ESS Instrumentation Task Group, Reflectometry

Helmut Fritzsche, HMI
John Webster, ISIS
Claude Fermon, LLB

General considerations about reflectometry at a pulsed source

1 The moderator

1.1 Which moderator is the best for reflectometry?

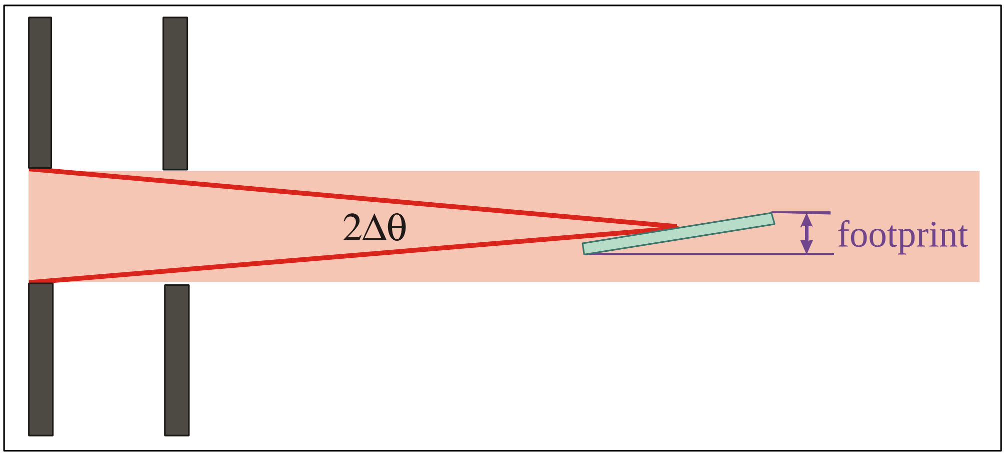
Comparing the different moderator types under consideration, namely poisoned, decoupled, and coupled, it is obvious that the coupled moderator delivers the largest intensity. Therefore, we strongly recommend the coupled moderator for neutron reflectometry.

1.2 Which wavelength is the best for reflectometry?

After having chosen the coupled moderator we have to discuss whether cold or thermal neutrons are better for reflectometry. To answer that question not simply the incoming flux *I* from the moderator has to be compared but the reflected intensity *R* at a fixed *q*-value, where *q* is the scattering vector:

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

with the neutron wavelength λ and the angle of incidence θ.



The reflected intensity *R* is proportional to the sample footprint ($R \propto IL\sin q$) and the angular resolution($R \propto \Delta q$) which is also proportional to θ for a fixed resolution Δθ/θ. As θ is proportional to λ for a fixed *q*-value we find for the reflected intensity:

$$R \propto Il^2$$

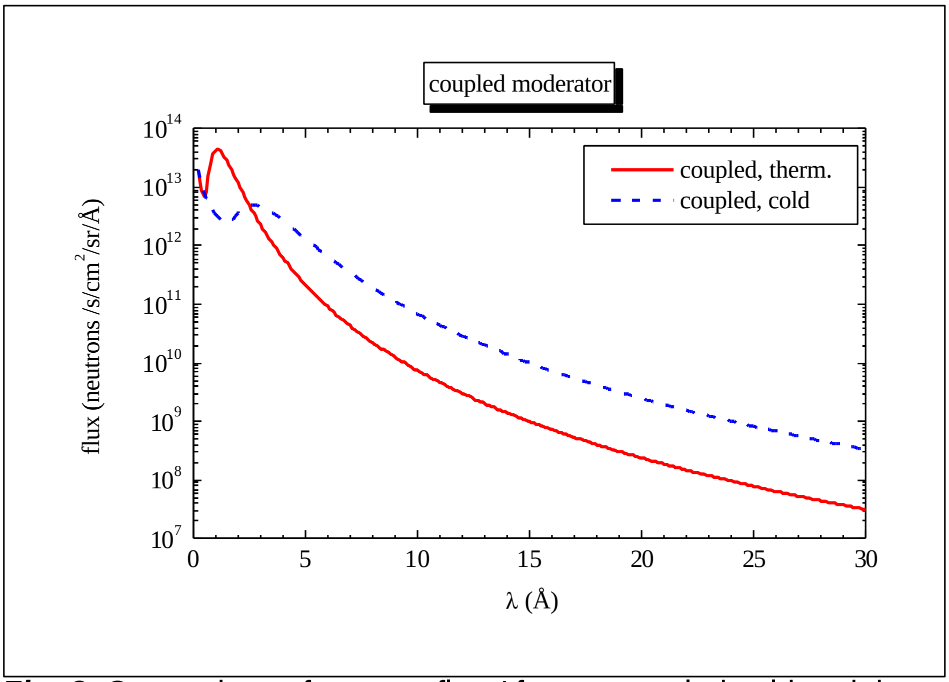


Fig. 2: Comparison of neutron flux *I* from a coupled cold and thermal moderator.

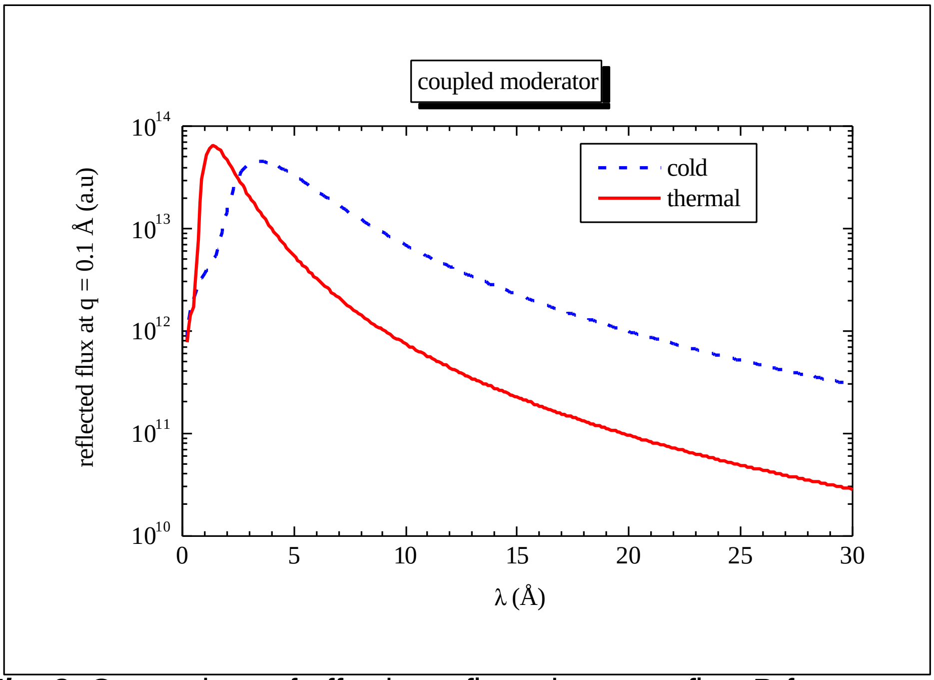


Fig. 3: Comparison of effective reflected neutron flux *R* for a coupled cold and thermal moderator

1.3 Discussion

Fig. 3 clearly shows that at a pulsed neutron source where a large wavelength band is used the coupled cold moderator delivers the largest effective neutron flux for reflectometry. In Fig. 3 only the flux from the moderator is considered. The performance at the cold moderator becomes even better when taking into account the neutron guides which favor the transport of neutrons with longer wavelength.
Therefore we recommend to build the reflectometer at a ***cold*** neutron source with a ***coupled moderator.***

2 Source frequency and pulse length

2.1 Influence of sample type

For reflectometry we can divide the samples in two groups: liquids and solid samples. To measure at different q-values solid samples can be rotated keeping the incoming beam constant Of course, the liquids cannot be rotated. Therefore, at a reactor the monochromator has to be tilted. At a pulsed source, a broad wavelength band can be used with a fixed angle of incidence. For the new liquids-reflectometer to be built at SNS a system consisting of a beam channel bender system together with a tapered guide will be realized. With that system a range from 0° to 8° can be achieved for the angle of incidence. Hence, liquids and solid samples can be treated in the same way with respect to the simulations in order to find the source parameters with which the reflectometer performs best.

2.2 Instrumental set-up

There are two parameters which have to be determined: the length of the instrument and the usable wavelength band. The length of the instrument depends on the moderator time constant, τ, the resolution r, and the wavelength λ:

$$D=\frac{t\,h}{r\,m\,l}=3956\frac{t}{r\,l}$$ (τ in s, λ in Å, D in m).

The optimum wavelength band is given by:

$$d\,l_{opt}=\frac{r\,l}{f\,t}.$$

For the three ESS sources under discussion (SPSS 50 Hz, SPSS 10 Hz, LPSS 16.6 Hz) we get the following parameters:

l (Å)	t (ms)	f (Hz)	r	D (m)	dl_{opt} (Å)
3	0.25	50.00	0.03	11	6.6
3	0.25	10.00	0.03	11	33
3	2	16.66	0.03	88	2.70

From these calculations the basic design criteria for a reflectometer at a pulsed neutron source are clear. Comparing the SPSS and LPSS the instrument at the LPSS needs to be much longer to achieve the same wavelength resolution. Comparing the 50 Hz and 10 Hz SPSS it is evident that the usable wavelength band is increasing for lower source frequency.

At a SPSS the wavelength band is typically defined either only by supermirrors or by a chopper for the short and supermirrors for the large wavelengths. A new idea to be realized a the SNS reflectometer is a bender system.

As has been shown earlier it is possible to perform successfully reflectometry experiments at a LPSS when using a set of choppers. The instrument design is discussed in Ref. [1].

The distance-time diagrams for the different instrument set-ups are shown in the figures below.

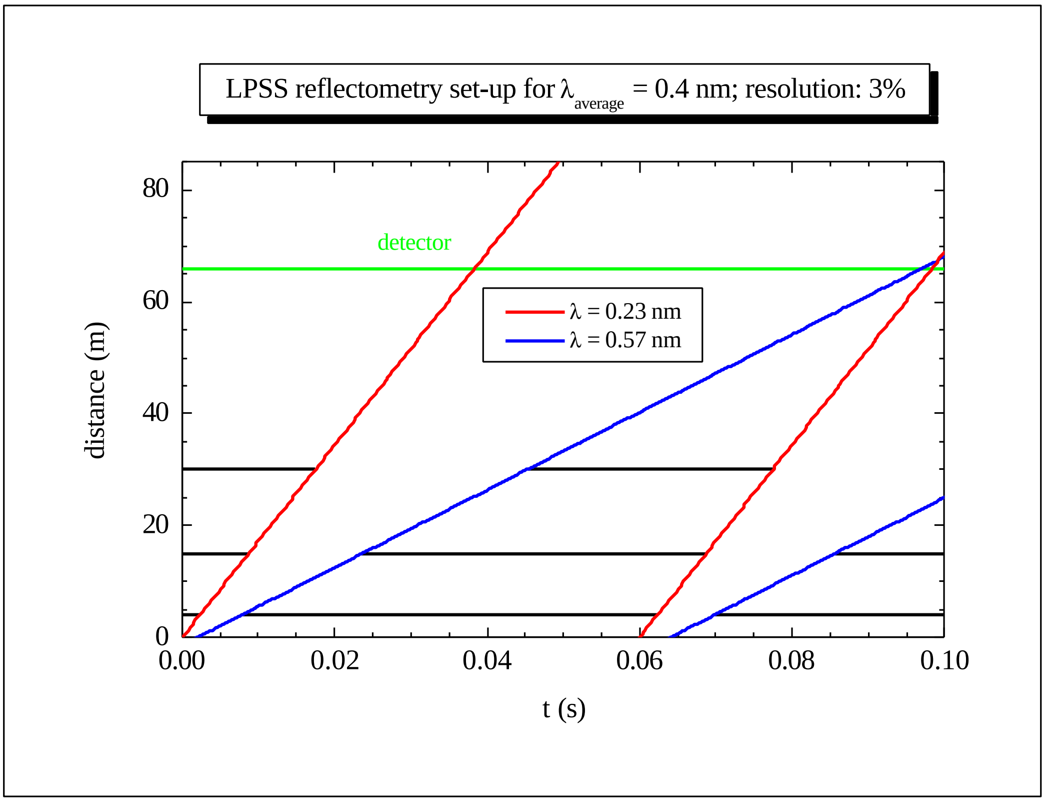


Fig. 4: instrumental set-up for a reflectometer at a LPSS.

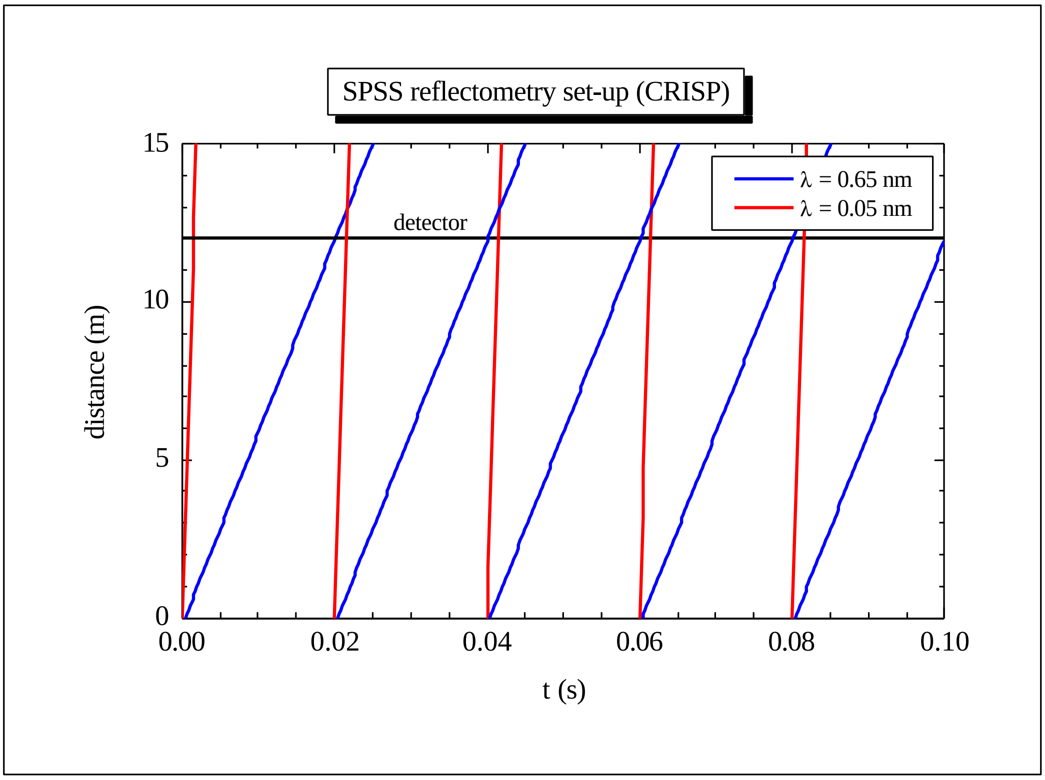


Fig. 5: instrumental set-up for a reflectometer at a SPSS.

2.3 50 Hz (5 MW) versus 10 Hz (1 MW)

As discussed above the source parameters define the usable wavelength band. The smaller 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 might be more effective than the data acquisition at a fixed angle of incidence using a large wavelength band.

To quantify our considerations we performed MC-simulations with a 5 MW SPSS running at 50 Hz and a 1 MW SPSS at 10 Hz. For the 10 Hz target the sample was held at a fixed angle of 2°, whereas for the 50 Hz target we used three different angles of incidence: 0.57°, 1°, and 2°. The neutron flux as a function of q is shown in Fig. 6. With three angles of incidence for the 50 Hz source the same q-range can be covered as with the 10 Hz source.

But even more interesting is the question: how long do you have to count for a typical reflectivity curve to get the same statistics for the 10 Hz and the 50 Hz source?

To answer that question we took a D_2O-surface as a typical liquid sample. For the 10 Hz source it takes 13333 s to acquire at least 1000 counts for each q-value whereas for the 50 Hz source one needs (2671 s + 0.5 s + 0.05 s) = 2672 s. This is a performance ratio of 13333 / 2672 = 4.99 and even when taking into account an overall time of 60 seconds for the motor movements the performance factor is about 4.9. So the performance just scales with the power of the source as already stated by Mike Fitzsimmons [2].

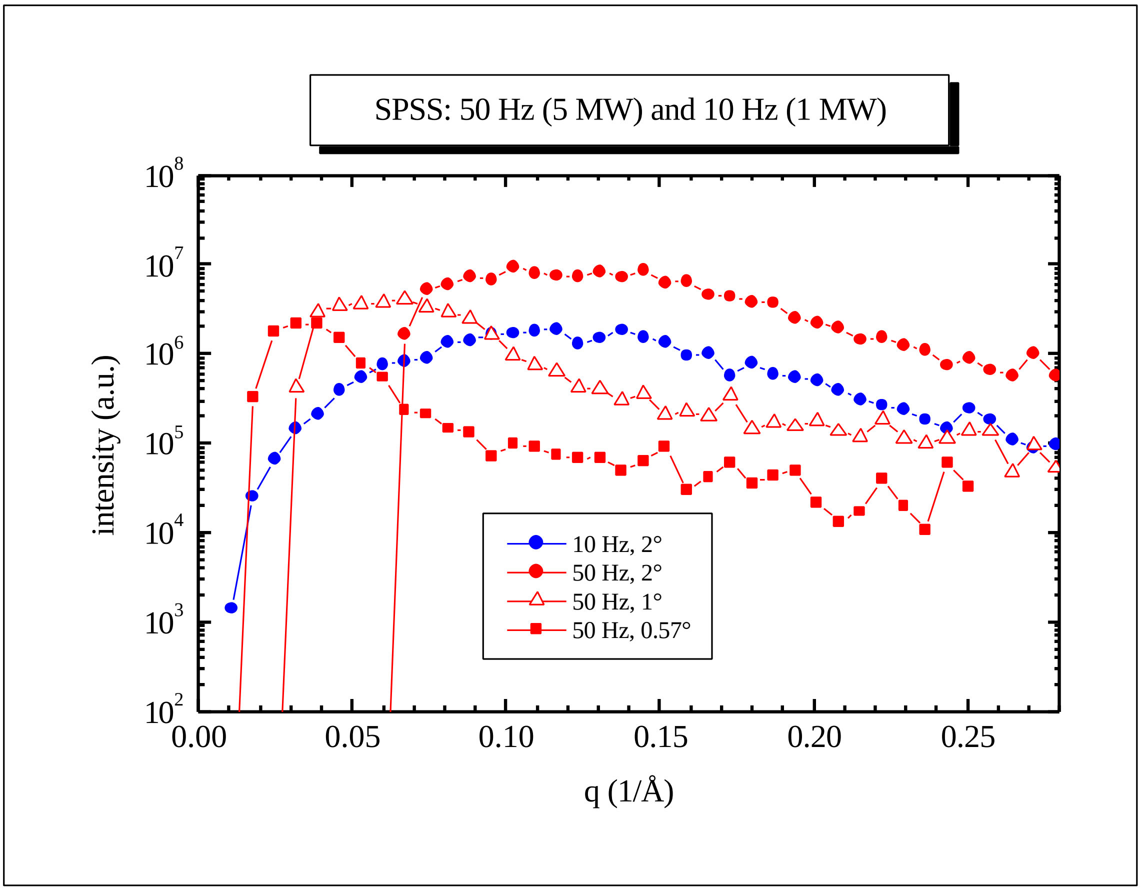


Fig. 6: reflected neutron intensity for a reflectometer at a SPSS with 5 MW, 50 Hz and 1 MW, 10 Hz from MC-simulations with the software VITESS.

2.4 Short pulse versus long pulse

Simulations show that for good resolution (better than 3%) the short pulse source performs better whereas for bad resolution both the long and the short pulse source have more or less the same performance if both instrumental set-ups are optimized.

2.5 Pulsed source versus reactor source

If we simply compare the flux of the 5 MW pulsed source and a coupled cold moderator to the cold source of the ILL we get a gain factor of about 20.

3 Conclusion

For neutron reflectometry the coupled cold moderator is the best choice from the ones under consideration for the ESS (cold or thermal decoupled, decoupled poisoned, coupled).

From our simulations can be concluded that the performance of a reflectometer is to a good approximation proportional to the power of the neutron source, what was already concluded by M. Fitzsimmons [2] in an extended study on the performance of neutron reflectometers. Therefore we strongly recommend to build a neutron reflectometer at a 5 MW source, either 50 Hz SPSS or 16.7 Hz LPSS.

4 References

[1] H. Fritzsche, C. Guy, J. Stride, and F. Mezei, J. Neutron Research **6**, 103 (1997)
[2] M. R. Fitzsimmons, Nucl. Instr. and Meth. in Phys. Res. A **383**, 549 (1996)