



Neutrons for science and technology



Imprint

Editorial Board

- C. Alba-Simionesco, ENSA and Laboratoire Léon Brillouin, France
- A. Desmedt, CNRS - University of Bordeaux, France
- M. Johnson, NMI3 and Institut Laue-Langevin, France
- K. Knudsen, Institute for Energy Technology, Norway
- J. Neuhaus, MLZ, Technical University of Munich, Germany
- D. Paul, University of Warwick, UK
- H. Rønnow, École Polytechnique Fédérale de Lausanne EPFL, Switzerland
- H. Abele, H. Rauch, Atominsttitut Wien, Austria
- A. Schneidewind, JCNS at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany
- A. Senyshyn, MLZ, Technical University of Munich, Germany
- M. Mühlbauer, Helmholtz Institut Ulm, Germany
- L. van Eijck, Delft University of Technology, Netherlands

Pictures

Cover and Page 4: Kindly provided by HZB, ILL, ISIS, LLB, MLZ, NMI3, PSI, Uni. Copenhagen and TU Delft.

Coordination / Edition / Design and layout

- Inês Crespo, NMI3 and MLZ, Technical University of Munich, Germany
- Ramona Bucher, JCNS at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany

Contact

European Neutron Scattering Association
<http://www.neutrons-ensa.eu/>

The elaboration of this brochure has been made possible thanks to funding from the European Union's 7th Framework Programme for research, technological development and demonstration under the NMI3-II Grant number 283883.

First edition: 2015
Second edition: 2017

Editorial

The European Neutron User Community, both academic and industrial, is large, accomplished and self-renewing, producing 50% of neutron scattering publications world-wide. Users are scientists from disciplines like physics, chemistry, biology, geology, medicine, archaeology, material science and engineering. The science they develop and the questions addressed span all societal challenges, promoting innovation and curiosity thanks to the extraordinary properties of the neutron.

These researchers have access to a vibrant ecosystem of world leading facilities, national and international and small, medium or large in size. Performance and value-for-money is achieved by supporting the facilities that co-operatively allow each to exploit their particular strengths, in particular via European Union programs. Scientists are currently preparing themselves to exploit the most intense neutron source in the world, the European Spallation Source, ESS, that started construction last year. However, the scientific success and return-on-investment of ESS is seriously threatened by an imminent reduction of 25 to 50% in capacity in the provision of neutrons in Europe in the next 15 years. It is therefore timely for the European Neutron Scattering Association to highlight the power of neutrons in the context of the impending threats and opportunities.

This brochure highlights some typical work from the academic and industrial user communities that has been chosen to illustrate the scope and potential of neutrons - it is far from being exhaustive. Dedicated websites of user associations, European projects and facilities can be consulted for more detailed information.



Christiane Alba-Simionesco
Chair of the European Neutron Scattering Association



Imprint	2
Introduction	6
Neutrons: an essential tool for science and technology	8
Europe leads neutron science	10
Neutron scattering centres in Europe	12
Addressing society's grand challenges	14

Energy	16
--------	----

Industry & Materials	18
----------------------	----

Health & Life	20
---------------	----

Environment	22
-------------	----

Arts & Cultural Heritage	24
--------------------------	----

Neutrons in the universe	26
--------------------------	----

Further Information	28
ENSA	29

Introduction

A bit of history

The neutron was discovered in 1932 by Chadwick (Nobel Prize). The use of neutrons to probe and understand matter and assess scientific theories was developed through the second half of the 20th century and neutrons have become a major analytical tool in the scientist's toolbox. Neutrons underpin spectacular advances in materials that are at the heart of new technologies in modern society.

The strength of neutron scattering resides in its simplicity

Neutrons do not possess an electric charge, they are neutral. They behave either as particles, waves or as microscopic magnetic dipoles. Using neutron beams with wavelengths corresponding to typical atomic distances (around 0.2 nm), they have energies equivalent to the temperature of the sample and are ideally suited to observe structures of materials and atomic movements. With their inherent magnet moment, they probe simultaneously the structure and dynamics of magnetism. The use of neutrons becomes more and more multi- and inter-disciplinary with complementary probes like the one provided by synchrotrons, NMR and numerical simulations. The diversity of the communities that use neutrons makes the centralization of scientific priorities impossible in the way that CERN does for the particle-physics community.

Facilities and the European Community

For neutrons there is no 'local laboratory'. You cannot prepare or carry out initial experiments at your home laboratory as can be done for photon-based techniques (X-rays, NMR, IR, Raman, etc). Training and expertise building in neutron techniques is gained at central facilities. Neutron users are totally dependent on access to the facilities for both capacity (*i.e.* availability of time to carry out research or training) as well as capability (*i.e.* availability of equipment with particular technical performance). The size of the user community is naturally limited by the number of facilities, the number of instruments and the operating schedules.

A high level of integration between facilities and the user community has been achieved through a series of European-funded projects, supporting dissemination, training and outreach as well as initiatives to harmonise the access to and use of facilities. In addition, a major, vital component of these projects has been trans-national access (TNA) which enables beam-time use for scientists outside their home nations and is of particular benefit to the majority of countries without neutron sources. An open access *modus operandi* of the facilities has thus emerged for all European scientists.

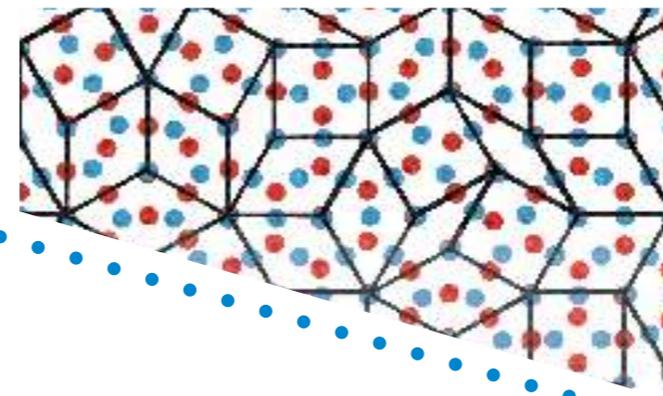
The future – threats and opportunities

Today Big Science serves materials science, life science, information science, and the overarching aim of promoting innovation for economic growth. Currently, small, medium and large scale neutron facilities collectively provide the experimental resources to underpin the work performed by researchers and engineers. Accordingly, the publication record is impressive – 1900 peer-reviewed articles per year. In the mid 2020's the European landscape will be completed by the most powerful neutron source in the world, the European Spallation Source, ESS in Sweden.

At a European Union level, a new project, SINE2020, has been funded for four years starting October 2015. One of two major goals of SINE2020 is to prepare for first neutrons at ESS, through its integration in the European ecosystem of facilities and the development of techniques specific to unprecedentedly high fluxes. A focus on data and industry users is designed to increase the innovation potential of neutrons – the second major goal of SINE2020. Europe, today, is in an apparently enviable position and the future for researchers should therefore be bright.

However first, discontinuous funding of the EU threatens the model of open access to facilities and mobility of scientists within Europe. It is crucial to maintain open access to sources for all European scientists in order to enable them to address the grand challenges of our society.

Secondly, several national facilities will close by 2020, long before the full operation of ESS: the overall capacity for neutrons in Europe will be greatly reduced. ESS will only cover at best 20% of all the needs, *i.e.*, focussing on advanced experimental capabilities, vital training resources, and important technical developments. Consequently, design studies for new, cost effective and energy efficient, accelerator-based sources must be initiated now in order to rejuvenate the ecosystem of European facilities by 2025. In this context, European scientists, their user associations and the facilities will combine forces to submit a new European proposal in 2016 that will focus on open access and address the future neutron landscape in Europe.



Neutrons: an essential tool for science and technology

Producing Neutron beams

Together with protons, neutrons form the nucleus of most atoms. Neutrons are therefore part of all the matter that surrounds us. To be used as a scientific probe and produce a beam they have to be released from the nucleus by a process called fission, as happens in a nuclear reactor using Uranium or by firing a high-energy beam of protons into a neutron-rich element such as lead or tungsten – a process called spallation.



Neutron scattering

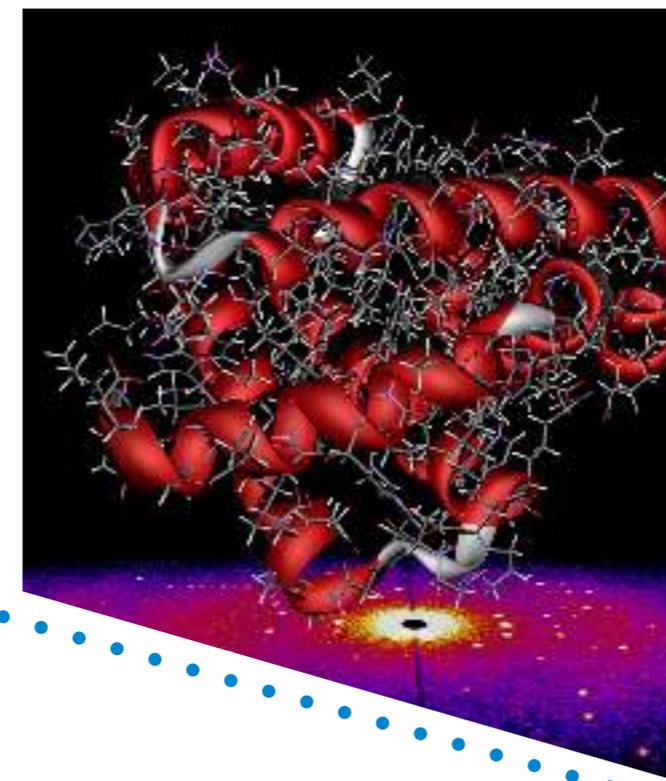
Neutrons as free particles have properties that make them particularly useful to look inside a wide variety of materials. In a neutron scattering experiment, a neutron beam passes through the sample or technical component under investigation. By observing how the direction or velocity of the neutron changes, researchers learn about the structure, composition or dynamics of the sample on an atomic scale. Having this basic information we can understand the physical, chemical or biological properties of a material.

The uniqueness of neutrons for research

Neutrons do not possess any electric charge, they are neutral. They behave either as particles, waves or as microscopic magnetic dipoles. Using neutron beams with wavelength corresponding to typical atomic distances (around 0.2 nm) they have energies equivalent to the temperature of the sample and are therefore ideally suited to observe atomic movements as well as to investigate atomic structures. By their inherent magnetic moment they probe at the same time the dynamic and structure of magnetism.

Looking into materials

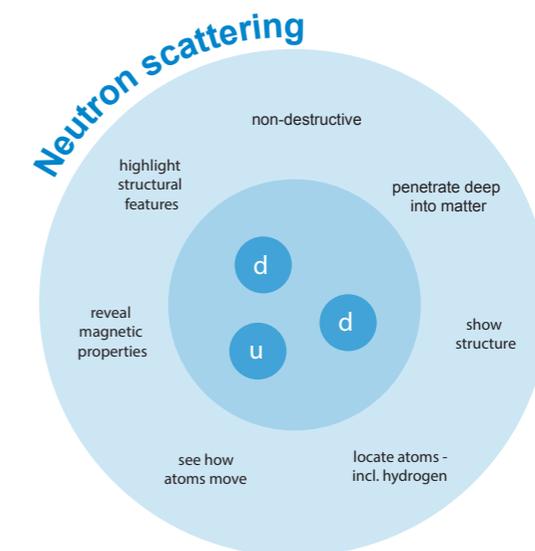
As neutral particles neutrons do not interact with the electrons of an atom, only with the nucleus. This enables them to penetrate material deeply and thus look into large technical objects. Furthermore neutrons can distinguish between different isotopes of the same chemical element. This leads to unique contrast for different materials in complex environments. For example, hydrogen containing rubber gaskets are visible even inside a big car engine or the exchange of hydrogen by the chemical equivalent deuterium can be used to label different sections in very complex biological macromolecules.



Investigating Neutrons

Bound to the nucleus, the neutron lives forever. As a free particle, however, it decays within about 15 min to a proton, an electron and an anti-neutrino. By investigating this decay in detail, especially the life time of the neutron, fundamental interactions can be studied which are relevant to the origin of our universe.

Besides the experimental activities mentioned above, neutrons are also used for (radio) isotope provision, irradiation (e.g. silicon), activation analysis and medicine.



Europe leads neutron science

Broad user base

A major challenge for neutron-based techniques is that neutron beams are only available in central research facilities. An ecosystem of sources sustains the vibrant, European neutron scattering community – the largest in the world.

Even though counting neutron users across Europe is a difficult task¹, today nearly 8000 researchers who use neutron centres for their scientific work could be identified. They rely on the open access and user programs at nine neutron sources across Europe and additionally eight smaller sources for specific applications. To a smaller extent neutron sources from abroad in America, Japan, Australia and Russia are used by European researchers.



Increasing demand of beam time

At the major neutron centres in Europe the demand for access in number of beam days exceeds the available amount by a factor of two. At all European centres substantial efforts are made in order to increase the performance and productivity of the neutron scattering instruments in order to react on the increasing demand of neutron research. European neutron centres currently provide a total of 32.000 beam days per year of open access to the scientific community.

Diversity strengthens success

For the European Research Area in the field of neutron scattering, the diversity of the neutron sources is crucial. 1900 peer reviewed publications each year underline the leading role of European scientists in the area of neutron research. This strength will be maintained by the new flagship neutron source ESS in Sweden. It will open up neutron science to new fields, which require even higher neutron fluxes and enable experiments that are not feasible today.

¹Data based on users registered at neutron sources (Pandata.eu)

²NMI3: Integrated Infrastructure Initiative of Neutron Scattering and Muon Spectroscopy

High mobility of researchers

Neutron sources are big research infrastructures. Scientists have to travel to find the best facility and instrument to address their particular scientific questions. Mobility and provision of access to sources in foreign countries is supported by infrastructure programs of the European Union like NMI3². During the last years around 600 scientists per year from all of the 27 European countries have been supported.

Sustainable future

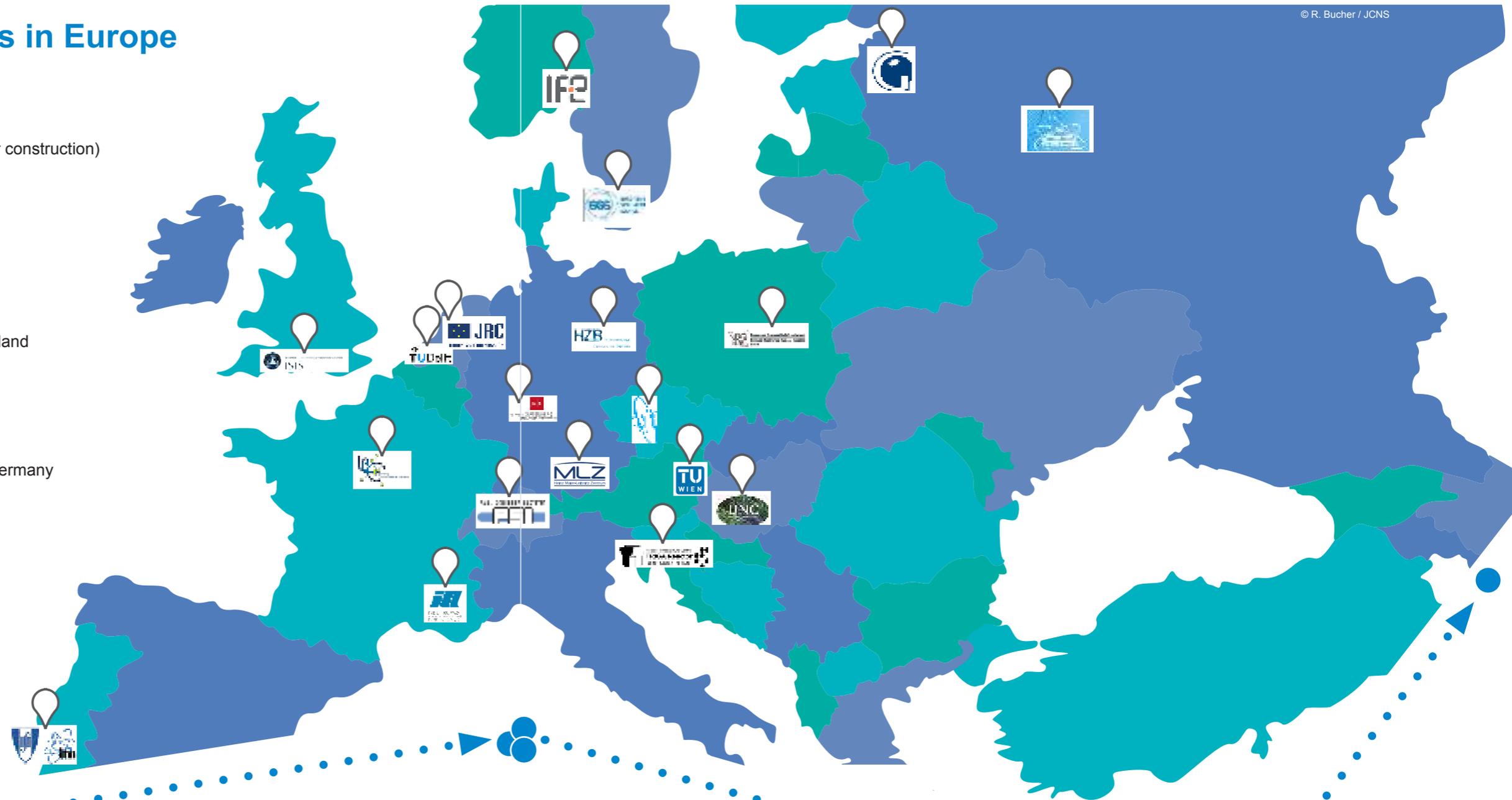
In order to exploit the full potential of neutron methods, specialised knowledge and training is mandatory. In collaboration with a number of universities nearly all neutron centres offer training courses and schools on the theory of neutron scattering, as well as hands on training at the facilities. European funding in the framework of the Integrated Infrastructure Initiative, NMI3, has stimulated exchange and coherence between these schools, grouping them in the NaMES programme (Neutron and Muon European Schools) of NMI3. As MOOCs become part of modern education, NMI3 is supporting the development of e-learning courses, which will be crucial to spreading education and training for neutrons.

- 8000 users
- 19 neutron sources in Europe
- 32.000 instrument beam days per year
- 1900 publications each year
- Collaboration and Flow
- New users welcome
- Supporting industry



Neutron scattering centres in Europe

- Budapest Neutron Centre (BNC), Hungary
- Demokritos, Greece (under extended shutdown)
- European Spallation Source (ESS), Sweden (under construction)
- Frank Laboratory of Neutron Physics, Russia
- Heinz Maier-Leibnitz Zentrum (MLZ), Germany
- Helmholtz-Zentrum Berlin, Germany
- Institute for Energy Technology, Norway
- Institut Laue-Langevin, France
- ISIS Pulsed Neutron Source, UK
- Joint Research Centre, Netherlands
- Laboratoire Léon Brillouin, France
- National Centre for Nuclear Research (MARIA), Poland
- Nuclear Physics Institute (NPI), Czech Republic
- Petersburg Nuclear Physics Institute, Russia
- Portuguese Research Reactor (RPI), Portugal
- Reactor Institute Delft – TU Delft, Netherlands
- SINQ – Paul Scherrer Institute, Switzerland
- TRIGA Facility, Johannes Gutenberg-Uni. Mainz, Germany
- TRIGA Mark II Reactor – TU Vienna, Austria
- TRIGA Reactor Infrastructure Centre, Slovenia



© R. Bucher / JCNS

Addressing society's grand challenges

Neutron scattering provides unique information, essential to solve the grand challenges of our society. The technique is used by researchers from a range of scientific fields and impacts on the efficient use of energy, the environment, pharmaceuticals and health care, computers, heritage, and innovation.

This section is a sample of the significant impact of neutron scattering in our society. We focus on five of the many grand challenges neutrons are helping to move forward.

Energy (page 16)

Energy storage, transport, conversion all benefit from neutron research. The investigation of properties of new energy storage materials rely heavily on neutron scattering. Suitable storage materials are analysed in operando using neutrons, for instance for transportation. Neutron scattering can help improve lithium batteries. The development of superconductors for energy transport relies on information from neutron scattering. In photovoltaics and solar energy research, neutrons are used to study the performance of solar cells.

Industry & Materials (page 18)

Neutrons contribute to the progress of industry in their materials development at all levels ranging from the atomic scale through to the visualisation of complete engines. The breath of applications of neutrons to industry can therefore also be found over the whole 10 orders of magnitude of material science length scales. On page 18/19 we highlight how the fundamental understanding of atomic magnetism helps to create the efficient refrigeration of the future and how sub-micrometer scale emulsions make efficient oil recovery possible. Foams are studied by industry for food and health care, covering foam structure from the sub-micron to millimeter scale, while with neutron imaging the cooling channels inside airplane turbine blades can be visualized, non-invasively.

Health & Life (page 20)

Research is fundamental to fight diseases. Neutron scattering provides vital information that cannot be acquired using any other technique. Neutrons provide structural information of relevance to degenerative diseases such as Alzheimer's. Biological function and enzymatic action benefit from critical detail provided by neutrons on hydrogen bonding and hydration. Drug delivery benefits from neutron scattering studies which may result in new therapeutic approaches in the future. Fast neutrons can be used for the treatment of malignant tumours. Neutrons are also used for the production of radionuclides that are used in medical diagnosis and radiotherapy.

Environment (page 22)

Thanks to their tremendous capabilities for analysis, neutrons contribute to the development of clean technologies. Neutron scattering helps scientists to fight pollution and develop eco-friendly processes that release fewer contaminants into the environment. Neutrons can provide information about rare elements and serve as a way to detect contaminants. Neutron techniques can help define the intrinsic nature of pollutants and its relationship with the substance they are polluting. Neutrons give insight into the role of clouds in global warming and play a role in the battle to curb carbon emissions.

Arts & Cultural Heritage (page 24)

Neutrons are an invaluable tool to analyse precious archaeological objects: they are non-destructive and can penetrate deep into cultural artefacts or beneath the surface of paintings, to reveal structures at the microscopic scale, chemical composition or provide 3D images of the inner parts of the artefacts. For heritage science purposes, whole artefacts can be placed in the neutron beam and analysed at room conditions, without sample preparation. Analysis can also be done under vacuum or other conditions, such as high or low temperature. The measurements are made in real time, which can be useful for testing conservation materials and methods.

Neutrons in the universe (page 26)

There are questions that have always puzzled mankind. Where do we come from? Where are we going? How did it all begin? Is there a primal force that is the cause of it all? And always the Faustian demand to detect the inmost force which binds the world. The goal is to get insight into the answers to fundamental questions and put to experimental test. Modern examples for neutron physics are: Why is the Universe made of matter rather than antimatter? Why was so much matter (the milky way, for instance) and so little antimatter left over after the big bang? Are there extra dimensions of space-time? Was nature left-handed from the beginning? Have the natural constants always been the same? Does antimatter follow exactly the same laws as matter? These are the questions pursued by the Neutron groups at different universities and research centres. All these questions are not invented ad hoc, but are essential for reaching a self-consistent description of nature.

Energy

New form of ice could help explore alternatives for energy production and storage

The discovery of a new form of ice could help understand Earth's geology, potentially helping to unlock new solutions in the production, transportation and storage of energy. Ice XVI, the least dense of all known forms of ice, has a highly symmetric cage-like structure that can trap gaseous molecules to form compounds known as clathrates or gas hydrates. Such clathrates are now known to store enormous quantities of methane and other gases in the permafrost as well as at the bottom of the oceans. To create the sample of Ice XVI, the researchers constructed a clathrate filled with molecules of neon gas, which they then removed by careful pumping at low temperatures. Images obtained by neutron diffraction allowed them to confirm when the clathrate was fully empty, and provided a complete picture of the resulting structure. Such research could help ease the flow of gas and oil through pipelines in low temperature environments. These conditions can lead to the production of gas hydrates within the pipes, which in turn form substantial blockages, the prevention of which costs industry approximately \$500 million a year worldwide.

User: W. F. Kuhs, Uni. Göttingen, Germany



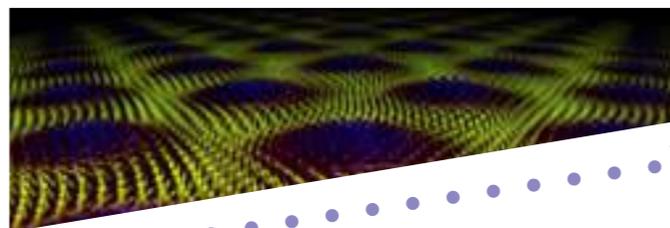
Energy consumption by computers could be drastically reduced by using skyrmions

A team of physicists from the Technical University of Munich and the University of Cologne discovered a physical phenomenon that could make computers use 100,000 times less current than existing technologies, and the number of atoms needed for a data bit could be significantly reduced. Using neutrons, they initially discovered an entirely new magnetic structure in a crystal of manganese silicon – a grid of magnetic vortices, so-called skyrmions. They were later able to prove that even the tiniest of currents is sufficient to move the magnetic vortices. Now the physicists developed a method by which skyrmions can be moved and measured in a purely electronic manner. At present a current is used in the read/write head of a hard drive to generate a magnetic field in order to magnetize a spot on the hard drive and thus write a data bit. Skyrmions, in contrast, can be moved directly and with very small currents. These findings have the potential to make saving data and processing it more compact and energy-efficient.

User: C. Pfleiderer, TUM, Germany

We can take the crystals generated in our laboratory and use neutrons to measure the magnetic structure, its dynamics and many other properties.

C. Pfleiderer, TUM, Germany



A promising alternative for natural gas storage and transportation

Methane hydrates are the Earth's largest natural gas reserve, but they are formed under very specific physical, chemical and geological conditions that can only be found in the bottom of the oceans or in permafrost. Now for the first time, researchers developed a technology to prepare artificial methane hydrates in just a few minutes. The team took advantage of the so-called "confinement" effect to artificially synthesise methane hydrates inside activated coal's pores. They then conducted inelastic neutron scattering (INS) experiments as it is the perfect technique to observe the self-dynamics of molecular hydrogen. Complementary synchrotron experiments were also conducted. While in nature the process to form methane hydrates takes a long time, the team made it in just a few minutes, thus making its technological applicability much easier. These results open a new pathway into the use of e.g. natural gas as fuel for transport, or for long-distance transport of natural gas at temperatures close to room temperature.

User: J. Silvestre-Albero, Uni. Alicante, Spain

These studies are the first evidence that it is possible to form methane hydrates in a smoother and much faster way than it happens in nature.

J. Silvestre-Albero, Uni. Alicante, Spain



Investigating a new material for rechargeable lithium batteries

A group of scientists discovered an interesting material that can be used for rechargeable lithium batteries. Analysis of data from neutron powder diffraction and synchrotron, combined with IR spectroscopy provided a precise determination of the crystal structure of the protonated hexatitanate $H_2Ti_6O_{13}$. The reversible capacity of this material is well maintained upon cycling, even at increasing discharge rates. Furthermore, this reversible capacity is similar to that obtained for other titanium oxides already proposed as anode material for lithium rechargeable batteries. Once its electrochemical performance is optimised $H_2Ti_6O_{13}$ can thus be used for batteries. The results obtained represent a significant step forward, furthering our understanding of the electrochemical behaviour of these materials and confirming their potential in the future development of rechargeable lithium batteries.

User: J. C. Pérez-Flores, Uni. San Pablo CEU, Spain

Neutron diffraction is indispensable for deeper investigations, as both Li and H atoms can be readily located within the structure using subtle intensity changes in the neutron diffraction patterns.

J. C. Pérez-Flores, Uni. San Pablo, Spain

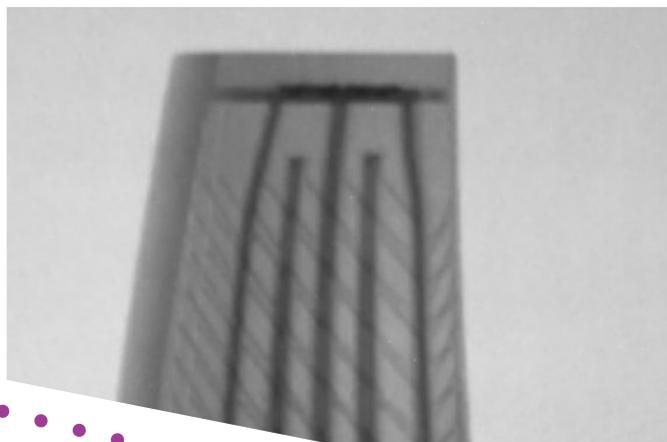


Industry & Materials

Neutron imaging on aircraft turbine blades

The turbine blades in jet engines operate at high pressures and temperatures and therefore each turbine blade needs to be carefully cooled. Modern turbine blades are hollow and are cooled by air flow from the inside, so the turbine itself can be fired above the melting temperature of the metal alloy of the turbine blades. The cooling air enters through the foot and escapes through tiny bores at the front and back of the blade. These holes are drilled with a laser, which must not touch the back side of the cavity in the blade. Therefore, turbine blades are filled with a dark wax before the laser drilling. The turbine alloy is semi transparent for neutrons, while the wax can be easily visualized, making neutrons the only non-invasive method to study the wax filling. Neutron radiography examination helped to fine-tune the temperature of the filling process so the wax reaches all parts of the cooling channels without forming bubbles. This example from the test series indeed shows a few remaining air bubbles in the blade.

Users: MTU Aero Engines AG, Germany



Oil emulsions

Only around 30% of the oil in typical fields flows easily up in wells. The rest of the oil is often trapped in micron diameter sized pores and is considered to be too difficult to recover. As the global demand for oil grows, the industry is developing new techniques to extract more of the remaining oil. Injecting water and surfactants is one way to increase the oil recovery. The oil will form microemulsions with the water and surfactants, which has a higher viscosity. With spin echo small angle measurement we have determined the structure and size of the microemulsion of crude oils with surfactants and water. The characteristic sizes are only an order of magnitude smaller than the pores, so the microstructure is of importance to the flow properties of the recovered oil-water mixture.

User: X. Li, Shell Global Solutions Int. BV, Netherlands



Magneto caloric materials for energy efficient heat pumps

Domestic refrigeration and air-conditioning contributes to more than 20% of the electricity bill of an US household. The majority of cooling devices nowadays utilizes the vapour refrigeration cycle and required refrigerant gases are the fastest growing source of greenhouse gas emissions. A similar but more energy efficient refrigeration cycle can be achieved with magnetic materials that show a large magneto-caloric effect. These materials heat up when a magnetic field is applied. After this heat is transferred to the environment, they cool down on removing the magnetic field and can take up heat from the substance that needs to be cooled. The processes as described are highly reversible and therefore very energy efficient, which can lead to a much lower utilities bill. Unlike the conventional compressor technology currently used for refrigerators, regenerators with magneto-caloric materials work without gaseous coolants. These magnetic materials are solids that can easily be recycled. Thus, this solid state technology has the potential to reduce the environmental impact of cooling technology. The commercial viability of magnetic cooling at and around room temperature requires an understanding of the structure and magnetism of the magneto-caloric materials down to an atomic length scale. Neutron diffraction is the unique tool to investigate the interplay between structure and magnetism at this atomic level, leading to better understanding the magnetic, and thus cooling, properties of this next generation of heat pumps.

User: L. Zhang, BASF, Netherlands



Foam lasting forever...or that collapse at will!

New soap foam, produced by "green chemistry" from a natural substance, is stable for several months even at 60°C. Moreover the foam can be destroyed quickly by a simple change of temperature. Foams act like a detergent thanks to specific surface properties of their molecules, so-called surfactants. By using neutron scattering, researchers observed and depicted the behaviour of a peculiar surfactant molecule, the 12-hydroxy stearic fatty acid extracted from castor oil. After adding a salt to make it soluble this surfactant has very advantageous properties: even in small amounts, it produces abundant foam which is stable for more than 6 months (usual it lasts only a few hours). The team showed that this process is reversible. Increasing the temperature of foam decreases its volume, and decreasing the temperature back to below 60°C stabilizes the foam again. The formation of stable foam with such a simple surfactant is a premiere. Thanks to their properties, foams have many applications in areas such as cleaning, decontamination, cosmetics, fight against pollution and fires, food, or extraction of natural resources.

User: A-L Fameau, L'Oréal Group, France



Health & Life

Neutrons make pregnancy tests more sensitive and cheaper

Scientists found how to make pregnancy tests more sensitive and cheaper. Thanks to neutron reflectometry (NR) experiments, they could investigate the interaction between antibody and antigens and the importance of a blocking protein, present in home pregnancy tests. NR is one of the few techniques that can accurately determine the surface coverage, density and thickness of adsorbed antibodies. The group used deuterated HSA which made it possible to better visualise how blocking proteins behaved. They observed that to achieve the required conditions for an effective pregnancy test, it is necessary to control the structural orientations of the antibodies immobilised. They also found that it is not worth to increase the quantity of antibodies above a certain level for an optimal performance. Thus, neutron studies can help not only to control the quality but also reduce cost considerably, as antibodies are very expensive.

User: J.R. Lu, University of Manchester, UK

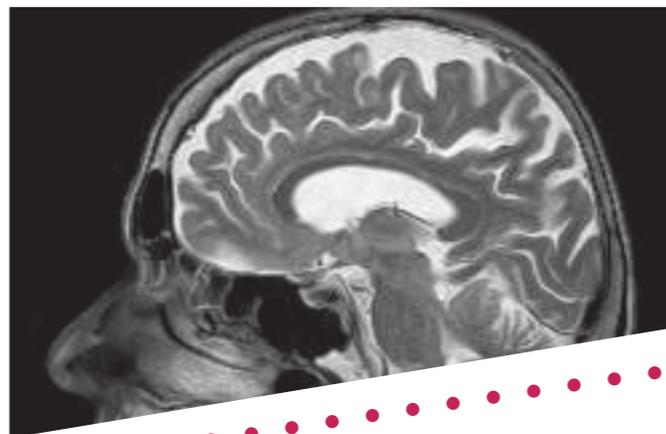


© Ceridwen, Wikimedia Commons

Towards a new tumour-specific contrast agent for MRI applications

Neutrons help in the search of diagnostic and therapeutic devices for cancer. Scientists investigated supramolecular aggregates formed by peptides as well as a new set of Gadolinium-based contrast agents for Magnetic Resonance Imaging (MRI), namely a non-invasive medical diagnostic procedure capable of giving high-quality images of the inside of the human body. Supramolecular aggregates allow cancer detection at early stages, through the recognition by the peptide that leads to a selective accumulation in some cancer tissues. Small-angle neutron scattering (SANS) and other techniques were used to characterise the devices. Results showed the ability of the aggregates to recognise specific cells that overexpress cholecystokinin receptors and behave differently depending on the pH. These receptors are overexpressed in certain human tumours. This scenario opens new opportunities for the development of diagnostic and/or therapeutic systems for the treatment of cancer pathologies.

User: L. Paduano, University of Naples Federico II, Italy

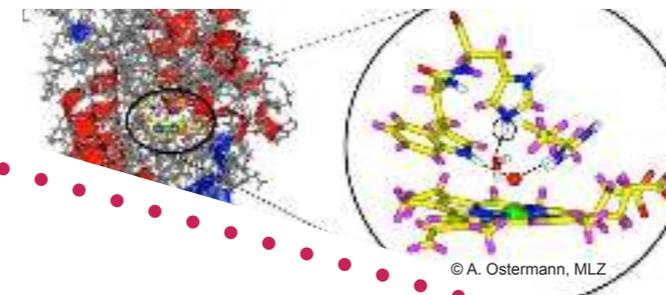


Neutron crystallography solves long-standing biological mystery

Researchers have solved a long-standing mystery in biology by identifying the structure of a vital enzyme intermediate. A family of enzymes, cytochrome c peroxidase (CcP), have a heme group in their active site with an iron atom, which becomes oxidised when a reacting heme is in an intermediate state called Compound I. One of the main, long-standing questions to unveil is whether the iron-bonded oxygen atom carries a hydrogen atom or not. Resolving this fundamental question has implications for understanding oxidative processes within living cells, which is critically important for drug development. They have used neutron protein crystallography, which is a unique technique to locate the positions of the hydrogen atoms. The answer turns out to be that the ferryl heme in Compound I is not protonated. But, unexpectedly, the results showed that one of the amino acid side chains on the molecule is doubly protonated, which raises questions of its own in terms of mechanisms for oxygen activation in heme enzymes.

Users: E. Raven and P. Moody, Uni. Leicester, UK

The ability to capture intermediates at cryogenic temperatures combined with the information available from neutron crystallography, means that we can finally see them.
P. Moody, Uni. Leicester, UK



© A. Ostermann, MLZ

Will we have stronger, enduring teeth? New material for tooth fillings is being investigated

Dental fillings are normally used to restore teeth, for instance after cavity formation. However the materials currently in use have a number of caveats. Scientists are testing glass ionomer as an alternative for dental fillings. They have the advantages of not requiring an adhesive as current fillings do, they release fluoride which makes teeth healthier, and have good biological properties. Furthermore their preparation requires no special equipment or illumination, which is a big advantage in remote areas without electricity. The team used neutron scattering to better see the hydrogen atoms in two different cements. X-ray experiments were also conducted. The results suggest that the strongest material that could be used is cement powder mixed with a polyacid. The liquid binds quickly to the cement, preventing free liquid to fill the pores. In fact glass ionomer cements could be stronger if we could control how the hydrogen atoms move within the material. By knowing this, the researchers can now infer on the material's durability and investigate further.

User: H. Bordallo, Uni. Copenhagen, Denmark



© Uni. Copenhagen

Environment

Healthy diet? Using neutrons to quantify selenium in cereal crops

Selenium (Se) is an essential micronutrient for human health, protecting, for example, against cardiovascular disease, asthma, male sterility and certain forms of cancer. Even though it is a common nutrient e.g. in cereals, it is lacking in the diet of at least 1 billion people around the globe. The few available data indicate that Portugal is one of the countries concerned. For this reason, a research project taking place in Portugal aims to assess the levels of Se in the country's cereals and soils. Samples were analysed in a slightly modified radiochemical neutron activation analysis (RNAA). This technique makes it possible to detect Se even when its concentration is very low. The results obtained give important insights into Se levels in Portuguese cereals, opening the way to future supplementation trials in the country, as already done in other countries.

User: M. C. Freitas, Inst. Tecnológico e Nuclear, Portugal



Where and how do plant roots take up water?

Have you ever eaten lupins? They are a common snack in Mediterranean countries. Scientists from the Georg August University of Göttingen in Germany have investigated where and how the roots of these plants take water from the soil. By using neutron radiography, they could trace the transport of deuterated water (D_2O) in the roots of the plants, which were grown in aluminium containers filled with sandy soil. The transport of water into the roots was then quantified using a convection–diffusion model of D_2O transport into roots. The results showed that water uptake was not uniform along the roots. The roots, mainly the lateral ones, took more water from the upper soil layers than from the lower ones. The function of the taproot (the plant main root) was to collect water from laterals and transport it to the shoot. According to the authors, lupin root architecture is well designed to take up water from deep soil layers.

User: M. Zarebanadkouki, Georg August Uni. Göttingen, Germany



From ash to eco-friendly solution for hazardous metals removal

The world's power plants produce about 600 million tones of coal ash every year that might damage the environment. A new method can turn those ashes into an eco-friendly solution. Ashes are chemically similar to volcanic precursors of natural zeolites, which are typical adsorbents in separation and refinery facilities. Through a simple, low-cost method scientists were successful to produce adsorbents from ash taken from a power plant. They modified the ash by hydrothermal treatment and ultrasonic activation in an alkaline medium. They conducted instrumental neutron activation analysis (INAA) experiments to characterise the materials. The results show that the new materials have enhanced properties with regards to the original ash and proved very efficient in removing hazardous metals from aqueous media. This method could be a cheaper alternative e.g. for nuclear waste treatment or soil remediation.

User: F. Noli, Aristotle University, Greece

The possibility to send samples to measure at the neutron sources give our students and new researchers the opportunity to complete the diploma and contribute to the research community.

Fotini Noli, Aristotle University, Greece



The cork viewed from the inside

Cork is the natural material stripped from the outer bark of cork oak. It was one of the first materials put under the microscope. The first depiction dates back to the years 1660, when Robert Hooke drew the scheme of its very characteristic cellular organization, giving the term cell to the basic biological unit. It is still the most used stopper to seal wine bottles and to preserve wine during storage. Cork stoppers are sorted in different classes according to apparent defects, named lenticels, which can be related to the cork macroporosity. The more lenticels there are, the worst the cork quality is. Neutron imaging combined with digital photography can investigate the defects of cork stoppers from two classes. Comparing the two qualities of stoppers, photography analysis and neutron tomography permit to differentiate these classes: around 4.1% and 5.9% of defects for class 0 stoppers, and 6.7% and 7.5% for class 4 stoppers, respectively. The next step to this work will consist in bridging the gap between structure investigated by imaging and functional properties of cork.

User: Régis Gougeon, Pôle Bourgogne Vigne et Vin, France

The unprecedented results obtained on the inner structure of cork stoppers clearly highlight the major inputs of neutron techniques for a deeper understanding of the bio-chemical processes involved in food and wine science.

Régis Gougeon, Pôle Bourgogne Vigne et Vin, France

Arts & Cultural Heritage

Remediation tools for conservation of artworks

In the past, synthetic polymers have been improperly applied as protective coatings to painted surfaces. Instead of preserving the paintings, these substances promoted a series of complex degradation mechanisms. The removal of these polymer films is one of the top priorities in conservation science. In order to design efficient nanofluids for cleaning artworks, it is necessary to understand their ability to remove given polymer films by determining both their structure and dynamics. Small Angle Neutron Scattering (SANS) is particularly suited for characterising complex nanofluids. SANS measurements were performed to investigate how two different nanofluids interact with the polymer to detach it from artworks. The results enabled to define a model for the interaction. A deeper understanding of the nano-structure and the mechanism that lies behind the cleaning process is the key of a more conscious approach to new conservation challenges.

User: P. Baglioni, Uni. Florence, Italy



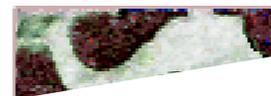
Neutron tomography of ancient lead artefacts

Ancient Roman lead ingots rescued from shipwrecks along the coast of Sicily in Italy were analysed by Neutron Tomography (NT). The artefacts date back to a period between the 3rd and 1st century BC. Neutron imaging is very well suited for investigation of samples of cultural heritage due to the high penetration depth of neutron radiation. Although the artefacts were heavily damaged the NT experiment showed, after a digital 3D reconstruction, the original mold marks and helped decipher hidden signs. The scientists could thus read the inscriptions on the ingots that feature name and surname of both the producer of the ingots as well as who they think is the mine owner from Carthago Nova in Spain, which dates back to the 1st century BC, when the Planius family (as the inscription suggests) was active in lead ingot trading.

User: F.L. Celso, Uni. Palermo, Italy

Neutron tomography seems to be the most successful method for non-destructive study of the inner structure of bulky archeological lead samples.

F.L. Celso, Uni. Palermo, Italy



Egyptian statuettes of Osiris: production unveiled by neutrons and laser

The world's museums exhibit ancient artefacts whose creation not much is known about. In the search for non-invasive methods, scientists have combined neutron tomography, time of flight neutron diffraction, and laser induced plasma spectroscopy to analyse copper alloy figurines, provided by the Egyptian Museum of Florence. They represent Osiris, the god of the afterlife, the underworld and the dead, with arms and legs bound to the body by mummy bandages, and holding the traditional insignias of kingship. The team discovered that even though the figurines come from different areas in Egypt, they were all crafted with similar core materials, same alloy compositions, and with a similar method for preparation of the casting mould. The statuettes were constituted by a sandy aggregate in a clayey matrix completely altered by the high firing temperature. The core was cast in a mould, and then coated with wax, which was directly modelled, and eventually covered with an earthy mantle. This innovative analytical approach proved very successful to analyse ancient artefacts and will be applied to other statuettes.

User: J. Agresti, Ist. Fisica Applicata Nello Carrara, CNR, Italy

The usefulness of neutron techniques in archaeometry has been proved through several successful investigations.

JA & SS, IFA "Nello Carrara"-CNR, Italy

Looking millions of years back with neutrons: the hearing of the *Kawingasaurus fossilis*

Let's travel back in time and imagine how life on Earth was before the biggest mass extinction, 252 million years ago. The *K. fossilis* was a small herbivorous living in the Late Permian period. A scientist investigated the mechanisms through which the *K. fossilis* could hear by conducting neutron tomography experiments and 3D visualisation. The results suggest the *K. fossilis* could hear through bone conduction and seismic vibration. It had much bigger inner ears than any other mammal. Even though the *K. fossilis* had only a skull length of circa 40mm, which is less than a third of the human skull, the ear vestibule had a volume about 25 times larger than that of humans. The animal had a fused triangular head with a snout shaped like a spatula, probably used for digging. This feature also enhanced seismic signal detection, which is how a number of animals sense information such as warnings about predators, courtship or group maintenance.

User: M. Laaß, Ruprecht-Karls-Uni. Heidelberg, Germany

Neutron tomography is suited to investigate the skull as neutrons are able to penetrate fossils very well and produce a good contrast between the fossil bones and the matrix.

M. Laaß, R-K-Uni. Heidelberg, Germany



Neutrons in the universe

Particle & Astroparticle Physics

The aim is to address basic open questions in particle and astrophysics. All in all, measurement precision has reached a level, where very fundamental questions of physics and cosmology come into reach for low-energy experimentation, most of which cannot be answered using experiments performed on high-energy accelerators because of their insufficient sensitivity. These include the understanding of natural forces and the associated symmetries as well as studies on gravitation at very small distances. The neutron, a very specific tool, allows the search for new physics becoming manifest itself as small deviations from expectations.

User: L. M. Heil, University of Leicester, UK; G. Konrad, Atominstitut TU Wien, Austria; B. Maerkisch, TU München, Germany



Neutron beta decay

A free neutron is unstable. Observables in neutron decay are the lifetime and correlation measurements between decay particles. These measurements give access to the weak interaction, and today, all semileptonic charged-current weak interaction cross sections needed in cosmology, astrophysics, and particle physics must be calculated from these neutron decay parameters. They enter in the prediction for the energy consumption in the sun via the primary reaction in the pp-chain and the solar neutrino flux, the light elements in the primordial nucleosynthesis, and the neutron star formation. They are also used for the calibration of neutrino detectors, and they serve as inputs for the quark mixing matrix. About a dozen new instruments are planned or are under construction for measurements of the lifetime of the neutron and the correlation coefficients.

User: P. Fierlinger, S. Paul, TU München, Germany

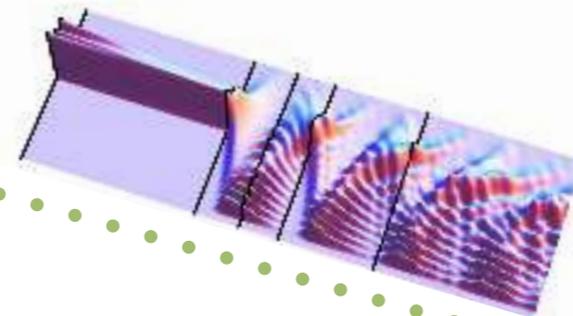


Quantum Physics

Quantum theory is being sensitively probed and developed through studies of single neutrons. From the very beginning, neutron interferometer experiments have been one of the useful tools for the investigation of quantum mechanical phenomena on a very fundamental basis. The dual nature of neutrons – in some respect a particle, in other respect a wave – is manifested by highly non-local effects observed in neutron interferometry. Recent progress has been made in investigating gravitation and related topics by a new quantum interference technique.

Many textbook experiments of quantum physics have been performed with the perfect crystal neutron interferometer where widely separated coherent beams can be produced and manipulated. It has been shown that neutron interferometry is powerful tool for neutron quantum optics experiments. The results contribute substantially to discussion about the foundation of quantum physics. Quantum contextuality and topological quantum effects deserve further investigations. Non-classical quantum states of neutrons can also be used for advanced diffraction work where higher order correlation functions can be measured.

User: Y. Hasegawa, H. Rauch, Atominstitut TU Wien, Austria



Test of Gravitation with Quantum Interference

Galileo Galilei would be somewhat surprised. At least, when neutrons become ultra-cold and fall in the gravity field of the earth. Today his famous fall experiment shows quantum aspects of the subtle gravity force in the sense that neutrons do not fall as larger objects do. Neutrons as quantum particles show characteristic departures from classical behaviour. We find them only on particular energy levels, when they come close to a reflecting neutron mirror, where only small quantum leaps are allowed. This phenomenon, known as quantum bouncer, is neatly explained by a general rule of quantum mechanics in the sense that bound states must have discrete energy levels. A gravitational bound neutron on the mirror corresponds to the electromagnetic bound electron in the hydrogen atom. But with neutrons, the energy levels have values that are smaller by many orders of magnitude compared with an electromagnetically bound electron in a hydrogen atom. Resonant transitions between several of the lowest quantum states have been observed recently. They demonstrate that Newton's inverse square law of gravity is understood at micron distance. A promising interest in such low-energy experimentation with neutrons is the unexplained role of gravity in modern theories and the realization that for basic open questions a deeper understanding of gravitation is needed. Neutrons do now test speculations on large extra dimensions of submillimetre size of space-time or the origin of the cosmological constant in the universe, where effects are predicted in the interesting range of such experiments and might give a signal in future experiments.

User: T. Jenke, Atominstitut TU Wien, Austria; V. V. Nesvizhevsky ILL, Grenoble, France

Further Information

Neutron users associations:

ENSA	www.neutrons-ensa.eu
Austrian Physical Society	www.oepg.at
Czech and Slovak Crystallographic Association	www.xray.cz
Danish Neutron Scattering Society	www.danssk.risoe.dk
French Neutronics Society (SFN)	www.sfn.asso.fr
German Committee Research with Neutrons (KFN)	www.sni-portal.de/kfn
Italian Neutron Spectroscopy Society (SISN)	www.sisn.it
Norwegian Neutron Scattering Association (NoNSA)	www.ife.no/en/ife/departments/physics/projects/nonsa
Spanish Society for Neutron Techniques (SETN)	www.setn.es
Swedish Neutron Scattering Society (SNSS)	snss.se
Swiss Neutron Scattering Society (SGN/SSDN)	sgn.web.psi.ch

Neutron websites:

NMI3	nmi3.eu
Neutronsources	Neutronsources.org
SINE2020	sine2020.eu

ENSA

The European Neutron Scattering Association (ENSA) is an affiliation of national neutron scattering societies and committees, which directly represent users. The overriding purposes of ENSA are to provide a platform for discussion and a focus for action in neutron scattering and related topics in Europe.



The European Neutron Scattering Association

The objectives of ENSA are the following:

- To identify the needs of the neutron scattering community in Europe.
- To optimise the use of present European neutron sources.
- To support long-term planning of future European neutron sources.
- To assist with the co-ordination of the development and construction of instruments for neutron scattering.
- To stimulate and promote neutron scattering activities and training in Europe.
- To support the opportunities for young scientists.
- To promote channels of communication with industry.
- To disseminate to the wider community information which demonstrates the powerful capabilities of neutron scattering techniques and other neutron methods.
- To assist, if appropriate, national affiliated bodies in the pursuit of their own goals.
- Affiliation to ENSA is open to bodies representing neutron scattering users in those countries who are members or associates of the European Union, Switzerland, and Russia.

Breaking news

Portable and stationary energy storage became a topic of increasing relevance - not only due to actual safety aspects. Rapid development of portable electronics, electrification of the drivetrain as well as the necessity to provide energy storage solutions enabling the effective use of renewable energy sources require energy storage devices, which are robust, safe, cheap and possess excellent performance and stability. Among various available technologies, Li-ion electrochemical energy storage offers the best compromise between energy and power densities along with its low cost, high cycling stability and low memory effect. Despite the simple principle of operation based on the separated migration of ions and electrons, modern Li-ion cells are sophisticated devices, where complex interactions between components occur on different scales dependent on internal and external

operating conditions. The fact, that the typical electrochemical cell is a closed/sealed system, calls for the application of characterization methods and tools capable to provide the information of processes occurring inside the Li-ion cell in a non-destructive way.

Due to its unique properties neutron scattering offers unprecedented sensitivity to various cell components, e.g. localization of lithium, oxygen and hydrogen. Neutrons yield contrast for transition metals which supply the charge balance in the battery. Their high penetration capability enables non-destructive probing of standard format commercial cells and batteries on different length scales ranging from sub-nanometers in diffraction experiments, near micrometers in small angle scattering up to millimeters and centimeters for neutron imaging. Complementary use of neutron scattering and electrochemical tools helps to gain deeper understanding of the complex interactions in electrochemical cells.

Figure 1: Neutron radiography of a fresh cell. The filling level of the „electrolyte“ reservoir (showed by arrow) changes upon charge/discharge due to cell „breathing“. By neutron radiography it was found that this stops working due to lack of liquid electrolyte in „fatigued“ cell.

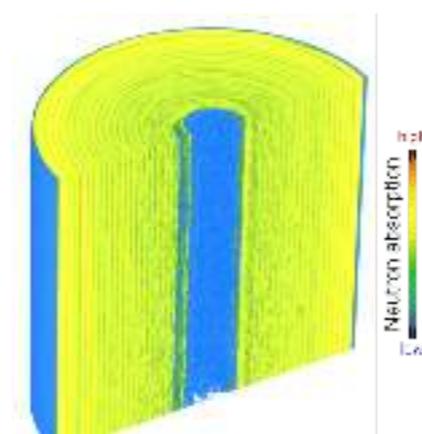
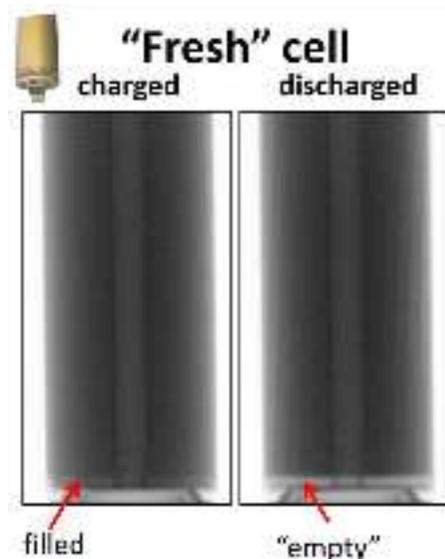


Figure 2: Neutron tomography reconstruction of the interior of cylinder-type Li-ion battery. Absorption levels are visualized by assignment to different colours.

In operando studies of Lithium – ion batteries

Neutron-based diffraction and imaging techniques are already widely utilized for ex situ and in situ experiments on electrochemical energy materials and systems of various kinds. They allow for life-time studies in various modes including changes observed vs. state-of-charge, state-of-health, chemical substitution or temperature. Neutron diffraction delivers details of the crystal structure or morphology of scattering domains (microstructure) and phase composition. Neutron imaging provides unique information about lithium distribution, gas formation, electrolyte dynamics in real Li-ion cells etc. Fracturing upon cell fatigue can be probed by small angle neutron scattering. Quasielastic neutron scattering has shown to provide unique information about structure and mobility of liquid electrolytes as well as the characteristics of the lithium transport in membranes and solid state conductors. Neutron reflectometry is highly suitable for studies of solid-electrolyte interphases and lithiation of intercalation kinetics into amorphous silicon, which becomes especially attractive for a new generation of electrochemical energy storage devices - all-solid-state batteries. Lithium concentrations, e.g. in electrode materials, are determined by neutron depth profiling on a nanometer length scale.



Figure 3: Layout of cylinder Li-ion cell of 18650-type showing jellyroll, positive and negative current tabs and centre ping.

There is rapid development in the field of instrument-adapted electrochemical cells, which are tailored with respect to the demands of neutron-based techniques and electrochemical needs. Furthermore, because of the high importance and request, dedicated instruments are available or under construction, e.g. SPICA - a Dedicated Neutron Powder Diffractometer for Battery Studies at J-PARC (Tokai, Japan) or a new powder option ERWIN - Energy Research With Neutrons at MLZ Garching, Germany.

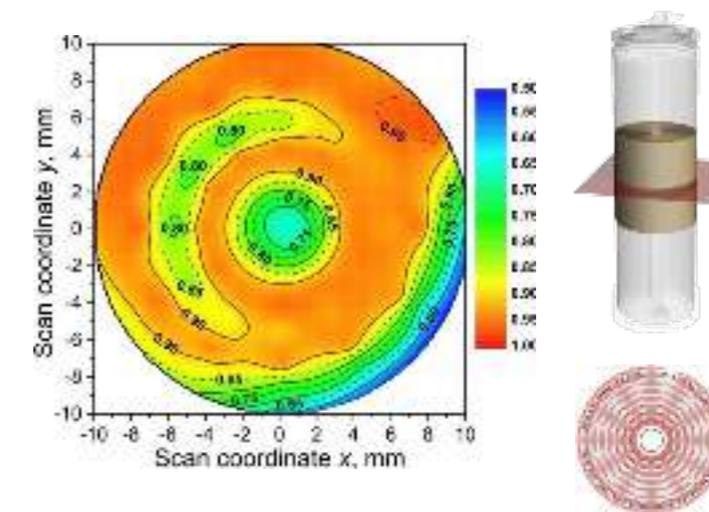


Figure 4: Lithium concentration in the graphite anode of charged Li-ion cell (type 18650) determined using spatially-resolved diffraction of thermal neutrons along the cut described by the right figures. Top: Investigated volume. Bottom: Distribution of gauge volumes.

