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Physica B 350 (2004) e687–e689

PHYSICA B

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Optimisation of guide exits by combining MC simulations and optimising routines

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Abstract

In many neutron scattering instruments a convergent guide exit is used to increase the flux on the sample. But at the same time, the divergence of the neutrons increases. The resultant flux on the sample can increase or decrease depending on its distance to the guide exit and the sample size (relative to the guide size). An optimum can be expected for an intermediate convergence. It was our aim to find this optimum for different distances and samples sizes. Therefore, we have performed MC simulations with the software package VITESS. We combined it with a numerical method to find the optimal values. Different kinds of shapes were tested. The influences of starting values and criteria for the optimal exit were checked. For long wavelengths and great distances between exit and sample, the maximum was obtained by diverging exits and not by converging exits. Funnels with a kind of elliptical shape perform better than linearly converging ones. Significant gains can be reached by adapting exits to a certain wavelength range—at the cost of losses in other ranges.

PACS: 02.70.Uu; 02.60.Pn; 61.12.Ex

Keywords: Monte Carlo simulations; Neutron scattering instruments; Guide exit; Optimisation

In many neutron scattering instruments, a focusing guide exit is used to enhance the flux at the sample and/or to improve the spatial resolution. The flux is increased by a converging guide, but at the same time the divergence is increased. A small guide exit increases the flux at the sample, whereas a high divergence decreases it. An optimum flux will be achieved by an intermediate convergence. Apart from the sample size, this optimum will depend on the distance between guide exit and sample, because the effect of divergence increases with rising distance between guide and sample. Furthermore, the optimum depends on the wavelength range, as the possible divergence and therefore its influence rises with wavelength.

We used the MC package VITESS [1,2] to examine these dependences. Moreover, we tried to find shapes of funnels giving a higher flux on the sample as a linearly converging funnel. We simulated a simple instrument consisting of a continuous source with a cold moderator, a guide of $6 \times 6\,\mathrm{cm}^2$ size and 20 m length beginning 2 m from the moderator, and a sample. The distance between guide exit and sample and the sample size were varied (details in Table 1).

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doi:10.1016/j.physb.2004.03.263

Table 1
Simulation data

Component	Position (m)	Parameters
Source	0	Continuous source $12 \times 12\,\mathrm{cm}^2$, 1–12 Å moderator temp. 45 K, total flux $3 \times 10^{13}\,\mathrm{n/(cm^2 s)}$
Guide 1	2–12	Straight, $m = 1$, $6 \times 6\,\mathrm{cm}^2$
Guide 2	12–22	Converging, $m = 3$, $6 \times 6 \rightarrow a \times b$
Sample	22.5/23.5/24.5/25.5	$1 \times 1\,\mathrm{cm}^2/2 \times 2\,\mathrm{cm}^2/4 \times 4\,\mathrm{cm}^2$

The first 10 m of the guide were of constant size, the second 10 m were varied. In most cases, the size decreased linearly over the 10 m. All components had the same sizes in horizontal and vertical direction. To compare the results, a transmission T was defined as the ratio of count rate on sample to count rate at the end of the straight guide. The simulation of the instrument was combined with an optimization routine to find sizes that yield optimal results. The criteria for optimal results were highest transmission T (for the whole wavelength range) or highest flux at the sample (for small ranges).

To perform this combination, the simulation is interrupted after the straight guide and the data of the trajectories are stored. The rest of the simulation is then performed several times with variations of the parameters of interest (reading the stored data as input). A numerical method is used to find parameter values with improved performance for the next simulations. This procedure converges after a few steps giving the optimal exit. This routine was already successfully used to optimize guide exits [3,4]. Here it is used to study more general features of guide exits.

Half a million trajectories were stored after the first part of the instrument; this number is sufficient to get results that are practically independent of statistical effects from the Monte Carlo procedure (see Table 2). Also the starting values have no influence on the result, if the number of fitted parameters is low (cf. Table 2).

Table 2
Influence of simulation and optimization parameters on optimal size of guide exit

Random seed	Initial Value (cm)		
	3	6	9
0	—	4.03	—
1	4.09	4.01	4.00
2	—	3.96	—

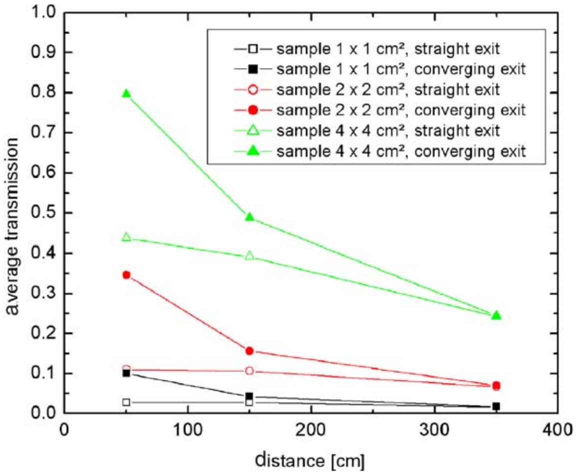

Fig. 1. Transmission T averaged over wavelength range 1–12 Å as a function of distance: exit–sample for different sample sizes.

Table 3
Optimized sizes of guide exits as a function of sample size and distance guide exit-sample

Sample size (cm^2)	Distance (cm)		
	50	150	350
1×1	2.53	3.82	5.21
2×2	2.65	4.01	5.17
4×4	3.46	4.32	5.60

The results show that large gains (up to a factor of 4) can be reached by converging funnels (compared to straight exits) for short distances between guide exit and sample, especially for small samples (see Fig. 1). The optimal exit size increases with distance to sample and sample size (see Table 3).

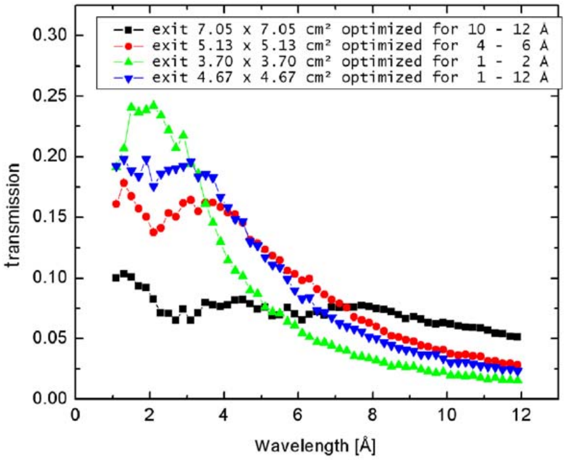

Fig. 2. Transmission T as a function of wavelength for exits sizes found by different optimization criteria (sample size $2 \times 2\,\mathrm{cm}^2$, distance 2.5 m).

The optimal exit size also increases with wavelength and can even reach values larger than the guide size for long distances to the sample, i.e. the exit is diverging (see legend of Fig. 2). Optimizing for long wavelengths yields a gain of about a factor of 2 (compared to a funnel for the whole wavelength range) at the cost of similar losses in the low wavelength range—or vice versa: improving the short wavelength performance gives losses for longer wavelengths (see Fig. 2).

We have found that there are better shapes than a linearly converging funnel (see Table 4). The optimal funnel consisting of 5 pieces of 2 m lengths (without any restrictions) is similar to an elliptical shape, slightly diverging within the first 4 m, than more and more converging to the exit. Similarly, the funnel consisting of 2 linear parts has a (6.87 m) long slowly diverging part followed by a short converging part.

Table 4

Properties of optimized exits for different shapes (sample distance 150 cm, sample size $2 \times 2\,\mathrm{cm}^2$, average transmission optimized)

Shape	Exit size (cm)	Average transmission (%)	Flux on sample (n/(cm^2 s))
Constant	6.00	10.6	0.99×10^9
Linear	4.01	15.6	1.77×10^9
Double linear	4.21	18.5	2.05×10^9
5 pieces, free	4.24	20.2	2.32×10^9

In general, funnels should be adapted to wavelength range, sample size and distance: guide exit–sample. Instruments can be improved by using 2 or more guide exits. More detailed studies including comparisons with analytical calculations are planned for the future. Combining MC simulations and optimization routines is a promising concept. In principle, this method can be extended to optimise other devices in the instrument.

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