Reflectometry instruments

H. Fritzsche[1], C. Fermon[2]

[1]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany
[2]Laboratoire Léon Brillouin, C. E. A. Saclay, 91191 Gif sur Yvette, France

We investigated the performance of a reflectometer for non-magnetic samples in a q-range from 0.01 to 0.5 Å^{-1} at a reactor source and a spallation source for a set of wavelength resolutions ranging from 1% to 8%. We considered an ambient water and liquid hydrogen moderator with different characteristics (coupled, decoupled poisoned, decoupled unpoisoned) at the three different target stations, which are currently under discussion for the planned ESS. The performed simulations 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 (5MW short pulse or 5MW long pulse) is the best choice for reflectometry. The 50Hz short pulse spallation source (SPSS) is the first choice for high resolution and the 16.6Hz long pulse spallation source (LPSS) is the first choice for high intensity. The performance gain is about 100 compared to a reflectometer at ISIS. This is due to the higher power (factor 33) and the usage of a coupled moderator (at least a factor of 3) and about a factor of 15 compared to ILL for high intensity.

In order to have optimized parameters for all reflectometry experiments we recommend to build two reflectometers: a high-resolution reflectometer at the 50Hz SPSS and a high-intensity reflectometer at the LPSS.

Basic instrument design criteria

The reflectometer is designed to measure small angle reflectivities down to 10^{-8} in a q-range up to 0.5 Å^{-1} for solid and liquid samples.

reflectivities down to 10^{-8}

q-range up to 0.5 Å^{-1}

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

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

$$v = \frac{D}{T} = \frac{h}{m\,l} \qquad (1).$$

The resolution r is defined as:

$$r = \frac{\Delta l}{l} = \frac{t}{T} \qquad (2)$$

with the pulse length t, which is just the uncertainty DT of the time of flight T.

If one wants to have a definite resolution, the distance between source and detector should be:

$$D=\frac{T h}{m l}=\frac{t h}{r m l}=\frac{h}{m}\frac{t}{r l} \qquad (3)$$

length of instrument is proportional to the pulse length and inversely proportional to the wanted resolution

For an optimum data acquisition time *dT*, i.e. *dT=1/f*, the optimum acceptable wavelength band $\delta\lambda_{opt}$ is given by:

$$d l_{opt} = \frac{h}{m D}\left(dT - t\right) = \frac{h}{mD}\left(\frac{1}{f} - t\right) \qquad (4)\ .$$

For a wavelength of λ = 3 Å and a resolution of 3% an instrument length of 88 m is needed for the LPSS, whereas 12m are enough at the SPSS. The usable wavelength band is 2.6 Å for the LPSS, 6.5 Å for the 50Hz SPSS and 33 Å for the 10Hz SPSS. From equations (3) and (4) the basic design criteria for a reflectometer at a pulsed neutron source are quite obvious. Comparing the short 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 at the 50Hz and 10Hz SPSS needs the same length of the instrument but the usable wavelength band is inversely proportional to the source frequency and hence, the 10Hz source has a five times larger usable bandwidth. For the SPSS setup the frame definition is realized by putting supermirrors into the neutron beam, whereas for the LPSS setup a chopper system is used.

usable wavelength band is inversely proportional to repetition rate and pulse length

Moderator assessment

As can be concluded from the above section only the pulse width but not the exact pulse shape is important. Therefore the best moderator for neutron reflectometry is the one which 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:

$$q = \frac{4p}{l}\sin q\ . \qquad (5)$$

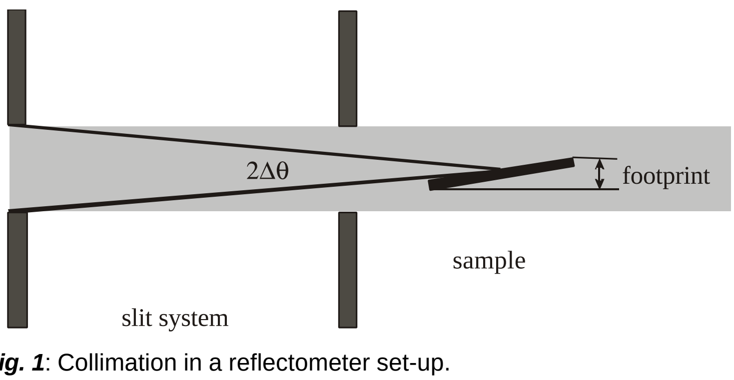

Fig. 1: Collimation in a reflectometer set-up.

As can be seen in Fig. 1 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:

$$R_q \propto I_0(l)\Delta q \cdot L\sin q \propto I_0(l)\cdot l^2 \qquad (6)\ .$$

reflected intensity is proportional to l^2

In Fig. 2 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.

coupled cold moderator is best for reflectometry

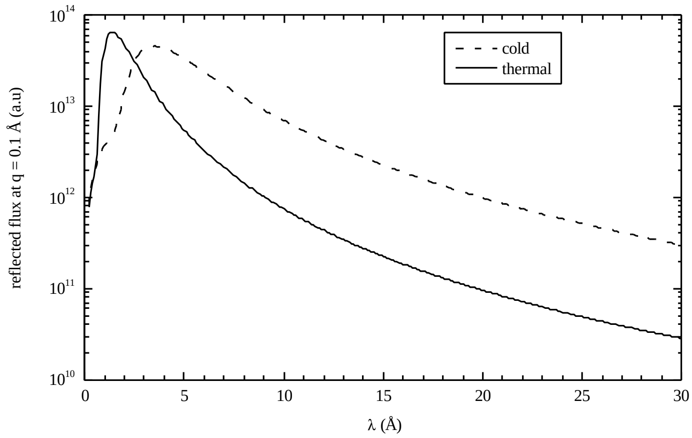

Fig. 2:: Reflected neutron flux at a fixed q-value for a coupled ambient water moderator (solid line) and a coupled liquid hydrogen moderator (dashed line)

Assessment of target stations

a) 5MW at 50Hz versus 1MW at 10Hz

As discussed above the source parameters define the usable wavelength band. The lower the source frequency the larger the usable wavelength band and hence, the larger the total intensity. But because of the Maxwellian distribution only a band of few Angstroms give valuable information – the other wavelengths give only a minor contribution to the intensity. Therefore a scan at three different angles with a shorter 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 5MW SPSS running at 50Hz with a 1MW SPSS at 10Hz. For the 10Hz target the sample was held at a fixed angle of 2.6°, whereas for the 50Hz 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.

Fig. 3 shows the reflected neutron flux from a D_2O-surface. The reflectivity curve was simulated using the Parratt-formalism [2]. It can be clearly seen that the 50Hz source with three angles of incidence can cover the same q-range as the 10Hz source with a fixed angle of incidence. To calculate the performance we calculated the time which is 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 10Hz 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. 3. There is no influence of the resolution on the performance and the SPSS with 5MW at 50Hz performs 4.4 times better than a SPSS with 1MW at 10Hz.

a 5MW source at 50Hz performs 4.4 times better than a 1MW source at 10Hz

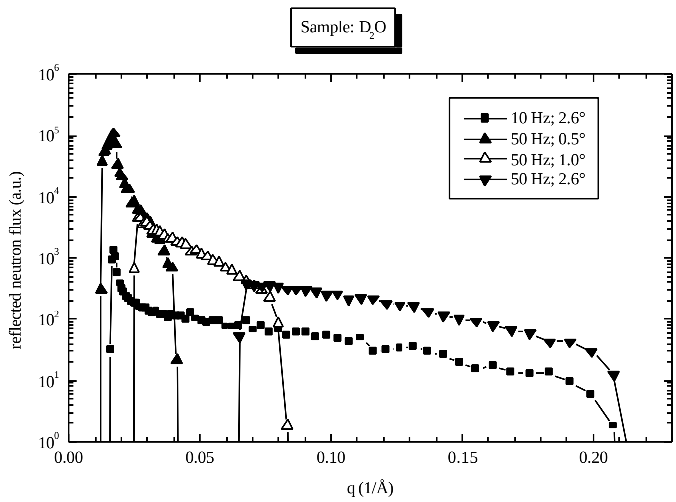

Fig. 3: Comparison of the reflected neutron flux from a 50 Hz SPSS and 10 Hz SPSS taking into account a D_2O-surface as sample.

b) SPSS versus 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. 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. The SPSS performs better for high resolution whereas a LPSS performs better for high intensity or low resolution, respectively.

The simulations performed by C. Fermon are in reasonable agreement with the VITESS-simulations.

high resolution:
SPSS performs better.

low resolution:
LPSS performs better.

a 5MW LPSS or a 5MW SPSS at 50Hz performs always better than a 1MW SPSS at 10Hz.

The conclusion is that the performance of a reflectometer is roughly proportional to the moderator brightness as already stated in a detailed study of M. Fitzsimmons [3]. The estimated gain factors are listed in the instrument performance sheet. In order to have the best performance for high and low resolution we recommend to build a high-**resolution** reflectometer at the 50Hz SPSS and a high-**intensity** reflectometer at the 16.6Hz LPSS.

Comparison to existing sources

A reflectometer at a 5MW 50Hz ESS-target station at the coupled cold moderator would perform about a factor of > 100 better than the same reflectometer at ISIS. The flux gain because of the higher power is 33 and the flux gain because of the coupled moderator is at least 3. Simulation results show a factor 10-20 source intensity gain for the 5MW stations compared to ILL, somewhat depending on wavelength resolution.

the source performance gain compared to ISIS is about 100

Technical issues

For both kinds of samples (solid and liquid) there is a need for an optimized reflectometer operating at high intensity as well as high resolution. Therefore, we recommend to build one reflectometer at the SPSS at 50Hz (high resolution) and one reflectometer at the LPSS (high intensity). Both reflectometers should provide polarized neutrons, either to investigate magnetic properties or to reduce the incoherent background of organic samples.

high resolution reflectometer at the 50Hz SPSS

high intensity reflectometer at the LPSS

both reflectometers with a polarized neutron option

As shown in the simulations experiments on liquid samples can gain a lot in performance when using different angles of incidence instead of using a broad wavelength band. The problems of calibration can be overcome as demonstrated e.g. at IPNS. A nice idea was presented for the new liquids reflectometer at SNS to realize the different angles of incidence by benefiting from the divergence of the neutron guide.

The 10Hz repetition offers the largest q range at a single angle of incidence, together with good wavelength resolution. This is advantageous for kinetic experiments. The same q range can be achieved at the 50Hz by using several angles of incidence. For kinetic experiments a fast switching between different angles (within a small fraction of a sec) needs to be realized.

References

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