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Modelling of wavelength cut-off filters and polarising mirrors in a neutron guide

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ABSTRACT

This paper details the modelling and parametrisation of mirror-in-guide neutron deflector devices used in transmission as wavelength cut-off filters and beam polarisers for neutron scattering instrumentation. The construction of so-called 'phase-space' or 'acceptance diagrams' allows a rapid and quantitative evaluation of parameters such as the critical angles of the mirror and guide coatings, mirror angle, and transmission properties of the mirror-in-guide system. Despite its apparent simplicity, mirror-in-guide devices result in surprisingly complex properties for their neutron transmission as a function of wavelength, divergence and neutron spin due to the possibility of multiple reflections from the surrounding guide walls and multiple strikes on the mirror. Depending on the choice of parameters such devices can be configured as low-pass wavelength filters, beam polarisers or periodic notch and band-pass filters for neutron scattering instrumentation. Geometrically constructed phase-space diagrams are compared with ray-traced neutron Monte-Carlo simulations to evaluate more detailed effects such as the weighting of the transmission probability which cannot be easily evaluated using phase-space diagrams. The results of phase-space modelling and simulations are used to define the specifications of the wavelength cut-off filters and beam polarisers for the new small-angle neutron scattering (SANS) instrument, D33, currently under construction at the Institut Laue Langevin.

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1. Introduction

Neutron guides are used to efficiently transport neutrons, sometimes over long distances up to $\sim$100 m, from source to instrument at almost all neutron scattering centres [1–3]. The inclusion of various neutron optical elements such as monochromators, collimators, choppers and polarisers allow the characteristics of the neutron beam to be tailored for a particular instrument in terms of the incident neutron wavelength or energy, beam divergence, time modulation or as filters to produce polarised neutron beams [4]. Elastic scattering time-of-flight (TOF) neutron diffractometers at both reactor and spallation neutron sources typically use chopper systems to shape pulses having a broad or continuous wavelength distribution or 'white' neutron beam such that final wavelength discrimination can be made by the time of arrival of neutron events at the detector. These instruments usually require a long wavelength cut-off in the spectrum such that the pulse repeat frequency can be optimised to maximise neutron flux while avoiding frame-overlap at the detector. A simple mirror in the neutron optical path can be used as an effective long wavelength filter based on the property that the critical angle, θ_c, for total reflection for neutrons is proportional to the incident neutron wavelength [5–7]. Thus, wavelengths greater than some critical wavelength, λ_c, can be reflected out of the neutron beam and absorbed while wavelengths less than λ_c are transmitted through the mirror. Similarly, polarising mirrors in neutron guides use the difference in critical angle for reflection from a magnetised mirror for neutrons polarised parallel or anti-parallel to the magnetisation to separate the two neutron spin states and provide polarised neutron beams [8]. In order to optimise the transmitted neutron flux and remove background due to scattering from the mirror such devices are best installed inside the neutron guide system before the final beam collimation for the scattering instrument.

In neutron optics it is common to define the (wavelength dependent) critical angle of reflecting surfaces relative to that of Nickel, which has the highest scattering length density and hence largest critical angle of any element. The critical angle for neutron reflection can be approximated by the relation:

$$\theta_c[degrees] = k \times m \times \lambda[\text{Å}] \quad (1)$$

where m is the ratio of the critical angles of the mirror and Nickel surface, $k=0.1$ [degrees/Å] and λ is the neutron wavelength [Å]. The value $m=1$ corresponds to a Nickel reflecting surface and, for example, $m=0.5$ for Silicon and $m=0.65$ for borofloat glass often

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used for neutron guides. Multilayer devices can be fabricated to enhance the critical angle beyond that of elemental or compositional surfaces to values of $m > 6$, albeit with reflectivities < 1 by using the diffraction properties of bi-layers of different spacing and varying neutron contrast in the 'supermirror' multilayer structure [9].

Here we consider neutron optical components consisting of a neutron guide of coating m_g containing a mirror of coating m_m that either spans the neutron guide as a single blade or arranged in a v-geometry with mirror angle ϕ relative to the walls of the neutron guide, as shown schematically in Fig. 1. It is demonstrated how to make use of, and how to construct, phase-space diagrams to make a simple analytical approach to the appropriate design of such mirror-in-guide wavelength and polarising filter systems. This geometric and analytical approach is compared with the results of neutron Monte-Carlo (MC) simulations. This work forms the basis of the specifications of the two wavelength cut-off and two polarising mirror filters that form some of the optical elements of the new small-angle neutron scattering (SANS) instrument, D33, at the Institut Laue Langevin [10].

2. Reflection processes for a mirror in a neutron guide

Fig. 2 shows schematically the introduction of a single-blade mirror into a neutron guide, at an angle ϕ to the parallel guide walls, and depicts some characteristic neutron trajectories that might be expected, depending on the specific choice of m-values. Fig. 2(a) shows possible trajectories for incoming neutrons with zero-divergence, i.e. parallel to the guide walls and for different wavelengths. Since the critical angle of the mirror depends on the neutron wavelength, short wavelength 'hot' neutrons may have incident angles below the critical angle of the mirror and as such are transmitted. Neutrons with longer wavelengths may be reflected by the mirror, as indicated schematically by the 'warm' and 'cold' neutron trajectories in Fig. 2(a). Reflection from the mirror results in an increased divergence (angle of the neutron trajectory relative to the neutron guide) and the reflected neutron subsequently heads towards the inside surface of the guide. A similar criterion now applies for reflection or transmission (and subsequent absorption) from the guide surface. The now increased divergence means that the neutrons of shorter wavelengths may not be reflected and may be absorbed by the guide, as depicted schematically by the 'warm' neutron trajectory in Fig. 2(a). The longest wavelength 'cold' neutrons, on the other hand, may still be reflected from the guide and head back on a trajectory towards the mirror. If its angle of incidence on the mirror now exceeds the critical angle these long wavelength neutrons may finally penetrate the mirror and exit the system. Fig. 2(b) shows the equivalent reverse process where an incoming long wavelength 'cold' neutron with a high divergence, θ, manages to initially penetrate the mirror only to reflect from the guide and then reflect again from the rear surface of the mirror. The above processes of transmission or reflection by the mirror, and reflection or absorption by the neutron guide continue upon subsequent reflections with the neutron divergence increased upon every mirror reflection. As illustrated schematically in Fig. 2, these usually unwanted processes result in a contamination of the neutron beam by long wavelength neutrons, albeit with a modified divergence. We show below that the characteristics of this long wavelength transmission through the mirror depend sensitively on the relative choice of reflecting surface coating, m_m and m_g.

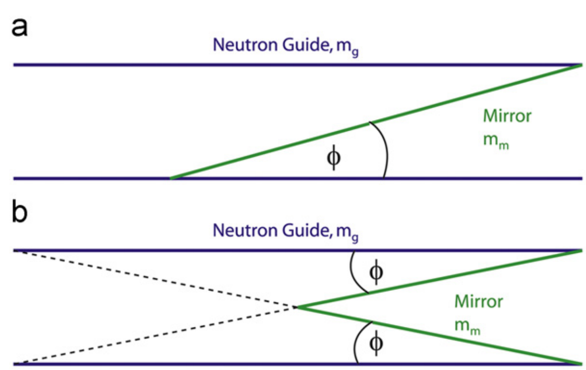

Fig. 1. Schematic diagram of a mirror-in-guide system for (a) single-blade mirror and (b) v-mirror of coating m_m inside a neutron guide of coating m_g.

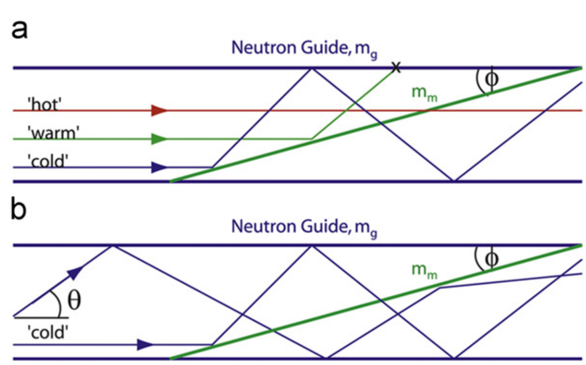

Fig. 2. Ray-traced neutron trajectories through the mirror-guide system showing processes such as reflection from the neutron guide, reflection from the mirror, transmission through the mirror and back-reflection from the mirror. Neutron trajectories labelled 'hot', 'warm' and 'cold' depict possible paths for neutrons of increasing wavelength.

3. Phase-space diagrams for a mirror-in-guide system

Neutron trajectories allowed through reflecting guide and mirror systems can be visualised using so-called 'phase-space' or 'acceptance' diagrams [11–22]. In general, neutron trajectories and properties can be characterised by as many as eight dimensions with three in space (x,y,z), three in divergence (θ_x, θ_y, θ_z), one in wavelength or energy (λ) and one in polarisation, (P). Such diagrams depict the regions of phase-space where neutrons can be present within the system [16]. A host of different phase-space diagrams may be constructed in order to graphically visualise the interplay between the various phase-space dimensions depending on the application. Most commonly plots of divergence vs. position have been used to describe neutron guide systems [11,12,14], monochromators [13,18], velocity selectors [15], chopper systems [19], assemblies of components comprising an entire instrument [17], and even, using computational acceptance diagram shading techniques, for optimising several neutrons guides and instruments in a neutron guide hall [20,22]. Recently, Copley et al. [21] have used such position vs. divergence phase-space diagrams to model neutron removal mirrors in guides that can be used as logic in a computer programme to quantify the transmission properties. Here, we show that for the application of modelling parts of θ_x and λ phase-space that is occupied, a much simpler first step is to graphically model part of phase-space using plots of wavelength vs. divergence, rather than the more usual position vs. divergence. Such diagrams produce useful insights into choosing m_m and m_g for devices such as wavelength cut-off filters and beam polarisers. Monte-Carlo ray tracing is then used to integrate phase-space to determine the transmission vs. wavelength properties of the device.

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