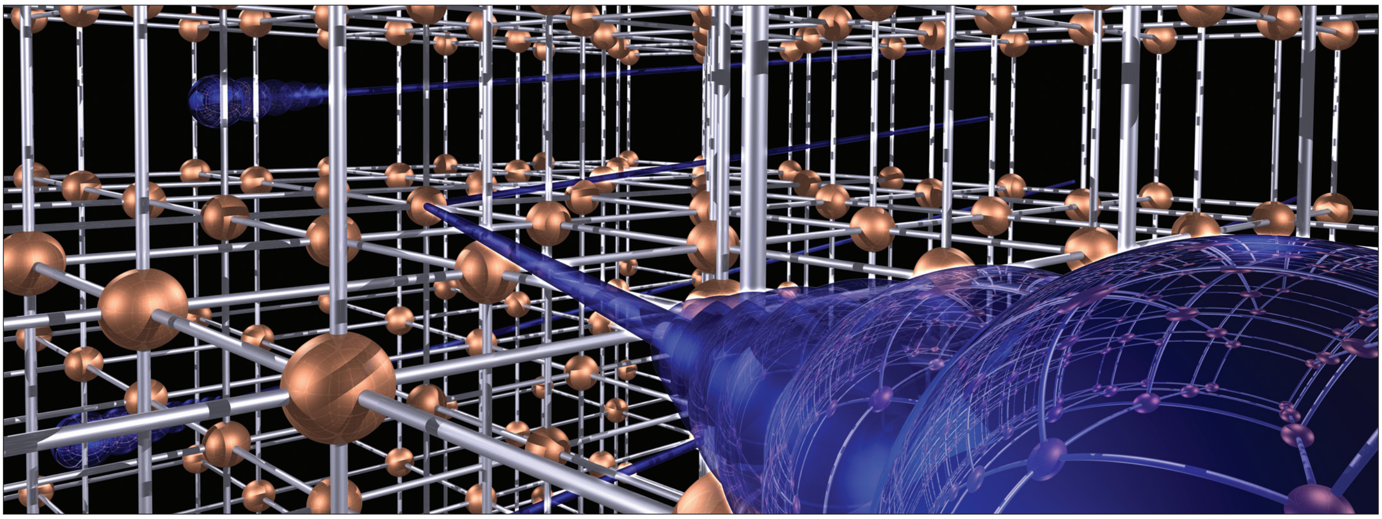
Neutron scattering

Neutron scattering is routinely used in modern science to understand material properties on the atomic scale. Originally developed as a tool for physics, the method has led to advances in many areas of science, from clean energy and the environment, pharmaceuticals and healthcare, through to nanotechnology, materials engineering, fundamental physics and IT.



ISIS NEUTRON SOURCE

What is neutron scattering?

The goal of modern materials science is to understand the factors that determine the properties of matter on the atomic scale, and then to use this knowledge to optimise those properties or to develop new materials and functionality. This process regularly involves the discovery of fascinating new physics, which itself may lead to previously unthought-of capabilities. Almost all of the major changes in our society, from the dramatic growth of computing and the internet to the steady increase in average life span, have their origin in our understanding and exploitation of the physics and chemistry of materials.

To investigate atomic-scale structure and dynamics, scientists use a variety of tools and techniques, often based on the scattering of beams of particles. An "ideal" probe might be one that has a wavelength similar to the spacing between atoms, in order to study structure with atomic resolution, and an energy similar to that of atoms in materials in order to study their dynamics. It would have no charge, to avoid strong scattering by charges on the electrons or the nucleus and allow deep penetration into materials. It would be scattered to a similar extent by both light and heavy atoms and have a suitable magnetic moment so that we can also easily study magnetism. The scattering cross-section would be precisely measurable on an absolute scale, to facilitate comparison with theory and computer modelling. This particle exists – it is the neutron.

Unfortunately, it is difficult to produce high-intensity beams of neutrons – which are normally only found strongly bound to protons in the nuclei of atoms. This can be done by fission in a nuclear reactor, where the release of neutrons is the fundamental process that produces heat. A research reactor, such as that at the Institut Laue-Langevin (ILL) in Grenoble, France, is optimised to produce bright beams of neutrons. Another way to produce intense neutron beams is using an accelerator-based source, such as the ISIS facility near Oxford in the UK, where a high-energy beam of protons releases neutrons from tungsten nuclei in a process known as spallation. Both research reactors and "spallation sources" are large and expensive facilities, so there are relatively few in the world. The UK is fortunate in having access to the world's best in each class – ILL and ISIS.

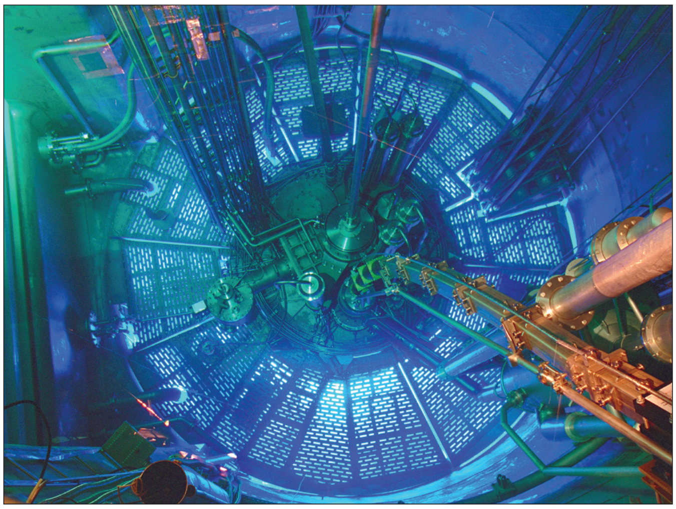
The science

Neutron scattering provides information that is highly complementary to that from other microscopic scattering techniques, such as those using photons (from visible light to synchrotron X-rays) or electrons (microscopy and diffraction), as well as to standard laboratory measurements. In modern materials science, it is normally the case that a variety of techniques are required to tackle any particular problem.

The ILL neutron beams are continuous, whereas those at ISIS are produced in short bright pulses 50 times a second, allowing different optimisation. Each facility operates some 30 separate experimental stations ("instruments"), which are individually tailored for a particular type of measurement and range of scientific applications.

Many neutron scientists use instruments at both ILL and ISIS and there is a large amount of knowledge sharing between the facilities, with advances in techniques and instrumentation benefiting both laboratories. This knowledge sharing extends across the international community, with smaller neutron sources providing input to the building of instruments and various national governments providing funding and expertise to particular projects. The network of European sources is complemented by international facilities at the Japanese Proton Accelerator Research Complex, and Oak Ridge National Laboratory, US.

Neutron scattering in the UK started at the Dido and Pluto reactors at the Harwell Laboratory in the 1960s. The ILL, jointly



ILL / J L BAUDET

owned by France, Germany and the UK, has 10 additional scientific member countries and began operation in the early 1970s. It has had several modernisation programmes, developing new neutron infrastructure and introducing new instrument concepts. The ILL's Millennium Programme continues to refresh its neutron guide infrastructure and instrument suite, increasing its effective performance overall by a factor of 20 since the year 2000.

ISIS is located at the Rutherford Appleton Laboratory, and is owned by the Science and Technology Facilities Council. It began operations in 1984 and has attracted scientific partnerships from across the globe. In 2009 it expanded its scientific capability and capacity for experiments by adding a second target station with additional instruments designed to study soft matter, advanced materials and bioscience. The second phase of this project aims to further increase the range of capabilities in soft matter, life sciences, neutron imaging and microchip irradiation testing.

Every year more than 1000 experiments are completed at ILL and ISIS, covering a wide range of research ranging from clean energy and the environment, pharmaceuticals and healthcare, through to nanotechnology, materials engineering, fundamental physics and IT. These facilities serve an international research community of more than 4000 scientists and each produces more than 500 research publications annually.

A future European Spallation Source, to start operation in the 2020s, is currently being planned by several European countries. The site for construction has been chosen as Lund in Sweden.

Applications

Neutron scattering is used in many different scientific fields. Neutrons can be used to study the dynamics of chemical reactions at interfaces for chemical and biochemical engineering, in food science, drug synthesis and healthcare. Neutrons can probe deep into solid objects such as turbine blades, gas pipelines and welds to give microscopic insight into the strains and stresses that affect the operational lifetimes of crucial engineering components. Neutron studies of nano-particles, low-dimensional systems and magnetism are used for the development of next-generation computer and IT technology, data storage, sensors and superconducting materials. Neutron scattering is a delicate and non-destructive measurement technique, making it ideal for use in heritage science.

● *Understanding magnetism*

The neutron is capable of seeing both the nuclei of atoms and at the same time the magnetic interactions of their electrons. Neutron scattering has made seminal contributions to our understanding of magnetism – from the early demonstration of anti-ferromagnetism in simple systems through to the complex magnetic structures found in hard magnets or the synthetic multilayer structures used for data-storage applications.

● *Investigating polymers*

Neutrons have been used to investigate polymers since the early 1970s. Originally, neutron research unveiled the structure and formation of polymers to understand how they assembled and bonded. Now neutron science is studying the dynamics of thin polymer films, further increasing their range of applications into areas such as anti-reflective coatings and time-release medications. The significant difference in the neutron scattering cross-section between hydrogen and deuterium allows selective "labelling" of chemically specific parts of complex molecular systems, giving a unique insight; this powerful technique is used for almost all soft-matter studies.

● *Revealing invisible worlds*

Neutron diffraction has been used to reveal the molecular structure of both crystalline and disordered materials since the early days of the discipline. Powerful computational modelling applied to neutron data allows accurate structures of pharmaceutical compounds to be derived, material structures in fuel-cell and battery electrodes to be optimised, and the orientation and packing of molecules in liquids and glasses to be understood. When materials bend, break or disintegrate it is their atomic structure that changes. Neutrons are used in a wide range of engineering applications to test the strength and suitability of materials under certain conditions, from studying the performance under strain of materials in aeroplane wings or train wheels to safely extending the operating life of nuclear power stations.

● *Biophysics: neutrons and the body*

A real understanding of the essential processes of life requires knowledge of how proteins and other macromolecules perform their roles. Techniques first used to investigate physics-based problems at ILL and ISIS have now been harnessed to identify water organisation in proteins and other biological systems. This is giving new insight into the way drugs and medicines move through the body and how they can be controlled and delivered to the specific area of concern. Neutron science continues to break new ground in investigating how drug-delivering polymers can move through membranes, how antibodies are structured and how active parts of medicines interact with lipids and proteins.

● *Unlocking the potential of hydrogen*

Hydrogen has the largest scattering interaction with neutrons of all the elements in the periodic table. Early experiments showing how hydrogen diffuses in simple metals have been built on to provide data supporting the development of materials for fuel cells and hydrogen storage. Hydrogen has been identified as a fuel with great potential for providing clean energy for transport, but its use is constrained by our inability to store it in a dense enough form suitable for vehicles. Neutron studies, currently being undertaken, will facilitate the understanding and development of materials that can store hydrogen safely and efficiently.

● *Unveiling our heritage*

The delicate, sensitive and deeply penetrating nature of

Timeline

1911	Ernest Rutherford develops the atomic model in which the nucleus carries most of the mass of the atom but occupies a very small part of its volume.
1923	Prince Louis-Victor P R de Broglie proposes that particles with mass may also show wave-like properties, now referred to as the de Broglie wavelength of a moving particle.
1932	James Chadwick discovers the neutron at the University of Cambridge. He receives the Nobel Prize in Physics in 1935 for discovering this missing part of the atom.
1938	Enrico Fermi receives the Nobel Prize in Physics for his work investigating the atomic scattering and absorption cross-sections of slow and thermal neutrons.
1946	Ernest O Wollan and Clifford G Shull, using the Graphite Reactor at Oak Ridge National Laboratory, US, establish the basic principles of the neutron diffraction technique. They prove the existence of antiferromagnetism, as predicted by Louis Néel who won the Nobel Prize in Physics in 1970.
1955	The first measurements of phonons from a prototype triple-axis spectrometer built by Bertram N Brockhouse confirm the quantum theory of solids.
1956	The Dido research reactor comes online at the Harwell Laboratory. It is the first reactor in the UK devoted to materials research and is instrumental in developing the use of neutron beams by university researchers.
1972	ZING-P and ZING-P' pulsed spallation neutron source concepts are demonstrated by Jack Carpenter at Argonne National Laboratory, US.
1972	The Institut Laue-Langevin (ILL) in Grenoble, France, one of the most intense thermal neutron sources in the world, comes into operation. It pioneers the use of neutron optics (guides) to substantially increase the experimental capacity of a neutron source and operation as a "user facility".
1974	Small-angle neutron scattering shows that polymer chains in the liquid state have a random coil conformation, as predicted by Paul J Flory who wins the Nobel Prize in Chemistry for his fundamental achievements in understanding macromolecules.
1984	The ISIS pulsed spallation neutron source opens at the Rutherford Appleton Laboratory, UK. It is the first major neutron user facility based on a high-energy proton accelerator.
1987	J Georg Bednorz and K Alexander Müller receive the Nobel Prize in Physics for the discovery of high-temperature superconductors. Later, neutron spectroscopy shows that magnetic interactions are crucial to understanding the mechanism of this phenomenon.
1991	Pierre-Gilles de Gennes receives the Nobel Prize in Physics for his work on liquid crystals and polymers. Neutron spin-echo spectroscopy was used to validate his models of polymer reptation dynamics.
1994	Clifford G Shull and Bertram N Brockhouse receive the Nobel Prize in Physics for pioneering the development of neutron-scattering techniques that can show "where atoms are" and "what atoms do".
2009	Next-generation accelerator-based pulsed neutron sources come online in the UK (ISIS Target Station 2), Japan (J-PARC) and the US (SNS).
2010	Lund, Sweden, is chosen as the site for the construction of the European Spallation Source. Construction is planned to be completed around 2018–19. The ESS will provide neutron beams up to 30 times brighter than present day neutron sources.

neutron beams enables heritage scientists to determine unique information from historic objects, museum artefacts or geological fossils with no risk to their value or integrity. Adapting techniques from crystallography and engineering, analysis of crystal structures in ceramic or pottery fragments can determine the period and region of manufacture and reveal ancient trade routes, while texture analysis of metal objects can identify manufacturing techniques and forgeries.

Impacts

Around half of all experiments at both ILL and ISIS have direct connections with industry, often through partnerships with university groups. Neutron scattering can be used to address the global challenges facing society, and to make developments that have immediate or long-term economic impact. Such applied research is built on a foundation of fundamental investigations and techniques developed over the last 30 years, so it is crucial to continue such basic work to underpin the theories and technologies of tomorrow.

Neutron experiments have provided definitive data to the chemical industry, which has enabled process optimisation and the saving of millions of pounds in energy costs and improved the environment by reducing waste effluent. Materials testing data have given aerospace companies confidence in new alloy compositions and manufacturing techniques. Health-based research has obtained key datasets required in preparation for clinical trials or to understand why certain drug treatments can be more successful than others.

Neutron facilities have unique requirements for advanced components and equipment that can challenge suppliers to innovate and develop new technologies. Partnerships with large research centres can support small businesses by giving them the security and confidence to embrace new areas of activity. UK businesses have benefited from work with neutron-scattering centres through technology development and knowledge transfer, which has led to substantial overseas exports.

Future developments

Neutron-scattering developments have not, historically, been driven by advances in source capability. Indeed, reactor-source brightness has increased by less than an order of magnitude since the 1950s. But instrumentation – large position-sensitive detectors, focusing optics, innovative exploitation of neutron polarisation – has produced enormous improvements in capability. The more recent development of accelerator-driven pulsed neutron sources has further stimulated advances in instrument design, which have now been implemented at continuous sources. This has fuelled an expansion of the field, originally focused on condensed matter physics, into materials science, soft matter and biomolecular systems, engineering, earth sciences, archaeology and the arts.

The simplicity of the neutron interaction, and the fact that it can be measured on an absolute scale with high accuracy, gives an easy and direct link to theory and computer modelling. In future it will be the norm for neutron experiments to be coupled with advanced computation.

The high scattering cross-section for light atoms means that neutrons are well suited to study many of the important topics in modern energy research – such as hydrogen storage, fuel cells and lithium-ion batteries. The performance of all of these materials and devices intrinsically depends on the motion of atoms (dynamics) and the structural changes this causes; neutrons are able to measure both aspects. They are also important in studying the tailored self-assembly processes that will be needed to improve the efficiency of organic photovoltaics. It is therefore clear that the use of neutron scattering in energy research, already significant, will continue to grow, with an increasing proportion of *in situ* measurements in real operating devices.

Fundamental studies of magnetism will remain a core topic of neutron scattering. For example, our understanding of correlated electrons, with its links to important practical applications such as magnetoresistance and superconductivity, is still in its infancy. The optimisation of devices increasingly makes use of thin films and nano-structuring, putting increased demands on instrumentation to make accurate measurements on ever smaller samples.

The unique information that can be obtained by isotopic labelling in soft matter and biology and health studies provides a powerful incentive to use these techniques, but the sample volumes required are relatively large and remain a hindrance to greater exploitation. A future drive will be to further develop neutron optics, possibly in combination with more powerful sources, to reduce sample volumes. The use of neutron reflectivity, where sample volumes are intrinsically small, to study, for example, biological membranes, is increasing rapidly. There is also an increasing demand to study kinetics, for example, processes and processing, which further drives technique development.

Neutrons can also be used at a more macroscopic scale – for example in radiographic and tomographic imaging. Neutrons can easily penetrate large objects, giving a picture that is effectively opposite (and hence complementary) to that provided by X-rays. Future development will include the use of neutron energy selective imaging, which allows distinction between different elements or even different crystallographic phases and textures – which can be extremely important in determining, for example, the strength of engineering materials. This can be combined with neutron diffraction to provide a three-dimensional map of residual stress, which in turn can be related back to the materials' properties. Potential applications range from improved gears for higher-power wind turbines to the advanced technology needed for Formula 1 motor racing.

Key facts and figures

- Neutron sources are a powerful creative hub for science and technology, bringing together a range of research disciplines from physics to earth science, medicine and engineering to solve current research problems and generate new research projects.
- There are around 15 neutron sources operating worldwide with significant capabilities for materials science research.
- The UK has the largest community of neutron-scattering expertise in the world, closely followed by Germany and France. In total, Europe has more than 4000 neutron users.
- More than 1000 experiments are completed each year at ILL and ISIS, and each facility produces more than 500 research publications annually.
- The US and Japan have recently built billion-dollar neutron sources to help develop their neutron-scattering expertise and user communities, and to gain parity with Europe.
- Industry use of neutron sources for product development, process optimisation and quality control can generate significant financial savings, export opportunities and reduce environmental impact.
- Neutron sources support a wide range of basic and applied research. Basic research today is rapidly moved to underpin the technologies of tomorrow.

Useful links

- www.isis.stfc.ac.uk
- www.ill.eu
- http://neutron.neutron-eu.net/
- http://j-parc.jp/matlife/en/index.html
- http://neutrons.ornl.gov/
- www.ess-scandinavia.eu

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