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SIMULATION OF VIRTUAL **SANS** SPECTROMETERS AT IBR-2 REACTOR

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1 INTRODUCTION

For over 15 years the time-of-flight SANS spectrometer YuMO has been operating at the IBR-2 pulsing reactor [1] in the Frank Laboratory of Neutron Physics, JINR, Dubna, Russia. The basic parameters of the spectrometer are summarized in Table I (see [2,3] for details).

TABLE I Basic parameters of YuMO at IBR-2.

Incident wavelength range	0.6 – 8 Å
Beam diameter at sample position	14, 18 or 22 mm (variable)
Momentum transfer range	0.008 – 0.5 $Å^{-1}$
Neutron flux on sample, time averaged	6×10^6-3.7×10^7 n/cm^2s (depending on collimation)

Recent successful tests of the solid methane moderator at IBR-2 prove that the parameters of the instrument can be improved considerably due to gain in the cold neutron flux of over a factor of 10 for 10 Å neutrons. The main directions of improving are to suppress the fast neutron and gamma backgrounds and extend the momentum transfer range, especially by reducing the minimum momentum transfer Qmin. The background is mainly caused by that the YuMO detector "sees" the IBR-2 moderator directly. As a result, weakly scattering samples are hard to investigate with YuMO. A relatively large value of Qmin does not allow studies of structures with a typical dimension larger than 250 Å (approximately).

To investigate various options to achieve the above stated goals, Monte Carlo calculations were performed. The aim of modeling 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 Qmin value.

The optimisation calculation is naturally restricted by the size of the IBR-2 experimental hall that limits the moderator-to-sample distance to approximately 18 m and the sample-to-detector distance to 15 m. So, the length of the simulated instrument is fixed.

2 MONTE CARLO SIMULATING PROGRAM AND RESULTS OF NEUTRON OPTIC ELEMENTS MODELING FOR VIRTUAL SANS INSTRUMENTS

The basic algorithms used in the Monte Carlo simulation programs are described in [4-6]. The new version of the program suite includes the gravitation effects [4]. A virtual neutron scattering instrument may incorporate the following elements: a moderator, neutron guide, bender, collimator, beamstop and a position sensitive detector. The entrance to the neutron guide or the bender can be arbitrarily shifted or/and tilted with respect to the plane of the moderator. The neutron guide may be a sequence of up to 150 straight, curved, and focussing sections whose cross-sections are rectangular, cylindrical or conical. Each section has its own neutron reflectivity and critical angle of incidence. A possibility is provided to install slits or collimators between sections.

The programs read in geometric configuration files describing the elements of the virtual instrument and their spatial arrangement. Neutrons are then generated and their passage through the instrument is modelled by the Monte Carlo method. The number of iterations for the given neutron wavelength depends on the respective number of such neutrons (specified by the user) registered by the virtual detector.

An output program gives the neutron flux distributions as a function of wavelength and/or coordinates at the exit of the neutron guide or neutron bender and at sample position. The spatial non-uniformity of the neutron flux and the angular divergence of the neutron beam are also specified. In addition, one can obtain the transmission coefficient for every section of the neutron optic system, average number of neutron reflections from the surfaces of the system, moderator to detector neutron time-of-flight uncertainty, and some other parameters.

Additionally, the momentum transfer range, neutron beam size on the beamstop, neutron losses per collimator, and the direct beam size on the detector were calculated for the small angle scattering spectrometer.

The neutron bender is a curved multislit neutron guide. Using natural nickel coated bender with radius of curvature 25 m, slit width is of an order of 1 mm, over a length of about 45 cm it is possible to remove fast neutrons and γ-rays from the neutron beam.

The neutron bender employed to construct our virtual SANS instruments is similar to the one used in the LOQ spectrometer at the ISIS spallation neutron source (RAL, UK) [7]. The length of the natural nickel coated bender is 60 cm by 3.1×6.1 cm^2 cross section. The slit width equals 0.9 mm. The number of slits is 31. The radius of curvature is 25 m. The characteristic wavelength for such a bender is 5 Å.

An analogous effect can be obtained with a curved neutron guide. Its total length, however, must be much larger than that of the bender. In our calculations we use a 10.1 m curved neutron guide with a radius of curvature of 1400 m. Its cross section is constant and equal to 2×2 cm^2. The characteristic wavelength is 3.1 Å for natural nickel coating.

The bender and the curved neutron guide both allow to suppress completely the fast neutron and gamma backgrounds from the IBR-2 reactor.

A comparison of transmission coefficients of the neutron bender with a natural nickel coating and a supermirror coating (m=2, $\gamma_c = 0.0034\lambda$ (Å)) and a natural nickel-coated neutron guide is illustrated in Figure 1. It is seen that the best results are obtained for the bender with a supermirror coating but only for short wavelengths. The supermirror-coated neutron guide is not included in the comparison because of a high cost of such device. However, to make the comparison more straightforward, below it is assumed that all neutron optic elements have a natural nickel coating. The reflectivity coefficient is equal to 0.98 for optic devices used in our calculations, which is comparable to the values obtained experimentally [8].

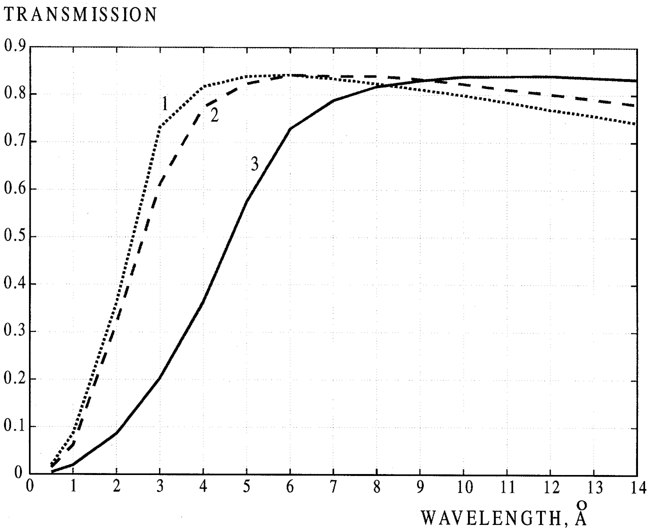

FIGURE 1 Line 1 (points) – transmission of the supermirror bender (m=2). Line 2 (dashed) – transmission of the natural nickel-coated guide. Line 3 – transmission of the bender with a natural nickel coating.

3 OPTIMISATION OF SANS INSTRUMENT

3.1 SANS Instrument with a Bender and a System of Collimators

The principle scheme of the instrument is shown in Figure 2. The first section is a straight guide with the length 0.5 m and the cross section 3.1 x 6.1 cm^2. The distance from the moderator plane to the entrance of the neutron guide is determined by the size of the existing biological shield around the IBR-2 reactor. The neutron guide “sees” a moderator surface area of 30 x 33 cm^2. The next element is the bender described above. At the output of the bender there is a 3 cm diameter pinhole collimator and at 15 m from it there is a 1 cm diameter pinhole collimator. Immediately behind the second collimator there is a sample with the diameter 1 cm. The position sensitive detector (PSD) with an outer diameter of 80 cm is installed at 15 m from the sample. In the center of PSD, an 8 cm diameter beamstop is installed. The collimators, sample and the detector are axially symmetric to the neutron beam. The diameters of the pinhole collimators are chosen on the basis of simulations to allow Qmin = $1.0 \cdot 10^{-3} \overset{o}{A}^{-1}$ for wavelength 10 Å.

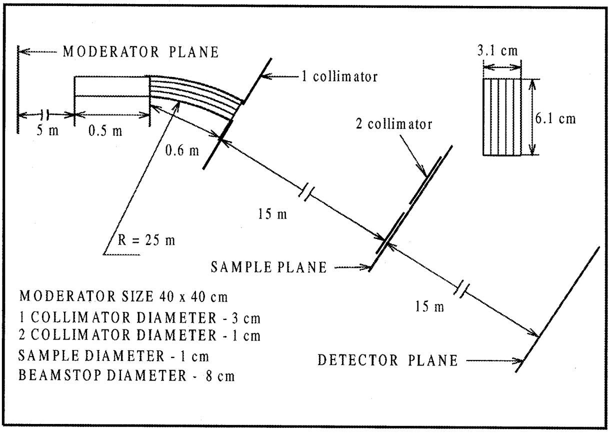

FIGURE 2 The SANS instrument with a bender and pinhole collimators.

The results of simulations without a sample are illustrated in Figure 3. The neutron wavelength range used in the simulations is 1-13 Å. One can see a significant effect of gravity at long wavelengths (>10 Å).

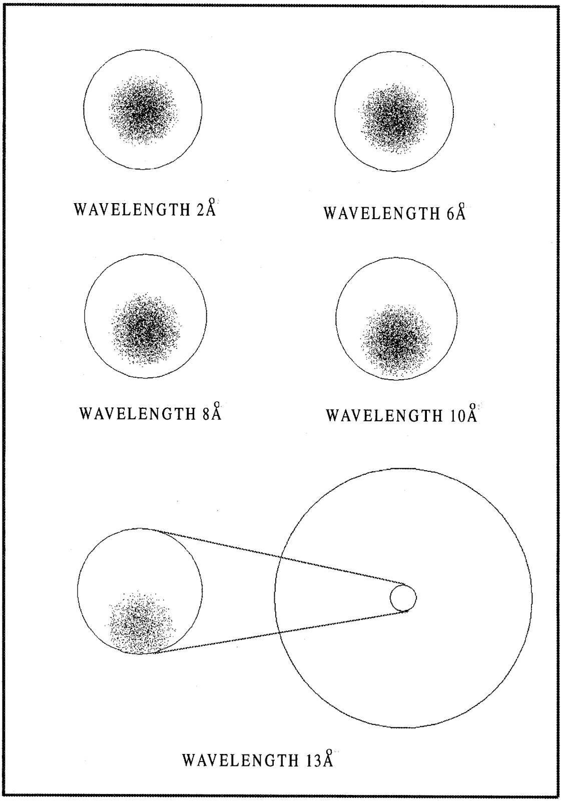

FIGURE 3 The direct neutron beam at detector and beamstop.

The distribution of the neutron flux on the sample in the horizontal direction is shown in Figure 4. The non-uniformity of the neutron flux is better than 7 % over the entire wavelength interval. The calculations are carried on until 4000 neutrons are counted for each wavelength in the sample. The estimated statistical error is equal usually 7% in our Monte Carlo simulation. So, this non-uniformity of the neutron flux is caused by a statistical error usual in Monte Carlo simulations.

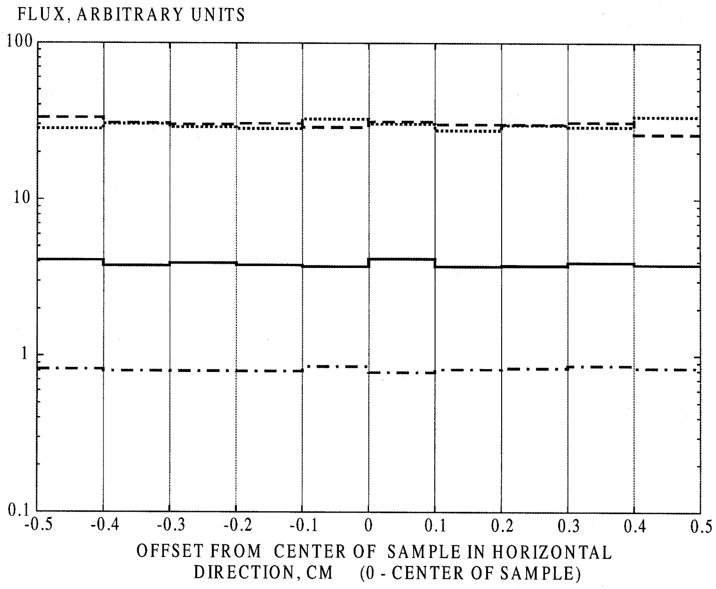

FIGURE 4 The horizontal profile of the neutron beam on the sample 1 cm in diameter for different wavelengths. The chain-dot line – for 1 Å, solid line – for 2 Å, dashed line – for 6 Å, and the dotted line – for 12 Å.

So, the SANS instrument shown in Figure 2 ensures a small background (fast neutrons and x-rays cannot pass through the bender), a high degree of neutron flux uniformity on the sample (< 7 %) and a good minimum value of momentum transfer Qmin = $1.0 \cdot 10^{-3} \overset{o}{A}^{-1}$ for wavelength 10 Å. The price to be paid is, however, a dramatic loss in neutron intensity due to extremely tight collimation. In addition, the large gravity effect has to be taken into account during data analysis. This fact can cause some uncertainties in interpretation of the results.

3.2 SANS Instrument with a Neutron Guide and a System of Collimators

The principle scheme is in Figure 5 showing a curved neutron guide with a length of 10.1 m and a radius of curvature of 1400 m. The cross section of the guide is constant and it equals 2x2 cm^2. This guide permits complete suppression of gamma rays and fast neutrons with $\lambda < 0.5$ Å.

To have Qmin = $1.8\cdot10^{-3}\overset{o}{A}^{-1}$ for wavelength 10 Å, there is installed a 2-cm diameter and a 1-cm diameter pinhole collimators at 6 m from each other at the output of the guide. Immediately behind the second collimator there is a sample 1 cm in diameter. The position sensitive detector (PSD) with an outer diameter of 80 cm is at 15 m from the sample. In the center of the detector there is a beamstop 11 cm in diameter.

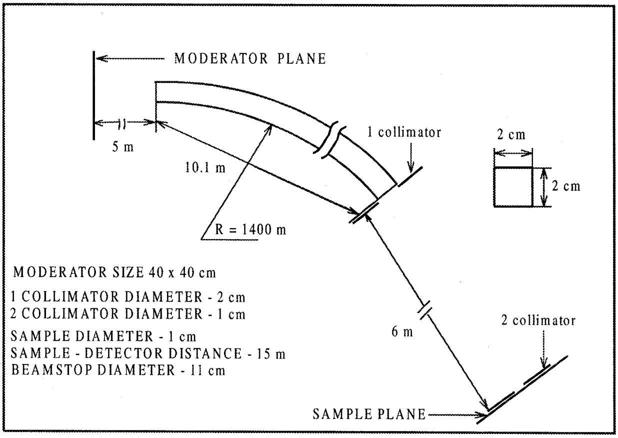

FIGURE 5 The SANS instrument with a neutron guide and pinhole collimators.

The results of simulation without a sample are shown in Figure 6. As above, the wavelength range used in the simulation is 1 Å to 13 Å. Interesting to note that the gravity effect in this configuration is much less pronounced than for the instrument discussed in the previous section. This is due to the use of a long curved neutron guide and a smaller distance between collimators. Neutrons are reflected from the walls of the guide (including the bottom wall) and as a result, the effect of gravity is reduced.

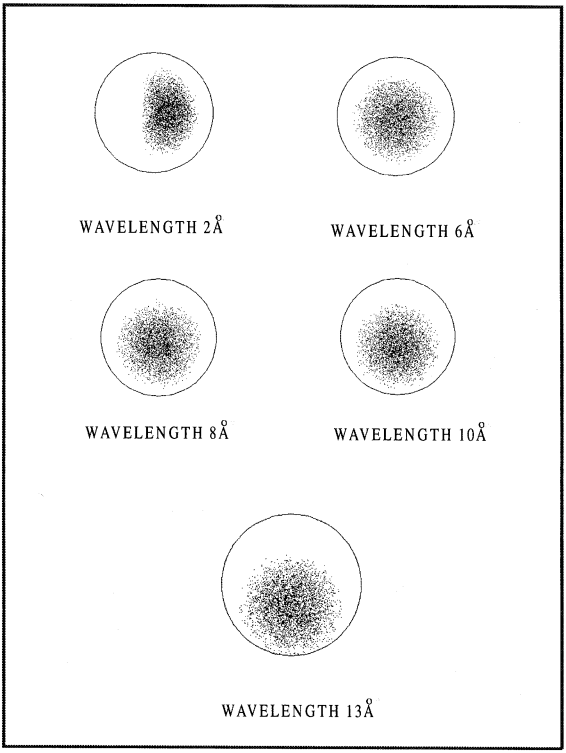

FIGURE 6 The direct neutron beam on the detector and the beamstop for the sample-detector distance 15 m and without the sample.

The distribution of the neutron flux on the sample in the horizontal direction is shown in Figure 7. It is seen that for small neutron wavelengths non-uniformity of the neutron flux is much higher than it is in the previous case. The non-uniformity of the neutron flux is better than 7 % only for the neutrons with wavelength $\lambda > 2$ Å. So, this non-uniformity of the neutron flux is caused by a statistical error usual in Monte Carlo simulations. The non-uniformity of the neutron beam becomes significant only for the neutrons with wavelength $\lambda \leq 2$ Å.

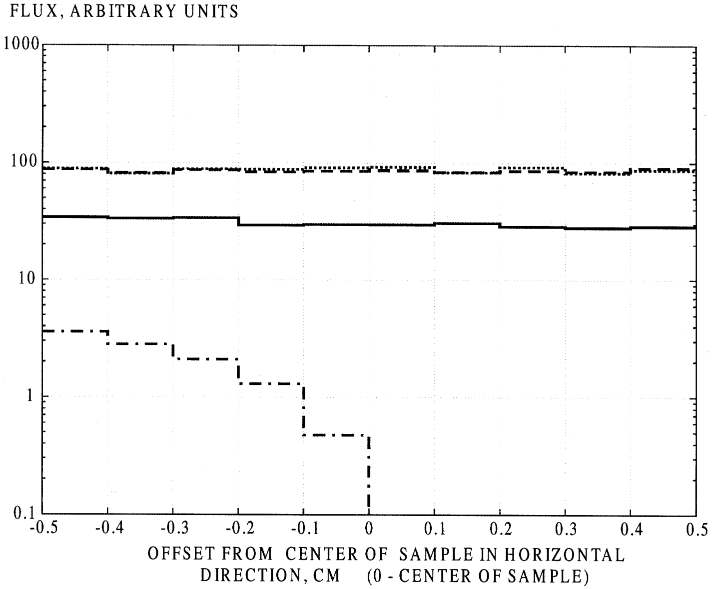

FIGURE 7 The horizontal profile of the neutron beam in the sample with the diameter 1 cm for different wavelengths. The chain-dot line – for 1 Å, the solid line – for 2 Å, the dashed line – for 6 Å, and the dotted line – for 12 Å.

This version of the SANS instrument allows to obtain higher neutron flux on the sample at the expense of a less uniform neutron flux and a larger Qmin value. The problem of intensity loss due to the tight collimation persists.

3.3 SANS Instrument with a Bender, Converging and Diverging Guides

Let us investigate another configuration of the SANS instrument. It incorporates the bender described above but with the cross section 3.1 x 3.1 cm^2 and a converging and a diverging neutron guides [9,10]. The converging neutron guide is 11 m long and has the inlet cross section 3.1 x 3.1cm^2 and the outlet cross section 1.96 x 1.96cm^2. This neutron guide converges at the center of the detector. The diverging neutron guide is 1 m long with an inlet cross section of 1.96 x 1.96cm^2 and an outlet cross section of 3.72 x 3.72cm^2. The diverging guide provides the possibility of compensating the divergence of the neutron beam from the converging guide. A diaphragm with a diameter of 1cm is at a distance of 3 m from the exit of the diverging guide. As before, a 80-cm diameter detector is installed at 15 m from the sample. The beamstop in the center of the detector has a diameter of 16 cm. The principle scheme is shown in Figure 8. The results of the simulation without a sample are illustrated in Figure 9.

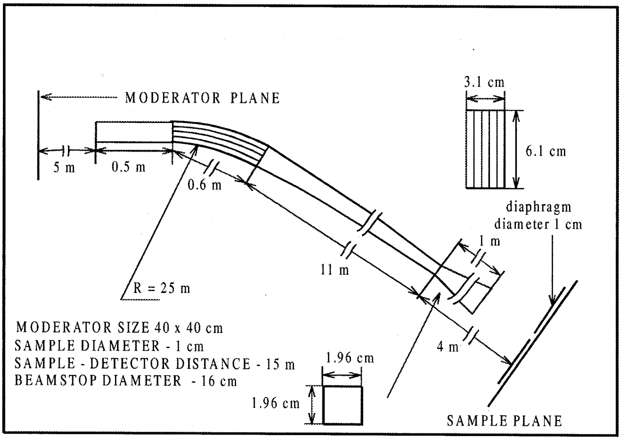

FIGURE 8 The SANS instrument with a bender, a converging and a diverging guides.

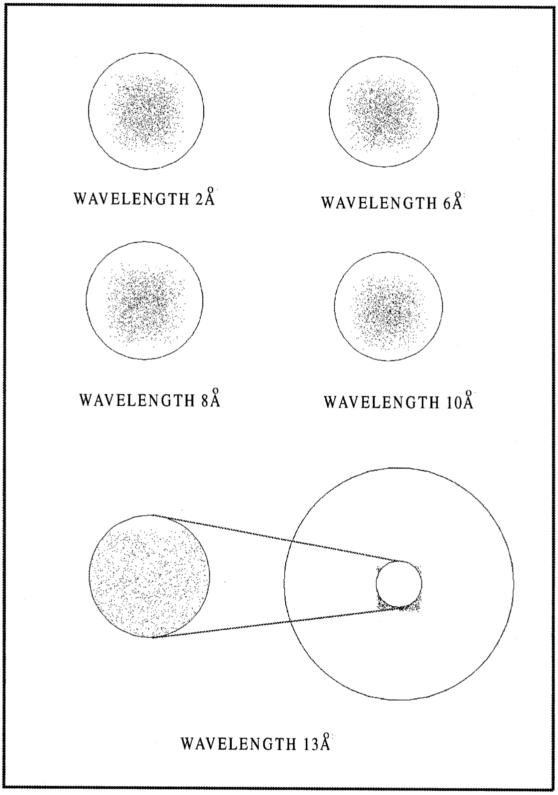

FIGURE 9 The direct neutron beam on the detector and beamstop for a sample-detector distance of 15 m.

The distribution of the neutron flux at sample position in the horizontal direction is given in Figure 10. The flux non-uniformity is smaller than 7 % for all neutron wavelengths considered and is comparable with the SANS option discussed in section 3.1. So, this non-uniformity of the neutron flux is caused by a statistical error usual in Monte Carlo simulations.

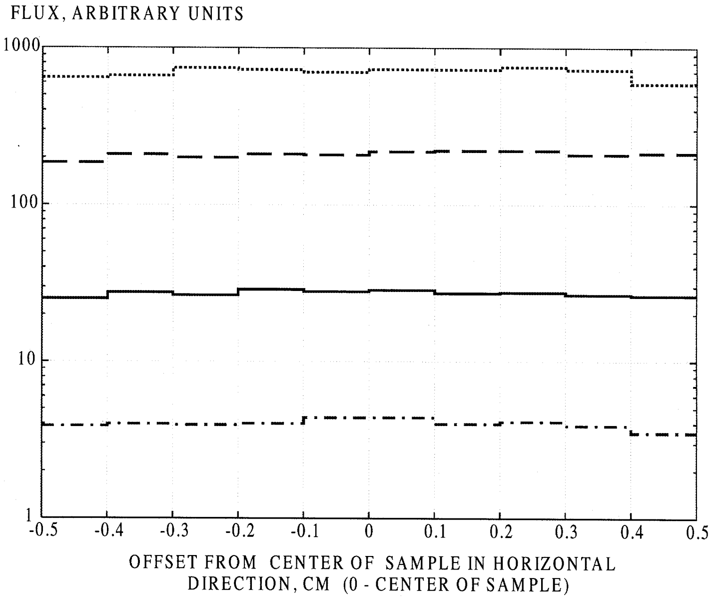

FIGURE 10 The horizontal profile of the neutron beam on a 1-cm diameter sample for different wavelengths. The chain-dot line – for 1 Å, solid line – for - 2 Å, dashed line – for 6 Å, and the dotted line – for 13 Å.

This instrument configuration appears to be optimal with respect to the neutron flux on the sample and a minimum value of momentum transfer. A detailed comparison of all three instruments is given in the next section.

4 COMPARISION OF DIFFERENT SANS CONFIGURATIONS

The thermal neutron spectra from the pulsed reactor IBR-2 with a solid methane moderator (T=60 K) and an ambient temperature water moderator are shown in Figure 11. The results of the calculation are shown in Figure 12. Using these two spectra the wavelength dependence of the neutron flux on the sample was calculated for all of the discussed virtual instruments.

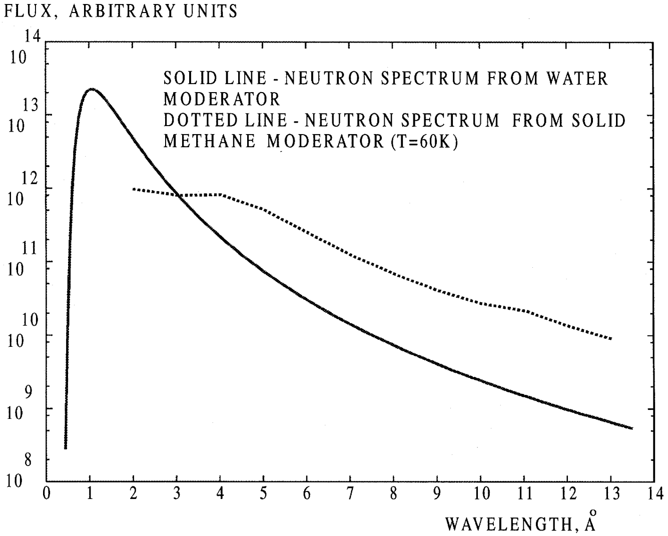

FIGURE 11 The spectra from the IBR-2 reactor with a solid methane (cryogenic) moderator and an ambient temperature water moderator.

One can see that for $\lambda \geq 3$ Å neutrons the instrument with a converging and a diverging guides is superior to the other options as to neutron intensity on the sample.

For all the discussed SANS versions, the solid methane moderator gives a larger gain for long wavelengths than the ambient temperature water moderator.

A comparison of minimum momentum transfers for different SANS options is illustrated in Figure 13. The momentum transfers were calculated using the beam spot size on the detector for a particular neutron wavelength. The effect of gravity was taken into account. The effect of gravity is illustrated in Figure 14 showing the displacement of the center of the neutron beam cross section with respect to the detector center versus neutron wavelength. The SANS instrument with a converging and a diverging neutron guides demonstrates a weaker gravity effect comparing to the other two options. The SANS instrument with a bender and pinhole collimation has the largest gravity effect.

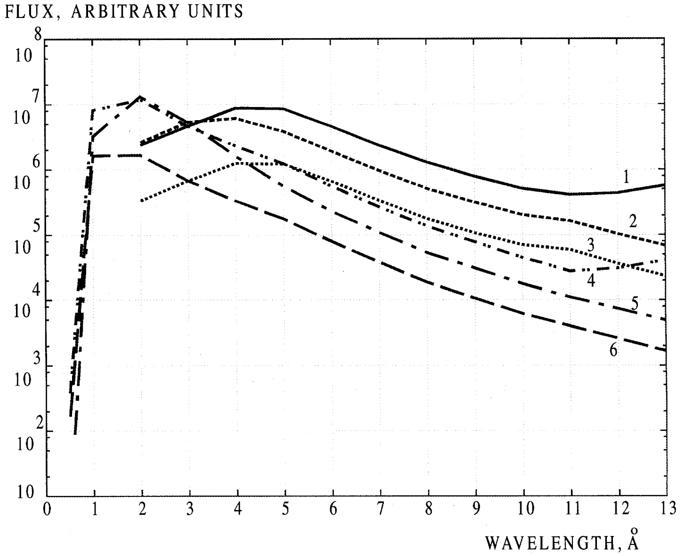

FIGURE 12 A comparison of the neutron flux on the sample with a diameter of 1cm for different virtual SANS instruments and different IBR-2 moderators. Line 1 is the spectrometer with a bender, a converging and a diverging guides and a solid methane moderator. Line 2 is the spectrometer with a guide and pinhole collimators and a solid methane moderator. Line 3 is the spectrometer with a bender and pinhole collimators and a solid methane moderator. Line 4 is the spectrometer with a bender, a converging and a diverging guides and a water moderator. Line 5 is the spectrometer with a guide and pinhole collimators and a water moderator. Line 6 is the spectrometer with a bender and pinhole collimators and a water moderator.

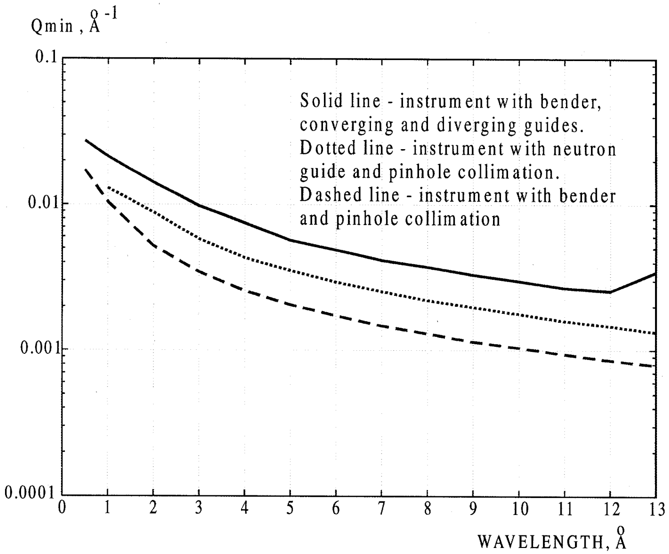

FIGURE 13 Qmin as a function of the neutron wavelength achievable for different virtual SANS instruments.

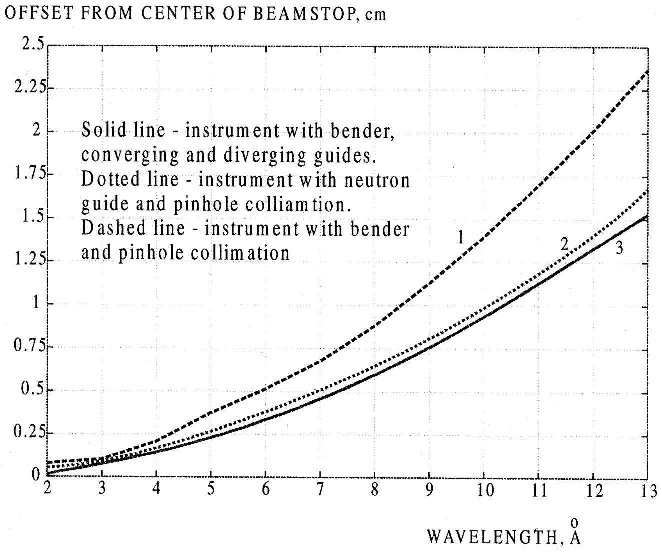

FIGURE 14 The gravity effect for different virtual SANS instruments.

Next, we estimate the resolution of the SANS instruments. A perfect scatterer was considered: every neutron was scattered with exactly the same magnitude (specified by the user) of the momentum transfer (δ - function of q) and random azimuth angles [11]. The width of the neutron spot on the detector is measured and the resolution is calculated. Also the average value of momentum transfer $\bar{q}$ is estimated. The gravity effect is compensated during data processing. The resolutions of the SANS instruments are given in Tables II, III and IV.

TABLE II The resolution of the SANS instrument with a bender, a converging and a diverging guides for wavelength 11 Å.

$q, \mathring{A}^{-1}$	$\bar{q}, \mathring{A}^{-1}$	$(\overline{q^2} - \bar{q}^2)^{1/2} / \bar{q}$, %
0.003	0.00315	27.9
0.004	0.00412	21.6
0.005	0.0051	17.6

TABLE III The resolution of the SANS instrument with a bender and pinhole collimation for wavelength 12Å.

$q, \mathring{A}^{-1}$	$\bar{q}, \mathring{A}^{-1}$	$(\overline{q^2} - \bar{q}^2)^{1/2} / \bar{q}$, %
0.0015	0.00157	19.4
0.002	0.00206	14.9
0.003	0.00305	10.1

TABLE IV The resolution of the SANS insrument with a guide and pinhole collimator for wavelength 12Å.

$q,\mathring{A}^{-1}$	$\bar{q},\mathring{A}^{-1}$	$(\overline{q^2}-\bar{q}^2)^{1/2}/\bar{q},\%$
0.002	0.0021	24.8
0.0025	0.00259	20.3
0.003	0.00308	17.1

5 CONCLUSION

On the basis of the Monte Carlo simulation of different SANS instrument configurations we conclude that most preferable is the instrument with a neutron bender and a converging plus a diverging straight neutron guides. Such SANS instrument allows obtaining of the highest neutron flux on the sample, full suppression of the fast neutron and gamma backgrounds and reach quite low Qmin values. When necessary, additional optional pinhole collimators can be used to reduce Qmin though at the expense of intensity.

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7 REFERENCES

[1] V.L. Aksenov, Physica B, **174**, 438-442 (1991).

[2] http://nfdfn.jinr.ru/flnph/fks/yumo.html

[3] User guide, neutron experimental facilities for condensed matter investigation at JINR, Edited by V.V. Sikolenko, Dubna, (1997).

[4] A.V. Belushkin, S.A. Manoshin, Monte Carlo calculation of mirror neutron guides, Communication of JINR, **P11-2000-56**, (2000).

[5] M.W. Johnson and C. Stephanou, MCLIB: A Library of Monte Carlo subroutines for neutron scattering problem, Rutherford Laboratory report, **RL-78-090**, (1978).

[6] M. W. Johnson, MCGUIDE: A thermal neutron guide simulation program, Rutherford and Appleton Laboratories report, **RL-80-065**, (1980).

[7] R.K. Heenan, ICANS-VIII. Proceedings of the Eighth Meeting of the International Collaboration on Advanced Neutron Sources, Rutherford and Appleton Laboratories Report, **RAL-85-110**, 523-525 (1986).

[8] V.V. Kornilov et al, The characteristics of neutron guides fabricated from FLOAT glass , Preprint JINR, **P13-80-496**, (1980).

[9] R.E. Lechner, Proceedings of ICANS-X, Los Alamos, 843-848 (1989).

[10] R.E. Lechner and F. Mezei, Proceedings of ICANS-XI, KEK Report , **90 - 25**, 919-929 (1991).

[11] P.A. Seeger, A.Williams, J. Trewhella, Proceedings of ICANS-VIII, Rutherford and Appletion Laboratories report, **RAL-85-110**, 441-453 (1986).

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Белушкин А.В., Маношин С.А. E13-2001-178

Моделирование виртуальных спектрометров
малоуглового рассеяния на реакторе ИБР-2

Более чем 15-летний период использования на реакторе ИБР-2 малоуглового спектрометра для изучения структур с большими характеристическими размерами показал, что некоторые параметры спектрометра могут быть улучшены. В особенности это касается уменьшения фона быстрых нейтронов и гамма-лучей для возможности изучения слаборассеивающих образцов. Другое направление модернизации — уменьшение минимального значения вектора рассеяния Q_{min} для возможности изучения структур с большими характеристическими размерами. Рассмотрены несколько конфигураций малоугловых установок на реакторе ИБР-2. Для вычисления параметров этих виртуальных инструментов использовался метод Монте-Карло. На основе моделирования представлен оптимальный вариант установки.

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Belushkin A.V., Manoshin S.A. E13-2001-178

Simulation of Virtual SANS Spectrometers at IBR-2 Reactor

The experience gained in the last 15 years of experimental studies of large-scale structures with the SANS instrument at the IBR-2 pulsed reactor in Dubna shows that some parameters of the spectrometer can be improved. In particular, it concerns reduction of the fast neutron and gamma backgrounds that limit the possibilities of studying weakly scattering objects. Another direction of improvement is to reduce a minimum momentum transfer value Q_{min} to study objects with larger characteristic dimensions. The paper investigates several configurations of the SANS machine at IBR-2. The Monte Carlo codes are used to calculate the parameters of such virtual instruments. An optimal instrument structure is proposed.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

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