NEUTRON & MUON
SCIENCE AND FACILITIES

A Strategic Review and Future Vision
Report from the Advisory Panel

Science & Technology
Facilities Council

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An Appreciation of the Review from Dr Brian Bowsher – STFC CEO

Providing access to facilities for neutron and muon-enabled scientific research for UK academics and industry is an important element of the Science and Technology Facilities Council's (STFC) activities. This includes operating the world-class ISIS spallation neutron and muon source at STFC's own Rutherford Appleton Laboratory, acting as the UK's associate partner in the international reactor source at the Institut Laue-Langevin (ILL) at Grenoble and managing the UK's contributions to the new European Spallation Source (ESS) under construction in Sweden.

In response to concerns expressed by the UK's user communities that the available neutron capacity across Europe was likely to be significantly reduced in the short to medium term, STFC commissioned an advisory panel to carry out a strategic review to assess how current and future priorities can best be met, taking into account the prevailing financial circumstances for STFC and its partner Research Councils (RCs), and the plans to establish UK Research and Innovation from April 2018.

STFC welcomes the panel's findings that are set out in this report. The conclusion that the UK is a world leader in many areas of neutron and muon science and that action needs to be taken to secure this position into the next decade is acknowledged as an important factor in future decisions. In particular, the panel's view of the major role that these science areas can play in supporting many of the pillars of the UK's proposed new industrial strategy is persuasive.

The panel has developed a number of options for securing future neutron and muon access, with differing mixes of access levels at ISIS, ILL and the future ESS source. These options represent a range of research capacity and cost outcomes for the UK. Two clear conclusions emerge from the panel's analysis. Firstly, that securing a sustainable future for the UK's ISIS facility is the most important element in all the options considered. Secondly, that all options will involve negotiating with our international partners on the future possibilities for life extension at ILL and the UK's level of involvement in scientific operations at ESS.

The panel's recommendations will be considered by STFC as it works with its partner RCs, the Department for Business, Energy and Industrial Strategy (BEIS), the international facilities and the user communities to develop a strategy for future neutron and muon access for UK researchers. The strategy will seek to achieve an optimal balance between managing the significant costs of the facilities needed and empowering the research communities to continue to achieve excellent outcomes for science, industry and society.

Foreword by the Panel Chair – Prof Philip Withers

It is certainly true that neutron scattering research is about to encounter interesting times. On the one hand, Europe's bright, new spallation source is starting to take shape; on the other hand, Europe is at risk of losing around two-thirds of its (reactor) neutron scattering capacity within the next eight years. Further, the nature of European collaboration going forward is also uncertain. It is clear, however, that a strong and well-equipped UK science base is critical if we are to play a full role both within Europe and beyond.

We can be proud of our pioneering contribution to neutron scattering, with the UK establishing the first reactor user facility and the first large spallation facility. This review demonstrates that the UK continues to exploit neutrons for high-impact science through its access to ISIS, the Institut Laue-Langevin (ILL) and other facilities across the world. In many cases, this is not only enabling world-leading science, but science that is also delivering economic, health or societal benefits. It is important to recognise the unique characteristics of neutron scattering, for example, in revealing magnetic properties, which enable it to provide insights unavailable through other means. Many scientists therefore use neutron scattering in harness with other investigative tools to build up a multi-faceted picture, and so funding for neutron science must be considered as part of a complex array of research infrastructure.

As we approach a period when older facilities are retired and new ones ramp up, gaps in facility access can have long-term effects on the science. Further, establishing a new 21st century facility brings new challenges and a significant spike in funding requirements. Given the many variables, it is not possible to precisely map out how the global provision of neutron beams will work out, nor how international funding and partnerships will realign. Consequently, this review explores certain options and looks at the opportunities and risks that each presents.

It is clear from this review that neutron scattering has contributed immensely to our understanding in the areas of health, digital technologies, energy, manufacturing and beyond. Many of the global challenges that lie on the horizon, from clean water to green energy, from an increasingly interconnected world to ensuring an innovative manufacturing base in the UK, will require the insights that future neutron experiments can bring. How we navigate through the significant drop in neutron availability and the realignment of international collaborations in the 2020s will be critical to the future of UK science. While the authors of this review are uncertain about what the future will bring, we are sure that the provision of world-class neutron and muon facilities will play a key role within the palette of investigative tools that are needed by the UK. This report is supported by the whole review panel and we commend the findings and recommendations to STFC and its partner Research Councils.

Executive summary

Neutron techniques that reveal the structure of matter and its magnetic properties are a vital part of many areas of discovery science. They are also core to the success of the UK’s future industrial strategy in such areas as advanced materials, low-carbon energy technologies, the digital economy and healthcare. Our review indicates that there is a continued need for neutron science as part of a broader toolbox of complementary research techniques.

The ISIS spallation neutron source and its suite of instruments is a world-class facility used by UK and visiting researchers. The UK is one of the three associates in the reactor neutron source at the Institut Laue-Langevin (ILL) and is contributing 10% to the construction of the new European Spallation Source (ESS). The next decade will be a time of significant change in the neutron landscape as a number of older sources reach the end of their operational life. This will certainly result in a reduction in available neutron capacity, and the UK needs to plan strategically if this is not to cause a slowdown in UK scientific advances.

This strategic review has looked at how current reactor and spallation facilities are used by UK researchers, and at what is needed to maintain the UK’s world-leading role in neutron and muon science applications. Three options are proposed for future access. It is important to note that none of these guarantees maintaining the current number of beam days in the long term, and that all involve fluctuations in funding as changes occur.

Central to all of the options is the need to maintain the UK’s internationally competitive ISIS facility. This will ensure that national scientific needs are met, give resilience to changes at other sources, and also provide a basis for building partnerships with existing and new collaborators across the world as the neutron map changes. The ILL source provides some complementary capabilities and important additional capacity, but it faces potential closure if a new protocol is not agreed. The ESS source is expected to bring significant new capabilities in the future but these are as yet unproven. The changing landscape of neutron sources and new user requirements will create a need for new funding and access models to broaden the user base and facilitate new partnerships and collaborations with industry and internationally.

In light of the significant changes over the coming years as sources close and the ESS comes on line, there should be a further detailed evaluation of the UK’s neutron needs in the mid-2020s, coupled with periodic instrument reviews to ensure continuing value for money from the investments in neutron capacity and capability.

1. Introduction

Significant breakthroughs and new insights in many science areas have been achieved using neutron and muon techniques. The ability of neutrons to reveal the nuclear structure of matter and distinguish between isotopes has made them a prime tool for research ranging from condensed matter physics through to soft matter biology. Muons provide a complementary probe to neutrons, particularly in the areas of magnetism, superconductivity and charge transport. This diversity of applications and the scale and cost of the facilities needed to enable neutron and muon-based research mean that it is appropriate to review and reassess the provision made to support this research.

The Science and Technology Facilities Council (STFC), on behalf of the UK research community and the relevant science-funding Research Councils (RCs), acts to provide access to major national and international facilities for UK researchers. In 2016, STFC commissioned an advisory panel to carry out a strategic review of neutron facilities (including muons) with the brief of making recommendations for:

- A 15-20-year vision for UK science requirements for neutrons and the facilities needed
- A ten-year strategy for UK access to neutron facilities, including underpinning technology, skills and community development

Central to the panel's approach to carrying out the strategic review has been the recognition that **meeting the needs of the science priorities for the UK must underlie the analysis and the recommendations made**. This report sets out the panel's findings, conclusions and recommendations. The panel has reviewed and assessed the evidence base for continuing to apply neutron (and muon) techniques in important science areas to generate beneficial economic, societal and knowledge outcomes for the next 20 years. It is recognised that maintaining a neutron scattering community per se is not a prerequisite. Given the cost of the facilities, it is important to justify the role that neutron scattering plays in the advancement of understanding and generating impact and to ensure that the right level of access is provided. The advisory panel's membership and terms of reference are set out in Appendix D.

2. Context for the strategic review

Small, laboratory-scale neutron sources do not exist except at very low neutron flux levels (see Appendix C for information on other sources). As a result, this research relies on the availability of large-scale facilities. These are typically based on fission reactors (such as at ILL) and accelerator-driven spallation sources.

The UK has been a pioneer in neutron science and the development of neutron sources. Indeed, the UK was the first country in the world to build a high-power spallation neutron source (ISIS) at the Rutherford Appleton Laboratory.

Making neutrons and muons

Spallation sources: The production of neutrons at a spallation source typically begins with a high-powered proton accelerator, which may be combined with a synchrotron or a cyclotron.

The neutrons are created by accelerating “bunches” of protons and colliding these with a heavy tungsten metal target. The impacts cause neutrons to spall off the tungsten atoms. Muons can be created by colliding a fraction of the proton beam with a graphite target, producing pions, which then decay rapidly into muons.

Reactor sources: Research reactors are nuclear fission reactors that serve primarily as a neutron source. They are simpler than power reactors and operate at lower temperatures. They need less fuel and less fission products build up as the fuel is used.

All sources use a system of moderators to change the neutron energies and guides to direct neutrons to the instrument arrays that surround the sources.

Credit: STFC

ISIS is a spallation neutron source based at STFC’s Rutherford Appleton Laboratory in Oxfordshire. Since it was built in the 1980s it has been the mainstay of the neutron provision for UK researchers.

Credit: ILL

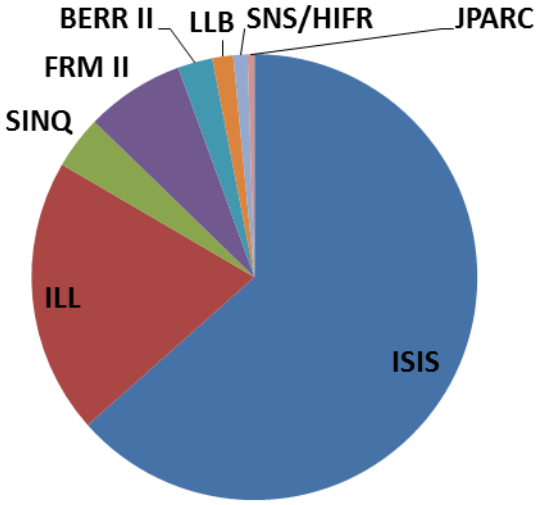
ILL is the European reactor source based at Grenoble in France. It has operated with high reliability since 1970. It is widely regarded as the best continuous neutron source in the world.

Neutrons from spallation and reactor sources have different characteristics and are, therefore, better suited to different types of experiments. For example, continuous neutron beams from reactors are generally better at focusing on specific details or following a fast temporal evolution. Reactor sources are better for protein crystallography experiments and produce the large fluxes of cold neutrons needed for nuclear physics experiments. They are also used to produce isotopes used in medical research and treatments. Spallation (pulsed) sources provide a global picture with a time resolution given by the time-structure of the source and often have lower background levels, which can improve the signal to noise level in the detectors.

As well as the existing sources, there is a major international project underway to build the ESS, which will be the world’s most powerful neutron source when it is fully operational in the late 2020s. Europe has two of only four muon sources in the world, with pulsed muons produced at ISIS and continuous muon beams generated at the SINQ facility at the Paul Scherrer Institute (PSI) in Switzerland. Approximately 80% of the current UK use of neutrons is at ISIS or ILL (see Figure 1) and these facilities account for an equivalent percentage of the UK's expenditure on neutron provision. The strategic review has, therefore, focussed on how the UK can make best use of the capacity and capabilities that these two existing sources and the future ESS can provide. It needs to be recognised that the future operation of the ILL and the establishment of operations at the ESS are managed within intergovernmental agreements in which the UK has significant influence, but not full control. The other sources used by UK researchers include:

- SINQ, Switzerland
- FRM II, Germany
- BER II, Germany
- LLB, France
- SNS + HFIR, United States
- J-PARC, Japan

Figure 1: UK use of neutron sources (by instrument-days used).



In most cases, there are reciprocal arrangements in place that make small amounts of time on these sources available at no cost. Any extended use has to be paid for from the researcher's funds (or by industry if it is commercial use).

An important driver for this review is the changing landscape of neutron facility availability over the ten-year timescale of the review's access planning. In Europe in particular, a number of reactor sources are closing (or are anticipated to close) in response to factors including increased operating costs, facility lifetime limits, more stringent safety requirements and fuel supply restrictions. The European Strategy Forum on Research Infrastructures (ESFRI)[1] study of 2016 analysed this in detail and forecast a baseline scenario, as shown in Figure 2.

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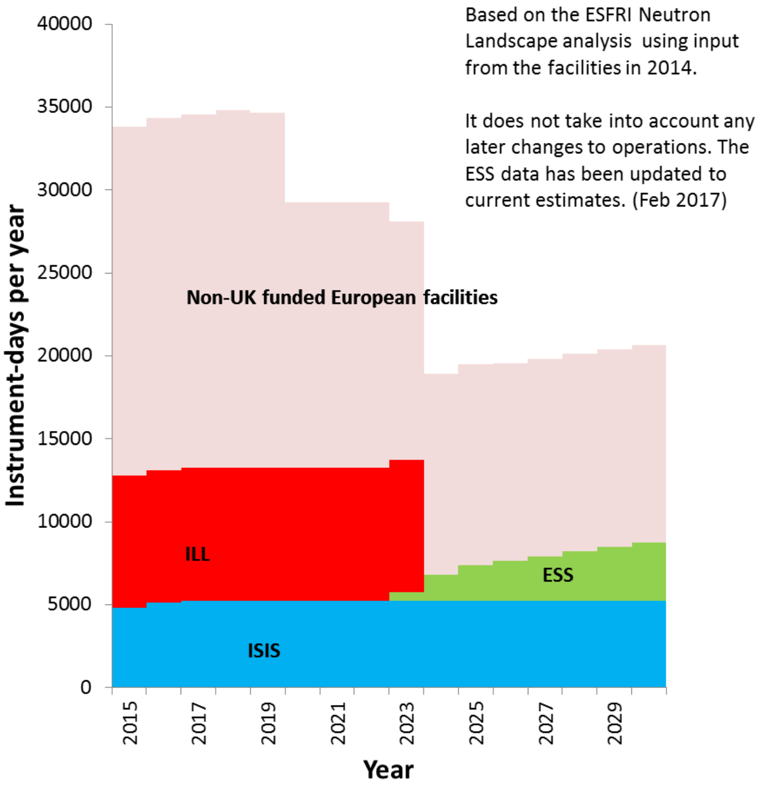
[1] ESFRI, *Neutron Scattering Facilities in Europe: Present Status and Future Perspectives*, 2016.



Based on the ESFRI Neutron Landscape analysis using input from the facilities in 2014.

It does not take into account any later changes to operations. The ESS data has been updated to current estimates. (Feb 2017)

Figure 2: Instrument-days chart (adapted from ESFRI 2016), showing the likely maximum capacity for all European facilities; note that the UK share of time at ISIS and ILL is approximately 75% and 25% respectively.

This shows that there will be a “neutron drought” with a 40% fall in capacity that will impact on the users of European facilities, therefore, reducing the access levels available to UK users. As is often the case, a time of change can also bring opportunities and act as a stimulus to drive innovation. The strategic review has looked for such opportunities in developing the recommendations in this report.

3. Properties of neutron probes and their complementarity with other probes

Neutron probes

In a neutron scattering experiment, a neutron beam passes through the sample or component under investigation. By observing how the neutron is scattered (i.e. how the direction and velocity of the neutron’s path changes), researchers learn about the structure, composition or dynamics of the sample on an atomic scale. Having this basic information gives insight into the physical, chemical or biological properties of a material.

The unique properties of neutrons (and muons) compared to other probes have made them an increasingly popular and important technique for experiments addressing fundamental and societal challenges (see Appendix A for more details).

Neutrons, as free chargeless particles, have properties that make them particularly useful to look inside a wide variety of materials. These properties include:

- Wavelengths and energies that enable measurements on the dynamics of structures over a very wide range of dimensions and frequencies, from 10^{-10} m to 10^{-2} m and frequencies from 10^{6} Hz to 10^{14} Hz respectively
- They are deeply penetrating, providing information from the hidden interior of a sample as well as from its surface, without damage to the sample
- They can provide isotopic contrast, providing a powerful way of deciphering the organisation of biomedical and soft matter systems
- They possess a magnetic moment, making them an ideal probe for the study of the structure and dynamics of magnetism
- How they are scattered can be calculated accurately, making them a precise, quantitative probe that can be used to directly benchmark computer simulations

Neutron instruments and techniques

- **Diffractometers**, which measure structure on the nanoscale (hard condensed matter)
- **Small-angle scattering**, which measures structures on the mesoscale (i.e. from groups of atoms up to micron-scale structures, such as polymers, macromolecules and biological complexes)
- **Reflectometers**, which study the surfaces of structures and layered systems (membranes, magnetic multi-layers)
- **Spectrometers** measure atomic and magnetic excitations (magnetic, lattice, molecular vibrations) and diffusion processes on timescales from the femto- to the microsecond
- **Tomography** and the direct imaging of matter down to the micron scale

Other probes

Neutron-based techniques complement a number of other experimental methods which are available in university laboratories or at other central facilities such as synchrotrons. In many areas (see section 4), neutrons have advantages and in others they complement other probes. Synchrotron radiation is now the method of choice to determine molecular structures, despite the fact that, generally speaking, the protons are rendered poorly. For phonon measurements, inelastic X-ray scattering enables the study of very small crystals, but the superior resolution and the ease of direct comparison with theory means that inelastic neutron scattering is still vital. Despite the many orders of magnitude increase in light source brilliance over the last 20 years, the vast majority of applications of neutrons have not been replaced by other techniques.

X-ray scattering (laboratory and synchrotron): X-ray diffraction is a very powerful structural probe. However, scattering depends on the atomic number of elements present in the material, which means that light atoms in the presence of heavier species can be essentially invisible to X-rays. It is often the light atoms (O, Li, H) that impart the key functionality, and this means that X-rays cannot properly probe the most important part of the structure. Compared to neutrons which penetrate deeply into matter (tens of cm), X-rays are essentially a surface probe (without resorting to high-energy potentially destructive beams), and this presents a significant limitation to their use as in situ and in operando probes.

X-ray crystallography: X-ray crystallography of individual proteins has dominated structural biology for four decades, but biomedical research is now moving towards the analysis of larger systems. Neutrons and X-rays can be combined, with the latter offering increased speed and resolution at the expense of beam damage and poor molecular differentiation. Neutron methods work on dynamic not frozen structures and can follow changes in structure or activity in solution over long periods without damage. Combining the data with cryo-electron microscopy creates a suite of methods that can tackle the very largest and complex structures, such as those involved in gene regulation, infection or bioenergy conversion.

Nuclear magnetic resonance (NMR): NMR can be a powerful probe of local structure and dynamics. However, only certain nuclei are NMR-active (some elements have no NMR-active isotopes) while others have NMR-active nuclei in such low abundance that materials need to be isotopically enriched to be studied; there are also complications associated with magnetic species. The range of non-ambient conditions accessible by NMR probes is also very limited.

Electron microscopy (EM): Advanced EM methods can provide ultra-high (sub-Å) resolution information about the structure and processes in functional materials. Relative to neutron-based techniques, however, capabilities for in-operando studies are still more limited. Electron microscopy does not probe the bulk of a material due to the statistics of measuring what will always be a statistically small fraction of the sample, whereas neutrons are a bulk probe.

4. Science applications

Neutron techniques have been used for over 60 years to explore the frontiers of basic science, and have enabled or validated ground-breaking discoveries of international importance, including many linked to Nobel Prizes.

- Small angle neutron scattering showed that polymer chains in the liquid state have a random coil conformation, as predicted by Flory who won the Nobel Prize for Chemistry in 1974
- Bednorz and Müller received the Nobel Prize in physics (1987) for their discovery of high-temperature superconductors. Neutron spectroscopy has shown that magnetic interactions are crucial to this phenomenon
- In 1991, de Gennes received the Nobel Prize in physics for his work on liquid crystals and polymers. Neutron spin-echo spectroscopy was used to validate his models of the snake-like polymer reptation dynamics of polymers
- Shull and Brockhouse received the Nobel Prize in physics in 1994 for pioneering the development of neutron scattering techniques that can show “where atoms are” and “what atoms do”
- Curl, Kroto and Smalley received the Nobel Prize in 1996 for their work on Buckyballs. Neutron techniques have been used to explore their unique properties and develop applications such as nano-tubes
- Thouless, Haldane and Kosterlitz received the Nobel Prize in 2016 for theoretical discoveries of topological phase transitions and phases of matter. Neutron scattering has found the evidence of the behaviours predicted by the topological theory

Neutron techniques are applied across a wide range of science disciplines, from condensed matter physics through to soft matter biology. The following research areas and applications have been selected to capture and showcase the capabilities and contribution of neutron scattering, but they are not intended to be fully comprehensive. These areas also align well with the themes in the Government’s recently published green paper on an industrial strategy[2] for the UK. This confirms the strategic importance of the research and its applications. Further examples of important applications and future opportunities are given in Appendix B.

Enlightening the manufacturing sector

Making advances in almost any industrial sector needs a profound understanding of the *processing-microstructure-properties-performance* relationships of materials. This requires materials to be characterised chemically and structurally, across many length scales.

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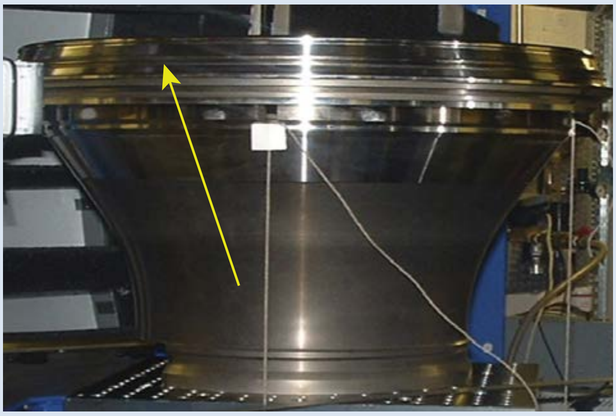
[2] BEIS, *Building Our Industrial Strategy, Green Paper*, 2017.

Materials can be chemically identical but structurally different, for example, in their crystalline form or as a result of strain-induced departures from their equilibrium state. These differences can have significant consequences for material properties and must be controlled during manufacturing. **Neutron scattering** can enable tuning and optimising of manufacturing processes, for example, by in situ monitoring during product creation, through studies of as-processed microstructures or the in operando assessment of the performance of manufactured articles. A critical advantage of neutrons over electrons and X-rays is their ability to **penetrate many centimetres into common materials** and their ability to differentiate isotopes of the same element or light elements in structures dominated by heavy ones. This means that they can probe deep inside materials to investigate, non-destructively, material that is representative of the bulk or buried interfaces.

Faster to market – inertia welded aero-engines

The higher the operating temperature, the more fuel efficient the aero-engine is. Since the newest higher temperature disk alloys cannot be joined by conventional welding methods, Rolls-Royce developed a new solid state welding method in which a rotating part and a stationary part are brought together and the resulting friction creates a weld with no melting (so-called inertia welding). Working with academics at Manchester University, Rolls-Royce used **neutron diffraction residual stress** measurements on full disk assemblies on the beam line (pictured) to ensure residual stresses were kept within safe limits. Trent XWB engines that adopt this technology have world-leading efficiency, driving their dominant market share and sales value estimated to be ~£22 billion.



The arrow marks the location of the inertia weld. Credit: P Withers.

Enlightening energy science

Neutron and muon scattering provides insight and understanding of the relationships between the macroscopic physical properties and the relevant processes to the microscopic structure, and in some cases the dynamics, of functional materials used in energy applications. The techniques have enabled significant advances in a wide spectrum of materials used in both energy generation and storage, including fuel cells, thermo-electrics, photovoltaics, batteries and hydrogen storage materials, and also for energy generation and transmission applications, such as high-temperature superconductors and permanent magnets.

Neutron diffraction is exquisitely sensitive to light elements in a material's structure and has made a high impact in, for example, the development of lithium conductors and storage electrodes used in batteries, proton and oxide ion conductors used in fuel cells, and hydrogen storage materials.

Neutron and muon spectroscopy provides complementary dynamical information on performance-critical parameters, such as ionic mobility and diffusion coefficients and their activation energies, in these highly functional materials. Neutrons interact weakly with matter, penetrating deeply into materials allowing the bulk structure and deep interfaces to be probed. This gives a significant advantage over other material probes by enabling **imaging** and **in operando studies** of devices, such as fuel cells and batteries (e.g. observing the water transport in polymer electrolyte membrane fuel cells and charge-discharge cycles in rechargeable batteries). This understanding is essential for making the crucial transition from the laboratory to a functional component in an operating device, and for optimising its performance. The weak interaction and attendant simplicity of the neutron-scattering cross section means that calculations have emerged as powerful ways to predict formation and stability, and to simulate the structures and behaviour of materials. This has helped accelerate improved performance in many advanced energy materials.

Improved fuel cell technology leads to more affordable power, lower emissions, and better reliability

Ceres Power, based in Horsham, West Sussex, started as a small spin-out from Imperial College 15 years ago and now employs around 100 people. It has won support from Innovate UK for a number of projects to develop its technology over the last ten years [1]. The company has begun licensing its technology to partners around the world for mass-market applications. The commercial potential of embedding this fuel cell technology into multiple power systems is enormous. Neutron scattering has been crucial in revealing key structure-property relationships in the cell's electrode and electrolyte materials.

Ceres Power "steel cell".
Credit: www.cerespower.com

[1] www.gov.uk/government/case-studies/ceres-power-fuel-cell-business-makes-manufacturing-breakthrough

Enlightening biological and medical innovation

Dramatic advances in medicine, public health, and economic and social progress have enabled us to live longer, healthier lives. Future innovations in science and technology are expected to further improve the quality and length of life. To fully exploit this exciting potential, a detailed understanding of biological structures as well as an understanding of the molecular and cellular basis of

Cleft palate repair

In Britain, 1 in every 700 babies is born with a cleft palate, making it the most common birth defect. Such congenital malformations are very debilitating. Until recently, surgery was the only option in severe cases. However, if the defect (or gap) in the cleft is very wide, there may be insufficient available tissue to close it without resorting to radical surgery, which can cause complications as the infant develops. Neutron studies were an integral part of the development of a novel hydrogel material (similar to that used in contact lenses) which can be used to cover the gap in the palate, thereby avoiding the need for complex surgery and all the distress and complications this can cause. This hydrogel is currently marketed by Oxtex.

Credit: Pixabay

disease is essential. **Neutron science** is playing a crucial role in obtaining this understanding. Significantly, and in contrast to X-rays, neutrons can sense the light atoms that comprise most biological molecules (e.g. ~50% of the atoms in biological molecules including proteins are hydrogen) and can discriminate between the two main isotopes of hydrogen, namely protium and deuterium allowing an understanding of the vital role of water in biological systems to be obtained. The gentle nature of neutrons means that it is possible to study living cells in the neutron beam and thereby determine the structure or dynamics of a biological molecule of interest or the passage of water into and out of cells. This exquisite ability to “see” hydrogen is allowing important discoveries not possible using alternative techniques such as X-rays. This is well evidenced by recent crystallographic studies of the interaction of an antiretroviral drug with its target enzyme, HIV-1 protease. **Neutron crystallographic studie**s allowed visualisation of the protons in the active site, something not possible with X-rays, thereby correcting the errors in the nature of the interaction proposed by X-ray scattering, and allowing drug designers to produce drugs that better interact with the target enzyme and improve retroviral therapy. Other significant advantages provided by neutrons, due to their weak interaction with matter, include the ability to measure samples within complex devices and environments, thereby mimicking in-use conditions of therapeutically active molecules.

Enlightening digital technologies

Neutron science has a crucial role to play in the development of new base elements on which our information and communications technology (ICT) infrastructure is built. Magnetic materials provide a natural home for digital infrastructure as, broadly speaking, the north and south poles can be correlated to binary 1s and 0s. To study magnetic behaviour on the atomic level, as is required for the development of modern digital needs, **neutron scattering** is the best, and sometimes only, tool available. In particular, neutrons can peer deep below the surface of a material to unlock the inner workings.

Neutron irradiation instruments are also used to test fault resistance in electronics against cosmic rays. The UK has invested £20 million in developing this capability, which will be used by companies such as Intel, NVIDIA, Airbus and Boeing.

Most of our current understanding of modern magnetism is based on neutron-scattering studies. The ability to see the individual magnetic moments, via **neutron diffraction**, and study their interactions, through **inelastic neutron scattering**, has been essential in the vast majority of discoveries of new magnetic phenomena and the corresponding applications (from the early understanding of simple anti-ferromagnetism to the understanding of extremely complicated 3D, multilayer or surface magnetic structures). Two of the most widely applied and important technology game-changers have been high-performance permanent magnets and giant magnetoresistance-based magnetic disc reading heads, both of which are the basis for multi-billion pound industrial markets.

To determine the atomic-level magnetic structure of a new material, neutron diffraction is overwhelmingly the technique of choice to get it and have a high confidence in the result. Typically, the investigation starts with a measurement on a powder, and in difficult cases, progresses to single crystal diffraction or the use of polarized neutrons.

Protecting aircraft systems from cosmic rays

The electronic systems in aircraft can be affected by high-energy neutrons, generated in the atmosphere by cosmic ray impacts. This can have serious consequences for safety critical systems.

Credit: Pixabay

By **bathing microchips in neutron or muon radiation** at the ISIS facility, companies are able to test their electronics at an accelerated rate, to develop strategies, designs and methods to mitigate the potentially catastrophic effects on control circuits. This has long been known to be an issue in avionics; increased miniaturisation, where structures are perhaps ten atoms wide, means this is now seen in ground-based systems as well.

The impact on UK science of curtailing neutron research activities

It is clear from the examples presented that neutron science provides unique and powerful insights into an extraordinary breadth of science disciplines. However, it is important to challenge the assumption that this necessarily justifies continuing to invest significantly in this area of scientific endeavour. What would be the strategic loss to the nation if the priority given to neutron research was reduced? The Advanced Materials Leadership Council[3] has identified a range of opportunities with significant potential for the UK to build its lead in. These are shown in the following box along with the critical roles that neutron research is and will continue to play in helping to bring these about.

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[3] See: https://connect.innovateuk.org/web/amlc.

Strategic materials-related opportunities for the UK

What if the UK could become a global market leader of energy storage and energy efficiency technologies, which are key in the transition to a lower carbon future? Materials can enable both cost-effective energy efficiency and energy storage solutions. These two sectors may be worth $215 billion and $590 billion by 2040 globally.

The new industrial strategy will support the intensification of research into energy storage – ***neutron studies established*** *the relationship between the structure and properties of alternative cathode materials, including lithium manganese oxide, lithium iron phosphate and lithium nickel manganese cobalt oxide.* ***Neutrons will enable*** *us to follow the critical changes that take place within operating energy storage devices non-destructively.*

What if healthcare treatments could be personalised using customised biomaterials that are responsive and not rejected by the patient's body? These would be effective and long-lasting, treating a range of diseases, delivering public health benefits and economic growth.

Small-angle neutron scattering *in combination with selective deuteration is enabling us to determine the solution structure of multicomponent biological systems as well as determining the interaction of drugs with biomolecules in solution and the nature of materials suitable for implants, amongst other things.*

What if our aerospace (£24 billion), land and sea transport (£55 billion) and oil and gas (£40 billion) sectors could exploit cheap, lightweight and strong materials that operate effectively in extreme conditions? This would revolutionise our use of structural materials and lead to efficiency and fuel savings with increased competitive advantage for UK industry.

In all these sectors, unexpected failures are unacceptable. ***Neutron strain scanning*** *is helping to safely introduce new engineering designs reducing the impact of air travel and extend the plant life of oil and gas and nuclear infrastructure. Neutrons are able to probe materials operating under extreme environments.*

What if the UK was the world-leader in developing and implementing a complete end-to-end materials research and development (R&D) ecosystem: from materials discovery through materials and component scale-up to high-volume manufacturing and system and service integration? The UK would be the place to develop and manipulate advanced materials faster than ever, and integrate these into devices and products effectively and efficiently to meet market demand and grow the UK economy.

To accelerate materials design and development, UK researchers need a wide palette of tools to characterise and probe materials behaviour. ***Neutron scattering*** *provides unique insights into the structure and dynamics of materials important to the health, digital, manufacturing and energy sectors.*

5. Industry users

Neutron research is very relevant to addressing many industry needs ranging from materials for new aero-engines and low-carbon energy storage technologies through to new drug delivery systems (see section 4). As a result, industry is well engaged in the neutron science programmes at all facilities, both through commercially funded proprietary experiments and as partners in open literature, academic-led, research projects. In recent years, industry has been linked with over 15% of the experiments carried out at ISIS and ILL. Proprietary use by industry at full cost is currently around 1%.

Key aspects for industry

Neutron studies allow the determination of material structure and molecular dynamics of solids, liquids and gases as a function of temperature and pressure. These characterisation studies use complex sample environments and are a capability that is often a key requirement of industrial users. These studies can closely approximate the situations and environments experienced by industrially important materials, components and devices during their active life.

Some of industry's science needs[4] relevant to neutron applications

- Increasing the durability of new materials and joining technologies
- Improving the cyclability of components and systems to extend lifetimes
- Understanding the causes of component failures
- Improving the properties of consumer and medical products, such as detergents and pharmaceuticals

Growing the UK industrial user community

While neutron characterisation can provide unique and unparalleled information on systems at operating conditions, there is a general ignorance of both the capabilities and costs of using these facilities amongst the wider industrial community. Growing the use by industry will need a programme of outreach to inform and advise them of the opportunities and the available means of access. Increasingly close liaison between sources, universities and industry, including exchanging staff, will help achieve this. The service to industry provided by facilities would be enhanced by:

- Helping industrial users through all the aspects of their use of the facilities: experimental design, sample preparation, experimental set up, data acquisition, data analysis, data storage and archiving and post-visit follow up
- Fostering partnerships between technique experts, industry and non-experts, for example, by providing a working environment that can encourage joint collaborative working

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[4] Drawn from recent collaborative research projects at ISIS and ILL.

- Facilitating preliminary experiments so that industry users can “test the water” and gain confidence in the techniques and what they can achieve using them
- Establishing more schemes by which industry can sponsor PhD studentships exploiting neutron techniques

The current activities to engage industry in neutron research[5] should be intensified, although it is recognised this may need additional resources. As well as promoting the opportunities and benefits to key sectors, operational factors that may impede industry’s willingness to commit to funded use of facilities should be reviewed and where possible removed. This will include reviewing the access modes open to industry so that an agile response to approaches by companies can be achieved that will meet their, often time-critical, requirements.

6. Capacity and capability

Neutron sources and their instrument suites have developed to facilitate specific scientific investigations and techniques. The differing source characteristics means that some are more suited to particular techniques than others, and facilities have sought to create the range of capabilities required to serve their user communities and to expand the use of the instruments to new science areas. In an environment of limited funding, it is particularly important that there is a rigorous prioritisation of what the facilities provide and what the future developments should be, to ensure the best overall value is maintained.

Matching capacity and capability with the science requirements is a dynamic process and it is recognised that ISIS and ILL carry out reviews of their instruments and demand levels. To gain more insight into this and to assess how well they matched user needs and demand levels, the panel asked ISIS and ILL to map the capacity available for specific capabilities and techniques. The approach to this is summarised in the following box.

The panel considers that this approach could be developed to inform a more detailed review of the capacity and capability landscape and to identify actions that should be taken. This would need a more in-depth picture of the particular capabilities and what trends there are in user demands and requirements and how these match science priorities.

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[5] Such as the EU’s Science and Innovation with Neutrons in Europe (SINE) 2020 project. See: www.sine2020.eu/.

Recommendation

The UK-funded facilities should continue to regularly carry out reviews of the capacity and capability provided. These need to be rigorous and transparent and include trends in demand in order to ensure that the supply matches the demand and changing priorities are identified early.

Mapping the capacity and capability

The instrument numbers in the experimental technique groups at ISIS and ILL were weighted by the current UK access levels (75% at ISIS and 25% at ILL). This gives, at an overview level, a picture of potential UK access and illustrates where there are commonalities in instruments and where there are divergent and complementary capabilities. Some instruments are more heavily used than others. There are many factors that influence demand levels (the need for specific capabilities, rolling programmes of experiments, changes in science priorities, etc.), so snapshots of demand for particular instruments have to be treated with care. To give a more robust picture of the available capacity, the success rates for user proposals at ISIS and ILL in 2015 were taken into account to give an indication of the **effective capacity** available to UK users for each technique group (see Figure 3).

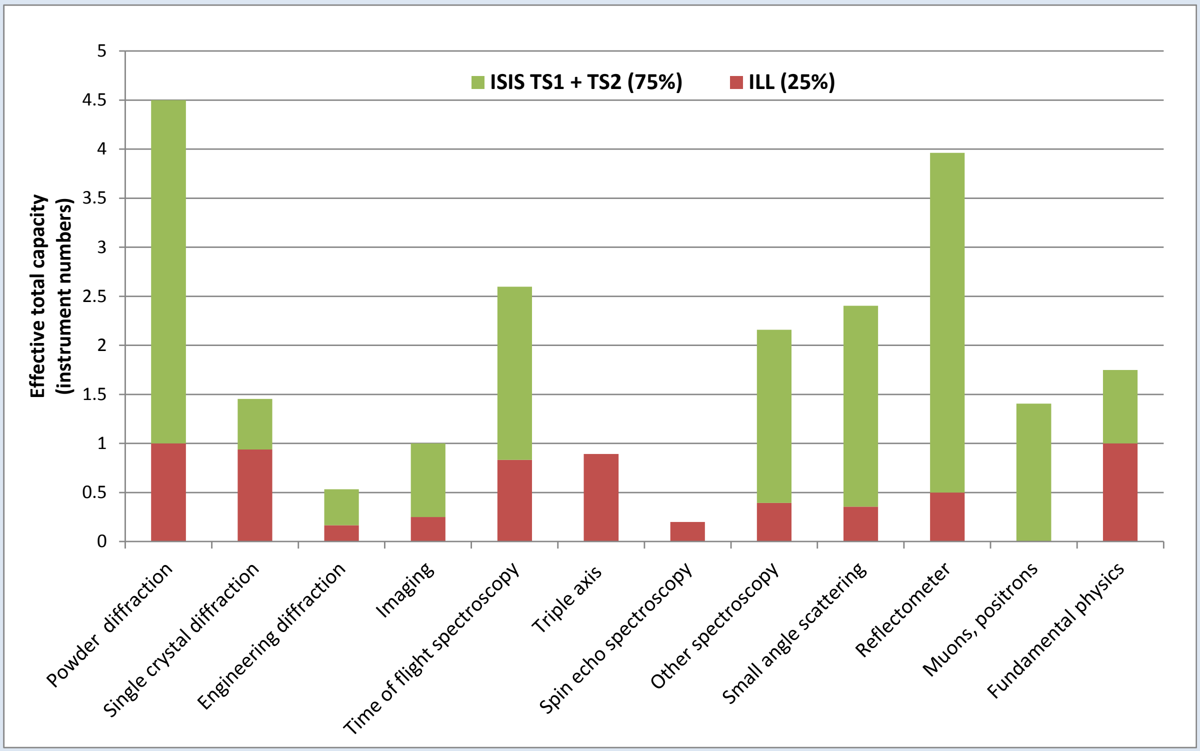

Figure 3: Total effective instrument capacity for UK users at ISIS and ILL

Note: Effective capacity is defined as number of instruments in a technique group multiplied by the average success rate of applications for those instruments.

There are many examples of beneficial collaboration between facilities – for example, in the areas of sample environment design and the development and use of analytical software to interpret neutron experimental data. The panel commend this collaboration and recommend that it should be adopted wherever possible.

Software and data handling and analysis, in particular, are important elements of the capability needed to maximise the outcomes from neutron experiments that can benefit from collaboration. Over the last 30 years, data acquisition rates have increased from KB per second to GB per second. As a result, the amount of data that must be processed, either in real time to monitor the experiment or subsequently to analyse the results, has become a significant hurdle. This can compromise the intelligent running of experiments and subsequently extracting value from the data collected. Also, the boundaries between the measurements and the software have become less distinct, and the experimenter experience is now often determined by the coupling between hardware and software. Developments in this area should be supported, especially where they enhance inter-facility collaboration – both between neutron facilities and also across other techniques, such as those using X-rays and electrons.

Recommendation

The UK-funded facilities should maintain and enhance their scientific and operational links to ensure best practice is shared and developments (e.g. in instrument design) benefit all and are not duplicated. A greater emphasis on computing and software is essential, and shared approaches to computing and software development should also be supported.

7. A vision for neutron research and the ten-year access plan

The importance of neutron facilitated science and the consequences of any significant loss of neutron capacity and capability

Sections 3 and 4 of this report have highlighted the high-impact science achievements already being made using neutron techniques and their future opportunities, both as a specific probe and in combination with other probes. In particular, neutrons are playing a key role in helping the UK realise an end-to-end materials R&D ecosystem: from materials discovery through materials and component scale-up to high-volume manufacturing and system and service integration. Losing a significant fraction of the UK's access to neutron techniques will unavoidably compromise this progress, which is increasingly reliant on the ability of academic and industry teams to rapidly carry out characterisation studies during the design and discovery process including in situ/ in operando studies of devices. This national capability is equally critical in the biosciences and soft matter disciplines as in the physical sciences and engineering areas, as illustrated in the range of case study examples.

The panel considers that relying on accessing increasingly scarce capacity at other national facilities (at which we would have limited influence) would create a very high risk to the UK’s ability to achieve its industrial strategy goals. In particular, it would be likely to result in a significant erosion of the national knowledge and skills base in key areas, including novel materials science; battery and other energy storage devices; structural materials; materials for demanding environments; catalysts; magnetic digital device structures and materials for information technology; and medical components including drug delivery systems and artificial organs and implants.

It is also clear that neutron experiments contribute to the UK’s high standing in research quality. *The ISIS Lifetime Impact Study*[6] noted that “ISIS publications outperform the UK average and it is not uncommon for selected ISIS publications to achieve several hundred citations within a three-year window”. An unpublished analysis of research grant holders by the Engineering and Physical Sciences Research Council (EPSRC) showed that, in 2015, ISIS users were the principal investigators for about 25% of the largest grants across the portfolio areas of physical sciences, energy, manufacturing and engineering. Experiments at ILL result in 500-600 scientific publications a year with typically one-third of these in high-impact journals[7].

It is clear there is significant synergy between neutron science and physically informed models that drive mechanistic understanding. Progress in this field is expanding at a nonlinear rate reflecting both the advances in experimental capability and modelling capability and capacity. There is every reason to believe we are a long way from a plateau with respect to science output, and the publication track record from the neutron community reflects this premise. The resulting industrial pick up and exploitation will follow a similar trend with very broad cross-sector applicability. The panel has, therefore, concluded that the need for neutron facilities to enable high-quality science that contributes to the national capability in high-impact science and technology applications will remain strong for the foreseeable future, and that the science opportunities will benefit from the unique ability of neutrons to provide insight into many aspects of materials and systems.

The vision for neutrons for the next 15-20 years

The above conclusion has been captured in a vision for the future provision and exploitation of neutron and muon facilities, as set out in the following box.

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[6] STFC, *ISIS Lifetime Impact Study*, 2017.
[7] See: https://www.ill.eu/science-technology/scientific-publications/list-of-publications.

The vision

Provide access to world-leading neutron and muon beams to:

- Exploit the unique capabilities of neutrons and muons and to complement other probes
- Achieve real-world impacts that contribute to meeting UK and global challenges
- Make best use of the reducing capacity by prioritising the highest quality science

Equip the UK science, industry and facility communities with the tools and skills to exploit the current and future capabilities by:

- Ensuring effective use of the ESS source and its capabilities as it comes on line
- Realising the skills benefits from the UK's campuses, in particular the ISIS centre of excellence in neutrons at Harwell

Achieving the vision

The panel judges that the need for neutrons will remain strong as many new and existing science challenges will continue to require the application of neutron techniques as part of the approach to addressing them. If actions are not taken, then there will be a significant reduction in neutron availability over the next ten years that may then be very difficult to recover from. This will have a consequent and lasting negative impact on UK science outcomes.

Recommendation

UK government and its agencies should continue to ensure adequate access to neutron facilities in order to meet the needs of important science areas.

The research programmes that will address the new science and technology challenges are going to need more agile experimental access as more complex and multi-probe investigations are required. Similarly, industry will need to be able to gain rapid access to investigate problems in new components and systems utilising novel materials that are increasingly going to form part of high reliability and safety- critical national infrastructure. This is likely to become increasingly incompatible with the main access modes currently employed that are still largely based on fixed application rounds. The Xpress route initiative by ISIS is a good start and can be built on.

Recommendation

Access modes need to evolve to ensure that agility is created so that academic and industrial users can effectively exploit the techniques to address high priority science and technology challenges. The UK can use its ISIS facility to lead on this.

Neutron sources are high-cost facilities and funding them and the science programmes that use them will continue to be a challenge. For spallation sources, such as ISIS and ESS, the highest costs relate to energy use and staff. Innovation will be needed in areas, such as improving machine energy efficiency and automating experimental procedures in order to minimise these costs where possible.

Recommendation

There needs to be a continuing focus on seeking reduced costs of beam time.

Neutron and synchrotron sources, and in the future X-ray free electron lasers (XFELs), are complex facilities. The co-location of facilities – such as at Harwell in the UK, Grenoble in France and PSI in Switzerland – can enhance the science opportunities and also create critical masses of expertise in technologies, such as detectors, accelerator systems, and data collection and analysis. There are considered to be further opportunities to achieve these benefits at Harwell.

Recommendation

Maximise the co-location benefits of ISIS being part of the Harwell campus, for example, in helping maintain world-class skills in the underpinning areas of expertise needed in topics, such as accelerator and detector technology.

A ten-year plan for UK neutron access

Over the next ten years, there will be significant change across many of the European neutron sources. In developing the access plan, it is important to have a clear picture of when major changes are expected to occur and the dates for key decisions and milestones. Some key dates include:

- 2018 – ILL has to secure an extension to its nuclear licence to operate
- 2019 – The BERR and Orpheus reactors are expected to close
- 2021 – Deadline for a decision on agreeing on a new protocol for ILL operations beyond 2023
- 2023 – ILL current protocol ends
- 2023 – Planned date for first eight instruments to begin user operations at ESS
- 2028 – Planned date for full suite of 22 instruments to come on line at ESS and the full 5MW beam power is reached

The research programmes that exploit neutrons are typically complex because of the nature of the science challenges being addressed and research teams that often span academia and industry within the UK and internationally. To allow effective delivery of these science programmes and ensure successful research outcomes are achieved in a timely manner, the access plan needs to respond to the expectations of UK users that they can have access to neutrons both on a suitable timescale – that is, the capacity is available, and with the necessary technical capabilities.

The reliance on large scale facilities means that this is an expensive area of scientific research. Affordability is, therefore, an important criterion that needs to be taken into account. There also needs to be an appropriate balance in the allocation of funds to provide the capacity and capability, and to support the specific research activities, since the bulk of both these funding streams presently come from the UK public sector support for science.

Recommendation

Neutrons are a key capability exploited by many research programmes supported by the RCs. Their provision needs to be considered within a balanced funding portfolio such that increases in funding for neutrons should not be at the expense of funding of the research programmes that exploit them. The panel recommends that the existing governance arrangements that STFC and the RCs have in place continue to tension this funding balance to ensure the best overall outcome for the UK is achieved.

Addressing this balance is set out in the following section where a number of options are developed.

8. Options for the neutron access plan

The diversity of the science areas that use neutrons and the associated measurement techniques means that it is a complex task to determine what the correct balance of capacity and capability should be. An additional level of complexity arises from the international nature of neutron provision, since changes in the availability of some sources and instruments are outside the direct control of the UK. As a basis to developing the access options, the panel summarised its view of the three major facilities and the roles they can play in the following box.

- **ISIS** is a world-class spallation neutron facility that must be the cornerstone of all future access arrangements. ISIS capabilities are well matched to many of the current UK science priorities and can be shaped to reflect emerging national needs going forward
- **ILL** is also a world-class reactor neutron facility, but the finite lifetime of the facility was recognised. ILL provides some novel and key capabilities, for example, in isotope production for cancer treatment and nuclear physics research and also for soft matter experiments. It should, therefore, be part of the access arrangements for as long as is feasible
- **ESS** has the potential to become a world-leading facility with the prospect of some new capabilities that will not be available elsewhere. Its long pulse characteristics will be a good complement to the ISIS short pulse system. However, ESS will not be fully operational with a significant suite of instrument stations for at least a decade

Three options have been defined for UK access to these three facilities over the next ten years: a **baseline option**, the panel’s **recommended option** and a **single source option**. These options are described subsequently, together with the associated risks, implications and opportunities that have been identified for each of them by the panel.

Baseline option

The baseline option comprises:

- **Maintaining operations at ISIS at the current level (150 user days/yr)**
- **Withdrawing from ILL at the end of the current protocol in 2023**
- **Taking up access at ESS at the same percentage level as our commitment to the construction costs (10%)**

Table 1: Baseline option risks, implications and opportunities

Risks	Some capabilities at ILL cannot be directly replaced at ESS and ISIS (e.g. those used by nuclear science).
	ESS may start up user operations late, or more slowly, than planned, exacerbating the loss of capacity.
	If ILL closes, well before the closure its ability to operate may be eroded through staff leakage.
	UK access at ISIS may be reduced if international use grows.
	The reduction in sources across Europe will mean less resilience to unforeseen changes in capacity.
Implications	There would be a permanent reduction in available beam days with a sharp reduction of 25% between 2023 and 2028.
	Science outputs will drop quickly (based on ILL experience).
	Some techniques and science areas will suffer from the loss of ILL capabilities (e.g. protein crystallography).
	Stopping further investment in ILL (the Endurance upgrade programme) could lead to strained relationships with ILL associate countries.
Opportunities	The sharp reduction in European capacity may increase international interest in use of ISIS.
	Retaining a UK capability may facilitate exchange-based access to other sources across the world.
	ISIS could strengthen its leadership role in neutron science in Europe.
	Access is secured to what promises to be the world's leading neutron source (ESS), benefiting UK science and giving access to future contracts for UK suppliers.

This option will result in a 25% reduction in capacity for the UK when access to ILL ceases in 2023. Although ESS is predicted to start science operations from 2023, the lost experimental capacity is unlikely to ever be fully recovered.

The impacts of capacity changes

The panel has reviewed evidence on the impact of facility capacity changes on the achievement of science outputs. This has been found to be significant, both in response to new capacity coming online and reductions in existing capacity.

Neutron sources are complex installations to commission and bring online. Information has been collected from several sources to show the rate of growth in science outputs in the years following their initial commissioning. This data (see Figure 4) suggests that it takes **ten years** for new facilities to reach a steady state in terms of outputs.

This gives a good insight into how quickly the new ESS facility can be expected to begin delivering significant levels of science outputs and start to offset the loss of ILL access.

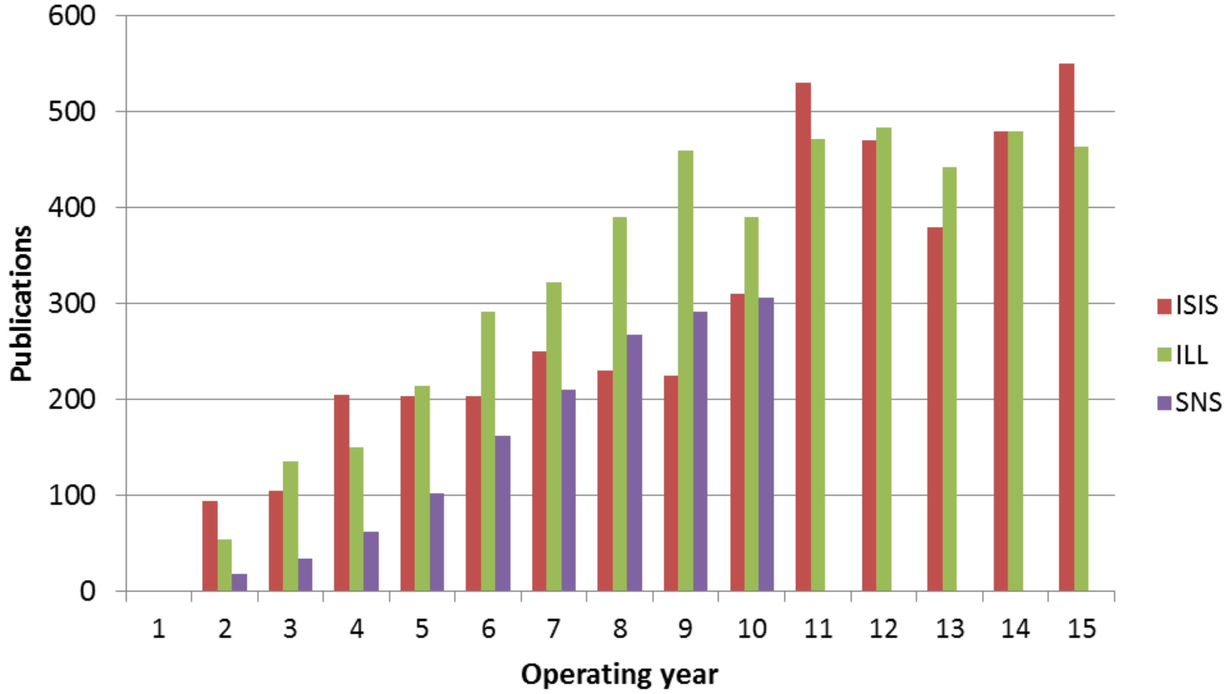

Figure 4: Publication ramp up at facilities after start up

The panel considered that ESS faces significant challenges in establishing its full complement of instruments (just 15 are currently funded). The spallation neutron source (SNS) facility of Oak Ridge National Laboratory in the United States is the nearest equivalent to the ESS in terms of power and complexity. The panel examined the detailed evidence of the SNS start up period (see Figure 5). This relates the science outputs to the increasing capacity and capability (in terms of instrument-days) as more instruments were brought into the user programme and more operational days were realised, and the beam power was ramped up.

The science outputs significantly lagged behind the growth in operational days as various technical problems had to be overcome, and the users gained familiarity with the new experimental facilities. It is very likely that ESS and its users will experience the same challenges.

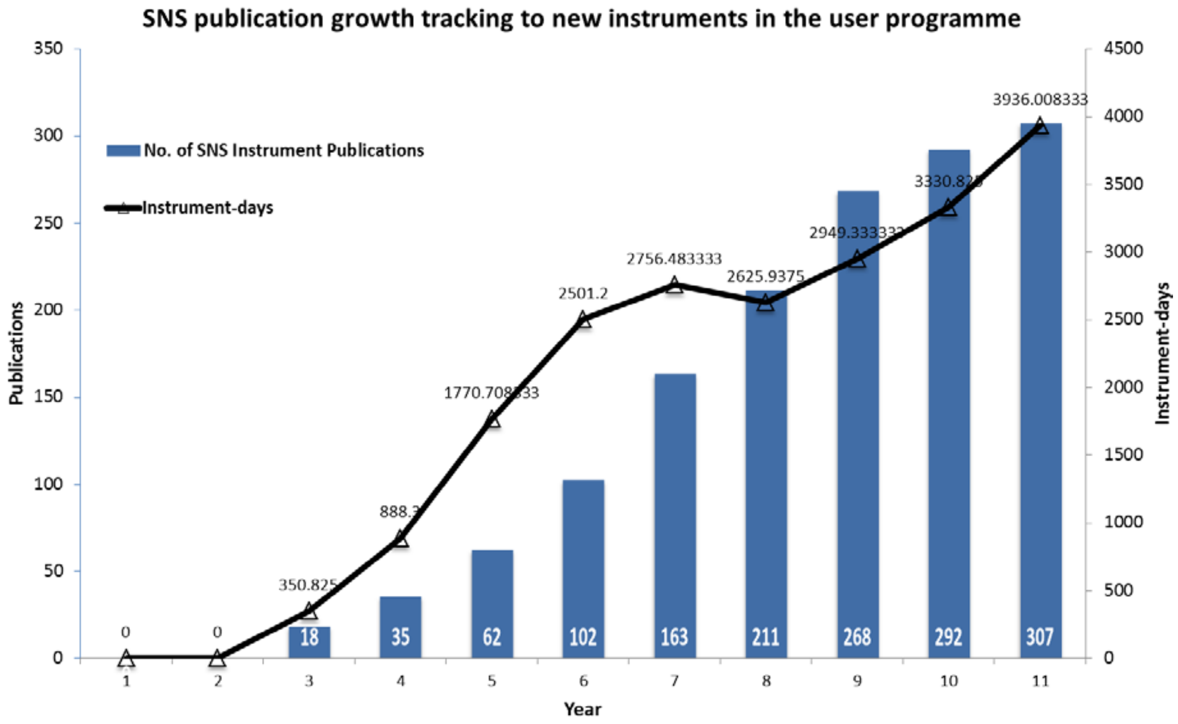

Figure 5: SNS publications and instrument-days[8]

Recommendation

As a completely new facility, ESS is the highest risk element of this access option and the panel recognises the challenges faced in bringing this large and complex new facility on line. The panel recommends that STFC actively monitors the progress with ESS construction and commissioning. If necessary the UK should renegotiate its costs and access if there are concerns about ESS performance, or if the scope for greater use is proven.

In the 1990s, the ILL source was shut down for several years for a major upgrade. Figure 6 presents the change in publication outputs over this period and shows the strong correlation between neutron availability and publications, with a very rapid decline followed by a ramped recovery after the source recommenced operations.

Based on this evidence, **the reduction in capacity in the baseline option is expected to result in a major slowdown in scientific progress**.

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[8] Oak Ridge National Laboratory, Neutron Science Research Publications. See: https://neutrons.ornl.gov/publications.

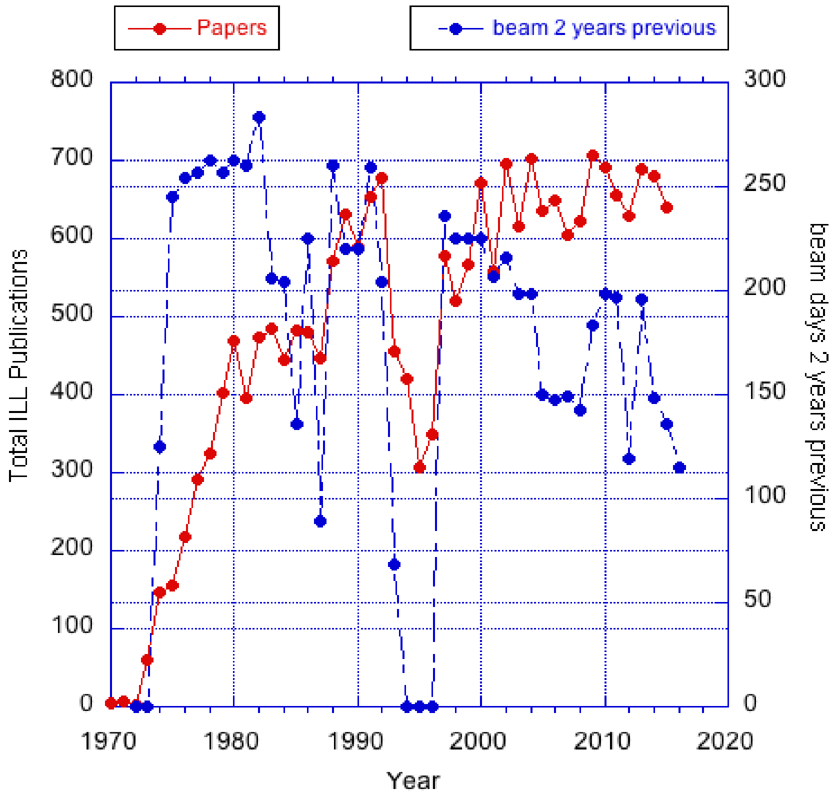

Figure 6: ILL publications in response to beam shut down (note the two-year time shift in the data sets to allow for the publication time-lag)

Recommended option

To offset the reduction in neutron capacity, the panel has developed an option that would provide continuity of beam time as ESS starts up by extending ILL access. This would ensure the UK community has the flexibility and opportunity provided by a national facility alongside access to the world's leading reactor source. Funding limitations over recent years have prevented ISIS from operating at full capacity, restricting the amount of high-quality science that can be performed. The panel considers that this should be redressed as soon as finances allow. This is the panel's recommended option which comprises:

- **Increase operations at ISIS to their full potential (180 user days/yr)**
- **Seek to extend operations at ILL for at least five years beyond the end of the current protocol in 2023**
- **Take up future access to ESS at least at 10%, and consider higher access up to 20%**

Table 2: Recommended option risks, implications and opportunities

Risks	ESS may start up user operations late or slower than planned. The impact on users would be greater if access level is increased.
	ILL's ability to operate may be constrained by fuel availability and may be eroded in the run up to any future closure.
	UK access at ISIS may be reduced if international use grows.
Implications	Long-term costs are approximately 75% higher than in 2016/17.
	The reduction in available beam days is delayed to 2028 and is less than 10%.
	Greater resilience to any unavoidable source down time.
Opportunities	Retaining a UK capability may facilitate exchange-based access to other sources across the world.
	ISIS could expand its leadership role in neutron science in Europe and across the world.
	Access is secured to the future world-leading source (ESS), benefiting UK science and giving access to future contracts for UK suppliers.
	If higher access is taken up, the UK would have a stronger influence on ESS operations and future development.

The operational capability and the scope of ESS's beamline expansion plan are uncertain. The panel, therefore, strongly recommends that, for the baseline and recommended options, a further review of access is carried out after two years' experience of science experiments at ESS. This would enable an assessment of how well ESS proves to be matched to UK science needs in terms of reliability, access modes and capability. The review could also consider revised options to meet the long-term future UK science needs, for example, by changing the level of access at ESS and examining the results of feasibility and design studies into other potential new facilities.

Recommendation

There should be a further review of neutron access once there is two years' experience of ESS operations. This review should address the extent to which ESS is proving to match the UK science requirements both in terms of capacity and capability and machine performance.

One source option

The panel recognised the need to consider an option that minimised costs, but had the least impact in terms of the reduction in access available to UK users and cost per beam day. Remaining within a flat cash budget over the ten-year period of the plan is not possible for our large national facilities without an unacceptable reduction in capacity and capability. The panel's view is that any significant change to ISIS in particular would be catastrophic for the UK science base since ISIS is the best matched neutron source for the majority of the UK's current science needs. The panel's preferred one source option is therefore:

- **Maintaining operations at ISIS at the current level (150 user days/yr)**
- **Withdrawing from ILL at the end of the current protocol in 2023**
- **Not taking up access at ESS**

Table 3: One source option risks, implications and opportunities

Risks	Some capabilities at ILL and ESS will not be replaceable at ISIS (e.g. those used for nuclear science).
	ESS operations may be significantly affected by the UK's non-participation.
	If ILL closes, well before the closure its ability to operate may be eroded through staff leakage.
	UK access at ISIS may be reduced if international use grows.
	The reliance on one source means less resilience to unforeseen down time.
Implications	The UK will have contributed £165 million to building a new source that we would have no access to.
	There is a large and permanent reduction in available beam days after 2023 (over 25%).
	Science output will drop quickly.
	Some techniques and science areas may suffer from the loss of ILL and ESS capabilities (e.g. protein crystallography).
	UK industry loses access to future ESS supply contracts.
	No further investment in ILL and ESS may lead to strained relationships with ILL associate countries and ESS participant countries and reputational damage for the UK.
Opportunities	The reduction in European capacity may help increase international interest in use of ISIS.
	Retaining a UK capability may facilitate exchange-based access to other sources across the world.

The panel gave detailed consideration to either ILL or ESS providing the single source option as these would enable a significant reduction in cost, although with commensurate reductions in capacity. The panel considered that both of these options were too high risk for the following reasons.

ILL has a finite lifetime and decisions on any future extension of operations will depend on factors outside the UK's control – for example, being able to meet the French authorities' regulatory requirements, access to fuel, and funding decisions by the other associates and science member countries. It was considered unlikely that

ILL will operate much beyond 2028 and so, if it was the only source, this would effectively become a **no-neutron strategy** in the medium to long term.

Were ESS the sole source for UK users it would severely limit the beamlines available and the number of instrument days would fall well below that needed to maintain science outputs at an acceptable level. Further, we would have limited control over determining the beamline suite and operation of ESS. This would restrict the opportunities for the UK to tune the beams and their operation to UK needs. In addition, many of ESS's technologies are still unproven and may not achieve their design performance. ESS will also be an expensive source in terms of instrument-day costs (estimated to be approximately twice ISIS instrument-day costs), at least until the instrument suite is expanded, which is not likely before the early 2030s.

Recommendation

The panel recommends that if budget limitations mandate adopting a one source option, then ISIS provides the best capacity and capability for the UK and secures a national research capability.

The wider family of neutron sources across Europe and the rest of the world provide a useful additional capacity, with typically 20% of UK neutron research currently making use of them. In the event that UK use of ILL does not extend beyond 2023, then opportunities should be sought to replace the gaps in capability that reactor sources are best able to provide. The European neutron access picture will radically change if ILL closes, as it currently provides a large fraction (~20%) of the total European capacity. Access to other European sources will become very competitive, at least until significant levels of access become available at ESS. It is likely, therefore, that the reactor sources in the United States and Australia will be the sources where the UK may be able to access small amounts of capacity to meet any pressing research needs. It may also be possible to adjust some instrument capabilities at ISIS to help reduce the impact of the loss of ILL access.

Recommendation

If UK access to ILL does not continue beyond 2023, then access to alternative reactor sources should be secured, with any necessary funding, to ensure that specific critical research needs can continue to be met.

Summary of the options

The relative costs and access levels (in instrument-days) for the three options are shown in Figures 7 and 8. These are indicative analyses and not accurate cost forecasts and give a broad-brush picture of the relative costs and access levels between the options.

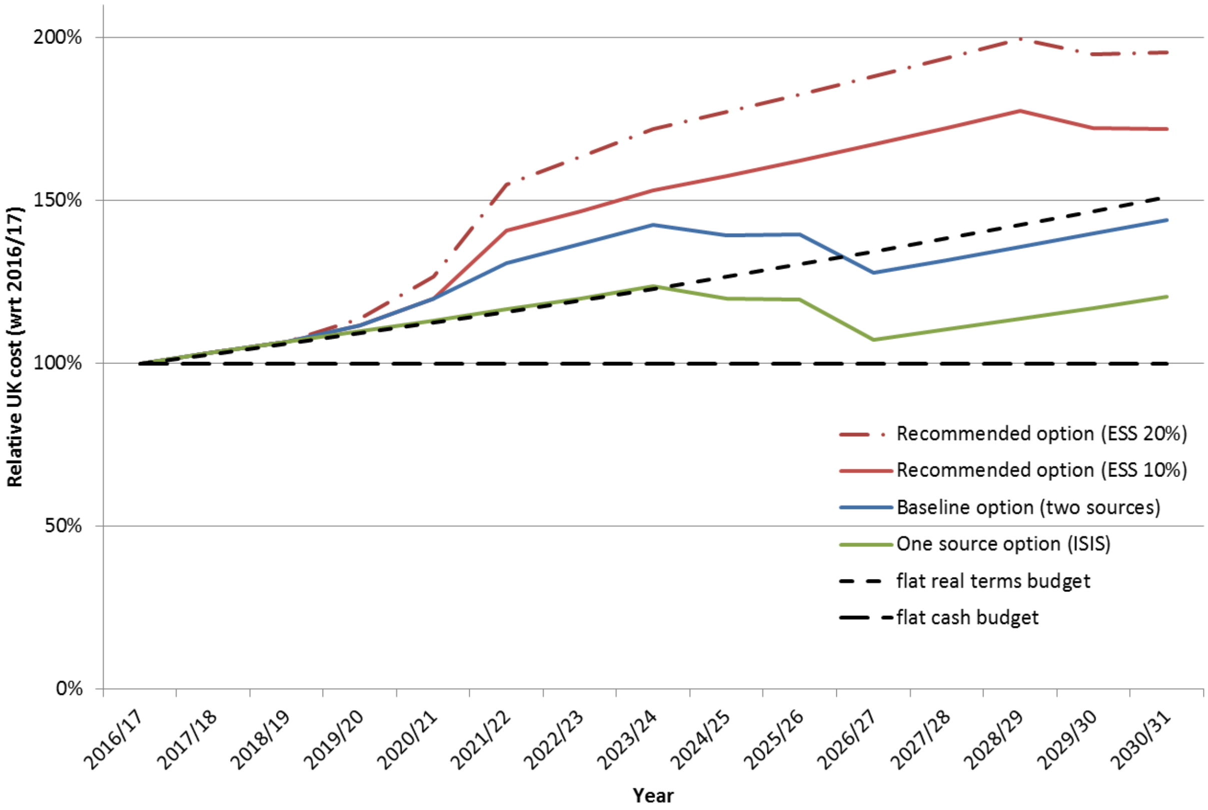

Figure 7: Relative costs of options

Notes: Inflation is included at 3%, costs are for operations only, i.e. no significant upgrade costs are included. Operational efficiency savings and decommissioning costs are also not included.

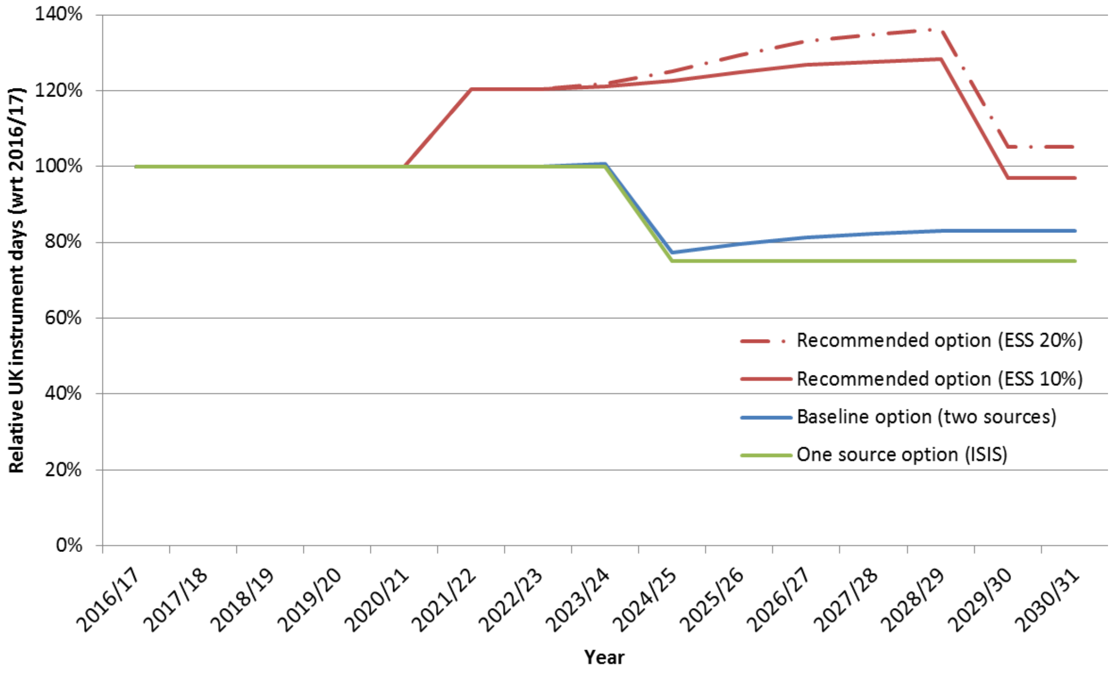

Figure 8: Relative beam days for the options

9. A sustainable future for the ISIS facility

ISIS is widely recognised as a leading neutron facility with a track record of innovation that has led to the deployment of new capabilities and the achievement of significant scientific advances. The recent impact study estimated £1.4 billion of past and future economic impacts from the research, innovation and skills that have been generated by the facility and the direct benefits to the local economy that come from employment and supply chain effects. As a key component of all the access options, it is important that ISIS reliability is as high as is reasonably achievable. The ongoing replacement of life-expired equipment (e.g. those related to the linac and synchrotron components) needs to be continued.

Recommendation

Ongoing investment in ISIS will be required to ensure it does not stagnate and also that UK science is equipped to fully exploit the new ESS capabilities as they come on line.

ISIS represents the largest proportion of UK expenditure on neutron access (as previously noted, it is also the source best able to meet a significant fraction of the UK's science needs). It is important, therefore, for ISIS to seek to diversify its funding base, particularly for the recommended option that includes an increase in ISIS operations. The decline in European neutron facility capacity over the next decade is expected to create an increased demand for access to the remaining sources that ISIS is well placed to help service. The government should **recognise and support the expanded role that ISIS can play** in building the UK's international leadership in important areas of science and technology.

There is a general international understanding around mutual open access to national facilities based on scientific excellence and this should not be lost. Funded access needs to be primarily based on long-term partnerships, and ISIS has been successful in securing a number of such partnerships over recent years. These have added to capability without impacting significantly on UK user access. This approach should be actively continued and expanded. Fully funded use by industry is currently around 1%. This could be significantly expanded – for example, up to say 5% – also without having a major impact on other users. The recently introduced industrial collaborative research scheme at ISIS has seen a quick ramp up to its target of 50 days/yr of industry involvement which supports the view that there is untapped potential in industry. The new IMAT (imaging and materials) and ChipIR (chip irradiation) instruments are both highly relevant to (different) industry sector needs, so they should be able to help increase the levels of commercial interest and use.

Other sources of UK funding include the Newton Fund, Global Challenges Research Fund and the new Industrial Strategy Challenge Fund. ISIS has already been successful in securing three Newton projects (with a value of £6.6 million). These other funding sources often have a skills and technology transfer theme. This is something that ISIS and the wider Harwell Campus Centre of Excellence is well placed to be able to deliver against.

Recommendation

ISIS should be supported and encouraged to actively seek to broaden its user and funding base internationally and with industry and other UK funding sources. This will be crucial to helping close the likely gap to the available public funding and will also ensure that there is continuing innovation at ISIS. A small loss in access for UK users is considered to be an acceptable element of a wider plan to securing a sustainable future for ISIS.

The current scoping activities exploring what is the full range of possible options for any long-term UK replacement for ISIS should be continued. It clearly makes sense for the UK to wait before making any decision on future options until there is experience of ESS. The findings of the recommended future neutron review would be an important input to any decision to launch an ISIS II in the late 2020s.

10. Skills and training

Neutron research programmes help train people in skills that are highly regarded by industry, particularly in the manufacturing and digital technologies sectors. This flow of skills from the research community into the economy also helps to strengthen the engagement of industry in neutron applications. Whilst this is a benefit to the wider economy, maintaining the skills base and expertise in the facilities and research programmes means that there is a continuing need to train new technicians, engineers and scientists.

The panel considers that there is a shortage of neutron competent or aware staff in industry which is impeding the growth of neutron use by industry. Even large companies such as Rolls-Royce have a very small pool of people with expertise in the use of neutrons. As a result, there is a high reliance on facilities to help industry users. This could be addressed by a closer collaboration between academia, the facilities and industry to recruit and train suitable students. On graduation, these students could significantly up-skill their employers as well as providing access to the benefits of neutron scattering to those companies during the course of their studies.

The Harwell Campus provides an excellent environment for developing skills both for visiting students and also training facility staff. It will be particularly important to ensure there is a suitable skills base in place to exploit the new ESS capabilities as they come on line from 2023 so that the benefits of the UK’s significant investment in constructing ESS can be realised.

Recommendation

Strengthen collaboration between industry and academia and upskill individual companies in neutron scattering by means of a significant cross research council and industry backed training scheme.

11. Conclusions

The use of neutron and muon techniques is and will remain a key requirement for UK researchers in academia and industry. The characteristics of these probes make their continued application critical to addressing important challenges for science and industry.

A proactive approach needs to be adopted to ensure that UK users can maintain the necessary access during a period of significant change in neutron facilities, especially across Europe. Core to this is maintaining and using the UK's ISIS facility to maximum effect. The establishment of the ESS and the potential closure of ILL may present significant risks to maintaining the science and also managing the costs.

The UK has an enviable reputation for world-class science and facility development. A strategic approach to delivering the optimal neutron capacity and capability mix is needed to ensure the UK's leadership in these areas of science and technology can be maintained and enhanced. This will require innovative approaches to broaden the access and funding arrangements and secure new partnerships and collaborations with international researchers and industry.

The strategic review has identified a vison for the long-term future of neutron-enabled science in the UK. The science case for neutron and muon applications has been reviewed, and future opportunities in strategic science and technology areas have been identified that support the continued investment in the necessary facilities and research programmes. A ten-year access plan has been developed with options to respond to a range of budget cases. It is clear that, with the necessary continued levels of investment, there are significant opportunities for continued UK success in science areas that are closely linked to the evolving national industrial strategy. If investment is constrained, resulting in reduced neutron availability, then there is a high risk that the UK will lose its leadership in some key areas of science and technology.

Appendices

A. Characteristics of neutron and muon probes
B. Science with neutrons and muons
C. Alternative neutron sources
D. Strategic review panel membership and terms of reference

The neutron – a powerful probe of matter, materials and systems

Many scattering probes, for example, photons (X-rays, light, etc.) and charged particles (e.g. electrons), interact with the electronic structure of matter. The neutron is a chargeless particle which is scattered by short-range interactions with nuclei. Using neutrons, the positions and motion of nuclei in matter are probed directly. The measurement process is precise and well-quantified (unlike many other probes), and neutron scattering provides the benchmark data for a wide range of simulations. Neutrons have the follow special features:

Neighbouring atoms in the periodic table can have very different neutron scattering powers – light atoms (e.g. H, Li, O) are just as visible as heavy atoms. Hydrogen and deuterium have large scattering powers for neutron diffraction, making neutrons an ideal probe of hydrogen in matter, in particular biological matter. Quasi-elastic neutron scattering is the only way to study both hopping vectors and frequencies of diffusing ions for hydrogen storage, battery and fuel cell materials. This is in contrast to probes such as X-rays which are scattered by electrons and see atoms according to their atomic number – for them, hydrogen is the least visible atom and other light atoms such as Li (important for battery science) and O (important in carbon capture science) in frameworks of heavier atoms are essentially invisible.

Isotopes of the same atom have different nuclei and, therefore, different neutron scattering powers enabling them to be distinguished from each other using a neutron probe. This enables matter to be selectively labelled without changing its chemistry so that parts of the system can be clearly highlighted whilst other parts are hidden. Hydrogen – deuterium exchange is highly effective for labelling and contrast matching. Nuclear magnetic resonance (NMR) is the only other analytical technique which can exploit isotopic labelling.

The neutron spin acts like an extremely small magnet and it probes the magnetism of matter by interacting with the spins of unpaired electrons. Neutrons are, therefore, the best direct, microscopic probe of magnetic structure and excitations of matter.

Weakly interacting with matter, neutrons penetrate deeply (up to 30cm in aluminium), allowing buried structures or interfaces to be studied non-destructively. As neutrons do not cause any significant radiation damage, they can be used to study fragile (e.g. archaeological and biological) samples.

Neutron wavelengths and energies are comparable with the nanoscale-to-mesoscale structures in matter and their excitations (dynamics) so that instrument resolution and dynamic range can be tuned to optimally probe structure and dynamics across very wide length and time scales.

Intense neutron beams are used to produce exotic, neutron rich nuclei and study their decay. Information about structure and stability is essential for understanding the nucleosynthesis of elements in stars and it is highly relevant to advanced nuclear technology for energy production and waste treatment.

The highest densities of ultra-cold neutrons allow neutron lifetime, decay and dipole moment studies to explore new science beyond the standard model of particle physics and probe fundamental asymmetries (parity, time-reversal, baryon number) in the Universe.

Muons

In an accelerator-driven neutron source, high-energy protons are hitting and disintegrating atomic nuclei in the target. The fragments from this disintegration consist of new, lighter nuclides, neutrons and gamma radiation and a number of short-lived radioactive particles that later decay into either radiation or other particles. One of these secondary particles is a heavy electron-like particle named a muon. The muon is unstable and will decay after 2.2 microseconds into an electron and two neutrinos. The muon lifetime is, however, sufficiently long for it to be used as a very powerful probe of matter and materials.

Muons from a target will penetrate into materials and can be used to study a wide range of magnetic systems, with the muon acting as a very sensitive microscopic magnetometer and probing longer fluctuation timescales than neutron scattering. Muons are suitable for studies of small-moment, short-range, random or dilute magnetism. In superconducting materials, muons can be used to explore the flux-line lattice generated when a field is applied to a type-II material, complementing small-angle neutron scattering measurements in some cases. Muons can be used to determine fundamental superconducting parameters, such as the penetration depth, coherence length, superconducting carrier density and effective mass. They can also be used to study various charge transport phenomena, including ion mobility in battery cathode materials, electron dynamics or charge carrier motion in conducting polymers.

The positive muon can act like a light proton. Where protons or hydrogen atom behaviour is difficult or impossible to study directly, observation of the muon response can enable models of its heavier counterpart to be produced; examples include investigation of hydrogen behaviour in semiconductors. In molecular materials, muons can form radical states sensitive to molecular dynamics and can be used to study chemical reactions.

In common with ultra-cold neutrons, very intense muon beams will allow muon lifetime, rare muon decay modes and dipole moment studies to challenge our current understanding of the Universe.

Manufacturing processes and materials of the future

Manufacturing turns materials into products. The selection, design and cost-effective, sustainable manufacture of materials can be the deciding factors between a successful launch of a new technology or not. Indeed, many materials have not reached the marketplace or realised their full potential because of one or more issues with the manufacturing stage. Furthermore, as the dimensions of many components need to be smaller (e.g. to exploit quantum technology) and the bespoke nature of products increases, driven by the possibilities delivered by additive manufacturing techniques, the manufacturing challenges are both increasing and becoming more diverse.

Illustrative neutron applications

Nearly all manufactured articles and components involve joints of one form or another. Welds have locked-in residual stresses and are sites of stress concentration and suboptimal microstructure. These three factors make welding a significant manufacturing issue from a structural integrity viewpoint. Further, new welding methods are needed to facilitate new engineering designs, leading to, for example, lighter, and more fuel efficient aero-engines.

Credit: Pixabay

Ensuring safe operation of nuclear power plant

The lifetimes of Hartlepool and Heysham I nuclear power stations have been extended from 2011 to 2019 as a direct result of **neutron residual stress measurements** made by the Open University. These support the life-extension case, maintaining jobs, ensuring security of electricity supply, and deferring the need for decommissioning and replacement of two nuclear power stations at a cost of several billion pounds each. The electricity generated during the life extension period has a market value of over £8 billion.

Neutron diffraction is the only method able to non-destructively map in three dimensions the residual stresses that become locked in when a weld is made. Obtaining unique information, gathered on both sub-scale prototypes and full-scale engines, has accelerated the safe adoption of inertia welding by Rolls-Royce. Further, the method is providing data that are critical to the safe life extension of existing plants. For example, **neutron diffraction** has had a direct impact on nuclear plants in the UK, being used by British Energy to validate predictions of the creep relaxation of residual stresses and hence the safe plant lifetime. This study represented the largest economic benefit to the UK of all the impact cases submitted as part of the recent Research Excellence Framework (REF2014) assessment of the quality of university research.

Additive manufacture (AM) allows components to be built directly from powders or wires using lasers or electron beam melting. Given its huge potential to manufacture innovative and/or bespoke designs in a resource efficient manner, AM has become a significant focus for government and industry alike. It is predicted to be a

£21 billion/year industry by 2020, and received >£25 million in research funding in the UK in 2015[9]. The high value end of this technology involves producing parts of complex geometry, made from materials that are impossible or hard to manufacture using traditional routes. Understanding the evolution of microstructure, crystallographic texture and residual stress is critical when making this sort of high-performance parts. Given the inherent complexity involved, a sound science platform is essential to unlocking the potential benefits of additive manufacture, and **neutron diffraction** will have a critical role to play. The importance of this has been recognised by national laboratories in the United States, Australia, Japan and France, where active neutron-based studies are aimed at improving the quality and cost effectiveness of AM. In the UK, the combination of industries (such as Airbus, Renishaw and Rolls-Royce) and the supporting academic community (e.g. Manchester, Nottingham, Oxford and Sheffield) is well placed to build on initial studies at ISIS to ensure best exploitation of the technology.

Catalysis is at the heart of many industrial production processes, including petrochemical refining and chemical production, with a turnover of ~\$19 billion per annum. **Neutron spectroscopy** provides information about reaction pathways during these chemical reactions allowing the development and optimisation of catalysts, such as those used in synthetic kerosene and methyl chloride production. Hydrogen is a key element so neutron scattering provides unique and significant insight in these processes. Catalysis is also used to reduce emissions from automotive exhaust systems. Studies at ISIS with industrial collaborators[10] have identified that hydrogen is mainly present as adsorbed water rather than palladium hydroxide as previously believed, paving the way for improved technology. A 3% compound growth is predicted[11] for catalytic converters meaning that they will account for >80% of Pd use and >50% of Pt use by 2020 and constitute a multi-billion-dollar industry.

Credit: Pixabay

A better catalyst for the chemical industry

Central to making a chemical commercially is the design of the catalyst that speeds up the relevant chemical reaction. It must be highly selective, directing the chemical pathway to maximise the amount of the final product at the expense of unwanted by-products. Ineos ChlorVinyls, which produces methyl chloride at its Runcorn complex, wanted a catalyst that would eliminate a by-product, dimethyl ether. Using **inelastic neutron spectroscopy**, tell-tale molecular vibrations could be detected and assigned to a particular molecular structure, revealing that a key intermediate compound was formed. Based on this information, Ineos ChlorVinyls was able to make its manufacturing process much more efficient.

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[9] Innovate UK, *Mapping UK Research and Innovation in Additive Manufacturing*, February 2016.

[10] Parker SF et al. Characterization of hydrous palladium oxide: Implications for low-temperature carbon monoxide oxidation, *J. Phys. Chem. C* 2010; 114 (33): 14164–14172. Available at: DOI**:** 10.1021/jp103847d.

[11] PGM, *Summary of Platinum Supply and Demand in 2015*, May 2016.Available at: www.platinum.matthey.com/documents/new-item/pgm%20market%20reports/pgm-market-report-may-2016.pdf.

Industrial biotechnology and synthetic biology: The use of living biological cells as factories and enzyme proteins as green catalysts is a growing area of manufacturing. At least 50% of new drugs in development are biopharmaceuticals and the bio-transformations sector is developing methods to use biomass as a feedstock for many processes including biofuels and plastics. Current research in synthetic biology will further expand these applications. Neutrons are unique probes of such systems being able, for example, via **small-angle scattering,** to view protein drugs within complex formulations and reveal how enzymes digest complex plant polymers, whilst **reflectometry** can reveal the means by which antibody drugs adhere to process surfaces.

New research topics and directions

The ever-constant driver in manufacturing is to increase profitability by considerably shortening the time and cost to market of new ideas. Critical to this is the close coupling of the computer-based design of new materials and manufacturing processes with experiments in an iterative manner. Multiscale models will be needed to design from the atom to the application; such models rely heavily on input data across all scales in order to refine them and to narrow the formulation and manufacturing process space to be explored, as well as for validation. In this respect, the ability of neutrons to penetrate materials and to provide unique information is critical and we envisage the need for further development of rigs able to replicate complex in-service conditions, aimed at replicating manufacturing processes on the beamline to generate real-time data on microstructure property relationships to enable us to identify the most promising manufacturing processing conditions.

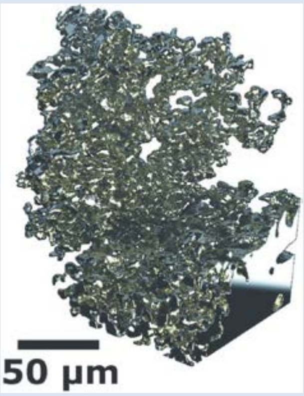
Smart and clean energy technologies

Our rapidly expanding demand for energy means that transforming the way we generate, supply, transmit, store and use energy is one of the defining global challenges in the 21st century. At its core, the challenge is a scientific one and one that neutron scattering will continue to make significant contributions in addressing. Energy systems of the future – whether they tap sunlight, store energy chemically or make fuel from splitting water – will revolve around materials and chemical changes that efficiently convert energy from one form to another. To control electrochemical reactions or to convert sunlight to electrons requires coordination of multiple steps, each carried out by customised materials with designed nanoscale structures. Such advanced materials are not found in nature; they must be designed and fabricated to exacting standards using principles revealed by basic science. Modern requirements will demand that these materials need to be more functional than the energy materials of today.

Illustrative neutron application areas

Solid oxide fuel cells (SOFCs) allow clean and efficient energy generation. They are a fuel-flexible and highly scalable energy solution, with applications ranging from small, mobile auxiliary power units to large residential and industrial combined heat and power systems. Conventional SOFCs, based on an yttria stabilised zirconia (YSZ) electrolyte, operate between 800 and 1000°C, and this has been a major obstacle to their more widespread use. A UK-based company, Ceres Power, has recently developed a micro combined heat and power module with an operating temperature around 600°C and electrical and overall efficiency of 45% and 90% respectively, saving the energy bill by 25% and about 1.5 tonnes of CO_2 per household per annum, compared to current generation methods. **Neutron diffraction** and **spectroscopy** methods have been instrumental in providing key insight into the relationship between structures, distribution of defects and ionic conductivity, first in YSZ and later in related materials, including the solid electrolytes and anodes used in the Ceres Power “steel cell”. This early insight has helped provide the design principles for the identification and development of new materials which outperform the current electrolytes, and neutron-based techniques are needed to help some of these candidates advance to applications stages. To develop SOFC cathodes it is essential to understand the ionic transport properties and their relation to the defect structure, particularly anion defects, as a function of temperature and atmosphere. Only **neutron diffraction and spectroscopy** offer this insight, especially through in operando techniques, probing stability of materials under applied electrical load. Particularly important neutron studies have been those on next-generation electrodes such as the layered perovskites, where accurate determination of anisotropic diffusion pathways has been critical in understanding ion transport. This work has been underpinned by computational modelling including advanced atomistic simulation studies, as well as total scattering and maximum entropy approaches.

Rechargeable lithium batteries: The global lithium (Li)-ion battery market is forecast to exceed $30 billion by 2020. Li-ion batteries are currently used in portable consumer electronic devices, but there is major interest in expanding the market into automotive applications and energy storage. The first-generation Li-ion batteries, introduced by Sony in 1990, used lithium cobalt oxide as the positive electrode. Powder **neutron diffraction** was crucial in establishing the arrangement of cations in the layers in the structure and the link between Li-ion distribution and the electrochemical performance of lithium cobalt oxides as cathodes. The issues around cost, safety and the amount of Li which could be extracted from the lithium cobalt oxide cathode have driven the development of more efficient lithium intercalation host materials. Neutron studies established the relationship between the structure and properties of alternative cathode materials, including lithium manganese oxide, lithium iron phosphate and lithium nickel manganese cobalt oxide. Although lithium cobalt oxide based rechargeable batteries still have the largest



Credit: Eastwood DS et al. Chem Comm 2015; 51: 266-268

Beyond Lithium-ion battery technology
Constraints of Li-ion batteries include low power and limited battery life, which can be significantly improved if lithium is used as the negative electrode or 'anode'. However, this creates well-documented safety issues as during charging and discharging of the battery, microscopic lithium fibres – known as dendrites – can form on the metal anode's surface. If these dendrites reach the cathode, or positive electrode, the battery can short-circuit and catch fire.

Research into sodium-ion and magnesium-ion alternative technology is accelerating; however, finding suitable cathode materials remains a challenge and one in which neutron scattering continues to play an important role.

share of the consumer electronics market, these alternatives are now being used in power tools and automotive hybrid systems. **Neutron reflectivity** and **neutron imaging** have also contributed significantly to battery materials research by helping the understanding of the formation of the solid-electrolyte interphase (SEI) which is buried in composite structures and devices. The SEI is critical to the performance and safety of energy storage materials (see inset), yet its formation is still poorly understood. These neutron-scattering techniques are well suited to the challenge of monitoring in situ the evolving SEI.

New research topics and directions

Energy science research will be continually challenged to develop and produce new and improved functional materials. The sustainability of these materials is of growing importance, and issues such as lifecycle costs, elemental abundance and the cyclability of particular systems present formidable challenges. Neutron and muon measurement techniques will remain critical in this evolving landscape, both for fundamental studies and for in situ and in operando studies where monitoring increasingly complex processes over a range of length scales and dynamics timescales will be essential. Neutron facilities have the myriad bespoke sample environments demanded by academic and industry users and these capabilities offer a competitive advantage over alternative techniques. Some examples of energy systems and materials development challenges that will need neutron techniques include the following.

New materials for SOFC components (electrolyte and electrodes) that will enable efficient operation at temperatures around 500°C and even lower. Neutron in situ studies using gas flow apparatus can probe SOFCs at their operating temperatures and under variable oxygen partial pressures.

High-performance thermo-electric converters which will require simultaneously maximising and minimising the competing quantities of electronic and thermal conductivity respectively through materials design and/or processing. High-stability (to moisture, temperatures and solar irradiation) lead halide perovskite based solar cells, have the potential to revolutionise photovoltaic technology. In addition to the high efficiency (over 20% currently), these materials are also particularly attractive owing to the low cost of the raw materials and low-cost, solution-based processing methods.

Rechargeable batteries with improved safety, higher gravimetric and volumetric energy density and improved long-term cyclability and sustainability. This requires the development of non-flammable electrolytes, improvements of the hierarchical approach to the electrode design in Li-ion batteries and further developments of the Li-air battery (a theoretical energy density 10 times higher than today's Li-ion batteries). Neutron scattering, including in situ and in operando studies using electrochemical cells or actual devices to study battery electrode materials during charge-discharge cycling, will enable these devices to be commercialised.

A grand challenge in condensed matter science is the development of room temperature superconductors. Very recent and significant advances in the fundamental understanding of the mechanisms of superconductivity in cuprates have rekindled the hope that this goal is achievable and neutrons will be key to making advances in this area. This technology would transform energy transmission by enabling loss-less power grids, and enable scenarios for electrified aviation.

Leading edge healthcare and medicines

Medicine and the health sciences are important both for the well-being of the population and the UK economy. They span from studies aimed at understanding the basic molecular and cellular mechanisms of both the healthy and the diseased person, through to the discovery of new therapeutic molecules, implants and biosensors. It is a rapidly moving area with increasingly complex drugs and other interventions being developed. Against this background, neutron science is fast becoming an essential tool because of the unique information it provides. Additional drivers for the increase in neutron use are the decrease in measurement times and reduced sample sizes plus improved neutron awareness amongst the relevant communities. All the large scale neutron sources worldwide now have growing programmes in the biological, medical and health sciences area.

Illustrative applications of neutrons

Perhaps not surprisingly, neutron studies on biologically relevant structures and processes for health and medicine exploit a wide range of neutron techniques. For example, **neutron diffraction** has been important in determining protein structure or examining biological membranes and fibrous biological molecules such as DNA, both in the absence and presence of drugs to aid in improved drug design. **Liquid neutron diffraction studies** are providing unique insights into the interaction of water with important biological molecules, such as peptides and lipids, and how this is perturbed by the addition of other biologically relevant materials. **Small-angle neutron scattering** (SANS) in combination with selective deuteration has been used successfully to determine the solution structure of multicomponent biological systems as well as determining the interaction of drugs with biomolecules in solution and the nature of materials suitable for implants, amongst other things. The ability of **specular neutron reflection,** again in combination with selective deuteration, to

Biosensors

The use of **neutron reflectometry** to probe the interaction of biomolecules with surfaces, yields detailed structural information not possible with other techniques. Such an understanding is essential in health and medicine, where interactions between a biomolecule and surface can be unwanted, for example as in the fouling of materials used in protein drug manufacture, or desired as is the case in highly sensitive biosensors. The latter case was exemplified by the work of Orla Protein Technologies, a UK biotechnology company, which developed a means to assemble antibodies on analytical devices to act as biosensors. The resulting very thin layers could only be measured by **neutron reflection** and the unprecedented detail obtained from these studies was used to justify the formation of a UK-based joint venture with the Japan Radio Company to convert their surface acoustic wave technology into a handheld wireless diagnostic device.

OJ-Bio's prototype medical diagnostic device.
Credit: OJ-Bio

probe surfaces and buried interfaces has allowed it to make a unique contribution in the study of model and actual cell membranes where more than 70% of drug targets reside. Elsewhere, neutron spectroscopies such as **inelastic neutron scattering** reveal important aspects of the molecular motion in complex systems such as the lipid-protein structures present in biological membranes; while **quasi-elastic neutron scattering** can be used to understand drug solubility and water diffusion within living cells, showing that water diffusion is much faster in living cells than had been envisaged. **Neutron imaging** methods are powerful tools for non-invasive in vivo imaging allowing, for example, cells to be seen when held in complex environments.

In exploring the physiological and sub-cellular mechanisms that underlie the origin and progression of diseases, it is critical that our understanding extends down to the molecular and sub-molecular level. In many cases, the interest is on large macromolecular and often supramolecular systems, and **small-angle neutron scattering** and **neutron reflectivity** – particularly when used in conjunction with H/D contrast variation – provide the ideal means by which it is not only possible to obtain the required structural information on selected parts of these highly complex systems, but also allows the study their dynamic behaviour over relevant timescales and without causing damage to the samples studied. This ability makes it possible to study the complex structures involved in, for example, gene regulation and infection, and to devise new means to combat inherited conditions like muscular dystrophy, find more effective drug delivery systems, and to find new ways to combat MRSA and other drug-resistant microbes.

Within the very near future, it will also be possible to routinely carry out membrane **neutron reflectivity** studies that probe the structure and dynamics of live cells. In 2013, experiments were reported[12] in which pluripotent stem cells were immobilized on gold/magnetic permalloy-coated silicon wafers functionalized with nickel-NTA with attached cell adhesion proteins. In this instance, the reflectivity measurements were made only to confirm and characterize the structure of the functionalized membrane support – but by extension the same system might readily be used in the near future for fully fledged mechanistic studies of cell differentiation – with benefits then afforded to tissue engineering and regenerative medicine. The following year, neutron reflectometry was used to examine the adhesion of various live cells to quartz substrates under different environmental conditions, including flow stress, in what is believed to represent the first successful visualisation and quantisation of the interface between live cells and a substrate with sub-nanometer resolution[13]. Such studies may have significant medical impact on the understanding of complex biological problems and their effective treatment, for example, for the development of targeted anti-invasive therapies.

Neutron diffraction and **quasi-elastic neutron scattering** studies are also relevant to medicines development because these techniques are uniquely able to provide information on the interaction of water with drug molecules, and on the dynamic behaviour of water in biological cells and membranes. An understanding of these

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[12] Körner A et al. PLoS One 2013; 8: e54749.

[13] Junghans A et al. *Mod Phys Lett B* 2014; 30: 10-28.

phenomena impacts the ability to manufacture solid medicines with good stability and dissolution properties, and also to design drugs with properties that allow them more readily to cross the blood-brain barrier to treat neurological disorders like Alzheimer’s and Parkinson’s disease.

New research topics and directions

The most significant advantage in the use of neutron techniques for biological and medical investigations could be gained by reducing the time for measurement to allow kinetic studies to be performed, as well as allowing precious, biological samples to be more effectively and efficiently used by performing real-time analysis and/or simultaneous measurement with other techniques.

Many important biologically relevant processes occur on the millisecond to minute timescale, including the fusion of membrane vesicles, the lateral diffusion of molecules in membranes and the binding of biologically relevant molecules with biological cells. However, at present it is not routinely possible to study these processes using neutron scattering. The ability to perform neutron experiments faster will open up the possibility of performing a wider variety of such measurements including the ability to perform kinetic measurements. Neutron experiments have historically been slow, frequently taking hours to days to complete; however, they can work on complex samples and have the significant advantage of avoiding the damage to fragile biological molecules that synchrotron X-ray sources often cause.

In many cases, it requires significant effort to prepare the amounts of biological material frequently necessary for study using neutrons. Hence the ability to rapidly obtain results, ideally from a real-time analysis of the data, would allow a much more efficient use of available material. Such analysis is especially important since many biological samples are assembled in situ and time can be wasted finding out if the preparation has been unsuccessful. Improvements in computer power and modelling mean that it should be possible routinely to analyse the neutron data generated during the experiment immediately following the data acquisition. By this means, it becomes possible quickly to identify potentially problematic samples and sample environment-related issues, allowing the experimental methodology to be modified to overcome these issues, and thereby ensuring that hard-gained and/or expensive biological materials are employed for maximum scientific benefit. An additional advantage to be gained from this possibility is the optimal utilisation of the instrument time, allowing the neutron equivalent of high throughput and the generation of a statistically robust output.

Another way to gain optimal information from precious biological material using neutron techniques is the simultaneous application of other techniques. This is possible because, unlike X-rays and some optical methods, neutrons are non-destructive and can probe inside complex, aqueous samples. This ability to observe, using neutrons, biomolecules in their native state can be combined with other experimental methods on the beamline to provide multiple readouts and more effective/efficient use of the biological sample. For example, the possibility of performing neutron reflectometry in combination with surface plasmon resonance and infrared spectroscopic measurements would greatly aid the study the binding of biological molecules to biological membranes. This approach can be applied to a number of neutron scattering techniques.

Transformative digital technologies

The digital economy is underpinned by the technological capabilities provided by hardware. The equipment and technologies behind the world's digital infrastructure are, by design, hidden from view, but make all of the difference in terms of competitive advantage for end users, as well as the supporting manufacturing and service economy. Developing the next generation of these technologies will open up new sectors of the digital economy.

Illustrative application areas

The ability to design one-, two- and three-dimensional structures has been absolutely critical in developing applications and testing fundamental physics models used in many other areas (see *The impossible monopole*). Such structures can be made artificially, for example, by depositing thin magnetic films on top of each other, giving rise to the giant magnetoresistance effect, the technology used in all hard disk read heads, or to set up the exchange bias memory effect, used in magnetic hard disks. Hard disk drives were a $32 billion market in 2016. To look at the sandwich-style structures, **polarized neutron reflectometry** gives you information on the layers and interfaces directly and non-destructively, no matter how deeply they are buried. For digital science, the key question is how the magnetic structure changes at the interface. To get the best out of these measurements, complementary X-ray reflectometry and/or low energy muon spin spectroscopy are really helpful when interpreting the data.

The impossible monopole

Magnetic monopoles are a key ingredient in grand unification theories but, to date, they have not been found in particle colliders or cosmic radiation.

Magnetic monopole excitations have been predicted to emerge from a frustrated magnetic system called spin ice, which maps onto the structure of water ice. The key experimental evidence in support of this theory was obtained using **diffuse neutron magnetic scattering** in back-to-back papers in Science[1]. This is the first time it has been possible to access and manipulate free magnetic charges.

Work is underway to develop artificial two-dimensional equivalents closer to real-world applications. In order to study these nanoscale systems, **neutron reflectometry** is the technique of choice.

[1] Science 2009; 326, 411 and 326, 415.

New topics and directions in the science area

The fraction of our electricity used for information technology (IT) – both processing and storage – is rising rapidly (annual growth rate ~5%) and has now reached about 5% of total electricity production[14], approximately equally shared between big data centres, office/home type computing and networks/transmission. Any new technology that lowers the energy cost per bit stored or manipulated will, therefore, be of huge monetary and environmental importance. Lower energy consumption will also allow higher packing densities and hence increased performance of electronic

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[14] Aebischer B and Hilty LM. The energy demand of ICT: A historical perspective and current methodological challenges. In Hilty L., Aebischer B. (eds), *ICT Innovations for Sustainability: Advances in Intelligent Systems and Computing*, vol 310. Springer, Cham: 2015.

components. Neutron scattering will be instrumental in the search for entirely new methods of storing and manipulating bits with minimal energy consumption. Several different paths are being explored in this area. One is the development of so-called multiferroics: materials where there is a strong coupling between electric and magnetic effects, so that the magnetic moments can be manipulated by electric fields, rather than magnetic fields or currents, reducing energy consumption. Neutron diffraction and inelastic scattering measurements were crucial in showing how electric fields affect the magnetic structure, and a room temperature material has recently been found, making device development much more likely. Another exciting possibility is the “skyrmion” state. Again, this was a concept from high-energy physics that was eventually observed, using **small-angle neutron scattering**, in manganese silicide (see *Using magnetic vortices as bits*).

An important new area is superconducting spintronics, another method of tackling the energy consumption problem. EPSRC is investing £2.7 million in testing whether it is possible to power spintronic devices with superconductors. Neutron reflectometry at low temperatures and in small magnetic fields will be important in establishing what happens across interfaces in these devices.

This technique will also assist with the drive to stack computing elements vertically, to increase efficiency and reduce energy consumption. Non-destructive testing during the development stage will also require the use of bulk imaging techniques. Neutrons provide a powerful tool that fulfils this requirement.

Using magnetic vortices as bits

Skyrmions are topological, vortex-like magnetic objects that come in two flavours (chiralities) that can be used to represent the two binary states, 1 and 0. They can be moved by small currents, and so present a very promising prospect for workable devices, which will work faster than current magnetic memory systems. They were first seen by small-angle neutron scattering in 2009 [1] and can now be made at room temperature using (Co, Zn, Mn) alloys – all cheap, easily sourced metals [2]. Neutron experiments have proved that these skyrmions respond to currents, and prototype devices are expected soon.

[1] Müehlbauer S et al. *Science* 2009; 323, 915-919.
[2] Tokunaga et al. *Nature Comms* 2015; 6, 7638.

Appendix C: Alternative neutron sources

Neutrons can be generated by a variety of mechanisms including:

- The spontaneous fission of radioactive isotopes such as californium-252 results in the emission of neutrons. All the spontaneous fission neutron sources are produced by irradiating uranium or another transuranic element in a nuclear reactor, where neutrons are absorbed in the starting material and its subsequent reaction products, transmuting the starting material into the spontaneous fission isotope
- Compact linear accelerators can produce neutrons by fusing isotopes of hydrogen together. The fusion reactions take place in these devices by accelerating deuterium, tritium, or a mixture of these two isotopes into a metal hydride target which also contains deuterium, tritium or a mixture of these isotopes
- Nuclear fusion plasma devices produce controlled nuclear fusion by creating dense plasma within which ionized deuterium and/or tritium gas is heated to temperatures sufficient for creating fusion with the associated release of neutrons
- Another type of neutron generator is the inertial electrostatic confinement fusion device or Fusor

For the majority of these systems, the useful levels of neutron flux available for experimentation are many orders of magnitude lower than from research reactors such as ILL or large spallation sources such as ISIS. Work is underway in several laboratories to develop compact accelerator-based neutron sources with sufficient performance to underpin the exploitation of the larger sources, for example, the Jülich 'high-brilliance' neutron source project[15] and the LLB SONATE project. Even if these prove to be successful in neutron generation terms, the associated neutron instrumentation needed would still be substantial in order to carry out useful experiments.

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[15] Rücker U et al. Eur Phys J Plus 2016; 131: 19.

Appendix D: Strategic review panel terms of reference and membership

Terms of reference

- Examine the key science challenges that require long-term access to neutron facilities based on inputs from the UK Research Councils, the UK science community via relevant STFC advisory panels and user groups, industrial stakeholders, and relevant facility directors
- Identify the requirements to address the key science challenges
- Identify means for meeting the UK's neutron facility access requirements
- Recommend a ten-year strategy for UK access to neutron facilities, including underpinning technology, skills and community development; and a 15-20-year vision for UK science requirements for neutrons and the facilities needed
- Estimate potential capital and operating costs to implement the strategy, and potential technology and instrumentation R&D costs. This should include an optimum strategy and options under financial constraint

Panel membership

Professor Philip Withers (Chair)	(University of Manchester)
Professor Jayne Lawrence	(King’s College London)
Professor Matthew Rosseinsky	(University of Liverpool)
Professor Julie Yeomans	(University of Surrey)
Professor Jeremy Lakey	(Newcastle University)
Dr Ivana Evans	(Durham University)
Dr Elizabeth Blackburn	(University of Birmingham)
Dr Richard Ibberson	(Oak Ridge National Laboratory, USA)
Dr Kurt Clausen	(Paul Scherrer Institute, Switzerland)
Professor David Rugg	(Rolls-Royce Plc)

Establishments at Boulby Underground Science Facility, Cleveland; Chilbolton Observatory, Hampshire; Daresbury Laboratory, Cheshire; Polaris House (STFC headquarters), Swindon; Rutherford Appleton Laboratory, Oxfordshire; UK Astronomy Technology Centre, Edinburgh.

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