Virtual design of the neutron guide for the TOF spectrometer NEAT

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Abstract. We present the results of a virtual design study based on Monte-Carlo neutron ray tracing techniques for the neutron guide of the time of flight (TOF) spectrometer NEAT. We studied several configurations with linearly or elliptically tapered compressors with different degrees of focusing and different guide coatings. The calculations were performed and cross-checked using two software packages which produced similar results. The geometrical arrangement of selected guide components was optimised with the Particle Swarm Optimisation algorithm. The results of the Monte Carlo simulations confirm an expected intensity gain factor of approximately 5, that can be achieved by the optimal configuration.

1. Introduction
NEAT is a direct time-of-flight cold neutron spectrometer designed to study the dynamics and structure in the time domain $10^{-13}$ s–$10^{-10}$ s and on the length scale ranging from microscopic (0.5 Å) to nanoscale dimensions (up to about 50 nm). To transport neutrons from the neutron source to the sample NEAT uses a neutron guide. The current guide of NEAT starts 1.5 m behind the cold source with a cross section 3 cm wide and 12.5 cm high (Figure 1). At a position 30.8 m behind the cold source the guide is horizontally split in half and only the upper half of the guide with a vertical dimension of 5.5 cm is used for the NEAT spectrometer. To monochromatise neutrons NEAT uses disc chopper devices which are installed in four chopper housings, located 35.1 m, 37.5 m, 42.6 m and 47.2 m from the cold source. The last section of the guide employs a so-called “eye-of-the-needle” section to optimise the intensity for the short chopper pulses. This device was invented in the course of the design process of NEAT [1]. In front of the last chopper the guide is horizontally focused to a width of 15 mm by a converging section and then decompressed towards the sample by using the diverging guide section. The neutron guide is coated with $^{58}$Ni, except for the converging-diverging sections which are made of supermirrors.

2. Simulations for the new configurations
Thanks to the number of important innovations at its conception, NEAT had equivalent flux, in spite of the medium flux of the reactor, and somewhat better ultimate resolution than the other best in class instrument worldwide, IN5 at ILL, for the first 10 years of operation. The fast evolution of TOF neutron spectroscopy in the last years resulted in an increase of the data rate of more than an order of magnitude at the world-wide leading instrument, and new developments at pulsed spallation sources promise a tremendous progress in performance. To maintain the
competitive edge of NEAT, a full upgrade of the instrument has recently been proposed [2]. The proposal includes the replacement of the existing neutron guide by modern supermirror neutron optics and a ballistic guide concept [3] to gain a factor of 5 in incident neutron flux compared to the present instrument. Here we present the results of the computer simulation study of the upgrade of the NEAT neutron guide. The new guide (Figure 1) is 12.5 cm high and 6 cm wide. The sample position has been moved 15.5 m downstream. To couple the neutron guide to the sample dimensions the neutron beam is compressed horizontal and vertically.

We conducted a computer simulation study of the new guide configurations using the VITESS software package [4]. To simplify the optimisation of the guide design, we decoupled the vertical and the horizontal dimensions in the calculations. For this purpose the neutron guide was simulated with perfectly reflecting mirrors in the dimensions of no interest, and the gaps between the different components, namely the guide exit and the sample position, were simulated with a perfectly absorbing mirror in the dimension of interest. Thus the total transmission is a product of the transmissions in both dimensions. For the verification we independently ran complete 2D simulations with final optimised parameters. Two detection windows were assumed in the calculations: one at the position of the guide exit and another one at the position of the sample. The intensity of the neutrons arriving at the sample was used as a final parameter for the neutron guide optimisation. VITESS calculations were combined with the Particle Swarm Optimisation (PSO) algorithm used to optimise the geometrical parameters of the guide and to maximise the total flux at the sample. PSO is a stochastic, population-based evolutionary algorithm used to find the optimum solution of a problem [5, 6]. As a final step, the calculated wavelength-dependent flux was divided by the flux delivered by the present NEAT guide.

2.1. Calculations of the horizontal configuration
As mentioned above the horizontal dimension of the guide equals 60 mm. It starts with a straight section 3.34 m long coated with supermirrors of $m = 3\theta_c$. To filter fast neutrons the guide includes a curved 40 m length long section coated with supermirrors with $m = 3\theta_c$ for the outer side and $m = 1.5\theta_c$ for the inner side. It is followed by a straight section and a compressor section. The length of the compressed section in the simulation was varied in the range of 2.01 m–7.34 m depending on the coating of the guide. For the optimisation of the guide configuration, we studied two options: (1) The neutron beam was compressed by a single linear part to deliver the beam to the sample. (2) This configuration included two parts, i.e., first a linear converging section that compresses the beam to 18 mm in front of the last chopper, which is placed 1.3 m from the sample, and then transports the neutrons by linear or diverging part to the sample. We simulated several configurations with different coatings and different compressor-decomposer distances (Table 1).

Figure 2 shows the gain factor and Table 1 shows the optimised geometrical parameters.
Table 1. Optimised exit width and converging length of the compressor part in the horizontal dimension for the cases of focusing on the sample and focusing on the last chopper, with samples of size 2.2/2.75/3.0 cm.

| m  | Focus on the sample | Focus on the last chopper |
|----|---------------------|--------------------------|
|    | Width (cm) Length (cm) | Width (cm) Length (cm)   |
| 3.5| 2.90/3.20/3.47 209.1/201.2/273.0 | 2.30/2.36/2.36 618.0/618.0/618.5 |
| 3.0| 2.91/3.24/3.47 208.4/234.9/266.9 | 2.57/2.35/2.57 604.2/620.6/604.4 |
| 2.5| 3.10/3.39/3.47 211.7/264.6/270.9 | 2.43/2.34/2.42 611.6/612.5/611.8 |

Figure 2. Gain factor for horizontal configuration with focusing on the sample (left) and focusing on the last chopper (right), for a sample width of 3 cm.

3. Discussion

Our calculations confirm an efficiency gain of a factor of even more then 5 of the new improved guide with increased dimensions for the neutron transport, as it was indicated by analytical approximations (Figure 3). The larger gain is observed in the short wavelengths range which is particularly important for low temperature and magnetism experiments, areas which are of strategic importance at Helmholtz-Zentrum Berlin.

The main problem with using a wider or higher neutron guide is the increased divergence of the beam when the neutrons are compressed towards the sample area with a smaller cross section and higher supermirror coatings. Because of the higher divergence fewer neutrons reach the sample, if they are not guided by the guide. Thus we identified the gap between the guide exit and the sample position as one of the main sources of the neutron losses. For the horizontal configuration with the guide-sample distance of 70 cm a gain factor of no more than 1.5 could be achieved. The gain increases up to the factor of 2.5 when the distance between the guide exit and the sample is decreased to 30 cm. The divergence can be decreased by increasing the sample width and height, which on the other hand spoils the resolution of the secondary spectrometer. Thus, we have two contradictory conditions which influence the guide configuration: On one hand the guide dimensions of the extraction part should be as large as possible to extract the largest possible number of neutrons, on the other hand the divergence should be reduced to avoid the losses. These conditions and the performance requirements of the secondary spectrometer motivated our choice for sample dimensions limited to a width of 27.5 mm and a height of 60 mm.

Furthermore, we observed that the intensity and the homogeneity of the beam on the sample improves if the dimensions of the guide exit are slightly larger than the dimension of the sample.
(Table 2). We observed this trend for all configurations in both dimensions. In the horizontal dimension the configuration with the neutron beam focused on the sample (a) proved to be more advantageous compared to the configuration with the compressor focused in front of the chopper (b). Thus, the gain factor of about 2.5 was observed for the configuration (a) while the configuration (b) only allows for a gain factor of 1.2–1.5. The configuration (a) is best optimised for the medium resolution of the primary spectrometer, when the chopper slit matches the guide width of 40 mm. However, it still allows the high-resolution experiments with chopper slits of 18 mm and delivers nearly the same intensity as in the case of configuration (b). Experience with NEAT user operation shows that about 80% of the experiments use the medium range resolution configurations which will optimally be realised by configuration (a).

4. Conclusions
Detailed simulations of the different guide configurations using an approach combining VITESS and Swarm Particle Optimisation were carried out for configurations possible for the time-of-flight spectrometer NEAT. The horizontal and the vertical configurations were split and analysed separately. Our calculations show that utilisation the neutron guide of $12.5 \times 6 \text{ cm}^2$ cross section coated with supermirrors of $m = 1.5\theta_c$ coupled to the sample of $2.75 \times 6 \text{ cm}^2$ dimensions by supermirror compressor part of $m = 3\theta_c$ results in substantial intensity increase. The gain factor of 5 and higher was calculated for the broad wavelength range of $2 \text{ Å}–15 \text{ Å}$.

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