Neutrons for Research:
The Spallation Neutron Source SINQ
at the Paul Scherrer Institute

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Neutrons for Research

Why neutrons are in such demand

How do certain alloys acquire the ability to «remember»? Which substances are best at storing hydrogen – the fuel of the future? What are the secrets of magnetic materials? Why does a material become superconducting? How can we cut the costs of the renovation of concrete structures?

The answers to these and many other questions can be found if we use neutrons as probes. If we scatter these uncharged particles at matter, they provide us with an insight into the dimensions of its atoms. Atoms are very small – their diameter is some hundred million times smaller than a centimetre – and therefore cannot be seen with the naked eye. Yet with the aid of neutron scattering we can make atoms «visible». Yes, neutrons not only tell us where particular atoms and molecules are located in a solid or liquid material, but even what they are doing there. No other experimental method gives us a similar wealth of information about the arrangement and movement of the atomic building blocks in the world around us. Thus neutrons have become an essential tool for many disciplines, such as physics, chemistry, biology and materials research. Their range of application is becoming increasingly broader, and extends, for example, from research into proteins or biological processes in cell membranes, through the study of catalysts, batteries, and magnetic substances, to the determination of the service life of turbine blades in gas turbines, as these are used in the utilisation of energy.

How the Polynesians discovered islands – without seeing them.

The extreme importance of neutron scattering can be illustrated, surprisingly enough, by the example of an invention by the Polynesian islanders. As early as the thirteenth century, these people were making long journeys in their outrigger boats between Tahiti, New Zealand, and the Fiji Islands. While methods of navigation in the Western world were based largely on the stars, the Polynesians relied on their observations of the ocean, which they set down in rod charts (Fig. 1). These were made from the ribs of palm leaves, which indicated the ocean currents and swell; mussel shells attached to these represented the positions of the islands. The locations of the islands created interference patterns on the ocean waves which were distributed across wide areas. At the points at which swell systems coincided, equalisation points or nodes were established, and the sea-going natives used...
these to find their way. In other words, when the Polynesians were on the high seas they observed the wave patterns, and this enabled them to locate islands without actually seeing them.

This gives us some idea of how we can find our way around in the world of atoms. We send out the right kind of waves into matter, and we observe the wave pattern after it has passed through the sample. We can then draw conclusions about the arrangement and movement of the atoms. Suitable for this are, for example, electromagnetic waves such as synchrotron light and neutrons.

What have neutrons to do with water waves?
The popular conception of neutrons is that they are particles. By this definition, the neutron is a point-like uncharged particle with mass, which rotates on its own axis, has a measurable speed, and, in addition, behaves like a tiny bar magnet. Neutrons, therefore, are ideal probes for the kind of research referred to above, because as neutral particles they penetrate deep into matter without disturbing it. An elementary particle like the neutron can, however, also behave like a wave (Fig. 2). Its reaction with atoms is then analogous to that of the water waves and the islands: we can measure interference patterns. The neutron accordingly manifests itself both as a particle and as a wave. This is amazing, but both concepts are correct; they are equivalent. We can both count individual neutron particles in a detector, as well as observe neutron wave patterns. The behaviour of the neutron which predominates depends on the process which is being observed. In the wave image, a wavelength is allocated to the neutron which depends on its mass and velocity as a particle.

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**Figure 2:** The concepts of the neutron as a particle and as a wave are equivalent.

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**The Neutron**

**As a particle**

- Neutron
- Proton
- Electron
- Particle with mass (mass = 1.07 \times 10^{-24} \text{ g})
- Rotates on its own axis (spin)
- Is a tiny bar magnet
- Measurable velocity
  - Thermal neutrons: ca. 2200 m/s
  - Cold neutrons: ca. 700 m/s

**As a wave**

- Wave
- Diffraction and interference pattern
- Measurable wavelength
  - Thermal neutrons: ca. 0.1 nanometre (1 Å)
  - Cold neutrons: ca. 0.4 nanometre (4 Å)

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Nanometre (nm): 1 nanometre is one millionth of a millimetre, or 10 Å (Angstrom).
How we can use neutrons for research into the building blocks of matter, without seeing them.

Thanks to the Spallation Neutron Source SINQ, since the end of 1996 researchers at the Paul Scherrer Institute (PSI) have a versatile and powerful neutron source available to them. The neutrons are «tapped off», in quantities of billions per second, by means of steel tubes and neutron beam guides (see page 31). Carrying this out calls for a lot of care, however, because in the process we are opening up a way to the outside for the neutrons, which are kept within the neutron source by iron, as if locked up within a bottle. This means that we have to trap the unwanted radiation, and this is performed by massive shielding, in which the monochromator is located. This functions as a kind of policeman, making sure that the speed limit is strictly adhered to. Neutrons which either speed along too fast, or dawdle along like «Sunday drivers», are captured. Only those neutrons which keep to the recommended speed are allowed to continue their journey. Outside the shielding they encounter the object being investigated, and are scattered in every direction; which is why we speak of «neutron scattering». The scattered neutrons are recorded by means of sensitive detectors, which we can position exactly, on air cushions, in any desired direction. The measurement results are plotted, and evaluated by means of computers. Figure 3 shows a schematic representation, and Figure 4 a photograph, of an experimentation instrument.
We shall describe here a few of the experiments which PSI researchers have been carrying out in the context of international co-operation. They make specific use of the special advantages of neutrons and neutron scattering, and provide excellent examples of the wide range of possible applications.

How do certain alloys acquire the ability to «remember»?

There are certain metal alloys which exhibit changes in their state which are associated with a «shape-memory» effect. Figure 5 shows an application of this effect; a clamp which is shaped at a low temperature «remembers» its original shape when it is heated up, in this case the smaller radius. It bends, and so acts as a clamp. This means that, when two metal items are joined, strengths can be achieved which are comparable to that of a welded seam. The bond can, if necessary (for example, for a repair), be released non-destructively simply by cooling it again to the low temperature.

What lies behind this ability to «remember»? To answer this question, we can consider in detail, for example, the «shape-memory» alloy of copper-zinc-aluminium, using neutron scattering. The scattering patterns (diffractograms) at the low temperature (20 °C) and at the high temperature (90 °C) differ dramatically (Fig. 6). From scattering patterns, we can unambiguously determine the structural differences of the two states (Fig. 7), which is a great help in understanding this remarkable material property, optimising it, and utilising it in technical applications. This experiment provides an impressive demonstration of the specific strength of neutrons; that is, their ability to make selective distinctions, even among elements which are next to each other in the periodic table – in this case, copper and zinc. This is not possible, for example, with X-rays.

Figure 6: The neutron scattering pattern of the shape-memory alloy, copper-zinc-aluminium (Cu-Zn-Al) varies a great deal at 20 °C from that at 90 °C.

Figure 7: Structures derived from the scattering patterns for the alloy Cu-Zn-Al, in its low-temperature and high-temperature states.

Figure 5: A clamp made of material capable of «remembering» its shape. Under high-temperature conditions it acts as a clamp, and releases at low temperature.
Which substances are best at storing hydrogen – the fuel of the future?

Hydrogen is a fuel which is unquestionably available in unlimited quantities. Hydrogen energy is environmentally friendly; if we burn hydrogen, apart from nitric oxide all we obtain is water. There are difficulties with the storage of hydrogen, however. There are certain metallic compounds which can store atomic hydrogen at up to three times the density of hydrogen in its liquid state, and release it again, under normal environmental conditions. Nowadays hydrogen storage media formed from iron-titanium or lanthanum-nickel compounds are the norm. For a large-scale technological breakthrough, however, the disproportionate ratio between the weight of the storage material and the stored hydrogen is still a major obstacle.

In other words, the task facing researchers is to find lighter storage substances, in particular those which are capable of absorbing more hydrogen. To do this, we need to understand precisely how the hydrogen is stored, and how it moves within the storage medium; and this is something we can achieve with the aid of neutron scattering experiments, because neutrons are scattered particularly strongly by hydrogen. The focus of research is on storage media created from light elements such as lithium and magnesium. As an example, the structure of the light metallic hydride LiMg$_2$RuH$_7$ is shown in Fig. 8. Whether this material is suitable as a reservoir for hydrogen depends essentially on the mobility of the hydrogen. This manifests itself in a neutron scattering experiment as a broadening of the scattering pattern. Initial results indicate that the hydrogen in the storage material moves in jumps, performing about a billion jumps every second and jumping at a speed of more than 100 km/h. This supports the suitability of this material as a hydrogen storage medium.

What are the secrets of magnetic materials?

The phenomenon of magnetism permeates our everyday lives almost unobserved, but in a vast number of ways, from the technical application of permanent magnets in engines through to medical applications. One particular strength of neutron scattering lies specifically in the investigation of the magnetism of matter, because the neutron is itself a «mini magnet» and can therefore «see» magnetic effects directly, by means of interaction.

On the other hand, it is not exactly easy to conduct experiments with magnetically-oriented (polarised) neutrons. With the development of a new type of super-mirror (Fig. 9), however, researchers at PSI have made a breakthrough in this field. Super mirrors such as these consist of up to 900 alternating layers of differing thicknesses of iron-cobalt-vanadium and titanium. They enable us to polarise neutrons more than 90 %. A special coating technique also makes it possible for the super-mirrors to be used even without an external magnetic field for the selection of the neutron polarisation, something which provides significant new advantages for experimental technology.
Why does a material become superconductive?

Even ten years after its discovery, the mechanism of high-temperature superconductivity (i.e. the transport of current without any resistance) is still largely not understood. Neutron scattering experiments have shown, however, that the electrical charge carriers behave differently from those in conventional superconductors. Basically, if we provide (dope) a copper oxide compound with charge carriers, they initially remain shut inside a kind of cage (Fig. 10). By increasing the number of charge carriers, these cages join together to make an interconnected network, in which the charge carriers can now move freely. As a result of this, superconductivity comes into existence below a critical temperature; in other words, a current flows without resistance. In technical circles, this phenomenon is called "percolative superconductivity", because the charge carriers in the cage network move in a similar fashion to the water in a coffee filter (a "percolator"). High-temperature superconductivity, in other words, is a non-homogenous property of the material. Experts can interpret this directly from the neutron energy distribution (Fig. 11). In this instance, a number of curves are overlaid on one another; with homogenous superconductivity, there would only be one visible.

![Figure 10: Schematic representation of high-temperature superconductivity in a copper oxide layer.](image)

![Figure 11: Energy distribution curves of neutrons after traversing a high-temperature superconductor (Pr$_{12}$Ce$_6$CuO$_{45}$). The overlaying of several curves indicates that the superconductivity is not homogenous.](image)
How can we cut the costs of the renovation of concrete structures?

The penetration of water into concrete and the renovation of buildings are well-known causes of some not insignificant financial burdens. For example, maintenance of the 3'088 bridges on the National Highway network in Switzerland costs about 100 million Francs a year. A more precise understanding of the spreading of moisture in concrete is therefore of direct practical use, in helping to reduce or avoid altogether the high cost of renovation, and in developing techniques for protecting structures of major cultural and historical significance. Again, it is neutrons which allow us to make the lighter water visible in concrete (Fig. 12), because they react with the hydrogen in the water more strongly than they do with the constituents of the concrete. Such transillumination with neutrons, known as neutron radiography, can in general be used for the non-destructive study of the different constituents inside materials. Because the ability to discern differs between neutrons and X-rays—such as, for example, synchrotron light—they complement each other ideally for these applications, too.

As these examples show, research with neutrons provides us with information about the order and movement of atoms and molecules in matter. And knowing these microscopic phenomena helps us to understand macroscopic material properties, as well as to influence them and put them to use in new applications.

The particular strengths of neutrons

**Neutron properties**

- Wavelength correspondence to the distance between atoms
- Energy correspondence to the kinetic energy of atoms
- Electrical neutrality, allows deep penetration into matter with hardly any damage
- Scatter contrast
- Identification of hydrogen
- Microscopic bar magnet

**Very well-suited for**

- Research into atomic structures
- Research into atomic motion
- Thick specimens, biological substances
- Differentiation between elements with very small mass differences
- Specimens containing water, biological substances
- Research into structures and motion in magnetic substances

Thanks to their specific properties, neutrons and synchrotron light are the ideal complement for many pioneering areas of research.
Where do we obtain neutrons from? As the partners of protons, they are the building blocks of the atoms of which matter is made. In contrast to the proton, the neutron carries no electrical charge. Its mass is a little higher than that of the proton, which means that it is not stable as a free particle, and decomposes with a half-life of some 890 seconds into a proton. Thus free neutrons do not occur in nature, but are stabilised in atomic nuclei by bonding forces. In order to use neutrons for experiments, we must first release them from the nuclei of the atoms. This means they are not easy to obtain, but there are two main ways of accomplishing this:

- **Splitting the nucleus** of fissionable material (uranium, plutonium) in a nuclear reactor. There are a number of research reactors in operation as neutron sources, such as at ILL in Grenoble, France.

- **A spallation reaction**, in which a heavy metal (such as lead) is bombarded with a proton beam from a particle accelerator. This is the basis for the sophisticated and complex technology of a spallation neutron source, such as SInQ at PSI (Fig. 13).

*Figure 13: The Spallation Neutron Source SInQ at PSI during the construction phase. The picture shows the steel tank, which encloses the whole inner region of the source, being lowered into place.*
**Spallation neutrons**

The Paul Scherrer Institute has been operating a proton accelerator with great success for more than 20 years, and, thanks to a number of special further developments in the past few years, this now holds the world record for power. The PSI proton beam is used by groups from all over the world for their research experiments on elementary particles, in solid-state physics, and on materials, as well as being employed for medical purposes such as tumour therapy. Alongside this, we direct the remaining, high-intensity proton beam onto the Spallation Neutron Source, SINQ. There, the protons strike a bar made of lead (known as the target) at high velocity. The protons colliding with the lead nuclei cause them to become highly excited ("nuclearly heated up"). This internal energy is released primarily by "evaporating" neutrons (Fig. 14); these are known as spallation neutrons. At the beam energy of the PSI accelerator, each proton releases about ten neutrons from a lead target, but, in contrast to nuclear fission, spallation does not result in a chain reaction, because the spallation process stops as soon as the accelerator is switched off.

**Thermal and cold neutrons**

The neutrons which are released escape from the target with a velocity of about 20'000 km/sec, which is much too fast for our purposes. For this reason we slow the neutrons down in a moderator material, which surrounds the target, by means of atomic collisions (Fig. 15). After this process, which lasts about 1–2 milliseconds, the neutrons have, on average, about the same velocity as the molecules of the moderator, ca. 2'200 m/sec., and we refer to these as thermal neutrons.

In addition to this, if we slow neutrons down in a very cold medium, the neutrons then become colder; in other words, their velocity becomes even lower, down to about 700 m/sec., and we then speak of cold neutrons. In SINQ, we create these in a separate volume of about 20 litres, which is embedded in the moderator tank and contains liquid heavy hydrogen at a temperature of −250 °C.
Extremely fast neutrons

Neutrons with very high energy, which are likewise created during the spallation reaction, can hardly be slowed down at all in the moderator. In order to protect the surroundings from them, the target and moderator region is surrounded by a massive five-metre-thick shielding, made of iron and special concrete. Even extremely fast neutrons are slowed down within this, partially reflected back again, or finally absorbed, whereupon their kinetic energy is converted into heat. Because of this, we must cool the inside of the shielding with water. This shielding allows research groups to remain safely in the immediate vicinity of the source for longer periods, while it is running.

The neutron source

Figure 16 shows a model representation of a section through SINQ. The target block and the beam guide of the proton beam are visible, the beam being directed from below onto the lead target in the centre. The target is surrounded by the moderator tank and this whole inner region of the neutron source is enclosed by a double-walled steel tank and a massive shield to provide protection against extremely fast neutrons.

Thermal neutrons: These result from deceleration in a substance at room temperature (20 °C), and have a velocity of about 2,200 m/sec.

Cold neutrons: These are produced by deceleration in a substance at very low temperature (e.g. in liquid heavy hydrogen, at −250 °C), and have a velocity of about 700 m/sec.

Figure 16: Model of the Spallation Neutron Source, SINQ, showing a section through the target block, and the beam guide for the protons, which emerge vertically from below.

Figure 17: Overall view of the target block, from a perspective similar to that of the model in Figure 16. On the left, the monochromator shielding for two experimental facilities with thermal neutrons is being installed and, on the right, a facility for irradiation.
Beam channels (on the left in the model), which can be closed off, lead out through this shielding to the experimental stations for thermal neutrons. On the right, embedded in the shielding, is installed the cold system for the cold neutrons. Figure 17 shows the actual facility from a similar perspective to that of the model, at the installation phase of the monochromator shielding for the experimental stations already mentioned. These, together with the shielding, can be moved on air cushions. While thermal neutrons escape from the system through the steel thimble-shaped penetrations of the moderator tank (Fig. 18) and the steel channels connected to them, we can transport cold neutrons out of the source and to the more remote experimental facilities by a more efficient method: using neutron guides.

Figure 18: The moderator tank, shortly before, and during installation. The lead rod (the target) is introduced into the central tube from above; the apertures in the tank wall are thimble-shaped penetrations which extend into the region of the tank centre, forming the innermost sections of the steel tubes from which the thermal neutrons emerge.
The neutron guides

Cold neutrons, with their lower velocity, exhibit a long wavelength. Their wave nature is so marked that we can influence them in the same way as light waves. In addition to wave superimposition, mirroring (total reflection) also occurs on suitable material surfaces. This means that we can transport cold neutrons in specially mirrored glass ducts, referred to as neutron guides, over considerable distances (50 metres and more) without significant losses. A bundle of such neutron guides is accordingly directed onto the cold moderator (Fig. 19), and led into the neutron-guide hall. Neutrons from these guides can be taken in, laterally or straight ahead, by the numerous different experimental installations.

Neutron super-mirror

A polished glass surface coated with a thin layer of nickel reflects neutrons completely, provided that their angle of incidence does not exceed a particular critical angle — in exactly the same way as for the total reflection of light. We are able to increase this critical angle substantially, and so bring more neutrons to the remote experimental installations, if we replace the nickel layer by a structured coating. This consists of several hundred alternating layers of differing thicknesses of nickel and titanium, from 5 to about 70 nanometres, and functions as a super-mirror, which we have developed and built at PSI. Figure 20 shows the composition of such a layered structure, viewed through an electron microscope.

Figure 19: Neutron guides, which transport cold neutrons to the experimental locations.

Figure 20: Neutron super-mirror. The picture taken by an electron microscope shows the nickel-titanium layer structure of a super-mirror developed at PSI; the thinnest layers are about 5 nanometres thick.
The Spallation Neutron Source SINQ at PSI

The experimental facilities

The flexibility and variety of the experimental facilities at SINQ are exceptionally large, of which Figure 21 gives an impression. The particular strength of SINQ lies in the field of cold neutrons. These make it possible to conduct experiments with substances such as macro-molecules and nano-crystals, which are of major importance in particular in the «growth areas» of biology, pharmacy, material sciences and earth sciences. Researchers at PSI make systematic use of the advantages of SINQ when installing their instruments for neutron scattering, and, by making use of innovative, unconventional concepts, they achieve maximum utilisation of the new SINQ neutron source, to the benefit of a broad international user community.

Figure 21: The arrangement of the different experimental instruments around SINQ and in the neutron-guide hall.

A successful 1996

As planned, we took SINQ into operation on 3 December 1996 – and with immediate success (Fig. 22). Thanks to optimum preparation and co-operation on the part of all concerned, the maximum intensity aimed at for sustained operation was almost reached by the second day; and the neutron yield more than fulfilled expectations. This was the reward for dedicated work on the proton accelerator, on SINQ, and on the development of new technologies for the experimental equipment. Thanks to this pioneering work by PSI, the research community now has the highest continuous flow of spallation neutrons in the world at its disposal, at SINQ.

Figure 22: Thanks to joint and committed effort on the part of a large number of PSI staff and future user groups, SINQ more than fulfilled expectations on its very first day. The blue curve shows how many cold neutrons passed into one of the measuring devices, and at which velocities (wavelengths) – and there were more than expected (red squares).
The PSI accelerator and its applications

Protons are raised to high velocity in the PSI accelerators, and then formed into a beam. After a wide range of applications for particle physics, medicine, and solid-state research, the beam reaches SINQ, where it produces spallation neutrons (lower right in the picture).
A Brief Overview of PSI

The Paul Scherrer Institute (PSI) is a multi-disciplinary research centre for natural sciences and technology. In national and international collaboration with universities, other research institutes and industry, PSI is active in solid state physics, materials sciences, elementary particle physics, life sciences, nuclear and non-nuclear energy research, and energy-related ecology.

The institute’s priorities lie in areas of basic and applied research, particularly in fields which are relevant for sustainable development, as well as of major importance for teaching and training, but which are beyond the possibilities of a single university department. PSI develops and operates complex research installations which call for especially high standards of know-how, experience and professionalism, and is one of the world’s leading user laboratories for the national and international scientific community. Through its research, PSI acquires new basic knowledge and actively pursues its application in industry.

PAUL SCHERRER INSTITUT

CONTACTS

- Information Officer: Dr. Myriam Salzmann
  Phone 056 310 26 71
  Fax 056 310 26 35

- Department Head: Dr. Walter Fischer
  Phone 056 310 34 12

- Head Neutron Scattering Prof. Dr. Albert Furrer
  Phone 056 310 20 88