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Study on s-shaped guide using mcstas software

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ABSTRACT

Monte Carlo simulations are performed for a vertical S-shaped neutron guide for the cold neutron sources of the FRM-II, HZB and PSI reactors through the McStas software. The aim of our study is investigate a relation between the cutoff in the cold neutron spectrum and the sources. Results for the neutron flux at the sample position are presented for different supermirrors with m = 1, 2 and 3. The vertical S-shaped neutron guides additionally provide a vertical displacement between beam hole and sample position, which can facilitate the implementation and manipulation of sample environments.

Keywords: **Neutron guides, Monte Carlo method, McStas.**

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1. INTRODUCTION

Small Angle Neutron Scattering (SANS) is a powerful technique for investigating the structure of polymers [1], food science [2], drug delivery [3] and biological [4] systems. SANS was developed by Shull and Brock-House (Nobel Prize in Physics, 1994) during the decade of 1950 and has gained new improvements until today. The instrument configurations has been continuously upgraded, from velocity selectors to modern optical systems. SANS was fundamental instrument in Florys predictions to random polymer walks (Nobel Prize in Chemistry, 1974) and the discovery of magnetic vortices in type II superconducting materials by Abrikosov (Nobel Prize in Physics, 2003).

Monte Carlo simulations are extremely useful in this scenario, because of the high cost and complexity of nuclear facilities. In this spirit, many studies have been done for components of SANS instruments through software McStas [5]. The neutron transport through curved guides allows the elimination of gamma rays and fast neutrons (λ < 1 Å), getting low background condition and transmission efficiency of about 90 % [6]. Studies on the transport of neutrons in curved guides with non-perfect reflectivity can be found in the literature [7]-[8], where the authors obtain analytical expressions for the angular and spatial distributions through acceptance diagrams.

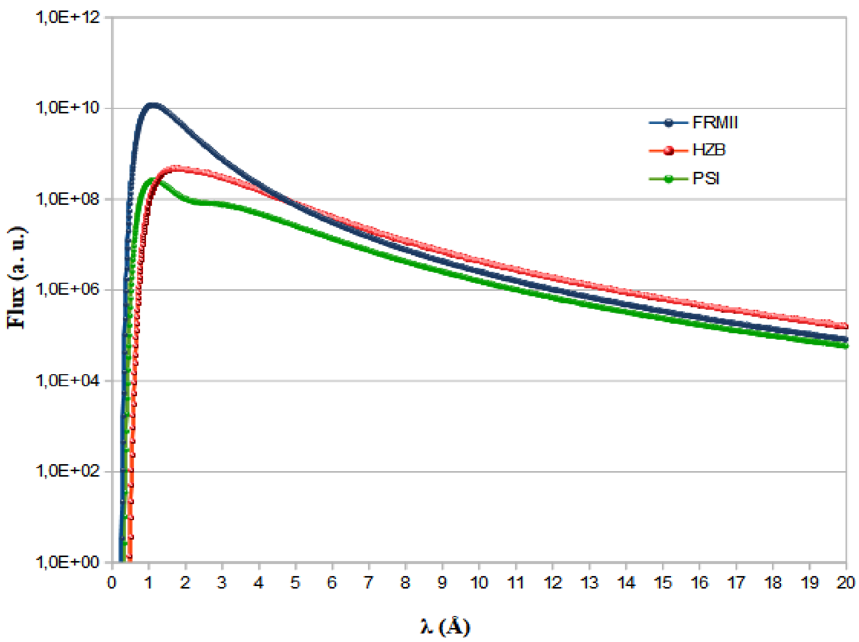
Considering the concept of SANS instrument at the FRM-II, Germany, Gilles and co-authors studied the transport of neutrons by a S-shaped guide [9]-[10]. The authors obtained the neutron flux values at the sample position for single-curved and S-shaped guides. It was observed a cutoff in the neutron spectrum using a vertical S-shaped guide type r = 480 m with coatings of Ni^{58} and supermirrors with m = 2. This configuration provides a sharp wavelength cutoff at λ_C = 3 Å. In this work the authors further observed that λ_C corresponded to the peak neutron flux in a single curved guide, which allows the transport of neutrons below 3 Å. The aim of our study is to investigate the dependence between different sources of neutrons and the cutoff in the cold neutron spectrum [9]-[10].

2. S-SHAPED GUIDE AND SIMULATIONS

The simulations were performed for the FRM-II, HZB and PSI cold neutron sources, which beam profiles are in the McStas software, a general tool for simulating neutron scattering instruments and experiments. The dimensions of the S-shaped guide were fixed, that is, two parts of length L = 16 m and radius R = 250 m, with openings of 50 mm x 50 mm. Additional straight guides 1 m long were implanted at the ends of the S-shaped guide, totaling a length of 34 m. The neutron flux was obtained at the sample position after a collimation length of 1 m.

The profiles of the neutron sources are shown in Figure 1, where we observe that the peaks of the fluxes are in the interval 0 < λ < 3 Å. The dominance of fast neutrons in this range was already expected, since the thermalization time of the cold source is not reached. Fast neutrons provide large values of transferred moments, being unable to reveal nanostructures, thus justifying their exclusion from the beam. We can observe that for a fixed supermirror, the wavelength cutoff of the neutrons is independent of the source.

Figure 1: *Cold neutron source profile of FRM-II, HZB and PSI reactors.*



3. RESULTS AND DISCUSSION

Figures 2 - 4 present the results of the simulations for S-shaped guides coated with supermirrors of m = 1, 2 and 3. The increase in the value of m implies the increase of the neutron transmission rate. Therefore, we can observe higher peak values for m = 3 than m = 1 and 2. For the same reason, the wavelength cutoff shifts to the low λ region where the increase of m restricts only neutrons with λ < 3 Å.

The results of the FRM-II source as a function of m is show in Figure 5. We can observe that λ_C shift at low wavelengths with the increase of m, according to adjusted equation λ_C (m) = 6.5 × $m^{-0.83}$, where λ_C is the wavelength cutoff in angstrons. This result is physically expected, as already seen, the neutron absorption increase for low m values (lower peaks). The same effect is observed for the other HZB and PSI sources, according to Figures 2 - 4. It is important to note that guides coated with supermirrors of m = 1 and 2 have peak fluxes of approximately 2 % and 29 %, respectively, at the peak value of m = 3. Therefore, the use of S-shaped guides coated with supermirrors of m < 2 should be avoided for the SANS instrument.

Figure 2: *Simulations of S-shaped guide with coating of Ni^{58} and supermirror with m = 1.*

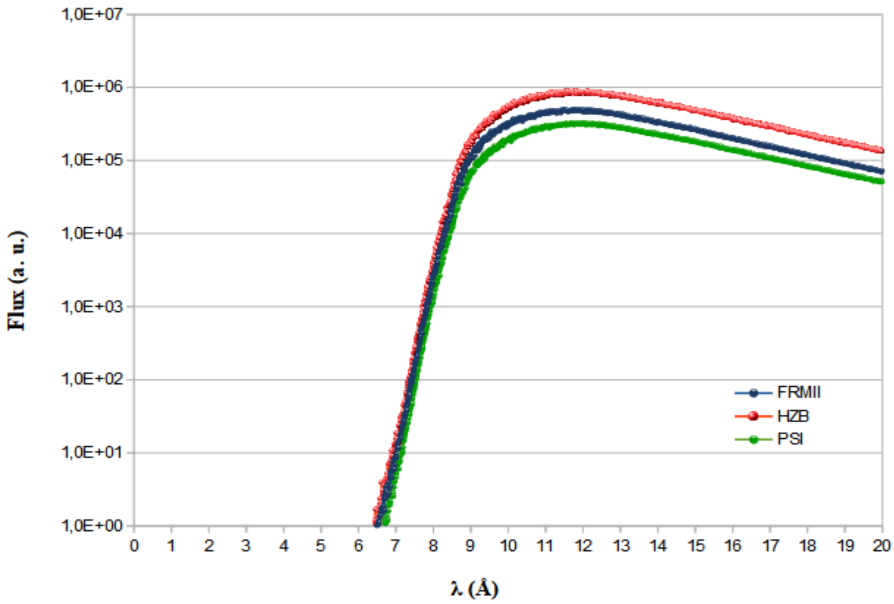


Figure 3: *Simulations of S-shaped guide with coating of* Ni^{58} *and supermirror with m = 2.*

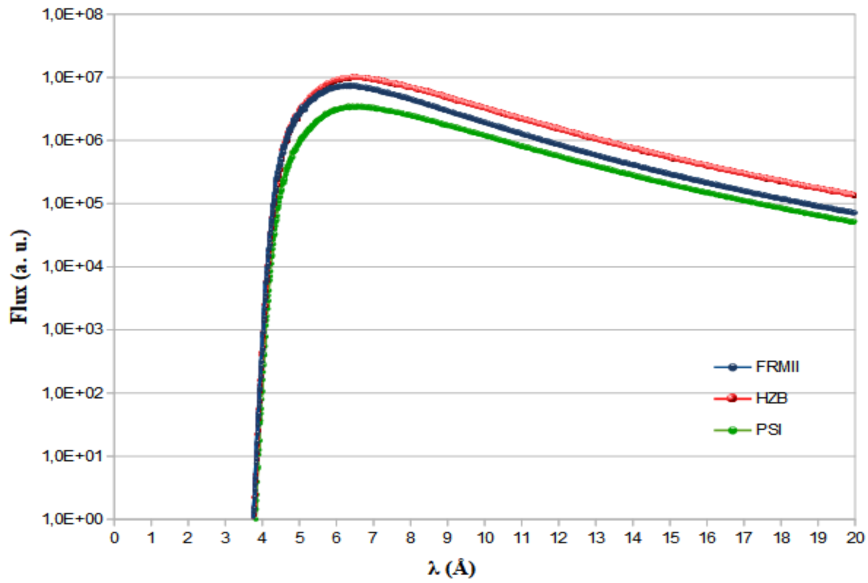


Figure 4: *Simulations of S-shaped guide with coating of* Ni^{58} *and supermirror with m = 3.*

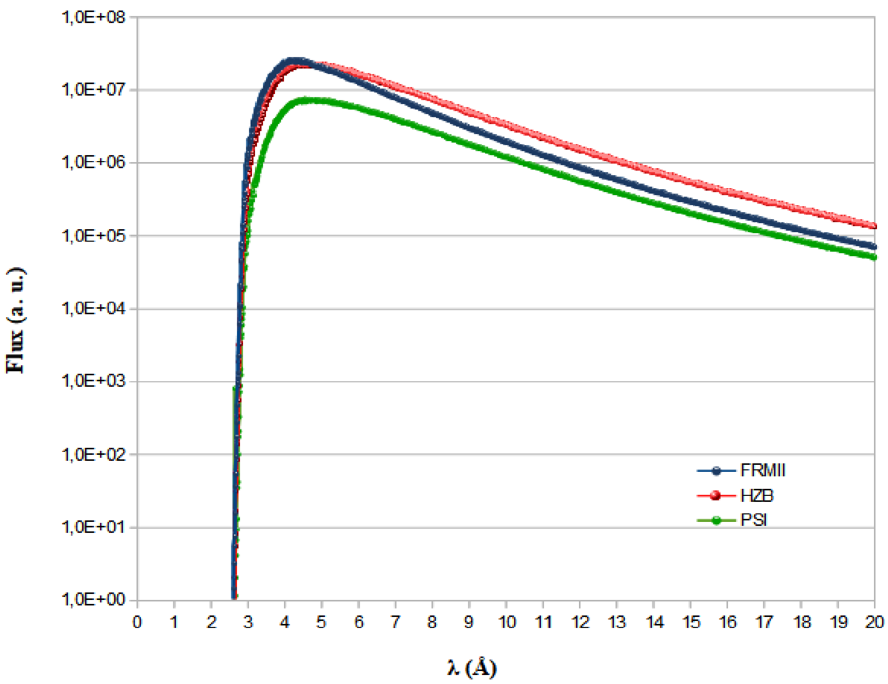
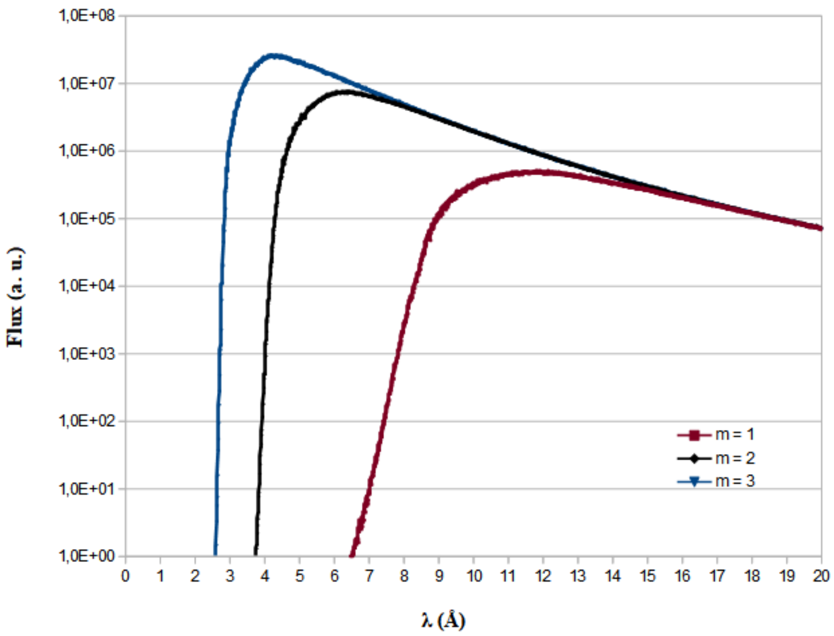


Table 1: Main parameters extracted from Figures 2-4. λ_{peak} (Å) is the wavelength at which the neutron flux (Φ_{max} (a.u)) is maximum and - α (a.u/ Å) is the slope of the distributions after the peak.

Source	*m*	λ_C (Å)	λ_{peak} (Å)	Φ_{max} (a.u)	- α (a.u/ Å)
FRM-II	1	6.5	12.2	5.1×10^5	5.6×10^4
HZB	1	6.5	12.1	8.8×10^5	9.5×10^4
PSI	1	6.6	12.3	3.3×10^5	3.6×10^4
FRM-II	2	3.5	6.5	7.6×10^6	5.6×10^5
HZB	2	3.5	6.5	1.0×10^7	7.5×10^5
PSI	2	3.5	6.3	3.6×10^6	2.6×10^5
FRM-II	3	2.5	4.1	2.6×10^7	1.6×10^6
HZB	3	2.5	4.4	2.3×10^7	1.5×10^6
PSI	3	2.5	4.6	7.5×10^6	4.9×10^6

Table 1 shows the main parameters extracted from Figures 2 - 4. We can observe the values of wavelength cutoff λ_C (Å) for the different supermirrors (m) and sources. λ_{peak} (Å) is the wavelength at which the neutron flux Φ(Å) is maximum and (– α) is the slope of the distributions after the peak.

Figure 5: *Simulations of S-shaped guide with coating of Ni*^{58} *and supermirrors with m = 1, 2 e 3, for FRM-II reactor .*



4. CONCLUSION

In this study we investigate the dependence between different cold neutrons sources and the wavelength cutoff for a S-shaped guide, inspired by the work of Gilles et al. [9]-[10]. We conclude that λ_C is independent of cold neutron source and dependent on the supermirror used in the guides. The S-shaped guide provides a filter for fast neutrons and gamma rays, undesirable in the SANS technique. Our results have a direct impact on the installation of a SANS instrument in facilities with space limitations, allowing the sample to be on a different plane from the beam hole.

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