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SMALL ANGLE NEUTRON SCATTERING FACILITY FOR LOW AND HIGH POWER REACTORS

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1. Introduction

Small angle neutron scattering (SANS) is one of the main techniques which can provide information on the size, shape, volume and interactions at distances from 5 to 1000 Å. Such a size interval represents a unique possibility for studying a variety of fundamental problems in biology, chemistry, polymers and materials science. SANS instruments could be built at steady state reactors and at pulsed neutron sources. In the latter case the time-of-flight (TOF) technique is used. SANS facilities usually used at steady state reactors provide data over a relatively small q-range with respect to the best resolution; whereas TOF techniques can provide a relatively wider q-range. This could be achieved when simultaneously using the white beam, TOF technique for t-scanning and the commonly known Θ-scanning.

Since 1984, a small angle neutron scattering spectrometer "YuMO" (named in honour of Yu.M.Ostanevich) has been successfully operating at the IBR-2 reactor in Dubna [1,2,3]. Although the construction of the "YuMO" instrument allows the choice between the slit or axially-symmetric geometries, preference was given to the latter. Both calculations and experiments have shown that the choice of axially-symmetric geometry leads to better luminosity and resolution [4].

This paper was stimulated by a discussion, concerning the experimental program for a SANS facility that could be used at low and high power reactors of the Egyptian Atomic Energy Authority (EAEA) under the auspices of the co-operation agreement between EAEA and the Joint Institute for Nuclear Research (JINR). This paper represents a proposal for the creation of a SANS instrument at the ET-RR-1 reactor which could be transformed to a SANS instrument for a higher power reactor.

2. Small-Angle Neutron Scattering

The earliest reference to SANS can be traced back to the end of the forties when Huges and co-workers observed the widening of the neutron beam transmitted through a piece of iron [5]. Now, SANS is considered one of the important methods for investigating materials and biological objects. Information about these objects is based on the fact that the differential scattering cross-section $d\Sigma/d\Omega$ depends on the scattering vector $\vec{q}$

$$\vec{q} = \vec{K} - \vec{K}_0 ,$$

where $\vec{K}_0$ and $\vec{K}$ are the neutron wave vectors before and after scattering. This coherent process is mainly due to the interference of waves scattered by nuclei, ignoring magnetic scattering. The dependence between q, scattering angle Θ and the wavelength λ is given by:

$$q=4\pi\sin(\Theta/2)/\lambda . \qquad (1)$$

The general theory of coherent scattering was described by Guinier and Fournet [6]. Accordingly, the total intensity of N nuclei occupying a volume Vo, including all possible N interferences, is given by:

$$I(q)= 1/Vo<\sum_{i,j} b_i b_j \exp[i\vec{q}(\vec{r}_i-\vec{r}_j)]>, \qquad (2)$$

where b_i, b_j are the coherent scattering lengths of nuclei i and j, respectively.

For the simple case where N monodisperse, homogeneous particles with intermolecular averages independent of intermolecular ones are embedded in a solvent, equation (2) becomes:

$$I(q)=n\,S(q)\,W(q), \qquad (3)$$

where n is the particles density,
S(q) is the structure factor, and
W(q) is the average of the form factor module square.

Even such strict conditions (monodisperse, homogeneous) are not enough to extract the particle shape. Fortunately, the asymptotic behaviour of W(q) is independent of particle shape. This important case is given by the Guinier [6] relationship:

$$W(q)=C^2\,V^2\exp(-q^2\,Rg^2/3), \qquad (4)$$

where C is the difference between the particle's coherent scattering lengths density and the solvent's one, Rg is the particle radius of gyration and V its volume. Thus, one can extract information about the radius of gyration and, thereby, about the particle's size.

The next important case is when the values of q are much lager than the inverse of the particle's smallest size. This leads to the Porod equation:

$$W(q)=2\pi\,C^2\,(S/V)q^{-4}, \qquad (5)$$

where S/V is the total area of the interface, per unit of volume, of the particle under investigation.

It follows from (1) that the dependence of $d\Sigma/d\Omega$ via q could be measured by changing either the scattering angle or wave length; or both. The "YuMO" SANS facility at the IBR-2 is based on changing, simultaneously, both the angle and wavelength .

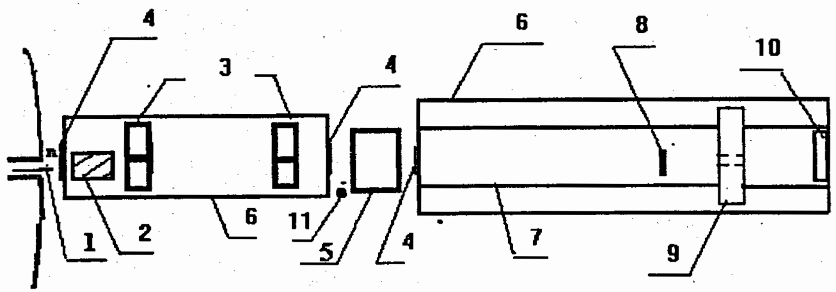

Fig.1.

1. Neutron beam from the ET-RR-1 reactor	**7. Railway for detector transportation**
2. Monochromator	**8. Vn internal standard**
3. Collimators	**9. Ring-wire detector with central hole**
4. Vanadium window	**10. Beam catcher**
5. Sample table	**11. Monitor**
6. Evacuated tubes	

3. The SANS Arrangement

The block diagram of the SANS arrangement is given in Fig.1. The neutron beam from the reactor channel (1) is transmitted, after the vanadium window (4), through the monochromator (2), where a certain wavelength range is eliminated. Such arrangement allows varying of the wavelength range of the chopped neutron beam. Neutrons, after the monochromator, pass through two successive collimators (3) and the first evacuated neutron tube (6). The collimating system (3) creates the required angular resolution, and the evacuated neutron tube reduces the neutron flux losses. The vanadium windows (0.15 mm thick) are practically transparent for neutron wavelengths from 1 to 8 Å.

The sample table arrangement (5) is computerised and can accommodate up to 20 samples. Automatic control of the sample table in two co-ordinate systems gives the possibility of adjusting the sample directly in the neutron beam. Besides, the sample table enables accommodaion of different instruments and arrangements required for materials science investigations at both variable pressure and temperature.

The second evacuated tube (6), also with a vanadium window, is placed just after the sample table. It is equipped with a railway for transportation of the ring-wire detector (9).

The tube itself is fixed on a special railway which allows the angle of neutrons incidence on the sample to be change. Such design allows studying a system in quite a wide q-range. The possibility of having the scattering detector in the direct neutron beam (without a sample) ensures the performance of the experiments with direct reference to the "direct beam".

3.1. Absolute calibration

Such design allows using two methods for absolute calibration:

1) "Internal standard" Vn method; a very efficient procedure and could be used without knowledge about the sample's transmission.

2) "External standard" method, where a standard scatterer is placed in the sample's position. Here, additional experiment is required for estimation of the transmission ratio between the sample and "external standard". The samples which could be used for absolute calibration must have several properties: a large cross section, stable in time and without inelastic scattering contributions. A vanadium sample can be used for such purpose. Vanadium is metallic, its scattering cross-section is almost incoherent with a negligible inelastic scattering contribution. Unfortunately the vanadium cross-section is not so high and it is more suitable as an 'internal standard'. Even then, it is placed very close to the detector. A water sample is a very good 'external standard' as its scattering cross-section is 20 times greater than the vanadium one. The choice of methods and samples, required for calibration depends on whether the sample is a strong or weak scatter. The 'internal standard' method also has the advantage that it removes the effect of long time fluctuation in the neutron beam intensity and without additional monitoring. The additional monitoring is only required in the case when the 'external standard' method is used; an additional account of the excess neutrons, before the sample table (5), is also required.

The intensity at the scattering detector, in the case of an 'internal standard' is given by

$$J_s(\lambda) = J_0\varepsilon(\lambda)T_s\left(\frac{d\Sigma}{d\Omega}\right)d_s\Omega_s,$$

where $\varepsilon(\lambda)$ is the scattering detector effectiveness,

T_s is the sample transmission,

$\left(\frac{d\Sigma}{d\Omega}\right)$ is the scattering cross-sections of a sample,

d_s is the sample thickness

Ω_s is the solid angle

J_0 is the spectrum of an incident beam

The intensity of the sample with vanadium is:

$$J_{V+S}= J_S+J_0\varepsilon\ T_ST_V\left(\frac{d\Sigma}{d\Omega}\right)d_V\Omega_V.$$

Then the scattering cross-section in "vanadium units" will be:

$$\left(\frac{d\Sigma}{d\Omega}\right)_{S_V} = \frac{J_S}{J_{S+V}-J_S}.$$

In the case when an "external standard" is used, equation (1) will be valid, but additional experiment still need to be performed in order to determine the sample's transmission. The scattering detector could be used when the neutron guide is rotated with the scattering detector. Consequently, by determining the beam intensity with and without the sample, its transmission could be determined. In such case, as given in external standard units will be

$$\left(\frac{d\Sigma}{d\Omega}\right)_{S_{ex}} = \frac{J_S}{J_{ex}T_S},$$

where J_S is the intensity from the sample,

J_{ex} is the intensity,

T_S is the sample's transmission.

The scanning, according to the scattering vector, as was mentioned above, could be performed in two ways: varying the wavelength through the monochromator or shifting the detector arrangement inside the neutron tube (6). The variation of the incident flux on the sample is realised by the collimating system.

3.2. The experiment's geometry

One has to choose between the slit (SG) and axially-symmetric geometry (ASG). It was found [7] that the use of ASG leads to serious improvement in the resolution function and increases luminosity. For slit geometry, the intensity is given by:

$$J \cong (L_1L_2)^{-2}\ X_1X_2X_3Y_1Y_2Y_3N_x\, d\sigma(k)/d\Omega\ , \qquad (6)$$

where $X_1X_2X_3Y_1Y_2Y_3$ is the dimension of the first and second collimators respectively,

L_1 is the distance between first and second collimator,

L_2 is the distance between the second collimator and the detector,

N_x is the flux incident on the sample.

In order to achieve maximum luminosity at a given resolution, the following optimisation conditions are required:

$$X_1/L_1=X_3/L_2=X_2/(1/L_1+1/L_2)\ , \qquad (7)$$

$$L_1=L_2\,. \tag{8}$$

In the case of axial symmetric scattering eq.(1) has the following solution [4]:

$$L_1=L_2\,,$$

$$R_m=2R_s\,,$$

where R_m, R_s are the first and second collimators radii, respectively.

The explicit shape of the resolution function was calculated analytically [7] and using the Monte-carlo simulation method [12]. The resolution could be approximated as a Gaussian one only in that case when eq. (7) and (8) are valid. This can be difficult in the case of a mobile detector.

For the slit geometry the resolution function is asymmetric and collimating distortion appears. The resolution function should be more or less symmetric. This could be realised in the case of ASG geometry, where collimation distortion is small compared with the SG. More details about the ASG analysis could be found elsewhere [8].

While the slit geometry, in the Guinier-region, acquires corrections up to 70%, the ASG correction is only 1%. Both geometries have been compared experimentally [10,12]. As a result it was found that the measuring time required for the slit geometry is 18 times greater than that of the ASG one; provided that q is same.

3.3 The detector system

The detector system consists of 8 independent wire detectors enclosed in a special arrangement filled with He gas (2.5 atm.), Ar (2.5 atm.) and CO (0.08 atm.). The detector arrangement is essentially the same as the one described before in [9]. Its efficiency should increase 80% for thermal neutrons. The detector system is insensitive to gamma background.

3.4. The parameters of the suggested SANS facility

Preliminary calculations were carried our for the SANS arrangement represented in Fig.1; with a ring-wire detector, filled with ^{3}He gas, and 8 wires giving 80% efficiency. The results of these calculations are summarised in Table 1.

Table 1

1	Thermal neutron flux at the reactor channel exit	10^7 n/sm^2 s
2	Thermal neutron flux on the sample	10^5 n/sm^2 s
3	Sample dimensions	10x5 mm
4	Q_{max} Q_{min}	0.6Å^{-1} 0.01Å^{-1}
5	The used wavelength range	1-8 Å
6	Resolution	0.09 Å^{-1}
7	Space resolution	2 sm

Conclusion

The present proposal presents a suitable SANS arrangement, for investigation of different materials .

- -The suggested SANS arrangement could be further developed for use at a reactor with flux higher than that of the ET-RR-1 reactor.
- -The suggested SANS arrangement allows both the slit and axially-symmetric geometries.
- -The axially-symmetric geometry, combined with a ring-wire detector, is the preferable one as it offers higher luminosity with a small correction for the resolution function.
- -The methods suggested for absolute calibration allow investigation of samples with different cross section areas.

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Установка малоуглового рассеяния нейтронов
для низко- и высокопоточного реактора

Обсуждается использование установки малоуглового рассеяния нейтронов на ET-RR-1 реакторе. Предлагаемая установка может использоваться на таком типе реактора, а также на высокопоточном и позволяет работать с щелевой и аксиально-симметричной геометрией. Показано, что аксиально-симметричная геометрия вместе с кольцевым проволочным детектором предпочтительнее по светосиле и по поправкам функции разрешения.

Работа выполнена в Лаборатории нейтронной физики им. И.М.Франка ОИЯИ.

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Maayouf R.M.A. et al. E13-94-257

Small Angle Neutron Scattering Facility
for Low and High Power Reactors

The possibility of using a small angle neutron scattering (SANS) facility at the ET-RR-1 reactor, is discussed. The type of SANS facility which could be used at such type of reactor, and higher power one, is suggested. The suggested arrangement allows both for slit and axially-symmetric geometries. It has been found that the axially symmetric geometry, combined with a ring-wire detector, is the preferable one as it offers higher luminosity and a smaller correction of the resolution function.

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

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