The HERMES reflectometer at the JULIC Neutron Platform

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Abstract. HERMES is a time-of-flight reflectometer that operated at the Orphée reactor until 2019. In 2022, HERMES was installed at the JULIC (Jülich Light Ion Cyclotron) Neutron Platform as part of a collaboration between the Laboratoire Léon Brillouin and the Jülich Centre for Neutron Science. The main goal of the current setup is to probe the viability of neutron instrumentation at a High Current Compact Accelerator-driven Neutron Source (HiCANS). As the flux at the JULIC neutron platform is several orders of magnitude lower than the original Orphée flux or the expected flux for a HiCANS, our current objective is to perform reflectivity experiments with supermirrors as a proof of concept. Nevertheless, Monte-Carlo simulations showed that the HERMES instrument's performance at a HiCANS such as HBS or ICONE could match that of reflectometry instruments operating at research reactors or spallation sources. An experiment with a supermirror carried out in December 2022 allowed us to preliminary prove the feasibility of this kind of experiments at an accelerator-driven neutron source.

1 Introduction

High current Compact Accelerator-driven Neutron Sources (HiCANS) have risen in recent years as a possible answer to the closure of various research reactors in Europe and the drop in beam time availability for the neutron user's community. This interest was motivated by the previous experience in compact accelerator-driven neutron sources [1, 2]. Several projects in numerous laboratories around Europe [3-6] are currently at different stages of their development and are merged within the European Low Energy accelerator-based Neutron facilities Association (ELENA) [7].

The Laboratoire Léon Brillouin is currently evaluating the use of HiCANS to provide the French neutron scattering community with a suite of world-class instruments. For that purpose, the performances of potential instruments at this novel type of source must be evaluated.

To achieve this goal and through a collaboration with the Jülich Centre for Neutron Science (JCNS), the HERMES reflectometer (see Fig. 1) has been installed at the JULIC neutron platform (JNP) at the JULIC accelerator [8] of the Institute for Nuclear Physics (IKP) Forschungszentrum Jülich.

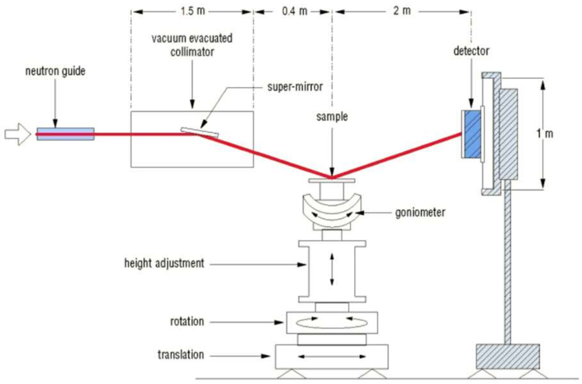

Fig. 1. Scheme of the HERMES reflectometer.

HERMES [9-11] is a time-of-flight horizontal reflectometer designed for soft-matter studies that operated at the Orphée reactor [12] until 2019.

The JULIC Neutron Platform (JNP) shown in Figure 2 is conceived as a technological test platform for the High Brilliance Neutron Source project (HBS) [13].

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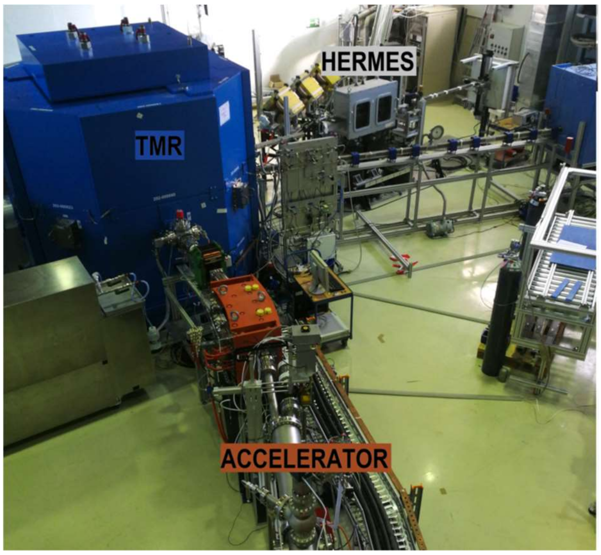

Fig. 2. The JULIC Neutron Platform at the FZJ.

Taking advantage of the JULIC proton cyclotron accelerator at Forschungszentrum Jülich, the Nuclear Physics Institute (IKP) has built a dedicated proton beamline to inject protons into the target-moderator-reflector (TMR) assembly built by JCNS.

Neutrons are generated by the impact of 45 MeV protons on a tantalum target and moderated by a polyethylene block surrounded by a lead reflector. The TMR assembly is embedded in a multilayer shielding with eight extraction channels designed to fit several instruments.

Furthermore, the TMR assembly can accommodate dedicated cold moderators for each channel. The source is able to deliver a cold spectrum with pulses in the 100 µs – 2 s range and is very well suited to evaluate the feasibility of reflectivity experiments at a HiCANS.

Reflectometry measurements are especially suited to evaluate the performances of a HiCANS source: (i) The operation in Time–of–Flight (ToF) mode is very efficient for reflectivity measurement; (ii) Some samples are very reflecting so that it is possible to perform demonstration measurements even with a very low incident flux; (iii) As the instrument is in principle built to measure reflectivity over 6 orders of magnitude in intensity it is very easy to assess the impact of the background noise on the measurements which is a key information which will determine the ultimate performances of instruments around HiCANS.

2 Monte-Carlo simulations

2.1 Neutron Source

Monte-Carlo ray tracing simulations were carried out to evaluate the instrument performance using McStas [14] software. In Table 1, the main parameters for the neutron source are shown for two scenarios. The first one is the projected flux for the High Brilliance Neutron Source (HBS) [4, 15]. The second one is the best-case scenario expected for the JULIC Neutron Platform which is currently only operating at a very low power.

Table 1. Neutron source parameters for HBS and the JULIC neutron platform (JNP) at the maximum projected current.

	HBS	JNP
ν [Hz]	24	50
Duty Cycle	1.6 %	4 %
E_{proton} [MeV]	70	45
$I_{proton,\ peak}$ [mA]	89.3	0.01
$\phi_{0,\ cold}$ (60 K) [n/cm².sr.pulse]	7.4 10^{10}	3.0 10^{6}
$\phi_{0,\ thml}$ (305 K) [n/cm².sr.pulse]	2.3 10^{10}	9.5 10^{5}
$\phi_{0,\ um}$ (UM unmoderated) [n/cm²sr.pulse]	1.6 10^{9}	6.5 10^{4}

The bi-spectral source is modeled with three components (Maxwellian) corresponding to the cold-moderated neutrons (60 K), the thermal-moderated neutrons (305 K), and the under-moderated ones (UM). This last component represents the neutrons that are not properly moderated by the thermal premoderator and the cold moderator. The flux corresponding to each component (cold, thermal, and under-moderated) is detailed in Table 1 and the simulated spectrum is shown in Figure 3.

Both for HBS and JNP, the flux is calculated considering a para-hydrogen cold moderator inserted in the extraction plug dedicated to the instrument.

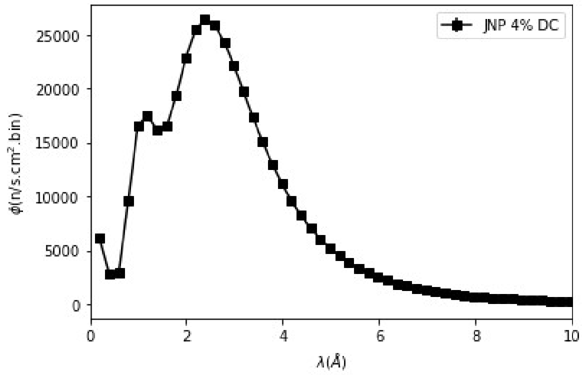

Fig. 3. Simulated source spectra at the JNP at 10 µA and 4 % duty-cycle (bin size: 0.2 Å).

2.2 Guide system

The design of the TMR allowed us to install a dedicated 2.5 m neutron extraction guide for HERMES. Being a horizontal reflectometer, only a minimum beam vertical divergence is useful, and therefore m = 1 coating for the top and bottom mirrors was chosen. Several geometries were analyzed for the lateral walls of the guide including semi-elliptical, trumpet, and straight ones (see Fig. 4). For the lateral walls, a higher m value would increase the total flux on the sample and thus m = 2 was considered for that purpose. Choosing a higher m-value (m > 2) would increase the horizontal divergence of the beam and thus the flux at the guide's exit. Nevertheless,

as HERMES was originally built with m = 2 guides along the instrument, the increase in flux wouldn't necessarily benefit the instrument's performance.
The case of a straight guide with m = 1.2 on all sides was also considered as it matches the current extraction guide configuration at JNP.

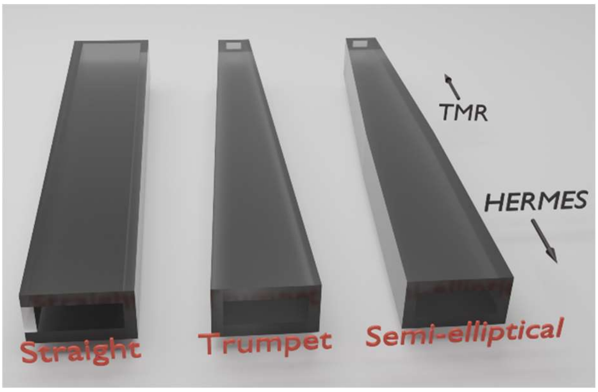

Fig. 4. Scheme of the different guide geometries evaluated to increase HERMES performance.

As it is shown in Table 2, except for the m = 1.2 guide, no major differences are observed for the different guide configurations. Due to the complications and costs associated with complex guide geometries, the choice was to stick to a straight guide.

Table 2. Estimated flux at the sample position for different guide configurations at JNP at 10 μA and 4 % duty-cycle.

Géométrie	ϕ_{sample} [n/s.cm^2]
Straight m = 1.2	2.16 10^3(1)
Straight	3.00 10^3(1)
Trumpet	3.27 10^3(1)
Semi-elliptical	3.40 10^3(1)

2.3 Instrument

A 20 cm gap was left between the end of the guide and the collimator to allow the insertion of a frame-overlap chopper. The HERMES collimator consists of four variable slits with a maximum collimation distance (d_{14}) of 1.5 m. The slits have a 3 cm horizontal opening and, for these simulations, a 2 mm vertical opening was selected corresponding to a vertical divergence of 0.15°.

Two horizontal m = 3.5 supermirrors sit between slits 2, 3 and 4 and can be used to deflect the beam for air-liquid reflectivity experiments. Also, vertical m = 2 supermirrors transport the beam along the collimator to take advantage of the beam's horizontal divergence. A schematic top view of the instrument is shown in Figure 5 including its principal dimensions.

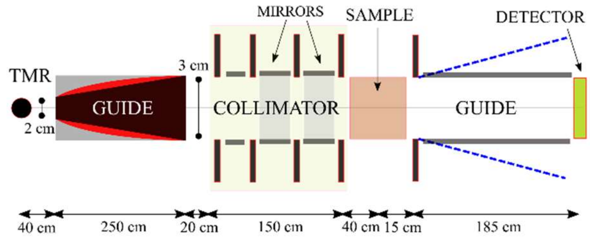

Fig. 5. Top view scheme of HERMES reflectometer at JNP with different guide configurations: straight (grey), trumpet (black) and semi-elliptical (red).

The sample sits at a distance of 40 cm from the last slit. An "anti-background" slit with an adjustable vertical opening is positioned at 15 cm from the center of the sample. Finally, a single He^3 tube detector (P = 10 bar) shielded with B_4C is located at 2 m from the sample position.

The beam reflected by the sample has a rather high horizontal divergence (see blue dashed line in Fig. 5) and thus a large detector would be needed to count all the reflected neutrons. A neutron guide with m = 2 supermirrors on the sides and B_4C on top and bottom is placed between the "anti-background" slit and the detector. This guide allows to harness all the horizontal divergence of the beam with a rather small detector area thus avoiding the background signal due to spurious neutrons arriving at the detector.

2.4 Reflectivity for a 20 nm Ni layer

For these Monte-Carlo simulations, we chose a 10 x 10 cm^2 sample consisting of a Ni layer (20 nm) on Si. Due to ToF resolution limitations with long pulses, a 200 μs pulse length was chosen for these simulations. This implies a duty-cycle of 1% for JNP and 0.48% for HBS.

In Table 3, the estimated flux at the source and at the sample position is presented for the two scenarios.

Table 3. Estimated flux at the source and the sample position for the JNP at 1% duty-cycle and HBS at 0.48% duty-cycle.

Source	ϕ_{source} [n/s.cm^2]	ϕ_{sample} [n/s.cm^2]
JNP	1.01 10^5 (1)	7.60 10^2(1)
HBS	1.42 10^9(1)	1.07 10^7(1)

If higher fluxes are needed, it can be easily increased by at least a factor 4 by just increasing the duty cycle.

In Figure 6, we show the simulated reflectivity curve for the JNP configuration for a θ = 0.8° incident angle.

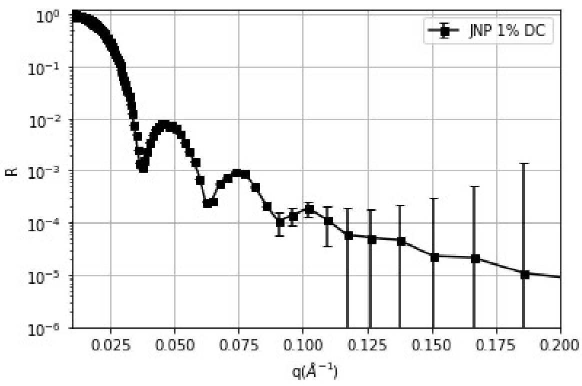

Fig. 6. Simulated reflectivity curve for a 20 nm Ni layer on Si on HERMES at the JULIC neutron platform.

Error bars were estimated assuming a 1 h collecting time. The Kiessig fringes are noticeable below q = 0.1 Å^{-1}, and reflectivities down to 10^{-4} should be measurable provided that the background noise is kept low enough. We can also extrapolate this performance to the HBS flux and, in that case, reflectivities below 10^{-5} should be easily achieved.

2.5 Frame-overlap

Count rate values in McStas are expressed in n/s, but actually, only one single neutron pulse is simulated by the code. If we want to consider the effect of frame-overlap (FO) in the case of the absence of a FO chopper, we need to add manually the frames. In this case, shown in Figure 7, the FO effect is clear for a 50 Hz frequency (20 ms frames).

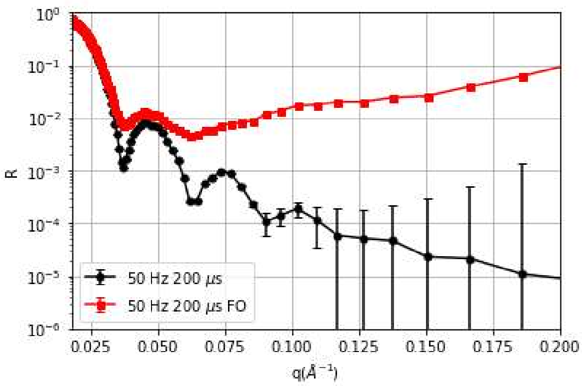

Fig. 7. Simulated reflectivity curve for a 20 nm Ni layer on Si with and without frame-overlap effect.

The effect of the FO entails that only one fringe is clearly observed, thus indicating that the use of a FO chopper or similar device is needed if we want to be able to resolve this kind of structure operating at those frequencies. Another simple solution would be to reduce the operation frequency, at the cost of reduced efficiency.

2.6 Pulse length and resolution

As it was mentioned before, an easy way to increase the flux at the sample position is to increase the proton pulse length. The tradeoff is that the instrument resolution is reduced thus limiting the samples that can be characterized.

In order to evaluate this effect, we simulated different pulse lengths ranging from 200 μs to 800 μs. The wavelength resolution for those pulse lengths is shown in Figure 8.

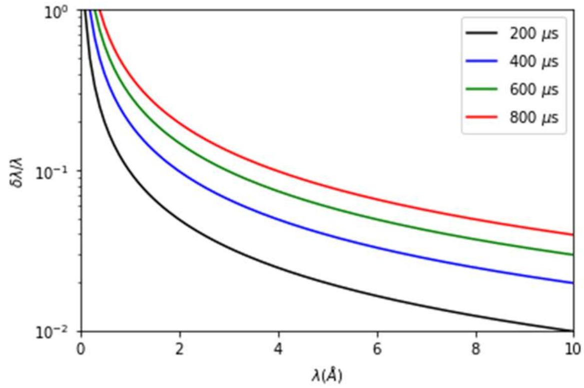

Fig. 8. Wavelength resolution for different pulse lengths.

The simulated reflectivity curves for the extreme cases are shown in Figure 9. For the reference sample (20 nm Ni on Si) and, assuming that there is no background noise or rugosity on the sample that could worsen the reflectivity curve, we are still able to distinguish the Kiessig fringes up to 0.1 Å^{-1} even for long pulses and gain a factor 4 in total flux.

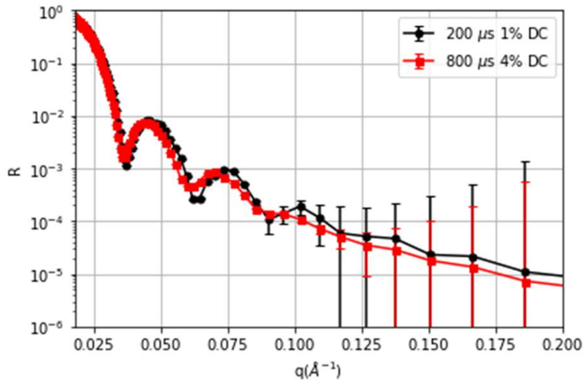

Fig. 9. Simulated reflectivity curve for a 20 nm Ni layer on Si for different proton pulse lengths.

3 First experiments at the JULIC neutron platform

HERMES was installed at the extraction channel 3 of the TMR in December 2022. Due to the lack of a cold moderator at that time, experiments were performed with thermal neutrons. The parameters for the JULIC proton pulse were $I_p \approx 250$ nA, $\tau = 400$ μs, $\nu = 125$ Hz corresponding to a power of 0.6 W on the target. The current neutron guide is an m = 1.2 straight guide with a 2.5 cm x 3 cm section and 2.5 m in length. A 40 x 250 mm^2 m = 4 supermirror provided by SDH was measured for 2.5 hours. The incident angle θ = 0.6º was chosen to match the peak flux with the expected critical edge. The direct and the reflected beam are shown in Figure 10, the high count rate at low ToF is due to the fast neutrons from the prompt pulse being moderated by materials close to the detector.

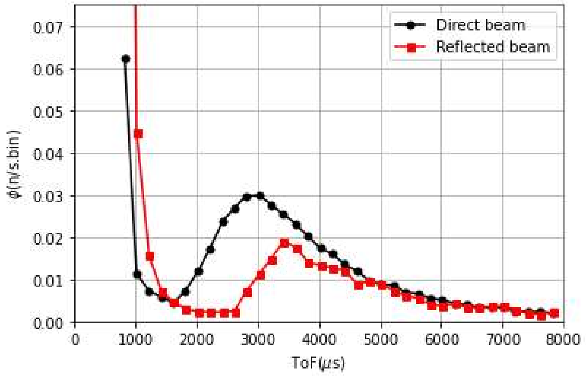

Fig. 10. Direct beam and reflected beam by an m = 4 supermirror measured at HERMES (bin size: 200 µs).

In Figure 11, the measured reflectivity curve along with Monte-Carlo simulations are shown. McStas simulations allowed us to distinguish the frame-overlap component from the contribution of the prompt neutron pulse.

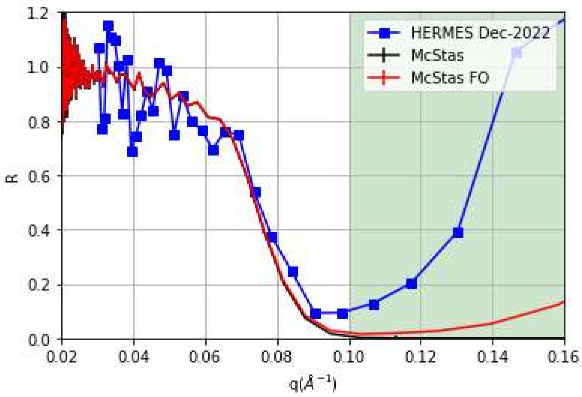

Fig. 11. Measured reflectivity curve for an m = 4 supermirror and McStas simulations.

It can be inferred that, although there is a contribution from the frame-overlap effect, the apparent rise in the reflectivity for $q > 0.1$ Å^{-1} is mainly due to the fast neutrons being moderated close to the detector creating an intense peak for short times. Dealing with background neutrons at HiCANS is one of the most challenging tasks and needs to be accounted for to reach reflectivities below 10^{-5}. For these experiments, the detector's shielding was merely a layer of B_4C that proved to be effective when the instrument was installed at Orphée. This might not be enough for this type of facility and additional shielding is currently being evaluated.

4 Conclusion and prospects

The very first experiments performed with HERMES at the JULIC neutron platform are encouraging. An operation at a power of 0.6 W allowed measuring reflectivities over one order of magnitude in reflectivity. A rough scaling to a power of 100 kW (HBS design) suggests that it should be possible to readily measure reflectivities below 10^{-5}. While these performances would not yet match existing state-of-the-art instruments, the current measurements have been performed in non-optimal conditions.

Several upgrades can be implemented to HERMES to improve its performance and are currently undergoing. The first major upgrade will be the installation of the para-hydrogen cold source, which should provide an increase of at least one order of magnitude in flux and would allow us to use higher reflection angles to avoid the direct beam.

The HERMES shielding was originally optimized for its position at the Orphée reactor in the guide hall, far away from the reactor's core. An improved shielding is currently being designed and built in order to improve the signal-to-noise ratio at JNP to reduce the influence of the prompt neutron pulse.

Although the background component is currently dominating over the frame-overlap effect, the incorporation of a frame-overlap chopper or a frame-overlap mirror to cut higher wavelengths is being evaluated.

Finally, the JULIC accelerator and the TMR are technically capable of significantly increasing the proton current, which would directly increase the neutron flux.

Based on the Monte-Carlo simulations we are confident that an optimized instrument at the JULIC neutron platform should be able to deliver sufficient performances to characterize large surface samples such as neutron mirrors, something that is currently demanded by the industry.

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