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An Instrument Suite for the HBS

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Abstract. We have investigated an instrument suite for the High Brilliance Source, a High-Current Accelerator-driven Neutron Source proposed by the Forschungszentrum Jülich, to explore the potential of this type of facility for the European and German neutron user community. The investigated instrument concepts cover most types of applications currently in operation at existing user facilities. Providing individual target stations with a frequency, a pulse length and spectral properties matched to the hosted instruments is the key feature of the proposed source, which ensures instrument performance that exceeds that at recently shutdown research reactors and thus a source competitive with modern neutron user facilities.

1 Introduction

A success of the European neutron community has been the network of low to high flux neutron sources, which formed a vibrant user community always pushing the limits of different neutron scattering methods. The creative power of the broad collective has led to the development of novel techniques, which often proved their potential and feasibility at smaller facilities before they reached full power at the high flux reactors such as the Institute Laue Langevin (ILL) in France. Now we have already entered the era of the MW spallation sources, but the tier of pulsed sources with low to medium flux with facilitated access for regional or national users is still missing, at least in Europe. Several projects explore the potential of High-Current Accelerator-driven Neutron Sources (HiCANS) [1–4] to cover the demands from the scientific field, but also to provide more capacity for industry by offering novel access schemes. They aim to provide national access to world class instrumentation and provide full user service in terms of sample environment, radio protection, etc. on the level of existing large scale facilities. Furthermore, HiCANS are scalable in size, in power and in price and can lead to the formation of a regional tier of neutron sources with immediate access to surrounding universities or industry, thus sustaining a user community with regular access to neutron instrumentation that is trained to make best use of the high power facilities.

The HBS project aims to be the national tier of such sources in Germany, filling the gap that was created by the shutdown of the research reactors FRJ II, BER II and FRG in Jülich, Berlin and Geesthacht over the last 20 years. At HBS, neutrons will be released from a Ta target, that is hit by a proton beam of 100 mA peak current and 70 MeV proton energy, well below the spallation threshold. This has several consequences:

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1. The proton accelerator becomes fairly straightforward and much cheaper than the high energy accelerators required for a spallation neutron source.

2. Each proton produces fewer neutrons at lower energy as compared to the spallation reaction. However, the neutrons are released (from the nuclei) within a very small volume, which can be coupled very efficiently to the thermal moderator. Despite the much lower source strength, the confinement of the neutrons in a small volume yields a high brightness of the moderators. Also the extraction system can move closer to the neutron source, giving access to large phase space volumes as required for many neutron instruments.

3. Shielding can be reduced as the amount and energy of fast neutrons, which are most difficult to absorb, is several orders of magnitude lower compared to spallation sources and research reactors. This makes the shielding less heavy and reduces the construction cost for a target station to a small fraction of the facility cost. Finally the lower radiation levels allow more flexible instrument designs, which can be easily adapted and upgraded in the future.

4. It is possible to provide individual target stations that match the requirements of the hosted instruments

   - in bandwidth by providing different repetition rates,
   - in pulse length to match different resolution requirements,
   - and in spectral properties by a choice of different moderators.

The HBS would offer one target station with repetition rate of $f = 24$ Hz and two target stations with a repetition rate $f = 96$ Hz to supply the appropriate bandwidth, resolution and spectral conditions: e.g. SANS and powder diffraction require a wide band of initial neutron wavelengths, while e.g. chopper spectrometers make use of a very narrow neutron energy band. Depending on the instrument length L the instruments can select the bandwidth, $\Delta\lambda$, of the incoming neutrons:

$$\Delta\lambda = \frac{h}{m_n}(f \times L)^{-1} \tag{1}$$

The different target stations are therefore vital to provide an optimized bandwidth for the individual applications.

Pulsed neutrons provide an intrinsic wavelength resolution that is defined by the ratio of the neutron pulse length τ_{Mod} to the time-of-flight, which depends on the wavelength and again the instrument length L. The wavelength uncertainty $\delta\lambda$ is given by:

$$\delta\lambda = \frac{h}{m_n}\frac{\tau_{\mathrm{Mod}}}{L}. \tag{2}$$

All target stations feature the same duty cycle to also have the same heat load on the target. For the 24 Hz target station, the proton pulse length of $\tau_{\mathrm{P}} = 667\mu$s and the moderated neutron pulse length τ_{mod} are nearly identical, while the 96 Hz target stations feature a fairly symmetric moderated neutron pulse of $\tau_{\mathrm{Mod}} \approx 250\mu$s as a result of equal contributions from the proton pulse, $\tau_{\mathrm{P}} = 167\mu$s, and the lifetime of slow neutrons in the water moderator. One of the 96 Hz target stations gives access to cold and thermal beams, while the second one is optimized to extract thermal, epithermal and even fast neutrons.

We can distinguish three groups of instruments making different use of the pulse and spectrum of the individual target stations. The first group requires a broad band and low resolution and will be

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

Table 1. Key figures for the instrument suite in the technical design report (TDR) for the HBS. Flux and resolution values are quoted for typical configurations of the instruments. Light blue: Large scale structure instruments, Dark blue: Diffractometers, Green: Spectrometers, Yellow: Imaging and analytics instruments.

therefore hosted at the long pulse 24 Hz target station. The second group has modest resolution requirements which are met by the natural pulse length of the 96 Hz target stations. Both groups require a chopper system only for the definition of the bandwidth and to prevent frame overlap. Instruments with more stringent resolution specifications require additional equipment to tailor the wavelength resolution by pulse shaping.

Recently the technical design report (TDR) for the HBS was published, which shows the technical feasibility of all key components for such a facility [5]. In the reminder of the paper we present a potential instrument suite that could be installed and operated at this HiCANS.

2 Large Scale Structure Instruments

Cold neutrons are ideally suited to probe structural correlations from nm to μm. These length scales are typically probed by Small Angle Neutron Scattering (SANS) instruments for 3 dimensional systems or reflectometers for layered systems. At existing neutron facilities, SANS is one of the most demanded methods with applications in life and material science, chemistry, physics and engineering. The sensitivity to light elements and magnetic moments and the option to control the contrast by isotope substitution provide insights on the mesoscopic scale complementary to more abundant methdods like SAXS. Both instrument types require comparably relaxed wavelength resolution, but very high collimation in either one or two directions.

Within the TDR, we have investigated a SANS instrument covering the range 0.001 $Å^{-1} < Q <$ 1.8 $Å^{-1}$. Using 2 detectors in different distances from the sample and a large wavelength band of 6.8 Å, the standard Q-range for SANS (0.002 to 1.8 $Å^{-1}$) can be covered in one shot. It is meant for high throughput and is therefore designed as a standard pin-hole SANS for a typical sample size of 1 cm^2 with a limited number of configurations and robot support.

The second instrument proposed for studies of large scale structures is an instrument optimized for grazing incidence SANS (GISANS), which allows one to probe lateral correlations in layered samples on the nm length scale. The GISANS instrument has the same size, wavelength band and Q-range as the SANS instrument. It is optimized for highest flux at the sample, because the scattering volume is small. A large Q-range in a single shot is achieved by the wide wavelength range, 2 detectors and 3 inclination angles that can be used simultaneously.

Both, the SANS and the GISANS instrument, have a better wavelength resolution than SANS instruments on reactor sources, which allows a better overall resolution that can result in new scientific results, e.g. on liquid crystal samples.

Two reflectometers have been investigated. One of them (OffRef) has an emphasis on the study of off-specular scattering accessing correlations up to μm length scale. As off-specular scattering is weak, a very low background is needed. This is achieved by getting out of the direct line of sight by using a curved guide and by choosing instrument length and wavelength band such that data acquisition does not take place during the proton pulse. A broad Q range is obtained by choosing the low frequency target station (24 Hz) and a short instrument length.

The other one (HorRef) is designed as a very short horizontal reflectometer of only 7 m length on the 96 Hz target station to provide a broad bandwidth. It combines a Selene guide system with direct beams from the thermal and cold moderators giving access to a very wide Q-range and high intensity, which will enable kinetic studies. The 3 beams can be used separately or simultaneously. The beam through the Selene has the longest wavelengths at the smallest inclination angle, the beam from the thermal moderator has the shortest wavelengths at the largest inclination angle; this results in a broad Q-range covered in one shot. The compact design guarantees that the Selene guides can be built with sufficient precision.

All these instruments use choppers for the bandwidth definition, requiring therefore choppers running at modest speed, which are readily available today. The key figures of the instruments are presented in the light blue rows in Table 1.

3 Diffraction

The HBS is well suited to host single crystal and powder diffractometers to explore the nuclear and magnetic structure of materials with atomic precision. Neutron time-of-flight resolved Laue diffraction is a perfect tool to explore large areas in 3D reciprocal space with particular sensitivity to the position of light elements and to the position and size of the spins in a sample. The HBS is particularly well suited for applications with modest resolution requirements, that can be met by the pulse length of the moderators. Examples are instruments for single crystal investigations or instruments for the study of diffuse scattering giving rise to broad signals in momentum transfer space. As the intensity variations across the band should stay reasonably small to measure different momentum transfer with comparable statistics, a bandwidth 1.5 Å$< \Delta\lambda < 2$ Å is perfectly suited for these applications. Hence these instruments are hosted at one of the 96 Hz target stations with moderator-to-detectors distances of 20 m$< L < 30$ m as calculated from eq. 1. The natural resolution of $\delta\lambda \approx 0.04$ Å matches typical resolution settings at existing instruments for similar applications. The instruments feature also similar chopper systems consisting of a bandwidth and a frame overlap chopper spinning with the source frequency.

For the study of small samples we have explored an instrument (MMD) employing a 2D Selene optic [7, 8] to illuminate a cross section of approximately 1 mm x 1 mm with potential applications for the investigations in macro-molecular crystallography or in combinations with sample environments that constraint the sample volume strongly. The former profits mainly from the sensitivity to hydrogen and other light elements in the sample, the latter from the penetration potential of the neutron. Tailoring both beam size and divergence distribution far upstream the sample, the instrument will be optimized for a high signal-to-noise ratio.

The second proposed instrument (PDNS) makes use of the sensitivity of neutrons to the magnetization distribution in a material. Hidden long and short range order often gives rise to emerging phenomena, e.g. skyrmions in non-centrosymmetric crystals. Polarization analysis can here be used to probe directly chiral correlations which are hidden otherwise. It has been optimized for the study of magnetic structures and dynamics with finite correlation length on the order of a few hundred Å and therefore has relaxed collimation requirements. The instrument is equipped with a polarizing transport system to provide the highest possible polarized neutron flux. As typical applications often involve weakly scattering samples, the illuminated area should be on the order of 5 mm x 20 mm, which is realized by an elliptically focusing guide. The polarization is analyzed in a large area of reciprocal space by a wide angle polarization analyser.

The third diffractometer (DENS) addresses disorder or short range order in novel materials, which are often key to understand the properties or the functional behavior. These give rise to weak diffuse scattering in the vicinity or between Bragg reflections. It is worth noting that in a diffraction experiment the inelastic scattering can lead to a signal of similar strength as compared to the elastic signal. By introducing a pseudo-statistical chopper close to the sample area in combination with cross correlation analysis, one can extract the elastic scattering only, again optimizing the signal-to-noise ratio.

A dedicated instrument to study disordered materials (DMD) with a emphasis on pair distribution function (PDF) measurements can be hosted at a short pulse target station with a dedicated moderator for the hot part of the thermal spectrum. It would be a comparably long instrument making use of the full pulse. Shielding would be required only for the detector, thus enabling the instrument to have a very open sample area, which allows the provision of extremely flexible sample environment. This is crucial for the use of a wide range of specialized sample environment, that can also be provided by external users.

To provide higher wavelength resolution, as required for a general purpose powder diffractometer or an engineering diffractometer for stress/strain analysis, one would have to apply pulse shaping. As the finite distance between the source and the pulse shaping choppers limits the accessible bandwidth, one could either realize a long instrument with a bandwidth matching the constraints of the chopper or build a shorter instrument making use of the wavelength frame multiplication [13] to fill the time frame. For the TDR, we explored both options, the short instrument at one of the 96 Hz target stations and the long instruments at the 24 Hz source. We could prove that the combination of an efficient neutron extraction and transport combined with large detector coverage and good access to the sample area can meet the demands for most experiments currently carried out at existing facilities.

The predicted capabilities of the diffractometer suite are presented in the dark blue rows in Table 1.

4 Spectroscopy

Neutrons are an indispensable tool to explore the nuclear and spin dynamics in an energy range 1 μeV< $\hbar\omega$ < 100 meV and a wide momentum transfer range and hence probe spin correlations and atomic motions in the time and length scales, which are an ultimate test for condensed matter theory. For pulsed neutron sources, direct geometry chopper spectrometers are a natural instrument choice. With the intermediate pulse length of the 96 Hz target station, the time frame defined by the source repetition rate matches perfectly the time frame of the proposed cold chopper spectrometer (CCS). The instrument would be ideally suited to study magnetic excitations covering the entire Brillouin zone, but also for quasi-elastic scattering to probe local motions of light elements, in particular, in the time range between ps and ns. In contrast to instruments at spallation sources, which have typically a lower repetition rate, there is no need to employ multiple initial energies, known as repetition rate multiplication. In this mode, a pulse shaping chopper assembly consisting of two counter-rotating discs tailors the wavelength resolution to the experimental needs, while a second assembly close to sample controls mainly the illumination time and hence the wavelength resolution after the interaction with the sample. The instrument requires a detector covering a large solid angle at a distance sufficiently large to allow investigations of quasielastic scattering with a resolution $\delta\hbar\omega \approx 20\mu$eV, leading to a sample to detector distance L_{SD} = 3 m.

A chopper spectrometer for thermal neutrons is not very effective at HBS due to the long distance required to achieve a good initial wavelength resolution. A narrow energy resolution can be provided by a focusing Bragg monochromator combined with a chopper just upstream to the sample to control the illumination time. At the HBS such an instrument (CRYSTOF) can be placed at 4 to 7 m distance from the moderator. With a large monochromator, one can transport a large phase space volume to the sample. The broad bandwidth enables the use of the different harmonics of the monochromator to multiplex the initial neutron energy.

While overview measurements of reciprocal space and the study of local motions can be covered perfectly by a direct geometry time-of-flight spectrometer, detailed investigations of a specific region in reciprocal space are the domain of triple-axis spectrometers (TAS) based at continuous neutron sources. Recently, novel concepts have been introduced based on multiplexing secondary spectrometers for TAS. Combining these with a time-of-flight primary spectrometer, new crystal analyzer spectrometers have been proposed at the ESS [9, 10] and the ISIS spallation source [11] to measure $S(\vec{Q}, \omega)$ in wider regions in reciprocal space. Adapting the concepts to the high repetition rate of the 96 Hz target station has enabled us to design a narrow bandwidth instrument (CAS), that concentrates the intensity into a narrow bandwidth $\Delta\lambda$ = 0.7 Å. This allows fast measurements of specific regions in reciprocal space, which can be extended by scanning of the wavelength band. The intensity variation across such a band are small providing similar statistics over the measured band. The natural resolution using the full pulse should be sufficient for most use cases. However, employing pulse shaping to improve the resolution in specific cases will be possible, as the time frame at the detector will still be nearly completely filled due to the large distance L_{Sam}. A very efficient transport with a relaxed collimation of 3° x 3° can be realized by a ballistic guide to provide a high sample flux.

To achieve higher energy resolution, which is needed to probe motions at longer timescales, requires a near backscattering crystal analyzer spectrometer (BSS). Making use of prismatic focusing, an instrument using an analyzer of highly oriented pyrolitic graphite can achieve a resolution $\delta\hbar\omega \geq 5\mu$eV [12] combined with a large acceptance of the analyzer. The proposed instrument for the HBS is designed to access a huge phase space as neutron optics can go as close as 50 cm to the moderator, enabling a collimation of 5º x 5º to be transported to the sample. The instrument will be equipped with polarization analysis to distinguish coherent and spin-incoherent scattering and accordingly enhance the sensitivity, in particular to cleanly probe the local dynamics of hydrogen and other elements with a reasonably high spin incoherent scattering cross section.

To extend towards even longer correlation times, one can use spin echo methods. We explored two options here: (i) A high resolution neutron spin echo (NSE) that can access Fourier times up to hundreds of ns to study the dynamics in polymers, bio-molecules or energy materials. (ii) Using the MIEZE technique in a neutron resonance spin echo (NRSE) instrument, one can also apply magnetic fields to a sample and probe spin correlation e.g. of topological spin textures, superconductors or ferromagnets. The spin-echo instruments would be hosted at the 24 Hz long pulse target station and profit in particular from the short distance at which the neutron guides can begin, allowing the extraction of a large phase space volume.

In Table 1 we show the key figures of the spectrometers in the green rows.

5 Imaging

To address the increasing demand for neutron imaging from a wide field of applications that range from arts and cultural heritage, to biology, geology and up to engineering applications, where the high penetration allows the investigation of entire devices in action, we explored the potential of different imaging stations. Most of them use different sample stages giving access to either high resolution or high intensity, e.g. for kinetic applications. The instruments make also use of the neutron polarization to image magnetic fields.

Imaging with cold and thermal neutrons (C-NI, T-NI) would profit in particular from the small cross section and short distance of the first aperture from the bright liquid para-hydrogen moderator enabling large L/D ratios.

A diffractive imaging station (D-NI) uses wavelength resolution in a narrow band to analyze the transmission around Bragg edges to gain e.g. local information about strain. The time-of-flight encodes the wavelength to enable Bragg edge imaging.

Furthermore, as one target station is dedicated to the use of high energy neutrons, imaging instruments using epithermal (EPI-NI) and high energy neutrons (HE-NI) could be built at the HBS. It would enable penetration into very large samples. For the latter, special pulse patterns can enable lock-in techniques to become sensitive to specific nuclear resonances and hence allow element or isotope specific investigations of specimen with unknown composition.

6 Analytics

There is a rising demand for the analysis of atomic compositions in samples, especially of chemically similar elements like rare earth elements. In contrast to other methods, prompt gamma neutron activation analysis (PGNAA) allows the determination of the atomic composition. It is a well established method to identify specific elements within crowded environments. The instruments suggested for the HBS refine this concept. We propose the following:

One instrument (ToF-PGA) would measure the wavelength dependent penetration of a sample to locate a specific isotope. For that, the wavelength of the absorbed neutron, that gives rise to the characteristic Gamma emission, is encoded by the time-of-flight.

A second instrument (PGAINS) would be used to measure the delayed gammas, to explore the composition of large specimen making use of epithermal and fast neutrons and their large penetration depths.

Furthermore, neutron depth profiling (NDP) will allow near-surface studies of light elements. Here the absorption of the neutron leads to an emission of an alpha particle with a well defined energy. From its energy loss upon the escape from the sample, one can deduce the escape depth and hence determine the depth profile of the respective isotope. The sample can be very close to the moderator thanks to the low radiation level and hence access a high neutron flux to become highly sensitive to the distribution of the element under investigation.

The parameters characterizing the imaging and the analytics instruments appear in the yellow rows in Table 1.

7 Conclusions

The potential performance of the instrumentation at the HBS is summarized in Table 1. It covers all neutron scattering, imaging and analytics applications that were available at the recently decommisioned research reactors. Despite the HBS source strength being significantly weaker, the instruments provide improved performances in terms of flux and resolution. The lower production of fast neutrons, which is furthermore limited to the duration of the proton pulse, provides the opportunity to increase the signal to noise ratio by at least an order of magnitude. The instruments also become more flexible due to the relaxed shielding constraints. This will enable shorter upgrade cycles for the instruments to adapt to new experimental challenges from novel scientific questions. The present target design was chosen to match the instrument requirements in bandwidth, resolution and spectrum. However, it should be noted, that the cost for a target station contributes only a small fraction of the overall cost of the facility. For this type of neutron source, it is straightforward to adapt or replace the instruments to account for new directions either in science or in neutron production, making this type of sources future-proof and sustainable. Last but not least, we hope that a new network of CANS and HiCANS sources will serve to train a new generation of neutron users that will be able to exploit the full potential of the upcoming MW spallation sources, where unprecedented capabilities can be expected.

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