Nuclear Instruments and Methods in Physics Research A 634 (2011) S1–S6

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Optimal shape of a cold-neutron triple-axis spectrometer

K. Lefmann [a,b,*], U. Filges [c], F. Treue [a], J.J.K. Kirkensgård [d,e], B. Plesner [d], K.S. Hansen [d,f], K.H. Klenø [a,b]

[a] Nanoscience and eScience Centers, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen Ø, Denmark
[b] European Spallation Source, University of Lund, St. Algatan 4, Lund, Sweden
[c] Laboratory for Development and Methods, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
[d] Institute of Nature and Models, Roskilde University, Denmark
[e] Department of Basic Sciences and Environment, Faculty of Life Sciences, University of Copenhagen, Denmark
[f] Mid-Greenland High School, Nuuk, Greenland

ARTICLE INFO

Available online 1 July 2010

Keywords:
Neutron instrumentation
Triple-axis spectrometer
Ray-tracing simulation

ABSTRACT

We have performed a McStas optimization of the primary spectrometer for a generic 40 m long, cold-neutron triple-axis spectrometer with a doubly focusing monochromator. The optimal design contains an elliptically focusing guide, a virtual source point before a low-grade PG monochromator, and non-equidistant focusing at the monochromator. The flux at 5 meV shows a gain factor 12 over the "classical" design with a straight $12 \times 3\,\mathrm{cm}^2$, $m = 2$ guide and a vertically focusing PG monochromator. In addition, the energy resolution was found to be improved. This unexpectedly large design improvement agrees with the Liouville theorem and can be understood as the product of many smaller gain factors, combined with a more optimal utilization of the beam divergence within the guide. Our results may be relevant for a possible upgrade of a number of cold-neutron triple-axis spectrometers—and for a possible triple-axis spectrometer at the European Spallation Source.

1. Introduction

The triple-axis spectrometer (TAS) is one of the oldest and most well-known types of neutron instrumentation; designed by the Nobel Laureate B.N. Brockhouse already in the 1950s [1]. Later ingenious instrument development has improved on the original design, most importantly the cold neutron moderator [2], and the neutron guide, which allows the transport of cold neutrons ($\lambda > 2$ Å) far away from the background-rich region around the neutron source [3]. An excellent recent textbook has been devoted to the description and use of the TAS [4]. However, there may still be some room for design improvements, which is the topic we investigate in this article.

Many cold-neutron TAS exist at continuous neutron sources around the world. Most of these instruments have adopted the 1990s design, where the neutrons are transported by a 30–50 m curved supermirror guide, and reflected down to the sample by a vertically focusing monochromator made by mosaic pyrolytic graphite (PG). Some examples of TAS of this design are IN-12 and IN-14 at ILL [5], TASP and RITA-2 at PSI [6], FLEX at HZB [7], and SPINS at NIST [8]. New developments in guide technology and the appearance of doubly focusing monochromators, implemented *e.g.* at PANDA (FRM-2) [9] and MACS (NIST) [10] have spawned ideas of upgrade of a number of cold-neutron TAS, *e.g.* at ILL, PSI, and HZB.

In this article, we will address the question of how to improve the configuration of the primary spectrometer of the cold-neutron TAS. We have simulated different instrument designs by use of the Monte Carlo ray-tracing package McStas [11]. We start by investigating the characteristics of the classical TAS design and then perform a number of controlled design changes. The optimal design is then found by a "free" computer optimization of all parameters, which is again restricted to find a realizable design. Finally, we explain the found results in terms of phase space densities and the Liouville theorem and discuss the optimal design of the complete cold neutron triple-axis spectrometer.

2. Design and simulation

The baseline design for these simulations is defined in terms of moderator, guide, and monochromator and can be seen as an idealization of the RITA-2 spectrometer at PSI. The moderator has a uniform neutron distribution over its $15 \times 10\,\mathrm{cm}^2$ area and follows a typical cold spectrum with an intensity corresponding to a medium flux source. We have chosen the parameters valid at 2002 for SINQ running at 1 mA current, as already used in Ref. [12]. The guide is 40 m long with $m = 2$ supermirrors and a reflectivity of 90.5% at $q = mQ_c$ ($\alpha = 4.38$ in McStas units) and has

* Corresponding author at: Nanoscience and eScience Centers, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen Ø, Denmark. Tel.: +45 35320476.
E-mail address: lefmann@fys.ku.dk (K. Lefmann).

0168-9002/$ - see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.nima.2010.06.273

a cross-section of $30\times120\,mm^2$. The guide starts 1.5 m from the moderator with a 5 m straight section, followed by a 20 m curved section with a curvature of $R=2$ km, and finally a 15 m straight section. The monochromator is placed 0.5 m after the guide opening and is made from PG with 30′ mosaicity and a reflectivity of 80%. The monochromator has five vertically focusing blades, each 30 mm tall and 200 mm wide, with a 1 mm gap between blades. The sample is positioned 1.5 m from the monochromator, the smallest distance achievable in practice due to shielding and sample environment requirements.

All simulations were performed with 5×10^7 neutron rays (2×10^7 when only flux numbers were required), corresponding to 5 min (2 min) processing time on a standard 2 GHz laptop for the straight guide. In most simulations, the monochromator was set to reflect neutrons of 5.0 meV ($\lambda=4.045$ Å). We recorded neutrons reaching the sample area, which is $1\times1\,cm^2$. The absolute flux value was for the baseline design found to $\Psi=4.03(2)\times10^6$ n/s/cm^2, with a spread (FWHM) of the incoming neutron energy of $\Delta E_i=127\,\mu$eV. These baseline results were used as the starting point for the optimization procedure, see Table 1.

Simulation of a very similar primary spectrometer has been performed for the RITA-2 spectrometer at PSI, and the results for both flux and (in particular) energy resolution of vanadium scans were found to agree well with the performance of the real spectrometer over a wide wavelength range [12,13]. This serves as a validation of the results of the present simulations, both in terms of absolute flux value and (in particular) on relative flux improvements and energy resolution. The energy spread of the incoming neutrons should be viewed in relation to the acceptance of the secondary spectrometer. For example, at RITA-2 this value is 141 μeV without collimation. The energy resolution of the complete spectrometer is found (for incoherent scattering) by adding the two contributions in quadrature.

2.1. Controlled design upgrades

Our initial simulations contained a series of individual optimizations to the design. The optimizations were performed in the order given below, and were mostly performed by optimizing the sample flux while varying a single parameter at a time. The gains mentioned should be understood as *additional* gain compared to last design change. The corresponding results are listed in Table 1.

- Improving the supermirror coating. This resulted in a surprisingly small flux increase (5%), reached at $m=4$.
- Increasing the guide width. This gave a large flux gain of almost 60% for $w=5$ cm, but a broadening in energy of around 40%.
- Increasing the guide height and inserting additional blades in the monochromator. This gave a further flux increase of 25% for $h=16$ cm.
- Increasing the PG mosaicity. A flux gain of almost 50% was found for $\eta=70'$, surprisingly without change in ΔE
- Doubly focusing monochromator, composed of $25\times25\,mm^2$ tiles. This resulted in an additional flux gain of 10% and an improvement of energy spread to almost the baseline design.
- Increasing the guide-monochromator distance to 2.4 m and the PG mosaicity to 45′. This gain was small, around 15%, and there was a small increase of energy spread.

Table 1
Results of the optimizations: flux (Ψ) and energy spread (ΔE_i) at the sample position.

Change	Ψ (10^6 n/s/cm^2)	ΔE_i (μeV)
Baseline	4.03(2)	127
Guide coating $m=4$	4.26(3)	130
Guide width 5 cm	6.62(5)	195
Guide height 16 cm	8.38(7)	195
Mosaicity 70′	12.24(8)	183
Doubly focusing mono.	13.52(8)	153
Fine-tuning mono.	15.82(6)	172
Elliptical guide, focus on mono.	26.7(4)	165
Virtual source, fine-tuning	35.7(3)	237
Free optimization	79.6(4)	137
Restrained, free optimization	44.9(2)	85

The individual steps are described closer in the text.

Increasing the monochromator-sample distance to 2.1 m to almost obtain equidistant (Rowland) focusing decreased the energy spread by 30%, but simultaneously lowered the flux by 40%. Hence, this idea was abandoned.

At the end of this simulation round, we received a flux gain of a factor 3.9 and an enlarged spread of the incoming energy of only 35%. This agrees rather well with earlier optimization studies for RITA-2 [14].

2.2. Optimization with an elliptical guide

The simulations in the previous section were performed with a conventional guide system with a constant cross-section. Recent developments in guide technology has enabled the construction of fully elliptical guides with strongly improved focusing possibilities [15]. Thus, it was natural to include elliptical guides in our design.

For truly elliptical guides, there is the complication that line-of-sight between moderator and monochromator will increase the fast-neutron background. At present a number of suggestion to circumvent this problem exist, none of which will cause substantial flux loss, including a bending of the elliptical guide, placing a beam stop within the guide, and accepting the (limited) additional background from the fast neutrons [16–18]. It is, however, at present not clear which of these solutions will prove most efficient in practice. Therefore, we here continue the optimization using only neutron flux and energy spread as optimization parameters, ignoring the line-of-sight complication.

We have continued the optimization, replacing the curved guide with an elliptical guide of the same dimensions. As a reassurance, we first reproduced the results below for a guide of infinite focal length. Next, we used focal lengths of 2.0 m—meaning that both the focal points were placed 2.0 m outside the guide. This provided a significant flux gain (65%) over the straight guide. Then, we created a virtual source by using 1.4 m focal length and placing the monochromator at 2.9 m to obtain Rowland focusing. This was accompanied by fine tuning of the monochromator parameters, and additional height to the monochromator. This scheme gave a flux gain of additional 35%, but again an increase in the energy spread. In total, this design gives us a 9-fold increase in flux at the cost of a factor 2 increase in energy spread.

2.3. Total computer optimization

Having obtained the encouraging results by the manual single-parameter optimizations, we went to explore unknown territory by performing a total computer optimization of most parameters describing the guide-monochromator system. The total number of parameters was 14, small enough to be achievable by the Simplex algorithm already implemented in McStas.