MLZ
Heinz Maier-Leibnitz Zentrum

Neutrons for Research

MLZ is a cooperation between:

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technical University of Munich TUM

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The Heinz Maier-Leibnitz Zentrum (MLZ):

The Heinz Maier-Leibnitz Zentrum is a leading centre for cutting-edge research with neutrons and positrons. Operating as a user facility, the MLZ offers a unique suite of high-performance neutron scattering instruments. This cooperation involves the Technische Universität München, the Forschungszentrum Jülich and the Helmholtz-Zentrum Geesthacht. The MLZ is funded by the German Federal Ministry of Education and Research, together with the Bavarian State Ministry of Education, Science and the Arts and the partners of the cooperation.

The Forschungs-Neutronenquelle Heinz-Maier-Leibnitz (FRM II):

The Forschungs-Neutronenquelle Heinz-Maier-Leibnitz provides neutron beams for the scientific experiments at the MLZ. The FRM II is operated by the Technische Universität München and is funded by the Bavarian State Ministry of Education, Science and the Arts.

Neutrons for Research

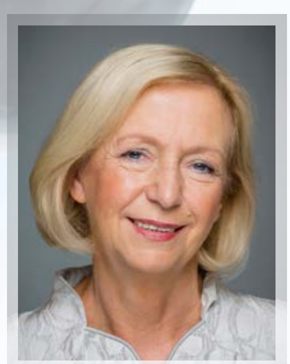
Foreword

For many years now, research using neutrons has made key contributions towards solving the great challenges that face science and society: in energy research, information technology and materials science, as well as in bio-medicine and tumor research. In order to strengthen neutron research, the Federal Ministry of Education and Research and the Bavarian State Ministry of Education, Science and the Arts foster collaboration between first-class partners, under the umbrella of the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching.

The Research Neutron Source Heinz Maier-Leibnitz (FRM II), a central scientific facility of the Technical University of Munich, offers scientists at the MLZ a cutting-edge research infrastructure. As one of the most powerful neutron sources worldwide, the FRM II is rooted in a unique environment, amalgamating the research campus of the Technical University of Munich, subject-specific institutions of the Ludwig-Maximilians-Universität München and several Max-Planck institutes. The founding of the MLZ in 2010 established a recognizable institutional framework for the common scientific use of the FRM II. The MLZ nurtures successful collaboration between the various participants in neutron and positron research and has rapidly evolved into a national and world leading centre in this area. As Federal Republic and State of Bavaria we support the work of the MLZ over the long-term.

The structure and aims of the MLZ blend seamlessly into a modern research landscape, where universities and non-university institutions involved in large-scale research engage in ever-closer cooperation. Stronger cooperation makes it possible to bring together the best minds and ideas and offer the best possible working conditions. The MLZ is a successful example of this, which we would very much like to see replicated. A unique opportunity lies, last but not least, in the closeness of cutting-edge research and university teaching. This opens up the perspective of supporting young academics in the future. Common recruitment procedures between the partners are an important element in promoting further networking.

The current brochure provides an illustrative overview of the high-powered and multifaceted research at the MLZ. We wish the MLZ every success for its future development.



Prof. Dr. Johanna Wanka

Federal Ministry of Education and Research

Dr. Ludwig Spaenle

Bavarian State Ministry of Education, Science and the Arts

MLZ – where big science and university merge

The rapid development of our industrial manufacturing capabilities, the ongoing extension of transportation, the massive increase in information technology and the constant increase in the average life-span of human beings – many of these large transformations and advances in our society have their origin in the understanding and utilisation of the physics and chemistry of materials and our growing insight into biological processes at a molecular level. One of the most important and most incisive tools for investigating these properties is the scattering of neutrons by these materials. The resulting scattering pattern can be directly connected to the physical and chemical properties that we experience in our daily lives.

Neutrons are one of the most universal and important probes for an understanding of the microscopic origin of the macroscopic functionality of present-day and future materials. Therefore, neutrons provide essential contributions to solving the Grand Challenges of our technological and scientific civilisation, e.g. in Energy, Information Technology, Life Sciences and Health, Nano Science and Engineering, as well as the Earth, Environment and Cultural Heritage. Moreover, the neutron as a quantum physical object grants insight into fundamental questions of our world such as the unification of fundamental forces and the origin of the universe.

The modern neutron sources of today, such as the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), are not built to solve just one single scientific problem, but rather they excel by being multi-disciplinary, covering almost the full range of science and technology. Within the family of worldwide and, in particular, European neutron sources, the FRM II ranks as one of the most prominent neutron facilities, combining a high flux reactor with a suite of the most up-to-date and diverse neutron instruments.

Scientific use, with some 1000 user visits per year, is organized jointly by the Technical University of Munich, Forschungszentrum Jülich and Helmholtz Zentrum Geesthacht. This cooperation is known as the Heinz Maier-Leibnitz Zentrum (MLZ). It is strengthened by collaborating groups from the Max Planck Society and nine further Universities, thus bringing together key-players in research using neutrons from all across Germany. The partners of the MLZ operate the instrument suite at the neutron source, thereby providing a service for the German, European and international scientific community. Where big science and the universities merge, the MLZ plays a special role in the education of young scientists and engineers. Within its international environment, the MLZ can claim to be preparing the future generation to meet the challenges of professional life in the global scientific and industrial world.

The MLZ sees itself as fulfilling a dual role – providing excellent service to the user community and performing cutting-edge in-house research. The instrument scientists at the MLZ, while pursuing their own research interests, reach out to the user community as local contacts. They anticipate future trends in their field of expertise together with the need for corresponding neutron instrumentation, and drive the instrument- and method development at the MLZ.

We very much hope that the present brochure goes some way towards explaining this ethos and provides a comprehensive overview of neutron methods and their applications, addressing the Grand Challenges of modern societies by the scientific work done at the MLZ.

Prof. Dr. Thomas Brückel

Scientific Director MLZ
Jülich Centre for Neutron Science, FZJ

Prof. Dr. Winfried Petry

Scientific Director MLZ
Forschungs-Neutronenquelle FRM II, TUM

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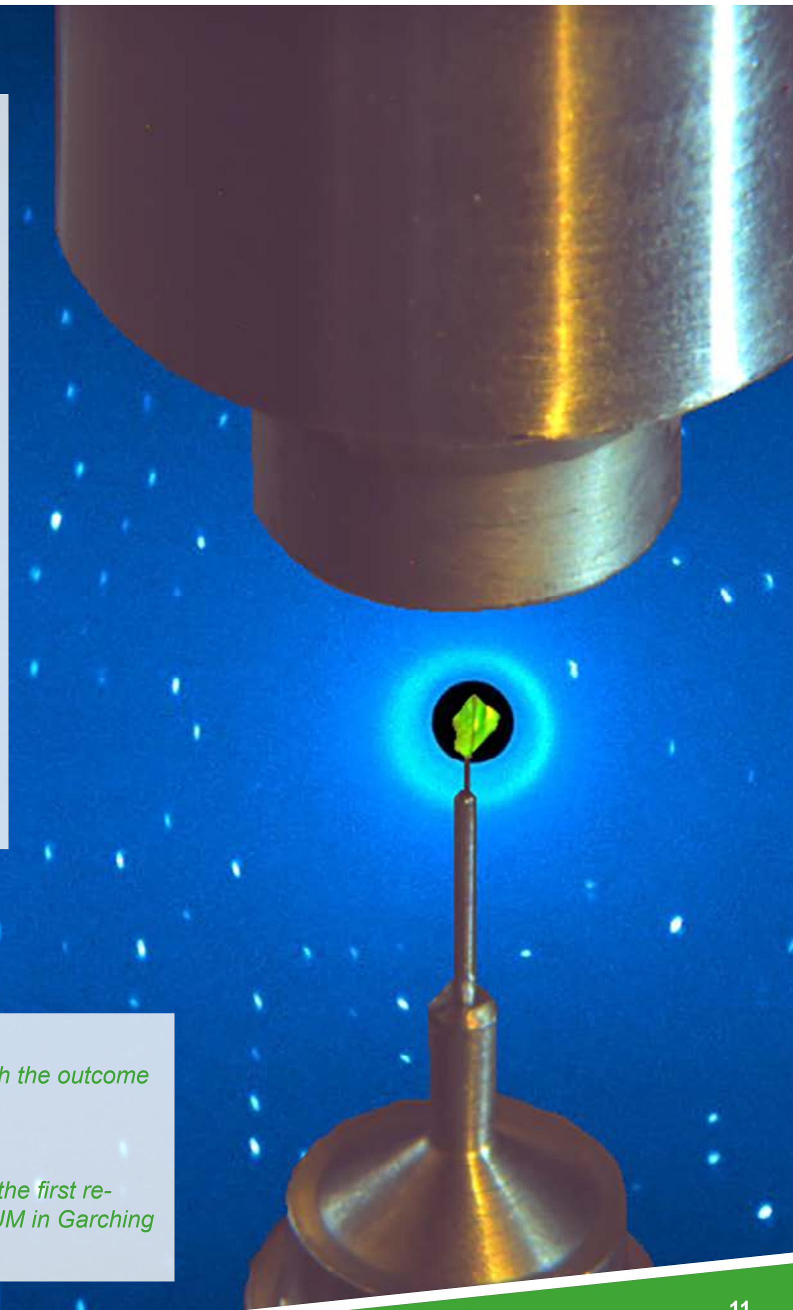
"The MLZ as one of the leading neutron research facilites in Europe has a bright future. In the network with the other neutron sources, the MLZ is developing new and improved scientific instruments and sample environment. The development is ongoing and will serve the next generation researchers. Another strong advantage of the MLZ is merging the expertise of facilities for neutron scattering with the science of universities. The European Neutron Scattering Association represents some 8000 scientists using neutrons. They produce 50 % of the neutron scattering publications worldwide, regularily exchanging ideas at the European and the International Conferences of Neutron Scattering. I hope to meet you there!"

Prof. Dr. Christiane Alba-Simonesco
Chair of the European Neutron Scattering Association

"Germany has a worldwide leading position in the research with neutrons. This particular strength has been achieved by the many excellent scientists educated, trained, supported, and served with neutrons by an intelligent network of small, medium, and flagship neutron sources. It is the Heinz Maier-Leibnitz Zentrum (MLZ) which plays a key role to continue this success story. Here, the Forschungszentrum Jülich, the Helmholtz-Zentrum Geesthacht, and the Technical University of Munich develop, operate, and provide neutron instruments at the highest level in close cooperation for the benefit of the national neutron community and beyond. I am convinced that this close cooperation of our national neutron centers which includes a variety of collaborating partners at universities, Max-Planck institutes, and other research centers is an indispensable prerequisite for the success of new flagship sources such as the European Spallation Source in Lund, Sweden."

Prof. Dr. Tobias Unruh
Chair of the 10th Komitee Forschung mit Neutronen

Neutrons –
a unique tool for analyzing and understanding matter



Why are neutrons so special? Neutrons are small, electrically neutral and magnetically sensitive particles. Neutrons penetrate all types of materials easily and can show where the atoms are, how they move and define their inner magnetic behaviour without damaging the materials. Their energy and, hence, wave length can be precisely tuned to investigate the structure and dynamics of materials simultaneously. Selecting the appropriate wavelength, these investigations range from the (sub-) atomic scale to complex molecules, from nano-structures up to macroscopic objects. This broad range of applications makes neutrons an indispensable tool for a multitude of studies in condensed matter research, physics, chemistry, biology and the engineering sciences.

“What is important is research, in which the outcome is unknown."

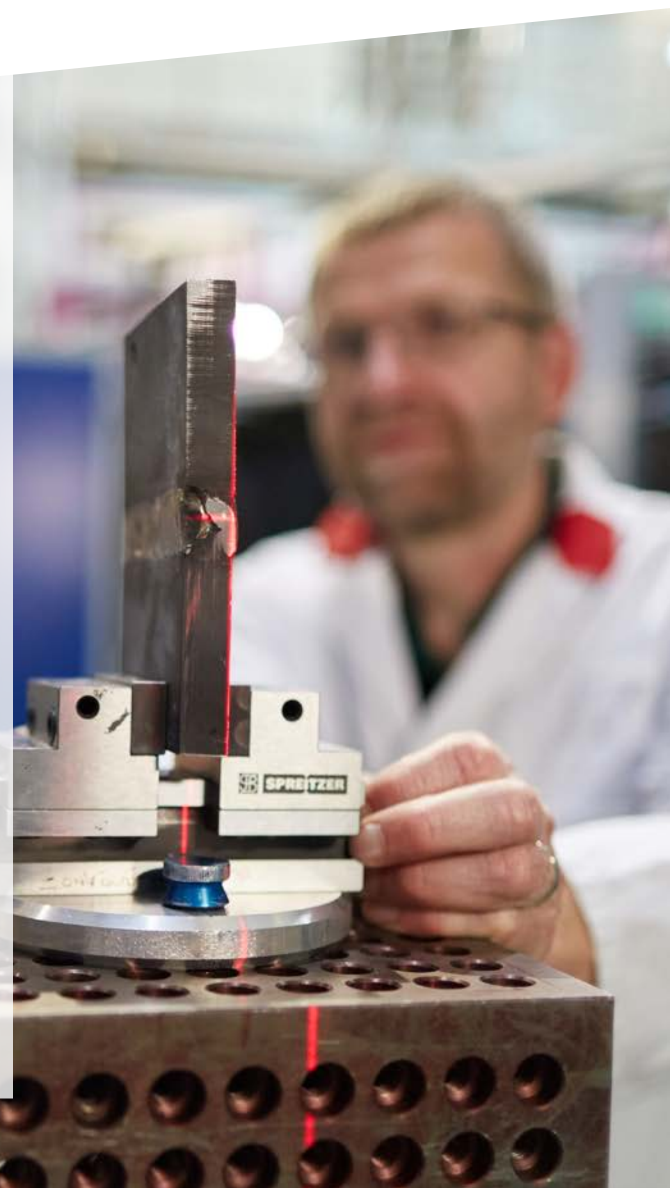
Prof. Dr. Heinz Maier-Leibnitz (1911 – 2000), initiator and director of the first research reactor in Germany, FRM at TUM in Garching

Diffraction

The wavelengths of cold, thermal and epithermal neutrons are comparable to the interatomic distances in the solid and/or liquid state, which lead them to diffract from the different ordered states. The phenomenon of neutron diffraction by crystals results from a scattering process, where neutrons are scattered by the neutrons of the atoms with no change in wavelength/energy (coherent or Bragg scattering). Such scattering results in a diffracted beam only if certain geometrical conditions are fulfilled. The resulting diffraction picture of a material, comprising both the intensity and position of diffraction response, allows the identification and complete elucidation of its structure.

Localisation of the individual atoms, determination of their concentration and thermal motion requires measurements and analysis of diffracted intensities, which are related through structure factor equations.

A broad band of neutron energies is typically utilized in neutron diffraction, e.g. cold neutrons are typically utilized in protein crystallography and magnetic diffuse scattering, thermal neutrons are standard for high resolution powder diffraction and/or stress, strain and texture determination in engineering materials while, for the sake of completeness, single crystal diffraction (with and without polarisation analysis) tends to apply to hot neutrons. By probing the atomic and/or magnetic arrangement, the localization of light elements near to heavy ones (e.g. hydrogen, lithium, oxygen etc), accurate determination of thermal displacements (Debye-Waller factors), investigations of microstructure (strain, stress, texture) – neutron diffraction gives clear and decisive answers to the long-standing and emergent scientific questions.



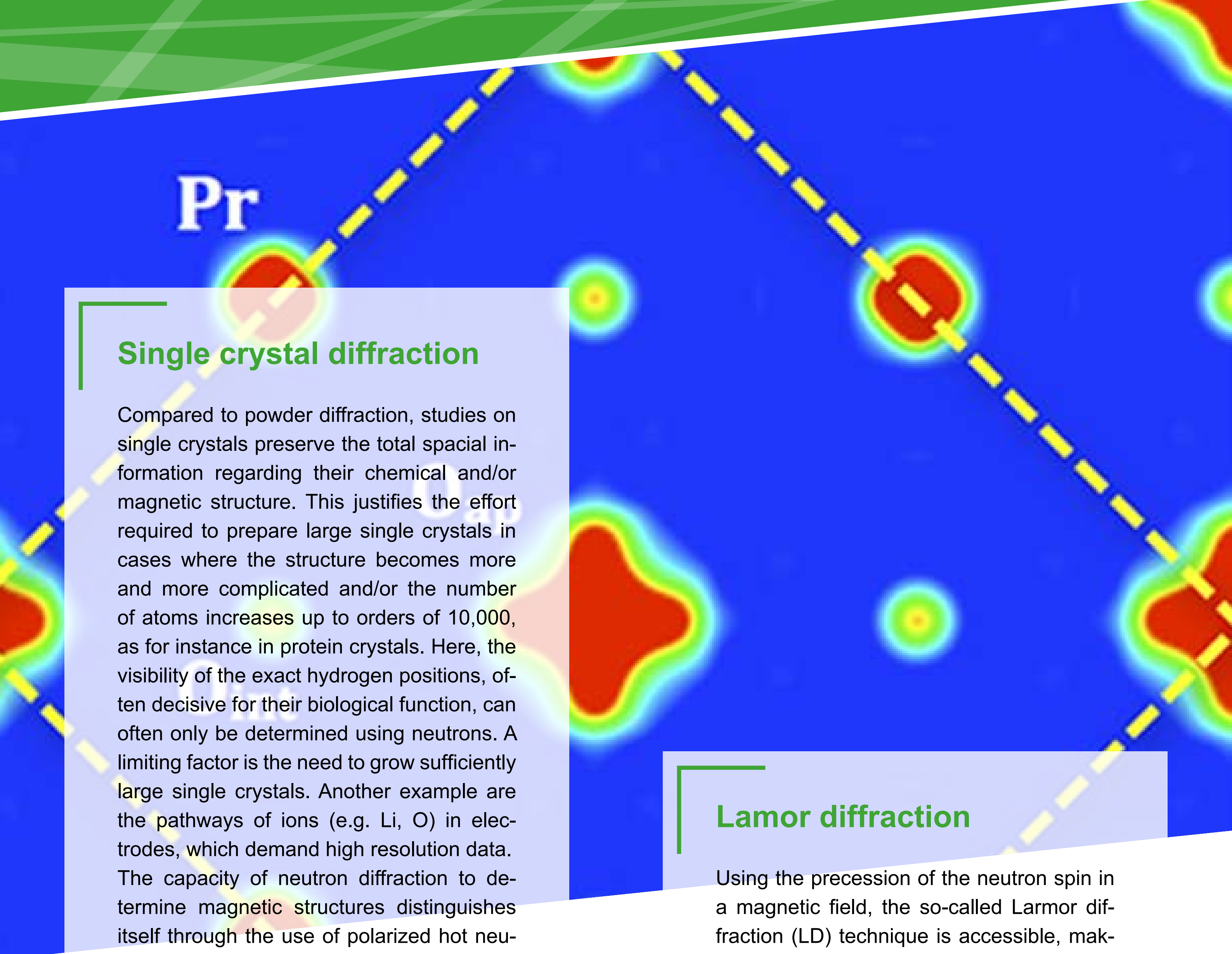
"The high resolution powder diffractometer SPODI has helped me to unravel the mystery of the composition of ice clouds. The crystalline structure of metastable nitric acid trihydrate could be explained for the first time and a heterogenous nucleation mechanism for these ice particles could subsequently be developed."

Prof. Dr. Hinrich Grothe,
Technical University of Vienna, Austria

Powder diffraction

In the field of new materials, growing large, single crystals of high quality is often a laborious task, while the effort required to obtain the majority of chemical compounds in the form of a powder or polycrystalline bulk sample is significantly less. Furthermore, for certain classes of materials, obtaining single crystals is generally not possible. This fact affords a great practical advantage to powder diffraction capable of yielding the structural details of materials in polycrystalline form enabling one to perform both qualitative and quantitative phase analysis. Being experimentally faster and simpler, powder diffraction is often used for the in-situ monitoring of structural changes vs. applying external parameters such as temperature, load (either mechanical or chemical), mechanical force, magnetic or electric fields and/or time (kinetic investigations). A number of aspects relevant to Materials Science can be addressed by different kinds of deformation, phase transformation, residual stress, texture, and microstructure studies.

Engineering diffractometers cover a wide range of applications in materials science and engineering, e.g. determination of residual stress in engineering components understanding the fundamental aspects of the behaviour of materials during synthesis, processing, and service; spatially-resolved studies of structural uniformities in a well-defined gauge volume (typically of the order of mm^3) inside a technical object; texture analysis and accurate determination of pole figures in mechanically deformed samples (technologically relevant alloys and composites, tectonically deformed rock minerals).



Single crystal diffraction

Compared to powder diffraction, studies on single crystals preserve the total spacial information regarding their chemical and/or magnetic structure. This justifies the effort required to prepare large single crystals in cases where the structure becomes more and more complicated and/or the number of atoms increases up to orders of 10,000, as for instance in protein crystals. Here, the visibility of the exact hydrogen positions, often decisive for their biological function, can often only be determined using neutrons. A limiting factor is the need to grow sufficiently large single crystals. Another example are the pathways of ions (e.g. Li, O) in electrodes, which demand high resolution data. The capacity of neutron diffraction to determine magnetic structures distinguishes itself through the use of polarized hot neutrons. Full polarization analysis, in combination with short wavelength neutrons using single crystalline samples, is the best way to obtain definitive answers to complex magnetic ordering phenomena in solids.

Lamor diffraction

Using the precession of the neutron spin in a magnetic field, the so-called Larmor diffraction (LD) technique is accessible, making it possible to measure lattice spacings with precision in the ppm range, i.e. one to two orders of magnitude better than conventional neutron or X-ray diffraction. Absolute distance values can be determined by calibrating the instrument against a Si standard. The main applications of LD include thermal expansion under pressure and at low or high temperature, and distributions of lattice constants (second order stresses). LD thus is unique in a parameter region, where standard methods such as dilatometry fail.

SANS

Going from the atomic to nano- or mesoscopic structures, the scattering angle of these particles becomes smaller with increasing size. To detect these small scattering angles, special instruments, the so- called Small Angle Neutron Scattering (SANS) machines, are provided at the MLZ. They make it possible to determine the mean particle size and their distribution in heterogeneous materials, as well as the form and structure of nanomaterials. As nano-composites, bio-molecules and other polymers often do not exhibit a homogeneous mass, but have differences in the (scattering) density, concentration or magnetism across the whole sample volume,small angle scattering can visualize the form and morphology of these complex molecules.

The unique feature of neutrons is their sensitivity to different isotopes of the same element which allows for variation of contrasts, especially with SANS. Here, the exchange of hydrogen by deuterium can, for example, mask polymers from a surrounding solution, yielding information on ordering phenomena such as the formation of micelles or layered membranes.

“Monitoring the precession of neutron spins in magnetic fields can greatly enhance the sensitivity and accuracy of neutron scattering experiments As an example, we have recently used spin precession techniques to measure the dimensions of magnetic domains in antiferromagnets, which is difficult to determine in any other way. These results provide important insights into the mechanisms underlying charge and heat transport in magnetically ordered solids.”

Prof. Dr. Bernhard Keimer, director of the Max-Planck Institute for Solid State Research, Stuttgart, Germany

Reflectometry

Neutron reflectometry measures how nanometre to micrometre thin films at flat interfaces reflect the neutrons when they impinge under very small incident angles. This makes it possible to study the properties of the film, such as its thickness, roughness, or internal structure. The MLZ instrument suite contains several dedicated neutron reflectometers which have different specialities, such as the capability to study magnetic layer systems or the surfaces of liquids.

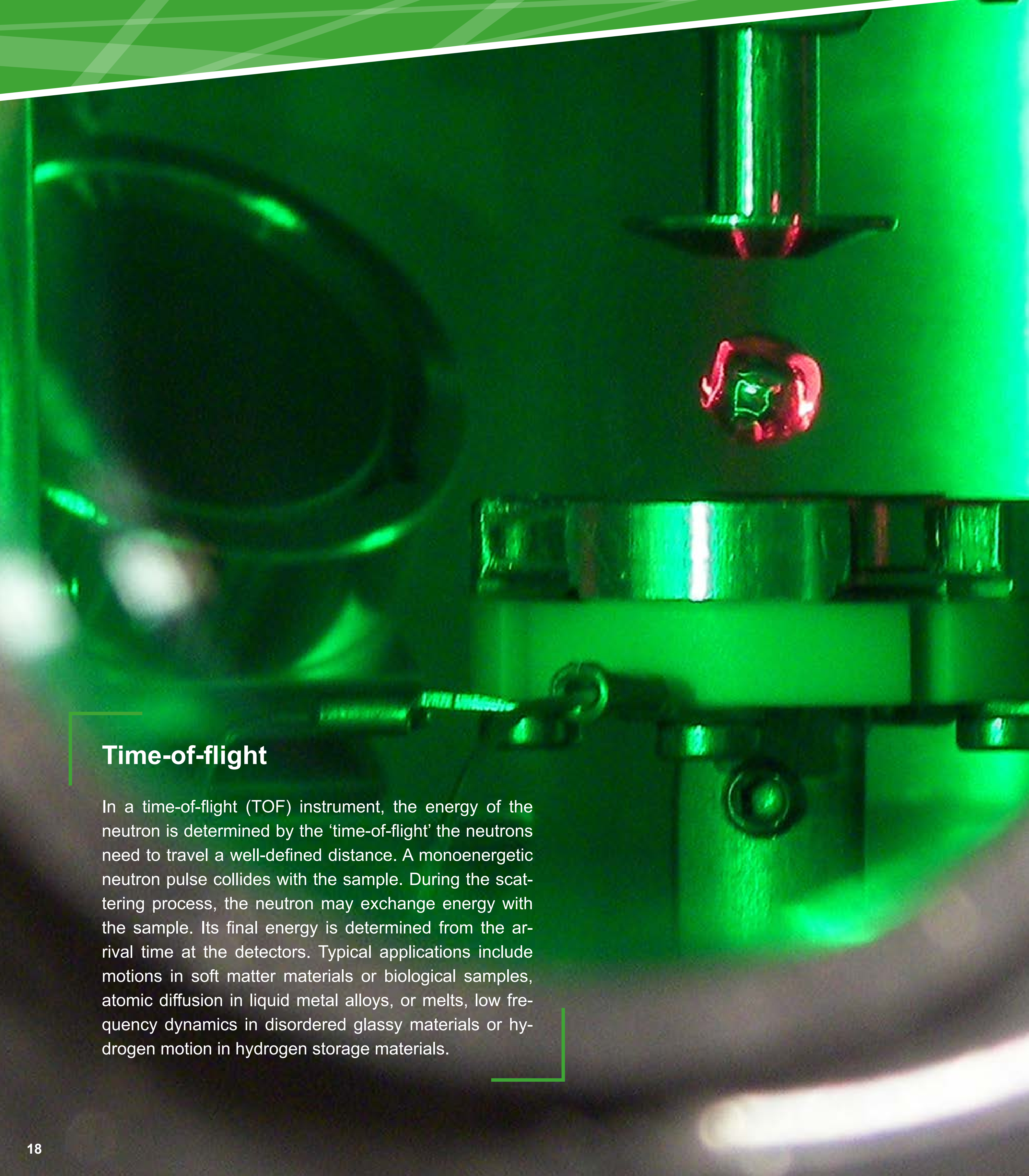
With reflectometry, it is possible to obtain valuable information for example on lipid bilayers in biological membranes and how e.g. other biomolecules adsorb to them. Also polymer coatings of hard surfaces can be studied; some of these polymers spontaneously form ordered patterns which could be used as template for other nanostructures to enhance the surface properties of materials.

Spectroscopy

Neutrons can be viewed in two ways – either as a particle or as a wave. In the latter picture, they have wavelengths similar to the movement of atoms. Thus, they can show how atoms move in different materials, when they exchange energy with a nucleus or a magnetic moment in the sample. This method is called spectroscopy. Neutron three axes spectroscopy is used for lattice dynamics or in order to explore the origin of magnetically mediated superconductivity. Time-of-flight spectrometers examine, for example, diffusion in metals or fluids. On a backscattering spectrometer and on spin-echo spectrometers, the motion in polymers or biomembranes can be probed.

Three axes spectrometry

Three axes spectrometers (TAS) are defined by the three independent axes of the instrument: monochromator (1st axis), sample (2nd axis) and analyser (3rd axis). At the monochromator, Bragg's law is used to select the energy E of the neutrons which hit the sample and interact with it. Due to the excellent resolution in momentum and energy (µeV…meV) as well as the low background of TAS, they are ideally suited for the investigation of collective excitations such as phonons (lattice vibrations) or magnons (spin excitations) in single crystal materials. Typical research topics include, for example, spin- und phonon dynamics in superconductors, multiferroics, thermoelectric materials and related compounds, spin waves in magnetic systems and low-dimensional magnets for quantum computing.



Time-of-flight

In a time-of-flight (TOF) instrument, the energy of the neutron is determined by the 'time-of-flight' the neutrons need to travel a well-defined distance. A monoenergetic neutron pulse collides with the sample. During the scattering process, the neutron may exchange energy with the sample. Its final energy is determined from the arrival time at the detectors. Typical applications include motions in soft matter materials or biological samples, atomic diffusion in liquid metal alloys, or melts, low frequency dynamics in disordered glassy materials or hydrogen motion in hydrogen storage materials.

Neutron spin-echo

Neutron spin-echo (NSE) spectroscopy uses the precession of the neutron spin in a magnetic field as a very precise stop-watch to detect tiny energy exchanges with the sample. When the polarized neutron beam (i.e. all the magnetic moments point in one direction) enters the magnetic field, the spins start to rotate around the field direction. Following the scattering at the sample, the neutrons pass through the exact opposite magnetic field. If elastic scattering takes place, the original polarization is recovered. Small energy losses and gains result in a reduced polarization that yields rather indirect information about the sample dynamics on a nanosecond scale. Typical applications of NSE include looking at the motion of polymer chains in the melt or in solution and domain motions of proteins or fluctuations of surfactant membranes in microemulsions in soft matter systems, as well as the dynamics of spin glasses in hard matter systems.

Backscattering

Backscattering spectrometers achieve an energy resolution below 1 µeV by filtering incoming and scattered neutrons through Bragg reflection under 180°. This gives access to molecular processes on a nanosecond scale. Typical applications include the study of hyperfine interactions, rotational tunnelling, hydrogen diffusion, the dynamics of supercooled liquids and relaxation in polymers and proteins.

Analysis

Chemical analysis of materials can be achieved by nuclear analytical techniques. Based on the interaction of neutrons with the atomic nucleus, both characteristic prompt and delayed gamma radiations are emitted and analysed. The energies measured identify the specific elements and the isotopes, while their intensities are proportional to their quantities. Thus, their detection can be used for the non-destructive analysis of a large variety of materials and extensive use of this is made in archaeology, geology, environmental research or medicine.

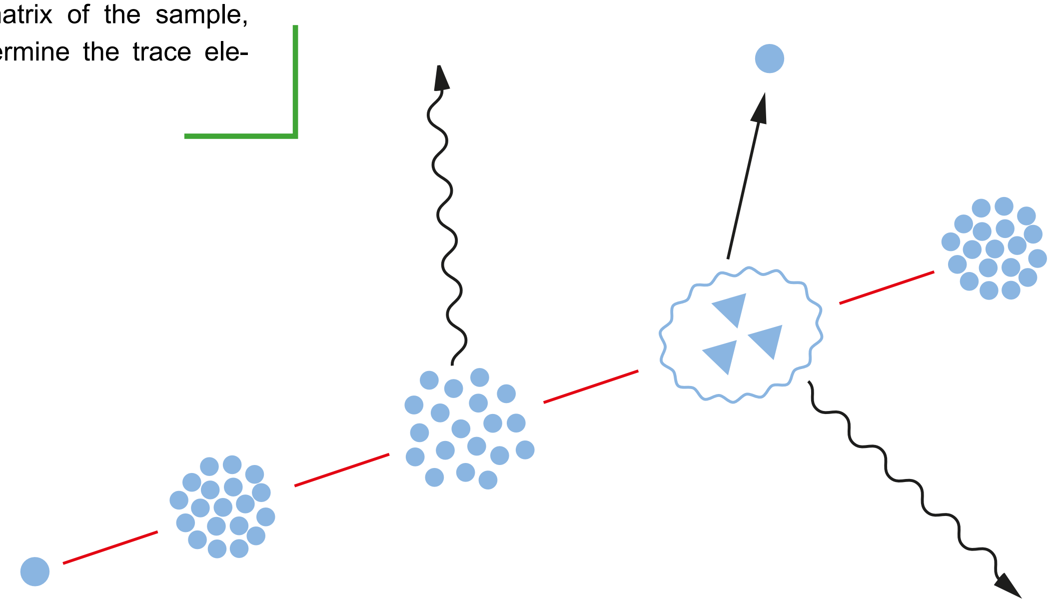
Irradiation

Neutrons are also used to irradiate samples and create specific isotopes. For example, silicon is irradiated with neutrons to dope it with phosphorus for use as a semiconductor in high voltage transport systems. Stable radioisotopes for technical and medical purposes are generated using the high neutron flux in the different irradiation facilities available in the reactor pool of the FRM II. Fast fission neutrons are used at a dedicated instrument for treating tumour patients directly. Scientists also use it for studying material resistance to neutron irradiation, for example for aerospace devices.

Prompt gamma and neutron activation analysis

Prompt Gamma Activation Analysis (PGAA) and Neutron Activation Analysis (NAA) are nuclear analytical techniques. They are based on the capture of neutrons by the atomic nucleus. Immediately following the capture process, the binding energy of the neutrons is released in the form of gamma rays (prompt gamma radiations). PGAA is typically used for the determination of the elemental composition of solid samples (approximately down to the ppm range).

When a radioactive nuclide is formed, delayed gamma radiation can also be detected (NAA). While PGAA is mainly used for the analysis of light elements and gives the composition of the matrix of the sample, NAA is useful to determine the trace elements in the sample.



Imaging

Neutron imaging is based on the various attenuation probabilities as a neutron passes through an object. Neutrons interact with the atomic nuclei, not with the electrons. Hence, they show contrast that is different from, and often complementary to, X-rays. Hydrogen, for example, has a much higher attenuation than many metals such as lead or aluminium, which makes it possible to visualize very small amounts of hydrogen-containing materials behind massive metal parts. The resulting radiographies and computed tomographies (CTs) give non-destructive insight into details which could not be observed using either X-ray or gamma CT. Typical applications include archaeology and cultural heritage, where organic materials in particular can be observed with high contrast, the investigation of pores in geological samples, or technical applications such as in-situ investigations of material transport in batteries, fuel cells and hydrogen storage systems

Positrons

The FRM II also operates the world's most intense mono-energetic positron source. These antiparticles of the electron are well suited to probe surfaces and the bulk of materials. As annihilating positron-electron pairs emit characteristic radiation which depends on the electron density in the sample, they can detect voids in the atomic lattice and distinguish different elements precisely. This method is non-destructive as the neutron methods do not activate the samples. As an example, the positron lifetime is slightly larger in vacancy-like defects than in the unperturbed crystal lattice. In this way, vacancy concentrations as low as $1:10^7$ can be detected.

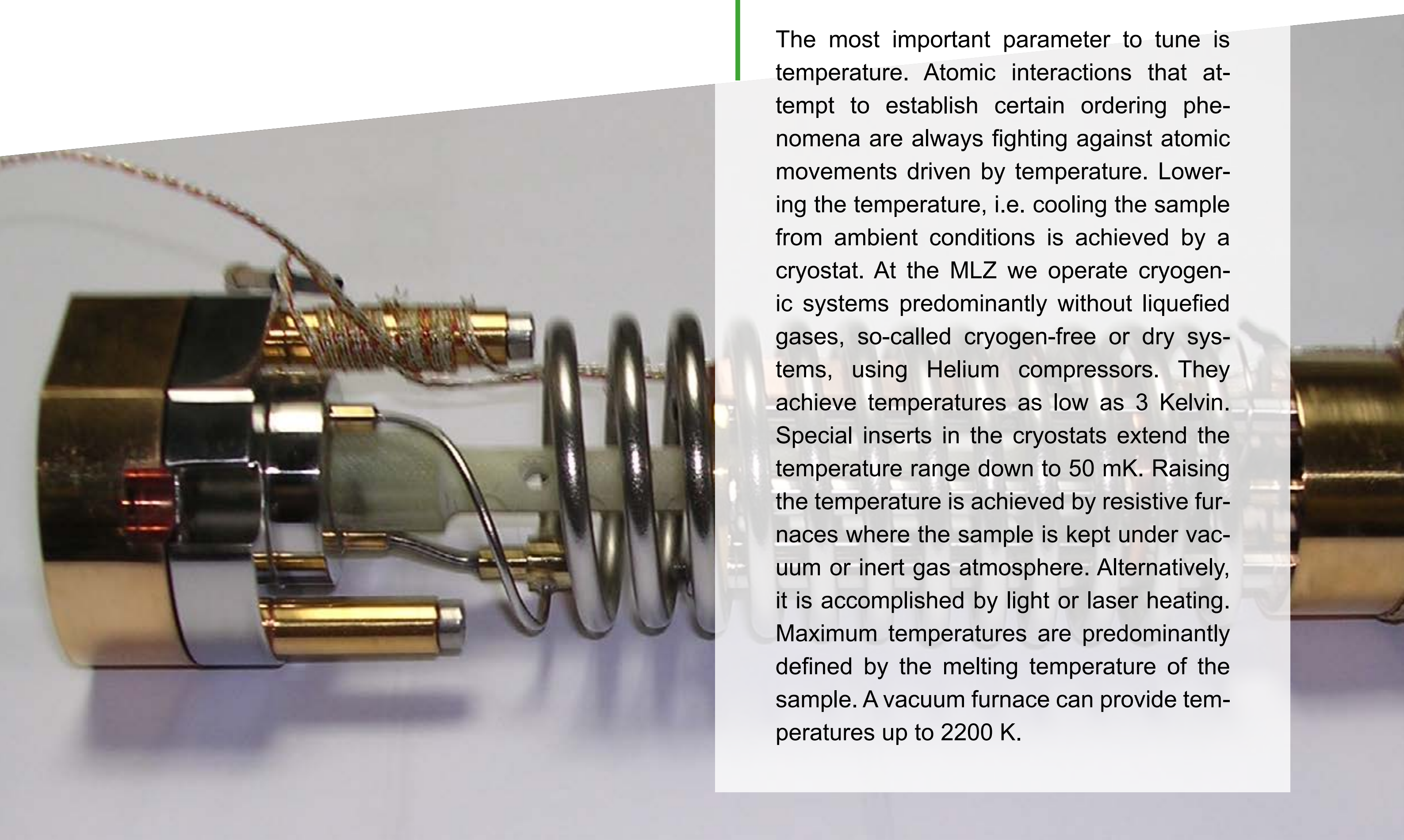
Nuclear and particle physics

The neutron itself is also the subject of investigations. For example, the decay of a neutron into a proton, electron and an anti-electron neutrino has still not been fully examined. For the most part, experiments in the field of nuclear and particle physics measure the correlation of energy and angle of reaction products. Theoretical models of energy levels in nuclei can be tested if all products of this reaction can be measured in coincidence. The results will help to further analyze what happened in the first moments following the Big Bang.

Ultra cold neutrons (UCN) can easily be stored for long periods of time (several tens of minutes). The storage and observation time is in principle only limited by the lifetime of the free neutron. These long observation times offer the possibility of investigating the fundamental properties of the neutron with the highest precision. In addition, the lifetime of the free neutron, an important parameter in the standard model of physics, can be measured with the highest precision. UCN are also used to observe quantum states of neutrons in the earth's gravitational field, which is a test of Newton's law in the µm-scale.

Sample environment

Experiments using neutron scattering aim to understand why physical, chemical or biological properties appear in condensed matter samples. In general, these properties exist under certain conditions such as temperature, pressure or applied magnetic or electric fields. Investigating the change of properties under varying conditions often provides a better understanding of the origin of these effects, especially the investigation of atomic arrangements and atomic movements. In order to tune these conditions for the sample material under consideration, special equipment, a so-called sample environment is provided by the MLZ at the different scattering instruments.



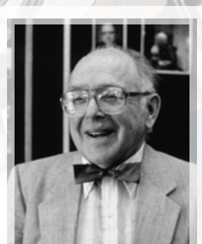
The most important parameter to tune is temperature. Atomic interactions that attempt to establish certain ordering phenomena are always fighting against atomic movements driven by temperature. Lowering the temperature, i.e. cooling the sample from ambient conditions is achieved by a cryostat. At the MLZ we operate cryogenic systems predominantly without liquefied gases, so-called cryogen-free or dry systems, using Helium compressors. They achieve temperatures as low as 3 Kelvin. Special inserts in the cryostats extend the temperature range down to 50 mK. Raising the temperature is achieved by resistive furnaces where the sample is kept under vacuum or inert gas atmosphere. Alternatively, it is accomplished by light or laser heating. Maximum temperatures are predominantly defined by the melting temperature of the sample. A vacuum furnace can provide temperatures up to 2200 K.

Another important parameter is the applied magnetic field, as neutrons are especially suited to the study of magnetic ordering or magnetic excitations. A large number of specialised magnets are available that use superconducting wires providing magnetic fields up to 14.5 Tesla. To study different magnetic ordering phenomena, the field direction with respect to the scattering experiment can be applied vertically, horizontally or parallel to the neutron flight path. The use of magnetic fields is frequently combined with the use of low temperatures where a superconducting magnet and a cryostat are combined.

Varying atomic distances through pressure is mainly appreciated by theoreticians as this parameter can be changed more easily during computer simulations than in real life. Depending on the type of sample material, pressure can be applied by compressed gases or liquids to achieve isobaric conditions or piston cells for uniaxial loading. A special, high pressure station can provide pressure up to 250 kbar. Special equipment is available to operate under constant stress or strain conditions.

Further parameters which can be controlled by the sample environment equipment include high electric fields, the humidity or the chemical composition in liquid-flow or stopped-flow cells or shear cells. A large amount of the equipment made available for neutron experiments is developed and maintained in-house, which ensures active development in this area. This strong in-house competence in sample environment allows for an optimal use, not only for investigations that involve varying all kinds of applied parameters but also for a large number of in-operando studies on complex objects, which presents an additional bonus when using neutrons for research and industrial applications.

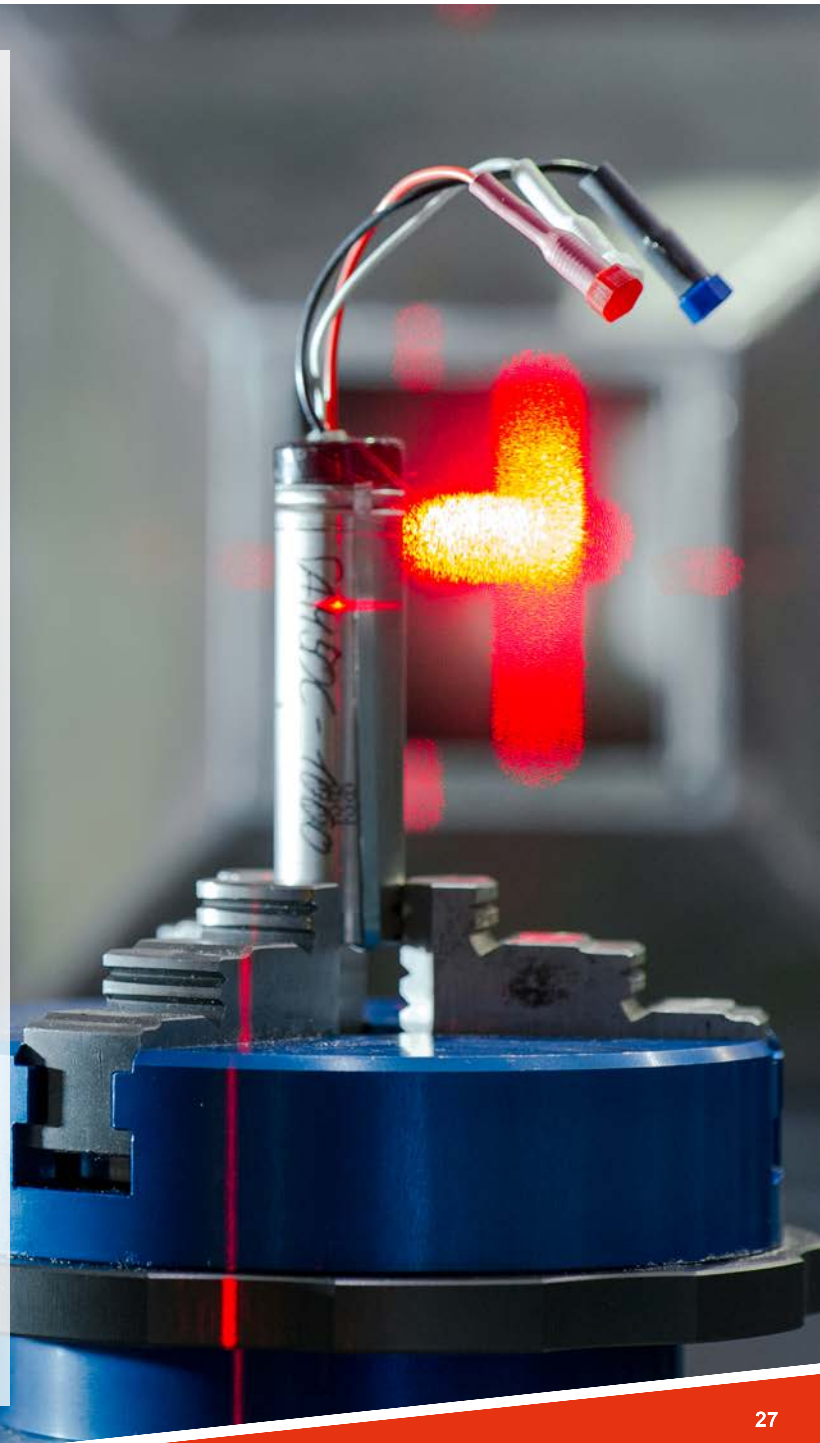
In order to support the user experiments, different laboratories can be used for the on-site preparation of samples, including a dedicated laboratory for biological samples, a chemistry lab, materials science lab and a thin film lab with MBE, TEM and X-ray tomography.



“Then we can think of how we can make better window glass, better semiconductors, better microphones. All of these things go back to understanding the basic science behind their operation.”

Prof. Dr. Clifford Shull (1915 – 2001), winner of the Nobel Prize in Physics, USA

Addressing the challenges



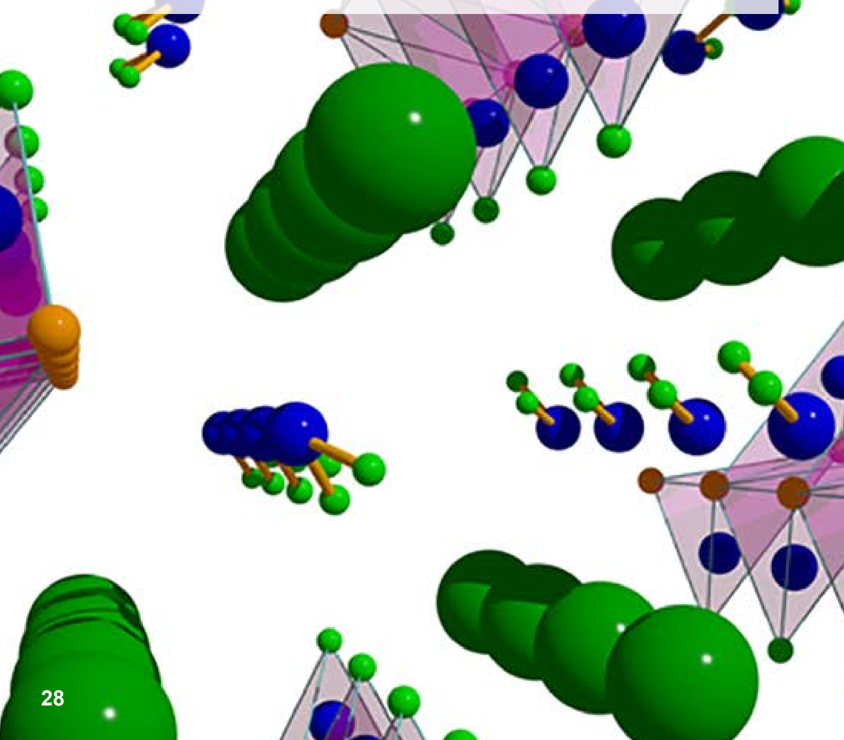
The MLZ, as the service provider for the scientific use of the FRM II, relies on the broad knowledge and extensive experience of expert neutron groups from all over Germany. To make best use of the rare neutron beam time, our users are supported by complementary methods to characterize and prepare their samples, including support on data evaluation and publication.

In order to provide open access to our infrastructure, twice a year the MLZ invites proposals for the entire instrument suite. The selection of these proposals is overseen by an international review panel which assesses the scientific merit of the proposed experiment. The provision of beam time is free of charge to our scientific users, on condition that the results obtained be published. Detailed information on procedures and deadlines is available via our web portal www.mlz-garching.de.

The neutron beams generated at the FRM II are not limited to scientific objectives. They are also used for industrial investigations and irradiation, for example to check the quality of automotive parts or provide transmutation doped silicon for high power electronics. Fast neutrons from the FRM II can also help to cure specific cancers by directly treating patients with neutron beams. And finally, the pharmaceutical industry uses neutron irradiation at the FRM II to produce radioisotopes to directly attack cancer cells, or for diagnosis.

Energy

The sustainable, environmentally-friendly and efficient production and use of energy is one of the major challenges that confront societies around the globe. In the search for new technologies for energy applications based on both soft and hard matter materials, neutrons offer a key analytical tool, providing deep insight into the structure and dynamics of new materials and an understanding of the underlying processes. For many energy-related materials, the presence of light atoms such as hydrogen, lithium or oxygen is at the core of their functionality and neutrons are ideally suited to elucidate the appropriate structures and dynamics. In addition, neutrons provide insight into electrochemical pathways, chemical reactions and mechanisms.



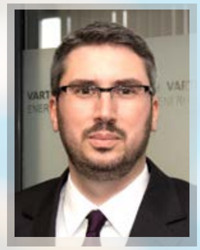
Hydrogen storage

In any hydrogen based fuel cell, storing and releasing hydrogen is a key process. Alkali amides that display this remarkable reversible process form new, unknown intermediate phases over absorption and desorption reaction pathways. This may constitute a severe limitation to an understanding of the basic mechanisms of the reaction kinetics. Combining the exchange of hydrogen atoms by deuterium atoms (deuteration) and neutron powder diffraction, the crystallographic structure of the compound $KMg(ND)(ND_2)$ has been solved. Knowledge of the structure of this amide-imide compound leads to a better understanding of the reaction pathway for amide based systems.

E. Napolitano et al., Int. J. Hydrog. Energy 39, 868 (2014)

As far as storing hydrogen is concerned, metal hydrides offer the highest volumetric densities and allow for safe and reversible storage. The compacted metal hydride was placed in an aluminium tank. In-situ neutron radiography is able to analyse quantitatively the hydrogen distribution inside the tank. However, to quantify the data, the correlation between the neutron beam attenuation and hydrogen content needs to be analysed. The researchers found a linear correlation between beam attenuation and the amount of hydrogen absorbed, providing the general basis for quantitative investigations of the hydrogen distribution in metal hydride systems and storage tanks.

S. Börries et al., Nucl. Instrum. Methods Phys. Res. Sect. A-Ac-cel. Spectrom. Dect. Assoc. Equip. 797, 158 (2015)



“Neutrons offer the direct view into the battery cells because of their low interactions. And contrary to other methods, we can conduct the measurements under more realistic conditions.”

Dr. Alexander Hirnet, Technical Manager at VARTA Storage, Nördlingen, Germany

Battery materials

Lithium-ion batteries need to be powerful, safe and fast-charging. However, one previously known, yet poorly understood phenomenon stands in the way of this goal: metallic lithium deposition or lithium plating. The cathode in lithium-ion batteries comprises a lithium metal oxide, while the standard material for battery anodes is graphite (carbon) with a layered structure. During the charging process, the lithium ions are stored in these layers. However, lithium ions occasionally form metallic lithium rather than intercalating into the anode, as desired. The lithium is deposited onto the anode and is no longer fully available. The result is a drop in battery performance. In extreme cases this can even lead to short-circuits. In addition, metallic lithium is highly inflammable. By installing a battery in the materials research diffractometer while it was charging and discharging, the neutron beam allowed the researchers to deduce indirectly how much metallic lithium had formed. The faster the charging process and the lower the ambient temperature, the more pronounced is the effect. If measurements are performed at -20 degrees Celsius, up to 19 % of the lithium ions normally involved in the charging and discharging process form metallic lithium.

V. Zinth et al., J. Power Sources 271, 152 (2014)

One of the limiting factors in battery lifetime is the loss of free movable lithium involved in the ion intercalation process. Using high resolution neutron diffraction, researchers were able to quantify the lithium concentration in the $LiCoO_2$ cathode and graphite anode of a 18650-type cell as a function of cell fatigue in a non-destructive way. A closer look at the lithium intercalation of graphite – the most commonly used anode material for state-of-the-art lithium-ion batteries – revealed a previously unknown signature of complex structures formed at the low lithiathion stages. The observed phenomenon might play a crucial role in the speed of charge (especially relevant for electromobility) and requires a reconsideration of the lithium intercalation/extraction mechanism into graphite.

A. Senyshyn et al., J. Electrochem. Soc. 5, 3198 (2013)

Renewable energies

Extracting energy and raw materials from plants usually requires a multi-step process and aggressive chemicals. To make these processes more efficient and conserve resources, researchers are looking for suitable enzymes to serve as catalysts. Using neutrons, researchers have investigated the reaction mechanism of the glycosidases.

The biomass is typically pretreated in a highly alkaline environment. However, the natural enzymes of the glycosidase family achieve their maximum activity in mildly acidic environments. To alter these enzymes in such a manner as to allow them to function effectively in a basic environment requires detailed knowledge of the reaction sequence of the enzyme, in particular the precise position of all hydrogen atoms in the active center of an enzyme.

The scientists analyzed the structure of the glycosidase using neutron scattering on enzyme crystals at the instrument BioDiff. They discovered that the decisive step depends on the orientation of a specific amino acid side chain: This important catalytic glutamic acid contains a carboxyl group. When it turns down and away from the substrate, the glutamic acid can take over a proton from a water molecule. When the chain turns upward, the acidity is strengthened and the proton is transferred to the substrate.

Q. Wan et al., Proc. Natl. Acad. Sci. U.S.A. 112, 12384 (2015)

Catalysis

Detailed knowledge of the elemental composition of surfaces is extremely important in understanding processes that take place at surfaces, such as catalysis. For instance, the chemical composition of a palladium surface decisively influences its catalytic ability and also plays an important role in the mechanical stability of thin membranes that are used for, e.g. hydrogen purification in industrial processes. The researchers used positron annihilation induced Auger electron spectroscopy (PAES) which allows the elemental composition of the uppermost atomic layer of a sample to be analysed. They analysed how nickel atoms migrate into the individual atomic layers of a palladium surface, which helps to understand the catalytic activity.

S. Zimnik et al., Surf. Sci. 643, 178 (2015)

"No one has ever observed hydrogen atoms in a glycoside hydrolase enzyme, and until now we did not know how the catalytic glutamic acid residue is protonated. Neutrons helped us enormously to elucidate the way this enzyme works."

Dr. Andrey Kovalevsky, scientist at the Oak Ridge National Laboratory, USA

Superconducting materials

The appearance of a magnetic excitation spectrum with an hour-glass shape in energy-momentum space is a characteristic property of high-temperature superconducting cuprates. Despite numerous studies, the origin of this peculiar excitation spectrum is not well understood. Using three-axis neutron spectroscopy, an isostructural but insulating cobaltate that also exhibits an hour-glass magnetic spectrum was studied. A fractal microstructure with a nanoscopic distribution of undoped and hole-doped regions within the cobalt oxygen planes was observed which unravelled the microscopically split origin of the hour-glass spectra on a nano scale.

Y. Drees et al., Nat. Commun. 5, 5731 (2014)

A coexistence of ferromagnetic and superconducting order rarely occurs because of the antagonistic nature of the two phenomena. This conflict can be resolved in the case of triplet superconductivity where electron pairs with parallel spins are not destroyed by the exchange field of ferromagnets. Using polarized neutron reflectometry (PNR), non-collinear magnetism on metal-oxide heterostructures has been investigated. The Josephson effect observed in these structures is explained by the penetration of the long-range triplet component of the superconducting correlations into the magnetic layer.

Y.N. Khaydukov et al., Phys. Rev. B 90, 035130 (2014)

High-quality crystals of $YBa_2Cu_3O_{7-\delta}$ (YBCO) are required in technical devices such as superconducting wires, fault current limiters or magnets, and to study the interplay between charge density wave and superconducting phases. A well-defined value and a homogeneous distribution of the oxygen in the films are highly important both for applications and fundamental research. Positron Annihilation Spectroscopy (PAS) uses the positron as a probe particle. Prior to their annihilation by surrounding electrons in YBCO, positrons are trapped in vacancies and other volume defects. The trapping in defects is observed by analysing the positron lifetime or the Doppler broadening of the electron-positron annihilation line at a characteristic energy. The localization of positrons leads to a strong correlation of observables to the oxygen content. The Doppler broadening of the annihilation line decreases with the oxygen content, which indicates that, even when positrons are trapped in Cu or Ba vacancies, PAS observables are still sensitive to changes in the oxygen content in the basal plane. This makes PAS an excellent technique for probing the oxygen content in superconductors and, hence, the local transition temperature in superconducting materials.

M. Reiner et al., Appl. Phys. Lett. 106, 111910 (2015)

Health & Life Sciences

Understanding complex biological processes requires the use of all the scientific and analytical methods available. The application of neutron scattering to the health and life sciences is often unacknowledged, but neutron scattering aims to provide very specific and unique information. The position of hydrogen in biological structures is established via atomic resolution using macromolecular neutron crystallography. Small-angle neutron scattering opens the door to structures on the nano- to micrometer scale, in particular in the natural environment of liquid solutions. Surfaces and interfaces are probed using neutron reflectometry, particular attention being paid to biomembranes. Neutron spectroscopy provides access to the motion of atoms and molecules on microscopic timescales.

Protein structure and dynamics

Cytochrome c peroxidases (CCPs) are members of the family of iron-containing heme enzymes. The heme group contained in the active centre of these enzymes is found, as well as elsewhere, in hemoglobin, which gives human blood its red colour.

The enzymatic reaction of the CCP proceeds in multiple steps during which the active centre of the enzyme adopts various intermediate states. The so-called intermediate state Compound I exists in many heme enzymes that transfer oxygen and play an important role, for example, in breaking down medication.

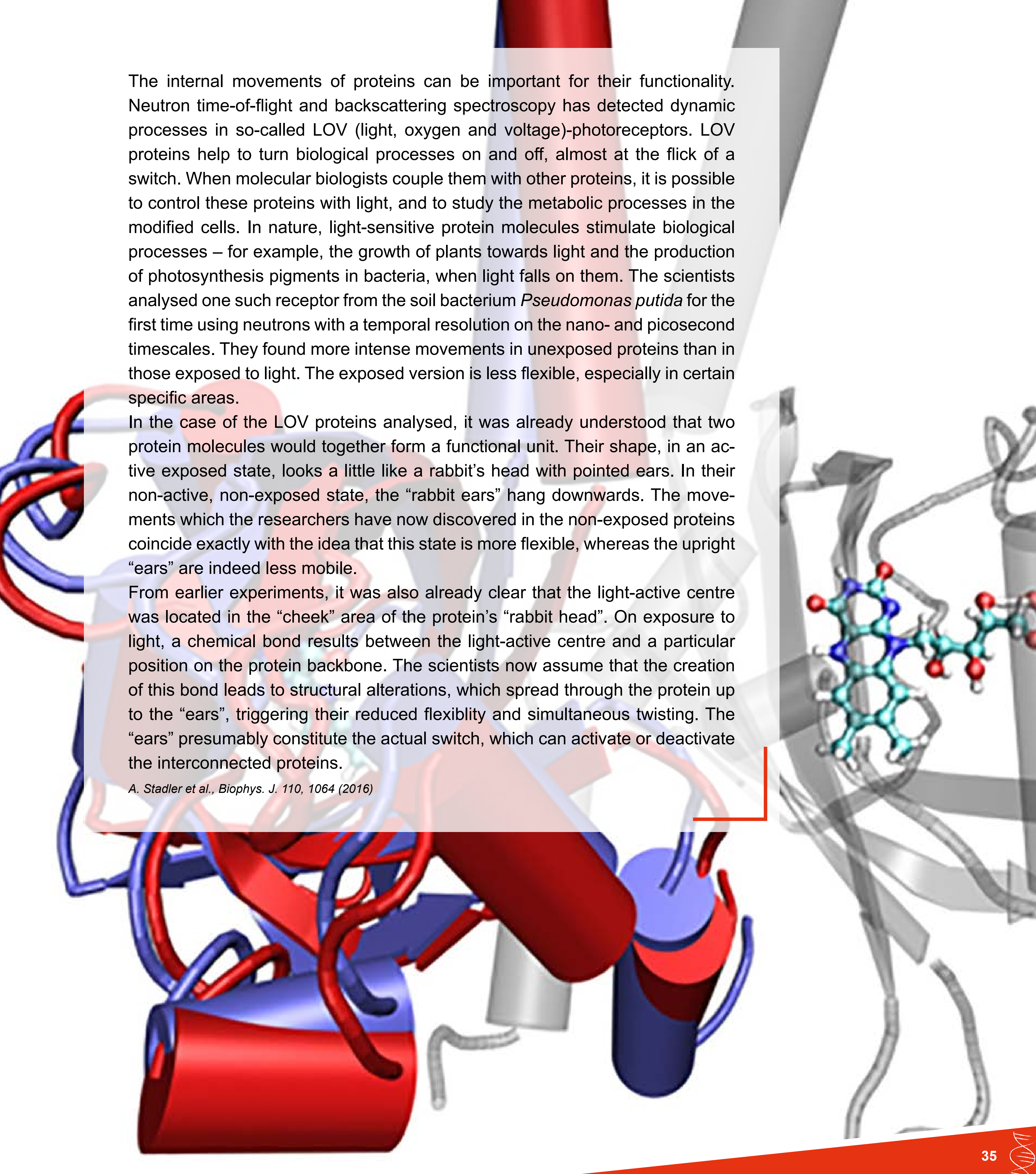
The researchers determined the structure of the Compound I state at a temperature of minus 173° Celsius in order to maintain the enzyme in its intermediate state for analysis.

Using neutron diffraction, the scientists discovered that, in the Compound I state, only a single oxygen atom is bound to the iron of the heme group. In other words, there is no hydrogen atom bound to the oxygen. This question has been under debate for 30 years. To their surprise, the scientists also discovered a group in the active centre that carries an additional hydrogen atom that was hitherto unknown. The reaction mechanism of the entire family of enzymes thus needs to be reconsidered.

C. M. Casadei et al., Science 345 (6193), 193 (2014)

"The exact nature of enzyme intermediates has been the subject of a long-standing controversy and conflicting interpretation of indirect evidence. At least we have been able to see these directly with the help of neutrons – this really is the "holy grail" of heme enzyme research."

Prof. Dr. Emma Raven, Biological Chemistry, University of Leicester, United Kingdom



The internal movements of proteins can be important for their functionality. Neutron time-of-flight and backscattering spectroscopy has detected dynamic processes in so-called LOV (light, oxygen and voltage)-photoreceptors. LOV proteins help to turn biological processes on and off, almost at the flick of a switch. When molecular biologists couple them with other proteins, it is possible to control these proteins with light, and to study the metabolic processes in the modified cells. In nature, light-sensitive protein molecules stimulate biological processes – for example, the growth of plants towards light and the production of photosynthesis pigments in bacteria, when light falls on them. The scientists analysed one such receptor from the soil bacterium *Pseudomonas putida* for the first time using neutrons with a temporal resolution on the nano- and picosecond timescales. They found more intense movements in unexposed proteins than in those exposed to light. The exposed version is less flexible, especially in certain specific areas.

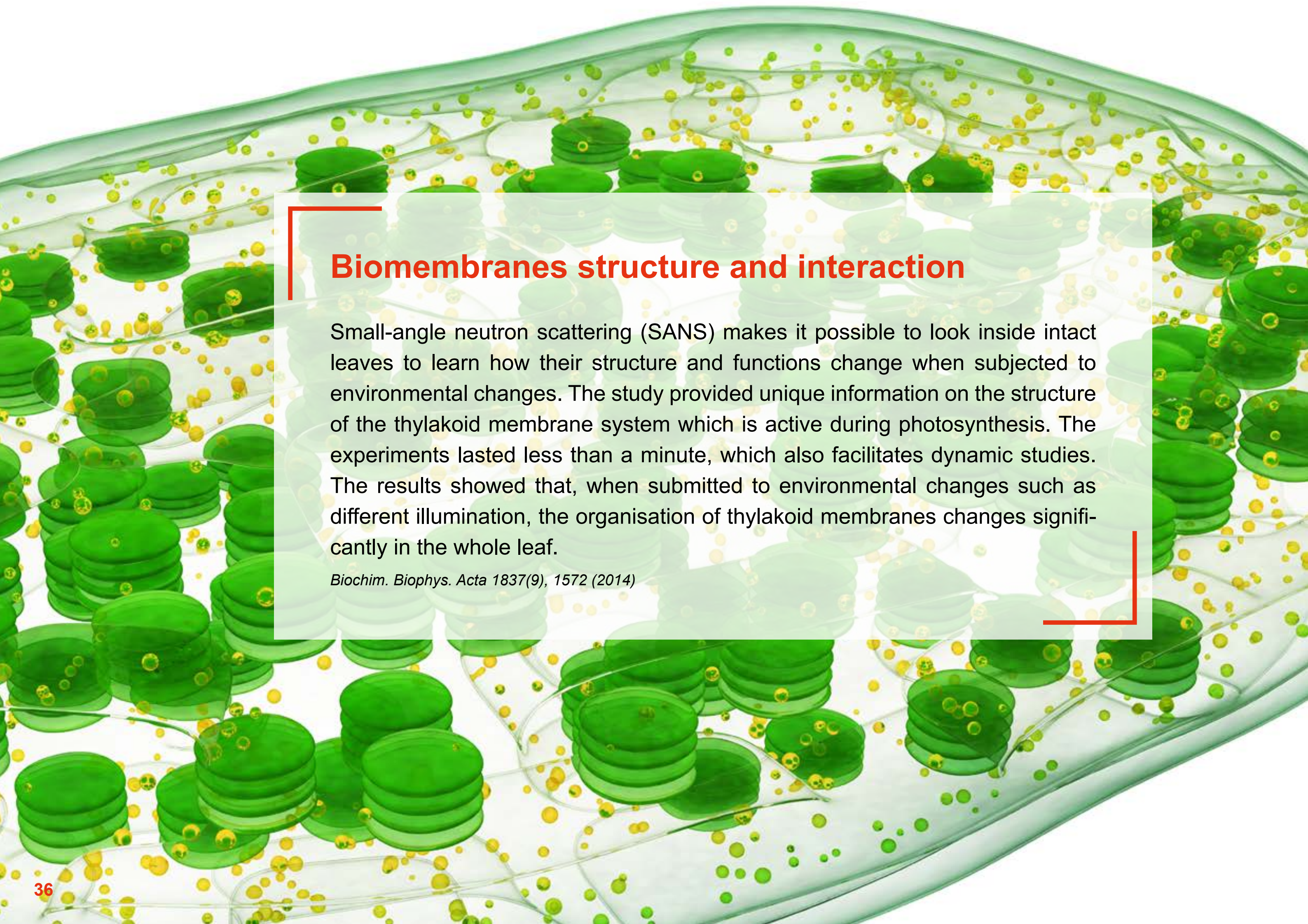
In the case of the LOV proteins analysed, it was already understood that two protein molecules would together form a functional unit. Their shape, in an active exposed state, looks a little like a rabbit's head with pointed ears. In their non-active, non-exposed state, the "rabbit ears" hang downwards. The movements which the researchers have now discovered in the non-exposed proteins coincide exactly with the idea that this state is more flexible, whereas the upright "ears" are indeed less mobile.

From earlier experiments, it was also already clear that the light-active centre was located in the "cheek" area of the protein's "rabbit head". On exposure to light, a chemical bond results between the light-active centre and a particular position on the protein backbone. The scientists now assume that the creation of this bond leads to structural alterations, which spread through the protein up to the "ears", triggering their reduced flexiblity and simultaneous twisting. The "ears" presumably constitute the actual switch, which can activate or deactivate the interconnected proteins.

A. Stadler et al., Biophys. J. 110, 1064 (2016)

"The use of the neutron techniques helped us to developments of effective theranostic nanosystems for application in nanomedicine."

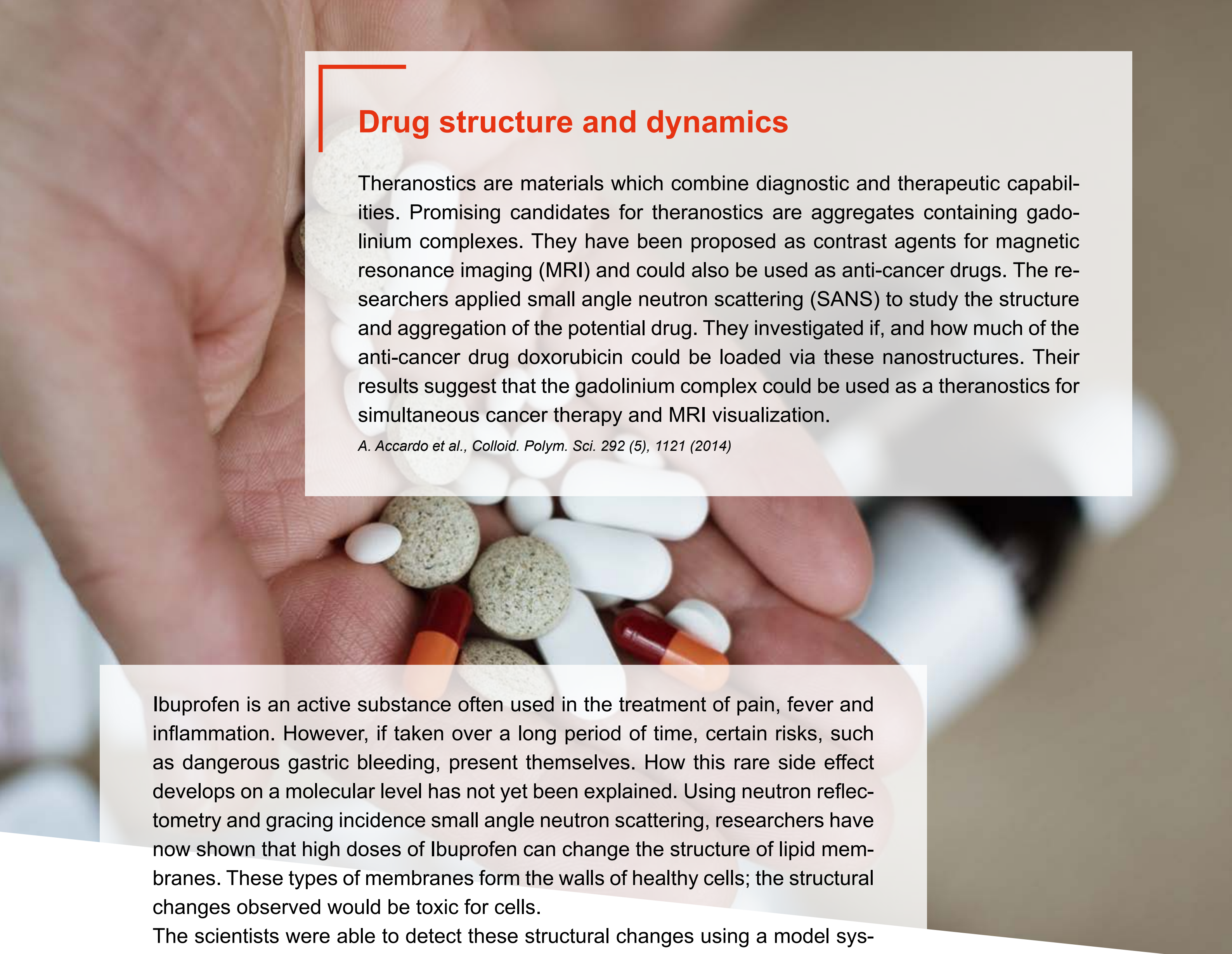
Prof. Dr. Luigi Paduano, Physical Chemistry, University Neapel Federico II, Naples, Italy



Biomembranes structure and interaction

Small-angle neutron scattering (SANS) makes it possible to look inside intact leaves to learn how their structure and functions change when subjected to environmental changes. The study provided unique information on the structure of the thylakoid membrane system which is active during photosynthesis. The experiments lasted less than a minute, which also facilitates dynamic studies. The results showed that, when submitted to environmental changes such as different illumination, the organisation of thylakoid membranes changes significantly in the whole leaf.

Biochim. Biophys. Acta 1837(9), 1572 (2014)



Drug structure and dynamics

Theranostics are materials which combine diagnostic and therapeutic capabilities. Promising candidates for theranostics are aggregates containing gadolinium complexes. They have been proposed as contrast agents for magnetic resonance imaging (MRI) and could also be used as anti-cancer drugs. The researchers applied small angle neutron scattering (SANS) to study the structure and aggregation of the potential drug. They investigated if, and how much of the anti-cancer drug doxorubicin could be loaded via these nanostructures. Their results suggest that the gadolinium complex could be used as a theranostics for simultaneous cancer therapy and MRI visualization.

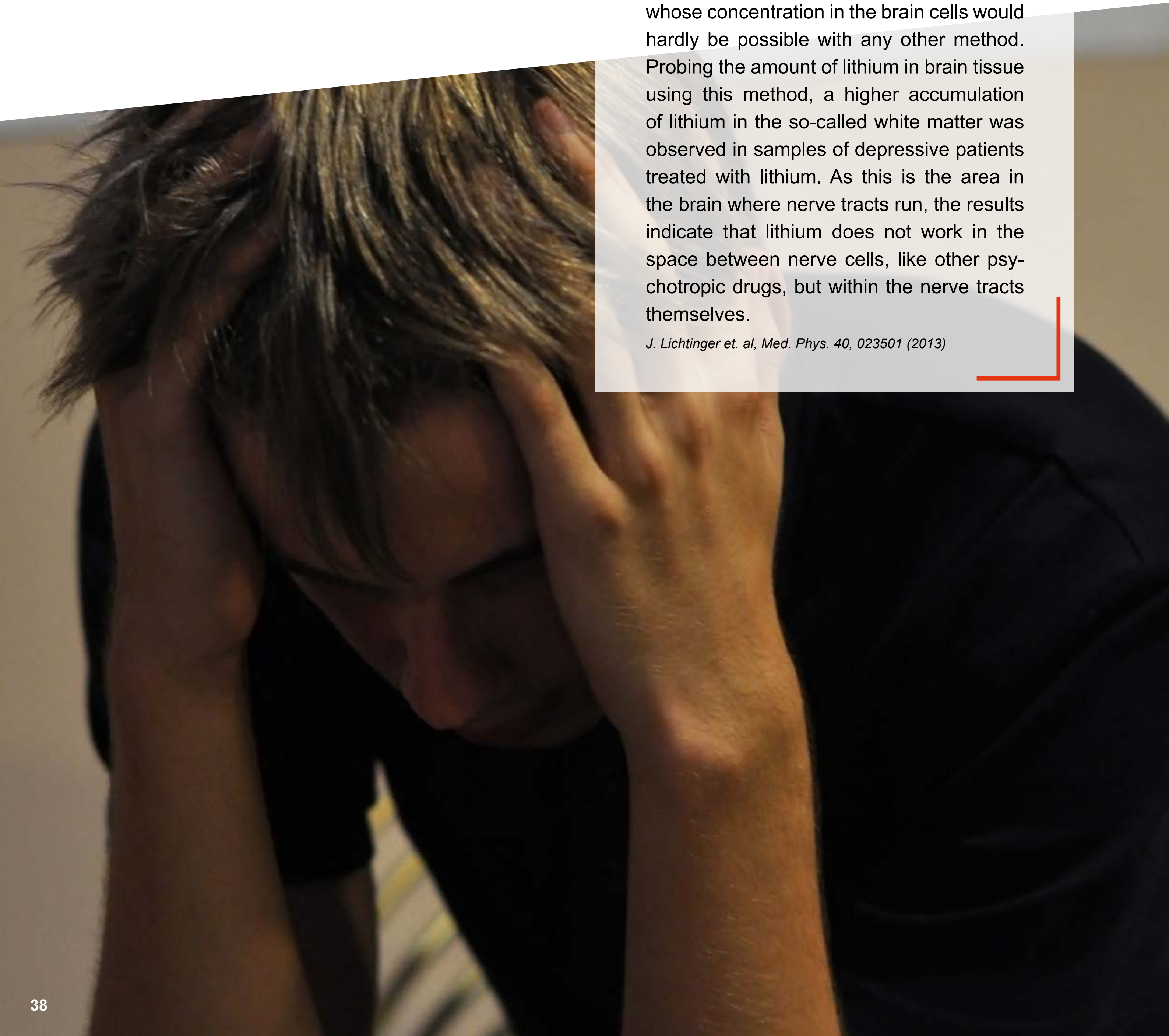
A. Accardo et al., Colloid. Polym. Sci. 292 (5), 1121 (2014)

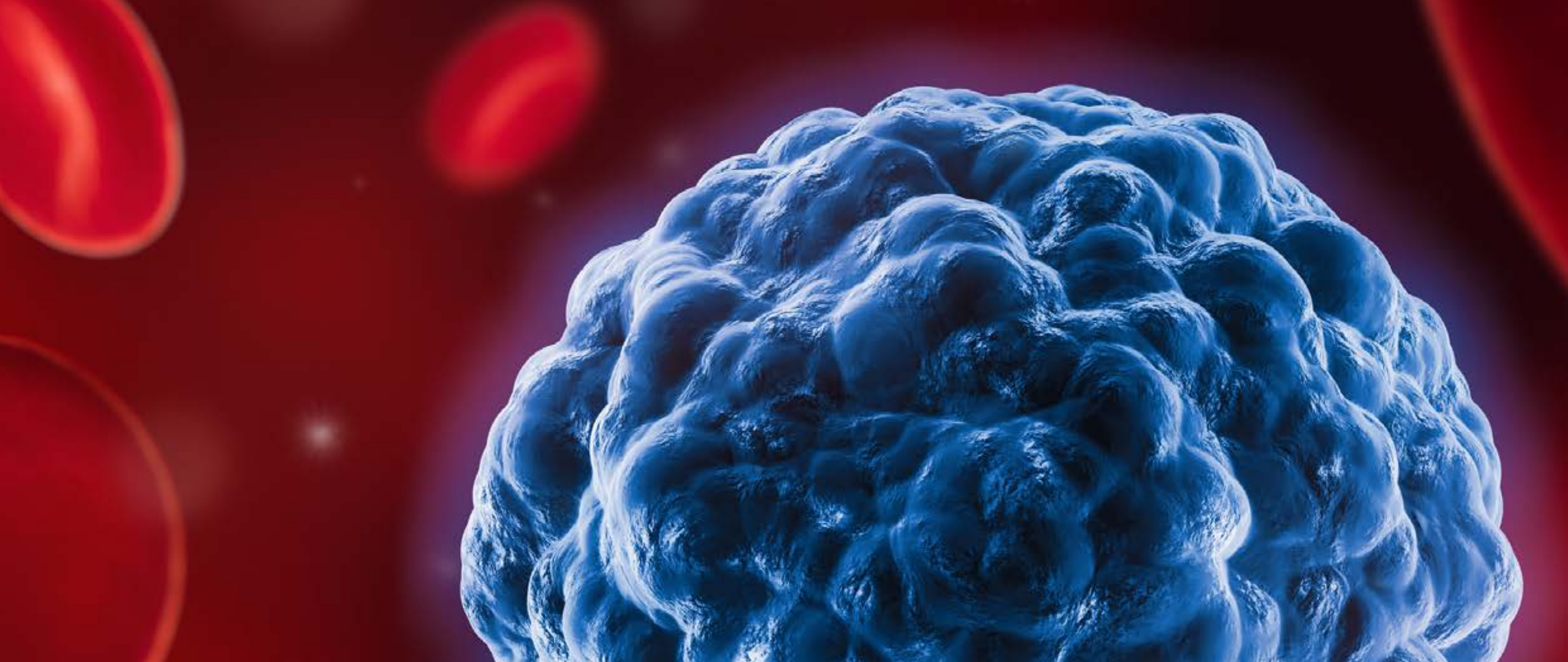
Ibuprofen is an active substance often used in the treatment of pain, fever and inflammation. However, if taken over a long period of time, certain risks, such as dangerous gastric bleeding, present themselves. How this rare side effect develops on a molecular level has not yet been explained. Using neutron reflectometry and gracing incidence small angle neutron scattering, researchers have now shown that high doses of Ibuprofen can change the structure of lipid membranes. These types of membranes form the walls of healthy cells; the structural changes observed would be toxic for cells.
The scientists were able to detect these structural changes using a model system of phospholipids from soy plants. Without ibuprofen or at low concentrations, the lipids examined formed parallel bilayers, which is usual for the cytomembrane of healthy cells. At high concentrations however, the membranes exhibited an ordered structure made up of holes.
The concentrations studied are far in excess of the estimated levels in medical applications. Researchers find it conceivable that, shortly after taking the medication, high concentrations may occur temporarily in certain places and – one might assume – this could be enough to cause tiny defects in the cell walls. Further studies should reveal whether this type of structural change can actually be observed in lipids of animal origin with complex structures.

S. Jaksch et al., Phys. Rev. E 91, 022716 (2015)

When absorbing a neutron, the lithium nucleus produces two charged particles. Detecting them at the same time offers an extremely low detection limit for this element, whose concentration in the brain cells would hardly be possible with any other method. Probing the amount of lithium in brain tissue using this method, a higher accumulation of lithium in the so-called white matter was observed in samples of depressive patients treated with lithium. As this is the area in the brain where nerve tracts run, the results indicate that lithium does not work in the space between nerve cells, like other psychotropic drugs, but within the nerve tracts themselves.

J. Lichtinger et. al, Med. Phys. 40, 023501 (2013)





Biomimetics

The teeth of chitons consist of a magnetite/protein-polysaccharide hybrid shell which displays remarkable properties such as outstanding fracture toughness, wear resistance and the highest reported hardness in biominerals. The mineralization mechanism of this material and the organic-inorganic hybrid structure were examined using small angle neutron scattering (SANS). The study revealed a strong interaction between ferric ions and gelatin molecules, leading to an inhomogeneous mineralization and a 'particle in matrix' structure, which will help to optimize the material for improved mechanical performance.

M. Siglreitmeier et al., Beilstein J. Nanotechnol. 6, 134 (2015)

Polymer drug carriers based on N-(2-hydroxypropyl)methacrylamide (HPMA) co-polymers have been developed for the treatment of tumors, with special focus on site-specific delivery and controlled release of anti-cancer agents into tumor tissues or cells. Such interest requires a detailed knowledge of the interior structure of the polymeric nanoparticles and structure evolution during drug delivery. Time-dependent SANS measurements following sharply changing pH levels have been applied to characterize the drug release and changes in the particle size and shape of HPMA. The change in pH simulates particle transport from the blood to the more acidic tumor environment. For most polymer-drug conjugates, nanoparticle growth or decay was observed within a time range of several hours in conditions mimicking the tumor microenvironment.

S. Filippov et al., Biomacromolecules 14, 4061 (2013)

Earth & Environment

Neutrons, thanks to their multiple applications and the prodigious possibilities for structural and chemical analysis that they offer, contribute to the understanding of environmental processes and the development of clean technologies. They also provide much needed insight into earth processes, geology, resources, and the properties of rocks and minerals.

Environment

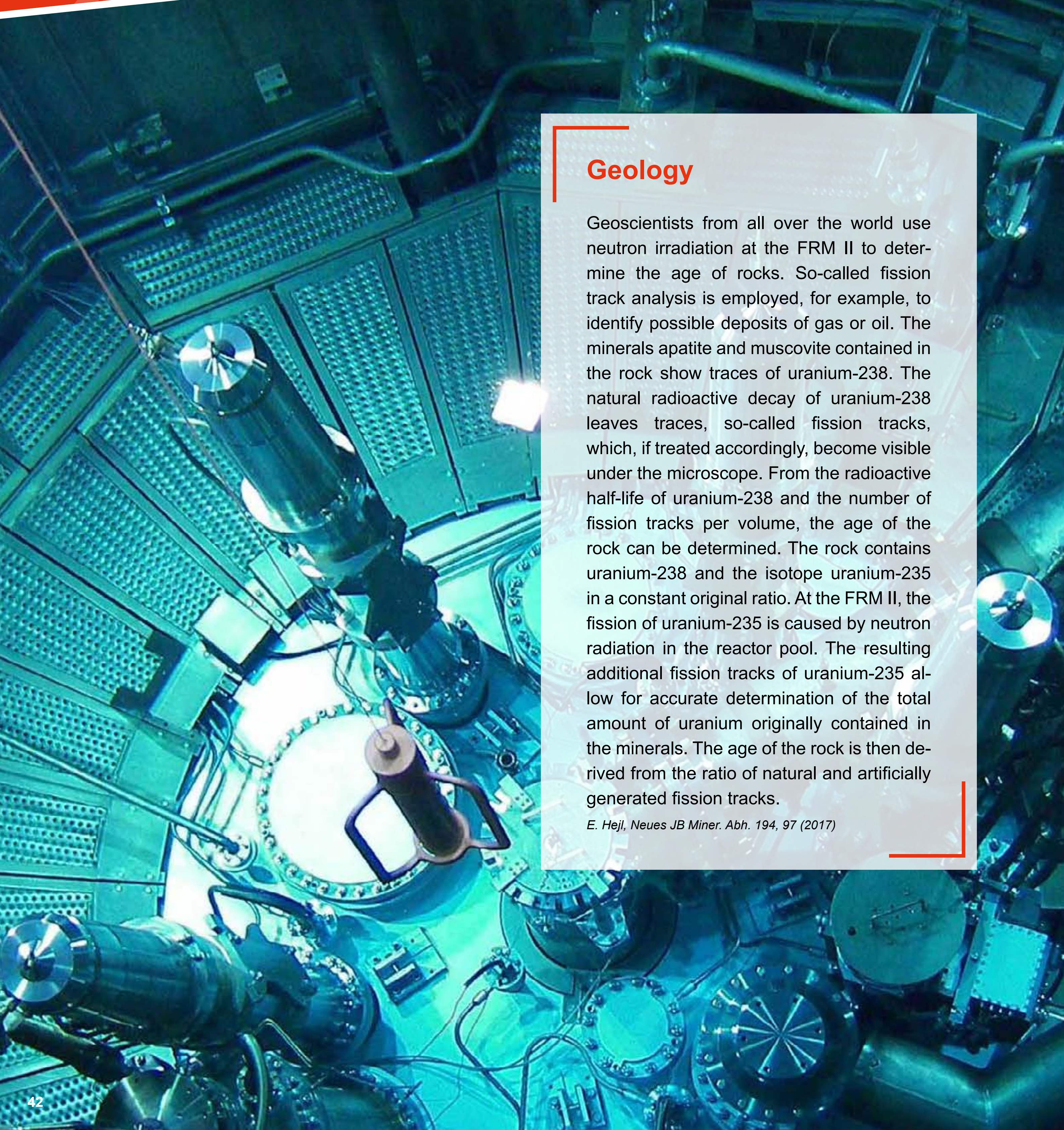
Reverse-osmosis (RO) desalination is an attractive technology nowadays, aiming to achieve high quality potable water from pretreated domestic wastewaters. One of the main limitations on cost-effective RO desalination is fouling of the membranes, mainly biofouling and scaling by calcium phosphate. SANS studies on the effect of the protein BSA on mineralization in a model salt solution were used to simulate the secondary effluent of a wastewater reclamation plant. The results will stimulate the development of chemical substances with similar organic functional groups which are sufficiently cheap and effective to be applied as coagulants in the process.

Y. N. Dahdal et al., Polymer 85, 77 (2016)

Climate

The long-term storage of carbon dioxide in porous layers of rock deep underground (carbon capturing and storage, CCS) could contribute to reducing the emission of climate-damaging gases in the atmosphere. With the help of small angle neutron scattering, an international research team investigating a natural 100,000-year-old carbon dioxide (CO_2) reservoir in Utah, USA, have shown that carbon dioxide dissolved in water remains stored in certain types of rock layers far longer than first envisaged. The storage of CO_2 in porous rock layers deep underground is a favoured solution. Before this can be achieved, there are many questions to be answered: Above all, how long can CO_2 remain stored in the rock? Thick layers of non-porous stone should prevent leakage, but the question arises as to how long they resist the acidic solutions of the liquefied gas. In the case of the natural reservoir in Utah, current experiments have found the top layer to be stable for at least 100,000 years, or ten times as long as once thought. Important information about the changes in the pore network structure was obtained using neutron small angle scattering instrument.

N. Kampman et al., Nat. Commun. 7, 12268 (2016)



Geology

Geoscientists from all over the world use neutron irradiation at the FRM II to determine the age of rocks. So-called fission track analysis is employed, for example, to identify possible deposits of gas or oil. The minerals apatite and muscovite contained in the rock show traces of uranium-238. The natural radioactive decay of uranium-238 leaves traces, so-called fission tracks, which, if treated accordingly, become visible under the microscope. From the radioactive half-life of uranium-238 and the number of fission tracks per volume, the age of the rock can be determined. The rock contains uranium-238 and the isotope uranium-235 in a constant original ratio. At the FRM II, the fission of uranium-235 is caused by neutron radiation in the reactor pool. The resulting additional fission tracks of uranium-235 allow for accurate determination of the total amount of uranium originally contained in the minerals. The age of the rock is then derived from the ratio of natural and artificially generated fission tracks.

E. Hejl, Neues JB Miner. Abh. 194, 97 (2017)

Cultural Heritage & Art

Neutrons are an invaluable tool in analysing 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, determine the 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.

"The research reactor offers a wide variety of possibilities for non-destructive examination of archaeological objects. Over many years, valuable information on the origin or production of objects has been gained, as well as new concepts for conservation."

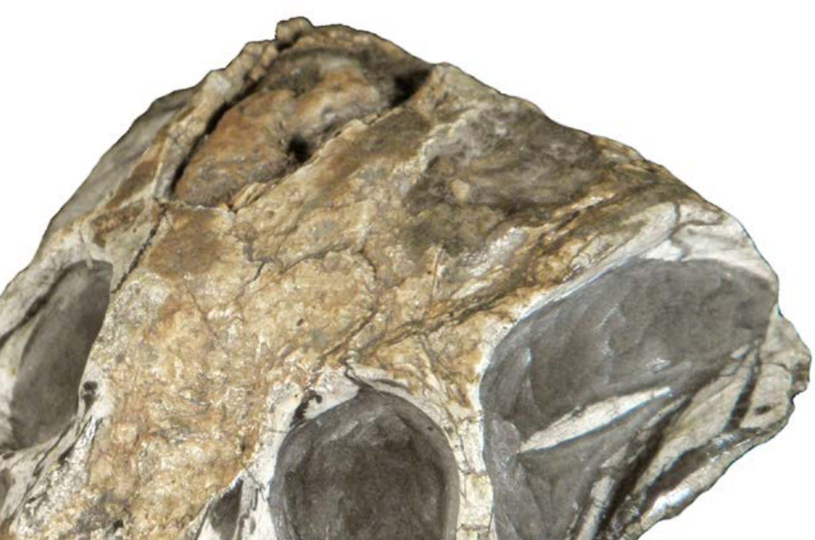
Prof. Dr. Rupert Gebhard, Director of the Archaeological Collection of the Bavarian State, Munich, Germany

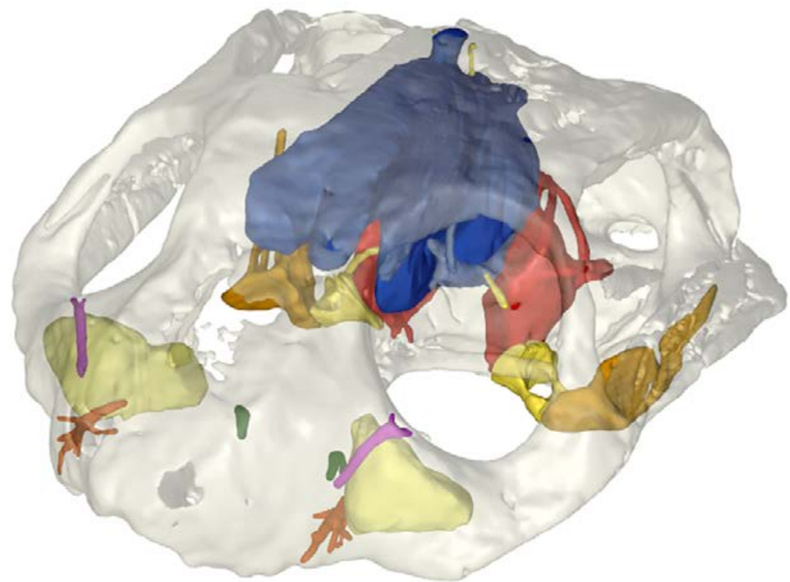
Archaeology

Iron has become one of the most important materials in the study of prehistoric and historic cultures. Therefore, the preservation of iron artefacts and the prevention of corrosion, in particular, plays a predominant role in the work of archaeological museums. Prompt Gamma Activation Analysis (PGAA) is ideally suited for determining the chlorine content of artefact pieces without destroying the valuable objects. With sensitivity in the ppm range, PGAA allows systematic, non-destructive tests of the efficiency of leaching procedures in the preservation of artefacts.

F. E. Wagner et al., Hyperfine Interact. 237, 30 (2016)

Thanks to neutron tomography, physicists were afforded a glimpse into a Roman god. Since neutrons penetrate metals much better than X-rays, they found that the figurine is hollow. Neutron radiography also showed that the legs were added after the first casting. A little door at the back seems to have been prised open after manufacture to remove the casting core.





Some 410-360 million years ago, the first vertebrates that developed from amphibians were not able to hear airborne sound, as this had not been necessary for life in water. Nevertheless, these animals were not completely deaf. It is believed that they could perceive ground vibrations on the body surface, the limbs, and especially via the jaw resting on the bottom, as do some snakes and crocodiles to this day. In order to hear the much weaker airborne sound, however, a drum, a middle ear apparatus with hammer, anvil and stirrup for amplification and a specialized inner ear are necessary, and up until now little has been known about the formation of these. Using neutron tomography, geoscientists have found that airborne sound listening began 30 million years earlier than previously thought.

M. Laaß and B. Schillinger, Physics Procedia 69, 628 (2015)

"Neutrons can easily penetrate iron-bearing rocks which shield X-rays, and provide excellent contrast between bone and rock."

Michael Laaß, Palaeontologist at the University of Duisburg-Essen, Germany

Art

Restorers employed two different cleaning methods on the 15th century head of the prophet that adorns the bronze Gates of Paradise at the Baptistery of San Giovanni in Florence: they cleaned a part of the bronze surface, blackened over the years, with a laser, another part chemically using salts and a third portion of the head remained uncleaned. It was hoped that neutron analysis would show nondestructively which cleaning method is optimal. In the case of the bronze head from the Paradise Gate in Florence, analysis with neutrons revealed that the chemical restoration method is more efficient. On the surface cleaned in this way, physicists found less residue of chlorine, which forms part of the black deposits.

Engineering & Nano Materials

Novel, high performance composite materials and devices that are organised from the meso to the nano-scale are being developed for applications in areas such as healthcare, information processing, energy, engineering or the environment. Developments in novel materials and 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. Neutrons cover all the length scales from the Ångström scale of the atomic structure of individual building blocks to the configuration of assembled, functional structures, making them essential tools for the elucidation of novel, smart materials and nanostructures.

Stress and strain

Metal matrix composites (MMCs) are widely used in advanced industries because of their outstanding properties. However, the poor weldability of MMCs is one of the major factors that limit the widespread application of MMCs. Friction stir welding (FSW) is considered to be a promising technique for joining MMCs. Using neutron diffraction, the multiscale residual stresses in welds were characterized and used to calculate thermal and plastic misfits.

X.X. Zhang et al., Acta Mater. 87, 161 (2015)

A mathematical model of the manufacturing process for large aluminium forgings used to machine compressor impellers weighing almost 150 kg revealed that the manufacturing process generated considerable mechanical stresses in the block's interior. Internal stresses of this kind can lead to material fatigue and cracks and, more importantly, may cause distortions in the impeller during the final machining process. Subsequently, the ability to calculate the tolerable limits of internal stress of components is of extreme importance to manufacturers. From strain measurements using neutrons, the residual stresses that verify the simulation models has been determined, leading to an improvement in the theoretical models used.

N. Chobaut et al., Finite Elem. Anal. Des. 131, 17 (2017)

"In our search for new materials for gas turbines, we have developed a new alloy system based on cobalt and rhenium. Neutrons help us to understand the stability and transformation of the microstructures at high temperatures."

Prof. Dr. Joachim Rösler, Institut für Werkstoffe, Technische Universität Braunschweig, Germany

Superalloys

The characterisation of early stage precipitation in Ni-based superalloys is an important issue as it strongly supports the development of new high temperature alloys. These alloys with single crystal precipitates embedded in a matrix are responsible for the strengthening of the blades in gas turbines. The formation of fine precipitates and their initial growth in an alloy system of a tungsten-rich Ni-based superalloy has been revealed by SANS due to the fact that this method makes it possible to characterize inhomogeneities of the order of 1-300 nm even in-situ at high temperatures, making it the perfect match to receive a size and volume fraction of these precipitates.

R. Gilles et al., J. Alloy. Compd. 612, 90 (2014)

Nowadays, researchers are looking for new materials for future gas turbines, as the current "work- horse" Ni-Superalloys are reaching their service temperature limit because of the melting point of the material. One candidate is the cobalt-rhenium-chromium (Co-Re-Cr) system that exhibits a higher melting point in the order of 100-200°C (depending on composition) than the Ni-based superalloys. Co-Re-Cr alloys are strengthened with nanoscaled tanatalum carbides (TaC). Complementary neutron diffraction and small-angle neutron scattering measurements, especially in-situ at high temperatures, were performed to study the stability of these TaC precipitates. It turns out TaC precipitates are stable at least up to 1200°C, making the important precipitates very interesting for alloy strengthening.

D. Mukherji et al., Mater. Lett. 64, 2608 (2010)

Nano materials

A currently active field of research is focused on the special class of soft colloids, i.e. elastic and deformable colloidal particles, which display a dual character associated with polymers and hard spheres. Due to their hybrid nature, soft colloids macroscopically show interesting structural and dynamic properties resulting from their unique microscopic structure. Small angle neutron scattering (SANS) revealed experimental structure factors S(Q) which, in combination with liquid state theory and simulations, lay the basis for understanding soft colloids.

S. Gupta et al., Phys. Rev. Lett. 115, 128302 (2015)

Glasses are part of the wide family of disordered materials. This means that their structure lacks any long-range order even if it is far from being totally random. Positron lifetime annihilation spectroscopy (PALS) represents a unique tool for looking into the interstitial voids in glasses and mapping their evolution as a function of density. PALS data allow us to describe with great accuracy the depth dependence of the density in absolute units, shedding some new light on the subtle nature of medium range order .

M. Zanatta et al., Phys. Rev. Lett. 112, 045501 (2014)

Soft materials

In engineering, bioengineering and medicine there is a huge demand for tailor-made polymeric materials that possess the ability to undergo massive changes in their volume, their elasticity or related properties when exposed to small stimuli. The working principle of these smart polymeric materials is based on a demixing phase transition, leading to massive changes in volume and elasticity. In order to elucidate the underlying mechanisms of phase separation, the dehydration of model thermo-responsive polymers in an aqueous environment was revealed using time-of-flight neutron spectroscopy.

M. Philipp et al., J. Phys. Chem. B 118, 4253 (2014)

Surface functionalization based on stimuli-responsive dispersed colloidal particles is an active area of research. The cooperative and inner dynamics of the dispersed particles were characterized by neutron spin echo spectroscopy while the inner properties of the adsorbed microgel particles were probed by neutron spin echo spectroscopy under grazing incidence. These microgels have a volume phase transition temperature close to body temperature (37°C). Adsorbed at solid substrates, such coatings could support implant integration into the body by minimization of infections and inflammation.

K. Gawlitza et al., Macromolecules 48 (16), 5807 (2015)

Tight packing leads to co-ordinated movements of larger groups of atoms within the melt. Neutron spectroscopy makes it possible to detect how long-chain molecules in their liquid melt move. The results contribute to a better understanding of mass transport in liquids, which plays a crucial part in many technologically relevant processes, for example in charging and discharging batteries, electrolysis, and chemical reactions such as catalysis in the liquid phase.

H. Morhenn et al., Phys. Rev. Lett. 111, 173003 (2013)

Information Technology & Quantum Phenomena

Advanced storage materials and technologies are needed to meet the ever-growing demand for increasingly fast and small devices such as computers, mobile phones and media players. The discovery of giant magneto-resistance (GMR) was the first application of spintronics to nanotechnology and resulted in the award of the Nobel Prize for Physics in 2007. It has given rise to a new field of research and led to important advances in wide ranging areas such as hard drive technology, magnetic-field sensors and transistors. Neutron scattering and the unique ability of neutrons to probe magnetic phenomena are contributing extensively in these areas.

Magnetic materials

Multilayers of rare earth such as gadolinium, dysprosium or terbium and ferromagnetic elements are known to show exchange bias effects. In these kinds of multilayer systems, a hard and a soft magnetic layer are combined and magnetically coupled at the interface. Polarized neutron reflectivity is an effective tool to probe such challenging ferrimagnetic systems. The temperature evolution of the coercivities and the reflectivity data, explain the magnetic behaviour of the system.

A. Paul et al., Phys. Rev. B 89, 14445 (2014)

The magnetocaloric effect describes the change in temperature of a material if exposed to a magnetic field and forms the basis of magnetocaloric refrigeration technologies. Compared to conventional vapor compression cooling magnetic refrigeration technologies have the potential for 20-30 % lower energy consumption. With neutron diffraction experiments two different magnetic systems were found in the compound $MnFe_4Si_3$, a promising candidate for ambient temperature magnetic cooling. This feature might be the key to the occurrence of a large magnetocaloric effect in other magnetocaloric materials too.

P. Hering et al., Chem. Mat. 27 (20), 7128 (2015)

Multiferroics

The emergence of ferroelectricity in representatives of the melilite family, including $Ba_2CoGe_2O_7$, below their magnetic ordering temperature is remarkable and the complex response of these materials to magnetic and electric fields can not be explained by the mechanisms commonly applied to the other multiferroics. Using spherical neutron polarimetry (SNP) the magnetic symmetry of the compound was refined precisely and the distribution of the magnetic domains in zero field and under the influence of the magnetic and electric fields determined, which made it possible to check the agreement with proposed models.

Using 3D polarization analysis the proportion of domain types in multiferroic crystals and the change when a magnetic and electric field is applied could be examined and accurately determined. With the help of this unique technique, it has been demonstrated experimentally that only one of the many theories fits the results measured.

V. Hutanu et al., Phys. Rev. B 89, 064403 (2014)

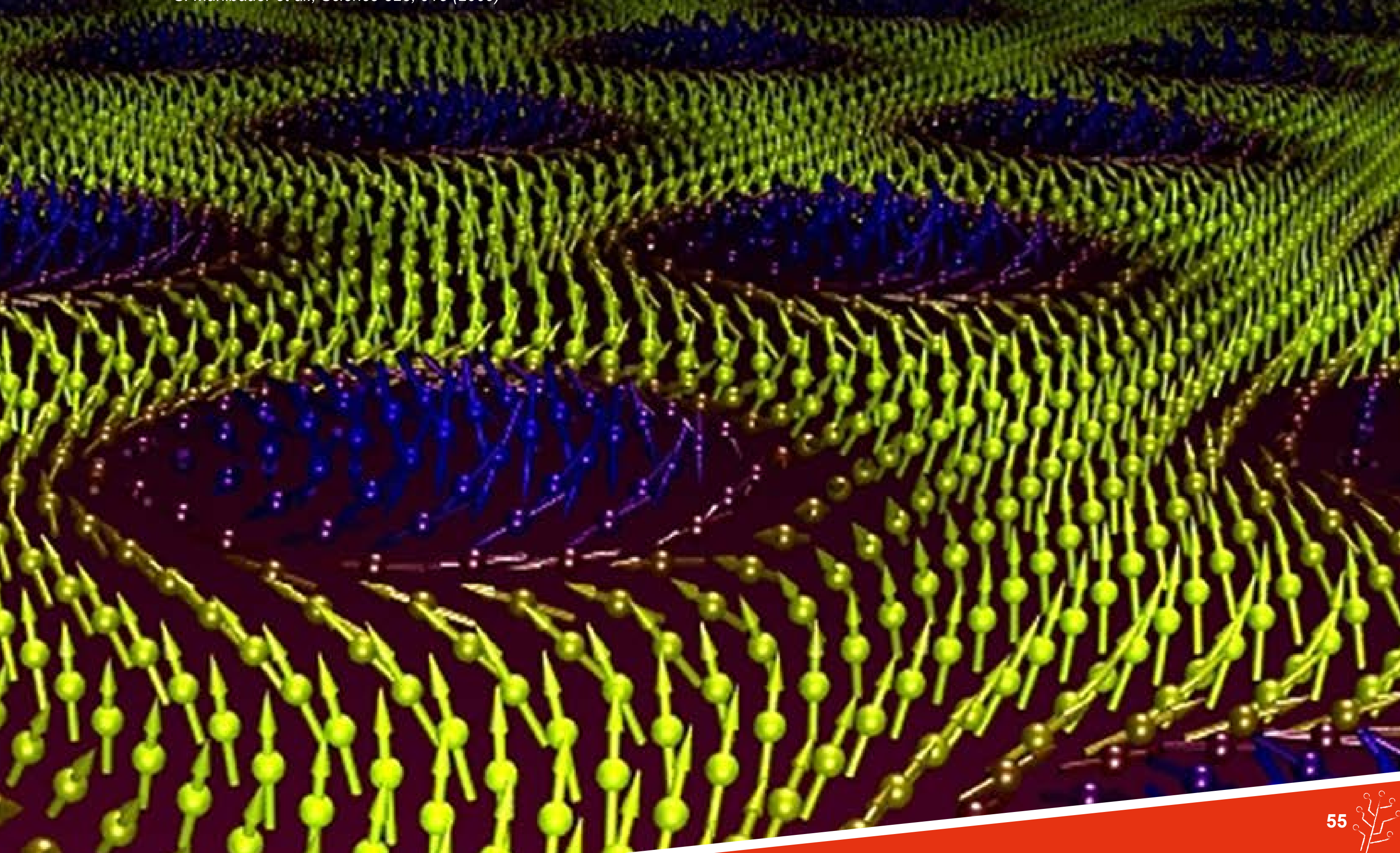
Skyrmions

In the case of magnetic monopoles in magnetic vortices, called skyrmions, information can be written and erased, which could provide a decisive step toward the realization of novel, highly efficient data storage devices. Whereas one needs around a million atoms to store one bit in a modern hard disk, the smallest known skyrmions in magnetic materials consist of only 15 atoms. At the same time moving such skyrmions requires 100,000 times less power than moving memory bits in devices based on conventional magnetic materials. The magnetic vortex structures were discovered through neutron scattering experiments on manganese-silicon.

S. Mühlbauer et al., Science 323, 915 (2009)

Skyrmion lattices – regular crystalline arrangements of Skyrmion lines found in chiral magnets provide an excellent showcase for the investigation of topological stability and phase conversion. Small-angle neutron scattering (SANS) is used to investigate the topological stability and decay of skyrmions. Bulk sensitive SANS data have proven the essential features of the topological unwinding of skyrmions in such samples.

P. Milde et al., Science 340, 6139 (2013)



Nuclei & Particles

Neutrons themselves are the object of study, because knowing their characteristics can contribute to the development of the grand theories of our universe. They are also probes for exploring atomic nuclei and for measuring fundamental constants. Neutrons are used to investigate the quantum effects of gravity or to test Einstein's mass-energy equivalence, for example.

Dark matter & the universe

Dark matter is invisible, but it acts on matter due to its gravitational pull, influencing the rotation of galaxies. If new kinds of particles or additional forces of nature exist, it should be possible to observe them. Neutrons are perfectly suited for this type of research. They do not carry electric charge and they are hardly polarizable. According to quantum theory, if very slow neutrons are used and funnelled between two parallel plates according to quantum theory, the neutrons can only occupy discrete quantum states with energies which depend on the force that gravity exerts on the particle. By mechanically oscillating the two plates, the quantum state of the neutron can be switched. In this way, the difference between the energy levels can be measured.

T. Jenke et al., Phys. Rev. Lett. 112, 151105 (2014)

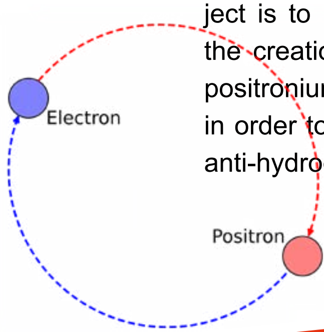
Antineutrinos

In addition to neutrons, the fission reaction of nuclear fuels such as plutonium or uranium releases antineutrinos. These are also electrically neutral, but can pass through matter very easily. Changes in the composition of nuclear fuels in the reactor can be determined by analyzing the energy and rate of antineutrinos. This is an additional option for monitoring reactors. The antineutrino spectra of three main fuel isotopes, uranium-235, plutonium-239 and plutonium-241, had already been determined. However, the antineutrino spectrum of the fourth main nuclear fuel, uranium-238, which accounts for approximately 10 percent of the total antineutrino flux, remained unclear. With an experimental set-up using fast neutrons at the MLZ the missing spectrum of uranium-238 could be measured.

N. Haag et al., Phys. Rev. Lett. 112, 122501 (2014)

Positronium

The characteristics of antimatter are still not fully understood. For example, it is not known whether or not anti-hydrogen is subject to the earth's gravitation or not. In order to produce anti-hydrogen efficiently from a reaction of anti-protons and positronium atoms at the European organization for nuclear research CERN, scientists need free positroniums. These particles composed of a positron and an electron exhibit a short lifetime of 142 nanoseconds. The positron source NEPOMUC at the MLZ, which boasts the highest monoenergetic positron intensity in the world, can produce a high number of positroniums. The aim of the project is to prepare a well-defined target for the creation of a high density of free cold positroniums at the FRM II positron source in order to enable the efficient formation of anti-hydrogen at CERN.



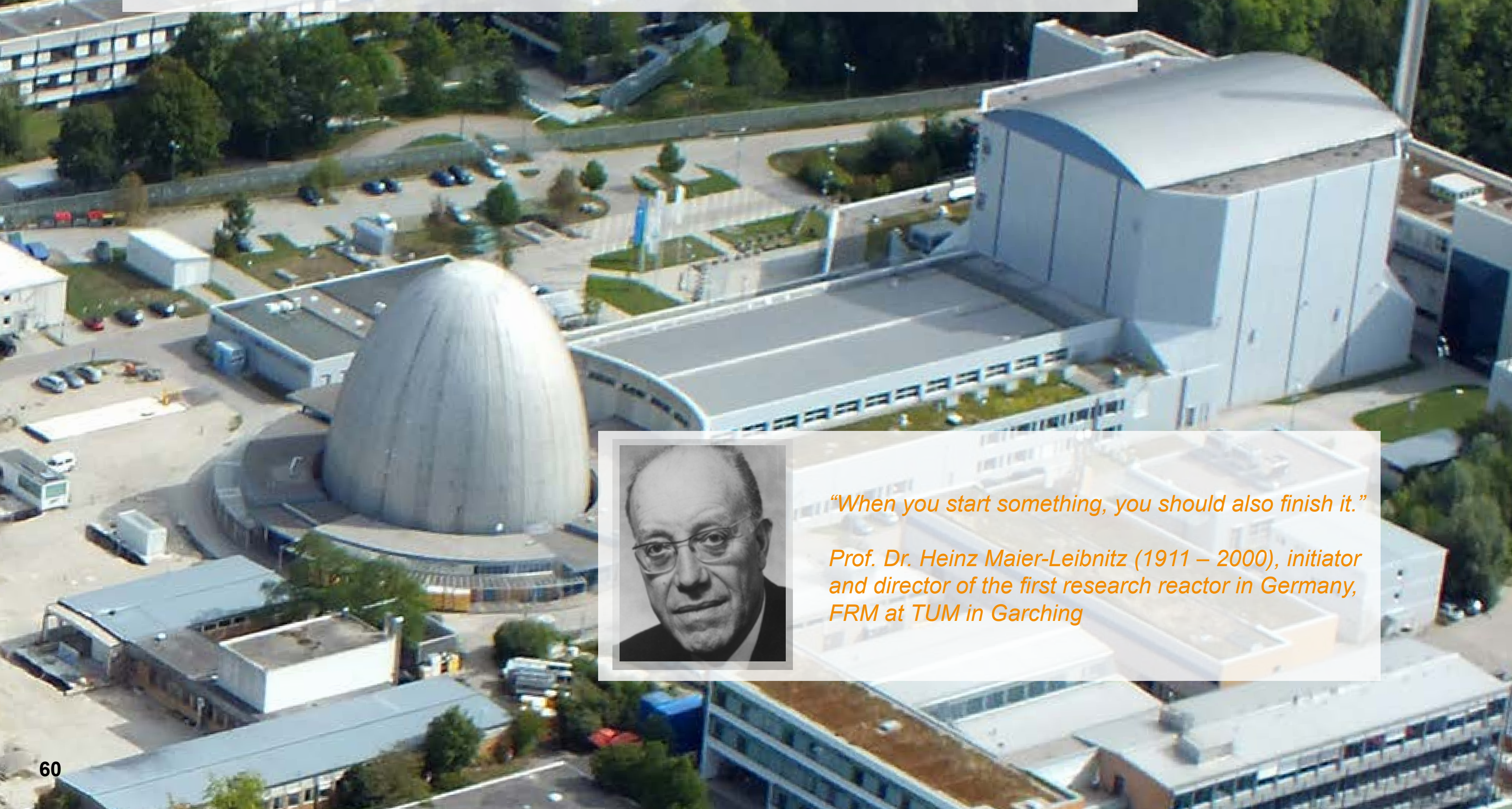
Facts & Figures

The Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) provides the highest neutron flux from a unique suite of sources ranging from ultra-cold (under construction), cold, thermal, hot to fast fission neutrons, covering neutron energies from nano to mega electron volts. In addition, one of the beam tubes serves as a positron source, offering the world's most brilliant flux of positrons for surface and defect analysis. About 30 scientific instruments are served simultaneously during the reactor operation of up to 240 days per year. Irradiation facilities for the production of radioisotopes, silicon doping or the analysis of samples by activation analysis extend the use of the FRM II for industrial clients in particular.

FRM II reactor

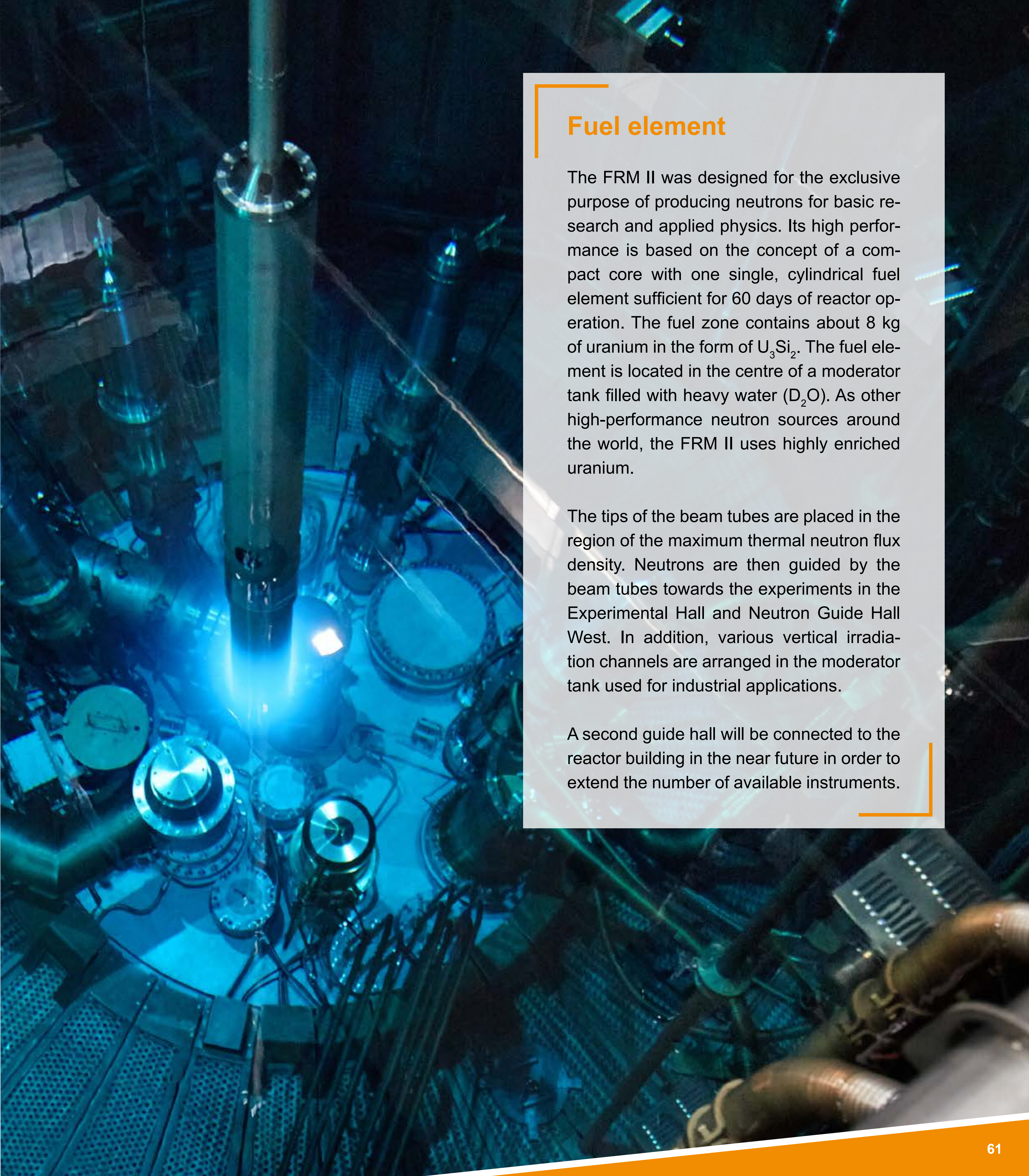
The Research Neutron Source Heinz Maier-Leibnitz (FRM II) is the most powerful neutron source in Germany and reaches the highest neutron flux density ($8 \cdot 10^{14}$ n/cm^{-2}s^{-1}, max. undisturbed flux density) relative to its thermal power (20 MW) world-wide. The FRM II is operated as a Corporate Research Center by the Technische Universität München (TUM) in Garching near Munich, Germany. Its first criticality was achieved in March 2004.

Some 30 experimental facilities are operated by scientific teams from German universities, research institutes of the Helmholtz Association, and the Max Planck Society. Today, 27 beam tube facilities are operational. A further seven irradiation facilities mainly for medical and industrial application are in service and an irradiation facility for the production of the medical isotope ^{99}Mo is under construction. The FRM II is equipped with cold, thermal, hot, and fast neutron sources and thus covers a broad range of applications, including a device for the continuous production of an intense positron beam.



"When you start something, you should also finish it."

Prof. Dr. Heinz Maier-Leibnitz (1911 – 2000), initiator and director of the first research reactor in Germany, FRM at TUM in Garching



Fuel element

The FRM II was designed for the exclusive purpose of producing neutrons for basic research and applied physics. Its high performance is based on the concept of a compact core with one single, cylindrical fuel element sufficient for 60 days of reactor operation. The fuel zone contains about 8 kg of uranium in the form of U_3Si_2. The fuel element is located in the centre of a moderator tank filled with heavy water (D_2O). As other high-performance neutron sources around the world, the FRM II uses highly enriched uranium.

The tips of the beam tubes are placed in the region of the maximum thermal neutron flux density. Neutrons are then guided by the beam tubes towards the experiments in the Experimental Hall and Neutron Guide Hall West. In addition, various vertical irradiation channels are arranged in the moderator tank used for industrial applications.

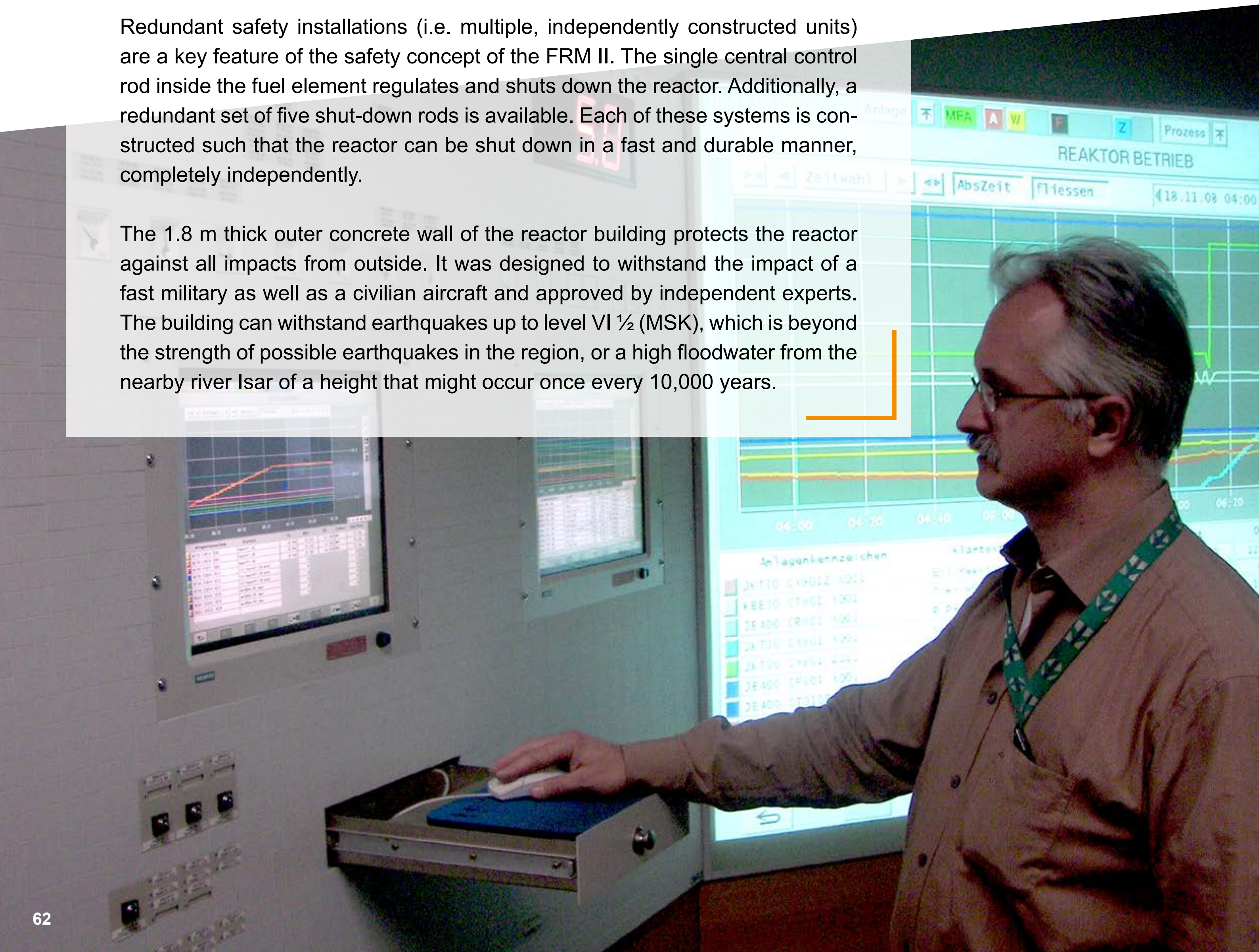
A second guide hall will be connected to the reactor building in the near future in order to extend the number of available instruments.

Safety over and above the standard

The highest priority is always given to safety at the FRM II. The inherent safety stems from its principle design. The fuel element, moderator tank, and beam tubes are located in the reactor pool filled with 700 m³ of highly purified water. On passing the fuel element, the temperature of the cooling water only increases from 37°C to a maximum of around 53°C. Neither steam nor high pressures are produced. Three subsequent cooling circuits guarantee the safe dissipation of the 20 MW thermal power via the air path.

Redundant safety installations (i.e. multiple, independently constructed units) are a key feature of the safety concept of the FRM II. The single central control rod inside the fuel element regulates and shuts down the reactor. Additionally, a redundant set of five shut-down rods is available. Each of these systems is constructed such that the reactor can be shut down in a fast and durable manner, completely independently.

The 1.8 m thick outer concrete wall of the reactor building protects the reactor against all impacts from outside. It was designed to withstand the impact of a fast military as well as a civilian aircraft and approved by independent experts. The building can withstand earthquakes up to level VI ½ (MSK), which is beyond the strength of possible earthquakes in the region, or a high floodwater from the nearby river Isar of a height that might occur once every 10,000 years.



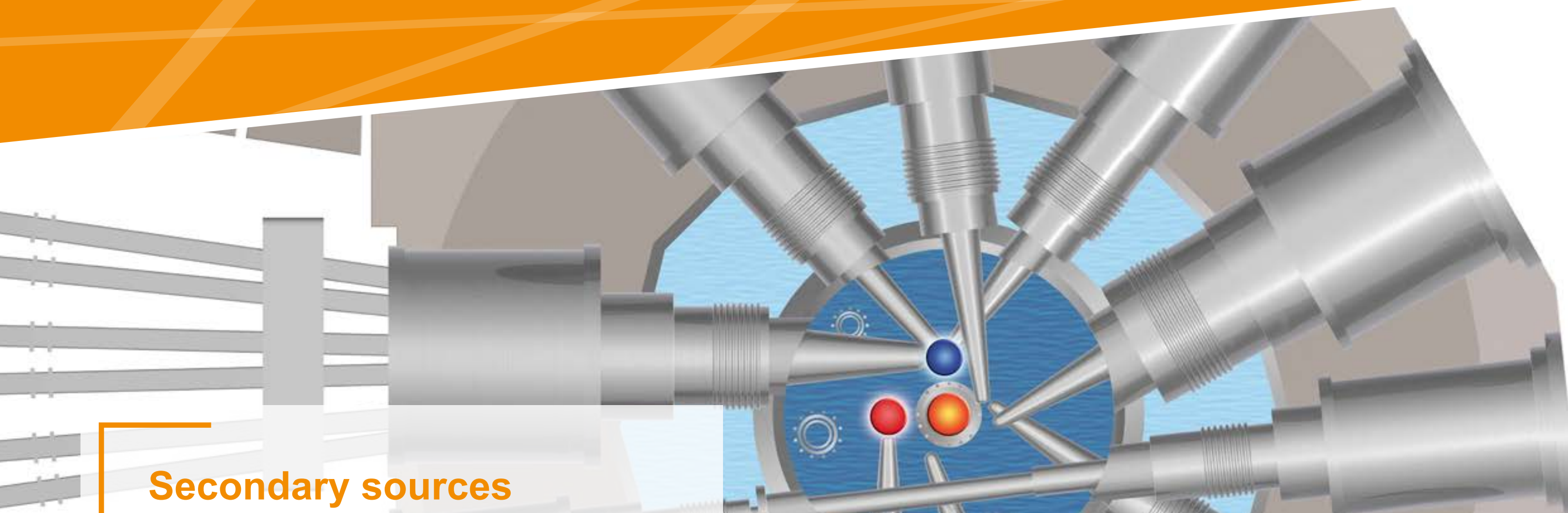
Reactor main parameters

- Thermal power: 20 MW
- Max. undisturbed thermal neutron flux density: $8 \cdot 10^{14}$ n/cm^{-2} s^{-1}
- 10 horizontal; 2 tilted beam tubes
- D_2O moderator
- H_2O cooling water

Staff and money

435 Mio€ construction costs (2003)

~ 400 employees on-site (MLZ + FRM II)



Secondary sources

The different instruments at the neutron source FRM II are supplied by various secondary sources that slow down or speed up the neutrons after thermalisation in the moderator tank. In total, five instruments, all in the Experimental Hall, are provided with thermal neutrons without further change to their energies by secondary sources.

At FRM II, a major proportion of the experiments is carried out using low energy ("cold") neutrons. This is achieved by three beam tubes being fed from the so-called cold neutron source, which is located within the moderator tank close to the maximum of the thermal neutron flux density. The moderator tank contains around 12 l of liquid deuterium (D_2) at a temperature of about 25 K. Neutrons interacting with the liquid D_2 in the moderator chamber lose their energy and their energy spectrum is shifted considerably into the low energy range in the order of 0.1 – 20 meV. Altogether 17 instruments are fed by cold neutrons, 15 of them in the Neutron Guide Hall West alone.

Neutrons with short wavelengths in the range of 0.1 eV to 1 eV are used to investigate the structure of condensed matter. As only a small fraction of this spectral range is present in the thermal neutron distribution, the neutrons are moderated upwards from about 300 K to 2200 K. This spectrum shift is performed by a hot neutron source. The hot moderator consists of a graphite block thermally insulated in the moderator tank next to the maximum thermal neutron flux density. Two instruments in the Experimental Hall are fed with neutrons by the hot source.

In order to obtain a high-intensity neutron beam with an unmoderated fission spectrum, an arrangement of uranium plates is inserted as a secondary source (a so-called converter). It supplies the tumour treatment facility MEDAPP and the radiography and tomography station NECTAR with fast neutrons. They have energies around 2 MeV. Furthermore, the reactor hosts the positron source NEPOMUC, where positrons are generated by pair production from absorbed high-energy gamma-rays. These gamma-rays are produced by the absorption of neutrons in a cadmium layer of the respective beam tube.

Neutron guides

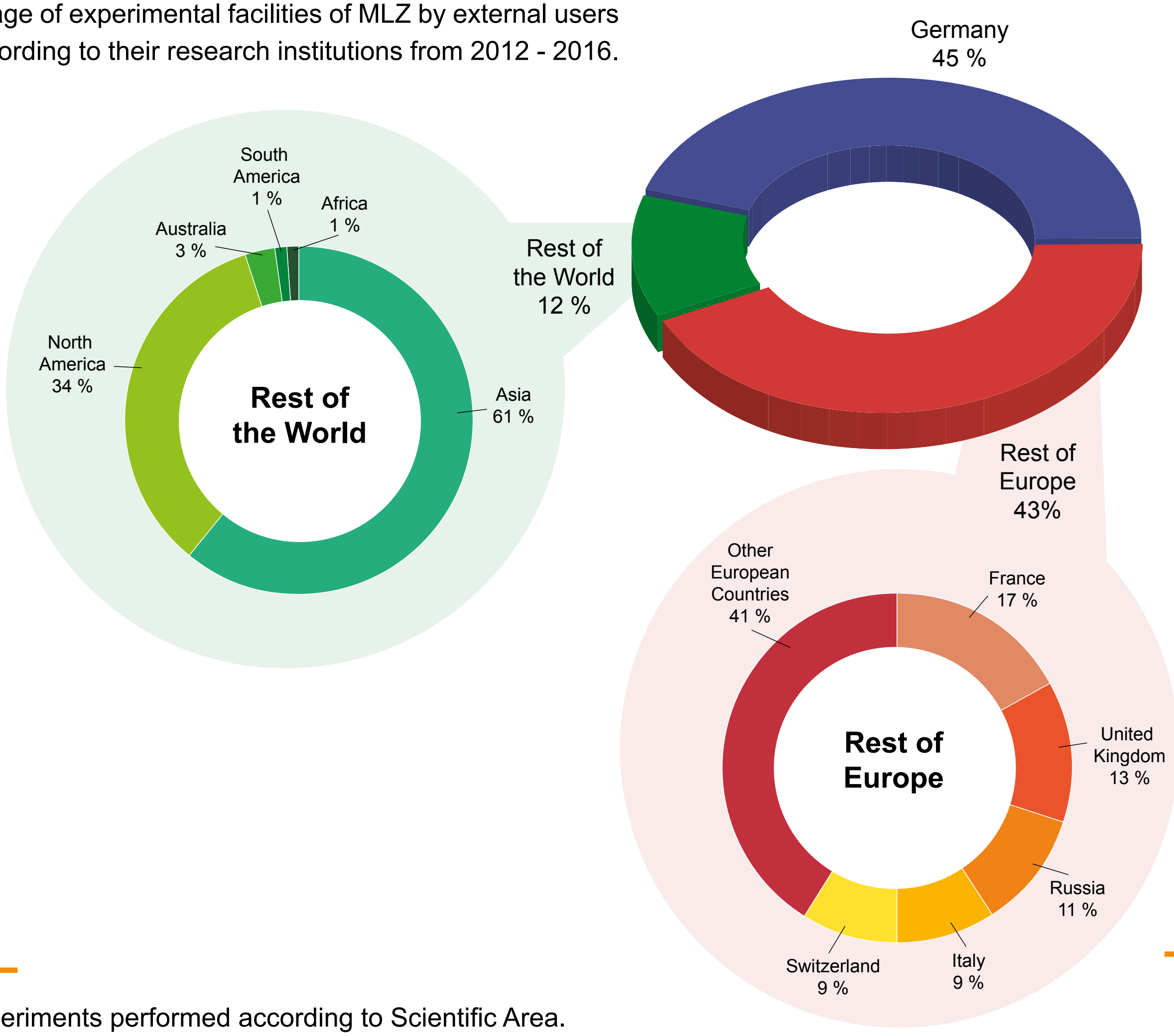
The MLZ makes extensive use of modern neutron guides to transport and distribute the neutrons over large distances in the Experimental Hall as well as in the Neutron Guide Halls. Adapted to the needs of the instruments with respect to wavelength distribution and angular dispersion the guide elements are coated with ^{58}Ni or supermirror coatings.

MLZ usage in numbers

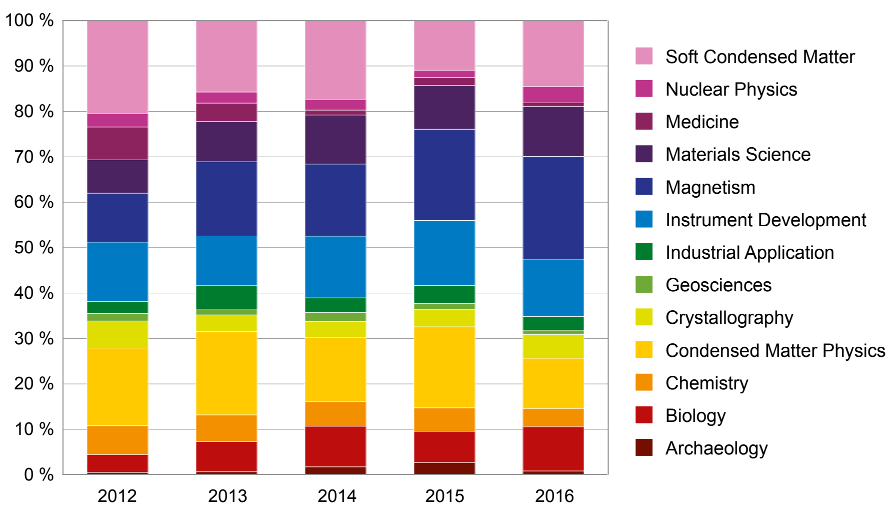
Access to the MLZ is open and free of charge to any scientist. Within the last 5 years, some 3000 external users have taken advantage of the experimental facilities at the MLZ. Two-thirds of the available beam time is devoted to these external users, while one-third is reserved for internal research. Of the external users about 45 % came from German universities and research institutions, 43 % from other European countries and 12 % from all over the world, mainly from Asia and North America, with some users from South America, Australia and Africa. Our European users came mainly from France, the United Kingdom, Russia, Italy and Switzerland. In each normal year of reactor operation, more than 1000 users make use of the experimental facilities at the MLZ.

More than 4500 experiments in total have been carried out in the course of the last 5 years by our users and our internal researchers. A variety of scientific questions covering different scientific areas have been addressed, ranging from Magnetism, Hard and Soft Condensed Matter Physics, Chemistry, Materials Science, Biology, Medicine, Geosciences as well as Nuclear & Particle Physics. At the MLZ, a strong focus is placed on Industrial Applications. Internal beam time is also used for Instrument Development in order to offer our users state-of-the-art instrumentation at all times. Interdisciplinary cutting-edge research at innovative high-class instruments, together with the high neutron flux of the FRM II and the overall engagement of numerous German universities and research institutions, make the MLZ the leading large-scale research facility using neutrons in Germany with huge international impact.

Usage of experimental facilities of MLZ by external users according to their research institutions from 2012 - 2016.



Experiments performed according to Scientific Area.



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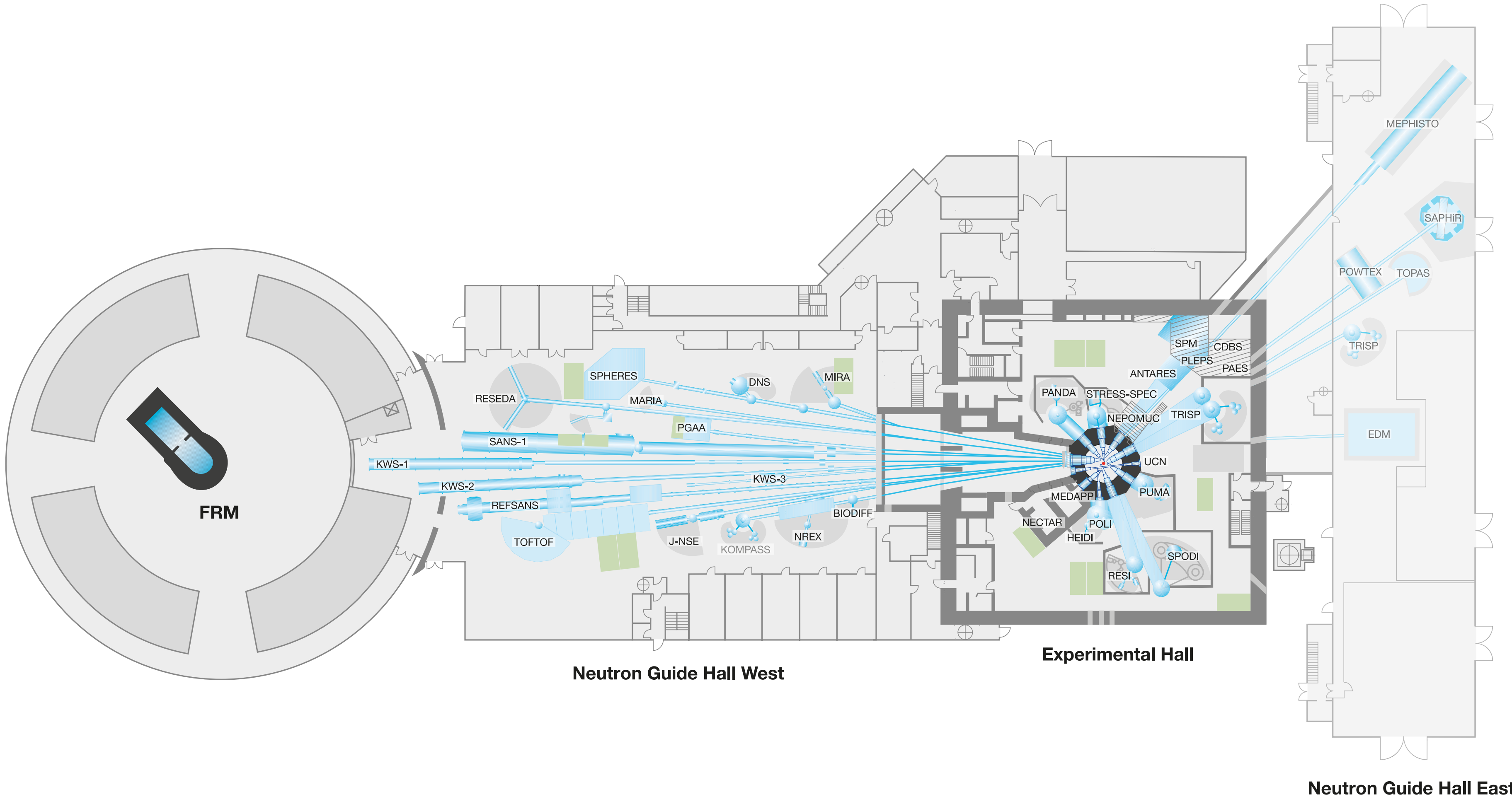

Instrument	Description	Neutrons	Operated by	Funding	Instrument group at MLZ
ANTARES	Radiography and tomography	cold	TUM	TUM	FRM II
BIODIFF	Diffractometer for large unit cells	cold	TUM, JCNS	TUM, FZJ	FRM II, JCNS
DNS	Diffuse scattering spectrometer	cold	JCNS	FZJ	JCNS
HEIDI	Single crystal diffractometer	hot	RWTH Aachen	FZJ	JCNS
J-NSE	Spin-echo spectrometer	cold	JCNS	FZJ	JCNS
KOMPASS*	Three axes spectrometer	cold	Uni Köln, TUM	VF	FRM II
KWS-1	Small angle scattering	cold	JCNS	FZJ	JCNS
KWS-2	Small angle scattering	cold	JCNS	FZJ	JCNS
KWS-3	Very small angle scattering	cold	JCNS	FZJ	JCNS
MARIA	Magnetic reflectometer	cold	JCNS	FZJ	JCNS
MEPHISTO**	Instrument for particle physics, PERC	cold	TUM	TUM, DFG	FRM II
MIRA	Multipurpose instrument	cold	TUM	TUM	FRM II
MEDAPP	Medical irradiation treatment	fast	TUM	TUM	FRM II
NECTAR	Radiography and tomography	fast	TUM	TUM	FRM II
NEPOMUC	Positron source, CDBS, PAES, PLEPS, SPM	-	TUM, UniBw München	TUM	FRM II
NREX	Reflectometer with X-ray option	cold	MPI Stuttgart	MPG	MPI Stuttgart
PANDA	Three axes spectrometer	cold	JCNS	FZJ	JCNS

Instrument	Description	Neutrons	Operated by	Funding	Instrument group at MLZ
PGAA	Prompt gamma activation analysis	cold	Uni Köln	TUM	FRM II
PUMA	Three axes spectrometer	thermal	Uni Göttingen, TUM	VF, TUM	FRM II
POLI	Single-crystal diffractometer polarized neutrons	hot	RWTH Aachen	VF, FZJ	JCNS
POWTEX*	Time-of-flight diffractometer	thermal	RWTH Aachen, Uni Göttingen, JCNS	VF, FZJ	JCNS
REFSANS	Reflectometer	cold	GEMS	VF, HZG	GEMS
RESEDA	Resonance spin-echo spectrometer	cold	TUM	TUM	FRM II
RESI	Single crystal diffractometer	thermal	LMU	TUM	FRM II
SANS-1	Small angle scattering	cold	TUM, GEMS	TUM, HZG	FRM II, GEMS
SAPHIR*	Six anvil press for radiography and diffraction	thermal	Uni Bayreuth	VF	FRM II
SPHERES	Backscattering spectrometer	cold	JCNS	VF, FZJ	JCNS
SPODI	Powder diffractometer	thermal	KIT	VF, TUM	FRM II
STRESS-SPEC	Materials science diffractometer	thermal	TUM, TU Clausthal, GEMS	TUM, HZG	FRM II, GEMS
TOFTOF	Time-of-flight spectrometer	cold	TUM	TUM	FRM II
TOPAS*	Time-of-flight spectrometer	thermal	JCNS	FZJ	JCNS
TRISP	Three axes spin-echo spectrometer	thermal	MPI Stuttgart	MPG	MPI Stuttgart
UCN*	Ultra cold neutron source, EDM	ultra-cold	TUM	TUM, DFG	FRM II

*construction
**reconstruction
VF: instrument construction funded by "BMBF-Verbundforschung" (Collaborative Projects)