

Future access to neutron sources

A strategy for the UK

Appendices

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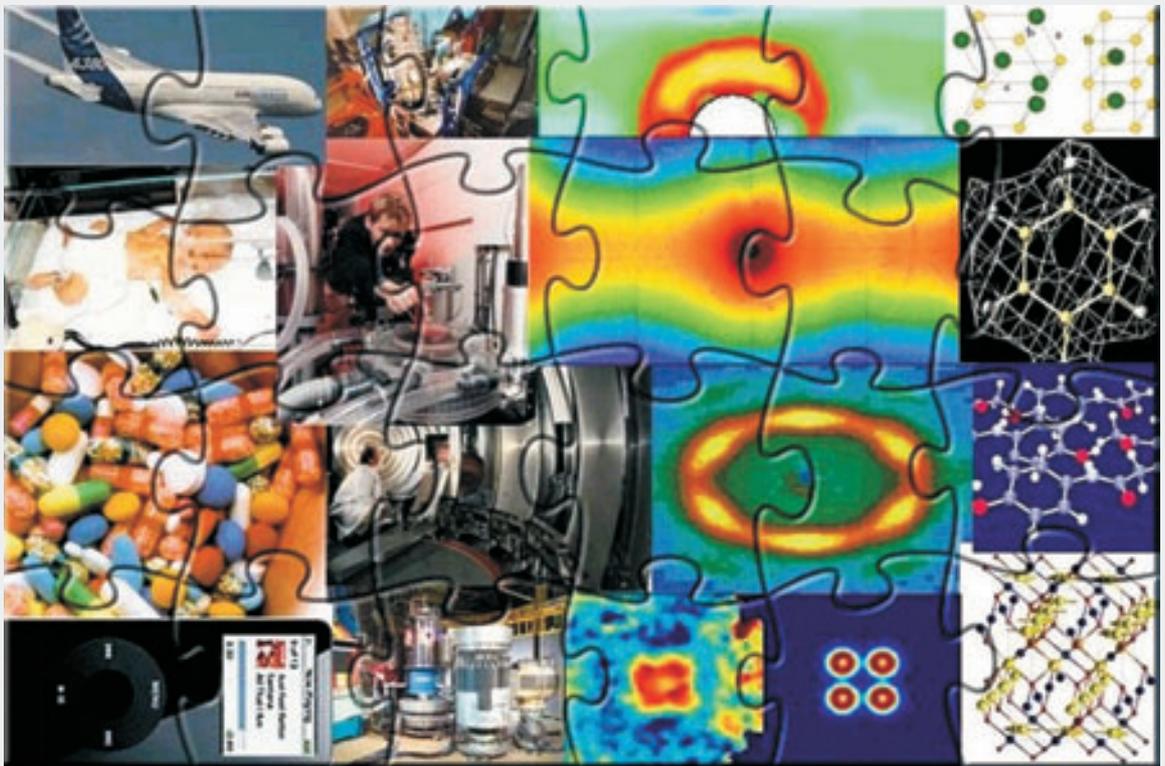
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The Science Case



Neutrons

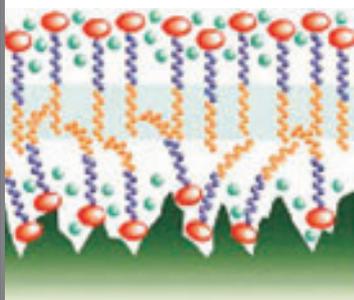
Neutrons for future science and technology



Neutrons

for future science and technology

Science in the early part of the 21st century is increasingly being driven by the need to expand and exploit a 'high value' technological economy. Society wants more and more complex and sophisticated materials that are lighter and stronger, devices that are smaller and cheaper, medicines that cure diseases quickly with minimal side effects, and everything must be energy efficient and environmentally friendly. This will require the development of, for example, new sensors and electronics, smart responsive structural materials and synthetic bio-materials. It will demand a detailed understanding of the relevant physical processes.



The increasing complexity means that scientists and engineers will need a range of complementary methods to unravel and optimise the properties of these new materials, and lead on to the next generation. Because of its unique abilities, neutron scattering will play a vital role in the portfolio of analysis techniques, in fields as varied as energy, nano-technology, materials processing, drug design, biotechnology, green technology and information technology.

Neutrons play a definitive role in our understanding of the material world around us, and have done so for the past fifty years. For example, the foundations of our atomic understanding of magnetism are mostly provided by neutron scattering. Our detailed knowledge of atomic and molecular dynamics owes much to pioneering research using inelastic neutron scattering.

The UK is a leading international player in the development of neutron based techniques. Starting from the early days of research at AERE Harwell, then through its key role in both the Institut Laue Langevin and the ISIS spallation neutron source, the UK has developed an outstanding academic user base for the broad scientific exploitation of neutrons across the scientific disciplines, from solid state physics and structural chemistry, through engineering and materials science, to the investigation of soft condensed matter and biomaterials.

Neutrons can show where atoms are and what atoms do. They allow scientists to look inside the structure of matter, from the vibrations of individual hydrogen atoms to the folding of proteins, from the high temperature and pressure needed to probe the properties of the earth's interior to the low temperature and high magnetic field needed to unlock the secrets of superconductivity.

Neutrons will, for the foreseeable future, continue to make significant, unique and necessary contributions to help solve numerous scientific and technological problems, from the understanding of fundamental physics to the optimization of industrial processes. Looking back over the last century, we can see that we are not very good at predicting, even 20 years into the future, which discoveries science will make or which directions technology will take. But we can clearly see that, given their unique abilities and the breadth and depth of their applications, neutrons will certainly be needed.

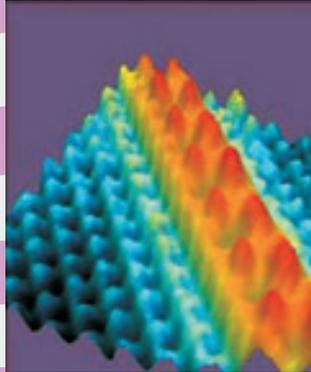
Because of their very wide range of applications, neutrons will provide underpinning scientific solutions in many of the current and future priority areas that are crucial for future technological solutions. and applications.

Drug design and pharmaceuticals



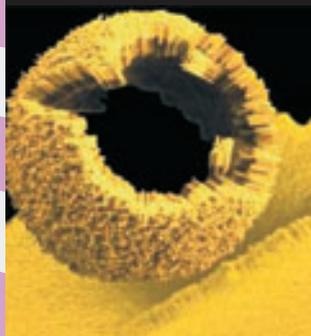
- Development of safe and efficient targeted drug delivery systems, such as in gene therapy
- Exploitation of natural antibiotics in the treatment of drug resistant pathogens
- Protein folding and mis-folding; degenerative diseases
- Understanding the associated processes at a molecular level

Nanotechnology



- Templating for the synthesis of new materials
- Nano-composites for lightweight structural materials
- Nano-fabricated magnetic clusters or molecular magnets or for quantum computers
- Atomic scale characterization of nano-particles

Sensors and smart materials



- Functionalised surfaces and interfaces
- Sensors and bio-sensors (lab-on-a-chip)
- Photoresponsive and polymer based materials for devices, displays and recording media
- Improved lubricants, adhesives and coatings
- Molecular electronics – beyond silicon

Bio-technology



- Bio-sensors (tissue based sensors)
- Synthetic bio-replacement materials with improved bio-compatibility and bio-lubrication – bio-mimetics
- Food technology

Environment and clean technology



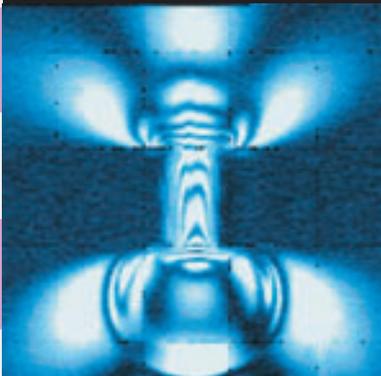
- Catalysts
- Materials for carbon sequestration
- Environmentally friendly materials, e.g. 'green' refrigerants
- Mineralogical origins of earthquakes and volcanoes
- The use of natural enzymes to break down environmental contamination
- Safe radioactive waste disposal

Energy for the future



- Hydrogen storage materials
- Fuel cell components; oxide ion conductors
- Clathrate hydrates for energy sources
- Light, high energy density batteries
- Energy efficient transport; superalloys, ceramics, fuel additives
- Next generation nuclear reactors

Materials and processing



- Processing of soft solids and complex fluids in extruders, mixers, pipe flow and micro-fluidics
- Controllable rheology for lubricants and oil extraction
- Structural integrity and safety: remediation of residual stresses in alloys, composites and welds
- Light weight, high strength alloys and composites; superconducting wires, bulk amorphous alloys
- In-situ measurements to understand materials synthesis, processing and treatments

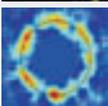
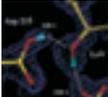
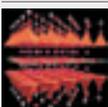
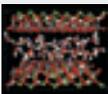
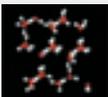
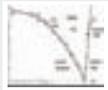
IT and quantum devices



- Giant magnetoresistance and exchange bias for spintronics and high density data storage
- Hard thin film magnets for micro-motors, -switches and -sensors
- Understanding magnetic roughness and phase diagrams – towards better electronic devices
- Understanding quantum complexity

Neutrons

50 years of scientific success



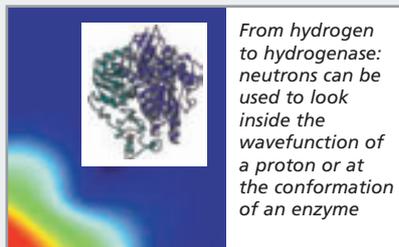
Neutrons have been making key contributions to our scientific knowledge for more than half a century. Continuous development of techniques and technologies has led to a continuous improvement in experimental capabilities, which has in turn led to a continuous broadening of the range of applications. Neutrons have been one of the first techniques of choice for detailed characterization of the atomic and magnetic structure and dynamics of many of the important new classes of materials that have been discovered or developed. They have also played a key role in validating many of the most important theories and models of the behaviour of condensed matter (and in disproving other theories).

- The first determinations of magnetic structures were made by Shull (Nobel Prize 1994) using neutron diffraction, confirming the theoretical ideas of Néel (Nobel Prize 1970). Without neutrons our microscopic understanding of magnetism would still be mainly theoretical. They remain the most important technique for determining magnetic structure and dynamics at the atomic scale.
- The development of triple axis neutron spectroscopy by Brockhouse (Nobel Prize 1994) led to the first measurement of phonons, confirming the quantum theory of solids. This provides the basis for our understanding of atomic dynamics in crystals.
- The elementary excitations in superfluid helium (^4He) - 'rotons' - were measured using time-of-flight neutron spectroscopy. Later 'tour de force' studies extended this to the 'Fermi liquid' ^3He . Such experiments provide stringent tests of our understanding of fundamental statistical physics.
- Small angle neutron scattering has been used to determine that polymer chains in the liquid state have a random coil conformation, as predicted by Flory (Nobel Prize 1974).
- Polymer reptation dynamics has been measured using neutron spin-echo spectroscopy, validating the model of de Gennes (Nobel Prize 1992).
- Bonding electron distributions have been determined using the combination of highly accurate neutron and X-ray single crystal diffraction data.
- Neutrons have made essential contributions to the understanding of phase transitions, for example in the measurement of soft modes.
- Neutron diffraction studies of ions in solution, using isotopic substitution to 'pick out' the arrangement of water around the ions, overturned textbook ideas of ionic solvation. Diffraction and reflectometry studies, using contrast variation to highlight the contributions of particular parts of complex molecules, have proved crucial to our microscopic understanding of the behaviour of soft matter systems such as polymers and surfactants.
- Neutron diffraction measurements determined the crucial importance of copper-oxygen arrangements in high temperature superconductors, discovered by Bednorz and Mueller (Nobel Prize 1987). Measurements of the magnetic dynamics have shown that magnetic interactions are crucial to understanding the mechanism of high temperature superconductivity.
- Neutrons have made significant contributions to our understanding of the structures and dynamics of fullerenes and fullerides, as discovered by Cull, Kroto and Smalley (Nobel Prize 1996).

See the world in a unique way

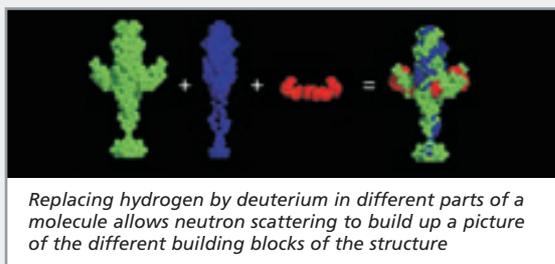
Length and time scales:

Neutron scattering enables us to study atomic and magnetic structure and dynamics over an enormous range of distances and times, from 10^{-11} m to 10^{-6} m and from 10^{-14} s to 10^{-6} s. While other techniques can provide information either within the same distance range or the same time range, this combination of both structural and dynamical information is unique to neutron scattering.



Sensitivity and selectivity:

The amount that neutrons are scattered by chemical elements of similar atomic weight, or even by different isotopes of the same element (such as hydrogen and deuterium), can vary significantly. This allows us to isolate or highlight particular atoms, or groups of atoms, in mixtures or complex materials.



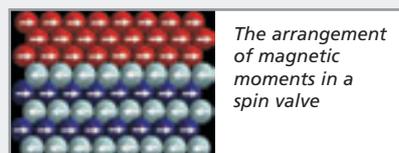
Penetration:

Neutrons pass easily through most materials, allowing us to study large or bulk samples, and buried interfaces, under extreme conditions such as high temperature or pressure. Neutrons are non-destructive, so delicate materials or precious objects can be studied without fear of damage. Neutron imaging techniques can be used to look inside objects as large as a car engine.



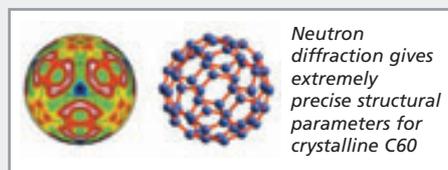
Magnetism:

The neutron acts as a tiny magnet, but has no charge, so we can use it to study the magnetic structures and dynamics of materials at the atomic scale, which underpin the properties we use in the everyday world.



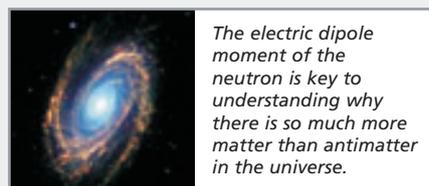
Precision:

Neutrons are a very precise tool. Their interaction with atoms is weak which makes analyzing the data, and understanding it, straightforward. We can easily compare neutron scattering results with computer simulations or models.



Fundamental properties:

Studies of nuclear and particle physics using slow neutrons probe the fundamental interactions in nature, helping us to understand events from the creation of the chemical elements during the first few minutes after the big bang of the universe to supernova explosions billions of years later.



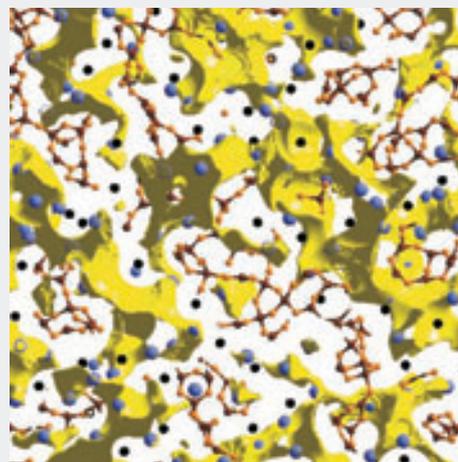
Providing pieces of the puzzle



The neutron is an indispensable tool for studying atomic structure and dynamics in condensed matter because of its particular unique properties. However, the value of neutron data can be considerably enhanced by combination with complementary data obtained by other methods, and similarly data obtained by other methods are enhanced by combination with neutron data. There is no single experimental technique that can provide us with all the

information we need to know about materials. Different techniques, based on different physical processes, provide different information. As the complexity of the materials under study increases, the approach needs to become 'problem based' rather than 'technique based'. The future trend is towards the use of multiple complementary experimental techniques, each of which gives us some pieces of the puzzle. Advanced techniques of computer simulation and modelling can be used to help put these together.

Developments in experimental techniques over the past decades have been amazing, and will continue to be so in coming decades. X-ray tubes have given way to 3rd generation synchrotrons with many orders of magnitude greater brilliance, and this trend will continue with the X-ray free electron laser. Optical lasers can now be used to investigate matter on the timescales of chemical reactions. Developments in neutron source power have been more modest, so why do an ever greater number of scientists use neutron scattering to study an ever wider range of scientific problems? On the one hand, neutrons offer unique characteristics as an experimental probe. On the other hand complementarity means that advances in the use of one probe, e.g. X-rays, produce an increased demand for information that can only be provided by another probe, e.g. neutrons. The combination of information means that the result is very much greater than the sum of the individual parts.



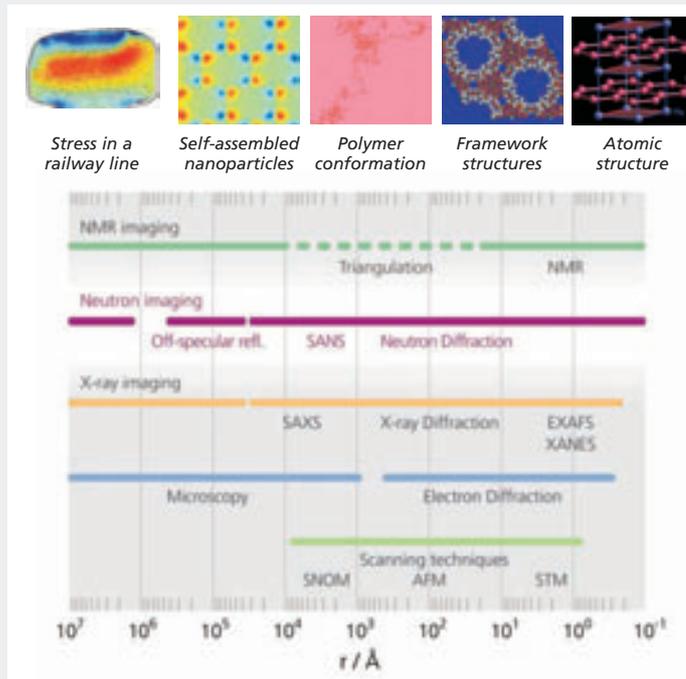
Structure of a glass, showing pathways for ion conduction. Such structures have been derived using computer modelling techniques directly based on the combination of complementary experimental data from neutron diffraction, X-ray diffraction, EXAFS and NMR

Because of the simplicity and weakness of the scattering interaction, atomistic computer simulations, models and theory can be used to straightforwardly calculate the expected neutron scattering data, and hence can be rigorously tested by experiment. This relationship is in general far more direct than with any other experimental technique. Neutrons therefore have a special role to play in the validation of both computational and theoretical techniques, and of the interaction potentials or other input parameters that may be used in them.

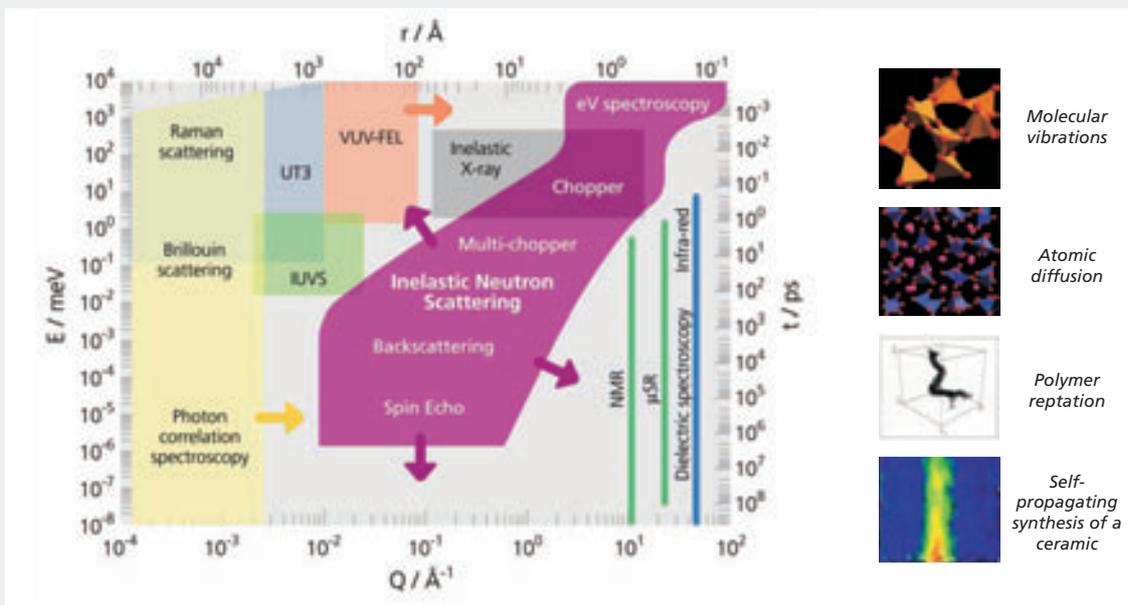
Filling the gaps

For structural studies there is considerable overlap in terms of the distance scales covered by different techniques, but the information obtained is nearly always complementary because of the different element specificity. Neutron scattering plays the major role in magnetic structure determination. Microscopy techniques are typically only applied to very small samples, which can be an advantage or a disadvantage depending on the application.

For dynamical studies the complementarity of inelastic neutron scattering and other experimental techniques is remarkable. The degree of overlap is small. Indeed, this is actually a disadvantage as it means that the differences in element specificity cannot be exploited as well as they can in structural studies. Instrumental and technique developments, both for neutrons and other methods, are currently tending to 'fill in the gaps', rather than providing more overlap.



Distance scales covered by some complementary experimental techniques. These vary by a factor of 10^6 , equivalent to the size difference between a football and the earth



Areas in distance-time covered by some complementary experimental techniques. Those that only probe time dependence, but do not directly provide distance information, are indicated as bars along the time direction. The time scale only refers to equilibrium phenomena. Non-equilibrium effects, such as those studied in 'pump-probe' experiments at very short times (fs) will always remain the domain of photon based techniques. With neutron techniques 'pump-probe' experiments may be possible down to μ s, covering the longer length and time scales important in soft condensed matter and biological systems.

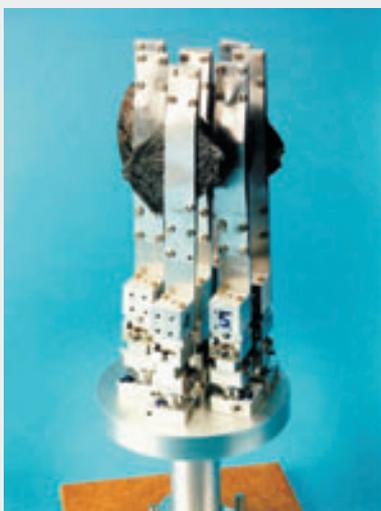
The future ... Neutrons

This science case gives a glimpse of what could be achieved, with the right investment at the right time. The breadth of applications of neutron scattering continues to grow, and advances in complementary techniques only increase, rather than decrease, this breadth. However, if the neutron facilities of today and tomorrow are really to realise their full potential,



they need to offer more than just neutrons, more than just the continued development of instruments, optics, detectors and techniques that has been so successful up to now. They must form a core part of a 'research super-centre' which provides a whole range of scientific capabilities, based on the 'user service' model which has been used so effectively at neutron facilities over the past 30 years. The majority of future 'users' will be experts in the particular scientific problem, not experts in using neutrons as a step towards the solution. Scientists based at neutron facilities of the future will act as the 'neutron expert' in a multidisciplinary approach to an increasingly wide variety of problems. This will require more than just neutron sources and neutron instruments. It will require a broad based scientific infrastructure located around the source, coupled with comprehensive scientific and technical support for using that infrastructure.

It is no coincidence that there has been deliberate co-location of neutron facilities with materials science or biological research centres, or with synchrotron or other facilities, at several sites around the world. There is a growing user demand for an increasingly wide variety of complementary measurement and characterization techniques to be available in conjunction with neutron experiments. The challenge will be to co-operate these facilities to achieve the maximum synergy, while maintaining the natural competition that drives scientific discovery.

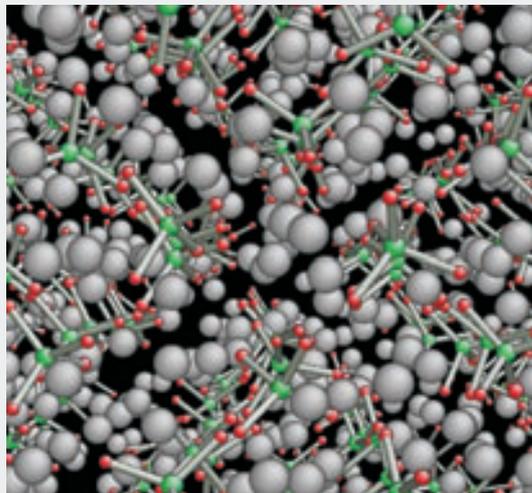


Scattering experiments need samples. In particular cases, because of the specialised nature of the synthesis and its close relationship to neutron scattering, it makes sense to co-locate the synthesis and neutron facilities and offer the combined capability to users. The most obvious case is deuteration; selective deuteration and contrast variation are absolutely central to the full exploitation of neutron scattering methods, particularly in the areas of soft matter, biology and disordered materials. The capability to synthesise selectively deuterated samples, from polymers to proteins, needs to be made available to a wide range of users, but this is by no means a trivial task. Another need is for crystal growth facilities, for example for the large crystals needed for inelastic scattering studies.



There is an ever increasing demand for a wide variety of sample conditions and treatments: temperature, pressure, magnetic field, electric field, stress, shear etc., often with more than one parameter being varied. The extreme conditions of this year become the standard conditions of next year. There are also demands for simultaneous measurements using techniques such as conductivity, magnetometry, heat capacity, X-ray diffraction and infra-red and Raman spectroscopy. Samples are synthesized and treated in-situ, sometimes under conditions relevant to industrial processes - 'bringing the laboratory to the beamline'. Experimental success depends on these services being provided with high reliability on a 24 hour basis, exactly the same as for the neutron source. This requires an increasing level of technical expertise and support.

Modern neutron instruments produce larger quantities of data, from more complex samples, at an ever faster rate. This data could either be used more qualitatively, or its analysis and interpretation could become the bottleneck in the research process. Given that one of the great strengths of neutron data is that it can be related directly and quantitatively to models and theory, it is clearly crucial that the analysis should be as quantitative as possible and make full use of all the data measured. This will require increased investment in the development of software, computing facilities and e-science. One goal is for sufficiently detailed analysis to be available on the same timescale as the experiment, so that the results can be used to guide the experiment interactively (and in some cases even automatically). This is particularly crucial as there are more and more non-expert users, from an increasingly wide range of scientific backgrounds, who no longer want to see 'data', but really want to see what neutrons can tell them - 'where the atoms are and what the atoms do'.

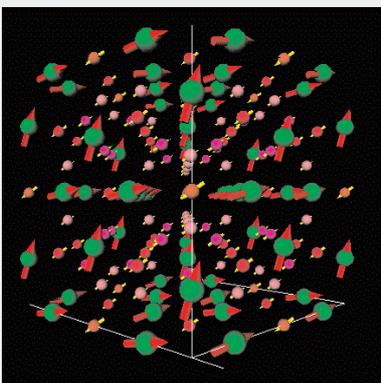


Neutrons and their applications

Neutrons are used for a multitude of scientific techniques and applications which are grouped together because, of necessity, they share the same neutron source. Given the breadth of applications it is impossible to cover them all within a short document, so this section contains only a selective view of some of the main areas of current research, and some of the likely future areas.

- Structural Chemistry and Physics
- Soft Matter
- Engineering and Materials Science
- Biology and Biochemistry
- Condensed Matter Physics
- Chemical Activity and Molecular Motions
- Fundamental Physics

Neutron diffraction has been central to many of the key advances in solid state chemistry and physics over the second half of the twentieth century. From the earliest experiments some fifty years ago on the magnetic structures of simple transition metal oxides, carried out at the first research reactors, neutron diffraction has impacted upon a broad range of research from hard condensed matter physics, through structural chemistry and the geological sciences, to pharmaceutical research. Much of our modern understanding of atomic and molecular magnetism began with these early neutron scattering experiments. Neutron diffraction plays a major role in the discovery and characterisation of novel magnetic materials that include very powerful hard permanent magnets, colossal magnetoresistance materials and molecular magnets.



The complex magnetic structure of Er_6Mn_{23} determined by neutron diffraction

Powerful hard magnets are found in all kinds of applications in the world around us from small motors used in automobiles and robotic devices to large medical devices and high powered particle accelerators. The next generation of magnets may well be made from soft materials or molecular magnets that are light, transparent and bio-compatible. Neutron diffraction is being used to map the magnetisation in these new materials, with the aim of adjusting the chemical structure to bring the magnetic transition temperature above room temperature. Colossal magnetoresistance (CMR) materials have generated great excitement over recent years because they exhibit an enormous change in electrical resistivity on application of a magnetic field. This

phenomenon has already found applications in magnetic memory devices such as computer hard disks. The neutron is an essential tool in the understanding of colossal magnetoresistance; neutrons are very sensitive both to magnetic behaviour and oxygen atom positions. Together this provides a deep understanding of these materials by unravelling their chemical nature, metal ion oxidation states and precise magnet structures.

Most real crystalline materials in their synthesis, processing and function form as polycrystalline aggregates and not as single crystals. Neutron scattering has contributed greatly to the powder diffraction technique, following the development of the Rietveld method some forty years ago, and has provided unique insights into the analysis of real materials. Perhaps the most significant contribution of neutron powder diffraction in this area has been in the synthesis and characterisation of new high temperature superconductors. Immediately after the discovery of $YBa_2Cu_3O_7$, the first high temperature superconductor with a transition temperature above the boiling point of liquid nitrogen, researchers at many neutron sources around the world were quickly able to show how the oxygen atoms were arranged and how oxidation of the material changed it from a semiconductor to a superconductor. Neutron diffraction measurements were also able to determine that the superconducting properties were controlled by a charge reservoir layer. Following this insight, chemists have been able to synthesise other new materials with even higher superconducting temperatures.

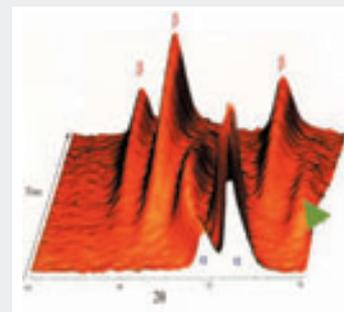
Energy storage materials have been the subject of intense research effort in recent years following the rapid development of portable electronic equipment such as cellular phones and laptop computers. Two kinds of lightweight rechargeable cells are now available: nickel-metal hydride (Ni-MH) and lithium-ion batteries. Both are charged by intercalating light atoms (H^+ and Li^+) into the electrode, and one of the keys to improving the performance of these batteries is a detailed

Neutrons

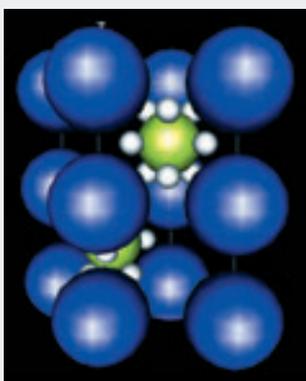
Structural Chemistry and Physics

understanding of these mechanisms. Since light atoms are involved, neutron diffraction is the ideal tool to characterise these materials. Moreover since neutron beams can easily penetrate large samples, real batteries can be studied in-situ and their detailed electrochemistry followed throughout multiple charge-discharge cycles.

Many of the key challenges that face mankind in the early twenty-first century concern our management of the environment around us. Efficient catalysis and cleaner fuels are two of the many crucial areas that impact upon our lives; they depend upon new materials advances. Neutron diffraction is playing a key role in the understanding of these materials issues. In-situ catalysis studies are revealing much about the interactions between small organic guest molecules and their host molecular sieve networks.



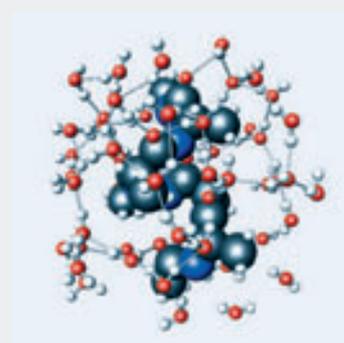
In-situ neutron diffraction during charging of a Ni-MH battery



The crystal structure of Mg₂FeH₆

Efficient, safe hydrogen storage is a key issue in the development of the hydrogen economy as an alternative to dependence on fossil fuels. Light metal hydrides such as MgH₂ and Mg₂FeH₆ act as hydrogen sponges, storing hydrogen at higher density than liquid H₂ itself. Neutron diffraction of deuterated materials is the optimal method for determining the location and behaviour of hydrogen as it absorbs and desorbs in these materials – this information is essential to the development of this field. Recently H₂ clathrate hydrates have also been mooted as potential hydrogen storage materials. Clathrate hydrates encage small gas molecules in a framework of hydrogen-bonded water molecules and have only recently been found to exist in nature. Marine sediments contain huge amounts of methane gas (CH₄) far exceeding the other known fossil energy sources of coal, oil and natural gas. A potential method for reducing carbon dioxide (CO₂) in the atmosphere may be entrapment as a CO₂-hydrate which is then submerged in the ocean, leading to a clean, closed CH₄-CO₂ carbon cycle. Again neutron diffraction has been key to the elucidation of these materials – even the compressibility of clathrates, which is necessary for sonic exploration of the sea bed, was largely unknown prior to neutron measurements of these light atom structures. High pressure studies of rocks and minerals using neutron diffraction are also giving insight into the behaviour of the earth's interior.

Neutrons have played a fundamental role in understanding the science of ice, water and aqueous systems. Neutrons not only scatter strongly from hydrogen but also from the other main components of these systems, such as oxygen, carbon, and nitrogen. Their sensitivity to the arrangement of water molecules in aqueous systems is further enhanced by isotope substitution techniques which allow the local order around particular atomic sites to be explored. Neutrons have led the field in providing quantitative measurements of the underlying structural signatures of hydrogen bonding, hydrophobic interactions and ion-water coordination, all of which are fundamental to our understanding of how much larger molecules, such as biologically relevant peptide chains, surfactant molecules, and other interfacial systems, function and fold. Equally they have probed the more



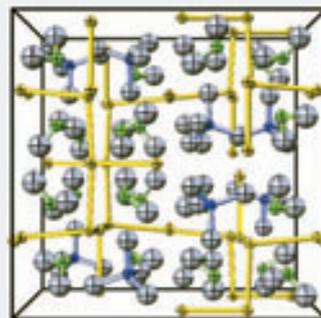
Water coordination around a ferrocene molecule in solution

esoteric aspects of water, particularly the question of how amorphous ice at low temperatures passes abruptly through an amorphous phase transition from an open tetrahedral structure like ordinary ice, to a much compressed high density structure. They have started to yield significant insight into the structural origins of the thermodynamics of aqueous mixing and dissolution – important factors in chemistry and engineering. Neutrons have been used to identify and characterise new forms of ice under extremes of pressure, and have been invaluable in explaining the paradox of how such a simple molecule as H₂O can have such a multitude of highly complex interactions when mixed with other materials and biological molecules.

Neutron diffraction has contributed immensely to a very broad range of structural physics and chemistry. The ability of the neutron to penetrate large distances in materials means that it is ideally suited to developing an atomic and molecular explanation of the behaviour and function of real systems operating under real conditions, from magnets and superconductors to batteries, fuel cells, catalysts and hydrogen storage materials. The development of high throughput neutron powder diffractometers has led to the parametric analysis of important systems ranging from CMR, superconductor and negative thermal expansion materials to fullerenes, fullerides and pharmaceutical compounds.

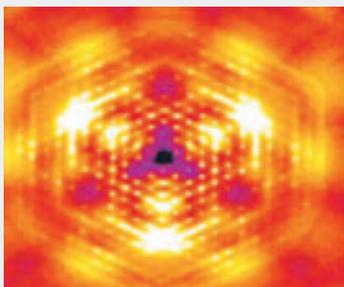
Future applications

The past two decades have shown unequivocally that neutron diffraction is central to the whole gamut of materials discovery. Whether the material is a high-temperature superconductor, a novel magnet, a fullerene or a colossal magnetoresistance material, past experience shows that neutron diffraction is a key element in the discovery and characterisation of these materials. The role of neutron diffraction will also undoubtedly be pivotal over the next two decades. It is impossible to predict the precise nature of the new materials that are yet to be discovered but it is certain, for example, that neutron diffraction will be of central importance in significant areas of future science and technology such as energy and environmental research. Breakthroughs will occur in battery research, oxide ion conductors for fuel cells, catalysis, lightweight materials, thermoelectrics, photovoltaics and hydrogen storage materials. In each of these material systems, neutron diffraction will be an essential tool and often, indeed, the definitive structural technique. For example, combinatorial methods are currently being developed in the search for new hydrogen storage materials; while synchrotron diffraction is the structural tool of choice for massive primary screening, neutron powder diffraction remains essential for hydrogen atom location and thus the definitive determination of the crystal structure. The lithium borohydride amide structure shown in the accompanying figure was recently discovered through medium throughput screening and its structure solved using neutron powder diffraction. Containing 11wt% hydrogen, developments based around this material may lead to a potential candidate for reversible on-board hydrogen storage.



Lithium borohydride amide: a new potential hydrogen storage system

One of the principal trends in materials discovery and development over the past two decades has been increasing complexity – this trend is certain to continue. The combined development of neutron sources, instrumentation and optics in conjunction with massive increases in computing power will enable substantially more complex experiments to be performed. Present experimental



Beyond Bragg peaks in benzil: diffuse scattering reveals molecular disorder

trends point to many forms of increased complexity. At its most obvious, complexity will be manifest in the chemical constituency of the materials under study; across the whole range of science from magnetism and superconductivity to molecular sieves and supramolecular chemistry, materials now synthesized contain many more independent atoms than two decades ago.

Pharmaceutical molecules are becoming more torsionally complex and molecular cages structures are being created with massive cavities. Developments in both single crystal and neutron diffraction instrumentation and analysis will enable these

techniques to play a central role in structural elucidation and interpretation. Complexity also comes in the form of heterogeneity. At an atomic and molecular level, much remains to be understood about disorder, crystallization and amorphization. Diffuse scattering and pair distribution function analysis has developed substantially over the past decade in large part as a consequence of increasing computational power and the concomitant improvement in analytical techniques. Over the next decade, the distinction between an amorphous and a heavily disordered crystalline material will disappear allowing, for example, deeper insights to be obtained in the mechanisms of amorphization of pharmaceutical compounds. Heterogeneity is also important in the development of new materials systems and in the operation of real materials devices such as batteries, fuel cells and catalytic converters. Increasingly new materials devices will be multicomponent in nature; catalysts intrinsically have this property and many novel hydrogen storage materials, for example, will involve hydrogen absorption and desorption between multicomponent end members.

Neutron diffraction studies of liquid and glass structure have increased in complexity over the last 15 years; this is principally as a result of the development of advanced modeling techniques based on experimental diffraction data. To date, this work has focused mainly on fundamental systems but with novel instrumentation and further increases in computing power, the focus over the next decade in glass research will move to more applied systems such as the complex glasses used in the telecommunication industry. Studies of liquids will also move to more complex systems that overlap increasingly with biology, where the fundamental role of water in many biological processes is poorly understood, and soft matter, where there is an urgent need to understand the behaviour of polymers at the atomic as well as at the mesoscopic level.

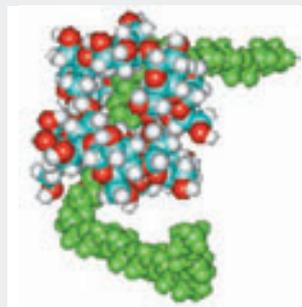
Higher neutron fluxes and increased detector coverage will facilitate real-time measurements of chemical processes. In the case of the multicomponent hydrogen storage system mentioned above, it will be possible not only to distinguish all the constituent compounds at full absorption and desorption but also to monitor the full hydrogen cycling process. Similarly, it will be possible to charge and discharge complete batteries in-situ; additionally through secondary collimation, it will be possible to monitor independently the processes that occur in the battery anode and cathode. In-situ materials synthesis studies in confined environments such as diamond-anvil high-pressure devices and hydrothermal cells will help optimize synthesis conditions. Catalysis studies and other important chemical engineering processes will all benefit from the detailed structural information that can be obtained from advanced neutron diffraction instrumentation. The generalization of this concept to bringing the chemistry laboratory to the neutron beamline with multiple ancillary diagnostic tools such as dielectric measurements, mass spectrometry and thermogravimetric analysis will enable neutron diffraction to play a very central role for the structural chemist and physicist across the scientific and engineering disciplines for the foreseeable future.

Soft Matter

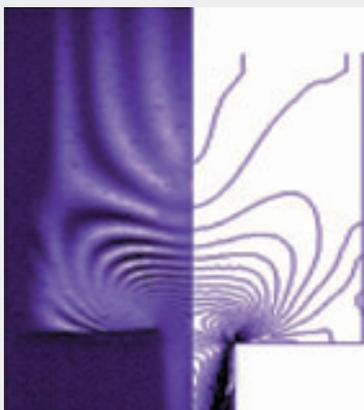
Neutrons

Soft Matter encompasses a wide range of molecular materials which includes polymers, surfactants and colloids. This is an area of research that is increasingly driven by the industrial and technological applications of highly complex mixtures and structures, many of which are not in equilibrium. The specific advantages of neutrons, in particular the use of contrast variation and the high penetration into materials, make neutron scattering a particularly powerful probe for studying the physical and chemical properties of such systems. These studies are providing key structural information in the complex mesophases that exist in many modern formulations, from personal care products to pharmaceuticals. Real time neutron studies of the processing of soft solids and fluids are making unique contributions to many industrial processes, from composites to colloids.

Indeed neutron scattering has developed into the primary tool for determination of the structure of self-assembling systems such as micelles, microemulsions, vesicles and other more complex mesophase structures. Composition, temperature, concentration, pH and ionic strength are all key factors in the development and evolution of their structures. Significant progress has been made in recent years in understanding equilibrium properties. For example, the penetrating power of neutrons enables scattering studies to be made in difficult environments. Such studies have provided much of the structural information that has led to the development of the CO₂-phobic molecules required for the emerging technology of super-critical CO₂ processing. They are also now providing important insight into the kinetics and structural transitions of self-assembling systems. For example, time resolved measurements have demonstrated that the worm-like micelle to vesicle transition on dilution of the lecithin-bile salt mixture evolves through the formation of non-equilibrium disk-like aggregates. A number of related studies are now further illustrating the richness and diversity of such non-equilibrium intermediate structures.



*Self assembled polyrotaxanes
(polymer complexes)*

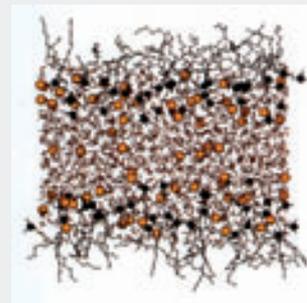


*Flow field for an entangled polymer
melt in an extruder*

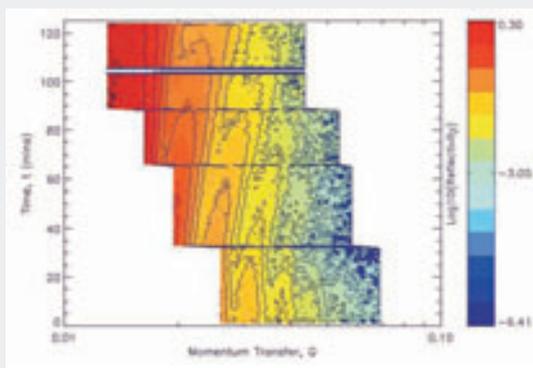
Recent spatially resolved scattering studies (currently possible on the millimeter length scale) have provided an important link between the evolution of microstructure and rheological properties, in conditions similar to those encountered in the processing of soft solids. The complex flow field of an entangled polymer melt was mapped out in a flow geometry similar to that encountered in extruders. Though measured on both the macroscopic and molecular scales, it is ultimately the molecular scale information that is important in terms of the rheological and solid-state properties. These studies have provided a quantitative account of the rich rheological behaviour in terms of the fundamental entanglement processes associated with reptation. Similar studies in both Couette and extensional flow geometries have provided temporal and spatial

information on the evolution of the complex mixed surfactant lamellar/liposomal/micellar microstructures associated with products such as hair and fabric conditioners. These studies are now providing a real opportunity to use molecular scale information to optimize processing conditions, formulation and product performance.

Surface studies have revolutionised our understanding of the adsorption of surfactants and polymers at interfaces, impacting upon applications as diverse as detergency, lubrication, adhesion and a range of specialised coatings. The behaviour of complex mixtures of surfactants, polymers and polyelectrolytes can be very different compared to that seen in the bulk, and this is the key to understanding many of the associated processes and phenomena. Much of what we currently know about the adsorption of surfactants and polymers at interfaces arises from neutron surface scattering studies. The structure of a range of important surfactants and surfactant mixtures has been determined at the air-solution and solid-solution interfaces to a resolution of 1 to 2 Å. This is providing the basis for an understanding at a molecular level of processes such as detergency and lubrication. Recent studies of the adsorption of polyelectrolyte/ionic surfactant mixtures have demonstrated how significant enhancements in adsorption can be achieved at surprisingly low solution concentrations due to strong surface polymer/surfactant complexation, resulting in an effective enhancement of four orders of magnitude. Related to this, scattering studies on the structures of polyelectrolyte layers have featured strongly in the development of polyelectrolyte multilayers in the formation of functionalized surfaces and novel microscopic structures for controlled encapsulation and release.



Molecular structure of surfactant molecules at the air-solvent interface, consistent with observations from neutron reflectometry



Temporal evolution of neutron reflectivity following solvent ingress into a polymer surface

Neutrons can provide important structural information on polymers from the atomic to the meso-scale. On the atomic scale this is epitomised by recent diffraction studies on crystalline polymers. Using the additional sensitivity that 'contrast' provides, it was shown that the structure of Kevlar, as accepted since the 1970's, was incorrect. The tailoring of modern polymeric based materials is highly dependent upon complex blends of polymers, and their surface or near surface properties are crucially important. Surface scattering studies

have provided the key structural information for the understanding of polymer-polymer interfaces, the role of compatibilisers and the effects of confined geometry. In-situ real time measurements are providing the opportunity to probe the early times of inter-diffusion at polymer-polymer interfaces and to access critical effects such as solvent ingress and the leaching or migration of plasticizers.

In addition to the information about static structures obtained from neutron scattering studies, dynamical studies have also played a central role in providing important information. One of the major theoretical developments in polymers in the past few decades has been the establishment of reptation as a key mechanism in the diffusion in polymer melts. The crucial experimental verification was obtained from neutron spin-echo spectroscopy. Similar techniques are now providing insights into membrane fluctuations and dynamics. This is becoming an important way of establishing the relative rigidity of a membrane, which is a key element in determining its microstructure, either as lamellar fragments or liposomes.

Future applications

Soft Matter research, primarily in colloid science, nanotechnology, surfaces and interfaces, encompasses many of the major high level themes and priorities identified as key future areas for UK research. This is especially true for aspects relating to environmental issues and the development of intelligent infrastructure. There is considerable overlap with the healthcare priorities relating to bio-materials. Three main areas of focus for the future applications of neutron scattering techniques are

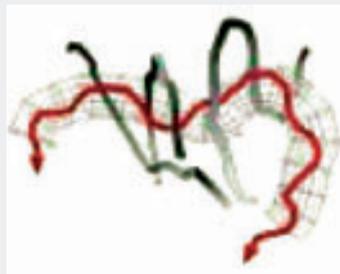
- directed self-assembly,
- the development of functionalised surfaces and interfaces and
- the processing of complex fluids and soft solids.

In these broad areas there will be increasing need to study complex multi-component and multi-phase systems in which there is a large diversity in the length scales of interest and importance, and systems that are not at equilibrium. It will be necessary to probe not only bulk structures, but also surface and near surface structures. Furthermore, there will be a demand to consider much more complex situations such as confined geometries, molecularly narrow pores and thin films, and a variety of interfaces such as liquid-liquid, liquid-solid and solid-solid. This will involve the use of more complex and difficult environments such as the complex flow fields encountered in extruders and micro-fluidic flow channels, and specialised cells such as electrochemical cells. These environments are more closely associated with those encountered in current and future industrial processes.

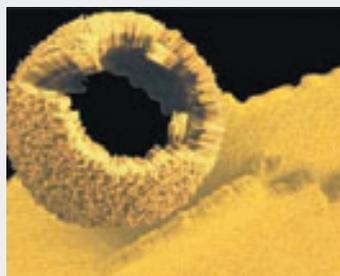
Although the structural information is of paramount importance, many of the key processes and phenomena that need to be understood and exploited are dynamic and not static. Hence kinetic and dynamical information will be required to unravel, at a molecular level, a variety of phenomena such as rheological properties, the kinetics of phase transitions (both in bulk and at surfaces) and the surface kinetics involved in phenomena such as drainage (Marangoni effects), surface viscoelasticity, and lubrication.

Directed self-assembly

Novel nano-structures in solutions, gels and soft solids, and acting as templates for mesoporous materials based on directed self-assembly, will form the basis of a diverse range of future smart materials. Complex fluids and soft solids designed as materials responsive to environmental changes such as temperature, pH, pressure and light, will have a hierarchy of structures. Neutron scattering will be a key structural tool required to probe the complex structures of these next generation materials and the kinetics of the transformations involved. Extensive deuterium/hydrogen contrast variation will be used to elucidate the detailed structure of these self-assembly systems over a wide range of length scales, from molecular to mesoscale. Specific contributions from a particular functional fragment or element of a structure can be identified



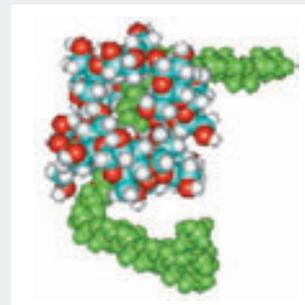
Schematic representation of polymer reptation in polymer melts



Self-assembled gold/polymer nanostructures

from such labelling experiments. Furthermore, the structural changes and response to environmental triggers, and the kinetics of those changes, will be accessible.

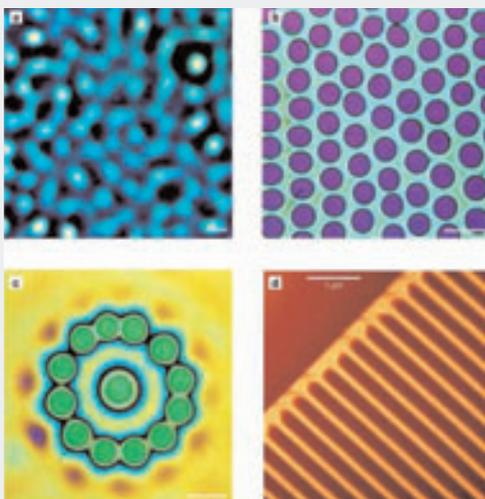
In solutions and gels, such complex fluids will exhibit tunable and controllable rheological responses, provide efficient solubilisation or encapsulation agents, and provide the opportunity for controlled and highly specific delivery properties. Such materials will provide new and efficient applications in areas as diverse as drug delivery, lubrication, oil extraction, detergency, and water treatment. In the solid state, and in soft solids, developments in self-assembly will lead to the evolution of new photonic materials, polymeric based devices and displays and micro-machines. They will provide the basis for the development of new mesoporous catalytic materials, ceramics and composite structural materials. To achieve these advances, new self-assembling structures will be developed, based on complex blends of surfactants, polymers, polyelectrolytes and bio-materials such as specific peptide fragments.



Self assembled polyrotaxanes (polymer complexes)

Functionalised surfaces and interfaces

The nature of the surface and interface, and the molecular structure and composition at or near the interface, is of increasing importance in a range of existing and emerging technologies. It is essential for our understanding and development of properties such as adhesion, lubrication and detergency, and in the recognition processes involved in a wide range of emerging sensor technologies and applications. Interfacial structure will play a critical role in the development of the next generation of polymeric based devices and displays. Surface structure has important consequences for the functionality of modern catalysts and catalytic cells, in electrochemical cells, and in other confined geometries such as pores in mineral/oil bearing strata and artificially generated mesoporous structures. The air-liquid, liquid-liquid, liquid-solid and solid-solid interfaces are all of importance.



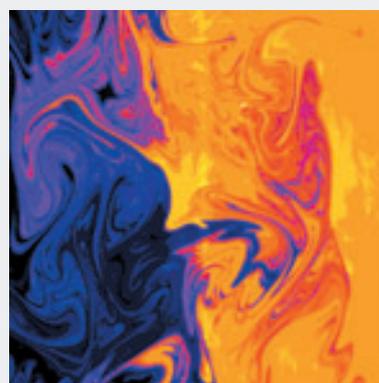
Patterned surface arrays generated by surface self-assembly

The use of complex mixtures of polymers, polyelectrolytes, proteins, peptides and surfactants to tailor the surface structure and composition, provides the opportunity to produce surfaces with specific functionality. A key element of the future direction of this approach will be the increasing use of bio-materials - bio-mimetics. Self-assembly at interfaces and in the near surface region will provide patterned surfaces and controlled lateral structure in the plane of the surface, with chemical inhomogeneity over a range of length scales. This will be crucial to further extend development of the range of functionalised surfaces. The nature of the new surface structures and phases that result, and their relationship to the equivalent bulk phases, will be of central importance.

Such novel surfaces will have an impact on the development of a range of new sensors, on the control of lubrication from bio-lubrication to engine oils, on adhesion, for decorative, protective and technological coatings, and in personal care products. Changes in the surface structure due to confinement, flow, pH and so on will be of increasing importance as the range and scope of novel functional surfaces develops. Neutron scattering will provide key information, that is not available from other surface probes, on surface and near surface structural information over the required length scales, from molecular to mesoscale, and with selectivity available through contrast variation. Although the static structural information is essential, the next step in many of these systems will be to probe the kinetics of the surface ordering and structural rearrangements, and dynamical surface effects.

Processing of complex fluids and soft solids

The processing of most soft solids and non-Newtonian fluids, found in products as diverse as amorphous and crystalline polymers, paints, and personal care products, involves complex flow fields and patterns in extruders, pipe flow and mixers. To understand, develop, and optimise these different processing routes, the rheological properties of these materials must be understood at a molecular level. Hence it is necessary to investigate their structural and conformational changes and spatial reorganisation in complex flow fields. This will be required over ever finer spatial and temporal resolution. To further develop emerging technologies, such as high throughput and 'lab-on-a-chip' concepts, requires the optimisation of micro-fluidics. Achieving the required spatial resolution represents a major challenge for the use of neutron scattering techniques. However, the penetrating power of cold and thermal neutrons makes many of the industrially and technologically relevant flow fields and geometries readily accessible for scattering experiments. The use of hydrogen/deuterium contrast, provides a sensitivity and selectivity not afforded by other structural probes.



Computer simulation of a complex flow field: interfacial mixing in two fluids

A related, but distinctly different, aspect of this area involves the study of even less well-defined flow geometries - the flow of non-Newtonian fluids in pores, fissures, and other porous media. The most obvious area is in enhanced oil extraction, where manipulation of the rheological properties can have a potentially enormous impact upon extraction efficiencies. There are also wider applications associated with a range of environmental issues and geological phenomena.

The accurate measurement of atomic separations as a function of position in a bulk sample, by means of diffraction, can be used to give information on macroscopic residual stresses. Neutrons have the particular advantage for such measurements that they can penetrate deep into most materials, for example metals or alloys, allowing non-destructive measurements of 'real' engineering components. The measurement of diffraction peak intensity as a function of sample orientation gives information on the distribution of crystallites - texture. Neutrons are particularly effective for spatially resolving bulk texture. For these techniques to be useful in engineering science requires that information can be obtained from realistic scale components, operating under actual environmental conditions and loadings over relevant timescales; this can now be achieved.



Measurement of residual stresses on the casing of a high pressure turbine and cone (Rolls Royce, Manchester)

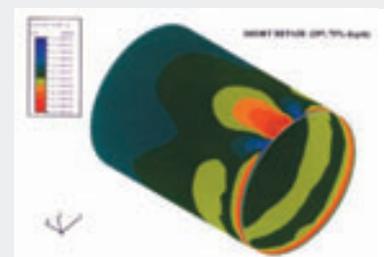
The use of neutrons for the study of engineering and materials science problems has expanded greatly in the last two decades. Originally most experiments were carried out as a 'parasitic' use of instruments designed, and mainly used, for other purposes such as powder diffraction. However, an increasing awareness of the capabilities of the method, and an increasing demand, has led to the construction of dedicated engineering diffractometers at most facilities during the 1990's. These have sample environments that can accommodate bulky and weighty components, together with the ancillary equipment needed to install and position them accurately. New software tools have been developed that allow for off-line experimental design and set-up, making more efficient use of beam-time.

Neutrons have been used to study a wide range of engineering problems, covering many different applications and industrial sectors. These range from the fundamental properties of plastic deformation of alloys and composites, and of phase transitions, through to the determination of internal stresses in production components for the aerospace, automotive, and power industries. While there is some commercial use of beamtime, most studies support basic engineering science, usually in collaboration with industry.

Examples of critical Engineering Science currently being investigated are:

- The development of unique integrated methodologies enabling, for the first time, the unambiguous quantitative identification of how residual stresses evolve during the manufacture of state-of-the-art aerospace components structures, directly impacting both UK aircraft (AIRBUS UK) and engine (Rolls Royce) manufacturing industries.
- The systematic determination of residual stresses in typical stainless steel power generation welds enabling

- (i) less conservative residual stresses estimates to be put into Structural Integrity Assessment evaluations and codes, enabling more efficient plant operation without compromising safety and
- (ii) validation of state-of-the-art finite element simulations allowing the residual stresses in difficult to access welds within the nuclear power generation industry to be predicted and used in Structural Integrity assessments

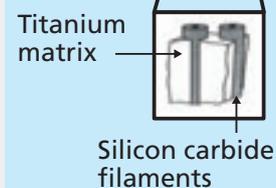


Finite Element Model stresses introduced by a repair on a girth weld (British Energy)

- Identification and modelling of how inter-granular stresses develop and influence the mechanical and physical properties of
 - light engineering alloys based on non-cubic (hexagonal) matrices, such as titanium and magnesium alloys, which are becoming increasingly important for energy efficient transport
 - nuclear materials such as zirconium and beryllium-based alloys which must be developed to give longer lives in higher neutron fluences if nuclear power is to make a significant impact on the development of a sustainable energy economy
 - the key factors affecting the fatigue life of shape memory and ferroelectric actuator materials.

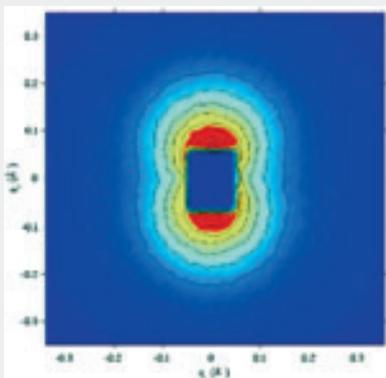


© Rolls Royce



'Bling' – a hoop-wound Ti-6Al-4V fiber integrally bladed ring. The inset shows the microstructure of the reinforced region

Small Angle Neutron Scattering techniques enable the structural

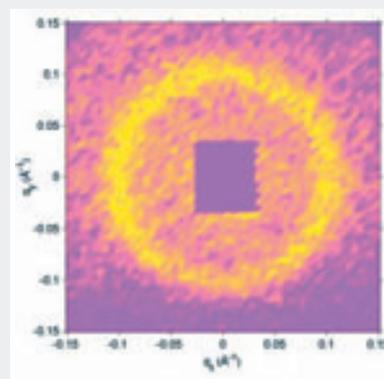


Anisotropic nuclear and magnetic scattering in irradiation damaged structural steel

characterization of materials over length scales of the order of a 10^{-9} to 10^{-6} m. SANS allows the study of microstructures in bulk materials while Grazing Incidence SANS probes in-plane surface structures. For example, SANS studies of reactor steels reveal the extent of radiation damage, void and precipitation formation, and the change in structure and composition as a function of radiation dose. These are technologically highly relevant factors with a view to next generation nuclear power generation or the construction of the ITER nuclear fusion test facility. Solidification, precipitation, grain growth and

refinement and grain boundaries in metals can all be studied - helping to understand the properties of metals from the atomic to the micro-scale for structural applications. Voids in open structured materials such as carbon nanotubes and zeolites reveal their structure, percolative connectivity, surface area and porosity. These are important parameters for gas adsorption for solid state storage of energy sources such as hydrogen, use as filter materials or for catalysis.

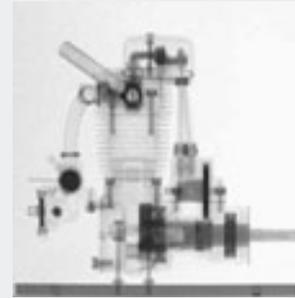
Using the magnetic moment of the neutron to provide an additional contrast mechanism, magnetic materials and microstructures can also be investigated using non-polarised or polarised neutron techniques. For example, melt-spun metallic ribbons, which are nominally amorphous and magnetically extremely soft, are actually shown to be nano-crystalline. Magnetic SANS shows that transverse internal magnetic fields persist well into the nominally magnetically saturated state. A new surge in SANS characterization and subsequent understanding of functional magnetic materials, as are used in magnetic recording media (hard disks), is aiding a deeper understanding of the magnetization process, inter-granular magnetic coupling and details of the local magnetic field environments. This allows the subsequent tailoring of artificially nano-structured magnetic components. For example, CoFe nano-particles are being deposited in regular



Neutron diffraction image from self-assembled FePt nano-particles

arrays using organic micelle templates, with the aim of producing materials with smaller magnetic domains or 'bit' sizes', thus giving higher storage capacity.

Neutron tomography is, as yet, an under exploited technique. The high penetrating power of neutrons, coupled with the relatively high scattering from light atoms (particularly hydrogen) allows imaging of, for example, lubricants in an engine.



Neutron tomograph of an engine (PSI)

Future applications

The future emphasis in engineering measurements is likely to shift more towards

(a) in-situ studies of various methods of processing and treatment:

- joining techniques such as friction stir welding; weld cooling;
- applied stress and fatigue testing;
- thermal treatments and the development of microphases;
- deformation of new materials, e.g. Co based superalloys.



Hoop stress components mapped across the tube cross section of a Ni superalloy inertia weldment for (left) as welded (centre) after conventional treatment and (right) after higher temperature post-weld heat treatment

(b) the study of materials under in-service conditions, for example:

- nuclear industry applications, such as reheat cracking and creep of pressure vessel plant;
- health care applications, such as prosthesis design or bone mechanics/interface growth.

Current applications that will continue to be important are:

- studies of welds in full engine assemblies and other large components;
- validation and optimisation of stress relief procedures.

There will be continuing development of

- Metals: superalloys, steels (high strength, high ductility), Ti alloys for aerospace applications and Zr alloys for future nuclear industry applications;
- Smart materials, including shape memory alloys and ferroelectric actuators;
- Ceramics;
- Composites: laminated structures and matrix composites;
- Nano-structured materials.

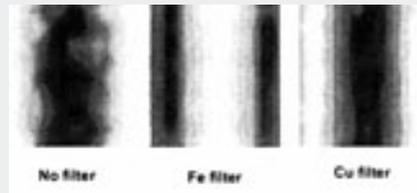


An application of a shape memory alloy

These will require study in terms of their fundamental properties, as well as the effects of forming them into components and any subsequent treatments.

Examples of new and developing experimental techniques will include:

- the use of position sensitive small-angle neutron scattering to study the size distribution of dispersoids and precipitates within engineering alloys and composites;
- ultra-SANS to measure e.g. the growth of voids to the point where they become catastrophic;
- the development of neutron tomography, with particular emphasis on non-destructive techniques that enable measurement of composition or chemical phase content (including magnetic phases) within the bulk of a sample; improved techniques using phase contrast.



Element and phase sensitive neutron radiography

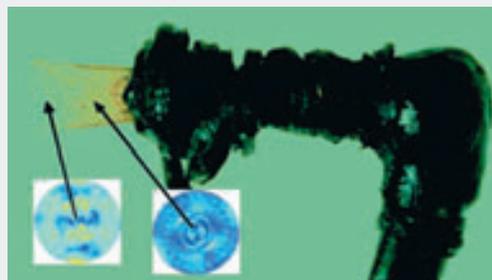
Neutron methods will become used ever more closely with computational methods such as Finite Element Modelling. These tend to be very effective for identifying trends rather than for giving absolute values, for which experimental data will continue to be required. Finite Element Models are already being used to plan and optimize experiments. Validation of these codes is especially important for safety cases in critical industries, such as the nuclear industry.

In parallel with developments in neutron methods, the use of synchrotron X-rays for engineering studies has also been a great success, with both diffraction methods for strain measurement and tomographic imaging techniques now being well-established. The flux available with synchrotron X-rays and the penetration available at high photon energies means that certain types of measurement can now be performed much more quickly than with neutrons. However, synchrotron X-rays at high energies are constrained to low diffraction angles, which means that in many components there is always one strain direction that cannot be obtained. The future of in-depth diffraction strain measurement, therefore, is likely to rely on neutrons just as heavily as before. For this reason, the development of integrated facilities that allow convenient access to both synchrotron X-ray and neutron beamlines will be highly-desirable in the engineering field.

Close collaboration between facility scientists, university users and industry has been of enormous benefit in developing instruments for engineering measurements. The cost of the technique is not dissimilar to many of the other techniques routinely used 'in-house' by industry, but in order for neutron techniques to be more commonly used they need to become more accessible, and the analysis and interpretation of experimental results has to become more routine and automated.

Cultural heritage

Exactly the same basic techniques can be used to study objects which are old rather than new - the major advantages being that the method can be applied without damage to delicate and precious objects, and the high penetration normally means that any part of the object can be studied. Texture pole figures can be used as 'fingerprints' of manufacturing techniques, for example whether objects such as coins have been cast or stamped.

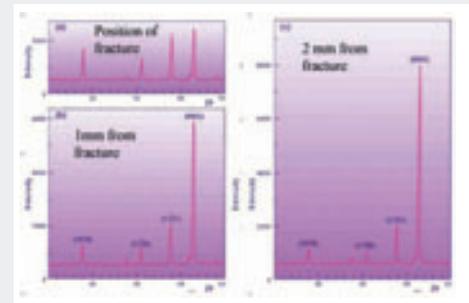


Texture measurements on the 'iceman' axes from the Italian Alps

Powder diffraction can be used to characterize the distribution of phases, e.g. in pottery, giving information on provenance or production methods. Small angle scattering can also be used to give information on the provenance of materials, for example the distribution of different crystalline phases is characteristic of different marbles. These applications are relatively recent, but are growing fast. It is likely that dedicated instruments for cultural heritage studies will be constructed within the next decade.

Other applications

Even more in their infancy are other applications such as medicine and dentistry (functional properties and healing of bones, dental implants), paleobotany and paleology (studies of fossils). These are likely to continue to be niche studies, but the unique abilities of neutrons mean that the limitations are often mainly due to the ignorance of scientists in other fields about the possibilities, and the ignorance of neutron scientists about these other fields, rather than to the technique itself. A significant effort in outreach activities is needed if these possibilities are to be exploited.



Neutron diffraction study of fracture healing in a sheep femur

Sources, instrumentation and standards

In all areas there is ultimately a need for higher flux sources, to enable

- faster measurements, e.g. to follow faster time-dependent processes;
- finer measurements, e.g. better resolution for near surface stress measurement;
- deeper measurements, e.g. non-destructive measurements on even larger components;
- new types of in-situ measurements, e.g. under processing conditions.

However there is still considerable scope for improved and expanded instrumentation at existing sources, for example by enhanced use of focusing techniques.

Two other specific aspects are also important for effective future exploitation of neutrons in materials science and engineering. The first is access to similar synchrotron based techniques. In the past few years these have developed considerably through the use of hard X-rays, and are now comparable with neutrons in terms of penetration into components, but much faster. However the need to use very small scattering angles means that only two components of stress can be measured. In many cases this missing information must be provided by a neutron experiment, which is only useful if it can be carried out on the same sample within a short period of time. The second aspect is that of standardization. For results to be acceptable for use in engineering design, particularly in relation to safety, measurement standards must be designed and implemented, preferably across many different neutron (and synchrotron) facilities.

Neutrons

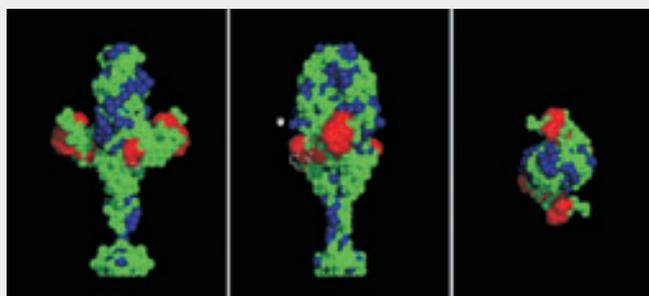
Biology and Biochemistry

Recent advances in molecular biology and biochemistry now mean that there are unparalleled opportunities for research in the structure and dynamics of complex biological systems. As the number of accessible problems increase, it is becoming clear that a whole host of different methods will be required for an understanding of these systems and of their biological function.

Neutron methods are non-destructive and can provide important information in biology that is not accessible by other methods. Central to this is the fact that different isotopes can scatter neutrons by vastly different amounts, and so (in the case of biological samples) selective deuteration can be a very powerful means of highlighting specific parts of biomaterials. So, if part of a molecule is deuterated, this labelled region will be very visible to neutrons in ordinary water, whereas conversely in heavy water its scattering power will be close to that of the solvent and the unlabelled region will stand out. This selective 'contrast matching' allows the organisation of complex systems to be probed in detail, and the relative positions and shapes of individual components to be accurately determined. This capability has important consequences for the study of biological macromolecules in solutions, interfaces, fibres, and occasionally as large single crystals for high-resolution crystallographic studies.

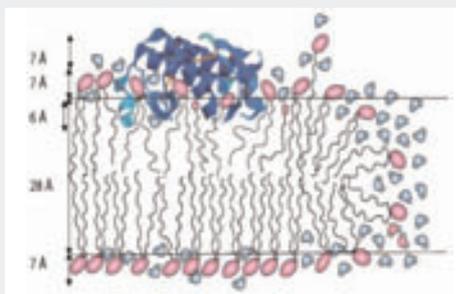
While neutron scattering methods have been available for some time, and have been refined and developed for non-biological systems, recent applications of the approach by the UK biological community are now producing a strong impact. This has arisen partly from developments in instrumentation specifically for biology at sources such as ILL and ISIS, and partly from an increasing

recognition of the power of deuteration methods, as well as new methods for sample production. Furthermore, as the amount of structural information continues to grow at a significant rate, and as analytical methods improve, there is growing awareness of the synergy that exists between X-ray, neutron, NMR and other spectroscopic methods for interdisciplinary studies of complex interactions at all levels of molecular organisation.



Selective deuteration used in conjunction with small angle neutron scattering reveals the arrangement of subunits in a Type 1 restriction-modification enzyme

Small-angle neutron scattering (SANS) is a powerful method that can be used to provide vital information at low resolution on the shape and inter-relationships between different parts of a macromolecule. Contrast variation can be used to highlight protein, nucleic acid or lipid

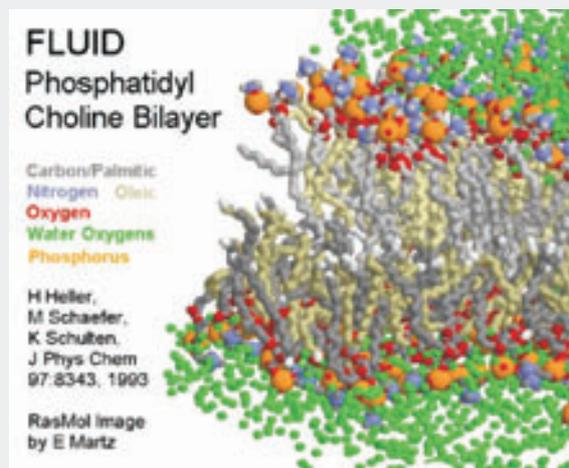


Schematic representation of Phospholipase A2 interacting with a phospholipid bilayer, derived from neutron reflectometry

components of complexes. Further insights into protein systems are possible if selective deuteration can be accomplished within a multi-subunit protein complex. Such an approach is now being routinely exploited using the facilities at the ILL-EMBL Deuteration Laboratory. A recent example is the determination of the subunit organisation in DNA modifying enzymes called Type I Restriction Modification enzymes. By individually deuterating the subunits, and studying reconstituted selectively deuterated analogues of the enzyme using SANS, it has been possible to determine

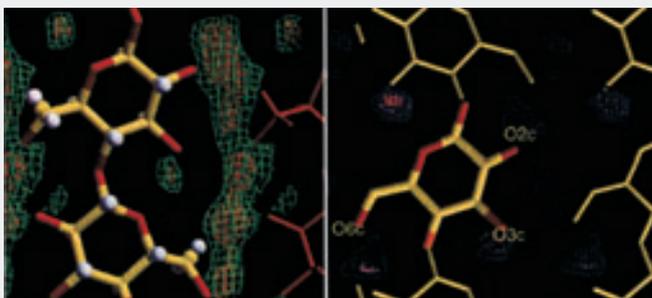
how the subunits organize to form the active enzyme. Work in progress aims to determine how these subunits move as the enzyme recognizes its target DNA sequence. Similarly, among many other examples, SANS has also revealed structural changes that occur in muscle proteins, and the way immune system proteins (immunoglobins) adapt their shapes to allow them to bind different targets. SANS, in conjunction with selective deuteration, is therefore emerging as a unique method. With developments in instrumentation currently underway it is likely to become a key technique for the study of proteins over the coming years.

A large number of key biological processes - from photosynthesis to the first interaction of cells with pathogens - occur in the region of the cell membrane. Of the estimated 30,000 proteins coded by the human genome, 30% are thought to be membrane proteins. Neutron reflectivity from selectively deuterated and contrast matched model membranes is emerging as a powerful technique for probing the structure and behavior of bilayer systems. The most detailed experimental structure of the phospholipid bilayer was obtained by combined x-ray and neutron diffraction from stacked bilayer systems, and the technique is being extended to ever more complicated systems. Neutron reflectivity has been used to understand the mechanisms by which toxins attack cell membranes, or how natural antibiotics affect the membranes of bacteria, possibly leading to new approaches in the fight against drug resistant pathogens. It is also yielding key insights into the delivery of genetic material across membranes, which is vital if gene therapy is to become a practical reality. Neutron reflection is also providing insights into the interactions between biological materials and coated surfaces. This will be essential in the development of new biocompatible surfaces for the next generation of medical implants and devices.



The structure of the phospholipid bilayer, at the atomic level

In fibrous materials, the advantages of using neutron diffraction for the investigation of solvent structure or hydrogen atom positions around molecules are clear. Here again selective deuteration can be powerfully used, as illustrated in recent neutron fibre diffraction studies of cellulose. This work was critical in establishing the nature of the hydrogen bonding in different forms of cellulose and in attempting to understand the conversion between these forms.



Density maps from neutron high-angle fibre diffraction reveal the hydrogen bonding network in cellulose.

Neutron crystallography can also provide important information at high resolution. Questions concerning hydration or the location of hydrogen atoms at the active sites of enzymes may warrant the growth of large crystals and the pursuit of a information not always available from X-ray diffraction. For example, Laue neutron diffraction has enabled the

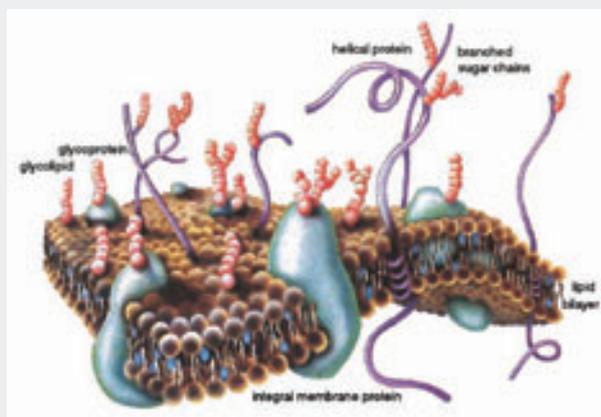
positions of water molecules in concanavalin A (a saccharide binding protein) to be pinpointed, therefore accurately determining the geometry of H-bonded networks in the active binding site. Similarly, the technique has been used to determine the positions of labile hydrogen atoms in the active site of Aldose Reductase, an important enzyme implicated in diabetic complications. This has provided further detail on residues in the active region of the protein, with potentially important consequences for drug design.

Biological macromolecules are nano-machines whose structures and internal motions have been selected by evolution to perform specific biological functions. Because neutron wavelengths and energies match vibration amplitudes and energies, respectively, neutron spectroscopy is uniquely suited to provide experimental data on atomic motions in such macromolecules under the influence of forces that maintain their stable and active structures. Current neutron instrumentation allows the measurement of functional dynamics in molecular biology over a variety of relevant time scales, from the picosecond scale of vibrations to the nanosecond scale of macromolecular diffusion. Experiments on protein solutions, membranes and whole cells, respectively, have allowed macromolecular dynamics to be related to protein stability and activity in different solvent environments, to the activity of bacteriorhodopsin, a membrane protein nano-machine with light driven proton pump activity, and to the adaptation of bacterial cells to extreme temperatures.

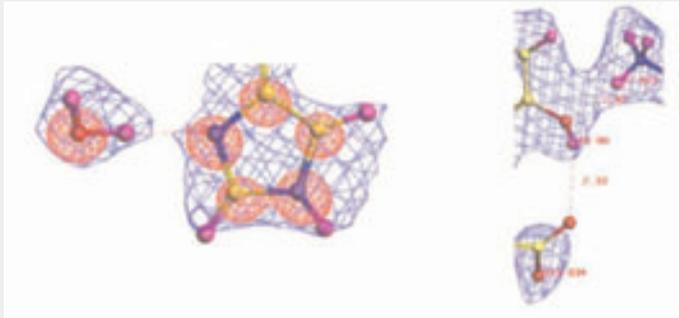
Future applications

Developments at existing UK-funded neutron facilities are producing major changes in the scope of neutron scattering for the study of biological systems. All this is occurring during a period when we are seeing a revolution in Biology comparable to that seen in the physical sciences in the early part of the 20th century. The sequencing of the genomes of many organisms, from simple plants and bacteria to humans, has provided a huge resource and allows modern molecular biology and biochemistry methods to produce large numbers of native and synthetic biological molecules and biomaterials in a variety of biological and biotechnological contexts.

It is becoming increasingly obvious to the biological community as a whole that as the questions in biology become more and more complex, real progress for biology and biotechnology will require genuinely multidisciplinary approaches. A large number of chemical, biochemical and physical techniques will be required to study complex biological systems, necessitating new collaborations between workers across a range of disciplines. Neutron methods will play a vital role giving novel information as well as providing strong complementarity with other techniques in which the UK has pre-eminence and major support, such as X-ray diffraction, both solid state and solution NMR, and electron microscopy.



The cell membrane, showing the location of proteins and other cellular material within the phospholipid bilayer



Density maps showing the positions of hydrogen atoms in protein crystals as determined by neutron crystallography

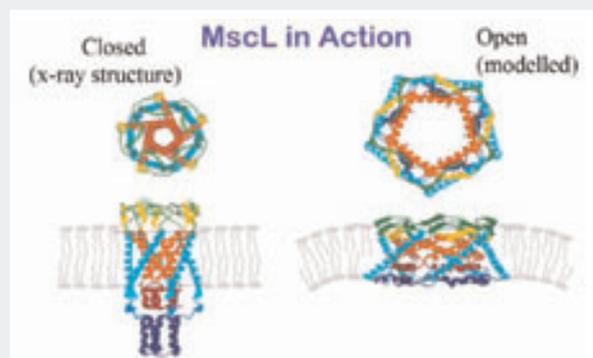
Neutrons have significant advantages for the study of biological systems. The fact that they are non-destructive means that delicate biological molecules, which can be destroyed by other methods, can be studied without damage. SANS provides a unique ability to study interactions between different parts of complex multicomponent systems.

Reflectometry allows novel access to the study of membranes and a large number of proteins, peptides and drugs that interact with membranes. Fibre diffraction methods can provide important information about hydration or hydrogen atom positions in partially ordered systems (eg cellulose, amyloid, DNA, muscle, collagen, filamentous viruses) as well as other functional materials. Neutron crystallography can be used to address specific questions relating to hydration or proton positions, for example where questions exist about protonation states at the active site of enzymes or in drug or ligand binding. While structural information is vital in understanding the properties of biomaterials it is important to emphasise that biological systems are not static, and that an understanding of the dynamics of these systems is becoming increasingly important. Neutron scattering is sensitive to the motions of molecules, from the scale of individual atomic atoms to the fluctuations of whole biopolymers, and can therefore provide information on dynamics on timescales relevant to biological function and complement rigid-atom information.

All of these techniques will have a major impact on the study of a wide range of biological systems, and can be expected to make a significant contribution to our understanding of fundamental biology, as well as in biotechnology, where the characterisation of new biomolecules/biomaterials will be essential. Some of the areas in which neutrons can be expected to make a key contribution include:

Membrane proteins

Membranes perform critical tasks in living systems including a wide variety of recognition functions and transport processes. Also the regulation of cellular viability is controlled through channels such as the mechanosensitive channel (MscL) which is being studied using neutrons to complement limited data from crystallography and NMR. Membrane proteins are also predicted to be the target for 50-85% of all new therapies for the next 10 years. Despite their prominence in all living systems, information on the structure and dynamics of such proteins is scarce, especially in functional description. SANS, neutron reflectometry and dynamics methods will all provide essential information on systems of this type to add to the knowledge base for this elusive class of biomolecule.



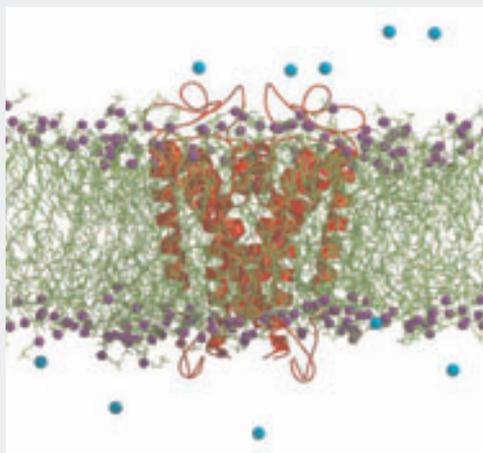
Schematic representation of the proposed mechanism of the MscL channel.

Gene delivery systems

The realization of the full potential of gene therapy will depend on the future development of safe and efficient gene delivery vehicles. Neutron reflection and small angle scattering will continue to be used to study the interaction of vectors and genetic material with membranes, exploiting the strength of the methods to study interactions between macromolecular complexes. Chemical diversity and physical size is being manipulated in drug delivery design for eventual therapeutic use. This is a commercial use of neutrons for which the UK-funded facilities are seeing an increase in use due to the lead in this area.

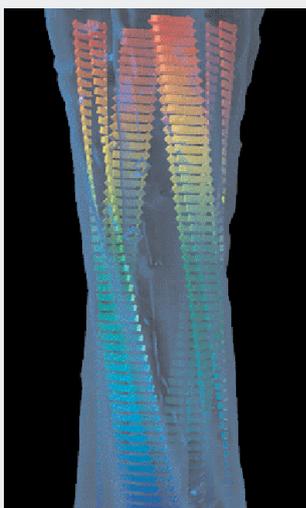
Natural Antibiotics

There have been many natural antibiotics isolated from plants, animals and microorganisms in recent years. In contrast to traditional antimicrobials, many are believed to act on the bacterial membrane, disrupting its integrity and function leading to cell death. Neutron reflectivity and small angle scattering will be crucial in determining their mechanisms of action, leading to new approaches to tackle drug resistant pathogens.



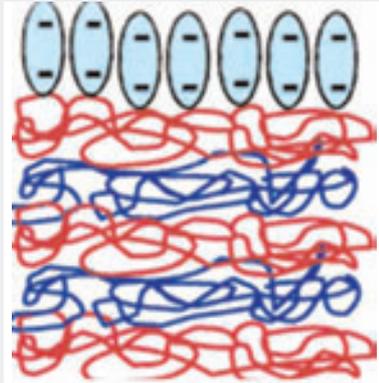
Molecular structure showing the location of an integral membrane protein

Folding and mis-folding of Proteins



Proposed arrangement of prion proteins in a 'fibril'

Protein misfolding has been implicated in many fatal amyloid diseases (eg Alzheimer's, prion diseases). Information on the structure of amyloid and on its assembly is becoming an urgent need given the public health issues involved. A variety of approaches are being taken to investigate these systems, including the study of a number of amyloid-forming synthetic peptide sequences as well as amyloid forming systems of 'native' origin. These studies have used electron microscopy, X-ray fibre diffraction, X-ray crystallography, solid state NMR and a variety of other techniques, with major progress in all of these areas. Neutron scattering, exploiting instrumentation that is currently being developed, can offer unique information here, complementing other approaches and allowing the investigation of amyloid systems both in solution and in partially-ordered samples. In both cases segmental labelling (deuteration) may be used to study ordered and disordered regions of these samples. Furthermore SANS methods can be used to study aggregation processes that occur during amyloid formation.



Polyelectrolyte multilayer, developed for biocompatibility and specific recognition

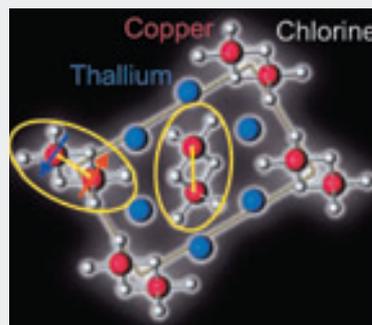
Bio-compatibility

Development of a wider range of bio-sensors (tissue based sensors) and of synthetic bio-replacement materials, and improvements in bio-compatibility and bio-lubrication, will contribute greatly to many aspects of modern health care. Neutron reflectivity, coupled with the manipulation of 'contrast', will be a crucial tool for these surface related problems, and the ability to probe a wide range of length scales will be essential for studying bulk bio-synthetic materials.

Introduction

The applications of neutrons as a probe of solid state physics range from investigations of concepts of fundamental physics to studies of near-application materials. Fundamental studies include those of physical realisations of simple theoretical models, but which nevertheless demonstrate novel or incompletely understood phenomena. One example is the study of magnetism in materials where quantum mechanics produces non-classical behaviour or novel states such as superconductivity and Bose-Einstein condensation. Another example of fundamental studies is that of strongly correlated electron systems. Here, well-established models of electrons moving in the 'average' background of the other electrons break down, and new concepts like quantum criticality need to be developed. These studies often require extreme experimental conditions - high magnetic fields, temperatures close to absolute zero, or pressures of thousands of atmospheres. Fundamental studies lead both to improved understanding and to the development of new materials. A comprehension of quantum magnetism is needed in order to understand the complex materials in which it plays a fundamental role, such as high temperature superconductors, or the molecular magnets that may become the components of future quantum computers. Strongly correlated electron systems can involve the coupling of the electron spin with the lattice vibrations or ordering of atomic orbitals, with concomitant coupling of, for example, resistivity with applied magnetic field, pressure and electric fields; these couplings can potentially be exploited in new materials with practical applications. Neutrons are an important probe as part of the effort to understand such materials, as they also are for investigating the magnetic nanostructures that already play an important role in data storage and sensors. There are huge materials science challenges to create the nanoscale devices for proposed future technologies such as spintronics. With enhanced capabilities, neutron scattering techniques will be a key tool for characterising and understanding these devices.

From fundamental studies to nanostructure materials science, improved neutron sources and instrumentation will offer new opportunities. A general need is for higher flux instrumentation to study samples that are smaller than presently studied, either because of difficulty in preparing large volumes, or because of intrinsic limitations imposed by extreme sample environment equipment. Alternatively, higher flux can be traded for better resolution; just as with the Hubble space telescope, better resolution will lead to new discoveries. The following sections expand on the science themes discussed above and the future opportunities in those areas.

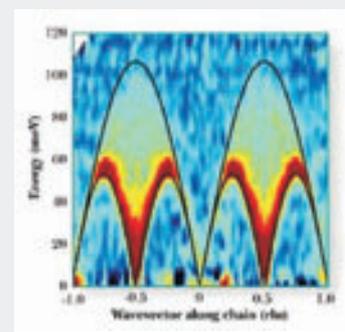


Atomic structure of $TiCuCl_4$. The copper ions form dimers (yellow rings) which weakly interact. The simple magnetic interactions make the material a model for studying Bose-Einstein condensation.

Quantum magnetism and molecular magnetism

Experimental realisations of model magnetic systems - those in which the interactions between magnetic ions have a particularly simple form - are test-beds for our fundamental understanding of magnetic phenomena. If we are to understand the properties of complex and potentially useful materials in which magnetism plays an important role, e.g. colossal magnetoresistive oxides or high-temperature superconductors, we must first understand the properties of model magnetic systems. The most sensitive and discriminating test of a magnetic model is its dynamics, which can only be probed using neutron scattering.

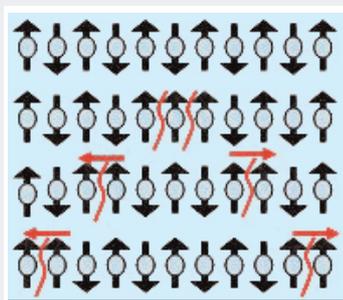
Simple interactions can lead to far from simple properties. When the quantum nature of the magnetic moment on atoms becomes important, entirely non-classical behaviour can result. One recent example is the remarkable observation of Bose-Einstein condensation in a magnetic system. In TiCuCl_3 , copper ions form weakly interacting nano-scale spin dimers. The ground state is non-magnetic with a non-zero energy gap to the excited magnetic states. An applied magnetic field reduces the gap until at a critical field one of the magnetised states becomes the new groundstate, at which point a non-magnetic/magnetic quantum phase transition occurs which is correctly thought of as the Bose-Einstein condensation of magnons. Thus, by studying arguably one of the simplest quantum magnets - coupled spin dimers - it is possible to test and develop fundamental concepts which have wide ranging applicability.



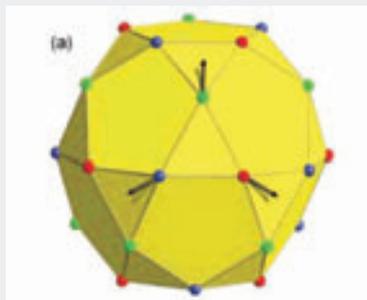
The wavelength-frequency map of scattering for the spin $1/2$ chain, measured in the model system KCuF_3

Another example of non-classical behaviour is a simple chain of spin $S=1/2$ ions. The classical picture of the magnetic excitations is a spin wave - the coherent precession of perturbed spins around their average direction. With spin $1/2$ the minimum perturbation on the chain is reversal of the spin, leading to defects on the chain which can only be created in pairs and propagate independently. The result is a continuum of energies for any given momentum of the defect pair. Neutron scattering was required to observe this phenomenon. The comprehensive data maps permit complete tests of predictions of the energy continuum and wider concepts such as energy-temperature scaling in this simple example of a one-dimensional system at the critical point between magnetic and non-magnetic ground state.

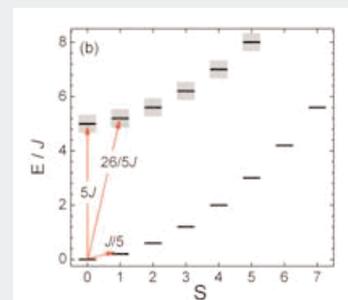
A topic of particular current interest, because of both fundamental physics and potential applications, is what happens when molecular systems are constructed with several magnetic ions to form molecular magnets. These are often constructed using organic complexes; the great flexibility and combinatorial possibilities of organic chemistry mean that molecular magnets can be found in a bewildering variety of shapes and geometries. Molecular magnets are widely heralded as likely components of any future solid-state realisation of a quantum computer. However, direct calculation of the exact quantum mechanical behaviour of such systems rapidly becomes complicated as the number of magnetic ions in the molecule increases. Instead, approximate or effective theories have to be developed to understand their behaviour. Neutron spectroscopy is proving to be invaluable in this burgeoning field as the most productive way to develop and test such theories. One of the largest magnetic molecules yet synthesised is $\text{Mo}_{72}\text{Fe}_{30}$, known as



The reversal of a spin in the spin $1/2$ chain causes a pair of defects in the arrangement of the spins, which can independently move along the chain



The near-spherical molecule $\text{MO}_{72}\text{Fe}_{30}$ showing the magnetic moments of three of the iron ions

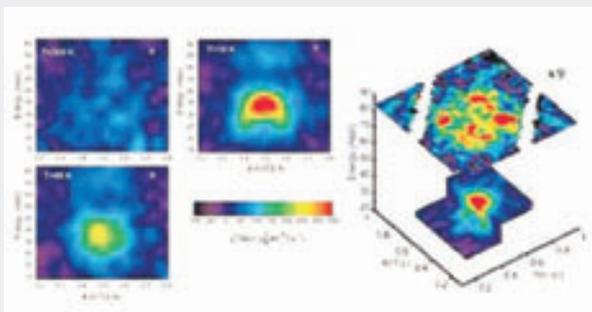


Energy levels of the higher energy states of the magnetic system, as probed by neutron scattering

Keplerate. This nano-meter sized polyoxomolybdate is a molecular quasi-sphere in which 30 Fe^{3+} ions ($S = 5/2$) occupy the vertices of an icosidodecahedron. The spins interact via an isotropic antiferromagnetic exchange coupling between nearest-neighbors. Neutron scattering data established that the low-energy physics of this complex molecule could be understood on the basis of an effective three-sublattice Hamiltonian mode.

Strongly correlated electron systems

Materials with incompletely filled d or f electron shells with narrow bands can display a plethora of unusual properties, including superconductivity at temperatures far higher than conventional theory can account for (high- T_c superconductors), certain oxides of manganese whose resistivity can change by many orders of magnitude in an applied magnetic field, and heavy fermion metals which behave as if the electron mass has been increased by a factor of 100 or more. The properties of these materials cannot be understood within the well-established framework of solid-state physics that explains simple metals, semiconductors or insulators. The essential difference is that any one electron cannot simply be considered as moving in a static 'sea' of the averaged motion of the others; the motion of an electron is too strongly correlated with that of



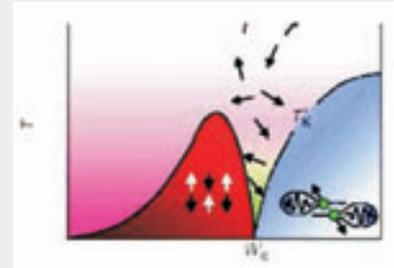
Portions of the wavelength and frequency dependent spectrum of magnetic excitations in the bilayer superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$

others. The outcome is an inter-play between the spin, charge, lattice and orbital degrees of freedom that can result in a host of exotic orderings, which in turn are responsible for the novel properties of strongly correlated materials, and the sensitivity to small changes in control parameters such as temperature, magnetic field, pressure or band-filling. As a consequence, strongly correlated materials form a major theme in current solid-state physics research.

Neutron scattering has had a huge impact in the field. One reason is that the magnetic properties of the materials are central to their the properties; neutron scattering is the method of choice for solving magnetic structure and is unique in being able to map the full momentum and frequency dependent correlations of the magnetism. Another is that many strongly correlated systems are oxides of transition metal and/or rare earth atoms, where the precise knowledge of the location of the oxygen atoms that neutron scattering provides is important to understand the properties. A good example that illustrates these points is the quest for the understanding of high temperature superconductivity. After more than 15 years of study, a full explanation has yet to be found. The general agreement is that the mechanism that pairs the electrons is magnetic, yet the nature of the magnetic interactions is unresolved. To discriminate between the host of theories requires a detailed knowledge of the magnetic fluctuations. Recent advances in techniques have enabled unprecedentedly comprehensive mapping of the spectra. In particular, in two different classes of high- T_c superconductor, one with isolated single Cu-O layers ($\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$) and the other with isolated Cu-O bilayers ($\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$), the similarity of the spectra strongly indicate a common mechanism for high- T_c superconductivity.

Heavy Fermions and quantum criticality

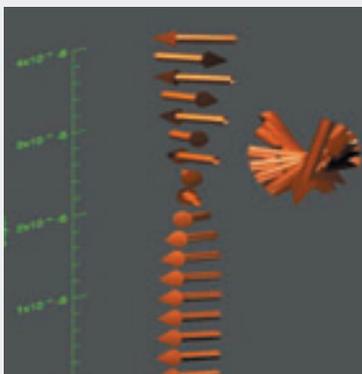
Heavy Fermion systems are distinguished from normal metals in that they exhibit extremely strong electron correlations. Often they can be understood mostly within the framework of Landau Fermi liquid theory, except that they must be attributed a very large effective electron mass. Recently striking evidence has been discovered that Fermi liquid theory breaks down in certain HF systems, and indeed in other strongly correlated materials. A commonly occurring case is in magnetic HF systems where the magnetic transition temperature tends to zero when some external control parameter such as magnetic field is applied. Here it is believed that a proliferation of low-frequency magnetic fluctuations in the vicinity of a quantum phase transition (QPT) leads to the non-Fermi liquid behaviour. The ability of inelastic neutron scattering to measure the momentum and frequency dependent spectrum of magnetic fluctuations enables definitive information about the nature of the QPT to be determined. A striking example is that of CeCu_6 , where the QPT is approached by substituting a small fraction of the copper with gold. Experiments were able to show that, as the QPT is approached, the mobile electrons of the metal localise at atomic sites, destroying the simple Fermi liquid picture.



At the critical coupling strength, W_c , between the mobile electrons and the atomic electrons at which there is a zero temperature phase transition between magnetic and non-magnetic order, local magnetic moments form at the atomic positions down to the lowest temperatures – distinguishing between two competing theoretical models

Nanostructured thin films, spintronics and interfacial phenomena

In recent years, the study of solid state magnetism has undergone a revolution in the area of magnetic nanostructures. This has been jointly driven by the discovery of the giant magnetoresistance effect (GMR) in 1988 and the development of advanced deposition techniques such as sputtering and molecular beam epitaxy (MBE). It is now possible to grow magnetic multilayers with atomic-plane precision and with tailor-made physical properties. In parallel, the transition from scientific discovery to commercial exploitation has been dramatic; numerous practical applications exist including magnetic devices for data storage, many types of sensor, next generation electronics - the so-called "spin electronics" - and potentially also quantum computing. Central to both fundamental and applied studies is the importance of the interface between materials in atomic proximity. Polarised neutron reflectometry is ideally suited for the study of such systems.

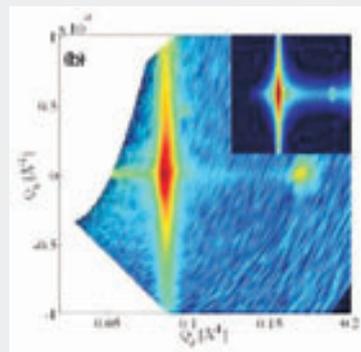


The spiral magnetic structure at the interface of antiferromagnetic and ferromagnetic layers.

Neutron reflectometry provides depth dependent information on both the chemical structure and the magnetic structure. This contrasts with more conventional techniques which provide an average over the entire sample (e.g. vibrating sample magnetometry) or only sample the near-surface region (e.g. microscopy). Real space models of the magnetic structure of systems can be reconstructed as a function of the distance from the surface, allowing tests of fundamental concepts such as the interplay between magnetism and superconductivity when placed in atomic proximity, or the origin of the magnetic exchange bias. This phenomenon was observed in the late 1950's but is still not fully understood, though it is exploited in

every modern computer in the hard disc read head. Exchange bias arises from the exchange interaction between an antiferromagnet and a ferromagnet, resulting in an off-centre coercivity loop, and is the method used to magnetically pin the reference layer in read heads. A partial explanation for the lack of understanding is the difficulty in characterising the buried interface between the antiferromagnet and ferromagnet. Neutron techniques uniquely have been able to reveal and quantify the proposed spiral magnetisation structure and the process by which the ferromagnetic layer reverses in an applied magnetic field.

The neutron technique is also able to probe in-plane structures on the micron length-scale. Conventional microscopy techniques, for example optical and atomic force microscopy, are easily able to probe such length scales, but only over small areas. The neutron technique samples a large area and provides a statistically significant measurement. For magnetic systems it is straightforward to apply a magnetic field to the sample, compared for example to electron microscopy techniques, so as to replicate in-situ conditions.

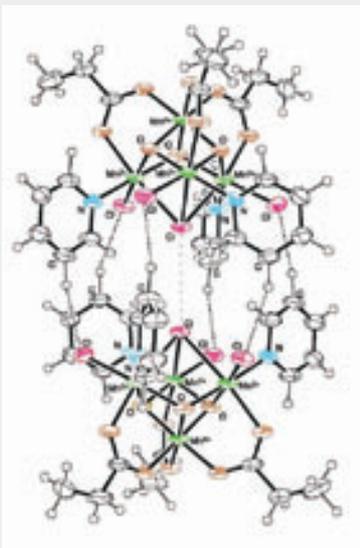


Neutron scattering intensity maps from a magnetically coupled multilayer. The inset shows a calculation revealing the details of the in-plane ordering

Future applications

Quantum magnetism and molecular magnetism

Future technologies will be based on our ability to engineer and understand the properties of materials at the atomic or nano-scale. Quantum effects become of increasing importance as this scale is approached, either by explicitly creating atomic scale objects or by reducing the dimensionality in one or more directions, giving rise to novel states of matter. Understanding the nature of such 'Quantum Matter' represents an enormous intellectual challenge, as well as requiring the development of new experimental techniques.



A dimer molecular magnet – two Mn⁴⁺ clusters

The continual discovery and synthesis of quantum magnets will enable tests of concepts of broad significance in systems with different interaction symmetries and geometries. These include quantum phase transitions (phase transitions at the lowest temperatures, that are driven by zero-point quantum fluctuations rather than thermal fluctuations), the stable multi-ion entities that can emerge where there are strong competing interactions ('quantum protectorates'), and models of quantum entangled systems interacting with decohering reservoirs of other degrees of freedom. All too often, good model systems can only be synthesised as small crystals, demanding better instrumentation than presently available. The energy scales that need to be probed, and the associated demands for high magnetic fields and low temperatures, go beyond current limits, requiring the development of instrumentation and sample environment with wider operating ranges.

Molecular magnets are widely considered to be likely building blocks for future quantum computers, as they are the smallest magnetic entities that can store a bit of information, and give the possibility of initialising and manipulating a coherent superposition of different quantum states of the molecule - the essence of quantum computation. Despite the invaluable contribution of neutron scattering to the field, progress is limited by the sensitivity of present day neutron spectrometers, which means that systems will only be investigated if they can first be produced in large volumes. Higher sensitivity and tighter resolution neutron spectrometers, coupled with larger magnetic fields to alter the magnetic ground state, will bring the unique capabilities of the technique to bear on the design of molecular magnets.

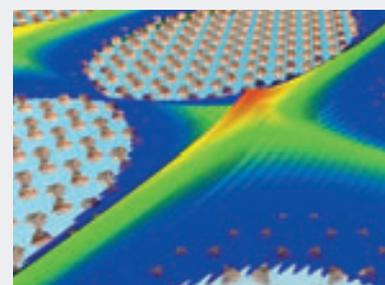
Strongly correlated electron systems

The study of strongly correlated systems will continue to be an active area of study in condensed matter research because of the host of interesting and unusual physical properties they can support, and the sensitivity of those properties to external control parameters. This richness derives from the coupling of a number of degrees of freedom, which makes understanding the systems a theoretical and experimental challenge. The neutron couples to both the atomic positions and magnetic degrees of freedom, which makes it a powerful tool in this field. To unravel this inherent complexity will demand more powerful neutron techniques for several reasons:

- The handle to understanding complex phenomena is the alteration of external control parameters, e.g. temperature, pressure, magnetic field or electron band filling. The time taken to conduct such parametric studies in several dimensions hampers investigations, so much higher throughput is required.
- With strong correlations and coupling between the different degrees of freedom it is becoming ever more important to make maps of the atomic and magnetic fluctuations, rather than sampling at special high symmetry points. For example, in high temperature superconductors the differences between predictions from competing theories can be subject to assumptions about the magnitude of parameters only within crude bounds - and correspondingly the locations of crucial regions in momentum and energy may not be known.
- Polarisation analysis is needed to understand the hybrid modes that emerge from the coupling of different degrees of freedom, yet is achieved at the price of large flux losses.
- Critical points at which defining phenomena are most pronounced - such as quantum critical points - often require sample environment that is restrictive on sample size, for example high pressure cells or large magnetic fields. Also, when new materials are discovered, they are frequently only available in small quantities. For investigations to be timely, or even feasible, improved capabilities are needed.

Spin electronics

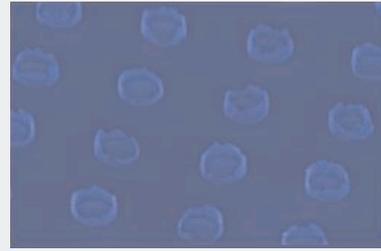
The ability to generate, manipulate and detect spin-polarised electrical currents in magnetic materials has resulted in the now burgeoning field of 'spintronics', which refers to the possibility of using the spin of the electron, as well as the



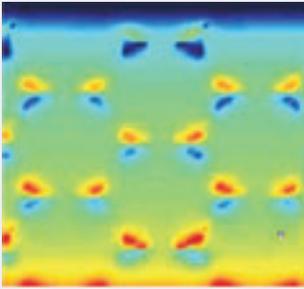
A schematic illustration of a patterned surface such as could be envisaged for high current density spintronic applications. The corresponding neutron scattering pattern is overlaid.

charge, to process and store information. The massive investment in spintronics-based research by companies such as IBM, Hitachi, Siemens and Seagate, is based on the huge revenue (billions of dollars per annum) that they are already reaping from early devices which exploit the basic GMR spintronic effect in hard disc spin-valve heads, and the revenue that is expected to come from magnetic RAM (MRAM).

There are huge materials science challenges if this concept is to be technologically relevant, for example in producing magnetic semiconductors that operate at room temperature. To incorporate these materials into useful structures it is essential that the interfacial chemical and magnetic structure is well characterised and understood. It is because of this requirement that neutron reflectometry will provide unique information, and the possibility of using this information to smart engineer new materials and devices.



Example of a patterned structure – cylindrical spin-valves



The calculated variation of the total magnetic field in the multilayer resulting from the patterning

For devices that rely on spin-injection for their functionality the systems will need to be nano-scale in all three dimensions, rather than nano-scale in a single dimension as is generally studied at present. For example, to continue the exponential increase in information storage areal density will require new approaches to circumvent the limits imposed by the nature of the physical interactions in the current technology. A promising technique is to produce regular grids of devices by patterning. Neutron techniques will be key to the characterisation and understanding of the operation of this new generation of materials and devices, but their increased complexity and three-dimensional nanoscale structure will demand improved capabilities.

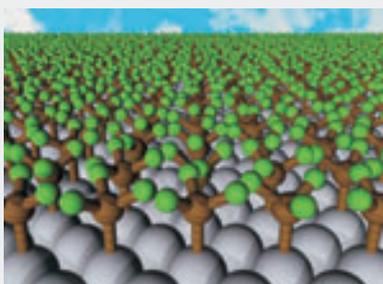
Neutrons

Chemical Activity and Molecular Motions

In studies of the dynamics of atoms and molecules, the great strength of neutron scattering lies in the availability of a range of techniques that not only cover time scales from 10^{-14} s to 10^{-6} s, but also simultaneously can provide distance information over length scales from 10^{-11} m to 10^{-6} m. Neutron scattering is unique in this respect.

Neutron spectroscopy can be used to study the molecular vibrational spectra of materials. Most applications so far have been to hydrogenous materials, taking advantage of the large incoherent cross-section for neutrons. The technique is very comparable to Raman scattering; it has the relative disadvantage that it is slower and larger samples are required, due to the low neutron flux, but the specific advantage that the peak intensities can be measured and calculated on an absolute scale and directly used to make vibrational mode assignments - there are no selection rules. In addition the use of isotopic substitution, particularly H-D substitution, allows the scattering from specific hydrogen bonds to be 'turned on and off', providing unique information. There have been significant improvements in the achievable resolution over the years. Neutron spectroscopy is now routinely used, in conjunction with ab-initio calculations, to provide unambiguous tests of detailed structural models of molecules and their local environment.

The measurement of rotational tunnelling spectra in model compounds has provided specific and reliable information, in combination with theoretical chemistry programs, on the interatomic potential surfaces surrounding particular molecular units (e.g. methyl groups). The effects of perturbations such as pressure or disorder have been studied in a controlled manner. The results form the necessary basis for the understanding of more complex systems, for example where coupling to other degrees of freedom becomes important.

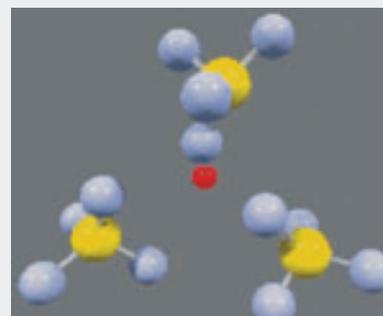


Artistic representation of methyl groups on the surface of a Pd catalyst

Neutron scattering has made key contributions to our detailed understanding of catalysts and other chemicals of industrial relevance. The technique has been used to identify the different hydrogen species present on a catalyst, determine their relative proportions and follow changes according to treatment. The state of the majority of adsorbed hydrogen on MoS_2 was determined to be molecular, while on RuS_2 , which is ten times more active, it was mainly atomic. Deactivation of an industrial Pd catalyst was found to be due to the presence of a layer of methyl groups on the surface.

Diffusion of molecules through porous solids such as zeolites, important in catalysis and separation processes, can be studied by quasi-elastic neutron scattering (i.e. low energy scattering where the elastic peak is broadened). Neutrons are particularly good at distinguishing light atoms, such as hydrogen, relative to the background matrix. When the size of the molecule is comparable to the size of the pore the diffusivity can be significantly reduced, but neutron spin-echo techniques can be used to study such slower motions.

Measurements of diffusion and charge transport in solid and liquid electrolytes and other ionic conductors are important for improved understanding of conduction mechanisms. Neutrons are particularly powerful for studying the motion of



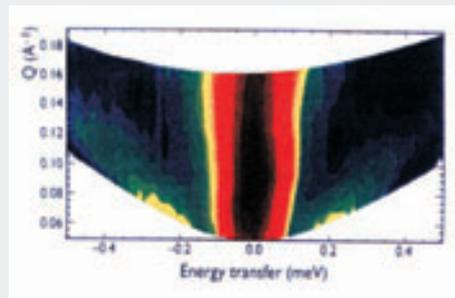
Proton conduction in $\text{C}_6\text{H}_8\text{SO}_4$

Neutrons

Chemical Activity and Molecular Motions

hydrogen because of its large incoherent cross-section, e.g. in metal hydrides for use in batteries or hydrogen storage materials, or in proton conductors for use in fuel cells. Oxygen ion conduction in fuel cell materials, or Li ion conduction in polymer batteries, can also be studied. Most work on non-hydrogenous materials has so far been on model compounds, but as techniques improve in-situ studies of ionic transport in real devices will become feasible.

Inelastic neutron scattering, closely coupled with theory and computer simulation, has provided much of our basic understanding of both single particle motions and collective modes in simple liquids. Experiments require measurements over as broad a range of energy and momentum transfer as possible due to the lack of any symmetry in the structure. Early measurements identified the existence of propagating acoustic modes in simple liquid metals (e.g. Rb), but which became overdamped at a Q value comparable to the first peak in the structure factor, i.e. a wavelength comparable to the interatomic spacing. In noble gas liquids, e.g. Ar, overdamping occurred at much lower Q, requiring the development of low angle inelastic scattering techniques, 'neutron Brillouin scattering', to access them. Recently developed inelastic X-ray scattering techniques both complement and extend the information that can be obtained with neutrons. A popular area of study has been the existence of 'fast sound' in liquids such as water.

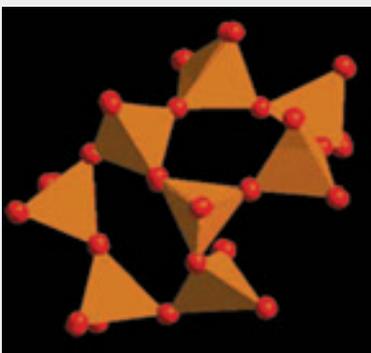


Dispersion of sound modes in liquid argon

Liquid He has been studied by inelastic neutron scattering since the very earliest days of the technique, initially driven by interest in the superfluid transition in ^4He . Neutrons provided the experimental validation of the dispersion of collective excitations, including maxons and the roton minimum. The recoil of high energy neutrons, 'neutron Compton scattering', can be used to probe the interatomic potential environment of specific types of atoms. This technique has been used to measure the Bose condensate fraction in liquid ^4He . Low energy inelastic scattering studies have been carried out on ^3He , which is the only readily accessible Fermi liquid, but these experiments needed an experimental tour-de-force because of the high absorption cross-section of ^3He . The elementary excitation spectrum was measured, showing spin fluctuations, a zero-sound collective mode and a quasi-particle-quasi-hole continuum. $^3\text{He}/^4\text{He}$ mixtures have also been studied. In recent years there has been a renaissance in the field with studies of quantum fluids in confined geometries, e.g. ^4He in Vycor glass, showing a range of new behaviours.

Our understanding of dynamics in glasses and amorphous materials is less well developed.

However the development of the mode coupling theory in the 1990's, together with concepts such as 'strong' and 'fragile' glasses, led to a considerable number of experimental studies of dynamics through the glass transition using neutrons. Initial validations of the basic scaling laws were made in systems ranging from elemental glasses such as Se to non-crystalline polymers such as poly-butadiene. Combination with data from light scattering and mechanical measurements in some cases gives data covering more than 10 orders of magnitude in time. Higher energy inelastic scattering has been used to show remarkable similarity between the density of states of network glasses such as silica and the corresponding crystalline phases, despite the lack of long



Low frequency modes in vitreous silica

Neutrons

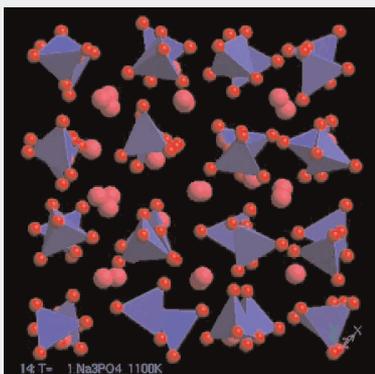
Chemical Activity and Molecular Motions

range structural order, or to provide additional information on complex structural units (e.g. boroxol rings in borate glasses) where results from structural data continue to be highly controversial. The origin of excess modes, the 'Boson peak' remains controversial.

Future applications

In chemical spectroscopy there are likely to be two emerging trends. Firstly, faster measurements on smaller samples will mean that the technique becomes more routinely applicable as a basic method for characterizing the internal modes of molecules. Raman and infra-red spectra may be measured simultaneously when possible, providing complementary information. The combination with ab-initio calculations will also become routine, though this will require the additional provision of high performance computing resources. Secondly, improved statistical accuracy and resolution, also coupled with increased computing power, will enable studies to move from internal modes to external modes. This gives the possibility to access more complex systems, i.e. to move from isolated molecules (model systems), to a molecule surrounded by many of the same type (e.g. in a crystal), to a molecule surrounded by many different molecules (e.g. in a chemical reaction medium or even a biological process). Despite the increasing complexity, the aim should be to maintain the advantage of neutrons in providing spectra that can be analysed on an absolute quantitative basis.

A particular early area of study will be strong hydrogen bonds, which are of interest for important biological mechanisms such as proton transfer. However they are not yet understood, even in model compounds. In studies of catalysis the emphasis will move from hydrogenous species to non-hydrogenous species, such as CO, SO₂ and NO_x.



Na⁺ ion conduction in NaPO₄

For quasi-elastic scattering studies of protonic and other ionic conductors the trend will again be to move from model compounds, in which the mobile species tend to have a high concentration, to 'real' materials (as used in e.g. fuel cells or high energy density batteries), where the concentrations tend to be lower. Studies of ions which are coherent scatterers of neutrons, e.g. Li and O, will be important. It is expected that these will be carried out in conjunction with other measurements (possibly simultaneously) such as conductivity and NMR. They will be complemented by structural (total scattering) measurements providing information on conduction pathways, and will be interpreted with the aid of computer

modeling and molecular dynamics simulation. Indeed, it is expected that molecular dynamics will be routinely used in conjunction with most neutron studies of chemical activity and molecular motions, and will be central to the exploitation of the technique.

While some neutron spectrometers already allow simultaneous measurement of structure and dynamics, this possibility is so far under-exploited. In the future it will be used more widely, for example to correlate changes in structure and vibrational spectra during chemical processes such as adsorption at a surface.

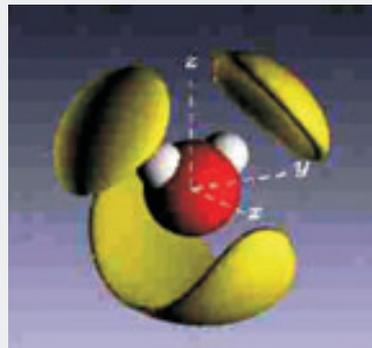
Pressure is another parameter that is not yet widely used in inelastic scattering studies, even though it is a very effective method for modifying potentials in a controlled manner and hence

Neutrons

Chemical Activity and Molecular Motions

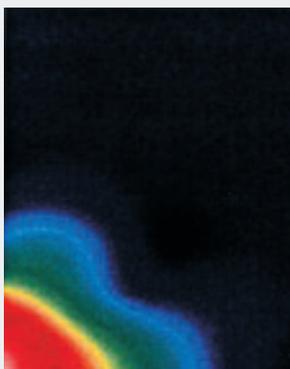
obtaining improved information on them. More widespread use will require higher beam intensities, either from higher flux sources or better use of focusing devices, in order to allow the use of smaller sample volumes.

As is indicated other sections, molecular magnets containing multiple magnetic ions offer the possibility to tune the magnetic interactions through organic chemistry, and are proposed as likely candidates for future quantum computers. The magnetic interactions can be very cleanly investigated through the measurement of low energy tunneling spectra.



The first oxygen coordination shell in liquid water

Aqueous and other solutions are clearly of enormous importance in chemistry and biochemistry/biology. However our understanding of the atomic dynamics is so far considerably less sophisticated than our understanding of the structure. Structural studies have become much more complex in recent years due to the combination of advanced computer modeling techniques and neutron diffraction data measured using multiple isotopic contrasts (H/D). The challenge for the future is to extend our understanding of water coordination as a dynamic process, including ionic, hydrophilic and hydrophobic interactions. This is likely to provide crucial underpinning knowledge for understanding of many dynamic biological processes such as protein folding.

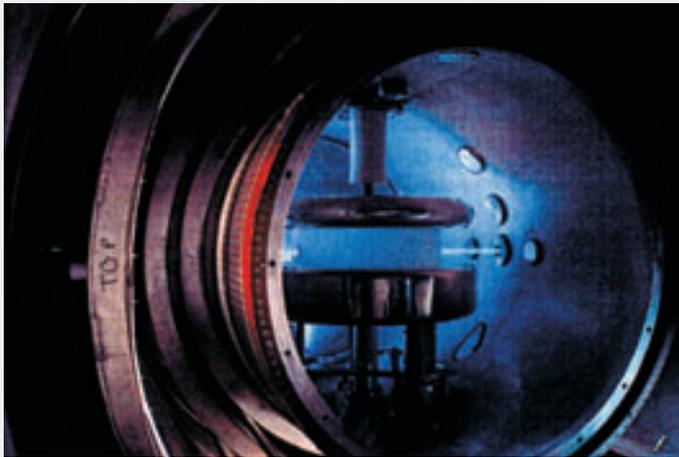


The wavefunction of a proton in KHPO_4

High energy spectroscopy using neutrons with eV energies has so far only been used at one instrument in the world. The technique has been slow in developing since it requires different technologies (e.g. detectors) to most other neutron instruments. However, it does offer the possibility to directly access information on potentials through measurement of the atomic momentum distribution, particularly for light atoms such as hydrogen. This is likely to be of increased use in future, for example in providing detailed information on prototype hydrogen storage materials. Recent developments have stretched the measurable energy and momentum transfer range into a region which is relevant for magnetic excitations, but is not readily accessible to chopper spectrometers. This will open up a new field of applications.

Fundamental Physics

Studies of nuclear and particle physics using slow neutrons contribute in various ways to a better understanding of the basis of our existence. They address fascinating questions ranging from fundamental interactions, to the creation of the chemical elements during the first few minutes after the big bang of the universe, to catastrophic cosmic events such as supernova explosions billions of years later. Some types of investigation focus on the properties of the neutron itself, while others employ the neutron as a versatile probe in nuclear reactions and scattering processes. Most experiments employ slow neutrons. Some are performed best using ultra-cold neutrons which have such a low energy that they can be trapped in bottles and observed for a long time.



Quartz storage cell for measurement of the neutron edm

A major goal of particle physics is to derive all of the forces appearing in nature from a unifying symmetry principle. This leads theorists to predict the existence of new, hitherto unobserved particles. Scientists working at particle accelerators try to produce these in high energy particle collisions and observe their decay characteristics. An alternative approach employs extremely high precision experiments at much lower energies. Manifestations of physics

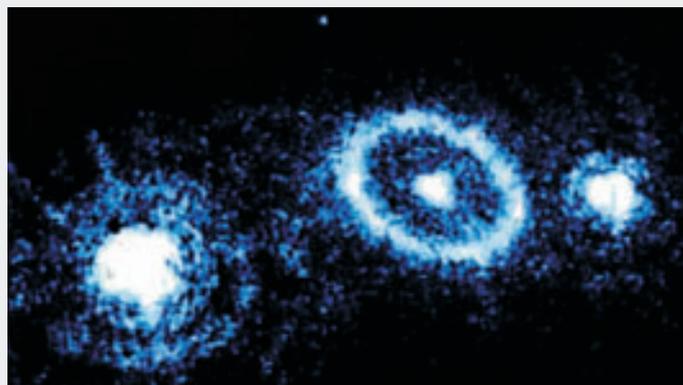
beyond the present theoretical framework should be detectable as tiny violations of some basic symmetries, either in particle properties or in well-selected interactions. Many observables are available in experiments with slow neutrons that are both sensitive to new physics and amenable to precision measurements. These complement experiments performed with particle accelerators. Perhaps the most prominent present example of this approach is the ongoing search for a non-vanishing electric dipole moment (edm) of the neutron. After more than 50 years of continuous improvement of the experimental techniques, and hence the accuracy, this experiment has now reached a sensitivity of the order of 10^{-23} eV for the energy of interaction of the neutron edm with external electric fields. Remarkably, this refinement has ruled out more theories beyond the standard model of particle physics than any other experiment. The property which renders the edm so significant is that its existence would show a violation of the symmetry with respect to the direction of time. By a deep theorem of particle physics this is related to a symmetry between particles and antiparticles, the so-called CP symmetry, with CP standing for charge conjugation combined with inversion of spatial coordinates. In high energy physics such effects have already been found in experiments with neutral kaons and B-mesons, which could be incorporated into the standard theory of particle physics. However, their small size is a major problem for cosmology: it cannot explain why the universe obviously contains so much more matter than antimatter. To solve this puzzle, a much stronger CP violation is required. Once a considerably more intense source of ultra-cold neutrons becomes available, as is presently being developed at various places around the world, CP violation beyond the standard model is expected to be observed as a non-vanishing neutron edm.

The neutron edm is not the only opportunity to search for time reversal invariance (T) violating processes. Two T-violating observables are presently being investigated in the decay of free neutrons, so far without any non-zero signal. Other experiments employ neutron-induced nuclear

reactions. Neutron optical methods have also been proposed. It is interesting that the various observables probe different mechanisms of T-violation. Such searches for tiny effects rely strongly on the availability of very intense cold neutron beams.

The experiments dedicated to revealing T-violation probe fundamental interactions relevant to the first microsecond after the big bang. Other observables employing slow neutrons relate to the question of the primordial origin of the chemical elements, which started to be formed about three minutes later. According to the standard model of cosmology, after the first second in the evolution of the early universe the density had already dropped below a critical value where weak processes could no longer maintain a thermal equilibrium between protons and neutrons. Neutrons then decayed freely into a proton, an electron and an antineutrino without re-conversion, which led to a continuous decrease of their number. This only came to an end after the temperature of the universe had dropped to such a low value that the deuteron, which is a non-radioactive nucleus formed by a proton and a neutron, was no longer subject to photo-dissociation by energetic gamma rays. A network of nuclear reactions subsequently led to the formation of some light elements. Obviously, one key property for understanding their primordial relative abundances is the lifetime of the free neutron, which is a direct measure of the strength of the weak interaction inducing this process. Combining this with the experimental value of one out of several decay asymmetries, one may determine the two coupling constants of weak interaction of the nucleon. These so-called vector and axial-vector coupling constants serve to determine many weak cross sections, also including those of important processes like the formation of deuterium via fusion of two protons in ordinary stellar burning, which is governed by the weak axial-vector coupling constant. Recent astronomical observations provide dramatically improved direct measurements of primordial element abundances together with a precise value for the number ratio of photons and nucleons in the universe. This progress calls for more accurate determinations of the neutron lifetime, together with some cross sections of reactions between light nuclei, in order to challenge the cosmological standard model.

It is not energetically possible to produce elements heavier than iron via nuclear fusion. It is relatively certain that these elements are formed in cosmic events like supernova explosions, where for a short time nuclear reactions provide strong neutron sources which induce reaction chains consisting of neutron captures and subsequent nuclear beta decays. The relative abundances of the various elements



Supernova 1987A

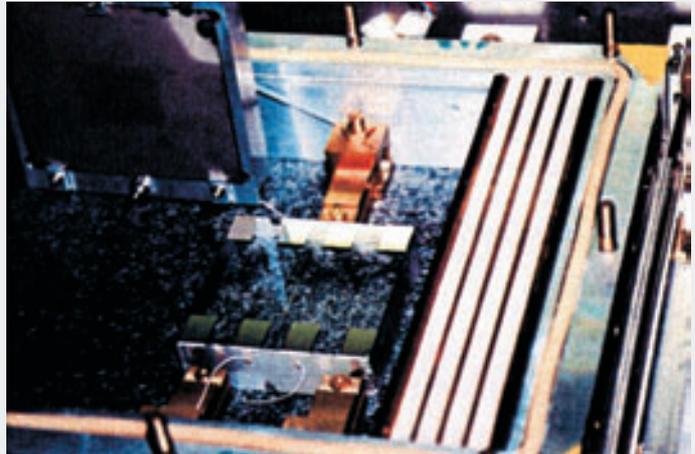
depend on the cross sections and lifetimes of extremely neutron rich nuclides, which are investigated using nuclear spectroscopy of fission fragments. Such studies are complemented by novel theoretical approaches to the nuclear many-body problem, where the ultimate aim is to understand interactions of bound nucleons in a model-independent way beyond existing nuclear theory with limited and rather uncertain range of applicability. This should result in firm predictions of cross sections of processes which either cannot be investigated directly in experiment or which will be amenable to experiment only in the near future, such as in investigations of exotic nuclei at new radioactive ion beam facilities. A first step is an effective

Fundamental Physics

field theory of nuclear forces, building on the fundamental symmetries of quantum chromodynamics. Full validation of this theory, and direct tests, require improved accuracy in measurements of the neutron scattering lengths and cross sections in nuclear few-body systems.

A completely new field of fundamental investigations with neutrons has just opened up with

the recent observation of neutron quantum levels above a mirror placed horizontally in the gravitational field of the earth. Although their existence was beyond any doubt - they are a straight consequence of ordinary quantum mechanics - a careful preparation of such states might lead to interesting applications. Particularly noteworthy is the search for deviations from the well-known ordinary Newton's law of gravity, which might occur at very short distances as a consequence of the hypothetical existence of folded extra dimensions. Within a certain range of small distances, neutrons are already now much more sensitive than the classical experiments with macroscopic test bodies. As in the search for the neutron edm, new sources of ultra-cold neutrons will be a key to further progress.



Apparatus for measuring quantum states of a neutron in a gravitational field

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