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Modeling of the focusing device and the elliptical neutron guide for the DN-6 diffractometer at IBR-2 reactor

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ABSTRACT

Possible options for modernization of the neutron beam forming system of the DN-6 diffractometer for the study of crystal and magnetic structures of microsamples at high pressures are being considered. It was demonstrated that for samples with the cross-section not exceeding 5×5 mm^2 the most efficient option would be the use of an elliptical neutron guide. It allows to deliver neutrons for large distances from the source to samples with minimal losses using, as a rule, just one neutron reflection per dimension i.e. one at a side and one at top or bottom. For the present moment due to technical difficulties of such option realization, the simplified solution was proposed. At the end of the curved neutron guide it is planned to install a vertical plane focusing 7-meter-long parabolic section. Such a modernization will increase the neutron flux at the sample by a factor 1.5–3.5 and reduce respectively the typical measurement times.

1. Introduction

Compared to X-rays, the neutron diffraction method offers some very important advantages for the studies of crystal and magnetic structures of materials depending on external thermodynamic parameters (temperature, pressure, magnetic field, etc.) [1]. For example, localization of light atoms (H, Li, O etc.) in the crystal structures is usually more precisely done with neutrons, especially if crystal structures contain also the heavy elements.

Neutron possesses the magnetic moment and, therefore, neutron diffraction is a powerful direct method for the study of magnetic structures and magnetic phase transitions in materials [1,2]. Additional factor is the large penetration depth for neutrons due to its charge neutrality and, as a result, the possibility to use complex sample environment for experiments, like cryostats, magnets, high pressure cells, etc.

An applied pressure is one of the most important thermodynamic parameters to address problems of structural and magnetic phase transitions at microscopic level as well as other physical effects in functional materials using neutron scattering. It allows vary the interatomic distances and valent angles in a controllable way to investigate their influence on the magnetic and other physical properties of materials [2–4].

Meanwhile such experiments are not at all trivial as the intensity of even advanced neutron sources is relatively low to perform measurements at pressures above 10 GPa. This is why not many centers in the world have instruments for high pressure studies. At the Frank Laboratory of Neutron Physics of the Joint Institute for Nuclear Research on the basis of high flux pulsed fast neutron reactor IBR-2 the DN-6 diffractometer for the studies at high pressure is successfully operating for several years already. The instrument is characterized by the high neutron flux on the sample and highly efficient multidetector assembly [5]. Design and neutronic parameters of the instrument allow performing experiments using the sapphire anvils with the typical sample volume of 1 mm^3 and maximum achievable pressures up to 10 GPa, as well as diamond anvils which allow to obtain pressures up to 40 GPa for sample volumes down to 0.05 mm^3 [6,7].

At present, to increase the range of pressures used in the experiments and to reduce measurement times considerably the problem of optimization and modernization of the neutron guide system becomes a very important issue for the DN-6 diffractometer. The present neutron guide configuration has the constant cross section 15×180 mm^2 along its whole length. The cross section of the sample used in high pressure experiments does not exceed 5×5 mm^2. To minimize the neutron flux losses for experiments at high pressures on samples it seems logical to introduce a focusing section for the existing neutron guide or, in an ideal situation, to optimize the whole neutron guide of the instrument.

It should be noted, that general questions of the optimization of the focusing design of the neutron guides for a triple axis spectrometer were considered previously in enough detail [8]. Short elliptic guides (2 m long) installed after tiny samples were presented in Refs. [9,10]. However, the case of the optimization of the existing neutron guides

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using neutron focusing devices, especially for pulsed neutron sources and for tiny samples, remains less highlighted [11]. The requirements on the precision of elliptic or parabolic guide manufacturing were not discussed before.

This work reports the results of modeling and optimization of the neutron guide system using Monte Carlo method. The simulations take into account the key technical factors influencing the neutron beam parameters on the sample, namely the focusing section for the existing guide and the completely new elliptical guide for the DN-6 diffractometer.

2. Description of DN-6 diffractometer

Currently the neutron beam forming system at DN-6 diffractometer consists of three parts, namely the straight 4.3 m long head part, 14.2 m long curved guide with curvature radius 1875 m and the 6.0 m long straight end part. The neutron guide sections are covered by natural Ni ($m = 1$). The present configuration fits well into the IBR-2 experimental hall and allows optimal suppression of fast neutrons and gamma background at the sample position. The final straight section serves for removal of the spatial asymmetry of the neutron beam intensity in transverse directions [12,13]. The sample having typical sizes not exceeding 5×5 mm^2 is placed at the distance 1.5 m from the exit of neutron guide system. For technical reasons, the sample center is shifted by 1.5 cm to the top with respect of the neutron beam axis.

As it is presented below, it is possible to increase considerably the neutron flux at the sample position by replacing the end straight neutron guide section by a parabolic focusing section. The optimal solution, for obtaining maximum possible neutron flux at the sample would be a completely new elliptical neutron guide. However, this is much more expensive and not feasible for technical reasons at IBR-2 reactor now.

The reliable way to optimize the neutron guide system and even the whole new instrument concept is the prior use of Monte Carlo simulations. It allows to consider every factor which can influence the parameters of the instrument. There exist several software suites to address the problem: VITESS [14], MCSTAS [15], RESTRAX [16]. Our modeling was performed with the use of VITESS 2.10 version. This package was previously used effectively for similar tasks [17,18]. The geometrical parameters of the modeled neutron guides have been optimized to obtain the maximum possible neutron flux on a sample with transverse dimensions equal to 5×5 mm^2.

3. Results of calculations

3.1. Modeling the focusing end part of the neutron guide

For the purpose to increase the neutron flux at the sample position the easiest and most straightforward solution would be the use of converging (focusing) neutron guide [19]. However, such a solution leads to a divergence of the neutron beam which can cause some consequences on spectrometer resolution.

The following parameters of the end focusing neutron guide section were analyzed:

(1) The reduction of the distance from the neutron guide exit to the sample down to 1.1 m, compared to 1.5 m for the existing configuration;
(2) The total length of the focusing section is 7 m;
(3) The width of the focusing section was kept constant equal to 15 mm, and the height of the section was converging from 180 mm at the entrance to 60 mm at the exit following either linear or parabolic shape (see the supplementary material);
(4) In the case of linearly focused section the top and bottom surfaces were considered as coated with supermirror having $m = 3$ or $m = 2$. For parabolically shaped section the coating with $m = 3$ was modeled.

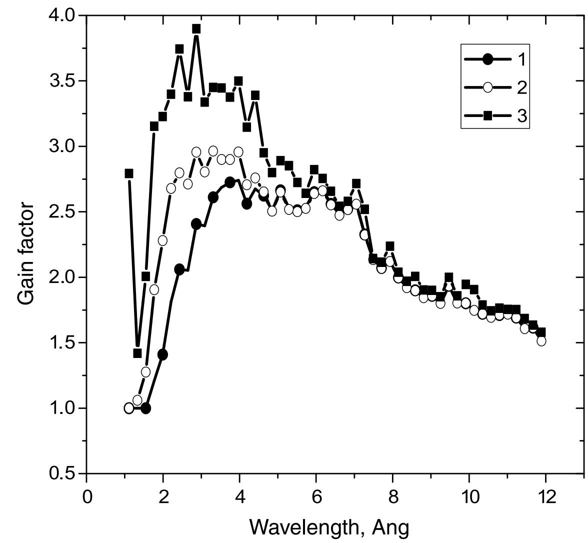

Fig. 1. Gain factor in neutron flux integrated over the sample of the size 5×5 mm^2 for different types of the focusing end part of the neutron guide compared to the existing guide. Line 1 corresponds to the linear focusing section with $m = 2$ coating, line 2—for $m = 3$ coating. Line 3 shows the gain for parabolically shaped focusing section with $m = 3$ coating.

Comparison of the results obtained for linearly and parabolically shaped focusing section are presented in Fig. 1. It is clearly seen that for the range of wavelengths 1–4 Å the parabolically converging section provides the best solution. While for longer wavelengths it shows no difference compared to linearly focusing section either with $m = 3$ or even $m = 2$ (see Figs. 1 and 2). But in any case the focusing section provides the overall gain in neutron flux by a factor 1.5–3.5 depending on the neutron wavelength.

As was expected, the parabolically shaped section with $m = 3$ coating shows better parameters compared to the straight section in the neutron wavelength range 1–6 Å. The modeling demonstrates that the manufactured precision of the cross section over the whole length of the neutron guide component which was assumed to be 50 cm long must be no worse than ±1.0 mm. The length of each such section must be kept within ±3.0 mm. Under such conditions the overall deviations from the ideal shape for the parabolical end part of neutron guide does not affect considerably the neutron flux at the sample position (Fig. 1 in the supplementary material).

Calculated vertical divergences of the neutron beam at the sample position for the existing neutron guide and the guide having at the end linearly and parabolically shaped focusing section are shown in Fig. 3. One can mention the triple peak shaped distribution of the neutron flux when focusing sections are used. Unfortunately, this effect can cause some problems with experimental data normalization and resolution corrections. It requires, therefore, the optimization and correct alignment of the axial geometry neutron detector system used at the DN-6 diffractometer. This problem disappears if one is using an elliptical neutron guide described below.

3.2. Calculations for the elliptical neutron guide

As mentioned above, the use of focusing section at the end of the neutron guide allows to increase the flux at the sample, however, it results in the considerable divergence and complex angular distribution. More uniform distribution of neutron intensity both in horizontal and vertical directions can be achieved by using an elliptical neutron guide. Additional advantage of using such a guide is the fact that neutrons experience small number of reflections from the neutron guide walls (just one per dimension i.e. one at a side and one at top or bottom).