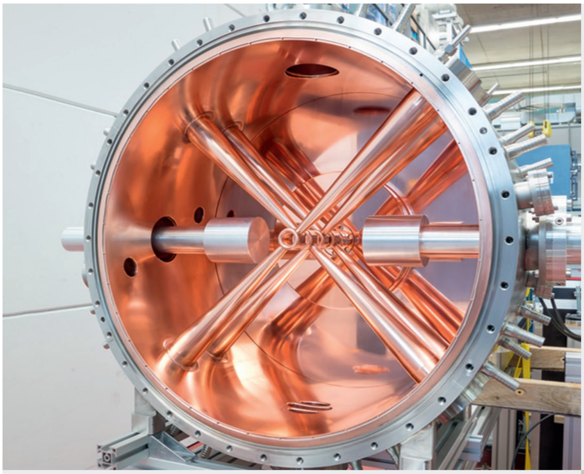

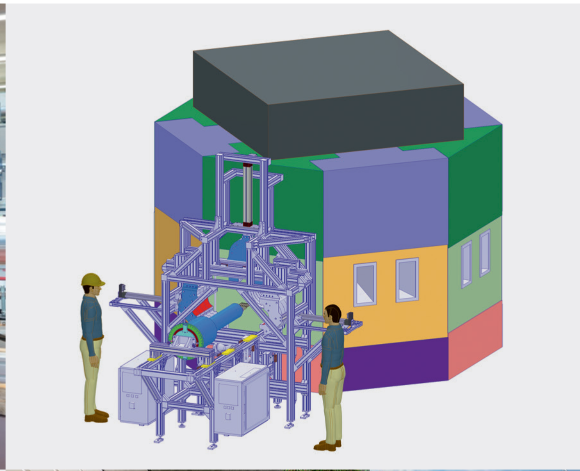

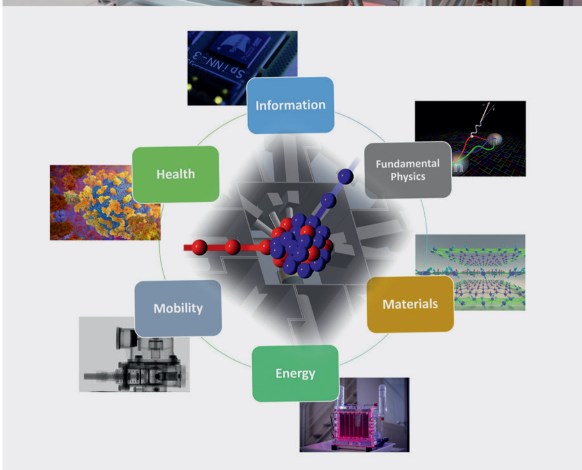

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T. Brückel, T. Gutberlet (Eds.)

Allgemeines / General
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”Wer nicht an die Möglichkeit glaubt, dass Utopien technisch zu verwirklichen sind, der arbeitet nicht daran und kommt auch nicht voran.”

Leo Brandt
Gründer des Forschungszentrums Jülich, Founder Forschungszentrum Jülich

CONTENTS

I.

ENABLING SCIENCE WITH A NEXT GENERATION NEUTRON SOURCE

The High Brilliance neutron Source HBS within the European and world-wide neutron eco system and its technical design.

The High Brilliance neutron Source (HBS) is a neutron scattering and analytics facility with high brilliance: it is a machine that sends intense beams of subatomic particles on samples to answer the question: "where are the atoms and what do they do?" This kind of research has a long and successful track record in Europe and it is well embedded in the landscape of various complementary techniques for non-destructive material characterization. It is key to the development of new materials, new drugs, new chemical processes, food technology, engineering, information technology and new energy capture and storage technologies. Three very topical examples of neutron research that are highly relevant to today's challenges and carried out right now include understanding the structure of lipid nanoparticles used as a delivery mechanism for mRNA therapy, essential for Covid-19 vaccines; discovery of quantum phenomena in quantum materials relevant for the second quantum revolution; and on understanding materials for future higher energy-density electric vehicle batteries as part of the European Union's Battery 2030 initiative.

I.1 Science Drivers

The development of functional materials and active agents is the key to the solution of many of the major challenges facing society, from energy technology to the environment, information and communication, transport and health. The special properties of neutrons make them an indispensable probe for the study of matter at the atomic level. To quote from the recent position paper of the League of advanced European Neutron Sources (LENS) [1]:
"The advanced analytical techniques provided by neutron research infrastructures allow unique insights into matter and materials by exploiting the characteristics of the neutron. The engineering sciences benefit from the ability of neutrons to penetrate very dense, heavy objects, the life science sector utilizes the heightened sensitivity of neutrons to hydrogen and water, condensed-state physics use the magnetic properties of neutrons to explore magnetic and electrical phenomena, while the non-destructive nature of neutron beams make them ideal for the study of rare cultural heritage and palaeontology specimens." (LENS position paper).
Neutrons are indispensable for (medical) radionuclide production. In curiosity-driven research, they enable the discovery of emergent phenomena in condensed matter systems, the ultimate test bed for our understanding of correlated many-body quantum systems. The neutron as a research object itself allows us to approach answers to questions about the existence of the universe and our own

existence.

The most important probes at the atomic level, neutrons, synchrotron X-rays, and electron-microscopy, complement each other; only together can they provide a complete understanding of the microscopic world of atoms and their processes leading to functionalities, just like we humans have several senses to orient ourselves in the macroscopic world. Neutrons excel

- as gentle, nondestructive probes e.g., in the life-sciences
- in operando studies of real size devices e.g., in energy conversion or energy storage devices
- in studies requiring complex sample environment e.g., of quantum materials under extreme conditions of ultralow temperature, high magnetic fields, or pressures
- wherever the relevant processes are driven by light elements e.g., hydrogen movements and bonds in biological systems; hydrogen, lithium or sodium in energy conversion and energy storage devices for the energy revolution e.g. fuel cells or batteries
- in studies of dynamic processes over a huge range of length and time scales; the ability of neutrons to measure the space-time correlation functions on an absolute scale enables direct comparison to ab-initio theories and serves as an experimental benchmark to test and improve such theories.

Neutron research not only plays a key role in the academic sector by creating new knowledge and educating young scientists, but it also generates innovation by translating research results into new and improved products.
"In addition to supporting the generation of new knowledge in academic and industrial research, neutrons are frequently employed by a range of industry sectors for quality control and the improvement of existing products and processes. The neutron facilities in Europe are used by several hundred different companies: from small and medium-sized enterprises to large global corporations across a wide range of sectors, such as the automotive, transport, pharmacological, food and consumer goods industries. The diversity of these companies demonstrates the significant contribution of neutron facilities not only to fundamental science within the academic sphere but also to innovation close to market in support of the knowledge-driven economy." (LENS position paper)
The LENS position paper concludes:
"Neutron techniques make significant contributions to scientific discovery, the creation of new technology and addressing society's greatest challenges."

I.2 European Neutron Eco System

"Over the last 50 years Europe has developed the largest community in the world of approximately 5,000 expert neutron users." (LENS position paper). Among European users, which publish about one half of all papers in the field of research with neutrons, the German community is one of the most productive in terms of the number of publications [2]. *"The world-leading ecosystem of neutron facilities in Europe, supporting a world-leading community of researchers, has been created by decades of investment, but the landscape is now undergoing major changes. Many of the national reactor-based sources have closed, reducing European experimental capacity to around 80% of that available in 2019. This will decrease further in the 2030's when ILL is likely to reach the end of its operation, at which point only 60% of the former capacity will remain. Other facilities may also close on a similar timescale. At the same time, the world's most innovative countries beyond Europe are planning to bolster their capacity and capability in this sphere. Some of these losses will be mitigated by the European Spallation Source (ESS) - a new, international, accelerator-based facility under construction in Sweden - and by the further development of existing sources. However,*

although ESS will be the most powerful neutron source in the world once fully operational, it will initially provide less than half the current capacity of ILL." (LENS position paper)

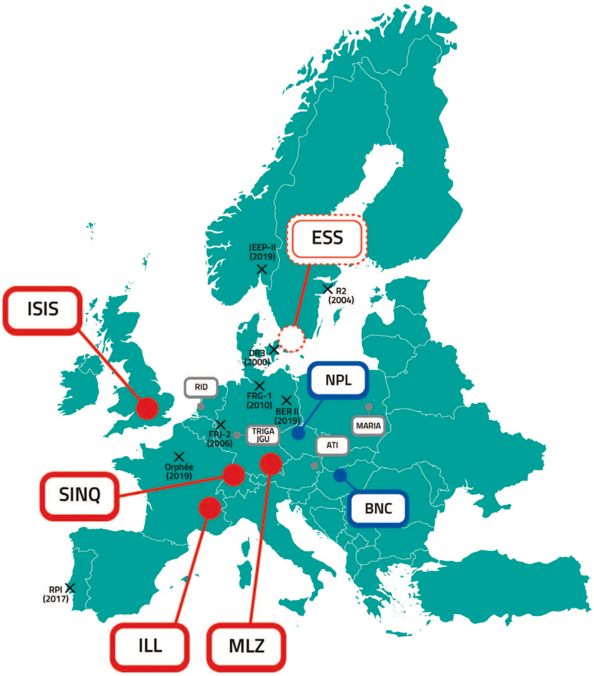

Figure I.1: *Neutron facilities in Europe [1].*

Neutron user facilities in Europe are based on two physical processes: fission and spallation. Older research reactors are reaching the end of their lifetime. In Germany, three such facilities, operated by national research centers in the past, have been permanently shut down: The FRJ-2 reactor in Jülich in 2006, the FRG-1 in Geesthacht in 2010 and the BER II reactor in 2019. In 2004 the FRM II reactor in Garching became critical, which is now the neutron source of the German neutron research facility Heinz Maier-Leibnitz Zentrum (MLZ). In 2019, two further research reactors were shut down, the Orphée reactor of the Laboratoire Léon-Brillouin (LLB) in Saclay and the JEEP II reactor in Kjeller, meaning that French and Norwegian neutron researchers lost their most important research tools. However, while many important neutron sources have been closed in Europe *"Critical national expertise in the development and application of neutron techniques has been maintained through 'neutron knowledge centres'."* (LENS position paper). These include the Jülich Centre for Neutron Science (JCNS), the German Engineering Materials Science Centre (GEMS) and the Laboratoire Léon-Brillouin (LLB), all operating instruments at the remaining neutron sources in Europe. In analyzing the changes in the European neutron ecosystem, taking into account societal resistance to new fission-based sources and the enormous price tag for new spallation sources, the League of advanced European Neutron Sources (LENS) concludes the following in its recent position paper:

- *"It is unlikely that research reactor-based facilities for neutron science will be built in Europe, so new facilities will need to be accelerator-based.*
- *Options for the development and expansion of the existing major facilities, such as ISIS-II and a new guide hall at SINQ, are in the design phase.*

- *Europe's new flagship facility ESS will come into operation with significant new capability, and with the potential to further increase the source power and the number of instruments available.*

- *The only route for entirely new facilities with significant capacity are High Current Accelerator-driven Neutron Sources (HiCANS), which could occupy the role played by national reactor-based sources in the past. Designs need to be demonstrated in practice through the realisation of an operational facility of this type."*

- *Different options have their own associated risks: though expanding existing facilities is technically low-risk, the centralisation of capacity in a handful of facilities increases the vulnerability of the ecosystem to the temporary shutdown or closure of one of them.*

- *Expertise based around 'neutron knowledge centres' can support both national and European user communities through the operation of instruments and the development of facilities.*

I.3 German National User Community

The Committee Research with Neutrons (KFN) [3] is an elected board with aim of fostering research with neutrons. It counts about 1500 regular neutron users in its data base. With financial support by the BMBF, the German neutron users have access to 25% of the neutron beam time at ILL, will have access to 20% of the neutron beam time at ESS, and have access to the instruments at MLZ, where national usage amounts to about 50% of the total beam time. Assuming for all these facilities about 200 days of user operation per year, this corresponds to 1700 instrument days for ILL (30 public instruments, plus more beam days accessible at CRG instruments), 600 for ESS (15 instruments), and 2700 for MLZ (27 instruments, about half beam time for German users) for German users. At ILL and MLZ together the average beam time per German user and year amounts to roughly 3 days. To use such beam time successfully it is important to be well prepared and explains why on average two beam times are needed to complete a publication based on research with neutrons. Note that for the currently funded instrument suite at the future Flagship facility ESS, a German user will have only one day of beam time every 2.5 years (=1500 / 600) on average. Competition for this prime-beam time will be extremely tough and only excellent preparation at national sources will allow efficient use and success. Just as neutron users from around the world can get beam time at MLZ, German users can have further access to beam time at other national facilities through their regular proposal systems (SINQ, ISIS, BNC, ORNL, NCNR-NIST, ANSTO, J-PARC).

- Risks in the provision of neutrons by reactor-based neutron sources are currently apparent for the FRM II reactor in Garching, which is the only remaining German neutron source after the reactor sources in Jülich, Geesthacht and Berlin were shut down. Necessary replacements of critical reactor components (e.g. central channel) and source components (e.g. cold source) as well as legal issues related to the supply and disposal of fuel elements and reactor operation with highly enriched uranium regularly lead to reactor down times. This makes it difficult to maintain a regular research program based on experiments with neutrons. Especially with regard to the training of the next generation of neutron scientists, it is of utmost importance that regular beam time can be guaranteed for PhD projects. Otherwise, there is a risk of loss of critical know-how and a dissolution of the user community for this specialized technique, which is not available on a laboratory scale.

- In view of (i) reduced neutron supply with the transition of the European flagship sources from ILL to ESS and (ii) reactor-specific uncertainties in future neutron supply, it is indispensable for the German user community that a reliably operating national neutron source is realized,

Figure I.2: *European Neutron Scattering Conference 2023 in Garching. © FRM II, TUM*

which, given the societal context, should not be fission-based but accelerator-driven. Such a source

- secures the access for German users to sufficient neutron beam time
- offers new techniques and globally competitive instruments to the German and international scientific community
- provides for the majority of beam time for the national user community
- enables specialized experiments that are rarely feasible at the flagship facilities due to lack of beam time
- prepares for the top experiments performed in future at ESS
- enables predictable research programs e.g., for PhD projects
- provides for user education and training and thus for a stable user base also for the other facilities
- allows for method and instrument development
- offers unparalleled capabilities to produce critical medical radionuclides through both neutron and proton induced reactions
- and, last but not least, enables short-term flexible industrial access without the restrictions of a facility operation under nuclear law.

1.4 High Current Accelerator-driven Neutron Sources (HiCANS)

In addition to fission and spallation, there are other nuclear processes that occur at accelerator-driven neutron sources below the threshold energy for spallation. Based on such processes, small, local sources, called Compact Accelerator-driven Neutron Sources (CANS), have been realized mainly in Japan, where the Japanese scientific community realized that the large investment in the J-PARC MW spallation source can only bear fruit with trained users and optimized methods. In the USA, there is another such facility, the LENS facility in Bloomington, Indiana. In Europe, there is no such source for use in materials research. However, with the concentration of European research with neutrons in a few major facilities (namely, the national facilities MLZ, ISIS, and SINQ, and the European flagships ILL or ESS), the risk associated with possible shutdowns and the need for diversification became apparent. Given the wide variety of research with neutrons and the fact that neutrons, unlike other probes, are not available on a laboratory scale, a healthy ecosystem requires the presence of a range of local, regional, and national facilities for method development, capacity and specialized capability, user recruitment, and training. In this context, the LENS position paper states:
Access to a range of neutron science facilities and expertise is essential if Europe's high technology nations are to continue their future materials research programmes and secure the resulting economic and societal impact. National facilities support the majority of research and provide a platform for skills and technical development. This enables optimal use of the specialised capabilities at international facilities, which lack the capacity to do everything.
And later in the same paper: *The ecosystem in Europe has been destabilised following the closure of a number of facilities causing decreased capacity and increased centralization. ... Though ESS will provide enhanced capabilities, these can only be fully exploited if the supporting ecosystem has sufficient strength, depth and diversity.*

Recognizing this challenge, the European Low Energy accelerator-based Neutron facilities Association (ELENA) [4] was formed, with members from eight European institutions collaborating on various projects. These range from a small CANS for a specific industrial company, to facilities with regional significance, to full-scale, competitive (national) user facilities. Such powerful facilities have only recently become realistic due to advances in accelerator, target, moderator, beam extraction, and neutron optics developments. They are based on high current accelerators and are referred to as High Current Accelerator-driven Neutron Sources (HiCANS). HiCANS pursue completely novel approaches; no such neutron source exists today. The importance of HiCANS is mentioned in the LENS position paper:
High Current Accelerator-driven Neutron Sources, that use lower energy than accelerator-based spallation facilities, have the potential to be a significant part of the future ecosystem through their scalability. This could enable a larger number of countries to become facility owners or operators and provide capacity and capabilities tailored to their local or national needs. Several projects/designs are being developed but experience needs to be gained through the construction and operation of the first HiCANS facility.

Within ELENA, several projects are being pursued for the realization of HiCANS facilities: SARAF at SOREQ (Israel), ARGITU at ESS Bilbao (Spain), ICONE at LLB (France), and HBS at Forschungszentrum Jülich GmbH (Germany). Among these projects, the HBS facility is the most ambitious and advanced. To quote the LENS position paper again:
The potential of High Current Accelerator-driven Neutron Sources (HiCANS) must be established by the construction and operation of a first HiCANS facility – Sonate (ICONE) or HBS.

Of all the HiCANS projects, the High Brilliance neutron Source (HBS) project is the clear technology leader. All critical components of the HBS have been designed, built and tested. A test station has been realized and the interaction of these components has been demonstrated. A Conceptual Design Report (CDR) was published in 2020, followed by this Technical Design Report (TDR). The main features of this facility are outlined below.

II.

SCIENCE AND INDUSTRY

The use of neutrons to probe and understand matter and assess scientific theories was developed through the second half of the 20th century and neutrons have become an essential analytical tool in the scientist's toolbox. Neutrons provide spectacular advances in science and technology promoting the sustainable development of modern societies.

The general science case for research with neutrons has been made for many occasions and by many organizations (e.g. LENS [1], KFN [5], ESFRI [6], ENSA [7] etc.). Looking at the modern trends in science, research is moving away from the investigation of simple model objects or the study of components of larger entities towards the understanding of entire complex systems, where various degrees of freedom are interacting and competing. Prominent examples are given e.g. in:

- **Life science.** In the protein data bank more than 200000 structures of proteins can be found, mostly solved by synchrotron x-ray scattering, NMR or more recently cryo-electron microscopy. Knowledge of the structure is an important first step towards understanding functionality.The next step requires an understanding of the dynamics of these macro-molecules, not only in dilute solutions, but also in the extremely crowded environment of real biological cells. Such knowledge does advance our ability to develop efficient pharmaceutical agents and thus to solve important challenges in health. Neutrons with their ability to cover the entire relevant phase space, to locate hydrogen and follow its movement, to vary the contrast between different components of such a complex system, are ideally positioned to take up the challenge and go beyond the study of the structure of single biological macro-molecules. The HBS, with its bright neutron beams two to three orders of magnitude smaller in cross section, will enable new science by reducing the need for materials and improving background conditions.

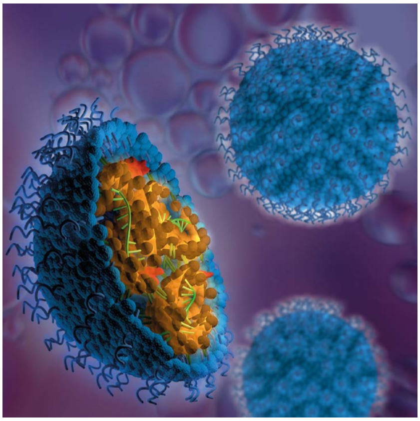

Figure II.1: *Neutrons are being used to improve the transfection of mRNA into cells through lipid nanoparticles for use in covid vaccines and more personalized drugs (BioNTech - Pfizer and AstraZeneca) [8, 9].*

- **Quantum technology.** Applications require specific quantum materials, e.g. for qubits for future quantum computers which are less prone to decoherence. The discovery of novel quantum materials with highly entangled quantum states and special topological properties is the realm of neutrons since the experimental setup requires complex sample environment for ultra-low temperatures, high magnetic field or high pressure. The spectrometers at HBS, with their ability for optimal phase space extraction, are ideally suited to the challenge of unraveling the complex dynamics of entangled spin quantum systems.

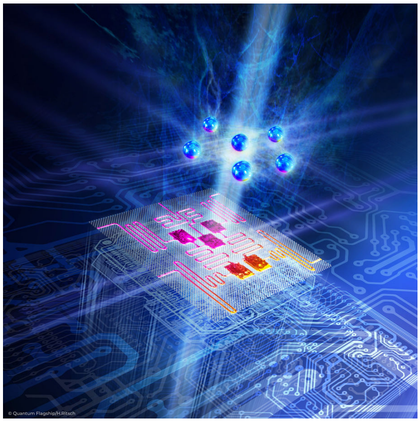

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Figure II.2: *Exploring and making quantum technology [10].*

- **Magnetism.** Because neutrons carry a nuclear spin, they are well suited for the study of magnetic materials. Neutron diffraction is the unique probe for magnetic structure determination. An estimated 95% of all magnetic structures have been determined with neutrons. Based on this, neutrons allow us to understand the spin dynamics and interface effects in thin film heterostructures that make up spintronic devices. They are used to optimize magnetic nanoparticles for in vivo applications such as targeted drug delivery, contrast agents for magnetic resonance imaging (MRI), or hyperthermia treatment of malignant tumors. The bright neutron beams of the HBS are ideally suited to provide the necessary knowledge for the design and optimization of complex multi-component spintronic devices and applications of nanomagnetic systems.

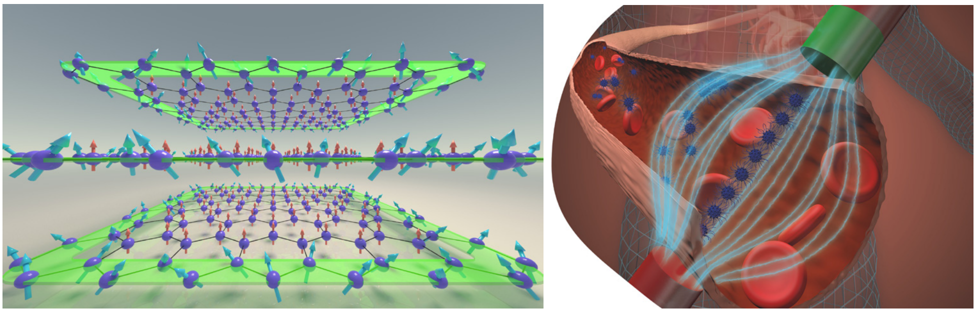

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Figure II.3: *Left: Novel spin excitations discovered in two-dimensional topological quantum materials with neutrons [11].*
Right: Optimizing magnetic nanoparticles for in vivo cancer treatment requires neutrons [12].

- **Energy technology.** The energy revolution toward renewable energy requires efficient energy conversion and storage devices such as fuel cells and batteries. These devices rely on the motion of light elements such as hydrogen, lithium or sodium. While other probes are blind to these elements in the presence of structural material consisting of heavier elements, neutrons are particularly sensitive to them. These light elements are the ones "doing the work" and are responsible for the functioning of energy conversion and storage devices. Neutrons are used to disentangle the water exchange mechanism and proton diffusion across the membrane in fuel cells or Li migration between the electrodes in Li ion batteries. Due to the penetrating power of neutrons, these studies can be performed operando, e.g. during the charging and discharging cycles of batteries, thus allowing the selection of the best materials, the optimization of the geometry, and the detection and control of the causes of aging and malfunction of the devices. Several instruments proposed for HBS are best suited for such studies, such as neutron depth profiling, diffraction or combined imaging and analytics.
- **Irradiation.** Radiation effects in electronics is a very important field of scientific and technological research for many applications of electronics. The study of neutron-induced single event effects (SEE) in commercial electronics with appropriate irradiation facilities is of strategic importance, in particular for digital electronics industries. Radioisotopes are used worldwide for various purposes in medicine, industry and science. A high-current accelerator-driven neutron source such as the HBS has the advantage that a wide range of radioisotopes can be produced by either proton or neutron capture reactions on a dedicated target station equipped with sample irradiation positions.

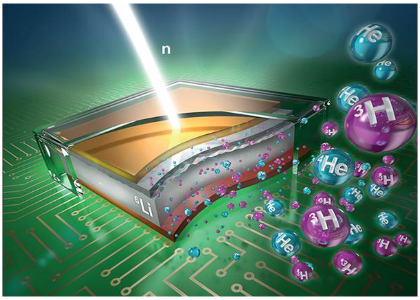

Figure II.4: Neutrons are used to improve lithium-ion batteries by following the movement of lithium between electrodes. This allows scientists to understand the aging mechanism of these devices, which is essential for further development [13].

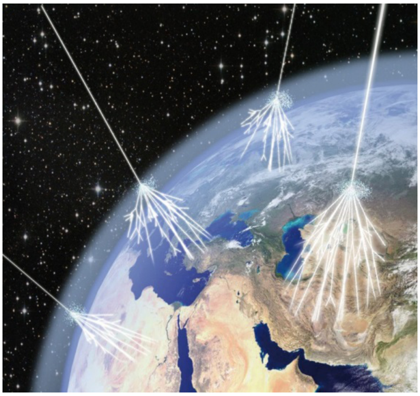

Figure II.5: Irradiation by cosmic rays [14].

- **Neutrons for Industry.** The development of mRNA vaccines and drugs, magnetic nanoparticles for cancer treatment, batteries or fuel cells for the energy revolution are examples of research conducted at neutron facilities in collaboration with or by industrial companies which directly translates into commercial products. Discoveries resulting from more fundamental studies, such as those in quantum materials or magnetism, have the potential to disruptively change technologies. A prominent example is the discovery of the Giant Magneto Resistance (GMR) effect by Peter Grünberg and Albert Fert, which revolutionized information technologies. But there are many other examples of research and development by commercial companies at neutron facilities. These include areas as diverse as the development of plant-protein based foods, the strengthening of engineering components (e.g., high-strength stainless steel screws or durability of nickel superalloys) for extreme applications, the detection of gas-hydrates in underwater pipelines, the optimization of brake discs, the development of lubricants, the quality control of nozzles and valves for the aeronautics and aerospace industry, the optimization and quality control of additive manufacturing - to name just a few recent examples. With its easy and fast access as a non-nuclear facility, its flexibility and its novel methods, such as element-specific tomographic imaging of large objects, the HBS will certainly strengthen the transfer of knowledge, methods and technologies from research with neutrons for use in commercial enterprises with positive impact on Germany as a business location.

What is presented here is a personal selection of examples by the authors and by no means an exhaustive list of the scientific discoveries and industrial innovations that are possible using neutrons as a powerful microscopic probe. Most of these applications are common to any powerful neutron source. However, an HBS type neutron facility is characterized by very bright beams, flexibility and ease of access without the cumbersome requirements for access to a nuclear facility. This makes the HBS particularly interesting for industry. Specific target stations can be operated with a dedicated access procedure for fast access on demand, highlighting applications relevant to industry, such as medical radionuclide production or neutron imaging and analysis important for quality control or the raw materials and recycling industries. It should also be noted that the technologies required to implement an HBS are at the forefront of today's technology and will give the companies involved an edge in know-how already during the construction phase.

To tackle all of the challenges in science and industry maximisation of the brightness of a neutron beam is highly requested. The HBS project will enable this as a new generation neutron source optimised for brightness. It will emphasis strongly:

- Science with neutrons to become accessible more easily and locally, far beyond the limited access to the world-leading facilities.
- Basic and applied research from material to life sciences, physics, engineering, food technology and industry or cultural heritage to be done more flexible and timely following specific scientific and societal demand.
- The capacity of neutron beamtime to be stabilized and enlarged by the establishment of new facilities with high-quality neutron instrumentation on a level complementing the high-flux reactor and megawatt spallation sources.
- Dedicated instruments for certain applications or specific scientific fields or industries to be realized on additional target stations e.g. irradiation stations.
- Research in many fields requiring high brilliance neutron beams, e.g. for life science, engineering materials science, quantum and nanotechnology, analytics will receive a boost.

III.

THE HIGH BRILLIANCE NEUTRON SOURCE (HBS)

III.1 Concept

The HBS project is being pursued under the leadership of the Jülich Centre for Neutron Science of Forschungszentrum Jülich GmbH (FZJ) together with partners from within FZJ, from national universities, from the Helmholtz Association or from international research centers. A conceptional design report (CDR) was published in 2020 [15]. The HBS project follows a new approach with several paradigm shifts:

- The basic process for neutron release from atomic nuclei in the HBS is neither fission nor spallation, but nuclear reactions based on the impact of low-energy protons on a metal target. This concept has already been realized in small accelerator-driven neutron sources (CANS) but is only now becoming feasible for a high-end facility through the application of the latest scientific and technological advances. No nuclear license is required for such a facility in Germany, and the shielding requirements are much less stringent.

- Rather than aiming for the highest source strength, HBS maximizes efficiency and brightness, the relevant physical parameter for most neutron beam instruments. "HBS produces fewer neutrons but uses them more efficiently." This approach translates directly into lower installation and operation costs.

- Rather than providing one neutron source/moderator for all instruments, which necessarily requires tradeoffs, HBS considers the source an integral part of the instrument and provides an optimal pulse structure and neutron spectrum for each individual instrument; "HBS provides individually tailored beam characteristics for each instrument, rather than one for all." This approach increases instrument performance.

- Rather than aiming for a specific size for a facility, the HBS concept is extremely flexible and scalable, from the size of a large laboratory for local university and industrial use to a full-scale and highly competitive user facility. The concept for the large laboratory facility has already been published under the name NOVA ERA [16]. A NOVA ERA has the potential to "bring neutrons to users, not users to neutrons." But it has not the potential to serve as a national neutron source with an internationally competitive instrument suite.

- HBS will provide additional capacity and new capability to research with neutrons. Optimizing for brightness makes the HBS well suited for research on small samples, important e.g., in the fields of life science, nanotechnology or engineering. It will offer novel techniques for industry, such as element-specific tomographic imaging of larger objects, relevant e.g. for quality control in manufacturing or for the raw materials and recycling industries.

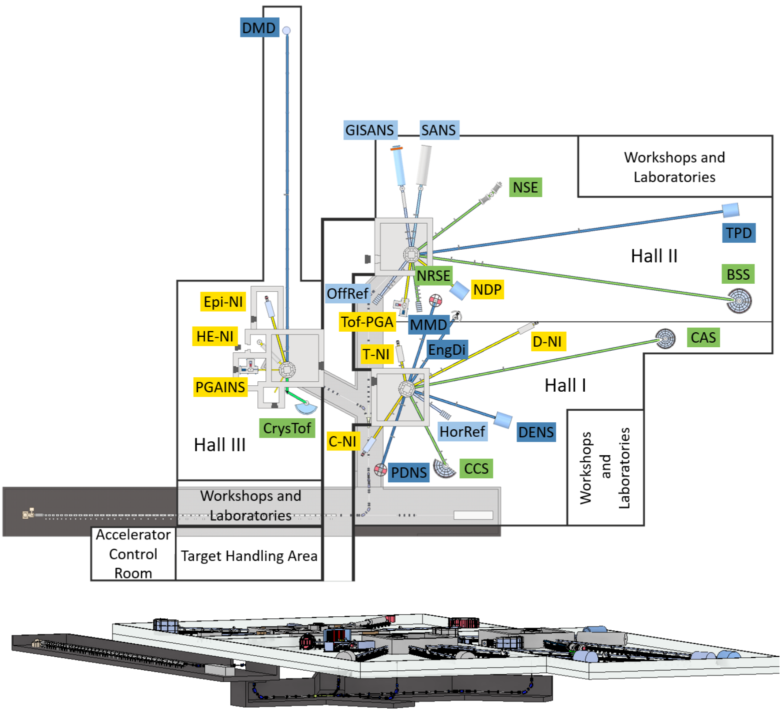

Figure III.1: *General layout of the HBS facility. The linac feeds the high-energy beam transport section with the underground multiplexer. It serves three target-moderator-reflector (TMR) units from below. The instruments are grouped around these TMR units in two experimental halls. This reference design contains a full suite of 25 instruments for diffraction, large-scale structures, quasi-, high resolution- and inelastic-scattering, analytics, and imaging. Additional instruments and TMR units can be added as needed.*

While HBS is aiming for a complete set of instruments, it will complement existing national facilities such as ISIS, MLZ, and SINQ. ISIS Target Station 1 houses spectrometers for high-energy transfer, a strength of a short-pulse spallation source. It focuses on hard condensed matter research and materials science. MLZ, with its efficient cold source, has a strong focus on high-resolution spectroscopy, large-scale structural studies (SANS, reflectometry), and the use of polarized neutrons for both magnetism and soft matter research. For the latter it provides excellent opportunities for studies of structure and dynamics. In general, the instruments at SINQ do not have the same flux as the other two facilities, but it nevertheless hosts a very strong scientific community in quantum materials research and has excellent capabilities in imaging. HBS will complement this ecosystem precisely where small beams are particularly important, such as in the life and nanosciences. The signal-to-noise ratio is expected to be unprecedented at HBS. Its novel indirect geometry spectrometers will provide special opportunities for inelastic studies of quantum materials and, in the backscattering geometry, of soft matter and life sciences. With its inherent flexibility, efficiency, accessibility and specific instrumentation, HBS will promote the use of neutrons in industry. For example, the combination of neutron analytics and imaging over a broad spectral range will be an asset for industrial use. Moreover:

- HBS is a novel and innovative approach to a neutron facility. Its modular design and avoidance of regulated materials ensure reliability and resilience.
- Sustainability during construction, operation and decommissioning is a driving objective for the design of the HBS. Concepts for operation with renewable energies are being pursued.
- The HBS concept is scalable and upgradeable: the reference design is conservative and, as with any first-of-its-kind installation, significant performance improvements can be expected as experience with such an installation is gained.
- HBS provides easy access without the administrative hurdles of a nuclear facility, thus expanding the user base and providing industry with convenient and direct access.

III.2 Layout and main features

The reference design of HBS comprises the following main components (Fig. III.1):

- a high current linear proton accelerator (linac) with an end energy of 70 MeV, a proton beam current of 100 mA in the pulse, a beam duty cycle of 4.8% and an average proton beam power of 420 kW.
- a high energy beam transfer system with a fast-switching multiplexer to distribute the individual proton pulses to three target stations. One will operate at a frequency of 24 Hz, two others at 96 Hz. The pulse structure of every target station will be optimized for a certain group of neutron beam instruments.
- compact target-moderator-reflector assemblies that offer pulsed neutron beams at optimal frequency, pulse duration and neutron energy spectrum to fulfill the needs of each individual instrument.
- a number of instruments grouped around each target station so that they receive the optimal pulse structure while individual one-dimensional "finger" moderators provide the adapted phase space volume to each individual instrument.

The technical details of these components are outlined in detail in the Technical Design Report HBS Volume 1 - Accelerator [17], Volume 2 - Target Stations and Moderators [18], Volume 3 - Instrumentation [19] and Volume 4 - Infrastructure and Sustainability [20] published in 2023.

III.3 The accelerator

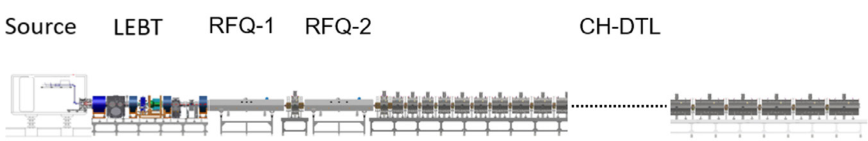

Figure III.2: *Conceptual layout of the HBS linac.*

The parameters of the high-power proton linac fall within a range of relatively low energy, high beam power, and low-to-medium duty cycle parameters that favor room temperature operation with respect to superconducting cavities. This choice eliminates the need for a cryogenic facility and allows recourse to the technology developed for the MYRRHA project. As depicted in Fig. III.2 the layout of the HBS-linac setup consists of

- an Electron Cyclotron Resonance (ECR) source, which provides a proton current above 120 mA.
- a Low Energy Beam Transport (LEBT) section to transport the beam from the source to the Radio Frequency Quadrupole (RFQ) and to match it into its acceptance.
- the 4-rod RFQ for focusing, bunching and accelerating the beam, consisting of two sections (RFQ1 and RFQ2) and an end-energy of 2.5 MeV.
- the Medium Energy Beam Transfer Line 1 (MEBT-1) between RFQ1 and RFQ2 providing beam matching of the phase space after RFQ-1 into the acceptance of the RFQ-2 at proton energy 1.272 MeV.
- the Medium Energy Beam Transfer Line 2 (MEBT-2) providing the beam handling after RFQ-2 and preparation for injection into the drift tube Linac at a proton energy of 2.5 MeV.
- the Drift Tube Linac (DTL) which will accelerate the 100 mA proton beam coming out of the MEBT-2 section up to an end energy of 70 MeV using CH-type normal conducting cavities. The design philosophy emphasis for a very modular design using proven technology and many identical parts (power couplers, pumps, tuner, LLRF) to minimize the number of required spare parts. In addition, the design will provide easy access for maintenance and repair to maximize the availability of the facility.
- solid state amplifiers feeding the accelerator structures at 176.1 MHz with powers between 100 and 600 kW. Solid state amplifiers offer significant advantages with respect to classical tube

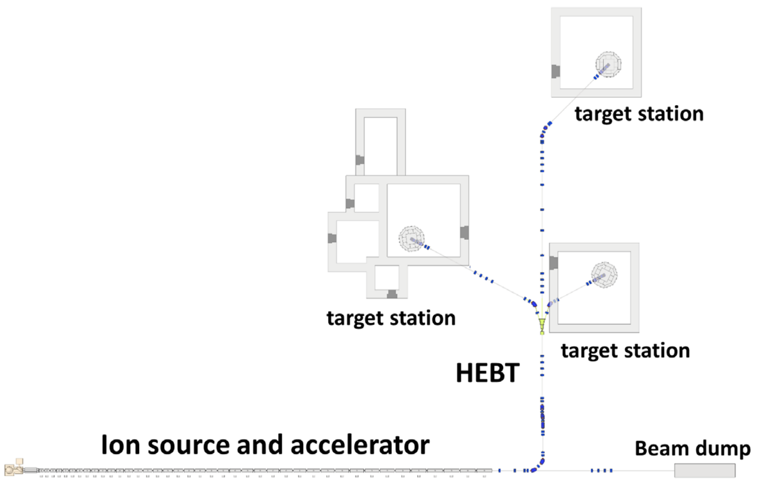

Figure III.3: Top view of the HBS High-Energy Beam Transport (HEBT) beamline to the individual target stations. The multiplexer is underground, and the beam is impinging on the targets from below.

amplifiers since they can be designed redundantly, so that in the event of failure of single amplifiers, the entire system is still ready for operation. In addition, they do not require high voltage and the footprint is much smaller compared with tube amplifiers.

- beam diagnostics and vacuum and cooling systems.

- a beam dump with a regular middle and irregular end segments distributing the proton beam of an average power up to P = 1 MW over a large cooling surface.

- a High-Energy Beam Transport (HEBT) including the beam multiplexer, which distributes the beam with appropriate frequencies of 24 Hz and 96 Hz and pulse lengths of 667 μs, and 167 μs, respectively, to three different target stations (Fig. III.3). The proton beam multiplexing system consists of a kicker magnet and a three-field septum magnet (TFSM). The concept has been tested experimentally at the COSY facility in Jülich.

III.4 The target stations

Target: The target releases free neutrons through the nuclear reaction of the incident protons with the atoms of the metal target. It is the heart of the facility and at the same time it's bottleneck, as it has to cope with as much deposited power in as small a volume as possible in order to achieve high brightness. The result of the target development process for HBS is a compact all-solid target without any moving parts made of pure tantalum. It is designed for a 70 MeV pulsed proton beam with a peak current of 100 mA, a peak and average thermal power of 6.3 MW and 100 kW, respectively, on a target area of 100 cm^2. Tantalum was chosen because it offers the best compromise of neutron yield, thermal, mechanical and thermomechanical properties, chemical, erosion and radiation resistance, hydrogen storage capacity as well as sufficient workability and an acceptable activation in a radiation field.

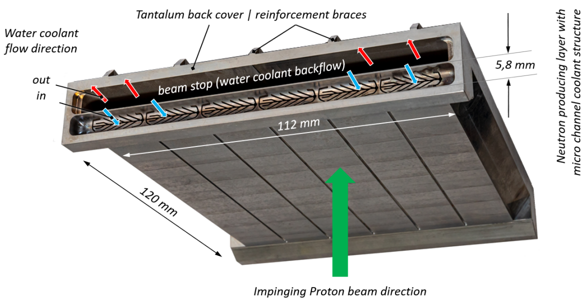

Figure III.4: Prototype of the 100 kW HBS target.

The neutron-producing layer is 5.8 mm thick and contains a "fishbone" microchannel cooling structure inside. The thickness of the layer as well as the arrangement of the microchannel structure are optimized so that about 96% of the incident proton beam completely penetrates this first layer and is stopped in the adjacent water layer (Fig III.4). This design, combined with the high hydrogen solubility of tantalum, minimizes the risk of blistering. Heat dissipation testing and the experimental verification of the thermo-fluid dynamic simulations were performed at an electron beam facility at FZJ. The target successfully withstood the design load of 1 kW cm^{-2}. This heat load experiment can be considered very conservative, leaving room for increasing the power and neutron source strength of the HBS in the future.

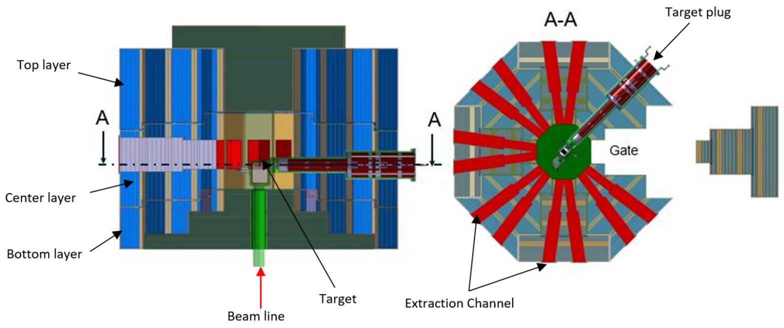

Figure III.5: *Vertical cut through the target station (left side) and horizontal cut through the center of the target station with opening (right side).*

Target station: The target is the heart of the target station, where neutrons are released from the target nuclei, moderated, and extracted towards the instruments. The target station is rather compact. It has an octagonal shape with an outer diameter of just below 4 m and a total height of 3.2 m. The primary shielding of the target station is made of alternating layers of lead and borated polyethylene (Fig. III.5). A mock-up of the HBS target station has been realized and tested at the COSY facility in Jülich.

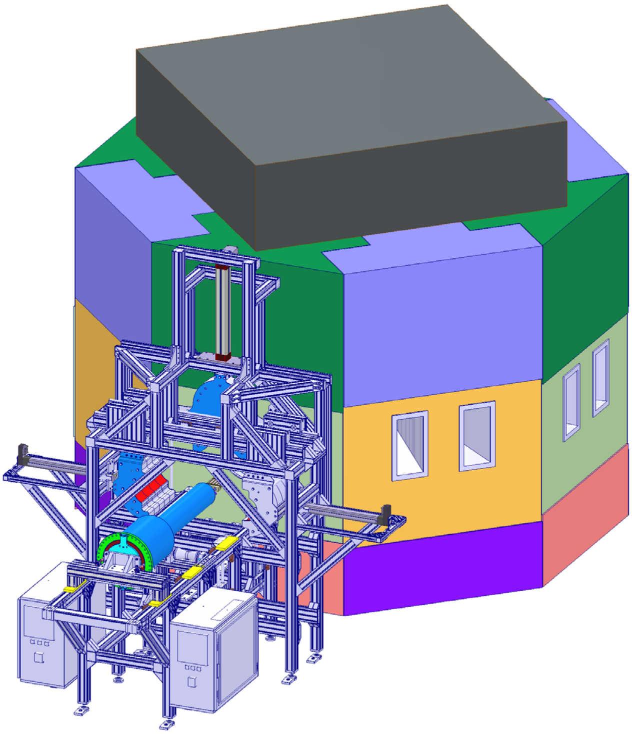

Figure III.6: *Handling tool in front of HBS target station, of which the target unit is pulled out.*

Target handling: The lifetime of the target is primarily limited by radiation-induced damage to the material by 70 MeV protons. Simulations, supplemented by literature, suggest a minimum lifetime for the target of 2.62 years for full power continuous operation. However, the operation time of the target will be limited to one year in order to keep the target activity, dose rate and radiation heat to reasonable levels to ensure safe handling and storage of the target. After one year of operation, the target will be exchanged with the help of a special fully automated target handling tool (Fig. III.6). The activity of the target, due to the radioactive isotopes built up in the target during the irradiation time, decreases by half within one day after the beam is turned off, mainly due to the decay of the short-lived proton induced isotopes. After one year of continuous, uninterrupted operation at full power and a waiting period of one week after the end of irradiation, the target activity is 0.2 PBq. This residual activity is mainly due to the decay of the 182 Ta isotope with a half-life of 114 days. Target cooling continues for the first week and is then turned off when the remaining decay heat is less than 37 W and the heat deposited in the target is less than 18 W. From this point on, no further active cooling is required. Using the target handling tool, the target is lowered into the storage position and decoupled. The intermediate storage consists of pits in the concrete ground floor. For an operating time of 30 years and an annual target change for all three target stations, a total of 90 pits, equidistant by one meter, are required.

Thermal moderator and reflector: The purpose of the thermal moderator-reflector unit is to convert the primary neutron energy spectrum into a thermal spectrum and to allow the extraction of the neutron beams to the experimental stations outside the shielding block. As the HBS is a pulsed neutron source, the materials of the moderator and reflector are chosen to moderate and store the neutrons on a time scale comparable to the proton pulse delivered to the target station. For the production of thermal neutron beams (10 - 500 meV) with high phase space density, light water is chosen as the main thermal moderator material (see Fig. III.7), since it allows active cooling of the remaining thermal load in the kW range during the operation of the target station. A lead reflector of about 20 cm thickness surrounding the thermal moderator returns a large fraction of the fast neutrons escaping from the moderator region on the timescale of μs, giving them a second chance to be moderated down to thermal energies. The reference design features a complex geometry of the moderator-reflector unit and allows the extraction of 12 beams (Fig. III.5).

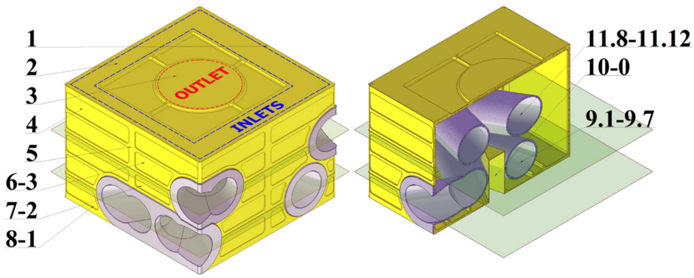

Figure III.7: Light water tank used as confinement of the liquid thermal moderator. Left: main view, Right: vertical cross section. For details see [18].

Cryogenic moderators: The HBS offers cryogenic moderators that feed one or two instruments with specific spectral pulse and angular emission characteristics. In this sense, the cold moderator is no longer part of the neutron source, but an integral part of the instrument and can be individually optimized during the design process of each instrument. The cryogenic moderators are a clear strength of the HBS design, as for the first time throughout the entire facility, so-called "finger" moderators with small dimensions are used. Compared to the cold sources of today's facilities, which typically have a volume of 10 to 20 liters, the finger moderators are an essential element for increasing beam brightness, as they are cylindrically shaped, typically less than 10 cm long, and have

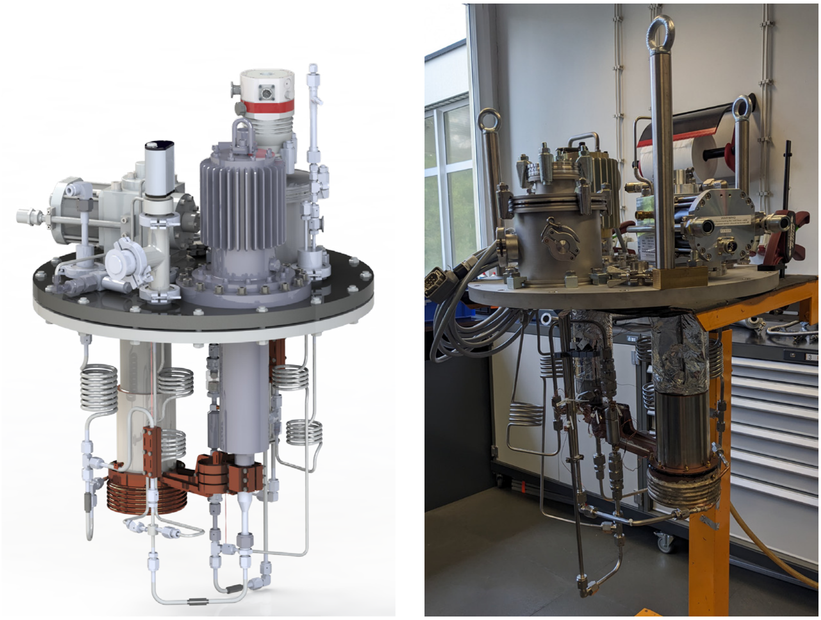

Figure III.8: Left: Design of the para-hydrogen main cryostat (courtesy of S. Eisenhut). Right: Assembly.

a neutron-emitting surface of only a few cm in diameter. Four different materials have been tested and improved at the JULIC neutron test platform, each with its own cryostat and moderator vessel: solid mesitylene C_9H_{12}, solid methane CH_4, liquid hydrogen H_2, and liquid para-hydrogen p-H_2 (Fig. III.8). A compact one-dimensional cold moderator can be placed inside the thermal moderator in a position where it is optimally supplied with thermal neutrons from all sides, while the cold neutrons are extracted in only one direction (one-dimensional) through an extraction channel towards the instrument. Bispectral extraction can be easily realized if the beam extraction system is designed to receive neutrons from both the cold moderator and the surrounding thermal moderator. The use of individual moderators for each instrument allows optimization of cold neutron extraction to the instrument. This modular design makes the facility resilient, as a failure of one cold source will only affect one instrument. In addition, this compact cold source can be easily replaced from the outside during the next one-week shutdown without opening the TMR shielding.

Epithermal, resonance, and fast neutrons: In addition to the extraction of thermal and cold neutrons also epithermal (0.5 - 2 eV), resonance (2 eV - 10 keV) and fast (> 10 keV) neutrons are released from the target and can be offered for experiments.

Target station control system: The target station control systems will be a subordinate systems of the overall accelerator control system, with the subsystems for (i) Target cooling, (ii) Target vacuum, (iii) Target diagnostics, (iv) Target handling, (v) Opening of the target shielding, and (vi) Personal Protection System.

III.5 Instrumentation

The HBS is a novel neutron facility that overrides some of the usual design criteria, such as striving for the highest source strength. Instead, efficiency, brightness and flexibility are maximized while keeping

	Instrument	τ_{pulse} [μs]	L_{tot} [m]	Det. Cov. [sr]	$\lambda_{\min}$ [Å]	$\lambda_{\max}$ [Å]	$\frac{\delta\lambda_{\text{pulse}}}{\lambda_{\min}}$ [%]	$\frac{\delta\lambda_{\text{pulse}}}{\lambda_{\max}}$ [%]	ϕ_{average} 10^6 [n/cm^{2}s]	Remarks
SANS	High-Throughput SANS	667	23.7	0.01	3.0	9.8	3.7	1.1	0.41	Low angle
			14.7	0.81	3.0	9.8	8.8	2.0	41	Wide angle
GISANS	SANS with GISANS option	667	23.7	0.01	3.0	9.8	3.7	1.1	0.41	Low angle
			14.7	0.81	3.0	9.8	5.9	1.8	41	Wide angle
OffRef	Offspecular Reflectometer	667	13.0	0.08	2.0	12.0	10.1	1.7	48	
TPD	Therm. Powder Diffr.	30	80.0	5.71	0.6	2.7	0.2	0.1	0.55	High Res., 2 frames
		667	80.0	5.71	0.6	2.7	5.5	1.2	160	High Int., 2 frames
NSE	NSE Spectr.	667	25.0	0.04	6.0	16.0	1.8	0.7	2.8	Very cold neutrons
NRSE	NRSE Spectr.	667	25.0	0.04	6.0	16.0	1.8	0.7	2.8	Very cold neutrons
BSS	Backscattering Spectr.	60	85.0	3.66	5.6	7.6	0.06	0.04	7	
Tof-PGA	TOF-PGNAA	667	12.4		0.03	9.0			130	
NDP	Neutron Depth Profil.	667	8.2		0.0	20.0			210	White beam
HorRef	Hor. Reflectometer	252	11.0	0.01	5.0	8.6	1.8	1.1	7	Small sample
		252	11.0	0.01	1.6	8.8	5.7	1.0	10	Multi beam
EngDi	Engineering Diffr.	35	21.8	2.52	0.8	2.7	0.8	0.2	0.23	4 frames
DENS	Diffuse Elast. Neutron Scat.	252	21.2	5.24	2.0	3.9	2.4	1.2	50	
PDNS	Pol. Diffuse Neutron Scat.	252	21.0	2.09	2.0	4.0	2.4	1.2	52	
MMD	Single Crystal Diffr.	252	21.5	9.39	2.0	3.9	2.3	1.2	18	for 0.8^o FWHM div.
CCS	Cold Chopper Spectr.	252	24.0	2.07	1.6	10.0	2.6	0.4	0.34	
CAS	Crystal Analyzer Spectr.	252	60	0.85	1.8	6	0.9	0.3	200	for 1.8 Å$< \lambda <$ 2.5 Å
C-NI	Cold Neutron Imaging	252	15.0		1.0	15.0	6.6	0.4	0.3	High Res.
		252	5.0		1.0	15.0	20	1.3	3	High Int.
T-NI	Thermal Neutron Imaging	252	10.0		0.5	4.5	20	2.2	0.35	High Res.
		252	4.0		0.5	4.5	50	5.5	10	High Int.
D-NI	Diffractive Neutron Imaging	252	30.0		1.0	15.0	3.3	0.2	2	
DMD	Disord. Mat. Diffr.	167	85.0	6.42	0.10	0.58	7.8	1.3		
PGAINS	PGAINS	167	8.6		0.00	0.37			16	
Epi-NI	Epitherm. Neutron Imaging	2	35.0		0.01	0.29	2.5	0.1	0.2	
HE-NI	Hi-Energy Neutron Imaging	167	10.0		0.00	0.01			80	
CrysTof	CRYSTOF	252	9.5	2.34	0.83	2.86	12.6	3.7	0.2	

Table III.1: *Key figures for the instrument suite presented. Flux and resolution values are quoted for typical configurations of the instruments. The colors indicate different instrument classes also used in Fig. III.1: Light blue: Large scale structure instruments, Dark blue: Diffractometers, Green: Spectrometers, Yellow: Imaging and analytics instruments.*

construction and operating costs as low as possible for such a powerful facility. The instrumentation, ancillary equipment, and laboratory needs must be defined by future users, tailored to the science that can be done with such a source. The reference instrumentation described here is the result of frequent interaction with users and their feedback. A full range of instruments for the most common applications is presented to demonstrate the capabilities of such a facility, although actual realization depends on many factors. While the reference instrument suite features 25 instruments, additional target stations could be readily added to host about 50 instruments in total, limited only by the accelerator characteristics.

Instrument suite: Overall, taking advantage of the particular source characteristics of the HBS, the performance of all instruments compares very favorably with that of corresponding instruments in existing facilities such as MLZ, ILL, ISIS. Polarization analysis is foreseen for most instruments of HBS as it provides distinctive additional information for soft matter, life sciences and magnetism. Among other applications, HBS offers particular strengths

- in combining the bright 1d finger moderators with advanced neutron transport systems based on SELENE optics, where beam spot sizes at the sample of less than 1 mm can be achieved. This is particularly useful for reflectometers when laterally inhomogeneous heterostructures are studied, e.g., in information technology, or for diffractometers for small single-crystal samples. The latter is important for protein crystallography in the life sciences, where usually only small crystals are available. In addition, the small beam size combined with pulsed operation leads to excellent background conditions.

- for novel indirect geometry spectrometers that combine the best of the worlds of three-axis- (TAS) and time-of-flight (ToF) spectroscopy. By using time-of-flight to decode the initial neutron energy, they can digest a large portion of the moderator spectrum and thus achieve extremely high sample fluxes. Crystal analyzers combined with position-sensitive detectors are optimized for small samples and higher acceptance, while prismatic focusing prevents energy resolution from being compromised. These concepts are ideally suited for the HBS with its small bright neutron source and provide excellent conditions for research on quantum materials. Similar concepts can be employed for near-backscattering spectrometers, which can probe hydrogen movements in energy technology devices or the life sciences. Such an instrument will be very competitive even to comparable instruments at MW short pulse spallation sources.

- for industrial research by combining neutron analytics and imaging utilizing the accessible broad spectral range up to resonance and epithermal neutrons. Moreover, the HBS offers the exceptional possibility to produce a remarkably wide range of (medical) radioisotopes through both processes, high energy, high current proton capture and high flux neutron capture, respectively. This will attract companies specialized in this domain.

Scientific Computing: HBS aims to address from the outset the challenges of data, metadata management, and high data rates. Figure III.9 presents a typical research workflow starting from an idea or a scientific question and finishing with an insight which usually leads to a new scientific question or to a publication or both. In order to achieve the goals in the area of data management, scientific computing and instrument support, the HBS will bundle these activities in a structure similar to the JCNS NeutronSimLab. This structure will be founded on the fields of action of the Helmholtz Digitization Strategy. Its task will be to coordinate science-, method- and technology-oriented digitization projects and to take over the management of the corresponding IT infrastructure for the HBS. Projects

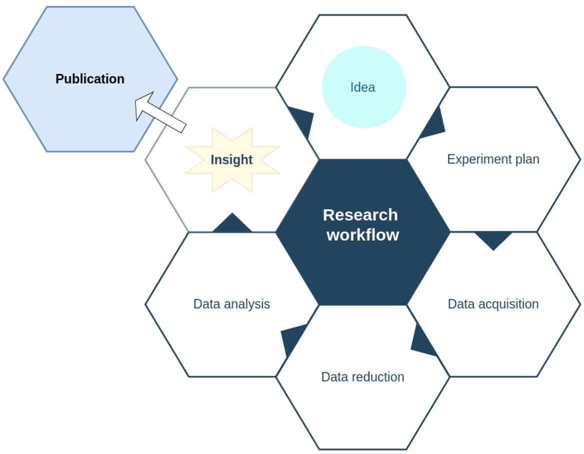

Figure III.9: *Research workflow at HBS: From idea to publication.*

include the development and maintenance of software for scientific data analysis, the design and implementation of new AI-supported methods, as well as the establishment of a cloud infrastructure and the development of digital twins for the remote control of instruments, the preparation of experiments, and efficient data analysis. A dedicated project group for data management will be established.

III.6 Infrastructure

A thorough structure of the organisation, management and construction of the facility based on accelerator, target, and instrumentation requirements has been developed. In addition to these organisational prospect, sustainability, environmental and socioeconomic impacts, decommissioning, and lessons learned from other facilities are considered. Companies specializing in sustainable construction and operation, power supply for large facilities, and architects, as well as experienced managers of existing facilities or facilities under construction, were brought in to provide sound solutions.

Because many of these aspects are subject to constant change, primarily due to societal demands, the description in this volume of the TDR differs from the technical volumes of the HBS TDRs. It provides a basic framework for considering and addressing the above issues for HBS as a large-scale research infrastructure [20]. The boundary conditions are highly dependent on the chosen location of the facility. In order to make concrete statements, it is assumed that the facility will be realized on the campus or in immediate vicinity of Forschungszentrum Jülich, where an administrative and scientific infrastructure is already in place and a widespread interest for scientific usage of the HBS exists in many different departments. Therefore, the schedule, costs and scope are described taking these boundary conditions into account and all costs are calculated in 2021 prices. Building such a facility "on a greenfield site" elsewhere would increase costs and construction time. Furthermore, to minimize possible risks associated with the realization of the project, it is considered to build the facility in several building blocks.

Estimated costs of the facility: In the following table costs are based on 2021 prices, no contingency and VAT are considered.

Installations	Block 1	Block 2	Block 3	Total
Accelerator	62.0	49.0	4.0	115.0
Target system	7.0	6.0	6.0	19.0
Instrumentation	32.2	46.0	37.1	115.3
Total	101.2	101.0	47.1	249.3
Buildings	**Block 1**	**Block 2**	**Block 3**	**Total**
	185.3	65.6	40.4	291.3
Total	286.5	166.6	87.5	540.6

Table III.2: *Cost estimates for HBS installations and buildings for the different construction blocks in Mio EUR based on 2021 cost reference. Contingency and VAT are not included.*

Buildings: State-of-the-art technology with low carbon emissions and suitable energy-saving technologies will be used for the design and construction of the buildings. Special attention will be paid to minimizing the amount of concrete due to radiation protection requirements e.g., by building the accelerator facilities underground. From the beginning of the project, consultations have been conducted with external service providers to aid in establishing minimized and CO2-neutral construction and operation of the HBS project. These consultations will continue throughout the life of the project to ensure a cost- and energy-efficient and CO2-neutral facility.

Energy consumption: It is assumed that the facility will be operated for 5000 hours per year. This corresponds to slightly more than 200 days of continuous operation. When in full operation, the total electrical energy demand is estimated to be ≈16 MW for the facility as a whole. Total annual consumption would be approximately 85.000 MWh. To ensure CO2-neutral operation, electricity demand will be met entirely from renewable energy systems e.g., by purchasing renewable energies through Power Purchase Agreements from external suppliers. During operation, specialized external agencies will provide continuous energy conservation and carbon footprint reduction support to maintain and further improve the energy- and cost-efficiency.

Staff: At full operation, a total of 230-240 full-time equivalents will be required for accelerator, target station and instrument operations, radiation protection and the user office and services. Special attention will be given to the commitment to Equality, Diversity and Inclusion (EDI). Since we assume that the site will be located in Jülich, it is anticipated that additional support will be offered by existing central providers for engineering, scientific computing, communications, etc. In case the HBS would be constructed as a green-field facility without access to the services and infrastructures of Forschungszentrum Jülich, and based on existing facilities such as MLZ, SINQ or ISIS operating at a similar scale, the HBS staff demand would be approximately 570 FTEs.

Organization / Management: To manage the HBS and the construction of the facility, a project management (PM) model will be used which was developed internally at JCNS for the particular case of the construction and management of research infrastructures. The model bridges the essential principles of PRINCE2® and the Project Management Institute (PMI) methodologies, adds a technique for measuring project performance and progress through Earned Value Management (EVM), and a stage gate approach. Different organizational charts have been developed for the construction and

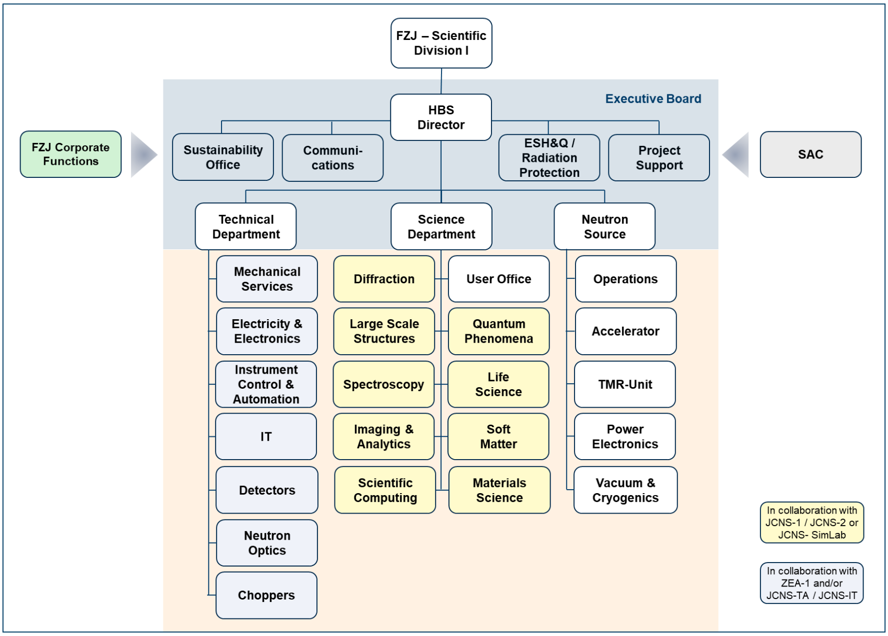

Figure III.10: *Proposed organizational chart for the operation phase of the HBS facility located at FZJ.*

operation phases of the facility. An example for the operation phase is shown in Figure III.10. During the construction phase, the project is divided into three main management departments dealing with the project itself, technical issues, and scientific issues. Together with the general project director, the project managers form the executive board where any routine decisions about the project are made. Dedicated independent advisory boards on project (PAC), technical (TAC) and scientific (SAC) topics will support and review any progress of the project. A steering board composed by members of the funding agency, members of the board of directors of FZJ and key institute leaders across the FZJ involved in the project will supervise the project director and the decisions of the executive board.

Safety and waste management: Non-radiological safety follows the principles established at Forschungszentrum Jülich GmbH. Both the accelerator and the instruments are equipped with state-of-the-art safety systems for personal and machine protection. Radiological safety follows the ALARA principle (As Low As Reasonably Achievable). The legal basis for the construction and operation of the HBS facility is the German Radiation Protection Ordinance (StrSchV); the HBS is not subject to nuclear law! Waste management for radioactive active waste will be done in cooperation with JEN "Jülicher Entsorgungsgesellschaft für Nuklearanlagen mbH", which bundles the entire nuclear decommissioning, dismantling and disposal expertise that has been built up in Jülich over five decades.

Socio-economic impact: HBS has the same general socio-economic benefits as most large research installations. In addition, some specific aspects result from the assumed location in Jülich. The construction and operation of HBS not only enables science to effectively address the grand challenges facing society, but also supports economic progress at the regional and local level in Germany and, in particular, in a former lignite mining region in North Rhine-Westphalia (NRW) undergoing massive structural changes. During the construction and operation phase, it offers countless opportunities for many high-tech and construction companies in NRW. During operation, the many thousands of guest visits per year will have a remarkable local economic impact. The education of students in a large facility with strong international appeal offers an opportunity for the many surrounding universities, e.g. in Düsseldorf, Cologne, Bonn, Aachen, all within max. 40 minutes drive.

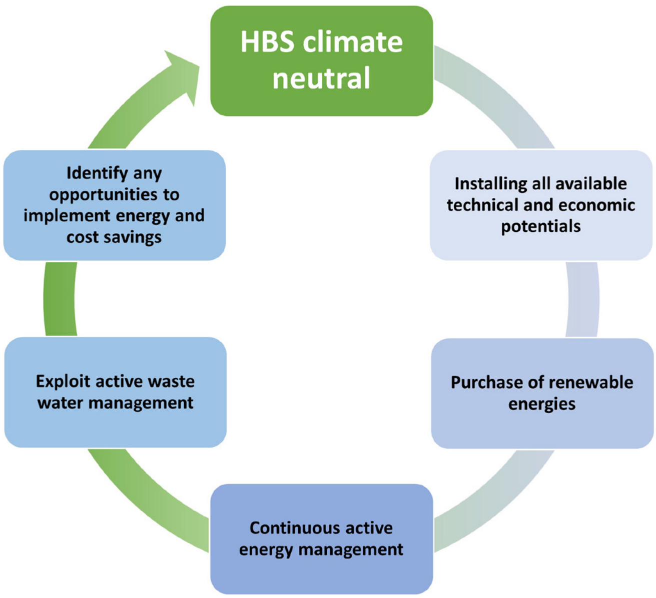

Figure III.11: *Activities to achieve HBS climate neutral operation.*

Decommissioning: Planning the decommissioning of the HBS facility is considered at the earliest stage of its development i.e., at the design and construction stages and will continue during the lifetime of the facility starting at the stages of commissioning and operation and potential upgrades. In order to ensure safe dismantling, the HBS facility will be designed and constructed to minimize the amount of radioactive and hazardous materials and to facilitate the management of activated materials employed by using modular shielding and technical components. As part of the facility's initial authorization, an initial decommissioning plan including risk analysis, is being developed to demonstrate the feasibility of decommissioning, to define a decommissioning strategy and to estimate costs.

A.

APPENDICES

A.1 Radionuclide production with HBS

Th. Brückel, B. Neumaier

The HBS is based on a proton linear accelerator, which shoots protons of an energy of 70 MeV with a peak current of 100 mA onto a tantalum target to produce neutrons. A multiplexer can be used to operate three target stations, each with 100 kW of power per target. The accelerator is operated in pulse mode. For the applications considered in the TDR Vol. 3 [19], a duty cycle of 6% is used, while 20% is the maximum possible for the present accelerator layout. Thus, a duty cycle of 14%, i.e. an average proton current of 14 mA at 70 MeV proton energy, is available for other applications. These applications can be carried out simultaneously in parallel with the intended use as a research and development platform for functional materials and active substances.

Of particular interest is the development and production of radionuclides for medical applications in diagnostics and therapy, or nuclear theranostics, the combination of both. In this field, the HBS has a unique selling point, since radioisotopes can be produced at HBS by both neutron- and proton-induced nuclear reactions. For this purpose, two additional dedicated target stations can be envisaged, one with a high-power target for neutron production, and one with a target for direct proton irradiation. These two target stations would be served by an additional multiplexer and could be integrated into the planned building structure, e.g. in the basement below the experimental hall. An additional multiplexer would allow several radioisotopes to be produced simultaneously at the target station for proton irradiation.

A.1.1 Radioisotopes by neutron capture

Among the radioisotopes produced by neutron capture, the radionuclide Mo-99 (molybdenum) stands out in particular. Mo-99 (half-life 66 hours) is the parent nuclide of Tc-99m (technetium) (half-life 6.1 hours), the most commonly used radioisotope for medical imaging and the study of pathological organ function. It accounts for about 80% of all nuclear medicine procedures, equivalent to about 40 million examinations per year worldwide, of which about a quarter are performed in Europe. In Germany, the demand is 60,000 examinations per week, which corresponds to almost 10% of the worldwide annual demand. Due to their limited half-life, interruptions in the supply chain of this medical isotope can lead to the failure or delay of important medical examinations, which are essential for further treatment and can have a negative impact on patient health.

Mo-99 is currently produced mainly by fission of highly enriched uranium U-235 with thermal neutrons. For this purpose, uranium targets are irradiated in a nuclear reactor with a high neutron flux.

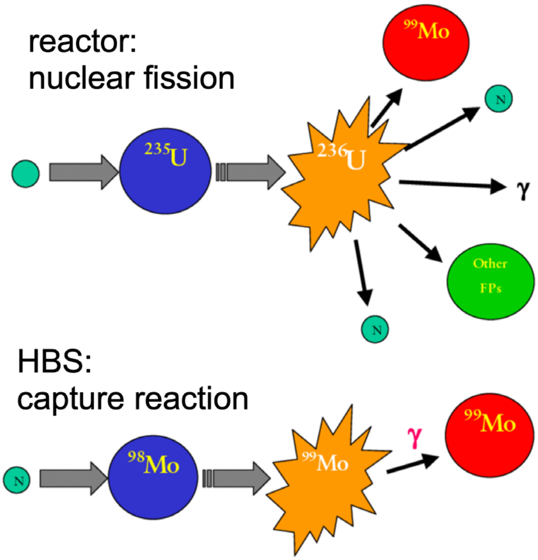

Figure A.1: Schematic of two possible routes to produce Mo-99, the parent nuclide of Tc-99m. Production in reactors by a fission reaction has a high cross section, but requires the use of nuclear fuel and leaves behind a significant amount of radioactive waste. Production by neutron capture at HBS has a lower cross section and results in less specific activity, but avoids the use of nuclear fuel material.

The production of Mo-99 in this way is very effective. Currently, 6 reactors in the world can produce this important radioisotope. Five of them are over 50 years old (source: Nuclear Medicine, World Nuclear Association, Feb. 2023 [21]). However, the radiochemical separation of Mo-99 from the uranium fission products produces significant amounts of radioactive waste that must be disposed of. In addition, strict nonproliferation measures must be taken. Moreover, several of the aforementioned reactors are scheduled to be permanently shut down in the coming years, while the licensing of new reactor-based plants is costly and takes a long time. Here, HBS can provide an alternative by obtaining Mo-99 from Mo-98 or natural molybdenum by a neutron capture reaction. Although the reaction is less efficient than uranium fission, it avoids the use of nuclear fuel with the aforementioned disposal and proliferation problems. In order to meet the demand of Mo-99 for Germany by HBS, a special high power target has to be developed. Furthermore, the nuclear chemical separation up to the production of a 99Mo/99mTc generator system has to be established and demonstrated. Exactly these challenges are currently (2023 - 2026) being addressed in the joint project "99Mo Best" in the "7th Energy Research Program of the Federal Government in Nuclear Safety Research and Radiation Research". Partners in this project are the University Hospital Cologne / University of Cologne, FH Aachen University of Applied Sciences, Leibniz Universität Hannover and Forschungszentrum Jülich (JCNS, INM, ZEA-1).

A.1.2 Radioisotopes by proton capture

For radioisotopes that can be produced via proton-induced nuclear reactions, HBS offers unique opportunities due to the high energy and high proton current and can open up a new terrain of high academic and application interest. Currently, radioisotopes formed by proton bombardment are produced at cyclotron accelerators. In commercial facilities, proton energy is typically limited to 30 MeV and current to 350 μA. Cyclotrons with higher final energy exist, such as the world's largest cyclotron at the Canadian research center TRIUMF, which has a maximum energy of 520 MeV. However, these facilities have a significant beam current limitation of a few 10 μA. In contrast, the HBS opens up the energy range from 30 to 70 MeV with possible currents in the mA range (up to 14 mA). In this energy range, the effective cross sections are often not precisely known, a problem that could be solved by measurements at the HBS. However, it is known that for many important isotopes the effective cross section, i.e. the production rate, increases significantly with energy, so that commercial production at HBS would be highly interesting. As an example, the following figure shows the important radioisotope copper-67. Cu-67 (half-life 2.58 days) is the longest-lived radioisotope of Cu. It is of outstanding importance for theranostics because of its simultaneous emission of β-radiation (mean β-energy: 141 keV; Eβ_{max}: 562 keV), useful for therapeutic treatments, and γ-radiation (93 and 185 keV), suitable for single photon emission computed tomography (SPECT). It can be prepared from Zn-68 by the (p,2p) reaction. The threshold for this reaction is above 25 MeV, so that relevant amounts of Cu-67 can only be produced in the 40-70 MeV energy range, since it is only in this energy range that the effective cross sections are correspondingly high (Fig. A.2). Furthermore, the figure demonstrates that cross sections in this energy range are insufficiently known and a wide scattering of data from different sources exists.

Some examples of other interesting radionuclides that could be produced at HBS are summarized in the table below (Fig. A.3). Of particular interest for theranostics, i.e. the combination of diagnostics and therapy, are four radioisotopes of terbium. These are 149Tb (α-emitter), 152Tb ($\beta+$-emitter), 155Tb (γ-emitter/SPECT), and 161Tb (β-emitter). These can all (except 161Tb) be produced at HBS by proton bombardment of Gd targets.

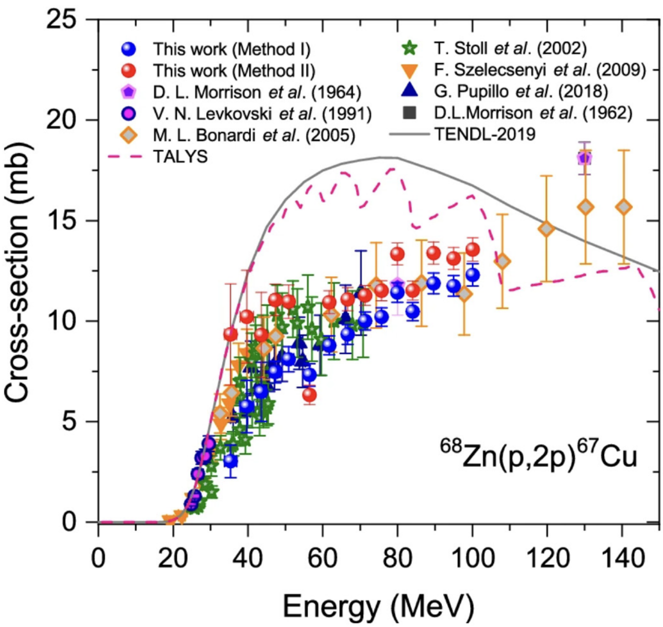

Figure A.2: Cross section for the production of Cu-67 from Zn-68 showing the scatter of the experimentally determined values and supporting the need for high proton energies around 70 MeV. [22]

Z	element	nuclide	T ½ [d / h]	conversion	av. energy [keV]	gamma-energy [keV]	application	production reaction
29	copper	Cu-67	2.6 d	beta-minus	141	93 185	SPECT, β-therapy	^{68}Zn(p,2p)^{67}Cu ^{70}Zn(p,α)^{67}Cu
50	tin	Sn-117m	13.9 d	Auger e$^-$	127	159	theragnostic for bones	^{121}Sb(p,αn)^{117m}Sn
21	scandium	Sc-47	3.35 d	beta-minus	162	159	SPECT, β-therapy	^{48}Ti(p,2p)^{47}Sc
65	terbium	Tb-152	17.5 h	beta-plus	1140	344	PET	^{155}Gd(p,4n)^{152}Tb
65	terbium	Tb-149	4.1 h	alpha beta-plus	3967	352 165	PET α-therapy	^{154}Gd(p,5n) ^{149}Tb
65	terbium	Tb-155	5,3 d	e- capture	-	87, 105	SPECT	^{158}Gd (p,4n) ^{155}Tb
65	terbium	Tb-161	6,9 d	beta-minus	500, 600		β-therapy	^{160}Gd(d,n)^{161}Tb
89	actinium	Ac-225,227	9.9 d	alpha	5800		α-therapy (prostate cancer)	^{232}Th(p, x)^{225}Ac

Figure A.3: *Examples of radionuclides that can be produced at HBS by proton-induced reactions*

A.1.3 Summary: Radionuclides at HBS

In summary, it can be stated that in addition to its planned application as a discovery and development platform for functional materials and active agents, the HBS also has great potential for the research and production of radioisotopes for medical applications. The possibility to produce a very broad spectrum of radionuclides both from nuclear reactions with neutrons (e.g. beta-minus emitters for tumor therapy) and from nuclear reactions with protons (e.g. beta-plus emitters for PET applications) provides the HBS with a unique selling point. Thus, the HBS can offer perspectives for the settlement of relevant companies in the surrounding area and contribute to the coverage of operating costs.

A.2 The HBS demonstrator: a first step to the realization of the HBS

The idea of a HiCANS like the HBS is completely new: there is no such facility in the world today. Many concepts are original and do not exist in other neutron research facilities. As a result, the HBS has been designed with a level of care unparalleled by most other large-scale facilities:

- All critical components have been optimized analytically.
- Their performance has been verified by extensive simulations.
- The components have been designed and prototyped.
- Their performance was tested experimentally.
- The interaction of all components was demonstrated on the JULIC neutron test platform in low power mode.

These steps are documented in the four volumes of the TDR, and the HBS facility could be built directly on this basis. This is the normal procedure for most other large scale facilities. On the other hand, the scalability of the HBS offers the possibility to realize a HiCANS in stages. A decisive step in this context is the construction of a HBS demonstrator based on a powerful high-current accelerator equipped with a versatile target unit and instruments.

At Forschungszentrum Jülich, the particularly fortunate position exists of having an infrastructure that allows to

- realize the demonstrator of the HBS without the need for extensive construction, i.e. the investment in the demonstrator "goes almost entirely into science and not into concrete".
- show the power of a HiCANS first time with the demonstrator with a set of instruments that allows one to produce world-class science and attract industry.
- build the building infrastructure for the HBS in the vicinity. This will be done concurrently with an ongoing experimental program at the demonstrator.
- reuse the demonstrator and instruments for the realization of the HBS by moving them into the newly constructed buildings during a relatively short shut down period of a few months.
- expand the facility to the full-fledged HBS, taking full advantage of the lessons learned from the operation of the demonstrator.

The advantage of this approach is that

- the performance of a HiCANS can be demonstrated.
- experience can be gained with its operation.
- improvements can be made based on experimental studies.
- users can already perform experiments without having to wait for the realization of the fully equipped HBS facility.
- the demonstrator and its instruments can be moved to the final location of the HBS, thus reusing the initial investment.

Following the approach described, the layout of the HBS demonstrator and its possible location will be discussed. Based on the TMR unit built at the Jülich Centre for Neutron Science, a corresponding high-current proton accelerator system with a proton current of 100 mA and a minimum energy of 35 MeV is to be realised. This accelerator will be connected to the present TMR unit and linked to corresponding instruments. With the chosen parameters, the technological basis for the efficient production of neutrons from tantalum and relevant medical radioisotopes will be achieved.

A.2.1 The HBS demonstrator in the COSY hall

Triggered by the concentration of the nuclear physics activities in Germany in the Facility for Antiproton and Ion Research (FAIR) in Darmstadt, it has been decided to move the nuclear physics activities of Forschungszentrum Jülich (FZJ) to FAIR and to discontinue the operation of the COoler SYnchrotron COSY at the Institute for Nuclear Physics of FZJ. As a result, a large experimental area under radiation protection supervision and equipped for the operation of accelerators with the corresponding radiation protection areas is becoming available for re-use in 2024. In fact, the JULIC neutron test platform of the HBS project is located in one of the external experimental areas of the COSY facility, directly supplied with protons from the JULIC cyclotron. In this area (so-called "Big Karl" area), the Target-Moderator-Reflector (TMR) station has been installed as a mock-up of an HBS TMR station for the aforementioned tests of the interaction of the different components (see Vol. 2 of the HBS TDR, [18]).

Compared to the design of the HBS TMR stations, there are three main differences: (i) the proton beam enters the test TMR from the side rather than from the bottom, (ii) the shielding is designed to operate at up to 1/10 the power of the HBS and (iii) the test-TMR has only 8 extraction channels instead of up to 12. Nevertheless, a demonstrator using this test TMR in combination with a powerful

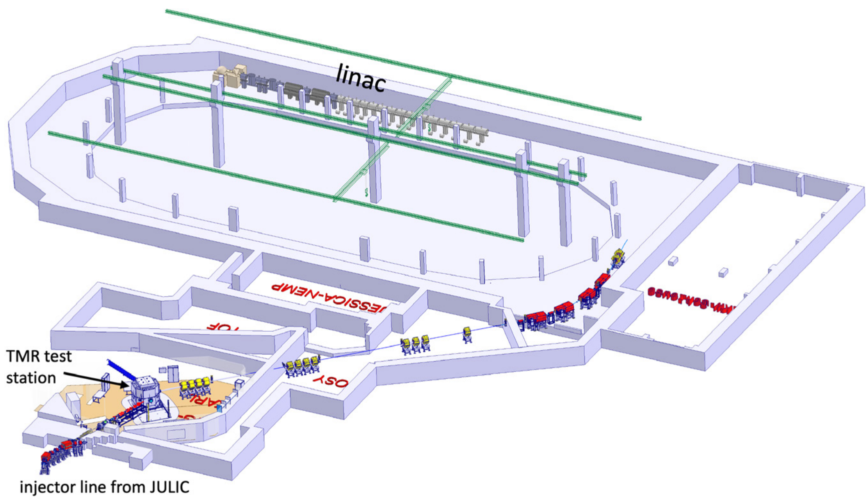

Figure A.4: Floor plan of the COSY facility. The width of the COSY hall is 37 m. The linac of the demonstrator is shown in the COSY hall, as well as the proton transfer line to the test TMR (lower left), where the current injector line of the JULIC cyclotron is still visible. The instruments can be placed around the TMR test station (in the so-called Big Karl area) and extend into the adjacent experimental areas, so that the instruments can have a maximum length of 30 m.

linac and equipped with a set of up to 6 well-selected instruments has an expected flux at sample comparable to that of medium flux research reactors, with several advantages such as small beam size and low background. Therefore, such a demonstrator will already enable world-class science and demonstrate the capabilities of a fully equipped HBS facility. Figure A.4 shows the possible layout of an HBS demonstrator in the COSY area.

An accelerator with 100 mA proton current up to a proton energy of 35 MeV requires 25 DTL cavities and has a total length of 58 m (including ion source, LEBT, RFQ and MEBT) [17]. As Figure A.4 shows, such an accelerator fits easily into the COSY hall. The neutron yield amounts to 12.5% of that of the HBS where the accelerator reaches 70 MeV [18]. Thus the performance of the instruments will be 1/8 of the performance of instruments at the full HBS and therefore quite comparable to instruments at medium flux research reactors. This is sufficient to achieve the goals of the demonstrator, namely to gain experience with such a new type of facility and to enable science based on the particular capabilities of a HiCANS, i.e. the high brightness beams at low background. Depending on available funding, the accelerator can be upgraded to higher proton energies by adding additional DTL segments. This will result in at least a quadratic increase in the neutron yield at the target station.

The cost of the linac for the demonstrator will be 53 Mio € for the 35 MeV version. The investment in high-energy beam transport and infrastructure modification is estimated at 28 Mio €. The total cost with the proposed instrumentation (see below, 23 Mio €) for the demonstrator sums up to 104 Mio €. The claimed values are based on the 2021 cost reference used for the entire TDR.

A.2.2 Proposed instrumentation of the HBS demonstrator

The demonstrator should not only enable world-class science, but also attract industry to a facility that is easily accessible and highly flexible. The instrument suite for the HBS demonstrator therefore includes workhorse instruments for a wide range of applications. Those instruments are particularly suitable for industrial use and produce a large number of high-impact scientific publications as known from other facilities. Based on these criteria, the following instrument selection is proposed for the HBS demonstrator chosen from Vol. 3 [19]:

Instrument type	Name	Vol. 3 chapter
Imaging	T-NI	VII.3
Analysis	PGNAA	VII.5
Diffractometer	MMD	V.3
Small angle scat.	SANS	V.7
Reflectometer	HorRef	V.9
Radionuclides	RN	Appendix 1

Table A.1: *List of instruments proposed for the HBS demonstrator. The name and chapter number refer to those used in Volume 3 of the TDR on instrumentation [19], except for radionuclide production, which refers to Appendix 1 of this volume.*

It is planned to involve University groups and industry from the very beginning in the realization of the instrument suite. The BMBF framework program ErUM ("Erforschung von Universum und Materie") to promote research at large-scale facilities and the action plan "ErUM-Transfer" to promote transfer of the results into commercial enterprises can be an important catalyst in this regard.

Prompt Gamma Neutron Activation Analysis PGNAA can be combined with the imaging beamline. Imaging and PGNAA Analysis, Reflectometer and Diffractometer were designed for the 96 Hz station, while SANS was designed for the 24 Hz TMR. However, the SANS instrument has a pulse shaping chopper that can be used for the demonstrator to suppress additional pulses, allowing the test TMR station to operate at 96 Hz for all proposed instruments. For the most demanding SANS experiments, the test TMR can be operated at 24 Hz. Radionuclide production requires separate run cycles as the internal part of the TMR station has to be changed. According to Table X.1 of the TDR Vol. 3 on instrumentation [19], the total cost for the scattering, imaging and analysis instruments amounts to 19.95 Mio €. Together with the additional investment for the radionuclide production and the sample environment, one ends up with 23 Mio € for the experimental stations.

A.2.3 Summary: HBS demonstrator at the COSY Facility

In summary, an HBS demonstrator can be realized using the existing building infrastructure of the COSY facility, which will be decommissioned in 2024. The HBS demonstrator forms the foundation for the future HBS neutron source, which is to be expanded and developed into a fully comprehensive research infrastructure for the scientific and industrial use of neutrons in Germany. Using the existing TMR of the JULIC neutron test platform, a facility supporting 6 applications can be realized. The instrument suite will be highly attractive to industry, allows users to perform world-class science, and demonstrates the capabilities of the HBS for radionuclide production. The total cost of the demonstrator will be 104 Mio €. Most of this investment can be reused for the final HBS, which can be built in parallel at a nearby location to provide a cost-efficient, powerful and innovative neutron source available for the German and international user community and the needs of industry.

B.

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