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# Bi-spectral moderator for spallation sources optimized for instrument requirements

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ABSTRACT

At a spallation neutron source, significant increase in the performance of neutron scattering instruments can be achieved if the target-moderator-reflector (TMR) and the following neutron guides are specifically tailored to the needs of different instrument classes. In order to define optimal quantities (e.g. positions of peak neutron flux, used wavelength band) for the Figure of Merit (FoM), a survey has been conducted at PSI covering the experience of the local instrument scientists. Based on this survey we introduce several FoMs which show the potential of tailoring the neutron spectrum to specific instrument needs. The developed methodology is adopted to optimize the top moderator in the conceptual design of the TMR of the European Spallation Source (ESS) Project. A parametrized geometry model of the ESS TMR is built in MCNPX and used within an optimization framework to study and optimize the moderator performance in the thermal and cold regions of the neutron spectrum. The results obtained with the optimized setup are compared to the ESS 2003 Project. Furthermore, experience is gathered while performing these simulations, e.g. the examination of the pulse shapes obtained with time-dependent calculations shows that for long-pulse target stations the peak brightness can with sufficient precision be obtained from time-independent calculations by scaling with the proton pulse duty factor.

## 1. Introduction

The neutron scattering community is constantly looking for smaller probes and shorter measurement times, thus higher intensity neutron beams. On the other hand, there are technological limitations from the neutron source side in producing these. First, in high flux reactors the power density, which is closely related to the neutron flux, cannot be further increased due to material constraints. Second, in spallation neutron sources, although there are still some improvements possible (e.g. higher proton current, rotating target), limitations due to accelerator design and coolability exist. However, considerable increase in the performance of the instruments can be achieved if the target-moderator-reflector (TMR) and the following neutron guides are specifically designed to meet the requirements of these instruments. Additionally, the performance of the instruments can be increased with proper shielding and positioning in order to decrease the background (e.g. by avoiding cross-talks). This paper focuses on the optimal design of the TMR with respect to the instrument requirements.

The only continuous spallation neutron source operating in the world is the SINQ at PSI [1]. The four high-intensity pulsed spallation neutron sources in operation today are the SNS at ORNL [2], the ISIS at the Rutherford Appleton Laboratory [3], the JSNS at J-PARC [4] and the one at LANSCE [5]. There are some small-intensity facilities as LENS, GELINA and NTOF. A future high-intensity neutron source is the European Spallation Source (ESS), planned to be built in Lund, Sweden, for delivering the first neutrons in 2019 [6]. The ESS baseline is a 5 MW long pulse (2.857 ms) facility at 14 Hz repetition rate, with 2.5 GeV protons hitting a solid rotating tungsten target. The envisioned coolant for the target is helium in contrast to the water cooling for the proposed second SNS target station [7]. The preliminary design of the TMR is based on the experience gathered from the operating spallation neutron sources. Due to the lack of detailed specifications for the moderators and the instruments desire for neutrons in the thermal and cold wavelength range, a bi-spectral box-shaped side-by-side moderator with liquid para-hydrogen at 20 K for cold neutron extraction and water at room temperature for thermal neutron extraction is investigated in this paper.

Due to the large variety of neutron scattering instruments and the possibility of providing a much broader wavelength band to them, bi-spectral moderators—whose spectrum is composed of two Maxwellians peaking at ~1 Å in the thermal and at ~2.5 Å in the cold part—are under consideration for future spallation

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**Table 1**
Evaluation of "desired" wavelength-band for different types of instruments.

| Instrument type | PSI instruments | Wavelength band Å |
|---|---|---|
| Reflectometer | AMOR | 4.1–10.0 |
| Diffractometer | HRPT, TRICS, DMC | 1.0–2.5 |
| Small angle scattering instruments | SANS, SANS2 | 5.0–13.0[a] |
| Cold triple axis spectrometer | RITA-II, TASP | 4.6–6.0 |
| Thermal triple axis spectrometer | EIGER | 1.0–2.5 |
| Chopper spectrometer (inelastic scattering) | FOCUS, MARS | 3.5–6.0 |

[a] Increase to 20 Å desired.

neutron sources. Ideas and calculations for transporting both cold and thermal neutrons to the instruments are already existing, e.g. a shortened extraction system with several mirrors is proposed in [8] which reflects cold neutrons from the off-axis moderator into the neutron guide while the thermal neutrons are transmitted through the mirrors. However, to our knowledge, optimization of the TMR based on Figure of Merits (FoMs) which quantifies the bi-spectrality of the neutron spectrum has not been carried out yet. Instead, the FoMs used for the optimization of the TMR included the integral of the neutron flux below a certain energy. This limit was set to 383 meV in [9] to optimize the thermal neutron flux by varying the thicknesses of back-to-back and side-by-side moderators. In [10], 413 meV was used as FoM for the thermal neutron flux to study the time distribution for different moderator thicknesses and pre-moderator extensions. 5 meV was adopted in [11,12] to maximize the cold neutron brightness with different moderator configurations and extraction schemes and to compare the time-integrated neutron flux from different targets, respectively.

In order to define optimal quantities (e.g. position of peak neutron flux, used wavelength band) for the FoM, a survey has been conducted at PSI. This comprehended the experience of the local instrument scientists which is based on the ~200 neutron instrument users visiting the institute yearly. Based on this survey we introduce several FoMs which show the potential of tailoring the neutron spectrum to specific instrument needs. The developed methodology is adopted to optimize the top moderator of the TMR of the ESS Project.

A parametrized geometry model of the ESS TMR (as described in detail in the conceptual design report [6]) is built in MCNPX version 2.7.0 [13] and used within an optimization framework that consists of the Monte Carlo code MCNPX for particle transport simulation, the stand-alone optimizer program that evaluates the FoM value and defines the optimization path in the parameter space, and the automatic generator of the input files together with enclosing control scripts [11]. The developed program is flexible enough to accommodate future changes.

Section 2 of this paper describes the methodology for formulating the FoM. Section 3 gives an overview of the geometric representation of the TMR used in MCNPX. In Section 4 simulation results are presented which, after proper normalization, are compared with data obtained in the ESS 2003 Project. Section 5 summarizes the paper.

## 2. Methodology and FoM

The survey conducted among the local instrument scientists is summarized in Table 1. The wavelength bands desired by the users range from 1 to 13 Å which encourage the use of a bi-spectral moderator. It should be noted that SINQ is a continuous spallation neutron source, thus the requirements of the users are more similar to those at reactors. Nevertheless, the presented method can be applied to pulsed spallation sources taking into account the specific features of these systems.

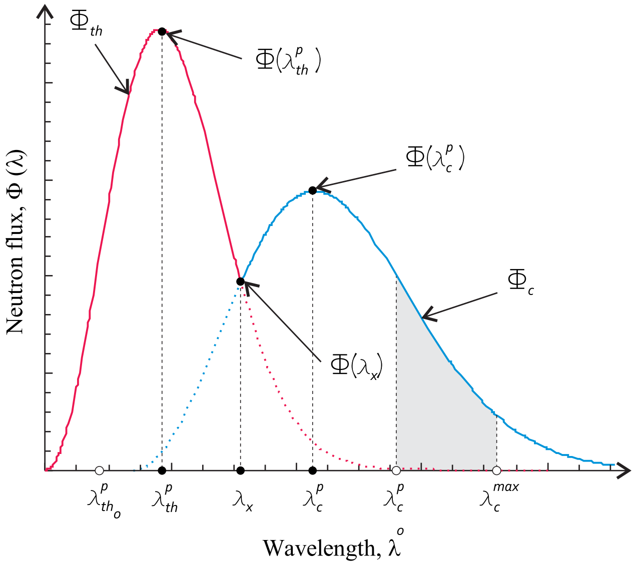

**Fig. 1.** Graphical representation of a bi-spectral spectrum. The following nomenclature is used: $\lambda^p_{th_0}$ and $\lambda^p_{th}$—user-desired and calculated position of peak thermal neutron flux, $\lambda^p_{c_0}$ and $\lambda^p_c$—user-desired and calculated position of peak cold neutron flux, $\lambda_x$—crossing point (local minimum) between the thermal and cold part of the neutron spectrum, $\lambda^{max}_c$—upper limit in the integral of the cold neutron flux; $\Phi_{th}$ and $\Phi_c$—thermal and cold part of the neutron spectrum, $\Phi(\lambda^p_{th_0})$ and $\Phi(\lambda^p_{c_0})$—thermal and cold peak neutron flux, $\Phi(\lambda_x)$—neutron flux at the crossing point.

**Table 2**
Baseline parameters of the ESS pulse.

| Parameter | Unit | Value |
|---|---|---|
| Proton kinetic energy, $E$ | GeV | 2.5 |
| Average beam power, $P$ | MW | 5 |
| Pulse repetition frequency, $f$ | Hz | 14 |
| Macro-pulse length, $\tau$ | ms | 2.857 |

Based on the survey, we propose an optimum bi-spectral neutron spectrum as a function of wavelength as depicted in Fig. 1. In our representation, the bi-spectral spectrum consists of a thermal part with its flux maximum ($\Phi(\lambda^p_{th})$) at $\lambda^p_{th}$ and a (more or less pronounced) maximum ($\Phi(\lambda^p_c)$) in the cold part of the spectrum at $\lambda^p_c$. Based on the user survey, the maxima should be located between 1.3 and 1.5 Å and at 4.1 Å for the thermal and cold part, respectively, i.e.

$$1.3\,Å < \lambda^p_{th_0} < 1.5\,Å, \quad \lambda^p_{c_0} = 4.1\,Å. \tag{1}$$

In the best case the relations

$$|\lambda^p_{th} - \lambda^p_{th_0}| \simeq 0 \quad \text{and} \quad |\lambda^p_c - \lambda^p_{c_0}| \simeq 0 \tag{2}$$

should be valid at the same time. It should be mentioned that the thermal neutron scattering instruments prefer a maximum at 1.0 Å. On the other hand, the limits given in Eq. (1) are acceptable as long as there is a significant increase in the thermal tail.

According to the neutron instrument scientists, an optimum bi-spectral moderator setup should ensure similar measurement times if either thermal or cold neutrons are used. To be more precise, a maximum factor of 3 between the peak values is acceptable. Thus, the peak values of the neutron flux in the thermal and cold parts of the spectrum have to be maximized

$$\Phi(\lambda^p_{th}) = \text{MAX}, \quad \Phi(\lambda^p_c) = \text{MAX}, \tag{3}$$