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Neutron guide system for small-angle neutron scattering instruments of the Jülich Centre for Neutron Science at the FRM-II

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Abstract

Following the shut-down of the FRJ-2 research reactor in Jülich a large part of the neutron scattering instrumentation operating there is currently being moved to the FRM-II research reactor in Garching-München. The installation of these instruments requires the design and set-up of new neutron guides with geometrical and optical features imposed by the positioning of the instruments in the neutron guide hall and by the foreseen significant improvement of the instrument performance. Particularly three SANS diffractometers require a special approach due to on one hand, their pre-determined size and on the other hand, the demanded neutron wavelength range. Expected characteristics of three neutron guides (currently under construction) optimized using VITESS and McStas simulation packages, namely the vertically "S-shaped" guides serving the KWS2 and KWS1 conventional SANS instruments and the horizontally "S-shaped" guide serving the focusing KWS3 instrument, will be reported on.

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Keywords: Neutron guide; Small-angle neutron scattering; Monte-Carlo simulations

1. Introduction

After shut-down of the FRJ-2 "DIDO" research reactor the Research Centre Jülich will continue the in-house research activity in the traditional fields of soft-matter and magnetism, as well as the instrument and method development and the user program at different external neutron sources. Eight instruments of the new founded Jülich Centre for Neutron Science (JCNS) that are currently being transferred from Jülich to Garching will operate at the FRM-II reactor in Garching-München and, at the same time are the subject of major upgrades. Planned significant improvements of the instruments performance, as well as their positioning in the neutron guide hall require the design and set-up of new neutron guides with particular geometrical and optical features. Particularly, three SANS diffractometers require a special approach due to on one hand, their pre-determined size and on the other hand, the demanded neutron wavelength range.

The KWS1 and KWS2 instruments are 42 m long conventional pinhole SANS diffractometers, which allow us to perform structural investigations within the momentum transfer range $Q = 10^{-3}$–$0.3\,\text{Å}^{-1}$ by the variation of the sample-to-detector distance from 1.25 to 20 m and a change of wavelength between 4.5 and 12 Å. Because of much higher neutron flux expected at FRM-2, wavelengths up to 20 Å are targeted that, in combination with neutron refraction lenses, will allow us to approach much lower values in Q. The incoming beam characteristics are defined by a 20 m long collimation base consisting of variable apertures at well-defined positions and 18 neutron guide segments each 1 m long, which move either in or out of beam in the front of those apertures. Both instruments were constructed to operate at the beam height of 1.5 m in Jülich and therefore, their reallocation in Garching requires a match to the beam height of 1.2 m at the FRM-II reactor.

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The design of the KWS3 focusing-mirror SANS and reflectometry instrument [1] is based on the one-to-one imaging of an entrance aperture on a two-dimensional position-sensitive detector by neutron reflection on a double-focusing toroidal mirror. The KWS3 is only SANS instrument in the world working on this principle, and its technical realization became possible only in the last decade, due to the development and production of very high-quality mirrors for X-ray space telescopes [2]. The 22 m long instrument is a pretty "1-dim" device and can therefore fit in narrow spaces, inappropriate for most of other instruments; a fact that was fully exploited during its re-allocation to FRM-II. For a fixed neutron wavelength $\lambda = 12.7\,\text{Å}$ and a typical entrance aperture of $2\times 2\,\text{mm}^2$ this instrument has already been permitted at the FRJ-2 reactor SANS studies within a Q range of 1×10^{-4}–$2\times 10^{-3}\,\text{Å}^{-1}$, thus perfectly bridging the "Q-gap" between the USANS double-crystal diffractometers and conventional SANS measurements [3]. Again, it is expected that the increased flux at FRM-II reactor will allow on one side, for the use of both SANS and reflectometry options with a high neutron intensity and on other side, for the use of wavelengths larger than 12.7 Å, both resulting in the extension of the lowest accessible Q-value down to $3\times 10^{-5}\,\text{Å}^{-1}$.

Al three SANS instruments will be placed at the ends of dedicated neutron guides emerging from the same initial neutron guide, namely NL3. Due to space and geometrical constrains in the guide-hall of the FRM-II reactor (the limited available place, safety regulations, easy approach to the sample positions, necessity to raise the beam height, placement of auxiliary equipment-shielded velocity selectors, pumps, etc.) but keeping the targeted instrument performance at the same time, we designed long vertical "S"-shaped neutron guides for the two conventional pinhole instruments, KWS1 and KWS2. KWS3 instrument can only be located in a much displaced position against the incoming beam axis of the NL3 guide, thus requiring the construction of a horizontal "S"-shaped neutron guide with a rather small radius of curvature.

Following these pre-imposed conditions the optimization of particular geometrical and optical features of the neutron guides was carried out using VITESS [4] and McStas [5] simulation packages. Expected characteristics of the vertical "S-shaped" NL3a-o and NL3b guides serving the KWS2 and KWS1 conventional SANS instruments and the horizontal "S-shaped" NL3a-u-S guide serving the focusing KWS3 instrument, are presently reported.

2. Calculations and discussions

The JCNS SANS instruments KWS1, KWS2 and KWS3 will be installed at neutron guides emerging from the NL3 cold neutron guide of FRM-II reactor. This neutron guide with the total cross-section of $50\times 170\,\text{mm}^2$ is split into two slightly curved neutron guides diverging from each other, NL3a ($50\times 110\,\text{mm}^2$) and NL3b ($45\times 50\,\text{mm}^2$) (see Fig. 1). The NL3b neutron guide designated to serve KWS1, is horizontally straight while vertically "S"-shaped, with characteristics that have to be determined by computer simulations. The NL3a neutron guide is split both horizontally and vertically into three guides: (i) the upper part (NL3-a-o), a $50\times 50\,\text{mm}^2$ in cross-section, that serves KWS2 and continues for 2.5 m with a horizontally curved section (same direction as before) followed by a horizontally straight guide, however "S"-shaped in the vertical plane; (ii) the lower part is divided into a narrow guide of $10\times 56\,\text{mm}^2$ in cross-section (NL3-a-u-S) that feeds KWS3, while the remaining part (about $35\times 56\,\text{mm}^2$ in cross-section) is a (reserved) guide NL3-a-u-N for a potential future instrument. The space constrain leads to the placement of the narrow KWS3 instrument in a much displaced position toward the incoming beam axis and therefore, to the construction of a "S"-shaped guide of a pronounced curvature ($R = 30\,\text{m}$) in the horizontal plane.

Geometrical parameters of the guides, namely the radius of curvature, length, symmetry ratio of the "S"-shape, as well as a possible combination of "S"-guides with subsequent straight guides is the subject of optimization by using VITESS and McStas simulation packages. The geometrical and optical features of the already built part of NL3 downstream the cold source are introduced in the simulations as fixed configurations. They provide particular wavelengths, angular and space intensity distributions which influence the intensity behavior through the following guide sections. In the first approach, the comparison between different configurations was done using the neutron source with constant wavelength distribution and a given flux while, once the guide configuration being optimized, preliminary quantitative estimations have been done using the flux measurements performed at another neutron guide NL-1 as reference [6]. The available space in the guide hall defines the maximal available guide length

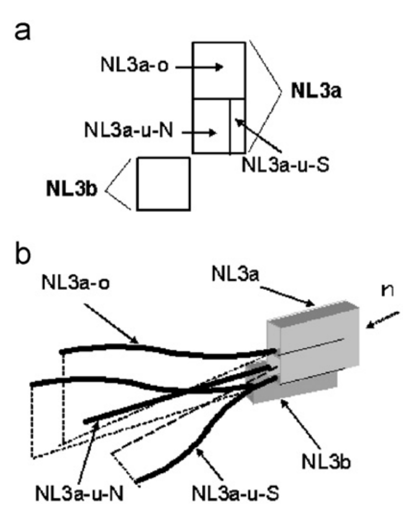

Fig. 1. Schematic representation of the splitting of the NL-3 neutron guide: (a) the front view of three guides serving three JCNS SANS instruments and the forth reserved neutron guide; (b) the shape and orientation of emerging neutron guides.

that is of 29 m for KWS1 and 22 m for KWS2. On the other hand, an increase in the critical wavelength of the neutron guides results in an enhancement of intensity for shorter wavelengths. Therefore a larger radius of curvature is desired, especially in the case of KWS1 and KWS2 instruments where shorter wavelengths (4.5–6 Å) are highly required. For the particularly desired vertical shift and for the total available length the "S" guide should have a radius of curvature of 800 m. Other different curvature radii between 500 and 800 m fulfilling the wavelength and beam height demands were also considered. In these cases, the shorter "S" guides are completed with subsequent horizontal straight guide sections up to the total available length. Fig. 2 presents gain factors for different "S"-shaped guides for a coating of the top and bottom walls with $m = 2$ supermirrors and of the left and right walls with ^{58}Ni. An overall ^{58}Ni coating of the additional straight segments to the shorter "S" guides was considered. The case of the 800 m curvature radius (thus a 29 m long symmetrical "S"-guide) is due to the intensity gain for shorter wavelengths very attractive. The important gain for "very short wavelengths" ($\lambda \leqslant 4$ Å) may be especially useful in the future when selectors that are able to operate with wavelength lower than 4.5 Å will be used. The "S" guide induces a rather inhomogeneous (vertical) intensity distribution at the guide output (Fig. 3). Simulations show that a 2 m long straight segment placed after the "S" guide is sufficient to smooth this distribution and lead to the conclusion that after the horizontal collimation flight base (either guides or apertures) the beam has again a completely homogeneous vertical distribution (Fig. 3). The optimal positioning of the mechanical monochromator (velocity selector) was also the subject of simulations. For an easy approach and to avoid disturbing other experiments in an emergency case, it is highly desirable to have the selector outside of the casemate. Therefore, several placements of selector—at the beginning or in different intermediate positions along the "S"-guide—have been checked from the point of view of intensity loss and modification of intensity distribution: although the break for selector brings losses, especially at higher wavelengths it makes no difference as to where to place the selector—either at the beginning or at the middle of "S" (Fig. 4).

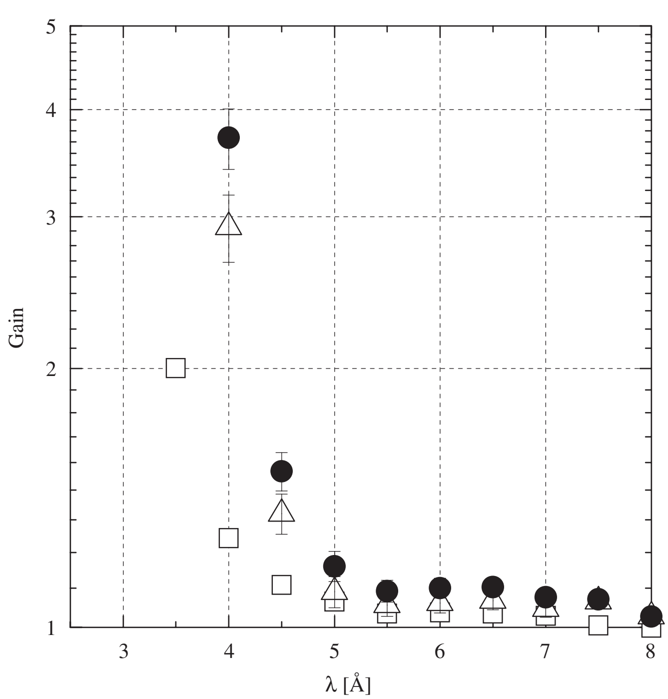

Fig. 2. Intensity gain factors at the output of "S" guides for different radii of curvature: open square—for $R = 800$ m vs. $R = 700$ m, open triangles—for $R = 700$ m vs. $R = 500$ m and full circles—for $R = 800$ m vs. $R = 500$ m.

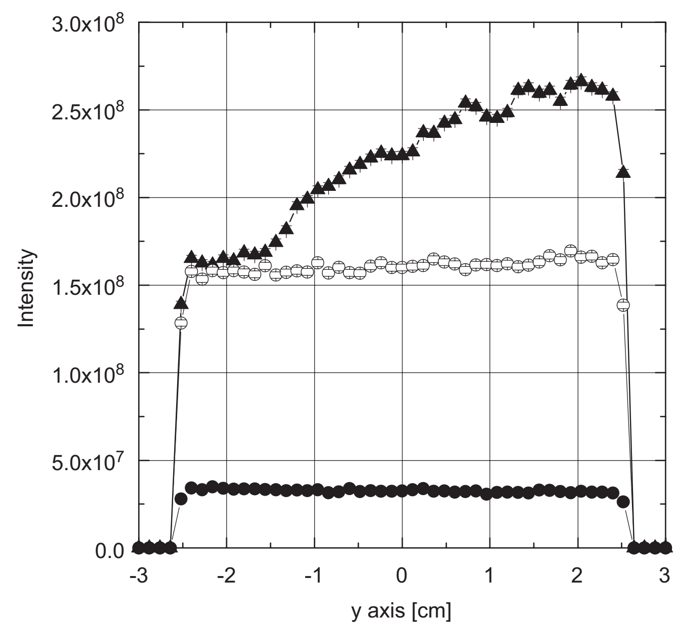

Fig. 3. The vertical distribution of neutron intensity after: a 29 m long vertical "S"-shaped guide with $m = 2$ supermirror coating of the top and bottom walls and ^{58}Ni coating of the left and right walls (full triangles); the "S" guide followed by 18 m straight guide (open circles)—the "2m-collimation" condition; the "S" followed by 20 m flight base with $50 \times 50\,\text{mm}^2$ apertures after 6, 12, 16 and 18 m (full circles, multiplied by a factor of 10)—the "20 m-collimation condition".

First quantitative flux estimation based upon the measured intensities at the end of NL1 guide [6] has shown that, with this optimized guide system, the KWS1 flux in the sample position is expected to be about 15 times higher at FRM-II, compared to that at FRJ-2 for the collimation length of 2 m and the wavelength spread $\Delta\lambda/\lambda$ of 10%. This factor applies in principle for the whole available wavelength range.

The KWS3 guide is designed as a horizontal incomplete "S"-shaped guide made of two sections, one which is 3.9 m long and shows a curvature radius $R = 30$ m and another one only 2.9 m long and curved in an opposite direction ($R = -30$ m). After this incomplete "S" guide a 1.2 m long straight section is installed. The simulations show that optimal beam characteristics are obtained by $m = 2$ supermirrors coating of the "S" guide for the vertical walls

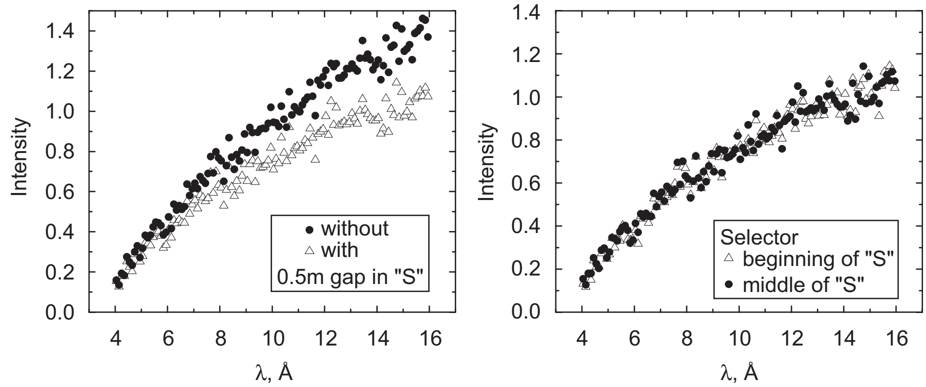

Fig. 4. Effect of the selector placement (0.5 m gap within the vertical "S" guide): a decrease in the intensity for longer wavelength (left); no influence for the selector placement at the beginning or in the middle of "S" (right).

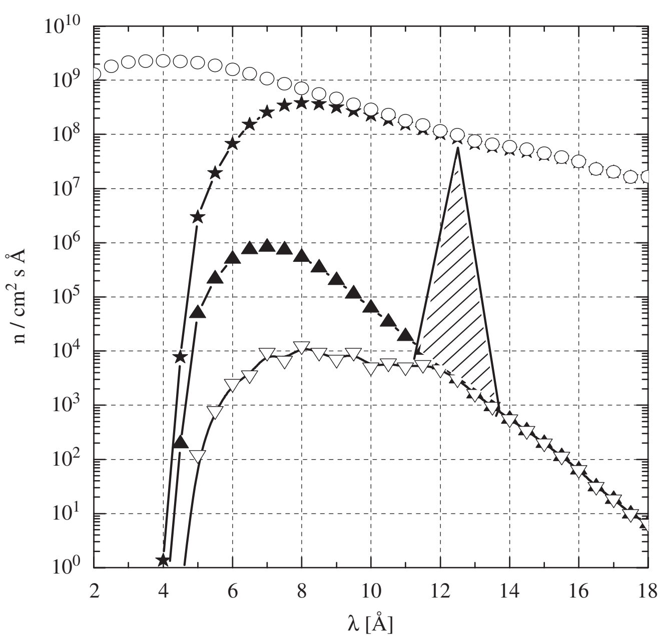

Fig. 5. Neutron flux delivered by the KWS3 guide calculated upon the measured intensity at NL1 [6]: open circles—at the entrance; stars—at the output of the anti-trumpet-like guide; filled triangles—the neutron flux transported through the selector blades; open triangles—the "background" in the sample position (reflected by the toroidal mirror); the monochromatic beam ($\lambda = 12.7$ Å, $\Delta\lambda/\lambda = 20\%$) is schematically represented by the large triangle.

and ^{58}Ni for the horizontal walls, while the following straight piece is overall coated with ^{58}Ni. The calculated background to monochromatized beam ($\lambda = 12.7$ Å) ratio after the focusing mirror is about 10^{-4} (see Fig. 5): this background is caused by short wavelength neutrons passing through the MgLi velocity selector blades (filled triangles in Fig. 5) and partly reflected further by the toroidal mirror (open inverse triangles). This optimized guide simulation shows that expected flux at KWS3 is about 100 times higher than that at FRJ-2 reactor (for $\lambda = 12.7$ Å and $\Delta\lambda/\lambda = 20\%$). This gain in flux will allow us to increase the Q-resolution up to 3×10^{-5} Å^{-1} by using smaller entrance apertures and larger wavelengths (16–20 Å) and thus, enter the Q-range that is traditionally accessed by the double-crystal diffractometry technique.

3. Conclusions

With a high cold neutron flux provided by the FRM-II reactor and a newly designed optimized neutron guide system the SANS instruments installed and operated by the JCNS will belong to the best instruments of such a kind world-wide. The expected increase in flux compared to the situation in Jülich is of about 15 times for the conventional KWS1 and KWS2 pinhole diffractometers and 100 times for the mirror-focusing KWS3 instrument. This significant gain in flux will allow for the successful use of the longer wavelengths up to 20 Å or even beyond and will permit, by combing both kinds of SANS instruments, to perform structural investigations within four orders of magnitude in the Q-range between 3×10^{-5} and 0.3 Å^{-1}.

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