Proc. Int. Symposium on Advances in Neutron Scattering Research, Tokai, 2000
J. Phys. Soc. Jpn. **70** (2001) Suppl. A pp. 451–452

Monte Carlo Optimisation of SANS Spectrometer at IBR-2 Reactor

Alexandre V. BELUSHKIN and Sergey A. MANOSHIN

Frank Laboratory of Neutron Physics, JINR, Dubna, Moscow region 141980, Russia

The operation of the YuMO small-angle neutron scattering time-of-flight spectrometer at the IBR-2 pulsed reactor has proved to be highly efficient for solving different structural problems in chemistry, biology and materials science. At the same time, it has become obvious that further development of the spectrometer may raise its performance to an even higher level. In particular, this concerns the background reduction and obtaining $Q_{min} \sim 10^{-3}$ Å^{-1} (in contrast to presently available 7×10^{-3} Å^{-1}) for a sample of 1 cm in diameter. To design an optimum configuration of the instrument, Monte Carlo simulations were performed. Several options of a virtual instrument consisting of a bender and/or neutron guide (curved, straight, focussing), collimation system, sample and detector were investigated. An optimum configuration of the small-angle scattering spectrometer at IBR-2 is proposed.

KEYWORDS: Monte Carlo optimization, small-angle neutron scattering, pulsed neutron sources

§1. Introduction

Small-angle neutron scattering (SANS) is a method widely used to study large scale structures with characteristic sizes of 1 - 1000 nm. At present, practically all research neutron sources are equipped with one or more SANS machines.

At the IBR-2 pulsed reactor of the Frank Laboratory of Neutron Physics o f JINR, Dubna, Russia [1] the SANS spectrometer YuMO has been operating for more than 15 years. Its main parameters may be found in .[2] Recent successful tests of the solid methane moderator at IBR-2 have shown that the instrument can be considerably improved because the moderator yields a 10 times gain in the cold neutron flux (neutron wavelength of about 10 Å). The main directions of the YuMO development are the suppression of the fast neutron and gamma background and widening of the momentum transfer range.

To investigate possible solutions of the above-mentioned problems, Monte Carlo simulations have been performed. The basic algorithms used in Monte Carlo simulation programs are described in. [3-5] The aim of modelling was to study the possibility of using different neutron optic devices such as neutron guides of different configurations, neutron benders, and collimators to improve background conditions and reach the lowest possible Q_{min} value.

The neutron bender is a multislit curved neutron guide. The length of the bender used in the simulations is 60 cm and the cross section is 3.1 × 6.1 cm. The slit width equals 0.9 mm, the number of slits is 31, and the radius of curvature is 25 m. The curved neutron guide used in the simulations is 11.5 m in length, the radius of curvature is 1400 m, and the cross section is 2 × 2 cm.

The bender or the curved neutron guide makes it possible to suppress completely the fast neutron and gamma background. Below, it is assumed that all neutron optic elements have a natural nickel coating to make comparisons more straightforward. The wavelength range used in the calculation is from 2 Å to 12 Å with a step of 1 Å. The calculation continues as long as 4000 neutrons are counted by the detector for each particular wavelength. The neutron spectrum from the IBR-2 solid methane moderator is used as an incoming spectrum.

§2. Monte Carlo Optimisation of the SANS Instrument at IBR-2

Three virtual instruments have been investigated. The first option is very similar to the existing YuMO spectrometer except for the fact that a straight 50 cm neutron guide section (3.1 × 6.1 cm in cross section) is installed at a distance of 5 m from the moderator, followed by the above described bender. At the output of the bender a pinhole collimator 3 cm in diameter is placed and at a distance of 15 m from it a pinhole collimator 1 cm in diameter is located. Immediately behind the second collimator is the sample plane and the sample-detector distance is 15 m. The Monte Carlo calculations have revealed that for this SANS configuration the uniformity of the neutron flux on the sample is better than 20 %. The fast neutron and gamma background is completely suppressed. The minimum value of momentum transfer is 1.5×10^{-3} Å^{-1} for the neutron wavelength 10-12 Å. Thus, the goals formulated in the introduction have been achieved. The price for this is, however, a dramatic loss in the neutron intensity because of extremely tight collimation.

To increase the neutron flux on the sample, another spectrometer configuration was studied, where a 50 cm straight neutron guide section is installed 5 m apart from the moderator and then it continues as an 11.5 m curved section described in the introduction and a 4 m straight section. The cross section of the neutron guide is constant and equals 2 × 2 cm. A pinhole collimator 2 cm in diameter is located at the output of the neutron guide and a pinhole collimator 1 cm in diameter is installed at a distance of 5.9 m from it immediately ahead of the

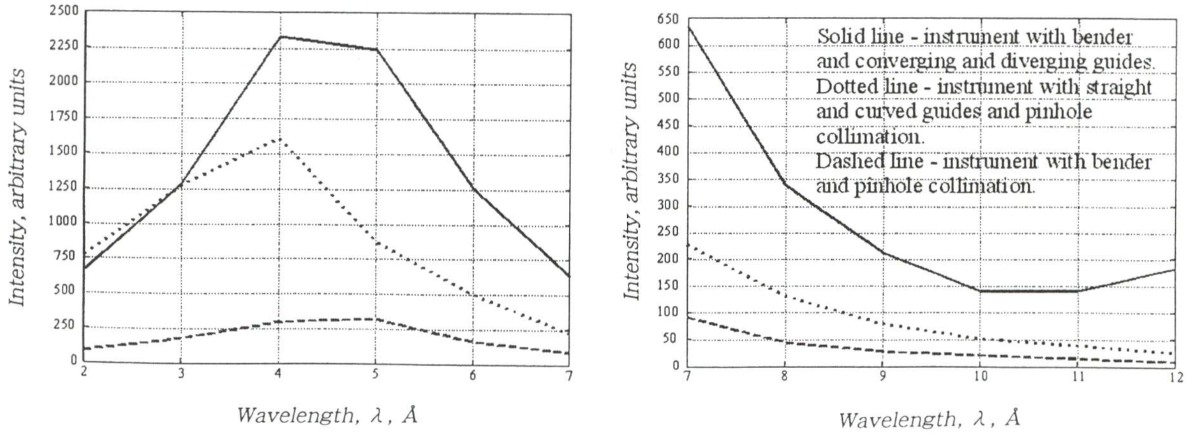

Fig. 1. Neutron intensity flux for three kinds of SANS instruments.

sample plane. The sample-detector distance is still 15 m. Using this configuration $Q_{min} = 2 \times 10^{-3}$ Å^{-1} is reached at neutron flux uniformity on the sample equal to that in the first option. A relative intensity gain on the sample of 8.4 times for 2 Å neutrons, 5.4 times for 4 Å neutrons, and 2.8 times for 12 Å neutrons is obtained.

The last investigated configuration consists of a 50 cm straight neutron guide section (3.1 × 6.1 cm in cross section) placed at 5 m from the moderator, followed by a neutron bender and 11 m long focussing neutron guide. The neutron guide has the inlet cross section 3.1 × 6.1 cm and the outlet cross section 2 × 2 cm. The focussing guide continues as a 4 m diverging guide with a 2 × 2 cm inlet cross section and a 9 × 9 cm outlet cross section. At the output of the assembly a pinhole collimator 1 cm in diameter with a sample behind it is placed. The detector is at a distance of 15 m from the sample. The last option gives a neutron flux gain of over a factor of 7 for the neutron wavelengths between 5 - 8 Å and of up to 20 times for the neutron wavelengths between 10Å and 12 Å. The minimum momentum transfer achieved using the last instrument configuration is 3×10^{-3} Å^{-1}. The uniformity of the neutron flux on the sample is again better than 20 %.

The intensity of neutrons on the sample for all discussed SANS instruments is given in Figure 1. Figure 2 shows Q_{min} achievable in different virtual instrument configurations as a function of the neutron wavelength.

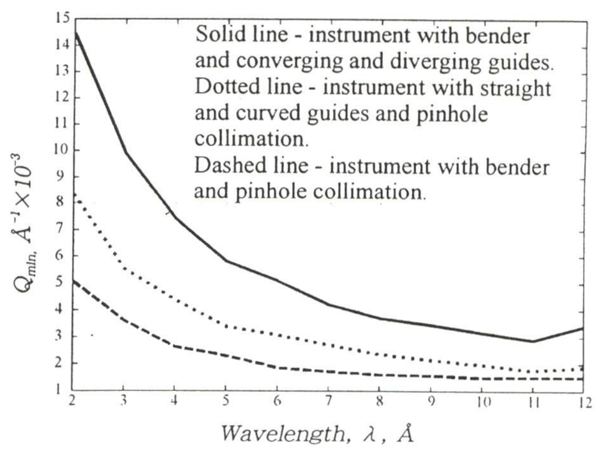

Fig. 2. Q_{min} for three kinds of SANS instruments.

§3. Conclusions

Modeling different SANS instrument configurations at IBR-2 one arrives at the conclusion that the most advantageous option is the instrument with a neutron bender and a focussing + defocussing straight neutron guide. It allows one to obtain the highest neutron flux on the sample, complete suppression of the fast neutron and gamma background caused by a neutron source and to reach quite low Q_{min} values. When necessary, additional optional pinhole collimators can be used to reduce Q_{min} though at the expense of intensity.

1) V. L. Aksenov: Physica B **438-442** (1991) 174.
2) V. V. Sikolenko: *User guide, neutron experimental facilities for condensed matter investigations at JINR* (Dubna, 1997) p. 18.
3) A. V. Belushkin, S. A. Manoshin: Communication of the JINR **P11-2000-56** (2000) 2.
4) M. W. Johnson and C. Stephanou: MCLIB, A library of Monte Carlo subroutines for neutron on scattering problem, Rutherford Laboratory report **RL-78-090** (1978).
5) M. W. Johnson : MCGUIDE, A thermal neutron guide simulation program, Rutherford and Appleton Laboratories report **RL-80-065** (1980).