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Performance of Reflectometers on Different Moderators and Target Stations of the ESS Project

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We have investigated the performance of a reflectometer on an ambient water and liquid hydrogen moderator with different characteristics (coupled, decoupled poisoned, decoupled unpoisoned) on different target stations, which are currently under discussion for the planned European Spallation Source (ESS): 5 MW short pulse at 50 Hz, 1 MW short pulse at 10 Hz and 5 MW long pulse at 16.67 Hz. The Monte-Carlo simulations performed using the software package VITESS show that the performance of a reflectometer is roughly proportional to the power of the source. Therefore, the coupled cold moderator together with the most powerful target station (5 MW short pulse or 5 MW long pulse) is the best choice for reflectometry. The repetition rate and pulse length are of minor importance.

Keywords: Neutron reflectometry; Pulsed neutron source; Monte-Carlo simulation; Time-of-flight

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INTRODUCTION

In order to provide quantitative data for the proposed design of the European Spallation Source (ESS), a reference instrument suite was chosen for which the performance on three possible target stations should be compared:

(a) 5 MW at 50 Hz repetition rate and short proton beam pulse (1 μs)
(b) 5 MW at 16.67 Hz repetition rate and long proton beam pulse (2 ms)
(c) 1 MW at 10 Hz repetition rate and short proton beam pulse (1 μs).

Additionally, different moderator types to be used are under discussion: coupled, decoupled poisoned, decoupled unpoisoned, all of them either working with ambient water or liquid hydrogen.

In the present paper, we discuss the influence of the different moderators, pulse lengths and source frequencies on the performance of a neutron reflectometer. Performing Monte-Carlo simulations using the software package VITESS [1] yielded quantitative data for the three

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different sources under consideration in order to come to a conclusion as to which kind of moderator and source is best for reflectometry. Starting with a given moderator spectrum, all other components like neutron guides or chopper systems were included in the Monte-Carlo simulations. In order to get real reflectivity data, we not only investigated the incoming intensity of the direct beam but also included a D_2O-surface as a sample. The reflectivity curve of that sample was calculated with the well-known Parratt-formalism [2]. In order to compare the performance of a reflectometer at different sources, we simply calculated the time needed to get the identical reflectivity curve with the same statistics.

BASIC CONSIDERATIONS FOR THE INSTRUMENTAL SET-UP

There are two basic parameters that have to be determined for the design of a reflectometer: the length of the instrument and the useable wavelength band.

The fundamental relation between neutron velocity v, wavelength λ, time of flight T and distance D between source and detector is:

$$v = \frac{D}{T} = \frac{h}{m\lambda}. \tag{1}$$

To a good approximation the resolution r is given by:

$$r = \frac{\Delta\lambda}{\lambda} = \frac{\tau}{T} \tag{2}$$

with the pulse length τ, which is just the uncertainty ΔT of the time of flight T.

If you wish to have a defined resolution, the distance between source and detector should be:

$$D = \frac{Th}{m\lambda} = \frac{h}{m}\frac{\tau}{r\lambda}. \tag{3}$$

For an optimum data acquisition time frame per pulse δT, i.e. $\delta T = 1/f$, the optimum acceptable wavelength band $\delta\lambda_{\mathrm{opt}}$ is given by:

$$\delta\lambda_{\mathrm{opt}} = \frac{h}{mD}(\delta T - \tau) = \frac{h}{mD}\left(\frac{1}{f} - \tau\right). \tag{4}$$

For a wavelength of $\lambda = 3$ Å (for $\tau = 2$ ms) and $\lambda = 2.7$ Å (for $\tau = 0.2$ ms) and a resolution of 3% and 8%, the values according to Eqs. (3) and (4) are listed in Table I. For the case of the 8% resolution, the instrument length was kept at a minimum length of 12 m because of geometrical boundary conditions. From these equations the basic design criteria for a reflectometer at a pulsed neutron source are quite straightforward. Comparing the short

TABLE I Instrument length D and usable wavelength band $\delta\lambda_{\mathrm{opt}}$ for a neutron wavelength of 3 Å (for $\tau = 0.2$ ms) and $\lambda = 2.7$ Å (for $\tau = 0.2$ ms) at a resolution of 3% and 8% respectively, for the three possible ESS target stations

Resolution (%)	τ *(ms)*	*f (Hz)*	*D (m)*	$\delta\lambda_{opt}$ *(Å)*
3	0.25	50.00	12	6.5
3	0.25	10.00	12	32.9
3	2	16.67	88	2.60
8	0.25	50.00	12	6.5
8	0.25	10.00	12	32.9
8	2	16.67	33	7.0

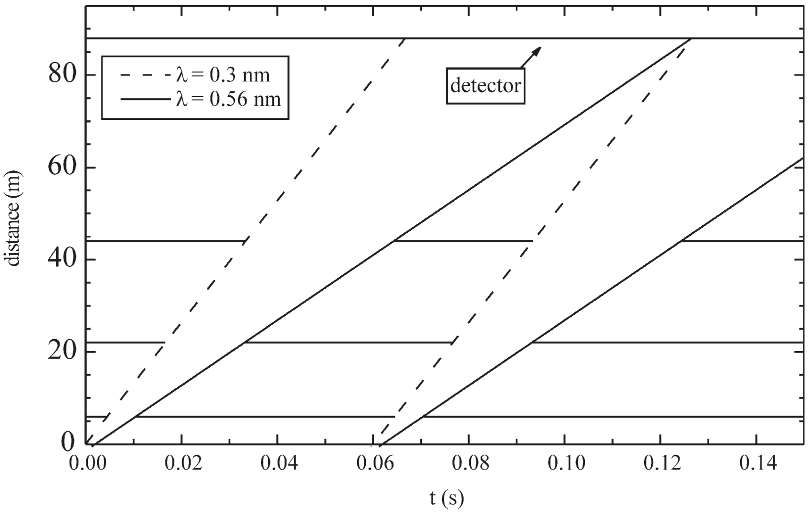

FIGURE 1 Distance–time diagram for a reflectometer at a LPSS.

pulse spallation source (SPSS) and the long pulse spallation source (LPSS), the instrument at the LPSS needs to be much longer to achieve the same wavelength resolution because of the longer pulse width. The reflectometer needs the same instrument length at the 50 and 10 Hz SPSS but the useable wavelength band is approximately inversely proportional to the source frequency, and hence the 10 Hz source has a five times larger useable bandwidth.

The instrumental designs used in the Monte-Carlo simulations for a resolution of 3% are shown in Fig. 1 for a reflectometer at an LPSS (16.67 Hz) and in Fig. 2 for a reflectometer at a SPSS (50 Hz). The SPSS-design corresponds to a typical instrument layout realised for CRISP at ISIS [3] and POSY at IPNS [4], whereas the LPSS-design is close to the one already used for MC-simulations [5]. For the SPSS set-up the time frame definition is realised by putting supermirrors into the neutron beam, whereas for the LPSS set-up a chopper system is

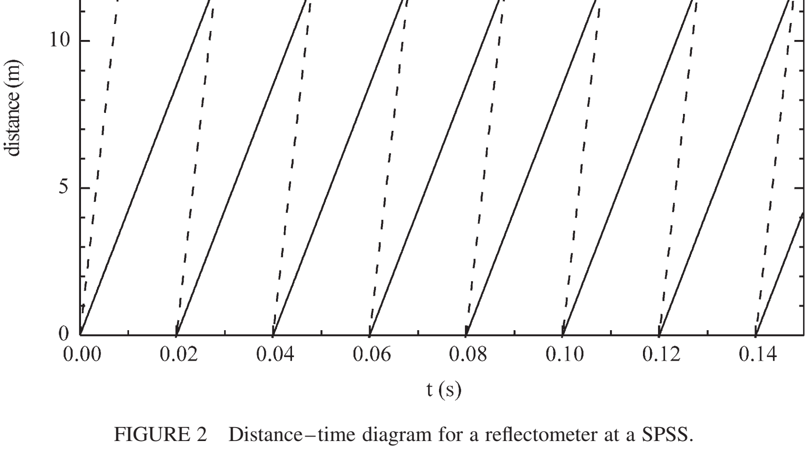

FIGURE 2 Distance–time diagram for a reflectometer at a SPSS.

used. For both instruments we used supermirror guides with $m = 3.5$, starting 2 m from the source and ending just in front of the slit system at a distance of 1 m from the sample position. The moderator had an area of $12 \times 12\,\text{cm}^2$, the neutron guides had a height of 10 cm and a width of 6 cm.

MODERATOR REQUIREMENTS FOR REFLECTOMETRY

For most reflectometry experiments, a medium (3%) or low resolution (8%) in wavelength is adequate. Only the effective width of the pulse but not the exact pulse shape is important. Therefore, the best moderator for neutron reflectometry is the one that delivers the highest flux, i.e. the coupled moderator. A point of discussion is whether an ambient water or a liquid hydrogen moderator is preferable. To answer that question, one has to consider not only the incoming intensity but the reflected intensity as a function of scattering angle θ and scattering vector q:

$$q = \frac{4\pi}{\lambda} \sin\theta. \tag{5}$$

As can be seen in Fig. 3, the reflected intensity R is proportional to the incoming intensity I_0 times the opening of the first slit (or the angular resolution $\Delta\theta$) times the sample footprint, which is proportional to the sample length L times $\sin\theta$. For a fixed q-value, $\sin\theta$ as well as $\Delta\theta$ are proportional to λ. Therefore, we get the following expression for the reflected intensity R_q at a fixed q-value:

$$R_q \propto I_0(\lambda)\Delta\theta \cdot L \sin\theta \propto I_0(\lambda) \cdot \lambda^2. \tag{6}$$

In Fig. 4 the moderator flux multiplied by λ^2 is displayed. Typically a bandwidth larger than 3 Å is used at a spallation source. Hence, the liquid hydrogen coupled moderator is the best for neutron reflectometry as it provides the highest integrated flux.

MONTE-CARLO SIMULATIONS

5 MW at 50 Hz vs. 1 MW at 10 Hz

As discussed above, the source parameters define the usable wavelength band. The lower the source frequency, the larger the useable wavelength band and hence the higher the total intensity. But because of the Maxwellian distribution, only a band of a few Angstroms gives valuable information—the other wavelengths give only a minor contribution to the intensity. Therefore, a scan at three different angles with a narrower wavelength band might be more effective than the data acquisition at a fixed angle of incidence using a large wavelength band. To quantify that consideration, we performed MC-simulations with the software package VITESS [1] comparing a 5 MW SPSS running at 50 Hz with a 1 MW SPSS at 10 Hz. For the 10 Hz target the sample was held at a fixed angle of 2.6°, whereas for the 50 Hz target we took three different angles of incidence: 0.5°, 1°, and 2.6°. In order to compare the flux at the same resolution we

(i) changed the slit size to keep the angular resolution $\Delta\theta/\theta$ constant
(ii) performed a data binning proportional to the inverse of the time of flight or proportional to λ, respectively, to keep the wavelength resolution $\Delta\lambda/\lambda$ constant.

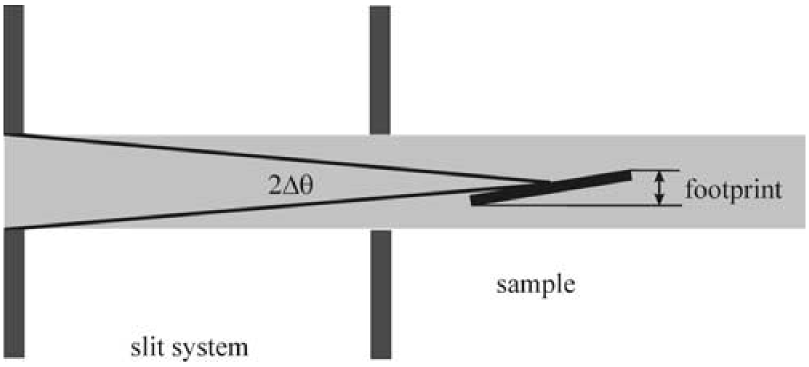

FIGURE 3 Collimation in a reflectometer set-up.

The reflected neutron flux as a function of q for the case of 3% wavelength resolution is shown in Fig. 5, where we assumed total reflectivity for all q-values in order to get the pure reflected neutron flux as a function of q without taking into account any special reflectivity curve of the sample. Figure 5 clearly shows that the 50 Hz source with three angles of incidence can cover the same q-range as the 10 Hz source with a fixed angle of incidence.

Of course, in the end the interesting issue is the performance of a reflectometer at these different sources. Therefore, we took a D_2O-surface as a typical liquid sample, simulated the reflectivity curve by the Parratt-formalism [2] and calculated the time needed to get the same statistics. The slit openings were adjusted for each scattering angle in order to have the same angular resolution at all q-values. For the 10 Hz source it takes a factor of 4.4 longer to acquire the reflectivity curve with the same statistics. The q-dependence of the reflected intensity is displayed in Fig. 6. There is no influence of the resolution on the performance and the SPSS with 5 MW at 50 Hz performs 4.4 times better than the SPSS with 1 MW at 10 Hz.

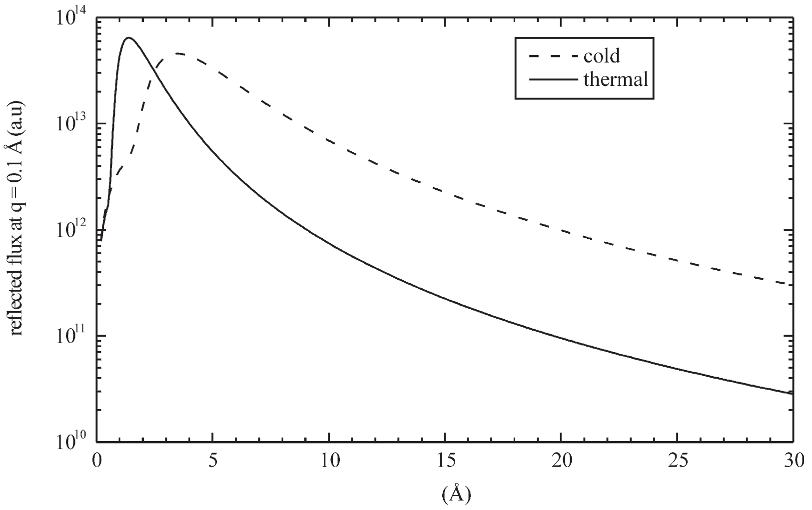

FIGURE 4 Reflected neutron flux at a fixed q-value for a coupled ambient water moderator (solid line) and a coupled liquid hydrogen moderator (dashed line).

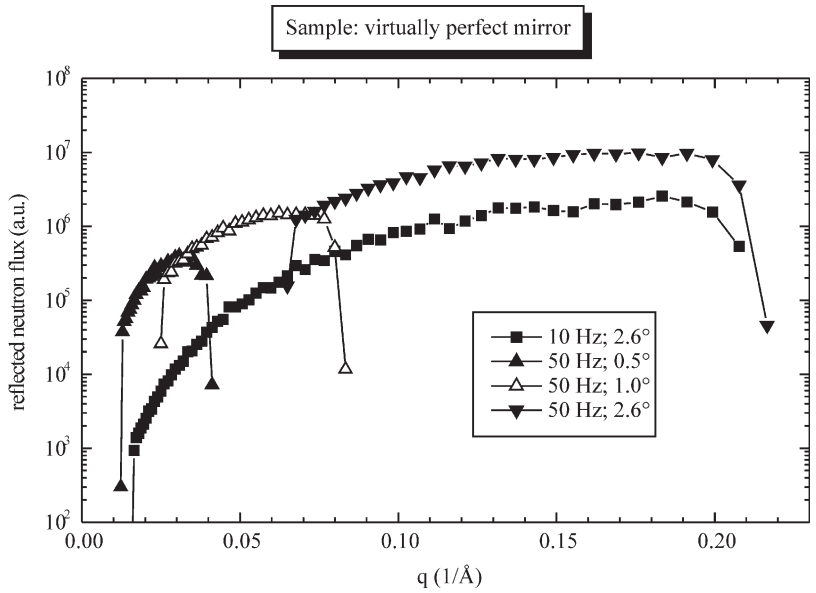

FIGURE 5 Comparison of the reflected neutron flux from a 50 Hz SPSS to 10 Hz SPSS as a function of *q*, assuming a sample with total reflectivity in the whole *q*-range. The simulations were performed with a wavelength resolution of 3%.

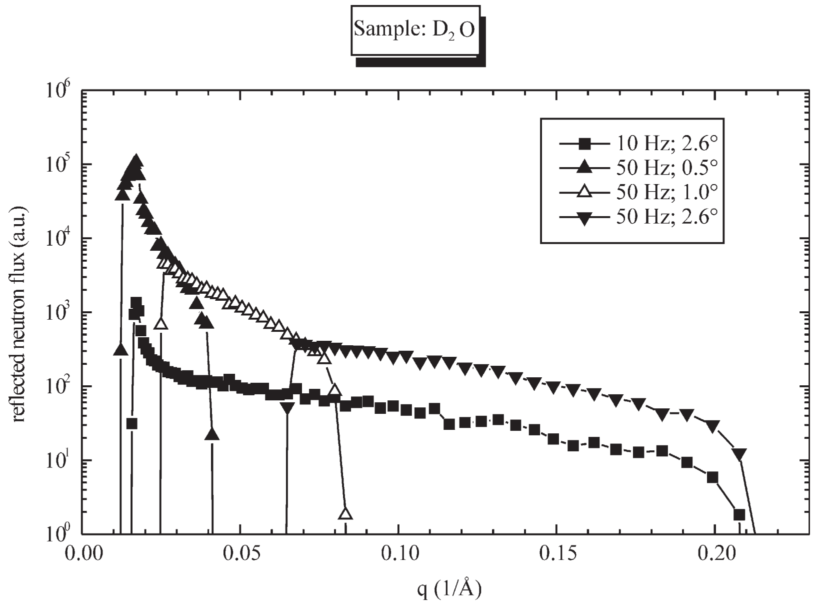

FIGURE 6 Comparison of the reflected neutron flux from a 50 Hz SPSS to 10 Hz SPSS taking into account a D_2O-surface as sample. The simulations were performed with a wavelength resolution of 3%.

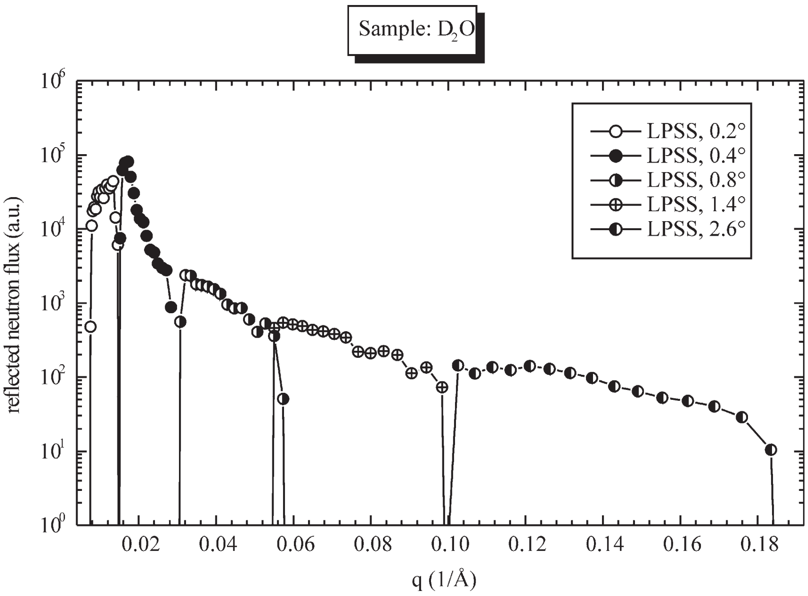

FIGURE 7 Reflected neutron flux from a 16.67 Hz LPSS taking into account a D_2O-surface as sample. The simulations were performed with a wavelength resolution of 3%.

SPSS vs. LPSS

Because of the smaller wavelength band used at the LPSS compared to the SPSS, one needs more angles to measure the whole reflectivity curve. That can be seen in Fig. 7 where the reflected flux for a LPSS instrument with a wavelength resolution of 3% is displayed. Instead of three different angles, one needs five angles of incidence at a LPSS to cover the same *q*-range. The performance depends on the resolution. At a wavelength resolution of 3% the performance ratio of SPSS to LPSS is 2.1, whereas at a resolution of 8% we find a ratio of 1.3. The main reason for the poorer performance at a LPSS is the intensity loss because of the need of longer neutron guides.

CONCLUSION

In the case of neutron reflectometry, the effectiveness of a neutron strongly depends on its wavelength. As shown above, the reflected neutron flux is proportional to the incoming intensity times λ^2. Therefore, the best moderator is the one that delivers the highest possible flux with a peak in the intensity distribution at the largest possible wavelength. So, from the moderators under consideration, the cold coupled moderator is the best for neutron reflectometry.

Concerning the spallation source parameters, the best source would be the one at the lowest possible frequency (delivering the largest possible wavelength band) and at the same time at the largest possible power. But, as the power per pulse is limited, one has to make a compromise on the power and the bandwidth, respectively. From our Monte-Carlo simulations it is clear that the larger bandwidth is of minor importance. The performance roughly scales with the power of the source, as already stated by Mike Fitzsimmons [6].

Therefore, a neutron reflectometer performs best at the 5 MW 50 Hz SPSS followed by the 5 MW 16.67 Hz LPSS. Because of the low power, the 1 MW 10 Hz SPSS shows the worst performance of the neutron sources under consideration for the ESS.

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