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MC simulations of reflectometers at reactor and spallation sources

K. Lieutenant*, **H. Fritzsche**, **F. Mezei**

Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany

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Abstract. We simulated spectra of reflectometers installed on pulsed sources as they are planned for the ESS (5 MW, 50 Hz short pulse, 1 MW, 10 Hz short pulse, and 5 MW, 16.67 Hz long pulse); for each of the sources a coupled moderator was used. For comparison of spallation and reactor sources, we simulated an instrument with equivalent parameters installed on a reactor source with a neutron flux of the ILL. For comparability of the data, constant wavelength and angular resolutions (of 3% and 8% were used for all instruments. The intensity at the detector was determined as a function of the momentum transfer for a virtual sample of total reflectivity and for deuterated water. Finally, it was calculated how long it takes for each source to measure the entire spectrum with a given statistical accuracy. Best results were obtained at the 50 Hz short-pulse source and the long-pulse source, while the 10 Hz short-pulse source performed worse. The measuring time calculated for the reactor source was the longest.

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The first task of the ESS instrument task group was to choose 2 of the 3 target stations suggested for the ESS: 1) short pulse spallation source (SPSS) 50 Hz, 5 MW, 2) SPSS 10 Hz, 1 MW, 3) long pulse spallation source (LPSS) 16.67 Hz, 5 MW. For all target stations, three types of moderators can be used: a) decoupled poisoned moderator, b) decoupled unpoisoned moderator, c) coupled moderator. Our aim was to decide, which combination of target station and moderator is best suited for reflectometry measurements and which wavelength band should be used in each case. This was tested for a reflectometer of low resolution (8% in wavelength and in angular distribution) and for one of medium resolution (3%). We tried to find ideal instruments for each source and resolution before comparing the results. The results were also compared to those, actually reachable at reactor sources. A range in momentum transfer q from 0.01 Å^{-1} to 0.25 Å^{-1} was examined.

1 Analytical considerations

As reflectometry does not need a high time or wavelength resolution, but a large reflected intensity I_R to measure small reflectivity values, the preferable moderator is the coupled moderator. For small reflection angles θ, I_R is proportional to the moderator flux j_0 times the sample footprint $A\cdot\sin\theta$ times the angular resolution $\sin\Delta\theta$. With

$$q = 4\pi\cdot\sin\theta/\lambda \tag{1}$$

one gets the wavelength dependence of I_R:

$$I_\mathrm{R}(\lambda) \propto j_0(\lambda)\sin\Delta\theta\cdot\sin\theta \propto j_0(\lambda)\sin^2\theta \propto j_0(\lambda)\lambda^2 . \tag{2}$$

Comparing an ambient water and a liquid hydrogen moderator, a higher integrated value of the reflected intensity is found for the liquid hydrogen moderator [1]. This moderator is therefore used in these simulations. For each instrument a wavelength band providing a maximal integrated value of $j_0(\lambda)\cdot\lambda^2$ was chosen. The wavelength bands are summarized in Table 1.

The uncertainty in θ is given by the widths of the slits and the footprint of the sample (cf. [1]). For a reactor source, $\Delta\lambda/\lambda$ is directly determined by the velocity selector. For a pulsed source, the wavelength is calculated from the time-of-flight t. Therefore, the uncertainty in λ is a consequence of

Table 1. Data of the simulated instruments for $r = 3\%$ (*upper part*) and $r = 8\%$ (*lower part*)

Source	λ/Å	t_p/ms	D/m	eval. time/ms
Reactor	4.59–4.73		15	
SPSS 10	2.7–35.7	0.25	12	8.19–106.19
SPSS 50	2.7– 9.3	0.2	12	8.19–26.19
LPSS 16.7	3.0– 5.7	2.0	88	69.23–125.23
Reactor	4.47–4.85		15	
SPSS 10	1.0–34.0	0.25	12	3.03–101.03
SPSS 50	2.0– 8.6	0.25	12	6.07–24.07
LPSS 16.7	2.5– 8.4	2.0	40	27.78–83.78

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*Corresponding author.
(Fax: +49-30/8062-2523, E-mail: lieutenant@hmi.de)

the pulse length t_p (and other effects having influence on the time of flight).

$$r_\lambda = \frac{\Delta\lambda}{\lambda} = \frac{\Delta t}{t} \approx \frac{t_p}{D/v_n} = \frac{t_p\, h}{D\, m_n\, \lambda}\,. \tag{3}$$

D: flight path = instrument length, v_n: neutron velocity
To get at least a resolution r_λ, the minimal wavelength has to be used. We estimated $t_p = 0.25$ ms for the SPSS and $t_p = 2$ ms for the LPSS (cf. [1, 2]). The instrument lengths can then be calculated from (3) (see Table 1). For the 50 Hz short pulse instrument with a resolution of 8%, the ideal total length is 6.2 m. But it is not possible to build such an instrument at the ESS because of the 6 m of shielding. We therefore used the 12 m instrument for this case as well, knowing that the real resolution (in wavelength) is about 4% and not 8%. With increasing instrument length the usable wavelength range decreases, because frame overlap must be avoided. (The slowest neutrons that can be considered must arrive before the fastest of the subsequent pulse.)

For negligible pulse length:

$$\Delta\lambda_{\max} = (hT)/(m_n\, D) = 3.956\ \text{Å} \cdot (T\,[\text{ms}])/(D\,[\text{m}])\,, \tag{4}$$

$T = 1/f$: time between two pulses.

2 MC simulations

To find out, which of the 3 target stations yields the best results, we performed Monte Carlo simulations of similar reflectometers at these sources. Additionally, an instrument with equivalent parameters installed on a reactor source was simulated. The neutron flux was that of the ILL (data taken from [2]).

The main instrument data are summarized in Table 1. The slit system, the sample position and the detector were identical for all instruments. The distances: 1. slit – 2. slit – sample – detector were 94 cm, 32 cm, 200 cm. (The sizes were taken from the V6 instrument at the HMI.) For the reactor source we used a velocity selector with a mean wavelength of 4.66 Å. The instruments at the short pulse sources work with wavelength filters using supermirrors as for instance CRISP at ISIS [3]. This monochromating system is not directly simulated; long wavelengths are cut in the 'source' module, short wavelength are cut by the choice of the evaluation time. For the LPSS reflectometers, a chopper system consisting of 3 single disc choppers with one opening rotating with the frequency of the pulse repetitions was chosen. For both instruments, a wavelength band chopper of 180° half way between source and detector was used. This is similar to earlier MC simulations [4].

The moderator had a size of $12 \times 12\,\text{cm}^2$ (as planned for the ESS). The preliminary moderator characteristics published inside the instrumentation task group were used [2]. For all instruments we used guides with a supermirror coating (m= 3.5) from 2 m behind the source to the first slit. The opening of the second slit is wide enough that angular resolution is determined by the opening of the first slit and the footprint of the sample. The first slit is adjusted for each simulation.

As samples we used a virtual sample of reflectivity $R = 1$ and D_2O. The reflectivity of D_2O was calculated with the well-known Parratt formalism [5]. The samples had a width of 4.5 cm and a length of 2.5 cm. More details are given elsewhere [1]. The simulations were performed with the VITESS software package [6].

3 Data evaluation

The intensities are compared in a plot intensity as a function of momentum transfer. As we used 180° choppers half way between source and detector, we got an overlap region, where neutrons of two successive pulses arrive. The neutron current in this time interval was not considered in the data evaluation. The time interval that cannot be used is thought to be 2 ms for the short pulse source and 4 ms for the long pulse source. The beginning of the time is calculated as the time of flight for the shortest wavelength that shall be considered. The times of evaluation are summarized in Table 1. To compare the results of the different sources, we calculated how much time it takes to measure the whole spectrum. Each single measurement is carried out for a time, necessary to get a minimal number of 10 000 counts for each measuring point. These times are summed up for all measurements necessary to cover the q range considered. This was done for D_2O as a typical sample (cf. Table 2).

4 Results and discussion

The results of the simulations of the low resolution instrument (8%) with the ideal sample of reflectivity 1 can be seen in Fig. 1. With the 10 Hz short pulse target station, a large q-range can be covered in a single measurement, but the intensities are much lower than those of the other pulsed sources, especially for low q-values. This is due to the low intensities of long wavelength neutrons. To cover the same q-range, 3 measurements are necessary using the 50 Hz short pulse target station and 4 to 5 measurements using the 16.67 Hz long pulse target station. But the intensities are a factor of 5 to 100 higher than those of the 10 Hz source. Comparing the 50 Hz

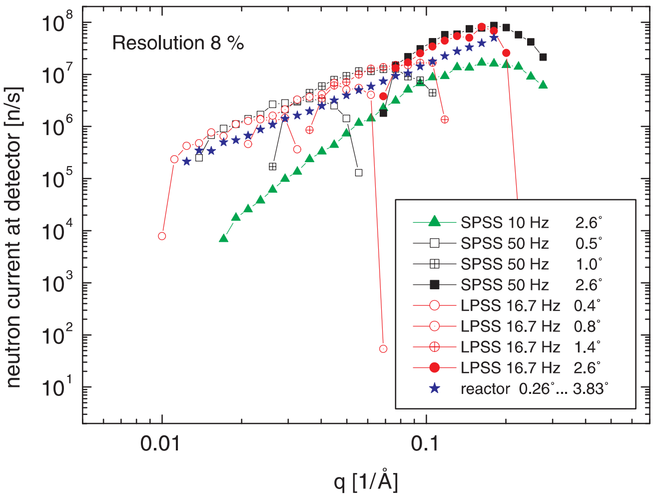

Fig. 1. Reflected neutron current from different sources as a function of q at instruments of resolution 8%, assuming a sample with total reflectivity in the whole q-range

Source	$r = 3\%$	$r = 8\%$
Reactor (ILL)	3700 s	160 s
SPSS 10 Hz	710 s	110 s
SPSS 50 Hz	170 s	25 s
LPSS 16.7 Hz	370 s	32 s

Table 2. Total times of measurements for a minimum of 10 000 counts per point ($q = 0.016\text{–}0.169$ Å^{-1} (3%), $q = 0.017\text{–}0.180$ Å^{-1} (8%))

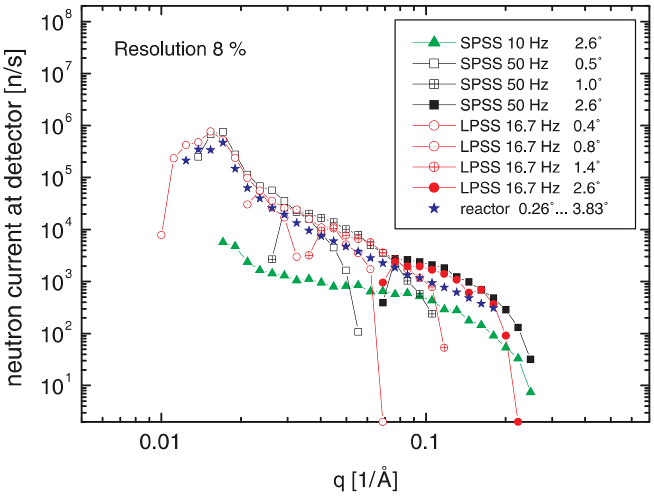

Fig. 2. Reflected neutron current from different sources as a function of q at instruments of resolution 8% after reflection at a D_2O-surface

SPSS and 16.67 Hz LPSS, one finds a little bit lower intensities for the long pulse source. This is mainly due to the losses inside of the longer guide system.

The simulation with the D_2O-sample yielded similar results (see Fig. 2). To compare the results of these simulations quantitatively, we calculated the measuring times for the whole spectrum as described above (see Table 2). This comparison shows that the additional measurements of the 50 Hz SPSS and 16.67 Hz LPSS (compared to the 10 Hz SPSS) are not a big disadvantage, because the reflectivity in the low-q-range is high and the measurements therefore do not need much time. The ratio of the times for all measurements is roughly 4 : 1 : 1.3 for 10 Hz SPSS : 50 Hz SPSS : 16.67 Hz LPSS. We expect improvements by using ballistic guides, especially for the LPSS, so that the difference between 50 Hz SPSS and LPSS may vanish. This will be tested in the near future.

The results of the simulations of the medium resolution instrument (3%) are very similar to those of the low resolution instrument. The only difference is that the intensities of the LPSS are significantly less than those of the 50 Hz SPSS. The reason is the long LPSS instrument (total length of 88 m). The same is found for the D_2O sample. The total measuring times have ratios of about 4 : 1 : 2 in this case (cf. Table 2, [1]).

The ratio between intensities of a reactor and a pulsed source depends on the q-binning. Here we have chosen a binning that directly corresponds to the examined resolution. The ratio of two neighboring q-values is 1+ total resolution. In this case, the intensities of the reactor source are higher than those of the 10 Hz SPSS and lower than those of the other pulsed sources. However, a total number of 63 measurements for the medium resolution instrument and 27 measurements for the low resolution instrument are necessary to cover the simultaneously recorded q-range of the single 10 Hz measurement. The time to measure the whole spectrum with 10 000 neutrons per measuring point is calculated again for the D_2O-sample to get a realistic comparison.. In the low resolution case, the time is a factor of 1.5 to 6.4 higher than that of the pulsed sources, in the medium resolution case a factor of 5.2 to 22 (cf. Table 2).

The results show that all pulsed sources under discussion yield much better results than the best reactor sources existing today, especially for measurements of higher resolution. For these measurements the 50 Hz SPSS is the best choice, whereas for low resolution reflectometers the 50 Hz SPSS and the 16.67 Hz LPSS provide the best results. The 10 Hz SPSS is the worst pulsed source under discussion for both resolutions examined, because the power of the source is too low.

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