In crystallographic studies of molecular compounds, both *neutron and X-ray diffraction* share a role with NMR and IR spectroscopy, though diffraction provides the most definitive answers to structural problems. Although the bulk of molecular crystallography will continue to be performed by laboratory X-ray techniques, neutrons will continue to make a unique impact through their ability to determine hydrogen positions and the fact that the chemical atom is a point scatterer of neutrons. Examples include the measurement of accurate positional parameters for all atoms for the determination of parameters for computational chemistry, the accurate determination of thermal motion and the investigation of materials in which hydrogen bonding plays a major role – an extraordinarily wide area which includes hydrides and hydrates, ferroelectrics, molecular and supramolecular chemistry, and structural biology.

With respect to *neutron stress measurements* in engineering use, destructive methods such as hole drilling and layer removal, as well as surface sensitive methods such as X-ray diffraction, will continue to provide additional information. Neutrons however provide perhaps the only way of refining and improving the reliability of the finite element models often used to predict residual stresses. Although very hard X-rays from some third generation synchrotrons may have penetrations that can begin to approach neutrons, their very short wavelengths result in low scattering angles, and hence restrict to a transmission geometry which is not suitable for many engineering applications. In radiography, the high penetration of neutrons gives clear advantages over synchrotron X-ray radiography. Furthermore, detection and inspection of hydrogenous materials, and materials containing neutron absorbers through walls of most of the technically important metals, is difficult or impossible with conventional X-ray or γ radiography.

In magnetic scattering, information from *neutron diffraction* is being complemented by *synchrotron X-radiation*, which is providing insights into magnetism through *magnetic dichroism, resonant magnetic scattering, extreme Q resolution, and the separation of orbital and spin contributions to the magnetic moment*. However, the weakness of non-resonant scattering and the absence of suitable resonances in the important 3d-transitional elements mean that neutrons have an important, if perhaps no longer unique, role to play. Magnetic single crystal neutron diffraction will still offer the best approach for the initial structure determination of a new magnetic structure, while, in spite of the advances in magnetic X-ray diffraction, magnetic neutron powder diffraction is, and will continue to be, the primary technique and the simpler tool for obtaining information about the arrangement of magnetic moments in crystalline solids.

In studies of ultrathin magnetic structures, *polarised neutron reflectivity* is the only method that provides a complete analysis of the magnetic structure, including the in-plane magnetic vector magnetisation profile and the coherence length of collinear and non-collinear spin structures in magnetic multilayers as well as magnetic disorder at buried interfaces. This information is necessary for understanding the basic interaction mechanisms in the multilayers, and for optimisation of devices such as spin valves. *Magneto-optic Kerr effect measurements* and *SQUID magnetometry* can be used in complementary experiments to determine magnetic reversal processes.

A complete understanding of magnetic properties requires the experimental characterisation of the 'imaginary' part of the magnetic susceptibility over a wide range of momentum and energy transfer (*inelastic magnetic scattering*). Of the potentially available local probes, NMR gives a momentum transfer average in the low frequency limit, while *light scattering* is too limited in momentum transfer space. The static part can now be studied using synchrotron sources (*magnetic X-ray scattering, spin-dependent X-ray absorption and dichroism*), but such studies are rather restricted to thin samples. Thus neutron scattering is today the only scattering probe that allows a full determination of the imaginary part of the susceptibility over the range in momentum transfer and energy that is of interest for magnetism in solids.

In contrast, *resonant magnetic X-ray scattering and dichroism* provide access to details in the electronic band structure that cannot be obtained from neutrons, and *magnetic X-ray scattering* is advantageous for small samples (including microcrystals), surfaces, or when high momentum transfer resolution is needed for critical phenomena studies. It is thus becoming increasingly clear that *neutrons and X-ray methods have to be combined* to optimise our studies of static microscopic properties. However, neutrons will remain the only probe able to study spin dynamics and magnetic fluctuations as a function of momentum and energy transfer in the energy range of μeV to hundreds of meV that is of interest to the physics of magnetism. Furthermore, the ease of performing neutron experiments under a wide range of extreme conditions remains a major advantage, as does the ease of interpretation of data resulting from the simple coupling between neutrons and magnetisation densities.

As in most areas of condensed matter, neutrons gain over X-ray methods where sample environment and the need to perform in situ measurements (e.g. of chemical reactions, physical transformations or where real-time materials processing is concerned). This is still the case when considering hard X-rays, where sample environment scattering is virtually unavoidable.

At very high pressures, synchrotrons can best measure lattice parameters and angles as a function of pressure; neutrons will be required to detect light atom positions.

When considering *reflectivity* in soft matter work of major industrial and environmental importance, X-rays can cover the same momentum transfer range, and offer higher flux than neutrons. However, in specular reflection, the ability to manipulate the refractive index makes neutron reflection more generally applicable for disentangling the quantitative elements of a complex interface. *Tunnelling and atomic force microscopy* probe the peripheral layer of atoms, giving little depth information and are, at the present state of development, generally qualitative. Understanding the various imaging processes is a current active research area. *Second harmonic* and *sum frequency generation* are very new techniques that give information about the orientation of groups in the interface, but no spatial information. They will be complementary to neutron reflection in some cases. Many of the qualitative surface analysis tools (*ESCA, SIMS, FABS etc*.) will remain high vacuum techniques, and hence are of little value in studying systems like soft solids where such environments are unacceptable.

The main techniques that 'rival' *small angle neutron scattering are light scattering* and *X-ray small angle scattering*. The ability to perform contrast variation, coupled with the weak interaction of the neutrons with materials, will continue to give neutrons a unique position in the armoury of techniques looking at these spatial scales. Furthermore, absolute measurements are straightforward with neutrons. For *light scattering*, although absolute measurements can be achieved, the inherent interaction strength finally limits the practical concentrations/thickness that can be achieved. *Light scattering* will continue to complement small angle neutron scattering in kinetics and dynamics areas associated with large (0.5 - 2 µm) scales. *Fluorescence methods* including *evanescent wave spectroscopy* are applied to similar systems in soft solids work, but on a different dimension scale, and so are complementary to other areas including neutron scattering.

In dynamical measurements of soft matter, the conventional electromagnetic probes (*photon correlation spectroscopy, fluorescence correlation and photobleaching recovery techniques and Brillouin light scattering*) operate on time scales that are long when compared to their neutron counterparts *quasielastic* and *spin-echo spectroscopy*. Similarly, the use of *multidimensional* NMR in the elucidation of local incoherent dynamical motions is often too slow and does not give long range correlations. Consequently, no technique can rival neutrons for the study of, for example, fast diffusional motion in porous media, segment dynamics and reptation, membrane fluctuations, or indeed the individual dynamics of molecules tethered to a surface. The methodologies therefore are complementary rather than competitive.

Neutron vibrational spectroscopy is strongly complementary to both optical (*Raman* and *IR*) and magnetic (*NMR*) spectroscopies. Again, the neutron technique gains from the relative simplicity of the neutron-nucleus interaction. Intensity information can therefore be analysed with greater confidence than the corresponding IR and Raman data. Moreover, optical studies are, in general, limited to a thin surface layer. In addition, the ability of the neutron technique to measure over a broad range of energy and momentum transfer yields spatial information that is related to the shape of the potentials. Its complementarity to optical techniques facilitates a better understanding of, and consequently more effective use of, *IR* and *Raman*. In proton transfer work, NMR studies are hampered by quantum effects and by strong motional neighbourhood interactions; inelastic neutron scattering is unique in being able to measure quantum tunnelling directly. In rotational tunnelling spectroscopy, neutron methods are complementary to *NMR*, *NQR*, *diffraction*, and *calorimetric measurements*.

In structural biology, the main complementary advantage of neutrons arises from deuterium labelling, contrast variation and the possibility of using a wide range of solvent conditions, in a range of (high and low resolution) *diffraction*, *reflectometry*, and *inelastic* measurements. There is also a much lower probability of sample radiation damage than for X-rays and electron microscopy. In studying functional dynamics in biomolecules, the wide range of time and length scales involved (femtoseconds – seconds; Å - 100 Å) of necessity requires a battery of techniques of which neutrons are an important one. *Quasielastic neutron scattering, two dimensional exchange NMR* and *quasielastic light scattering* methods are the best choice for increasing the width of the time window for the observation of dynamical processes in membranes. As their space and time resolution are very different, by combining the three methods, we can study selectively dynamical membrane processes over more than ten orders of magnitude. *Fluorescence* and *Mössbauer spectroscopies* also provide nanosecond time scale information on dynamics in proteins, while *IR* and *Raman* give femtosecond scale information on local vibrations. There is possible future potential in *quasielastic X-ray scattering*, which could complement *neutron spin echo* and *incoherent inelastic measurements*. As in liquids and disordered materials, computer modelling and molecular dynamics will be increasingly used in interpreting the results of both neutron and other measurements on complex biomolecular systems, as the methods increase in reliability and computing power and methodology improve.

In structural studies of liquids and disordered systems, the wide momentum transfer range accessible on pulsed sources, together with the simplicity of the neutron-nucleus interaction, makes neutrons the diffraction method of choice when accurate results are essential. Third generation synchrotrons promise to increase the momentum transfer range accessible using hard X-rays, and will ease the difficult correction problems associated with X-ray studies of liquids. Although a few demonstration experiments have been performed, it has not yet proved possible to determine partial pair correlation functions using X-ray anomalous scattering, though we should expect the outstanding problems to be tackled in the next decade. The fact that X-rays see electrons, however, means that the two techniques are genuinely complementary. The precision of nuclear data the ESS will provide, when combined with X-ray data, will yield, for the first time, accurate information on electron distributions in disordered materials. The element-specific local structural information that can be obtained from EXAFS and XANES methods again underlines the complementarity with neutron methods, especially as quantitative accuracy of measurements and theoretical calculation capability are improving.

NMR-based structural methods mostly provide information on local bonding in disordered materials, so may be considered as equivalent to EXAFS or to the very high momentum transfer part of the diffraction pattern. Although element specific, only a restricted range of elements is suitable, though these tend to be the important ones technologically. *Solid state NMR* is playing an increasing role in materials studies, and is now a truly useful complement to neutron scattering. However, adequate interpretation of NMR data is still a problem, with apparent inconsistencies remaining between indirect NMR and direct neutron results. More work seems to be needed on theoretical calculations of e.g. quadrupolar couplings and asymmetry tensors.

New developments in *inelastic scattering of synchrotron X-rays* are starting to achieve an energy resolution of a few meV, with further developments promising 1 meV as a likely resolution limit. Although initial results on liquid systems have attracted much attention, current experience is still too limited to know how quantitative a technique (in the sense of an absolute measurement of $S(Q,\varpi)$ as from neutrons), inelastic X-ray scattering is likely to be. The fact that it is being done at all underlines the importance of this particular region of space and time. The early results also show that it should be considered as a complementary technique. The fact that inelastic X-ray scattering sees electrons rather than nuclei is an important aspect of this complementarity, borne out by the early results on liquid lithium. Here, comparison with the neutron results suggests great promise in combining the X-ray and neutron techniques to extract higher order electron correlations. There thus appears great potential from the two techniques working together, though we should expect, in future, X-rays to be the choice for some studies, and neutrons for others, depending on the relative weighting of the mode(s) of interest and the resolution required. The absence of incoherent scattering of X-rays will, however, remain a fundamental disadvantage of inelastic X-ray scattering, preventing the motions of individual atoms being studied by the technique.

Light scattering will always be the fastest method of studying atomic dynamics, with techniques now covering a tremendous range of time scales, from 10^{-15} to 10^{2} s. However, all information is confined to very low momentum transfers, and there are problems of unknown matrix elements and high sensitivity to impurities or surface effects. There are in general clear advantages of studying dynamics of disordered materials with both neutron and light scattering techniques. *Field gradient NMR* should probably be the technique first used (where applicable) for studying diffusion of, e.g. H, if purely macroscopic information is required. However, because of the different time scales (10^{-4} to 10 s for NMR, 10^{-12} to 10^{-8} s for neutrons), the information obtained can be different. NMR spatial resolution is limited to momentum transfers $Q < 10^{-2}$ Å^{-1}, while neutrons cover the range 10^{-3} to 10 Å^{-1} . There is also a subtle difference between the macroscopic diffusion coefficient measured by NMR and the chemical diffusion coefficient measured by neutrons.

The opportunities of really effective exploitation of complementarity are dramatically increasing with our improving ability to use *computer simulation or modelling* to 'combine' the results from different techniques to obtain an interpretation consistent with the different sets of data on disordered systems. Techniques such as reverse Monte Carlo and their increasingly imaginative developments allow the optimal use of each individual technique where it provides most data and has least problems. Demonstration studies have been performed that combine data from neutron and X-ray diffraction, EXAFS, and NMR to give a consistent interpretation. Such approaches will become routine.

Despite many claims, the number of *molecular dynamics* simulations on the structure of disordered materials that agree within errors with the experimental results is tiny. Even fewer agree with experimental dynamics results. If molecular dynamics simulation is to realise its full capability as a predictive tool, accurate interatomic potentials that reproduce experimental data must be used. The central role of neutron scattering here is obvious, and the implied complementarity will be even more powerful with future increases in computing power that will make it routinely possible to 'tune' potentials by comparison with neutron scattering results. Such approaches are already beginning to make significant impact on the interpretation of neutron scattering results on relatively complex disordered systems. Examples include biologically-important interacting ligands in solution, as well organic and inorganic materials which are increasingly important to modern technologies, allowing a revolution in materials design and optimisation.

Societal needs and the ESS

The proposal to build the ESS reflects the growing need for new and improved tools that will deepen our understanding of the material world and enhance our ability to utilise effectively this understanding, to the benefit of societal needs across Europe. Neutrons are a vital component of the sophisticated array of such tools that probe the structures and motions of matter at the molecular and mesoscopic levels, a knowledge of which provides the essential clues in our understanding of both life processes and the functioning of modern industrial materials. The ESS will enable European Science and Technology to advance further together in the understanding, control, and sustainable exploitation of material properties on submicron scales to the benefit of mankind.

The science case for ESS is packed full of specific examples, some of which are summarised below. These are relevant, generally to fulfilling increasing societal needs along a widening front, and specifically with respect to the Foresight Themes of the various European countries, and to those generic technologies applicable to a wide range of industries.

The physics and chemistry of soft solids – an area of scientific endeavour often driven by the commercial significance of products that are a highly complex mixture of components and structures – will see major advances with the exploitation of ESS that will meet many future industrial needs. An understanding the molecular response of a wide range of relevant (often food-related) systems to deformation, shear, etc. is needed if we are to optimise *manufacturing processes and their control*. In surfactant systems, information will be gained relating to the production of new materials such as the synthesis of inorganic nanocrystals in inverse microemulsions and the formation of porous inorganic materials from sol-gel reactions in bicontinuous phase. Furthermore, many of the most important industrial products are connected with porous materials, with the behaviour of the contained fluid being a critical feature in reactive control. Examples which will benefit from the capabilities of ESS include oil-bearing rocks, water-saturated soils, separation materials, heterogeneous chemical materials such as silicas and zeolites, as well as an enormous range of foodstuffs, cleaning powders and pastes, building materials and cosmetics. The number of Foresight Priority themes relating to these systems is considerable, including *health and lifestyle, workplace and home, biomaterials, catalysis, chemical and biological synthesis, materials process technology, agriculture, environment, energy, and food and drink*.

Interface studies are a particularly powerful technique through which ESS will make major advances possible in a wide variety of areas important to societal needs. Obvious examples include detergent development, paints, inks, coatings, composite materials such as polymers and alloys (including understanding the bonding between the different components), areas of *food technology* such as the stability and structure of emulsions, foams, gels, etc., as well as the physics of lubricants and adhesion, fuel additives and aspects of oil recovery. In 'harder' materials, we instance the need to understand magnetic multilayers, including those with giant magnetoresistance properties, that will be a major player in the future of the *control* and *information storage* device industries. ESS will also perform surface work relating to functional layers in electronic packaging, gas adsorption and reaction processes involved in both gas *sensors* and *catalysis* processes. Advances in understanding corrosion – including stress corrosion – could contribute to reducing annual losses from these processes of billions of ecu.

The kinds of studies of interfaces ESS will enable will have a particular influence on electrochemistry, where buried interfaces will be accessible, together with *in situ* studies of many relevant processes from those involved in battery technology, phase transfer catalysis, biological systems, and the corrosion of metals and alloys. Access would also be possible to electrochemical processes in exotic media such as supercritical fluids, or liquid sulphur dioxide or ammonia, areas which are becoming extremely important in industrial applications. There are clear implications here for areas such as *energy technology, clean process technology, waste management, catalysis*, and *future transportation systems among others*.

Materials research itself – both on new structural and functional materials, and on their properties and processing (including 'decommissioning' and disposal) – is a common priority in Europe. Here, ESS will have major effects, both with respect to classically crystalline materials and less-ordered ones such as glasses. In the *energy technology* field, work on systems such as fast ion conductors and hydrogen-storage materials could influence the development of new battery systems and fuel cell technology, while molten salt and liquid metal research and development relating to radioactive waste processing, advanced reactor coolants and electrolytic production of aluminium also relate clearly to *environmental integrity*. In *transportation*, in addition to batteries, fuel cells, and hydrogen storage, developments will also relate to sensors (of very general applicability in control and monitoring systems), *coatings* for engine components and hard and soft magnets (e.g. for electric motors). In *information technology, microelectronics*, and *telecommunications*, developments ESS will be involved in include optical fibres, electro-optic materials, sensors (again), semiconductors, solar cells, magnetic recording, magnetic media and smart windows. In 'general' *materials and chemicals development*, we can example ceramics and ceramic coatings, composites and catalysis. In *structural materials*, ESS studies will contribute to satisfying the increasing demand for lightweight high temperature materials, particularly for *new generation aircraft*. Not only will the intrinsic properties of these new materials gain from neutron studies at ESS, but also their response to in-service use will benefit from the facilities in the Engineering Research, Development and Test Centre.

Biomaterials developments will build on work on increasingly complex systems that ESS will be particularly well suited to deal with, in terms of understanding complex synthesis procedures, property tailoring, surface interactions in contact with generally highly corrosive biological fluids and materials ageing. Obvious examples are dental materials and implants.

Understanding life behaviour and degradation of materials in general is an important issue, and here again the science case for ESS heralds significant contributions. Much work remains to be done on 'old' *structural materials* such as cements, as well as on the behaviour of materials under severe irradiation conditions, both in service, and during subsequent long term storage as vitrified waste. Corrosion, being an electrolytic process, has already been mentioned in an earlier context.

There is major potential in developments relating to liquid systems. Understanding interactions in solution will be a major element in improving our present poor understanding of such a basic process as solubility, of vital importance to the chemical industry (including *food technology*) and to *biotechnology* development. The way is open to the tailoring of specific liquid media to allow processing at lower temperatures than at present, and with reduced adverse *environmental load*. The implications here for *health and lifestyle, food science, clean processing* and *environmentally sustainable technology* are obvious.

ESS will open up opportunities in biology and biotechnology. High resolution structural work will be of relevance in *pharmaceuticals, agriculture* and *biotechnology* generally: structure based protein and drug design both require high precision structures with location of hydrogen atoms and water molecules if the nature of the important interactions that control binding and association are to be understood. Work on supported membranes and polymer films will feed into biosensor development. Further *pharmaceutical* applications include structures and dynamics of drug delivery systems such as vesicles, improved understanding of membrane transport and the structures of artificial cells. In *medicine* also, information will be delivered on basic biomolecular structures and dynamics, while work – in solution and in crystal environments – on supramolecular structures such as viruses, the signal recognition particle and the ribosome, will complement X-ray studies. *Agriculture* will benefit in terms of studies of structures and interactions of pesticides and herbicides, interactions with plant cells and membranes and the study of plant viruses. *Environmental quality* will gain from the development and characterisation of biodegradable materials, while a range of other applications in *biomaterials* has been discussed above.

The Engineering Research, Development and Test Centre will, as already indicated, play a major role in, among other Foresight priority areas, *structural materials*, *design optimisation* of components for their performance requirements, *risk assessment*, and *health and safety*. In addition to inspection and performance assessment of the materials themselves, the Centre will give the process engineer a unique capability to both monitor and develop processing performance and technology, through a versatile array of real-time radiological and element and temperature specific tomographic techniques. The latter kind of work will be particularly relevant in following bearing lubrication and oil transport in running (both aircraft and auto) engines, evaporation processes and coolant transport, improved pump, valve and clutch operation. In nuclear engineering, the Centre will be equipped for a variety of work relevant to the integrity and performance of nuclear materials. Overall, the unique insights the centre will offer into the performance of industrial components and industrial processes will be ever more necessary if European industry is to compete in increasingly competitive global markets.

In Earth and Environmental Sciences there are contributions that work at ESS will make that are of major *environmental* significance. Mechanisms behind phase transitions that are thought to be relevant to earthquakes can be studied, with obvious implications for earthquake prediction. Similarly, work on rheological properties of magmas is needed to obtain an understanding of volcanic eruptions. Less dramatically, but also important to the *quality of life*, improved methods of building and art monument preservation are likely, as are significant reductions in present-day losses (up to 70%) in quarrying of high quality stone. *Environmental issues* relating to the transport of pollutants in the Earth's crust and the inhibition of fouling growths in e.g. marine environments, will also benefit.

Predicting the future is always fraught with uncertainty. Whilst all the scientific dreams may not be realised, the vast amount of new science which would be achieved with the ESS, and its importance on societal needs, is beyond any doubt.

3. Neutron instrumentation at the ESS

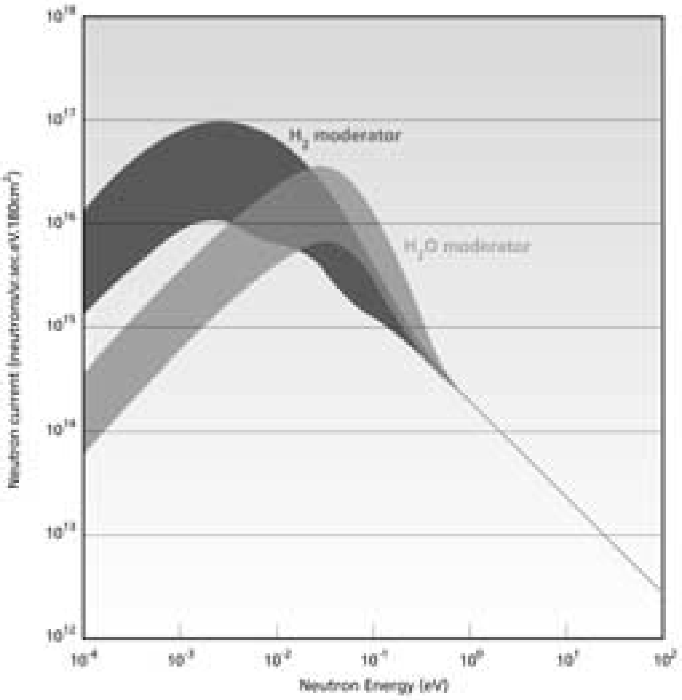
The past twenty years have seen a rapid development in the performance and sophistication of neutron instrumentation on pulsed sources which has rivalled the growth in source strength itself. The first generation of pulsed source neutron scattering instruments, which were built at modified high energy physics accelerators and electron linacs, were superceded by second generation instruments at purpose-built facilities such as ISIS. By incorporating advances in detector design and data acquisition technology, these instruments have become quantitatively different from those on reactors, and software developments have led to visualisation capabilities unthought of a generation ago. Further developments are continually taking place.

The ESS will be furnished with third generation pulsed source instruments designed with the aid of sophisticated Monte Carlo methods, based on the experience at existing sources and incorporating advanced optics and the latest detector and polarisation techniques. This will have a multiplicative effect on the performance of the source. Gains of three orders of magnitude in performance can be anticipated in some cases through the combination of source enhancement and instrumentation development.

A reference instrument suite for the ESS

The source parameters at a pulsed neutron facility play an integral part in defining the characteristics of the instrument. The repetition rate of the pulses at the target determines the time frame over which data are collected and hence the dynamic range explored in an experiment. Two target stations, delivering high and low frequency sharp pulses respectively, allow a broad and balanced coverage of the whole scientific programme envisaged in Chapter 2. The material, temperature and neutronic properties of the moderators and reflector dictate the trade-off between spectral intensity and pulse characteristics which play an important part in defining instrument resolution. Accordingly, in the reference design one neutron target (and the muon target) will operate at 50 Hz, and the second neutron target will operate at a lower frequency, say 10 Hz. The two neutron targets will provide qualitatively different beams, the high frequency target concentrating on thermal and epithermal neutrons with moderators decoupled from the reflector, thus maintaining the sharpest pulse possible. The low frequency target will have two moderators, both at liquid hydrogen temperature for the generation of cold neutrons. One moderator will be tightly coupled to the reflector to maximise the intensity of the beams and the second will be decoupled to provide high resolution. The parameters of the low frequency target will be specifically chosen to allow high band-pass instruments to operate optimally (see figure 2).

Figure 2: ESS neutron current. The neutron current (neutrons per steradian per second per electron Volt times moderator surface) from cryogenic and ambient temperature moderators. With appropriate choices of decoupler and poisons, flux and pulse width characteristics can be optimised.



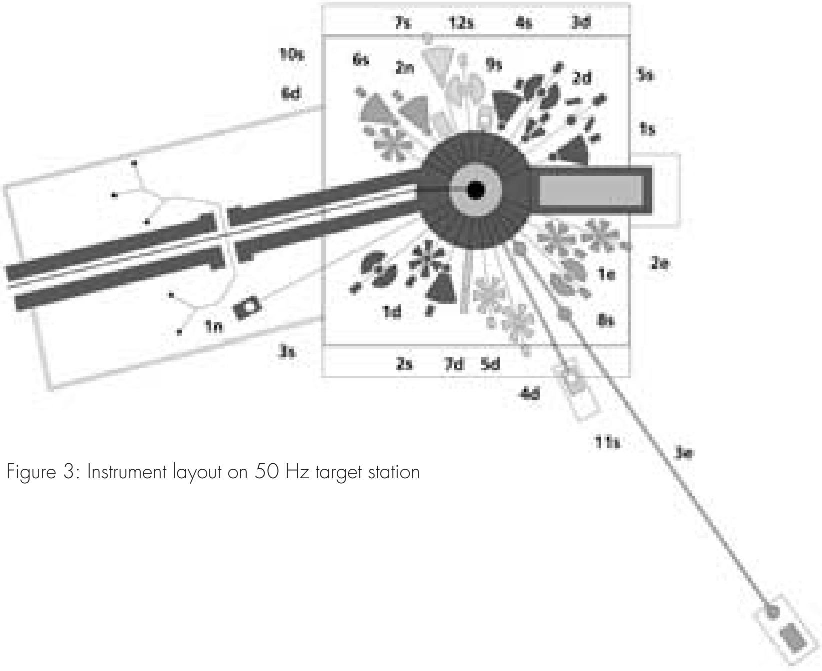


Figure 3: Instrument layout on 50 Hz target station

Table 1: Target Station 1 – High Frequency 50 Hz

Ambient High Resolution Moderator (9 Instruments)

Name	Description	Length
1d	High Intensity Powder Diffractometer	15 m
2d	Liquids & Amorphous Diffractometer	10 m
3d	Single Crystal Diffractometer	10 m
1s	High Energy Chopper Spectrometer	10,6 m
2s	Polarised High Energy Chopper Spectrometer	10,4 m
3s	Electron Volt Spectrometer	15 m
4s	Medium Energy Chopper Spectrometer	10.3 m
5s	Molecular Spectrometer	15 m
1n	Nuclear Physics Instrument	50 m

Cold High Resolution Moderator (15 Instruments)

Name	Description	Length
4d	Biology Diffractometer	20 m
5d	High Pressure Powder Diffractometer	12 m
6d	Special Environment Single Crystal Diffractometer	15 m
7d	High Intensity Small Angle Scattering Instrument	10 m
6s	Low Energy Chopper Spectrometer	10,6 m
7s	Polarised Low Energy Chopper Spectrometer	10.3 m
8s	Polarised Crystal Analyser SX Spectrometer	25m + guide
9s	Crystal Monochromator Spectrometer	10,2 m
10s	Multi-Chopper Low Energy Spectrometer	15 m + guide
11s	Near-Backscattering Spectrom.	40 m + guide
12s	Backscattering Spectrometer	15 m + guide
1e	Engineering Diffractometer	15 m
2e	Engineering Diffractometer	15 m
3e	Radiography and Tomography Instrument	10,30,100 m
2n	Ultra Cold Neutron Nuclear Physics Instrument	10 m

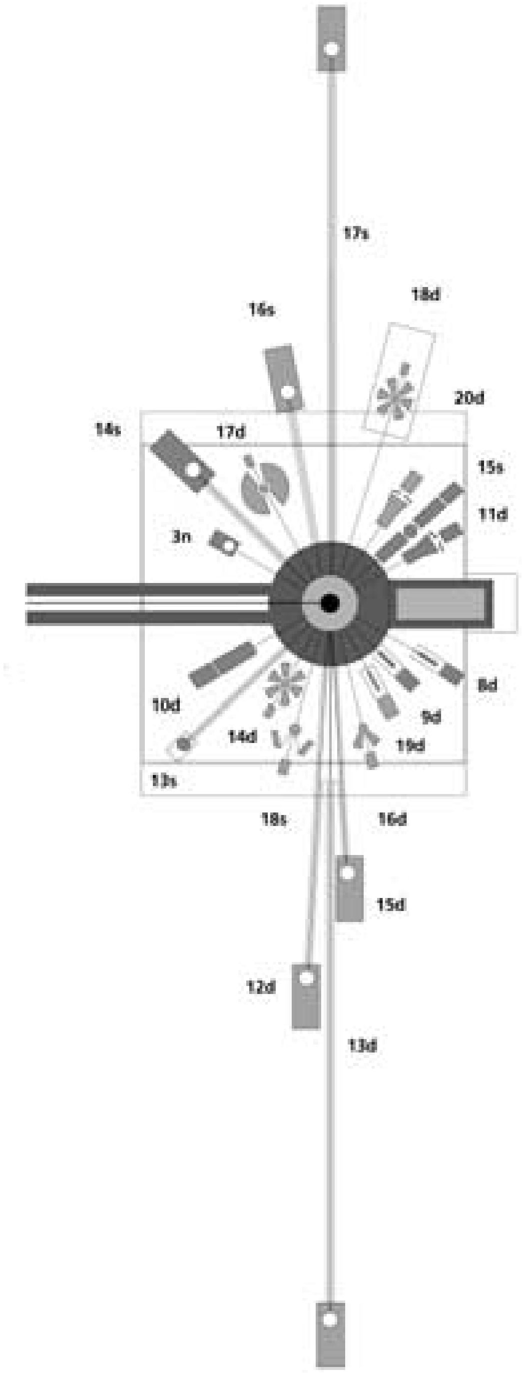


Figure 4: Instrument layout on 10 Hz target station

Table 2: Target Station 2 – Low Frequency 10 Hz

Cold High Intensity Moderator (8 Instruments)

Name	*Description*	*Length*
8d	High Intensity Reflectometer	10 m
9d	Chemistry Reflectometer	15 m
10d	Small Angle Scattering Machine	20 m + guide
11d	Polarised Beam Small Angle Scattering Machine	10 m
13s	High Intensity Single Crystal Spectrometer	40 m + guide
14s	Polarisation Analysis Near-Backscattering Spectrometer	35 m + guide
15s	Spin Echo Spectrometer	12 m
3n	Nuclear Physics Instrument	20 m + guide

Cold High Resolution Moderator (12 Instruments)

Name	*Description*	*Length*
12d	High Resolution Powder Diffractometer	75 m + guide
13d	Ultra High Resolution Powder Diffractometer	150 m + guide
14d	Polarised High Intensity Powder Diffractometer	10 m
15d	Magnetic Powder Diffractometer	50 m + guide
16d	Liquids & Amorphous Diffractometer	25 m
17d	Magnetic Structures SX Diffractometer	20 m
18d	Extreme Conditions Diffractometer	40 m + guide
19d	Physics Reflectometer	15 m
20d	Small q Diffractometer	20 m + guide
16s	Polarised Crystal Analyser SX Spectrometer	40 m + guide
17s	Backscattering Spectrometer	90 m + guide
18s	Molecular Spoectrometer	25 m + guide

A unique feature of both target stations will be the provision of bundles of neutron guides feeding a larger number of instruments than would otherwise be possible. Confidence gained on existing spallation sources has demonstrated clearly the viability of neutron guides, which were previously the preserve of reactor sources. Effective utilisation of guides will allow (i) increased source utilisation, (ii) the effective use of shielding and (iii) the optimum siting of instruments.

On a pulsed source, distance from the moderator is a fundamental factor influencing the instrument performance. Altogether 44 neutron scattering instruments will operate around the facility, with capacity to expand as demand determines. The same consultation exercise which was used to explore the scientific potential of the ESS has produced a balanced set of instruments – spectrometers, diffractometers and reflectometers – with which to deliver the anticipated programme. In parallel, four instrument groups considered what specialist developments were needed in the areas of Single Crystal Excitations, Large Unit Cell Crystallography, Small Angle Scattering and High Resolution Spectroscopy. From this process, the reference instrument suite for ESS emerged and R&D requests were identified.

The reports of the scientific and instrument working groups have identified a generic set of instruments – 62 in total – which cover the whole parameter space accessed by neutron scattering and fully satisfy the needs of the scientific programme. This is an important and significant statement which could not have been made with confidence prior to this study. In particular the four instrument groups – specifically charged with a critical review of instrument areas in which an insufficient demonstration of potential had yet emerged – were resoundingly positive. Three of these areas depend upon high fluxes of cold neutrons where a recognition of the intense beams available has been slow to reach a wider consciousness, and the fourth relates to the standard-bearer of the measurement of collective excitations in single crystals – the triple axis spectrometer. For a large proportion of these instruments, improvements in data rates of between one and three orders of magnitude will result compared to the present world's best instruments – regardless of whether they are reactor or spallation source based.

These 62 generic instruments have been distilled down to 44 instruments – the reference set of instruments – which will cover the scientific programme well. Some instruments, for example polarised versions of chopper spectrometers, are kept in reserve pending advances in technology.

The 44 instruments are assigned almost equally between the two target stations. Five instruments are devoted to fundamental neutron and nuclear physics and the remainder cover elastic and inelastic scattering, with the elastic instruments slightly in the majority. A set of these instruments will form the proposed Engineering Research, Development and Test Centre – a novel concept which bridges the gap between scientific and industrial applications of neutron scattering. The reference set of instruments is listed in Tables 1 and 2 and an instrument layout for each target is shown in Figures 3 and 4.

A complete report on the proposed instrument suite is presented in the ESS Report, *Neutron Instrumentation for the European Spallation Source*. This report contains descriptions of each instrument, layouts around each target station and costings, as well as the full reports of the four specialist Instrument Working Groups.

Experimental infrastructure and support facilities

Dealing with 2500 visiting researchers in a year with 250 on site at any one time demands excellent user facilities. These will include a purpose-built accommodation block and restaurant facilities run on commercial lines and available seven days a week. Users will have electronic access from their study-bedrooms to data collection and analysis facilities and to the site library system. Lecture theatres and seminar rooms appropriate to a large international facility will be needed. The ESS campus will be a focus for European scientific endeavour, will have the ability to host major international symposia and will be a natural meeting place for scientists from all over the World.

A full set of experimental support facilities will be an essential aspect of the efficient operation of the facility. These include:

User liaison centre

The lubricant for the whole scientific programme will be the User Liaison Centre. It will be the focus for user needs – registration, accommodation, and transport; beam time applications and their review; information, training and experimental safety. The co-ordination of information flow, statistics and performance figures, will be a central role for the User Liaison Centre.

Instrument operations and support

The programming of instrument schedules will be a co-ordinated task involving the User Liaison Centre, instrument scientists and the Instrument Operations and Support group. Sample environment equipment – cryostats, furnaces, pressure cells, magnets etc. – will be developed, supplied and operated by the Instrument Operations and Support group. Instruments will be maintained, and upgrades implemented through this team.

Specialist technical support

The optimisation of instrument performance will be software driven with sophisticated monitoring processes for detectors, electronics, compressors, choppers and vacuum systems. Sample preparation laboratories covering all major disciplines, from engineering to biology, and experimental safety in all its aspects, will come under the wing of Specialist Technical Support. It will also house essential development laboratories.

Dedicated support laboratories are crucial, especially to facilitate the exploitation of new frontiers as set out in Chapter 2. The Engineering Research, Development and Test Centre will be paralleled by appropriate facilities in other areas. The specific needs of biologists, where sample sensitivity is particularly critical, are recognised in the provision of a specialist Biology Support Laboratory.

Data management and flow

The ESS will generate an immense amount of data – up to 10 Terabytes per annum. Streamlining and managing the flow of this information will be the role of the Data Management & Flow group. An integrated team will supervise the data acquisition, data visualisation, and data analysis. Totally radical solutions will be necessary to manage this task.

R&D for neutron scattering instrumentation and techniques

Although present knowledge and experience will allow the construction of third generation instruments that will deliver the projected ESS scientific programme, a range of R&D issues have been identified which will provide a stronger platform from which to launch the instrument construction programme.

Some of these involve identified improvements in component performance which, in addition to being essential for ESS, will also yield dividends on the present generation of sources. These include faster, less expensive detectors, improved optics for neutron guides and focusing devices, white-beam polarisers such as 3 He, compact beam shaping devices and improved software for data visualisation and analysis. The development of a better theoretical understanding of correction factors is also required in specific areas such as reflectometry.

Other areas requiring R&D are the development and prototyping of novel instrumentation. Particular examples have been identified: a white-beam neutron spin-echo spectrometer, a fully operational 300 neV resolution backscattering instrument, a cold neutron coherent excitations spectrometer and a single crystal diffractometer using cold neutrons.

Background suppressing techniques, including a full understanding of potential cross-talk between the instruments, also need to be explored.