

# Conceptual Polarization Setup at CENTAUR, the SANS/WANS Instrument at the Second Target Station of SNS

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**Abstract.** CENTAUR is a multifunctional general purpose small-angle and wide-angle neutron scattering instrument with diffraction and spectroscopic capability in the future Second Target Station at the Spallation Neutron Source of the Oak Ridge National Laboratory. To fill a gap in neutron polarization capability, the instrument will be designed to provide polarization analysis. Here we present the conceptual polarization setup at CENTAUR, as well as the Spin Echo Modulated Small-Angle Neutron Scattering setup which will further expand the length scale covered by the instrument.

## 1. Introduction

CENTAUR is a small-angle and wide-angle neutron scattering instrument with diffraction and spectroscopic functions currently under design as one of the first eight selected instruments to be built at the Second Target Station (STS) of the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory (ORNL). As the only instrument capable of small-angle neutron scattering (SANS) among the selected instruments, it was optimized to be a high-performance SANS instrument with wide Q coverage up to diffraction region by leveraging the broad wavelength band and high brightness source at STS.

In many science areas, including soft matter, polymer science, geology, biology, quantum condensed matter, and other material sciences, there is a gap in performing in-situ and operando experiments for kinetic and out-of-equilibrium studies of phenomena. With the consultation from a broader user community, the instrument specifications and requirements are derived to fill this gap. Briefly, CENTAUR will be a high-performance SANS instrument, reaching  $Q_{\min}$  as low as  $0.001 \text{ \AA}^{-1}$ . Most notably, it can cover  $0.001$  to  $20 \text{ \AA}^{-1}$  simultaneously to provide measurements from mesoscale to atomic-scale. The time resolution for relatively strong scattering samples needs to be in the seconds range for time-resolved studies over this wide length scale. Typical sample sizes are from 1 to 10 mm in diameter. The high-flux beam will ensure less sample material is needed, e.g., biological samples, or smaller samples that can speed up discovery of new materials.

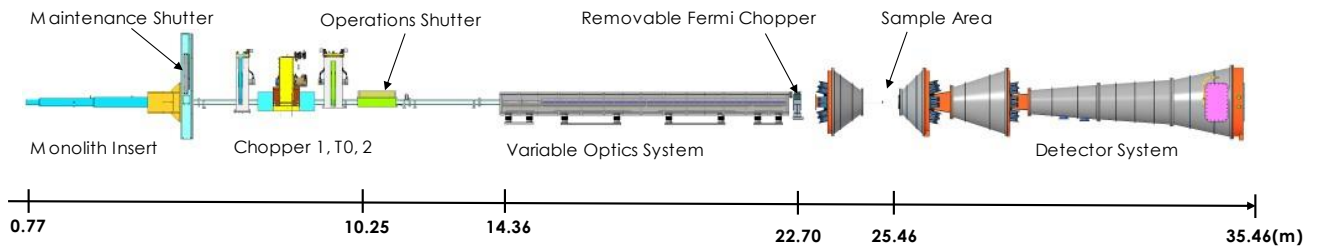
As a general-purpose instrument, the sample environment at CENTAUR will be designed to accommodate a wide user community with convenient access and expandability. With the increased throughput, we envision equipment such as in-line flow cells similar to those at synchrotron SAXS beamlines, robotic sample handlers, and multi-modal sample holders integrated with additional complementary measurement tools will be designed. In addition, closed-cycle refrigerators, low-temperature cryostats, and superconducting magnets that are typical for quantum condensed matter research will be available and conveniently accessed.

In our survey with the user community, the lack of polarization capability at the current ORNL SANS instrument suite is an outstanding capability gap [1]. Polarized neutrons with polarization analysis can be used to separate nuclear and magnetic scattering. This technique is very sensitive to the direction of magnetic moments because only the component of the magnetic moments perpendicular to the scattering vector  $\mathbf{Q}$  contributes to magnetic scattering. In polarized SANS, the structural scattering (coherent nuclear scattering) does not flip the neutron polarization  $\mathbf{P}$  while the magnetic scattering can cause the neutron polarization to flip if the magnetic interaction vector  $\mathbf{M}_\perp$  is perpendicular to  $\mathbf{P}$ . Therefore, polarized SANS is a great tool to study magnetism and magnetic materials on nanoscopic and mesoscopic scales, which include magnetic nanoparticles, magnetic oxides, non-collinear structures, skyrmion-like systems, etc. In addition, for soft matter samples, incoherent scattering mainly from hydrogen atoms may dominate the SANS signal at high  $Q$ s. It is possible to use polarized SANS to separate the coherent nuclear scattering and the spin-incoherent scattering because for spin-incoherent scattering 1/3 of the scattering is non-spin-flip and 2/3 spin-flip [2]–[6]. Then by applying polarization analysis, the coherent scattering can be extracted from the total scattering signal. To fill this gap, we will design CENTAUR to be capable of polarization analysis. We are also considering implementing an additional advanced analysis mode called Spin Echo Modulated SANS (SEMSANS) to further extend the length scale that CENTAUR can probe. In this paper, we present the concept for the polarization setup.

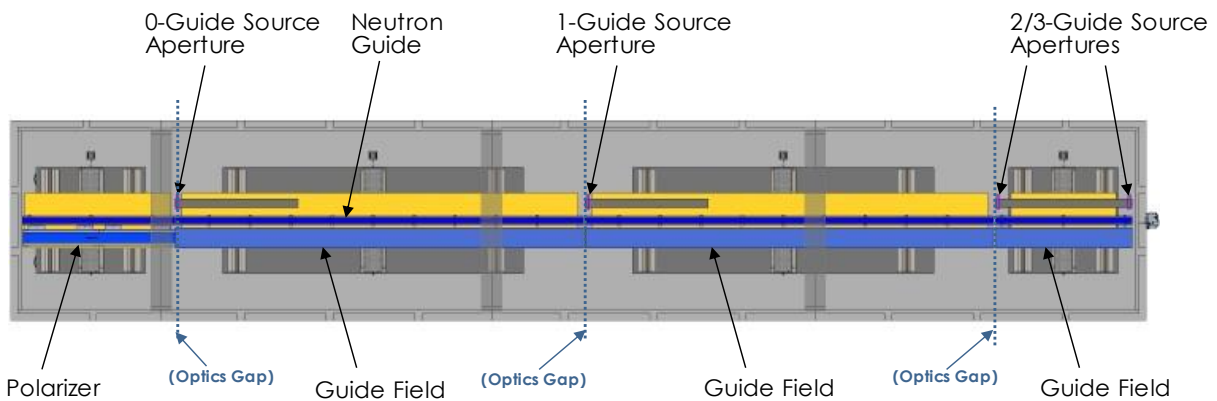
## 2. Overall instrument design

CENTAUR will be a pin-hole collimated instrument with a variable neutron guide insertion system to provide adjustable divergence and flux. The design closely follows the instrument concept that was published recently [7]. Here we briefly go over its source characteristics and instrument components (Figure 1) before discussing the polarization setup. The instrument will be located at beam port position viewing a tube parahydrogen coupled moderator. It is noteworthy that the compact sources at STS provide the highest peak brightness of any current or planned neutron sources that translate into excellent flux at the sample position. These characteristics are favorable for experiments including those using polarization. The source is 3 cm in diameter, which dictates the downstream neutron supermirror guide size. As of the end of 2022, the optimum non-polarizing guide option to match the source is an octagon shape with each side being 1.24 cm in size. Compared to traditional square guide of 3 cm by 3 cm, it increases overall flux by about 15% and results in more uniform phase transport. All fixed neutron guides will be straight from about 1m away from the moderator face to the variable guide system. A few gaps will provide locations for bandwidth defining choppers 1 and 2 and a T0 chopper, which suppress fast neutrons and prompt gamma rays from the source. All choppers are inside the target bunker, which is a heavily shielded structure which surrounds the target monolith. Figure 1 shows the design as of the end of 2022, which has evolved from the earlier publication [7].

A variable optics system will start at about 14.36 m from the source, next to the bunker wall (not shown in Figure 1). The system will include interchangeable components, such as neutron guides, polarization V-cavity mirrors, open space, and source defining apertures (Figure 2). The system consists of interconnected vacuum boxes based on the proven GP-SANS and Bio-SANS collimation box design that was derived from the original NIST SANS design [8]. The generous space inside also provides additional positions for different polarization supermirrors in the future upgrade for possibility to optimize polarization for certain wavelength bands.



**Figure 1.** Key instrument components of CENTAUR as of the end of 2022.



**Figure 2.** A top view of the Variable Optics System. The dashed blue lines separate the system into 4 sections as detailed in the description.

The first section of the box will be about 1 m long with interchangeable optics between a V-cavity polarizer and non-polarizing guide. After that are variable collimation sections with length of 3 m, 3 m, and 1 m, supported on individual motorized stages for inserting into the neutron beam path as necessary. Three sections of non-polarizing neutron guide with lengths of 3 m, 3 m and 1 m can be inserted into the beam path to provide different collimation and source-to-sample distances of 10 m, 7 m, 4 m and 3 m (designated as Number of Guide (NG)=0, 1, 2, 3, respectively). This is the major mechanism to adjust the flux and divergence on the sample. The source defining apertures, 30 mm in diameter, will be mounted at the end of neutron guides in the vacuum boxes and can be inserted as needed. Additional smaller apertures can be provided within reserved positions along the beam path.

After the polarizing supermirror, a magnetic guide field will be presented along the entire beam path to the sample position. We will describe the setup in more details in the next section.

At the end of the variable system, outside the optics box is a translatable high-speed chopper, tentatively a Fermi chopper, for the spectroscopic mode. An evacuated flight tube will extend the beam to the nominal sample position at about 25.46 m from the source.

Larger sample environment devices can be accommodated by slightly offset from the nominal sample position by a small distance upstream. The sample area will be an open walk-in space inside a radiation-shielded cave. It will offer flexibility for smaller and larger sample environments, such as a robotic sample changer, a cryo-magnet, and importantly, for polarization devices such as  $^3\text{He}$  analyzers, Wollaston prisms, etc. While the detector configuration at CENTAUR allows large, continuous solid angle coverage from SANS to WANS (forward scattering detectors) and diffraction (backscattering detectors), large sample environments and polarization device will shift the actual sample position slightly depending on their size and cause shadows restricting some scattering geometries especially the backscattering diffraction, only allowing for SANS/WANS experiments. The Q range for polarization requested by the user community is limited to within  $0.002 - 0.4 \text{ \AA}^{-1}$ , which can readily be achieved with the forward detectors at CENTAUR. For diffraction polarization analysis, another STS instrument VERDI will provide full polarization analysis at larger scattering angles for diffraction for its own scientific missions [9].

For maximum compatibility between the instrument's diffraction and SANS/WANS capabilities, a typical flat SANS sample geometry is recommended. It was used as the primary test sample geometry in the performance estimations. This geometry has influenced the location and geometry of the detectors, especially the location of the backscattering diffraction detectors. However, other geometries can be supported depending on the needs of a given experiment.

The configuration is one of the unique features at CENTAUR. In contrast to a typical SANS instrument in which detectors are located inside a large vacuum detector vessel and move back and forth to collect data at different  $Q$  ranges, CENTAUR will have 4 banks of detectors at fixed positions to provide simultaneously small-, wide-angle and diffraction angle coverage. In the forward direction, detectors at 10.00 m, 3.33 m, and 1.11 m will provide large solid angle coverage. The backscattering detectors will be 1.25 m away from the nominal sample position upstream. The backscattering detectors will be mounted in a movable rack and can be moved to enlarge the sample area, enabling potentially more space for possible polarization setup around the sample position. The backscattering detector geometry is considered instead of, e.g., 90 degree scattering angle detector, due to the compatibility with the typical flat SANS sample geometry. The post-sample scattering path will be under vacuum, provided by a large, segmented but interconnected, evacuated chamber for all forward detectors and an additional chamber for the backscattering detectors. The detectors will be scintillator-Anger cameras with silicon photomultiplier (SiPM) arrays. The physical pixel size of the SiPM will be 6 mm by 6 mm, and the Anger readout method will augment the effective spatial resolution to at least 1 mm by 1 mm [10]. SiPM-based Anger cameras have been demonstrated to be insensitive to magnetic fields. However, with the limited diameter of the polarization analyzer after sample, the higher angle banks will be shadowed and not used in most polarization experiments.

### 3. Basic Polarization Setup

The polarization system at CENTAUR will provide the capability to separate incoherent and coherent nuclear scattering, or magnetic scattering and nuclear scattering. Based on the science drivers, the required  $Q$  range for polarization analysis is  $0.002 \text{ \AA}^{-1}$  to  $0.4 \text{ \AA}^{-1}$  under a magnetic field higher than 1 T. With a typical wavelength bandwidth of  $7.44 \text{ \AA}$  from the 15 Hz source and the beam defining chopper system, e.g.,  $2\text{--}9.44 \text{ \AA}$  or even longer wavelength, the  $Q$  range from the forward detectors (mostly the low-angle and mid-angle banks) can provide more than this  $Q$  coverage (Table 1).

The basic setup will consist of the following major components:

- A neutron V-cavity supermirror polarizer at the entry of the variable optics system box (Figure 2). It will generate a polarized neutron beam before the sample and can interchange with a regular non-polarizing supermirror guide. The cross-section will be 3 by 3 cm. The  $m = 4$  coating will ensure efficient reflection of neutron wavelengths longer than  $2 \text{ \AA}$ . With the length of the supermirror  $\sim 1$  m, the system provides up to 10 m source to sample collimation distance, sufficient to reach  $Q_{\min}$  as low as  $0.001 \text{ \AA}^{-1}$  at the 10-m detector array, like the non-polarization guide sections configuration. The interchangeable system will have high accuracy and repeatability to ensure no realignment is needed during switching of in experiments.
- A magnetic guide field will start after the supermirror throughout the neutron path to maintain neutron polarization. The field will be a minimum of  $1.5 \times 10^{-4}$  Tesla with stacks of permanent magnets between steel plates. The neutron guides and other components along the path will be nonmagnetic to prevent interference with the polarized neutron beam.
- A radio frequency (RF) adiabatic fast passage spin flipper will be installed along the beam flight tube ahead of the sample position (Figure 3(a)). It allows flipping the neutron beam polarization relative to the applied magnetic field at the sample. It encloses the beam flight tube, which allows 3cm x 3cm beam cross-section to go through. We require the flipping efficiency to the opposite direction of the polarized neutron to be higher than 99% for neutron wavelength  $> 2 \text{ \AA}$  with the flipper on. Without the RF signal, the neutron will go through the flight tube without changing its polarization direction.

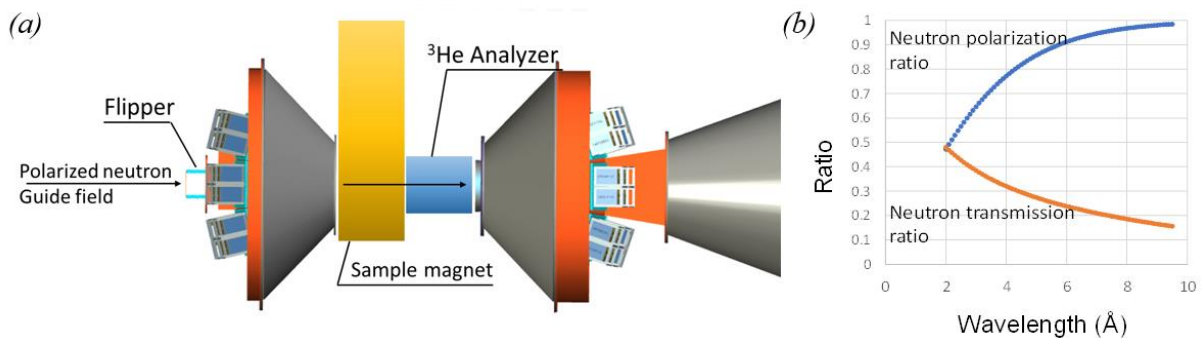
- A  $^3\text{He}$  neutron spin analyzer selects the polarization direction of the neutron beam scattered by the sample between the sample position and the detector vessel (Figure 3(a)). The  $^3\text{He}$  analyzer can also serve as a high efficiency neutron spin flipper such that all four neutron cross sections ( $++$ ,  $+-$ ,  $-+$ ,  $--$ ) can be measured.

**Table 1.** Scattering angle ( $2\theta$ ) and  $Q$  coverage limit with  $^3\text{He}$  analyzer housed in a system including the holding field and magnetic shielding with length of about 50 cm and 15 cm in diameter. The sample position is assumed to be right in front of the  $^3\text{He}$  analyzer system.  $Q_{\min}$  is  $0.0016 \text{ \AA}^{-1}$  at  $9.44 \text{ \AA}$  at  $\text{NG}=0$  guide collimation

	Maximum $2\theta$ (rad)	$Q_{\max}$ with $2 \text{ \AA}$ neutron ( $\text{\AA}^{-1}$ )
$^3\text{He}$ analyzer	0.15	0.47
Low-angle detector bank (at 10 m)	0.063	0.178
Mid-angle detector bank (at 3.33 m)	0.19	0.597

As polarization analysis will be implemented at many of STS instruments [9], [11], [12], we anticipate both ex situ and in-situ  $^3\text{He}$  analyzer systems will be developed and deployed across the facility. An ex situ system can be used for routine short experiments at CENTAUR for its simplicity and practicality [13]. Multiple  $^3\text{He}$  cells with different diameters of up to 15 cm can be prepared outside the instrument for the needed  $^3\text{He}$  polarization and then be moved in before the experiment. Because of the polarization decay, the  $^3\text{He}$  cell may later be swapped to a fresh one as needed to ensure the analyzer's performance. For example, with a 70%  $^3\text{He}$  polarization ratio, the  $^3\text{He}$  cell can be optimized to provide a good balance between the neutron transmission ratio and polarization within the wavelength band (Figure 3(b)). They can be used effectively typically for tens of hours or even days. CENTAUR sample area allows in-situ spin-exchange optical pumping system to be deployed for longer or more sophisticated experiments. Regardless of which system, magnetic shielding will be used to prevent stray field from degrading the decay time constant of  $^3\text{He}$  polarization.

Last but not the least is an instrument data acquisition and integrated control software that can flexibly and conveniently configure and perform experiments with different polarization options. As demonstrated recently, careful considerations will be implemented to ensure the functionality and user experiment [14].



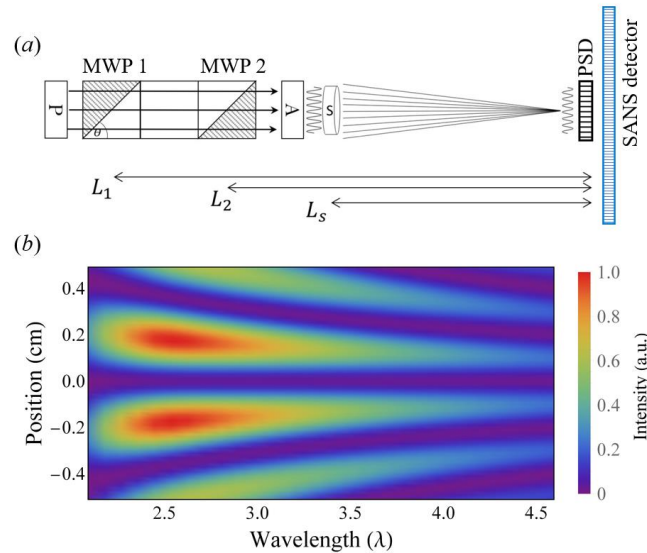
**Figure 3.** (a) The conceptual setup of the polarization system at the sample area, adapted from reference [7]. (b) Estimated neutron transmission ratio and polarization ratio at different wavelengths for a  $^3\text{He}$  cell with a thickness of 5 cm and a pressure of 1 bar with a 70%  $^3\text{He}$  polarization.

#### 4. Spin Echo Modulated SANS Setup

With the polarized neutron capability at CENTAUR, SEMSANS can also be implemented, as shown in Figure 4(a). While more details can be found in references [15]–[17], the fundamental principle of SEMSANS is to use magnetic Wollaston prisms (MWPs) to modulate the neutron beam profile on the

detector [18]. With such intensity modulations, the conventional SANS signal can be encoded via Fourier transform into a change in the amplitude of the modulations. Therefore, the very low Q signal that is contained in the footprint of the direct beam can be used to extend the length scale measurable significantly. To implement this and resolve the modulation, a position sensitive detector (PSD) with high spatial resolution is required, which will be installed in the direct beam position where the beam stop is located. Since the sample is located on the downstream side after the polarization analyzer, SEMSANS can allow us to use the direct beam, which is usually dumped at the beam stop in a conventional SANS instrument, to recover some of the signals that are beyond the length scale resolution limit of conventional SANS. With the additional PSD at the beam stop position only, the Q range of the conventional SANS will not be affected. Therefore, by combining SANS and SEMSANS, the length scale probed can be greatly expanded to tens of microns.

In SEMSANS, scattering signal from the sample will be Fourier transformed from reciprocal space (Q) to real space, the scale of which is termed spin echo length.  $\xi = \lambda L_s / P$ , where  $\lambda$  is the neutron wavelength,  $L_s$  is the distance from the sample to the detector and  $P$  is the period of the intensity modulation on the PSD. With TOF, it would allow us to probe a wide-band length scale in one single measurement, which is unique compared with a constant wavelength neutron source. Moreover, the higher wavelength resolution of TOF source will greatly minimize the aberration in the intensity modulation and therefore benefit the contrast of the modulations.

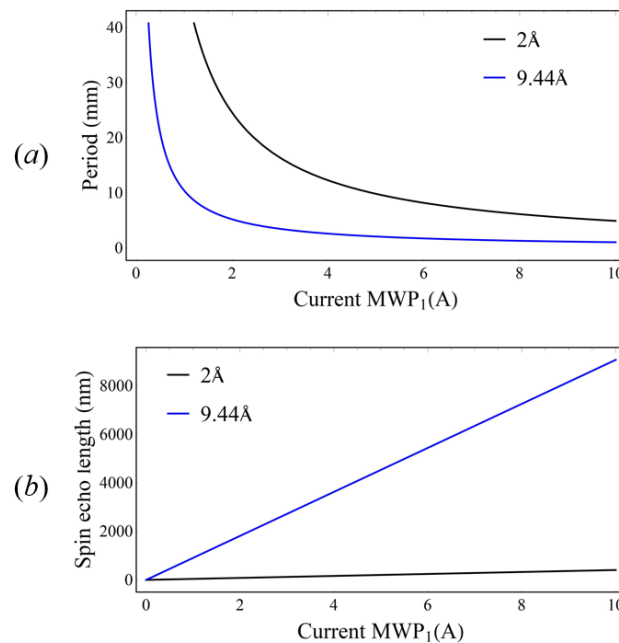


**Figure 4.** (a) the proposed SEMSANS setup combined with a SANS detector and such setup has been realized at the polarized SANS instrument of Larmor at ISIS [16]. The scattering of conventional SANS has been omitted for clarity purposes. The backscattering detector bank of CENTAUR will be designed to be movable to provide the necessary space in the sample area, P: polarizer; A: analyzer; s: sample. (b) the intensity modulation on the PSD, simulated by McStas, at the beam stop position as a function of wavelength at 10A of current applied inside the first MWP.

To access long length scales, it is critical to minimize the period of the intensity modulations. The period of the intensity modulation is calculated and shown in Figure 5(a) for two different neutron wavelengths, e.g., in CENTAUR's typical 15 Hz wavelength band. Correspondingly, the accessible length scale in real space is also calculated and plotted in Figure 5(b). With 10 Å of current inside the first MWP, the smallest period of the intensity modulation is for 9.44 Å is  $\sim 1$  mm.

The proposed detector used for this setup is an Anger camera with an increased spatial resolution. In order to clearly resolve the modulations, a resolution of 0.2 mm or better is needed, or at least 5 data points in each period. This can be achieved using an Anger camera with 3-mm SiPM pixels and a bright

scintillator. With the hardware currently available, this would result in a detector area of 53.2 mm x 53.2 mm with 266 logical pixels. Note that the high spatial resolution is only required along the vertical dimension. A scintillator detector based on a similar principle operates at LARMOR [19], successfully reaching the 0.2 mm resolution in 1 dimension. The proposed Anger camera will also be able to improve on the count rate capability, increasing the throughput of the detector and the ability to measure at the direct beam. The high-resolution Anger camera can be integrated within the central part of regular Anger camera for SEMSANS or as a separated retractable module which translates into the location of the beam stop in front of the 10 m low-angle detector bank. The R&D needed to increase the Anger camera resolution as above is underway. An imaging detector may also be considered to further enhance the rate and spatial resolution performance.



**Figure 5.** (a) the calculated period of the intensity as a function of the current inside the first MWP two different neutron wavelength, (b) the calculated accessible length scale (spin echo length) for various current setting in the first MWP for two different neutron wavelengths.

With the combination of SANS with SEMSANS, the dynamic range of the CENTAUR instrument can be greatly expanded and therefore, it would allow the study of high throughput kinetic processes of the formation of large structures on the nano- and micron scale in a single instrument and the same sample environment setup [16].

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