Industrial Employment of Neutron Scattering

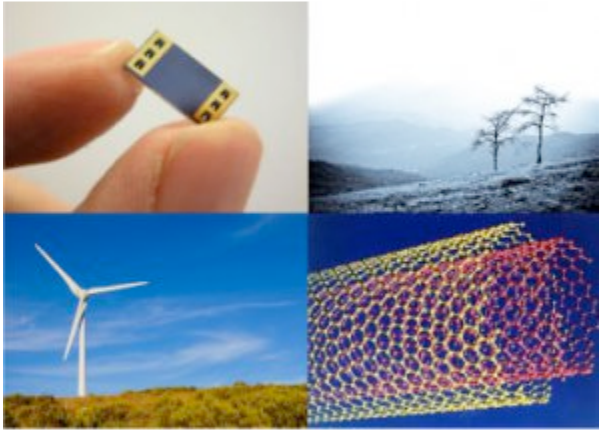
The unique properties of neutron beams increasingly attract the attention of industrial R&D. In traditional industrial sectors such as manufacturing, petrochemical and conventional energy production, neutron scattering techniques have helped develop materials for novel data storage devices and nano-sized additives in the petrochemical and polymer industry. Neutron methods have been used to elucidate the role of surfactants in preventing pipeline clogging by waxes, to enhance the understanding of chemical reactions in catalytic processes, to improve the fatigue life and structural integrity of engineering components, and even to tailor the tastiness of ice cream. More recently in the health and life science sector, neutrons are becoming a tool of choice in the understanding of drug delivery mechanisms and early drug development and characterisation, due to amongst other things their low energy deposition on organic matter, nano-metric resolution, and sensitivity to light elements, see BOX. Neutrons have also played an important role in the growth sectors of renewable energy and clean technology, e.g. fuel cells and the hydrogen economy.

Thus, neutron scattering techniques are employed in industrial R&D where the competitive advantage derives from the know-how that defines the cutting edge of technology in the relentless product development race. Small improvements in the understanding of materials and processes often translate directly into significant cost savings and gains, e.g. by prolonging the lifetime of a catalyst, lowering maintenance costs in power plants, or increasing the optimal performance temperature of turbine materials. To be able to do that in a safe and reliable way, scientists and engineers need detailed and accurate knowledge about the material properties in service. The limits of laboratory-based materials characterisation techniques are frequently at the very transition from laboratory conditions to service conditions.

Computational techniques such as molecular dynamics simulations allow simulation of materials under service conditions, but they require extensive benchmarking and experimental verification. Hence, only by testing materials and processes in real service conditions can one reveal and verify the empirical and analytical development. This is one of the many areas where neutron scattering techniques excel.

Grand challenges of today´s modern societies

Using neutrons to address today´s issues



Today´s societies are faced with serious challenges in myriad areas. To better address these issues, the European Union has grouped them under the label **Grand Challenges of our civilisation**.

Although they haven´t yet been rigorously defined, these overarching 'Grand Challenges' encompass issues that can be addressed by scientific and technological research.

Essentially, they involve the development of new materials with better, or even completely new, functionalities, which could allow to build new technical devices, or improve process technology.

Out of the wide range of applications of neutron and muon research, we have chosen to focus on the following Grand Challenges: Energy, Health and Life Science, Information Technology, Nanoscience and Nanotechnology, Environment and Earth Sciences, Heritage Science

Neutrons and muons are also invaluable tools for blue skies research at the forefront of basic science, enabling the advancement of our knowledge of fundamental principles of condensed matter, well before any technological applications.

Energy

Energy storage, transport, production - neutrons are multi-faceted tools contributing to different areas of energy research

Figure 1 (Right) A mirror consisting of a $Mg_{0.7}Ti_{0.3}$ thin film after applying a hydrogen containing gas, the mirror changes into a light absorbing $Mg_{0.7}Ti_{0.3}H_x$ film.

With the growth of the world population, basic needs such as food, clean water and health care are becoming more and more difficult to meet. Although technological solutions exist for many problems, all of them rely on a continuous supply of energy in the form of electrical power or heat. In view of limited resources of fossil fuel, other high-grade forms of energy, such as electricity will gain more and more importance. However, the production, distribution and storage of electrical power need substantial improvements in order to meet the world´s future needs.

Neutrons and muons probe the atomic structure and are therefore well suited to investigate materials for energy research. Furthermore, neutron can penetrate massive material easily, which allows to study complex components in-situ under technical conditions.

One of the major challenges in energy management is to increase dramatically our capacity to store energy for subsequent use as electric power. Nickel-metal hydride (Ni-MH) and lithium ion materials are replacing less efficient heavy-metal batteries based on toxic cadmium and lead. The properties of these new energy storage materials depend on light-weight atoms such as hydrogen and lithium. These are difficult to see with X-rays, but they scatter neutrons strongly.

Examples in the field of **energy storage** research comprise the use of neutron diffraction to study the phase analysis of anode and cathode materials during charging and discharging of batteries and radiographic imaging of the filling level of batteries. Quasi-elastic neutron scattering can help explain the dynamics of the lithium ions inside such batteries and the thin films and their interfaces inside the batteries are also being investigated with neutron reflectometry.

Hydrogen storage is another important topic to overcome the limitations of energy storage in general. Due to the high sensitivity of neutrons to hydrogen atoms, their transport properties in solid storage materials can be analysed in detail. The filling of hydrogen in real devices under usage conditions reveals the technical details of the charging/discharging process. Suitable storage materials are being been analysed in detail using neutron diffraction, especially for light weight materials as possible hydrogen storing materials for mobile applications.

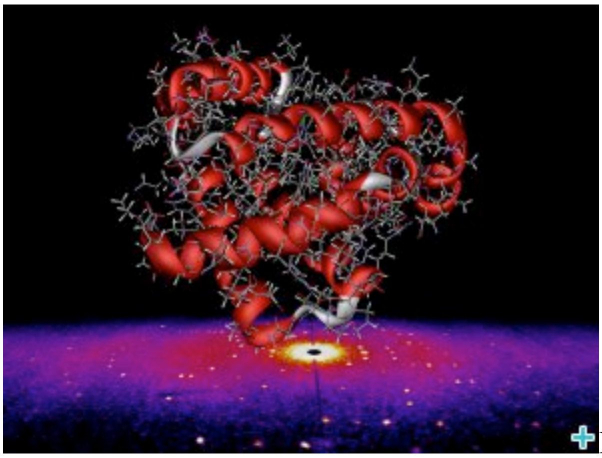
See this scientific highlight about the use of neutrons to study Magnesium-Titanium (Mg-Ti) alloys for hydrogen storage.

In the field of **energy transport**, the development of high temperature superconductors benefits from the basic understanding of material properties achieved by neutron scattering.

In **photovoltaics** and solar energy research, reflectometry is used to study the performance of solar cells.

Health and Life Sciences

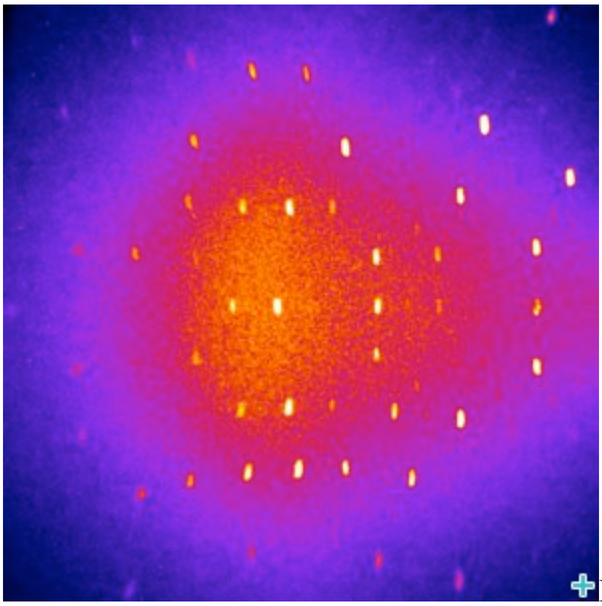
How neutron scattering can contribute to life sciences and health


Myoglobin Artistic representation of the protein myoglobin. The red ribbon model shows the alpha-helices. The floor of the picture is a neutron diffraction pattern of a myoglobin crystal. Author: Andreas Östermann FRM II/TUM

The increase of life expectancy, the growth of the world´s population and the changes in the Earth´s climate mean that we are today faced with major health challenges. In recent years there have been spectacular advances in the understanding of the molecular and cellular basis of disease, thanks to fundamental discoveries in chemistry, physics and biology. Fighting disease doesn´t only involve developing treatment, but also relies on a better understanding of fields such as genetics, environmental factors and nutrition.

Research in diverse areas is being carried out today that may have an impact on the future of the world´s population health: not only biomedicine but also food science, water science, environmental science, materials science and biotechnology. Molecular-level information is crucial in all of these areas. It is becoming increasing obvious that the most effective approaches involve the combined use of a wide range of techniques linking length scales from the atomic/molecular levels to macromolecular levels at which function/properties are manifested. Neutron scattering is an invaluable tool that can make vital contributions through the provision of novel information that cannot be acquired using any other technique.

Neutrons can see the elements and molecules of life in a way that is not possible using X-rays – for example critical detail is provided on hydrogen bonding and hydration, which are aspects of macromolecular systems that are critical to biological function and enzymatic action. This type of information on biological structures and on the pathways associated with protein assembly (or mis-assembly) is critical to understand the molecular and cellular basis of disease. For example, neutron scattering data are providing important structural information of relevance to degenerative diseases such as Alzheimer's disease and other conditions that are associated with the deposition of insoluble fibrils in the body.


Myoglobin diffraction Neutron diffraction pattern of a myoglobin crystal. Picture Andreas Ostermann and Tobias Schrader.

Neutron techniques are also being used to study drug molecules and their interactions with a variety of biological molecules. Such studies are of interest in drug discovery and delivery and may result in new therapeutic approaches in the future. Neutrons are also used for the production of radionuclides that are used in medical diagnosis. There is also increasing interest in the development of approaches whereby neutron beams can be used to target and destroy tumours.

Neutrons are gentle probes and penetrate materials easily without damaging them. They are very precise and extremely sensitive to the detailed structure of synthetic materials. They are powerful tools for the characterisation of new materials – for example recent neutron scattering work is providing data that are of central interest for the development of new biomaterials for dental and bone implants.

Key neutron techniques in this area include Neutron Small Angle Scattering (SANS), which provides information on the dimensions, shapes and morphology of large molecules and macromolecular complexes. Neutron Macromolecular Crystallography (NMX) gives unique structural information at high resolution, inclusive of vital detail relating to hydration and protonation states of key functional areas of proteins. Neutron Reflection (NR) can be used to study interfaces such as surfaces and membranes. Other areas such as inelastic neutron scattering and elastic incoherent neutron scattering can reveal important aspects of molecular motion. Neutron imaging methods are powerful tools for non-invasive in-vivo imaging.

Information and Communication technology (ICT)

Research with neutrons

Our knowledge-based societies are dependent on modern technologies for the storage, exchange and processing of digital information. Advanced technology is needed to meet the ever-growing demand for increasingly fast and small devices such as computers, mobile phones and media players.

Nanotechnology and the field of **spintronics** are greatly contributing to this area, thanks in part to neutron scattering and muon spectroscopy. Spintronics refers to technologies that exploit both the spin of the electron and its charge. Most current devices such as amplifiers only utilise the charge of the electron. The discovery of giant magneto-resistance (GMR) was the first application of spintronics to nanotechnology and resulted in the Nobel prize for Physics in 2007. It has given rise to a new field of research and enabled important advances in wide ranging areas such as hard drive technology, magnetic-field sensors and transistors.

Spintronics is key to the next generation of digital devices.

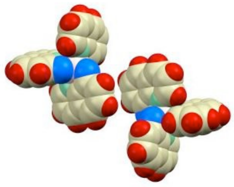
By exploiting both the intrinsic spin of the electron in addition to its charge it will be possible to improve the energy efficiency, speed and memory storage density.

Many materials, which exhibit properties that are beneficial to the design of spintronic devices, are called “smart materials”. A smart material is a material that reacts to an external stimulus, such as stress, temperature, electric or magnetic fields by significantly changing one if its materials properties. For example smart glass can change its degree of transparency with the application of an electric field or magneto-resistive material change their electrical resistance in the presence of a magnetic field would be considered smart materials.

Understanding the internal details of how smart materials work is essential for their technological exploitation and the ability to predict / engineer new smart material behaviors. Characterising the internal details requires a multifaceted probe like those provided by various neutron scattering techniques.

The magnetic properties of materials can be investigated using techniques such as magnetic neutron diffraction and inelastic neutron scattering. Neutron reflectometry and small angle neutron scattering are also powerful tools to identify the structure of organic materials for new electronic devices such as organic light-emitting diodes and electroactive polymers.

Organic spintronics and muons


OLED The propellor-shaped molecules of Alq3, which are used as an active constituent of organic light emitting diode (OLED) displays.

Electronic devices based on organic semiconductors such as Alq3 (tris[8-hydroxy-quinoline] aluminum) are revolutionising display screens and large-area electronics. They are economically favourable, can be easily processed in large areas, their electronic properties are easy to tune, and they are simple to grow into high quality thin films.

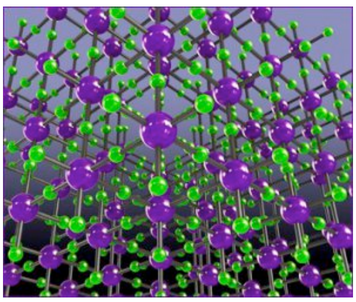
Many aspects of charge transport in organic semiconductors remain poorly understood and making progress in this area is needed to use these materials to their fullest extent.

Implanted muons provide a powerful local probe technique for studying the dynamics of mobile spins.

Muon spin relaxation studies at ISIS have been used to probe the charge carrier motion in Alq3 as a function of temperature. The charge mobilities obtained in this way are significantly larger than those obtained from direct transport measurements in polycrystalline films and thus provide an estimate for the intrinsic upper limit for the mobility that might be achievable in high quality bulk material.

Nanotechnology

Overview



Nanotechnology is the engineering of functional systems at the **molecular, or nano-scale** -from 1 to 100 nm. Novel, high performance composite materials and devices that are organised at the nano-scale are being developed for applications in areas such as healthcare, information processing, energy, and the environment.

Developments in nanotechnology rely on the determination of structures over a wide range of length scales, as well as grasping how the combination of structure and dynamics leads to unique properties.

Both x-rays and neutrons cover all the length scales from the Angstrom scale of the atomic structure of individual building blocks to the configuration of assembled, functional structures, making them essential tools for the elucidation of nanostructures.

Neutrons, however, have some built-in advantages compared to X-rays; namely their spin, mass, and the strong scattering cross section for the hydrogen isotope deuterium.

Neutron techniques

In neutron reflectometry (NR) experiments, the neutron spin is used to study thin films or planar interfaces; such as magnetic effects in ultrathin films used in storage or spintronics applications for example. In these cases, NR can help to determine magnetic moments in monolayers and coupled layers. Due to the high sensitivity towards hydrogen, NR is also employed to study biointerfaces such as lipid bilayers. It can reveal minute structural changes in the lipid bilayer in response to protein binding. These experiments aim to reveal the molecular mechanisms occurring at the nm scale.

An even more ambitious challenge is to understand cellular contacts at nanostructured interfaces, which may allow to improve implant technology for example.

Other applications of neutrons to nanotechnology from the soft matter world include plastic electronics, in particular solar cells and sensors. Here, interface morphology is key for optimising efficiency.

Small angle neutron scattering (SANS), on the other hand, is a non-destructive method ideal for the study of nanoparticles, such metal nanoparticles, or proteins. SANS is used to study polymer chains growing or aggregation on nanoparticles and polymer/nanoparticle interaction, for application in materials science or medicine such as drug delivery or contrast imaging. SANS can also be used to analyse the aggregation of nanoparticles, for example protein aggregation, which is a phenomenon related to neurodegenerative diseases.

NR and SANS have been combined in a technique called grazing incidence SANS or GISANS. Here, structural correlations at interfaces are studied, for example the phase separation of two polymers as in organic solar cells or protein aggregation at membranes.

Environment and Earth Sciences

Overview

The increasing world population density, together with global urbanisation and industrialisation are putting a real strain on the planet and the environment. To keep on growing and prospering, or simply maintain a livable standard of living, countries need to minimise this strain and protect their environment. Neutrons, thanks to their multiple applications and the tremendous capabilities for analysis that they offer, can contribute to the development of clean technologies and processes. They can also provide much needed insight into Earth processes and the properties of rocks and minerals.

Fighting pollution

Neutrons scattering is helping scientists to fight pollution and develop environmentally friendly processes that generate and release fewer contaminants into the environment. Neutron activation analysis and prompt gamma activation analysis can provide information about rare elements and serve as a way to detect contaminants. Neutron reflectometry and neutron diffraction can help define the intrinsic nature of pollutants and its relationship with the substance they are polluting .

Neutrons are able reveal the short range order of ions sequestered in minerals like clays. In particular, when the clays are in contact with water neutrons can determine the hydration of these ions, a key element to determine whether the ions could be released in nature or not. This is true for any pollutant, but it is particularly pertinent for actinides in nuclear repositories.

Neutron research is also helping scientists understand what materials, such as plastics, can be blended into useful products, while being efficiently manufactured and recycled with the least effect on the environment.

Atmospheric science

Clouds Brownish gray cloud (dust pollution) over the Tasman Sea just off the coast of southern Australia. True-color image taken by the Sea-viewing Wide Field-of-view Sensor [(SeaWiFS)]. Image courtesy the [SeaWiFS Project], NASA/Goddard Space Flight Center, and ORBIMAGE, on Wikimedia Commons

Neutron diffraction can also contribute to atmospheric science and the study of ice crystals in clouds, and give valuable insight into the role of clouds in global warming. Neutrons have their role to play in the battle to minimise carbon emissions.

One area in particular is in the manufacture of cement, which contributes 5-7% of man-made (and 4% of total global) CO_2 emissions. Neutron scattering techniques can help understand the process of cement aging – and thereby help to extend the lifetime of cement. This will in turn reduce overall cement production requirements and the carbon emissions it engenders.

Small angle neutron scattering can also be used to analyse materials for carbon capture and storage, another way to reduce CO_2 emissions into the atmosphere.

Research into alternative energy sources can also benefit from neutron scattering techniques: hydrogen storage, solar cells are only a few of the technologies that neutrons are contributing to develop, please see our Energy page for more details.

Earth sciences

Neutrons can be applied to several fields of Earth sciences. They provide a unique tool for the understanding of both surface and deep Earth processes.

In the former case, which is dominated by the effects of water, the sensitivity of neutrons to hydrogen allows precise measurements to be made of the structure, synthesis and dynamics of hydrous mineral phases.

In the latter case, which utilises the penetrating power of neutrons to study large volume samples coupled with the sensitivity of neutrons to light atoms, the field can be subdivided into either petrophysics, the understanding of the properties of rocks at high temperatures and pressures, or mineral physics, the detailed study of the individual constituent mineral phases.
In space, neutrons can help detect water on planets and also make possible the study of comet cores via earth hydrates and the study of meteorites via earth ice.

Heritage science

Overview

Ancient vas studied by neutron tomography at ANTARES@FRMII

Vase2 Picture courtesy of Petra Kudejova, FRMII / TUM Vase3 Picture courtesy of Petra Kudejova, FRMII/ TUM

All crystalline material – metal, pigments, rock, ceramics – can be analysed by neutron diffraction.

Neutrons are an invaluable tool to analyse precious archaeological objects: they are non-destructive and can penetrate deep into the cultural artefact 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.

Neutron tomography and radiography provide information about interesting inner parts of the object, which can be subsequently analysed by other neutron techniques for more detailed information.

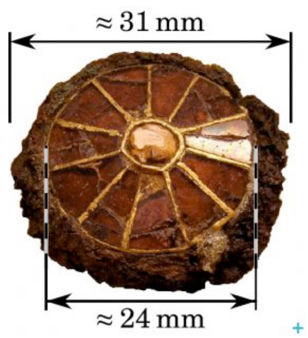
Activation analytical methods allow to study the elemental composition of virtually any material and object, which can be used to determine the geographical origin of an object.

Neutron scattering methods

For archaeology and cultural heritage studies, crystallographic analysis by time-of-flight neutron diffraction allows to quantitatively determine the crystallographic parameters and phase content of a material.

Neutrons have much greater penetrating power than X-rays, so whereas X rays are useful for small powder samples and surface analysis, ToF-ND can go right through thick samples of bronze or steel for example.

Small-angle neutron scattering has been used for studies on samples of different types of paper and ancient paper. These studies have yielded details of the surface morphology of cellulose fibres, the spatial distribution of water-filled pores, and the increasing dimension of water domains in cellulose as degradation occurs, and allowed for methods for the prevention of paper ageing to be developed.



Disc fibula from the 6th century, with 3D elemental maps for gold and silver.

Fibula 3D elemental maps for silver. Picture courtesy of FRM II Fibula Disc fibula from the 6th century, 3D elemental maps for gold. Picture courtesy of FRM II.

Nuclear analytical techniques such as Prompt Gamma Activation Analysis (PGAA), Neutron Activation Analysis (NAA) or Neutron Resonance Capture Analysis (NRCA) are used routinely in cultural heritage studies. They allow for non-destructive chemical analysis of historical artefacts, with little or no sample preparation. For example, PGAA and NAA can give useful information about the origin of the findings based on the ´fingerprints´, or typical patterns in the trace element compositions of the raw materials and of the object, while NRCA can be used for studies of bronze and brass objects.

Combining these methods provides invaluable information for cultural heritage studies. The EU Ancient Charm (FP6) project brought together large scale neutron facilities and museum scientists in order to develop new methods and techniques for the analysis of cultural artefacts and resulted in the development of new imaging techniques with neutrons.

A new technique called Neutron Tomography-driven Prompt Gamma Activation Imaging (PGAI-NT) is a powerful tool for the investigation of complex precious cultural heritage objects. It combines the advantages of both neutron imaging and prompt gamma activation analysis: the internal structure can be investigated using neutron imaging, and then the internal details can be analysed with PGAA.

Using this method, this fibula from the 6th century found in western Hungary (see figures) could be investigated. Without disassembling the precious jewel, its internal structure and composition could be studied in detail. Its origin, most probably a German workshop, could also be determined using this technique.