The MLZ MORIS program

Pre project description

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Document prepared by the MORIS working group

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1 Executive summary

Continuous improvements and the development of new additional instruments enabled world-class research with neutrons and positrons at the MLZ in Garching over about 20 years now. Competitiveness on an international scale on one hand, implies major upgrades if new technologies in neutron instrumentation is available. Limited availability of spare parts after two decades of operation on the other hand, increases the risk of failures after such a long time of ongoing user service. This motivates the MLZ to launch a substantial upgrade and refurbishment program for the second half of the 2020's decade, the MORIS program.

With the recent commissioning of new instruments in the guide hall-East, the major focus of MORIS is not to increase the number of instruments in user operation even further. However, new perspectives are presented to complement the instrument suite at the MLZ by new type of instruments, which are so far not available, but which would satisfy a need identified by our wide spread user community.

This document summarizes the state of development of 26 individual projects to refurbish and improve our instrument suite. This second version of a pre project documentation has a focus on the discussion of the science case of the renewal program. Having addressed our advisory bodies, the discussion with experts from our user community in April 2023 will strengthen and guide our project.

Gathering all this input we aim for a more detailed project plan to be presented to our funding bodies by the end of 2023. As this list still has to be consolidated during the year, first estimations of costs and schedules are already included at this stage. So far we calculated an investment of about 57M€ in addition to project related manpower in the order of 7.7M€ taking into account an overall duration of the MORIS project of 5 years.

2 Overview

The Heinz Maier-Leibnitz Zentrum (MLZ) is a leading center for cutting-edge research with neutrons and positrons. Operating as a user facility, the MLZ offers a unique suite of high-performance neutron scattering instruments. This cooperation involves the Technische Universität München, the Forschungszentrum Jülich GmbH and the Helmholtz-Zentrum hereon GmbH. The MLZ is funded by the German Federal Ministry of Education and Research (BMBF), together with the Bavarian State Ministry of Education, Science and the Arts (StMWFK) and the partners of the cooperation. Based on the Forschungs-Neutronenquelle Heinz-Maier-Leibnitz (FRM II), which provides neutron and positron beams for the scientific experiments, the MLZ plays an important role for application of neutrons within the European landscape of research infrastructures.

The user operation with its first 14 instruments started in the year 2005. The instrumentation and user operation is based on a close cooperation with external user groups from universities, research organizations and Helmholtz centers from all over Germany. The open call for scientific use attracted right from the beginning an international user community in the range from 40-50% of beam time applications.

The close cooperation of the TUM with the Helmholtz centers in Jülich and Geesthacht to exploit the scientific use of the FRM II was established by a cooperation agreement in 2011 and financially supported by the BMBF. This cooperation has led to the inauguration of the MLZ in 2013 in order to present a single entry point for the user service offered by the cooperation partners. After a first ten years period, the funding of the cooperation was prolonged for another 5 years in 2021. Continuous development of the instrument suite, including the transfer and refurbishment of 6 instruments from FZJ after the closure of their neutron source in Jülich, as well as building of new instruments led to 27 neutron and positron instruments in user operation today. With the extension and commissioning of the new neutron guide hall East, four additional instruments will be available. The transfer of two instruments from the Helmholtz Centre Berlin will bring another additional powder diffractometer to the MLZ and allow for the replacement of an obsolete setup in the guide hall West.

After about 20 years of user operation, the refurbishment and performance upgrade, as proposed in the MORIS (**M**LZ **O**rganized **R**efurbishment of the **I**nstrument **S**uite) program, aims to enable the MLZ to serve continuously as an international competitive neutron center. Being the main neutron source for the German scientists, the number of beam days it will provide every year plays a crucial role for the sustainability of neutron and positron research in Germany

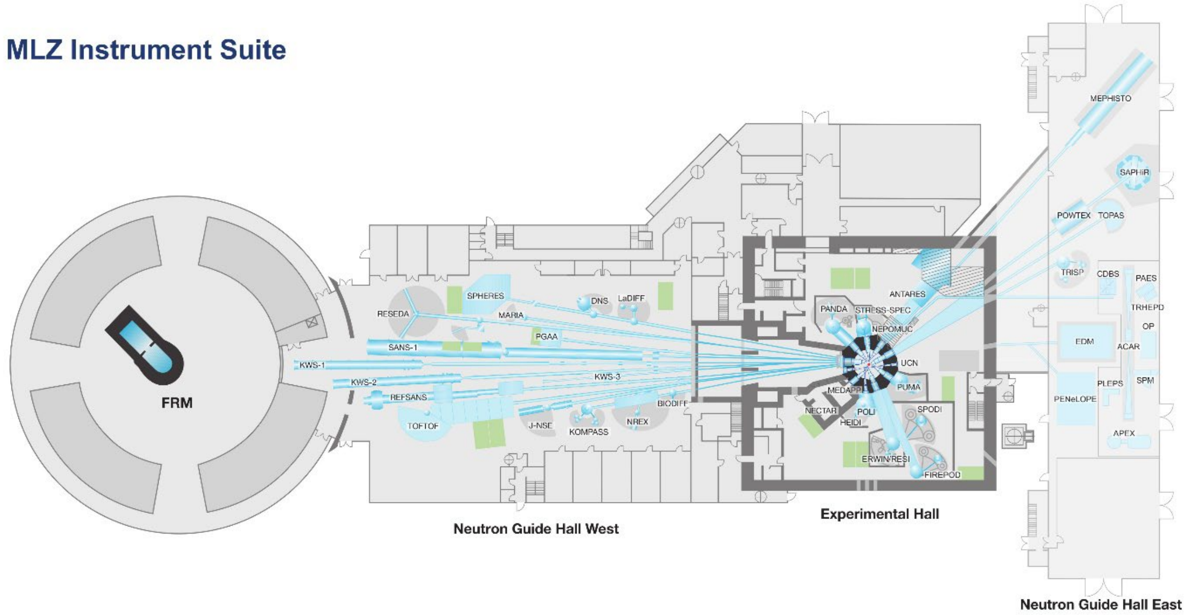

Figure1: Layout of the instruments at the MLZ as planed of end 2022. The additional instrument Firepod from the HZB will be placed at the beam channel SR8a near to SPODI. The second instrument from HZB, former FLEXX will become LADIFF at the MLZ and replace the instrument MIRA in the guide hall west. The instruments shown in the guide hall east including the ones using the future ultra-cold neutrons (EDM and PENELOPE) are under construction, transfer or commissioning.

3 Structuring refurbishments and upgrades

Based on an in-depth in-house analysis of the requirements regarding refurbishments and possible upgrades, projects were defined and discussed in an open MLZ retreat, taking place in July 2022 on the premises of Kloster Holzen. Consolidated projects will be discussed with our users in a workshop in Garching in April 2023 in order to strengthen the scientific case of the numerous projects. The requirement of a refurbished instrument suite should take the opportunity to include updated needs from our broad user base. Advice from the MLZ advisory committees (IAC and SAB) will be included in the final selection process in July 2023 and guide us to the final project description until the end of 2023. Figure 2 shows the overall time line and outlook to a possible implementation up to 2029.

Figure2: Time line of the MORIS program.

To structure the entire MORIS program the individual projects are classified into five different categories in the following sections. They are grouped to elaborate possible synergies, motivate future prioritizations if necessary, or put them in an optimized time line for the realization in view of available resources for the development teams. The MLZ as a hub of neutron research and instrumentation in Germany comprises not only instruments from the cooperating partners. Within the MORIS program, all instrumental developments are discussed for now in the pre project phase in view of the science case and benefit to our user, without taking into account possible future funding schemes

3.1 Building new instruments

Any upgrade program motivates to discuss the instrument suite by itself. Even though the focus of the MORIS program is not to enlarge the instrument suite of the MLZ, the science case of new instruments to extend the usage of neutrons beyond existing possibilities is worthwhile to discuss with our user community. A main issue to overcome in view of a possible realization is the very limited space in the existing halls. By purpose, we aim to discuss the proposed new instruments in a first step without considering these technical issues. New instruments might replace outdated ones in a further instrument development phase if a strong science case given by our user community drives these changes.

3.2 Renewals

After a long time of user operation, several instruments suffer from substantial risks, that major spare parts are not available any longer. These are for REFSANS the neutron guide, for BIODIFF the imaging detector is no more available and for TOFTOF the detectors and the detector electronics as well as the Choppers are on high risk to fail. The risk of failure will be mitigated by the renewals of critical components or the rebuild of the entire instruments if appropriate. The science case for these major changes is revised in the modernization program to ensure a future continuous and long-term operation. These significant investments include numerous performance improvements to keep the instruments internationally competitive.

3.3 Upgrading Instruments

Major upgrade on existing instruments are proposed to achieve significant improvements of the performance or extensions of their applications to numerous scientific questions. The projects cover the optimization of neutron fluxes by renewing neutron optics, extending the dynamic range of measurements in momentum transfer and energy range up to boosting the signal to noise ratio in order to address even smaller sample sizes or investigate weak signals at highest resolution. These projects are strongly instrument specific and offer new possibilities of the application of neutron and positron beams. The upgraded instruments will allow to address new scientific questions, however, it might sacrifice previous optimizations. Especially for this new focus, the discussion with our users is of utmost importance, as it will go for a significant modified offer of beam time.

3.4 Upgrading Techniques

Without changing the major focus of the instrument, the adaptation of key components, taking advantage of recent technological developments, enables significant increases in the performance or optimized capacity for the user operation. In this section, we gathered projects aiming to invest in technical developments serving more than one instrument, such as large area detectors, improved neutron optics, the use of modern robotics technology or extensions of the method itself.

3.5 Sample environment

The provision of sample environment equipment is essential for most of the experiments performed at the MLZ. Dedicated devices at the instruments together with a pool of standardized equipment cover a broad range of experimental parameters including temperature, pressure, external field or very specialized ones like humidity or composition. A significant upgrade in the application of high magnetic fields including new technological developments like high-Tc superconducting wires will enable to address new question in the research of quantum phenomena beyond today's possibilities. The high density of instruments in the areas at the MLZ, however, defines a strict magnetic field policy in order not to disturb neighboring instruments when using these extreme fields. This requirement imposes a special optimization of the high field magnets in view of active compensation of stray fields.

4 MORIS projects profile

The short descriptions of the projects are grouped according to section 3.

4.1 Building new Instruments

4.1.1 FLASH-NT – A new imaging instrument on a cold neutron guide

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Science Case

Neutron imaging is an invaluable tool for many applications where X-rays fail to provide sufficient contrast, or do not penetrate at all. Together with recent achievements in high-resolution detectors and the development of advanced imaging techniques, many novel fields of applications become possible. For example, high resolution neutron imaging has shown great potential in the optimization of the water management in anionic exchange membrane fuel or electrolyzer cells, which is a key feature for their large-scale application in a fossil-free chemical industry. Similarly, the visualization of lithium transport phenomena and dendrite growth with highest possible spatial resolution provides novel insights for the improvement of safety and lifetime of Li-ion batteries. The use of modern and advanced neutron imaging techniques helps to find solutions for many important scientific challenges, e.g. the study of magnetic domains in electric steels using neutron grating interferometry (nGI) with the aim of developing electric drives with higher efficiency or the spatially resolved investigation of magnetic properties of weakly ferromagnetic materials using polarized neutrons that may eventually lead to the development of novel storage devices. Additionally, the spatially resolved determination of phase composition or strain mapping in alloys using Bragg edge imaging provides tremendous potential particularly for industrial applications.

Technical realization

We propose to build the additional neutron imaging instrument FLASH-NT, which is complementary to the higher energy spectrum at NECTAR and ANTARES, at an end position of a cold neutron guide. FLASH-NT will provide a small beam cross section of maximum 10 cm x 10 cm, a fully moderated cold neutron spectrum with a minimum wavelength of ~2 Å, combined with an extremely low background. The instrument will be optimized for applications requiring highest possible spatial resolution down to the single µm range and applications using advanced imaging techniques that will benefit most from the broad spectral range and the low background at a neutron guide, thus adding new possibilities to the portfolio of neutron imaging applications at MLZ. The end section of the guide should be focusing to an adjustable pinhole. A prominent example of such a concept is the instrument NeXT at ILL. The pinhole is followed by a collimation flight path of ~6 m length that can be relatively narrow and is used to house instrument components such as a velocity selector, a double crystal monochromator, the source grating for nGI or a polarizer. After another beam scraper to reduce the background, the experimental cave needs a wider footprint in order to accommodate the sample (including sample environment) on a motion stage and the detector. The minimum footprint of the cave should be ~3 m x 4 m. In addition to the neutron velocity selector, a chopper system consisting of at least three disc choppers will be installed along the neutron guide, providing finer wavelength resolution of ~0.5%.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase																
Procurement																
Manufacturing																
Installation/commissioning																

Cost estimate:

Invest Shielding, neutron guides, velocity selector, cave interior, white beam detector, motion control, double crystal monochromator, choppers, TOF detector, infrastructure	3 330 kEUR
Additional personnel (1 Scientist, 1 engineer)	800 kEUR

4.1.2 Instrument concept - Bonse-Hart Ultra Small Angle Neutron Scattering, BOUNCE

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Science Case

The ability to probe internal structure to 10's of μm, quantitatively, statistically and non-destructively, presents the USANS technique as a way of bridging the gap between the real space capabilities of neutron imaging and the mesoscale interrogation by SANS. As a complement to the traditional pin-hole type SANS instrument slit-smeared USANS extends the structural perspective over many orders of magnitude in length-scales. These considerations are critical to the understanding of soft hierarchical materials where transport properties can be related to levels of structure from the mesoscale up. Scientific questions with compositional heterogeneity over many length-scales are common in geophysics and soil science, food digestion and chemical engineering problems such as filtration. Chemical reaction may be dominated by the interfacial area, and thus small pores, but mass transport is dependent on the number, size and connectivity of larger pores. In suspensions and emulsions bulk rheology is largely controlled by the shape of constituents and organization around the micron scale. The mechanical properties of dairy gels (food texture), where a percolated network is formed by the aggregation of structural sub-unit 100's of nm in size, casein micelles, are dependent on organization of the network. This perspective could be used on the formation of vegetable protein based gels, and may lead to an enhanced consumer uptake through manipulation of texture properties with potential environmental, less reliance on animal-based protein, and health, benefits. Furthermore, USANS has the usual advantages over conventional experimental techniques in the ability to selectively visualize sample components, e.g. fat or casein micelles separately in milk, and in the case of living samples the non-ionizing nature of neutrons allowing cellular processes to continue.

Technical realization

The proposed Bonse-Hart USANS instrument, BOUNCE, would be sited with a pre monochromator in a guide. Two modes of operation are foreseen, a high flux mode and a high-resolution mode where instrument flux is sacrificed for a smaller q-min. We plan two modes of detection for scattered neutrons for the high flux mode, the conventional point-by-point mode (rotation of analyzer crystal) and a bent crystal analyzer, in which the scattering pattern is collected on a linear detector. The former mode is for optimized lowest q-value, the latter mode is suitable for kinetic measurements with the accessible q-range determined by the bending of the analyzer crystal. The instrument will enable flexibility in sample presentation, particularly with respect to sample thickness and range of contrasts, and enable a range of sample environments, complementing the existing instrument and sample environment suite at MLZ. The innovation in the design from existing instruments will be the exchangeable bent and rotating crystal analyzers. The control of background through appropriate shielding is critical for the instrument's q-max and the overlap in q-range with the existing SANS instrument. The overall perspective on the instrument is simplicity in design and maintenance and ease of use with particular emphasis on ease and flexibility of sample presentation.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Preliminary design																
Procurements																
Detailed design																
Installation																
Commissioning																

Cost estimate:

Invest Pre-monochromator, shielding, bent crystal analyzer, 2 pair channel cut quintuple bounce Si crystals, sample table, detectors, sample changer	2 000 kEUR
Additional personnel (1 Scientist, 1 engineer)	800 kEUR

4.1.3 Indirect-geometry crystal spectrometer Mushroom

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Science Case

Magnetic systems are a fertile ground for the design of novel quantum and topologically non-trivial states characterized by exotic excitations. Recent examples include spin chain and square-lattice low-dimensional antiferromagnets, quantum spin liquid candidates, spin-ice compounds, and unusual spin textures. These systems are not only of fundamental interest, but may also pave the way to new technologies. For example, skyrmion spin textures open new possibilities for data storage and electronic applications. Key features of the ground state and finite-temperature behavior of a magnetic system are captured by the spectrum of its excitations. All of the aforementioned systems reveal exotic excitations dissimilar to standard magnons that form narrow bands in conventional ferro- and antiferromagnets. The detection of exotic excitations is by far more challenging, as they show broad distribution in the energy and momentum space. One typical example are helimagnons, the excitations of helical magnets like in MnSi. They are extend over a wide range of momentum and low energies. The spin-ice and spin-liquid candidates among the 4f oxides entail weak magnetic interactions, thus showing spectral features at typical energy transfers of 1-2 meV. These features are intrinsically very broad, as they often reflect fractionalized excitations carrying spin-1/2 in contrast to spin-1 for conventional magnons. These latest trends are often combined with the fact that the systems are magnetically very dilute, and the samples are getting smaller and smaller in physical size.

Technical realization

Such complex dispersion relations require long measurement times and great effort when measured on triple-axis spectrometers that can only scan through the (Q, E)-space point by point. Compared to this the proposed indirect-geometry spectrometer Mushroom with a time-of-flight primary chopper spectrometer, a large spherical crystal analyzer covering the upper part of the instrument and a large flat detector area below the sample position for the secondary spectrometer, can measure the excitations over a broad range in the (Q, E)-space at once. It is worth mentioning that in the current instrument suite of MLZ there is no such instrument for providing a fast out-of-plane full coverage of (Q, E)- space. Mushroom would provide all necessary information within a much shorter time frame, only at the cost of a slightly reduced energy and momentum resolution as compared to a triple-axis spectrometer, but significantly better than direct TOF instruments. Furthermore, it can be built relatively compact as the main dimension of the secondary spectrometer is only given by the dome of PG crystals above the sample, and only the sample is rotated. The accessible wavelength band is foreseen to be 1 – 10 Å with an adjustable wavelength resolution of 1%- 5%. The instrument including shielding would be in total 20 m long and 5 m wide.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase																
Procurement/Construction																
Installation/commissioning																

Cost estimate:

Invest PG crystals, shielding, detectors, choppers	3 000 kEUR
Additional personnel (1 Scientist, 1 engineer)	800 kEUR

4.1.4 BIODIFF-2: Optimized for large unit cells

Andreas Ostermann[1], Tobias E. Schrader[2]
[1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München; [2]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH

Science Case

The science case for the new protein crystal diffractometer BIODIFF-2 is identical to that of the BIODIFF, but concentrates on larger unit cells which are coming up more and more often. Up to now, only one other instrument in the world, MaNDi at ORNL, can perform high resolution structure determinations using neutrons on crystals with unit cells of that size. Recently, more and more proposals have been submitted with interesting projects that exceed this unit cell size, such as the structure determination of membrane proteins which typically have unit cells sizes above 200 Å. As the user community grows, the number of projects/proposals with larger unit cell crystals will continue to increase in the future. In this way BIODIFF-2 is a real investment into future instrumentation at the MLZ.

Technical realization

At the moment, the detector-to-sample distance at BIODIFF is fixed by the cylindrical Image-Plate-Detector. However these detectors are no more available and therefore a new instrument has to be equipped with a new detector technology. Furthermore, we propose a detector concept with a variable detector-to-sample distance. This will allow to compensate the reflex overlap on the detector for larger unit cells by increasing the detector-to-sample distance.

The detector type we propose here is the newly developed "event-mode" detector type based on a TPX3CAM camera. It is characterized by high efficiency and intrinsic time resolution. The intrinsic time resolution will enable the possibility to follow structural changes within the crystal after an external trigger in the time domain. In addition, the variable sample-to-detector distance will allow more space for micro-spectroscopic tools to determine the UV-visible spectrum of the crystal on the beamline. This UV-visible spectrum contains information on the state (radical or redox-state) the protein is in. The new detector concept also alleviates future problems in the procurement of spare parts for the Image-Plate-Detector, which carries the risk of long instrument downtimes.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase	■	■	■	■	■	■										
Procurement				■	■	■	■	■	■	■						
Manufacturing							■	■	■	■						
Installation									■	■	■	■	■			
Commissioning												■	■	■	■	

Cost estimate:

Invest Monochromator, shielding, velocity selector, collimator, sample holder, detector arm Detector modules + mechanical parts (identical to BIODIFF renewals)	 2 000 kEUR 1 000 kEUR
Additional personnel 1 Scientist (2nd Instrument responsible)	400 kEUR

4.2 Renewals

4.2.1 Renewal concept TOFTOF

Marcell Wolf, Christopher Garvey
Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München

Science Case

As a cold time-of-flight spectrometer, TOFTOF's impacts are felt across scientific areas including: biophysics, materials science; fundamental hard and soft condensed matter physics, chemistry and biology. The upgrade addresses both the competitiveness of the instrument around existing scientific areas and aspires to address new questions/areas stemming from all the grand challenges for the MLZ and its user community. Specifically we seek to enhance the sample area, angular resolution and number of neutrons analyzed by increasing the flux at the sample, decreasing background signal and increasing solid angle and angular resolution.

Neutron spectroscopy provides insights in molecular mobility in energy storage. Such as novel anode or cathode materials, electrolytes and the study of ion mobility in batteries under in-operando conditions may provide for improved electrochemical storage. Studies of hydrogen mobility and binding characteristics in solid-state hydrogen storage material characterize both chemisorption and physisorption. The perspective may enable efficient, sustainable and cheap catalysts in fuel. The perspective on hydrogen dynamics, and the accompanying molecular dynamics, from TOFTOF on biological or soft matter material such as proteins, peptides, lipids and polymers is important for, e.g. gels, new drug release systems, polymer blends, and liquids in confinement or organic solar cells. In health and the life-sciences dynamics are proving an important step from the structural view enabled by crystallography in understanding function. For materials science, the possibility to probe low-lying excitations (e.g. the phonon density of states) and measurements of diffusion coefficients will help to improve the understanding and development of novel materials.

The study of quantum spin liquid and quantum spin ice phenomena in low dimensional and/or frustrated materials reveals rich physics and new concepts emerging from the quantum behavior of many interacting particles.

Technical realization

We plan to upgrade:

Primary spectrometer: The focus for the upgrade of the primary spectrometer is to improve the delivery of neutrons to the sample and to renew the chopper system that after its long years of operation is in need for a replacement. For higher flux an the sample and to adapt for smaller sample sizes, an elliptical neutron guide option is considered, with better compression towards the sample, and divergence profile adapted to a position sensitive detector.

Secondary spectrometer: A position sensitive detector (PSD), with out-of-plane Q resolution and with increased total solid angle coverage will enhance the application of TOFTOF to inelastic scattering on single crystals and the efficiency of neutron use. In addition, we plan to renew the sample chamber to move to an evacuated flight path and to increase the area available for sample environment, such as high field magnets.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase																				
Procurement																				
Detailed Design																				
Decommissioning																				
Installation																				
Commissioning																				

Cost estimate:

Invest Primary spectrometer, sample and detector chamber, detector (assuming a reuse the TOFTOF ^{3}He)	6 500 kEUR
Additional personnel 1 Scientist (4 years)	400 kEUR

4.2.2 BIODIFF detector array renewal: tackling even larger unit cells

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Science Case

At the instrument BIODIFF, the incident wavelength can be freely selected between 2.7 Å and 5.6 Å. This is an essential unique feature of BIODIFF and allows it to adapt the wavelength to the unit cell size of the sample crystals. At a wavelength of 4.7 Å, unit cells with lattice constants up to 200 Å can be measured at BIODIFF. Up to now, only one other instrument in the world, MaNDi at ORNL, can perform high resolution structure determinations using neutrons on crystals with unit cells of that size. Recently, more and more proposals have been submitted with interesting projects that exceed this unit cell size, such as the structure determination of membrane proteins which typically have unit cells sizes above 200 Å. As the user community grows, the number of projects/proposals with larger unit cell crystals will continue to increase in the future. In order to serve such needs, it is essential to extend the capabilities of BIODIFF.

Technical realization

At the moment, the detector-to-sample distance at BIODIFF is fixed by the cylindrical Image-Plate-Detector. When using a longer wavelength - to counteract the reflex overlap on the detector in case of large unit cells - the maximum achievable resolution, will inevitably be cut. For this reason, we propose a detector concept with a variable detector-to-sample distance. This will allow to compensate the reflex overlap on the detector for larger unit cells by increasing the detector-to-sample distance.

The detector type we propose here is the newly developed "event-mode" detector type based on a TPX3CAM camera. It is characterized by high efficiency and intrinsic time resolution. The intrinsic time resolution will enable the possibility to follow structural changes within the crystal after an external trigger in the time domain. In addition, the variable sample-to-detector distance will allow more space for micro-spectroscopic tools to determine the UV-visible spectrum of the crystal on the beamline. This UV-visible spectrum contains information on the state (radical or redox-state) the protein is in. The new detector concept also alleviates future problems in the procurement of spare parts for the Image-Plate-Detector, which carries the risk of long instrument downtimes.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Benchmark detector																
Design /Procurement																
Manufacturing detector																
Install. /Commissioning																

Cost estimate:

Invest Detector modules + mechanical parts	1 000 kEUR
Additional personnel	- kEUR

4.2.3 REFSANS Beam Delivery Refurbishment and Upgrade of the Secondary Optics

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Science Case

The horizontal reflectometer REFSANS fulfills the needs of the soft-matter and materials science communities in terms of interface characterization at the nano- and meso-scales[1] including the case of free liquid-air interfaces[2]. TOF operation together with event mode acquisition prove to be very useful for kinetic measurements (typ. time resolution 20-30 s) e.g. for in situ studies of thin film structure evolution[3]. Beside conventional specular reflectometry, off-specular measurements give access to in-plane correlations over large distances[4]. A special feature of the instrument is the unique capability for TOF GISANS, which has been used to characterize e.g. electrodes for photovoltaic systems, or nanoparticles[4,5].Since its operational start, the performance of the neutron delivery system has degraded significantly. Replacing this guide in order to insure the future of the instrument is the primary aim of this proposal. Additionally, options to improve the instrument performance for modern experiments which usually involve relatively small samples have been explored. Nested Mirror Optics (NMO)[6] offer the opportunity to horizontally focus the very wide beam of the instrument (170 mm) onto samples narrower than 30 mm rather than the 80 mm as of today. Overall, the proposed refurbishment/upgrade would allow REFSANS to perform measurements on time scales competitive with those possible at Figaro (ILL), the *de facto* benchmark horizontal reflectometer.

Technical Realization

The primary delivery beam system includes a twisted guide which delivers a 170mmx12mm (WxH) beam. Measurements have shown that restoring the initial performance of the guide would bring an intensity increase close to a factor 2. Simulations of alternative technological options showed that, given the geometric constraints, a twisted guide is actually the optimal configuration to feed REFSANS. Additionally to this refurbishment, we propose to install a horizontally focusing parabolic NMO at a distance of ca. 2m upstream of the sample. This optional device would be used for reflectometry, where the in-plane divergence can be arbitrarily increased. For GISANS measurements, the focusing optics would be translated out of the beam and the existing radial collimator would be used instead. A sample slit package will be placed on a 30 cm translation stage parallel to the beamline axis. This will enable optimization of the slit position according to the actual sample size or allow the use of bulky sample environments. An optional Soller collimator will be installed upstream of the NMO in order to better control the lateral footprint for small samples. McStas simulations using an accurate description of our present optical configuration starting from the cold source show that intensity gain factors 2 can be expected using this setup. Additionally and independently, a new set of vertical slits will be installed at the center of the instrument in order to allow for a shorter vertical collimation length (4 m vs 8.6 m) thereby increasing the available intensity by a factor 2 when measuring at incidence angle 2° or above. This is especially important since it affects the configuration where the lowest reflectivities are usually measured. In a longer-term perspective, the experience gathered during the operation of the NMO setup will be useful to design a new primary beam delivery system.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design												
Procurement												
Production /Installation												

Cost estimate:

Replacement of twisted guide	2.0 MEUR
Invest NMO + mechanical parts	300 kEUR
Additional personnel	- kEUR

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[4] Physical chemistry, chemical physics N/A, 10.1039.D1CP03201A (2022) [10.1039/D1CP03201A]
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4.3 Upgrading Instruments

4.3.1 Passive Magnetic Shielding for the J-NSE “PHOENIX”

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Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH

Science Case

The current J-NSE represents at the moment the best known design of a Neutron Spin Echo (NSE) spectrometer, enabling measurements with correlation times up to several 100 nanoseconds in routine operation. An important area of science at the J-NSE is the investigation of domain motion in large proteins under physiological conditions, a unique capability of NSE, requiring extremely high precision measurements since deviations in relaxation from diffusive behavior needs to be quantified.

However, a major source of instrument downtime or increased sources of noise and systematic error in the data are magnetic field variations in the area of the J-NSE spectrometer coming from sources like magnets, the crane, relocated steel plates, moving polarization analyzers. Measures have been started to reduce the influence of those stray fields, which affect the NSE signal already on the order of a few mG. Some technical aspects of actively compensating varying fields are evaluated at the moment, but will never provide the robustness of a passive magnetic shielding. Precision measurements of small effects at highest resolution in the dynamics would gain significantly in quality with a passive magnetic shielding.

Technical realization

The most elegant and robust solution, which proved to work excellently for NSE instruments, is the double layer μ-metal housing as it is provided for the SNS-NSE in Oak Ridge. It has to surround the full instrument, also the floor needs to be included into the housing, and the housing needs to be large enough such that the mirror fields inside the cage do not reduce the resolution of the instrument. This has been worked out for the SNS-NSE and it provides an incredible phase stability, enabling measurements of small effects with a very good precision. Two options will be evaluated, either a relocation of the instrument into a new position at the end of the neutron guide hall, or installing it at the current position, which would require coordination with the neighboring instruments due to the restricted space available. The exact design of such a μ-metal housing needs to be developed with FEM calculations as it has been done by ZEA-1 also for the SNS-NSE.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design/procurement																				
Installation																				
Recommissioning																				

Cost estimate:

Invest Double wall μ-metal housing, granite floor, neutron guide, relocating infrastructure	3 000 kEUR
Additional personnel	- kEUR

4.3.2 DNS-WAPA

Yixi Su
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Science Case

Frustrated and topological quantum magnets, such as quantum spin liquid and magnetic Weyl semimetals etc., have become a focus of intense research in condensed matter physics, owing to the remarkable possibilities to realize emergent quasiparticles that do not correspond to any theoretically known elementary particles, e.g., magnetic monopoles in spin ice, Majorana zero mode, and Dirac and Weyl fermions. Realization and eventual manipulation of these exotic quasiparticles in condensed matter, often manifested as continuum-like fractionalized excitations, can lead to potential applications in future quantum technologies such as decoherence-free quantum computing. Furthermore, due to complex interactions in these many-body quantum spin systems, that are often beyond the well-established description with only Heisenberg exchange interactions, such as bond-direction dependent Kitaev exchange interactions, spin-orbit coupling (SOC) and DMI mediated strong spin anisotropy, dynamical spin chirality and topological magnons, the conventional collective excitations like magnons may become highly unusual. The detection of these emergent excitations and exotic quasiparticles in frustrated and topological quantum magnets thus represents a tremendous challenge experimentally, since the relevant inelastic scattering signals are very weak, often very broad in Q-space, and may be highly anisotropic in spin-space or strongly bond-direction dependent. A dedicated cold-neutron TOF spectrometer that combines with a new-generation wide-angle polarization analysis (WAPA) can meet this challenge. The primary consideration of the DNS-WAPA project is to upgrade DNS to a more dedicated cold-neutron X-TOF spectrometer that would become internationally competitive among similar instruments for the measurement of magnetic excitations, meanwhile, to retain its world-leading position in polarized magnetic diffuse scattering.

Technical realization

The targeted major upgrades include such as a new in-vacuum detector tank with $L_{S\text{-}D}$~2 m, a new-generation Fe/Si gapless wide-angle polarization analyzer system covering an angular range of 120° (horizontal) × ±10° (vertical), and the enlarged PSD detector arrays. DNS-WAPA should be easy-to-switch between polarized and non-polarized TOF mode, and will be fully compatible with the XYZ polarization analysis method and high magnetic field. The estimated gaining factors comparing to the current DNS: x 10 in polarization analysis efficiency, x 5-10 in signal-to-noise ratio due to the much-reduced background. DNS-WAPA would be competitive to the upgraded D7 (ILL), and to the polarized LET (ISIS), POLANO (J-Parc) and HYSPEC (SNS) in the domain of polarized inelastic neutron scattering in the respective cold-neutron regimes, and to SHARP (LLB/ILL) and FOCUS (SINQ), both cold-neutron X-TOF instrument, in the domain of non-polarized inelastic neutron scattering. Meanwhile, DNS-WAPA would be complementary to other cold-neutron spectrometers such as TOFTOF and KOMPASS etc. at MLZ, since it is dedicated to the polarized cold-neutron TOF spectroscopy and polarized magnetic diffuse scattering.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase	■	■	■	■	■	■														
Procurement				■	■	■	■	■	■	■										
Detailed Design							■	■	■	■	■	■	■	■						
Installation														■	■	■	■	■	■	
Commissioning																	■	■	■	■

Cost estimate:

Invest In-vacuum detector tank, Fe/Si based WAPA system, addition ^{3}He PSD tubes, chopper	4 500 kEUR
Additional personnel (1 Scientist, 4 years)	400 kEUR

4.3.3 Polarized Backscattering with high Resolution

Earl Babcock, Michaela Zamponi, Stefan Mattauch
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Science Case

Typical QENS studies address hydrogen rich samples featuring a dominant contribution from the spin-incoherent scattering cross section. But for samples with low hydrogen content among other elements or isotopes with smaller incoherent cross sections (e.g. Li), the distinction of coherent and incoherent scattering is not straightforward. Polarized backscattering can enable the study of materials or composites where the portion of incoherent scattering compared to coherent scattering is much smaller. This could especially be interesting for functional materials under ambient conditions and perhaps even in-operando study where the signals can be highly dominated by the coherent scattering of the materials used. Moreover, the ability to study the dynamics of incoherent and coherent scattering contributions separately gives unique information on the cooperative vs local dynamics of a system. Polarization analysis for QENS has been implemented on direct geometry chopper spectrometers and efforts are underway to design polarized backscattering instruments on pulsed sources. However, none of these instruments will be able to approach the sub-μeV energy resolution of a reactor based backscattering spectrometer in true backscattering geometry. To enable the unique combination of high energy resolution and polarization analysis for QENS, new instrumentation ideas as an upgrade to the SPHERES backscattering spectrometer shall be explored.

Technical realization

The realization will require several phases. The first stage is a detailed study of the design constraints. Incident beam polarization should be accomplished through a SM cavity polarizer, the optimal location of such a device and incident beam flipper, given the existing constraints of the primary SPHERES spectrometer will be studied in simulation. Pending the eventual location of the SM polarizer, a plan for guide field of the incident beam and secondary spectrometer can be achieved. It is expected, that the secondary spectrometer would need field over the whole neutron flight path between the sample and the energy analyzers. Next, detailed modelling of the strategy for polarization analysis will be done. Solutions using wide-angle SM technology and wide-angle, in-situ polarized ^{3}He spin filter cells will be considered and calculated for positions both directly before the detector, and between the sample and the energy analyzers where the scattered beam would pass the polarization analyzer device twice due to the backscattering condition needed to preserve sub-μeV resolution. Neutron studies on the effects of the different polarization elements on contributions to resolution and background will be undertaken. If the ^{3}He option is considered best, efforts to design a wide-angle in-situ polarizer compatible to SPHERES would proceed, if the SM analyzer option is optimal, its detailed design and construction would need to follow. A challenge will be to fit in the polarization analysis with the given constraints and might require modifications of existing components. Any new elements will be optional and do not effect unpolarized measurements.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase	■	■	■	■	■	■	■	■												
Procurement					■	■	■	■	■	■	■	■								
Installation									■	■	■	■	■	■	■	■				
Commissioning																	■	■	■	■

Cost estimate:

Invest Polarizer, Analyzer (^{3}He or super mirror option)	1 000 kEUR
Additional personnel (1 Scientist, 4 years)	400 kEUR

4.3.4 SANS-1MAX: Massive Q-Range Upgrade

Sebastian Mühlbauer[1], Abdel Al-Falou[1], Andreas Wilhelm[1], Andre Heinemann[2]
[1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München; [2]German Engineering Materials Science Centre (GEMS), Helmholtz Zentrum Hereon

Science Case

The SANS-1^{MAX} proposal aims both at ***extending the dynamical Q-range*** and ***increasing the maximal momentum transfer Q***. Both upgrades will enable the access to new fields of research, particularly ***for modern materials science applications***. The increased ***dynamical Q-range*** is particularly beneficial for the growing demand of in-situ measurements of irreversible processes, e.g., precipitation growth in high performance alloys, quenching of alloys, rapid heating and cooling processes and the mimicking of metal process chains, in particular in combination with sample environment like the dilatometer. ***Accessing larger Q*** allows measuring even smaller correlations of a few atoms to study the early growth of precipitates. A maximum momentum transfer of 2.2 Å^{-1} of the SANS-1^{MAX} proposal will finally allow covering the first Bragg peaks of typical alloys like e.g. Ni or Co based superalloys and their main precipitates. This option will enable coherent investigations of early stage precipitation covering the SANS and diffraction region in a single measurement. It hence allows an analysis of the size, size distribution, shape and ***the crystalline properties of precipitates***. Besides materials science, SANS-1^{MAX} will also tremendously increase the overall efficiency of SANS-1.

Technical realization

The SANS-1^{MAX} proposal consists of two independent two subprojects. The replacement of the S-bender neutron guide with an optimized version will shift the wavelength cut-off down to ~2.5 Å. There are two possible concepts of achieving this goal whilst keeping both *end points* and *end vectors* of the existing guide system: Increasing the m-values, and alternatively, separating the guide into two horizontal channels while keeping the m-values. The latter system owns the advantage of no increased divergence and lower (cheaper) m-values at the expense of a more complex mechanical design. Extended McStas simulations have tested both options. This project includes the installation of a new selector adopted to shorter wavelengths and a new chopper disk for the existing TISANE chopper for a flexible tuning of the wavelength spread for the diffraction regime. The installation of a second, high-*Q* detector bank at short detector distances on a second, independent detector carriage is made possible by the large existing detector tube of SANS-1. This new detector will consist of 3 identical detector banks, each 0.5mx1m, arranged in a window frame scheme around the primary 1m^2 detector.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design Phase																				
Procurement																				
Optic installation																				
Det installation																				
Commissioning																				

Cost estimate:

Invest Neutron guides, chopper, selector, auxiliaries, ^{3}He detector	3 000 kEUR
Additional personnel (1 Scientist, 4 years)	400 kEUR

4.3.5 Rapid Spatially Resolved and Element-Specific Defect Analysis with Positrons

Christoph Hugenschmidt
Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München

Science Case

The Coincidence Doppler Broadening (CDB) spectrometer with its monoenergetic scanning positron beam allows the investigation of defect distributions in three dimensions (3D) and of the elemental surrounding of open-volume defects. It is designed to address the following scientific questions:

(i) Homogeneity of samples, i.e. depth and lateral distribution of lattice defects. Examples are (laser beam or friction stir) welded technical alloys, irradiated materials, superconducting and (doped) thin semiconducting films; (ii) Defect kinetics and fast defect annealing at high temperatures, e.g. of samples after severe plastic deformation or plasma-facing materials for fusion reactors;
(iii) Vacancy-solute complexes and nano-clusters in, e.g. doped semiconductors or precipitation-hardened alloys; (iv) *In-operando* defect analysis of samples, which are not stable in vacuum, exposed to gases and/or during application of el. fields. Examples are electrode materials or aging of thin polymer films in various atmospheres; (v) fundamental research with ortho-Positronium (o-Ps).

Technical Realization

The CDB spectrometer at NEPOMUC provides the only scanning positron micro-beam in routine operation worldwide. The typical lateral resolution of ~250µm can be improved to ~50µm by using a transmission-type remoderator (100nm Ni(100) foil). Challenges of this remoderator are reliable long-term operation, mechanical stability, surface conditioning, and comparable low efficiency (~5%).

In order to cope with the forefront research questions and to extend the capabilities of the instrument we plan to upgrade the CDB spectrometer by considerably enhancing its performance in terms of (i) spatial resolution, (ii) measurement time and signal-to-noise, and (iii) high sample temperature. The upgrade project comprises three work packages (WP's):

WP1: By implementing a novel two-fold positron remoderation stage we envisage a **spatial resolution of 1 µm**. This brightness enhancer basically comprises beam optics with two solid rare-gas remoderator units. Due to its high efficiency the beam intensity will be increased by a factor of 4-5.
WP2: For optimum coverage of the field-of-view, the detection system will be extended by additional 12 HPGe-detectors that immediately increases the instrument performance by a factor of two. Total **gain in measurement time** (see (i)) will be **one order of magnitude**. Moreover, the efficient coincidence detection of 3-γ events (free o-Ps) will allow the study of open porous structures.
WP3: For **high-temperature measurements (up to 1200°C)** we want to install an infrared laser (140 W) for contact-less sample heating; the temperature is measured by using a pyrometer.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulations																				
Procurements																				
Cold setup																				
Setup at CBDS																				

Cost estimate:

Invest Remoderator, detectors, furnace	700 kEUR
Additional personnel (1 Scientist)	500 kEUR

4.3.6 Neutron velocity selector on thermal three axes spectrometer PUMA

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[1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München; [2]IQMT, Karlsruhe Institut für Technologie

Science Case

The thermal-neutron three axes spectrometer PUMA at MLZ is designed to achieve high neutron flux at the sample position, making it a leading instrument in the worldwide research community for performing experiments with low inelastic scattering intensity, such as magnetic or phononic excitations. To further enhance its capabilities, the installation of a neutron velocity selector is proposed. The neutron velocity selector will improve the control of background levels by effectively eliminating unwanted higher-order neutrons and provide greater flexibility in inelastic neutron scattering measurements by allowing for more flexibility of choosing outgoing neutron wave vectors. Alongside the upcoming nested mirror optics on PUMA, the neutron velocity selector will bring a significant synergy effect particularly in measuring a small-size sample under an extreme sample environment.

Technical realization

The applicable neutron velocity selector on PUMA with the maximum rotation speed of 26,000 rpm (≈ 5.4 $Å^{-1}$) and the screw angle of 11.7° (corresponding beam divergence ~ 2.5°) can be readily produced by the company Airbus. Based on a given beam path and distances between axes, the neutron velocity selector should be installed in between the virtual source and the monochromator of PUMA. The velocity selector should be motorized for an automatic removable since it cannot operate for the highest neutron energies available on PUMA. Depending on the actual space limitation inside the monochromator drum, a slight design modification could be required.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design confirmation																
Order + Procurement																
Installation & test																

Cost estimate:

Invest 2 x Velocity selector	550 kEUR
Additional personnel	- kEUR

4.3.7 PANDA upgrade primary spectrometer: neutron channel - PUNC

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Science Case

PANDA is a world-leading cold three-axis spectrometer complementing TOF instruments in case of specific requests for resolution and related signal-to-noise ratio or demanding sample environments. Providing experiments with highest reliability since 2005, PANDA is always requested for newest scientific aspects in strongly correlated electron systems and on quantum magnetism, but serves for studies on phonons and their interaction with electronic degrees of freedom, too. There are only five comparable instruments in Europe, all of them being continuously overbooked. Recent improvements focused on the secondary side with the BAMBUS multi-channel-system and on the development of artificial intelligence (AI) assisted mapping modes for better efficiency. However, PANDA keeps limited by its primary flux. Higher flux, and concurrently, a better signal-to-noise ratio will allow more and better experiments. At the same time, it would address the increasing demand for high-end experiments, e.g. on spin-liquids / spin-glasses (see e.g. PRL 122 137201, Nature Comm. 10 4530, PRL 120 087201) or topological systems (e.g. Nature 586 37), would allow new science (e.g. spectroscopy under high pressure, e.g. NPHYS 4190), and would improve the efficiency of high-field studies.

Technical realization

The PANDA primary spectrometer with a short source-to-monochromator distance of 7.8 m is optimized for high-resolution cold spectroscopy with overlap to thermal wavelengths, but does not allow the installation of a velocity selector (VS). Introducing a velocity selector will improve the peak-to-noise ratio significantly and increase usable flux by avoiding filters. For flux improvement there is an estimate of gaining a factor of two (with negligible loss in resolution) by keeping the focusing monochromator unchanged but adding three nested-mirror elements in the beam path (C. Herb, TUM). To make the necessary space, we suggest to **build a new neutron channel (beam port to drum)** to install of a velocity selector and at the same time, adapt the shielding to improve the maintenance accessibility of the primary components close to the source (collimation, sapphire filter, etc.). A careful analysis of all aspects in changing the phase space over the wide energy range and testing new ideas needs an extended study. Shielding will be adapted in result accordingly.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
McStas Simulations																
Detailed design																
Procurement																
Installation																
Commissioning																

Cost estimate:

Invest Velocity selector, new shielding	1 300 kEUR
Additional personnel	- kEUR

4.4 Upgrading Techniques

Boosting Instrument performance by detector upgrades

4.4.1 HEiDi: Large Area Detector for High Q Studies

Martin Meven, Piotr Fabrykiewicz
RWTH Aachen University, Institute of Crystallography, Head: Prof. Mirijam Zobel

Science Case

The single crystal diffractometer (SCD) HEiDi at the hot source of FRM II offers high neutron flux down to short wavelengths < 1 Å (max. gain ~10 at 0.55 Å compared to thermal spectrum). The high penetration depth for studies on strong absorbing rare earth (RE) compounds or with complex sample environment like high pressure cells and the large Q range up to ~22/Å at 0.55 Å improve studies on complex magnetic or partly disordered structures and yield very detailed/precise information for many grand challenges, like quantum materials for information technology or new materials for energy storage. To fully exploit these advantages to as many science cases as possible, we propose a large 2D position sensitive detector (PSD) in order to extend the instrument's efficiency for faster and more accurate data acquisition (full coverage of reciprocal space, signal-to-noise correction, speed-up of data collection by up to one order of magnitude). In addition, by using a large PSD for sophisticated detection/separation of Bragg and diffuse scattering from the sample vs. modulated background HEIDI will be able to handle new scientific cases (e.g. disorder in battery materials) that benefit from modern methods like total scattering / pair distribution analysis (PDF) with neutrons for both powder (nPDF) and single crystals (3D-Δ-PDF) (e.g. T. Whitfield et al., IUCrJ (2016), Dove & Li, Nucl. Analysis 1 (2022), Weber & Simonov, Z. Krist. (2012)).

Technical realization

Based on our experience with a recently for HEiDi designed small ^{6}Li-glass scintillator based PSD with high efficiency for short wavelengths (2 mm ^{6}Li-glass > 50% at 0.55 Å, 15 photomultipliers (PM) with 48*48 mm² sensitive area each, 16*16 pixel, collaboration with JCNS detector group) and after studying the designs of e.g. D4@ILL, WAND²@ORNL, we favor currently a large ^{6}Li-scintillator PSD (130° horizontal coverage, 13° height) with 30*3 (w*h) conventional PM or Si-PM/ONRL. The restricted space of the experiment field of HEiDi limits the max. radius of this detector to 1150 mm. Including shielding, the heavy load of this detector will require a separate support on air cushions. An optional oscillating horizontal radial collimator will suppress spurious scattering from sample environment to minimize background.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4				Year 5			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Design	■	■	■	■	■	■														
Procurement			■	■	■	■	■	■	■	■	■	■	■	■						
Manufacture						■	■	■	■	■	■	■	■	■						
Assembly														■	■	■	■			
Commissioning														■	■	■	■	■	■	■

Cost estimate:

Invest PSD detector, radial collimator, mechanical support & shielding	2 700 kEUR
Additional personnel (1 Scientist, 4 years)	400 kEUR

4.4.2 Magnetically induced texture and mPDF– pushing the state of the art of the polarized neutron single crystal diffractometer POLI

Jianhui Xu, Henrik Thoma, Martin Meven, Mirijam Zobel
RWTH Aachen University, Institute of Crystallography

Science Case

Polarized neutron diffraction is a powerful tool for studying magnetism-related physics, typically using large single crystals to compensate for the relatively low polarized neutron flux. However, for modern science topics such as quantum topological materials, available single crystals get increasingly smaller, their magnetic moments get weaker, and the number of measured data points rises as required to solve the advancing complexity. This leads to very long measurement time to achieve reasonable precision. What is more, quite often only powder samples are available and the flipping ratio (FR) method with a single counter detector is not applicable. An area detector allows to scan the reciprocal space of single crystals with significantly fewer steps and measure a large continuous Q-range in a single shot, which is highly desirable for powder samples. In turn, more time can be dedicated to weak signals and small samples. Remarkably, it was recently shown that the FR method with a 2D detector can be applied to powder samples with magnetically induced textures and the measured data precision is surprisingly close to that obtained using single crystals [1]. A 2D detector also opens the possibility to measure magnetic pair distribution function (mPDF) of powder samples which is a new analysis tool recently developed for studying magnetic correlations and showed its potential to study magnetic topological phase [2-3].

Technical realization

As the first step towards the usage of a large 2D detector on POLI, a small 25x25cm^2 ^{3}He position sensitive detector (PSD) of the former 6T2 instrument in the LLB is currently being transferred to POLI. This allows us to optimize the design of the proposed large area detector and to develop the dedicated data acquisition and evaluation software. The ^{6}Li-glass scintillator design of the PSD under construction for HEiDi is preferred to use on POLI as well. We propose PSDs with a radial collimator located at 0.7 m away from the sample with a 130° horizontal and 30° vertical acceptance. The horizontal coverage provides Q_{max} = 10 Å^{-1} for λ = 1.15 Å which is sufficient for measuring magnetic signals. The wide vertical coverage compensates for the limitation of the only horizontal sample rotation and is compatible with the magnet opening. This design will boost the measurement efficiency of 3D single crystal data by a factor of 5-20 and enable the measurements of 2D magnetic-field-texturized powder data (FR method) and powder mPDF.

Schedule and Cost

High level Schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulations																
Design																
Procurements/Assembly																
Commissioning																

Cost estimate:

Invest Detector, mechanical support, shielding	5 060 kEUR
Additional personnel (1 Scientist, 4 years)	400 kEUR

References

[1] I. A. Kibalin, et. al., Physical Review Research 1.3 (2019), 033100.
[2] B. A. Frandsen, et. al., Acta Cryst. (2014). A70 (2014), 3.
[3] Z. Dun, et al., Physical Review B 103.6 (2021), 064424.

4.4.3 Improved neutron detection for high-resolution diffraction applications

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Science Case

Neutron detectors are a key component of every neutron instrument, defining sensitivity, resolution and efficiency/speed of measurement of the entire setup. Among various experimental techniques involving neutron scattering, neutron powder diffraction (especially its high-resolution version utilizing monochromatic neutrons) is one of the most demanding with regard to neutron detection typically requiring high detector efficiency, large solid angle of the detector along with a positional sensitivity in horizontal and vertical directions. The instrument SPODI is a classical representation of a high-resolution powder diffractometer operating with monochromatic neutrons with a near-to-classical peak profile, a high peak resolution and a stable, flat and low background. The SPODI multidetector consists of 80 vertical position-sensitive ^{3}He tubes (1´ ∅, 0.3 m effective height) arranged on the arc of 160° 2θ with 1.1 m radius. A stack of Soller collimators (L/D=344) in front of each detector tube supplies the high resolution over a broad range of momentum transfer and mitigating the self-collimation effect, relevant for large diameter samples, e.g. Li-ion batteries of cylinder-[Senyshyn, 2011] and/or prismatic- [Baran, 2019] types, modern ferroelectrics [Hinterstein, 2010], functional alloys [Saubert, 2016] etc.

The data collection at SPODI in its state-of-the-art configuration proceeds through the stepwise positioning of the detector, requiring typically 40 steps, thus leading to the exposure time multiplied by the equal factor. A reduction in step number along with the increase of detector coverage in both vertical and horizontal dimensions will have a multiplication effect on the speed of data collection, and, overall efficiency increase of the entire instrument by a factor x3.5 in nearly every application without significant compromise in the profile shape and instrumental resolution.

Technical realization

A new multidetector design adopting 200 vertically position-sensitive ^{3}He tubes (1/2´ ∅, 0.5 m in effective height) arranged on the arc of 160° 2θ with 1.3 m radius will be implemented. Loss of detection efficiency upon a reduction of the tube diameter from 1´ to 0.5´ will be compensated by the doubling of the ^{3}He gas pressure. An increase of vertical detector solid angle by 40% will be achieved by the increase of detector tube length from 0.3 m to 0.5 m. A new set of Soller collimators adapted to detector specifications needs to be designed and manufactured.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Order 3He gas												
Design and production of multidetector												
Procurement detector tubes												
Procurement Soller collimator												
Validation of individual components												
Procurement of detector electronics												
Integration in instrument infrastructure												

Cost estimate:

Invest 3He gas, detector tubes/electronic, collimation, mechanical support	2 000 kEUR
Additional personnel (1 Scientist)	300 kEUR

References:

Senyshyn, 2012: J. Power Sources, 2012. 203 126-129
Baran, 2019: J. Energy Storage, 2019. 24 100772
Hinterstein, 2010: J. Appl. Cryst., 2010. 43 1314-1321
Sauber, 2016: J. Appl. Cryst., 2016. 49 923-933

4.4.4 Faster Kinetics followed by SANS

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Science Case

In the past, the exchange kinetics of polymers between different polymer micelles have been resolved using SANS. The option of selective deuteration has a huge potential to look at any exchange process in the future. Usually, one starts with two differently labelled, but otherwise structurally the same entities that by the time exchange their building blocks and, therefore, lose the contrast between them. The science field is now moving to smaller molecules like lipids that have much faster exchange kinetics than the slow polymers. Therefore, experimentally shorter time scales have to become accessible for kinetic measurements. Apart from kinetic measurements, even in static measurements, one wants to measure much faster in order to explore a larger parameter space at a given time. The results will be fed to industrial optimization processes that often are supported by artificial intelligence that even require much more experimental data.

One prominent example of the past is the Covid vaccine using mRNA embedded in lipid particles. Here, one needed to study the drug delivery processes and the ideal compositions (with many more ingredients). So, lipids as formulation component and as interacting material are becoming more and more important for the industry.

Technical realization

To follow kinetic processes using SANS, the provided intensity if often not enough. One either has to perform many repetitions or is limited to rather to the minimum time of the one shot experiment (~10s+). Therefore, it highly important to optimize the beam preparation section of an instrument (including the velocity selector and the collimation) and maximize the detector area (for optimal data collection).

Beam preparation part will already be tackled in the course of 2023 on internal funding including a tilt option for the selector for 20% wavelength spread and an exchangeable beam stop to allow for sample apertures of 2.5 x 2.5 cm^2 (instead of 1 x 1 cm^2). The intensity gain will be 2 x 6 = 12.

In a second upgrade step, we propose the extension of the detection area by implementing a near-field detector with a hole in the center for the small-Q information. This additional detector will cover an area of 1 x 1m^2 and, therefore, will allow for an approx. 2-fold higher detection of neutrons.

Schedule and Cost

High level schedule:

	Year 1				Year 2			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Detector production	■	■	■	■	■	■	■	■
Housing installation				■	■	■		
Instrument integration					■	■	■	
Commissioning								■

Cost estimate:

Invest SoNDe detector, housing and tube installation	4 800 kEUR
Additional personnel	- kEUR

Improving Instrument by Neutron Optics

4.4.5 A dedicated polarization analysis setup for ANTARES

Michael Schulz, Burkhard Schillinger, Aureliano Tartaglione
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Science Case

The outstanding transmission characteristics of the neutron combined with its magnetic moment render it a unique probe for the determination of magnetic properties of bulk ferromagnetic materials. While neutron scattering techniques probe magnetism from an atomic length scale up to a few 100 nm, neutron imaging has been shown to provide complementary information from macroscopic length scales down to a few 100 µm. Imaging with polarized neutrons can be employed to directly visualize large individual magnetic domains as e.g. found in grain oriented electric steel typically used for transformers. Moreover, the spatial variation of magnetic properties of samples arising e.g. from stress introduced during manufacturing or chemical inhomogeneity can be probed. Recently this technique was extended to the three dimensional measurement of vectorial magnetic fields.

Currently, the spatial resolution with polarized neutrons at ANTARES is limited to ~0.5 mm mainly by the large distance between the sample and the detector that is required for the placement of the polarization analyzer, which has a length of ~500 mm. Moreover, since the polarizer and analyzer available at ANTARES are not optimized for the spectrum of the instrument, the polarization reaches only ~70% at a wavelength of 4.3 Å, where the flux is only 10% of the peak flux. We propose to design and acquire dedicated polarizers and analyzers for ANTARES in order to strongly improve the spatial resolution, flux and polarization at the same time. In combination with 3D polarization analysis setup this will significantly enhance the scientific possibilities at ANTRES. The same setup could in the future also be used for polarized imaging experiments at the proposed new imaging instrument FLASH-NT.

Technical realization

Analyzer: We propose to design and purchase a solid state bender with a Si wafer thickness of 50 to 100µm as an analyzer for ANTARES with a design wavelength of ≤3 Å and a length shorter than 5cm, thereby significantly reducing the distance between sample and detector and consequently improving the spatial resolution.
Polarizer: The polarizer must not affect the beam collimation and should therefore be a transmission polarizer. Multi-V-cavities will provide high polarization in combination with good beam homogeneity. Special care needs to be taken to introduce smallest possible effects on the degree of polarization at the V-joints, which will otherwise be visible in the acquired images. The length of the polarizer is less crucial as it does not affect the spatial resolution. A length of 1m seems reasonable, which will require only a few v-joints to cover the required field of view.
3D Polarization Analysis Setup: A dedicated setup for 3D polarization analysis allowing to rotate the spin to an arbitrary direction before and after the sample including a magnetic shielding around the

sample region will be designed within the project. Special care will be taken to reduce the distance between sample and detector as much as possible.

Schedule and Cost

High level schedule:

	Year 1				Year 2			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Optics simulations								
Procurement, manufacturing								
Installation & tests								

Cost estimate:

Invest Solid state bender Analyzer, V-cavity polarizer, 3D Polarization Setup	350 kEUR
Additional personnel	- kEUR

4.4.6 Fast hydrogen kinetics in thin films

Laura Guasco, Thomas Keller, Bernhard Keimer
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Science Case

A rapidly developing field of research is based on charging hydrogen into solids and solid-state devices to modify their magnetic and electronic properties in a specific and reversible way. Prominent examples include targeted modification of the lattice architecture and doping level of quantum materials, modulation of the exchange coupling and magnetic anisotropy of magnetic multilayers and devices, and solid state gas sensors. Artificial neural networks, the key component for machine learning algorithms, will gain efficiency by a synapse design with ultra-low power consumption. The synapses are programmed by a gating voltage charging or discharging a thin conductive layer with hydrogen to modify its resistivity.

Currently, there exists a gap in the available nondestructive measurement techniques for the quantitative detection of hydrogen in thin layers. Available methods provide insufficient sensitivity, time resolution, and in-operando applicability. The proposed upgrade will close this gap and provide better understanding of the microscopic processes involved in the aforementioned hydrogen based technologies, and has the potential to attract a new neutron user community from this rapidly growing field of research.

Technical realization

We propose to upgrade and optimize NREX for studying the interaction of hydrogen with surfaces and thin film structures. The main goals of the upgrade are: (i) to increase the sensitivity and time resolution for single shot experiments by one order of magnitude compared to existing neutron techniques, with the aim to detect changes of the hydrogen concentration with a sensitivity better than 1%at. in less than one second, and (ii) to improve the time resolution for periodic gating experiments by two orders of magnitude, from currently 1 ms to 5 µs.

We will implement a new beam modulation scheme based on one radio-frequency (RF) spin flipper with a subsequent polarizer to modulate the beam intensity, and a fast time resolved detector. The performance of the polarization analysis is not affected by this intensity modulation, this means that both the kinetics of the hydrogen concentration and of the magnetization reorientation can be studied simultaneously.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulation	■	■	■	■	■	■						
Construction			■	■	■	■	■	■	■	■		
Commissioning & tests									■	■	■	■

Cost estimate:

Invest 2D position sensitive detector, RF flipper, neutron optics focusing device, small detector, sample gas handling system	570 kEUR
Additional personnel (1 Scientist)	300 kEUR

4.4.7 Multi-angle high resolution spectroscopy and Larmor diffraction

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Science Case

High-resolution spectroscopy is one of the few domains of neutron scattering that is not expected to be accessible by X-ray techniques. Neutron spin echo plays a prominent role in this area, with TRISP optimized to study excitations in the thermal region. The basic information accessible by TRISP is the intrinsic lifetime of excitations that carry the information about their interactions. One hurdle for such experiments is the availability of sufficiently large crystals, which could be relaxed by significantly increasing the flux and detection efficiency at TRISP. The second unique feature of TRISP is the high-resolution Larmor diffraction (LD), which will in future be extended by LADIFF to even better resolution and small momentum transfers. The interest in LD is continuously growing, especially for the study of small lattice distortions related to spin and charge ordering phenomena, and in the measurement of the thermal expansion in specific directions of the crystal lattice. Larmor diffraction is also possible on poly crystalline samples (powders). This is an essential feature, as most interesting new materials only can be synthesized as powders.

Technical realization

The main limitation of TRISP is the flux and the detection efficiency. For increasing the neutron flux, we will increase the beam divergence in the secondary spectrometer between monochromator and analyzer. The beam divergence in the secondary spectrometer will be increased by reducing the length of the spin-echo units from currently 1m to 50cm, and by using focusing guides close to the sample. The technical challenge is here to develop new superconducting radio frequency spin flippers with twice the effective field.

Challenging is also the design of a spin-echo multi-analyzer. The basic structure is the same as for other TAS multi-detectors, with multiple identical channels covering a range of scattering angles. Each channel hosts one PG analyzer with variable k_f reflecting the beam upwards similar to the BAMBUS or CAMEA detectors. We plan to start with a design with 10 channels, each hosting (from sample to detector) a focusing ellipse, a superconducting spin echo unit, a variable k_f analyzer (PG), a solid state polarizer, and a 1-inch detector.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulation																
Construction																
Commissioning & tests																

Cost estimate:

Invest Superconducting spin echo units (incident beam), superconducting multidetector channels (10 channels)	2 800 kEUR
Additional personnel (1 Scientist)	400 kEUR

4.4.8 Upgrade of the chopper system for the thermal spectrometer TOPAS

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Science Case

Thermal chopper spectrometers are typically used to study condensed matter excitations in the energy range between 5 and 200 meV. The lower energy part of this range is presently served by the PUMA three axis spectrometer. TOPAS is at present designed to extend the energy range as high as the source provides high enough brilliance with a good energy resolution over the entire energy range. Neutron wavelength $\lambda > 0.6$ Å will be accessible thanks to the straight elliptic neutron guide. It will add mapping capabilities for high energy excitations in condensed matter, but also open a novel spectral range for molecular spectroscopy in the so called fingerprint region of H vibrations above 100 meV energy transfer. The present upgrade will make use of the Repetition rate multiplication or Multi E_i developments for instruments at spallation sources, which we label below polychromatic illumination. The continuous neutron source adds flexibility to this concept as the bandwidth can be controlled by means of choppers. It allows to optimize the instrument consequently towards high relative energy transfer, but still probing a large dynamic range with optimized conditions due to the multiple initial neutron energies used.

Technical realization

The present projects aims at upgrading the TOPAS chopper system to optimize it further for measurements of excitations in the high energy loss region. For that, the upstream Fermi chopper FC1 should be replaced by a pair of disc choppers significantly further downstream. Preliminary simulations place the chopper pair in the experimental hall, but the final placement of the chopper would be part of the first phase of the project, a detailed conceptual study of the renewed chopper system. The replacement of the Fermi chopper provides modest intensity gains, but the mayor gain is expected to arise from improved resolution conditions in the dynamic range of high relative neutron energy loss $\hbar\omega > 0.7E$. The polychromatic illumination assures, that still the entire dynamic range profits from the improved resolution. It also requires a bandwidth chopper that we intend to place at the position of the present Fermi Chopper 1. Via changes of the repetition rate of the P-chopper pair and the frequency of the bandwidth chopper we can adjust the overall bandwidth to the actual experiment. Finally, we consider a change of the second Fermi chopper slit package, which features straight channels, with curved channels to increase the timeframe, enhance the suppression of long wavelength neutrons and improve the transmission of the neutron band in use. For all this changes we will assess the effects on the neutron performance and on the engineering layout of the instrument.

The gains of the upgrade in terms of flux are modest and due to the slightly better transmission of disc choppers as compared to Fermi choppers. The gain of upgrade is due to consequent optimization for large energy transfer in combination with the polychromatic illumination. The polychromatic data acquisition promises a significant enhancement of the data quality. The measured spectra contain redundant information as the lower energy transfer regions are sampled several times, but always with different time windows. By appropriate data processing combined with a detailed modelling of the resolution function from the digital twin of the instrument, it will be possible to extrapolate the high resolution from the measurements with long initial neutron wavelength λ to the high energy transfer regions.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Concept: Simulation and design																
Engineering Design: chopper/guide																
Procurement / Manufacturing																
Installation																

Cost estimate:

Invest Choppers & support, shielding, Fermi package, beam monitor	950 kEUR
Additional Personnel (1 Scientist, 3 years)	400 kEUR

Optimized Instrument Performance with state-of-the art robotics

4.4.9 Automated sample change systems for SPODI/FIREPOD/ERWIN

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Science Case

At neutron and synchrotron facilities an increasing demand for automated measurements in the frame of mail-in services of samples has long since been observed, and is also already clearly stated in the long-term goals of the Vision MLZ 2030 program. Automatic sample changers not only improve the efficiency in the usage of measurement slots, they also widen the scope of scientific applications. In particular, robotic systems enable to measure large series of samples prepared by different processing routes or by varying the chemical composition. Exemplary small series of such measurements on Li-ion batteries [Mühlbauer 2020], solar-cell [Ritscher 2016] or engineering [Povstugar 2016] materials at room temperature have already been carried out using a semi-automated 10-sample carousel. This sample changer is also the basis for the very successful rapid access program at SPODI. There is a high demand to extend rapid access measurements to cryogenic temperatures, in particular for measurements that, e.g. only require one measurement above and one below a certain phase transition temperature. Most proposals involving a large number of samples with only a few temperature points each would therefore benefit greatly from a cryogenic or a high temperature sample changer. Prominent examples from user operation on SPODI are measurement series on metal-organic-frameworks [Bon 2019] and magnetic systems [Neibecker 2022]. An automatic sample changer systems for cryogenic temperatures becomes especially prudent with the two new additions to our powder diffraction suite at SR8, ERWIN and FIRPOD, complementing the instrument SPODI.

Technical realization

All instruments at SR8 should use one common pool of sample environment including automatic sample changing systems. We plan to use a multi axis robotic arm (Stäubli TX 60) as flexible sample changer for all temperatures. The basic concept is the combination of a robot equipped by a sample magazine with dedicated sample environment for automatic sample change. Thus, the robot could be combined with ADR type cryostats from Kiutra that offer options for automatic sample change and enable low base temperatures. Hence, we envisage two ADR type cryostats for the pool. For high temperatures, another oven is required in addition to the SPODI furnace. The furnace design must be adjusted to allow for automated sample changes by a robotic arm.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3				Year 4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Procurement robot Spodi																
Integration into NICOS																
Design/ Procurement cryostat																
Design /Manufacture furnace																
Integration into NICOS																

Cost estimate:

Invest Robot, cryostats, furnace	1 300 kEUR
Additional Personnel (1 Scientist / Instrument Control)	400 kEUR

References:

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Extended Applications for Analytics

4.4.10 PGAI with gamma detector cluster

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Science Case

Prompt Gamma Activation Imaging (PGAI) has been proven to be used for the non-destructive 3-D element mapping of complex archeological objects and artifacts. Further applications include scanning of closed capsules or holders containing harmful materials. The method is based on the sharp collimation of the neutron beam and the emitted gamma radiation so that a predefined 3D voxel is detected only. The optimum size of such a voxel is a few mm^3, while in normal PGAA the beam and the gamma-ray collimator have a diameter of about 2 cm. The acquisition from such a small volume means of course a drastic reduction of the count rates and makes the experiment by measuring the voxels one by one extremely slow. This limitation can be overcome with a new concept in the detection: The narrow neutron beam irradiates the sample along a whole line, and the gamma photons will be collected from many points at the same time. Using multiple detectors and collimators, containing several channels focused to the same voxels, could increase the efficiency by two orders of magnitude. A cluster detector system could be used for other purposes, as well, the cross-talk between the segments could be used for Compton-suppression or for the reconstruction of the original signal energies using the so-called add-back technique and it also broadens the nuclear-physics applications.

Technical realization

The main component of the setup is the detector cluster. One possible arrangement looks like a flower: a hexagonal HPGe detector is surrounded by six others. They have a common cooling, but all 7 detectors have individual preamplifiers and high-voltage supplies. Other geometrical arrangements are also possible, and they must also be considered before the final decision. Each detector must collect the photons from different voxels. Using one single collimator channel in the shielding obviously reduces the signal strength too much, so several channels will be focused on the same voxel in the case of each detector. This needs a machining of the heavy-metal shielding with a high precision.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulation, selection of cluster detector	■	■	■	■								
Procurement, installation, collimation					■	■	■	■				
Commissioning									■	■	■	■

Cost estimate:

Invest Cluster detector, spectrometer, collimation system, shielding	500 kEUR
Additional personnel (1 Scientist, 1.5 years)	150 kEUR

4.4.11 Beta-gamma correlation NAA

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Science case

In instrumental neutron activation analysis (INAA), typically, the detected particles are the characteristic γ rays emitted by the radionuclides produced during activation. So far, coincidence/anticoincidence counting has scarcely been exploited, although, with a few exceptions, activation products emit several particles at once: γ rays, mostly in a cascade, and β particles. Their simultaneous detection drastically increases the selectivity and thus broadens the range of detectable elements. A unique setup based on the near 4-π detection of both β and γ radiation combining HPGe detectors and scintillation counting using list mode is recommended for the determination of difficult-to-measure radionuclides. Besides β-γ coincidence, anticoincidence mode used in the case of pure β and γ emitters facilitate the determination of such important elements as phosphorus which is not detectable in standard INAA. Possible application include the determination of trace phosphorus in silicon, often asked for by semiconductor industry, the determination of sulfur in concrete, air filters or crude oil and petroleum products.

Technical realization

The setup must detect the beta and gamma quanta with nearly 100-% efficiency. For this purpose, a plastic scintillator counter is needed for beta particles, which is surrounded by a gamma-ray detector, either by a large inorganic scintillator (BGO, LYSO, $LaBr_3$) or by a well-type HPGe detector. The first solution has a smaller energy resolution for the γ rays, while the second one facilitates the counting of very small samples only. The signals are combined using a digitizer with a multi-channel input, enabling logical operations and list mode acquisition for both coincidence and anti-coincidence modes.

Investments: HPGe detector (well-type and coaxial with cooling, preamplifier and high-voltage supply), scintillator detectors (scintillators with special geometries, photomultipliers and high-voltage supply), digitizer.

Schedule and Costs

High level schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulation, finalization of concept	■	■	■	■								
Construction and Installation					■	■	■	■				
Commissioning									■	■	■	■

Cost estimate:

Invest detector, spectrometer, electronics	200 kEUR
Additional personnel (1 Scientist, 1.5 years)	150 kEUR

4.4.12 GRAINS - Gamma-Ray Analysis from Inelastic Neutron Scattering

Adrian Losko, Zsolt Révay
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Scientific case

The major reaction of the fast neutrons at imaging instrument NECTAR is inelastic scattering, in which a lower-energy neutron and a medium-energy gamma photon is produced. The gamma rays are characteristic, i.e., they identify the emitter nuclide. Using the coincidence detection of these particles, the elemental mapping of complex samples would be possible which will be exploited in GRAINS project. Applicability of GRAINS is aimed at a broad range of scientific fields, providing a worldwide unique capability to determine bulk isotope concentrations. Examples range from archeology, where the samples composition could be determined in 3, batteries and fuel cells, where the chemical composition could be mapped in full size cells or industrial applications, where e.g. scintillators could be inspected for inhomogeneity in composition, or all the way to inspection of hazardous materials that cannot be opened, e.g. nuclear waste forms.

Technical realization

The facility is planned at NECTAR, where the gamma-ray background is sufficiently low to enable short sample-detector distances. The setup will consist of (i) a neutron detection unit, i.e. a scintillator screen behind the sample and a fast camera suitable for time stamping, and (ii) a gamma ray detection unit, similarly suited for time stamping and located perpendicular to the neutron beam. The gamma-ray detectors are connected to a multichannel digitizer collecting all the gamma-ray in list mode and also establishing the coincidence between them and the neutron events. Only the n-γ coincidence events are collected, whose positions are given by the neutron scintillator, while the characteristic energies detected by the gamma detectors identify the emitter elements providing the elemental map across the sample. For the gamma detection, scintillators like $LaBr_3$ or LYSO should be investigated whose timing characteristics are better than those of HPGe detectors, at the same time their lower energy resolution should be enough for these types of characteristic gamma rays. The improvement of timing characteristics of HPGe detectors should also be investigated.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulation and test measurements	■	■	■	■								
Technical specification, procurement					■	■	■	■				
Installation, commissioning									■	■	■	■

Cost estimate:

Invest Gamma ray detectors, electronics, shielding, beam scrapers	650 kEUR
Additional personnel	- kEUR

4.5 Sample environment

4.5.1 New Magnets for Correlated Electron Systems at MLZ

Sebastian Mühlbauer[1], Markos Skoulatos[1], Christian Franz[2], Marcell Wolf[1],
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Science Case

Strongly correlated electronic systems are one of the key fields of research where neutron scattering played and continues to play a pivotal role. At MLZ, several high impact discoveries have been achieved over the last decade exploring new physics and revealing new functionalities towards future data storage or logical devices. Besides new instrumental concepts and even more brilliant neutron sources to detect even weaker, often diffuse signals, a key step towards the exploration of new physics is extending the available parameter range of the sample environment – particularly for (quantum) disordered systems, exotic electronic ordering phenomena or collective electronic excitations. Here, temperature, pressure and electrical field and particularly the application of ***magnetic fields*** are crucial to tune the properties of strongly correlated electronic systems. With the MORIS program, we propose the purchase of three new magnets, all based on the new, cryogen free high temperature superconducting (HTS) technology.

Technical realization

A 10T high performance compensated, asymmetric horizontal magnet optimized for small angle neutron scattering (SANS), reflectometry and the resonance spin echo technique MIEZE (Modulation of IntEnsity with Zero Effort) is focused on the use of polarized neutrons and polarization analysis in forward scattering direction. Feasibility studies show that a field of 9T-10T can be achieved using the novel HTS materials at reasonable weight (~700kg) and size (75cm x 75cm) enabling the use on a large number of beamlines at MLZ with minimized interference and stray fields. This compares to fields of ~3T that are achieved in existing systems dedicated for polarized neutrons. The magnet will be optimized for lowest possible parasitic background scattering with the least possible amount of material in the beam. Together with a dedicated integrated cryostat, it will offer a wide temperature range of 50mK to 350K. Its specifications are designed to fit in the instruments SANS-1, KWS-1, KWS-2, KWS-3, NREX and RESEDA.

A ultra-low background vertical field magnet for time-of-flight (TOF) neutron scattering is required with the commissioning of the thermal TOF TOPAS in the guide hall east and after the upgrade of the cold TOF TOFTOF with a pixelated 2D detector. Both instruments require a compact design with a diameter less than 800mm to fit the available sample space. A large horizontal opening of -35° → 155° and a vertical opening of ±20° allow efficient measurements using the full detector coverage. A high magnetic field of 10-14T and ultra-low background allow the investigation of the most pressing questions in quantum spin liquids, functional materials, high-Tc superconductivity and many more. A dedicated cryostat is probably needed due to the space restriction.

Finally, a dedicated horizontal magnet with a dilution unit for triple-axis-spectroscopy and of a moderate strength of H=5T is envisaged, in order to meet the user needs for continued cutting edge research performed at the MLZ. An emphasis is placed in keeping a nearly 360°-free access window within the scattering plane of such a magnet, at the expense of reducing the maximum possible magnetic field. This enables then a routine operation and avoids complex planning of experiments due to large sections of dark angles.

Schedule and Cost

High level schedule:

	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Technical specification												
Procurement												

Cost estimate:

Invest 10T horizontal SANS, 10-14T vertical TOF, 5T horizontal TAS	5 000 kEUR
Additional personnel (1 Engineer)	300 kEUR