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Spectrometers for compact neutron sources

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ABSTRACT

We discuss the potential for neutron spectrometers at novel accelerator driven compact neutron sources. Such a High Brilliance Source (HBS) relies on low energy nuclear reactions, which enable cryogenic moderators in very close proximity to the target and neutron optics at comparably short distances from the moderator compared to existing sources. While the first effect aims at increasing the phase space density of a moderator, the second allows the extraction of a large phase space volume, which is typically requested for spectrometer applications. We find that competitive spectrometers can be realized if (a) the neutron production rate can be synchronized with the experiment repetition rate and (b) the emission characteristics of the moderator can be matched to the phase space requirements of the experiment. MCNP simulations for protons or deuterons on a Beryllium target with a suitable target/moderator design yield a source brightness, from which we calculate the sample fluxes by phase space considerations for different types of spectrometers. These match closely the figures of todays spectrometers at medium flux sources. Hence we conclude that compact neutron sources might be a viable option for next generation neutron sources.

1. Introduction

Neutron scattering has proven to be one of the most powerful methods for the study of dynamics in condensed matter. This is due to the fact that the neutron energy in cold and thermal moderators matches the energy scale of atomic and molecular motions and of spin excitations, whereas the neutron wavelength is of the same order of magnitude as the typical length scales in condensed matter. Therefore, to resolve atomic, molecular and spin correlations in space from sub-Å to μm range and in time from the ps to the μs range requires only a modest resolving power from 10 to 1000 as compared, e.g., to X-ray methods.

However, many applications of neutron spectroscopy are flux limited and therefore any new generation of neutron sources has boosted the development of new instrumentation. With the latest development of MW spallation sources the source brightness has reached a new level, exceeding the brightness of the formerly most intense research reactors by more than one order of magnitude. Accompanying these brightness gains with an optimized transport and analysis systems, the new instruments at the MW spallation sources promise efficiency gains between two and three orders of magnitude as compared to existing instruments and therefore will enable completely new science. Beside these new bright opportunities, many of today's applications will still be requested by the users. As many research reactors face the end of their operational time, the demand for future medium flux sources is hence pressing. Recently we have suggested a pulsed source based on low energy nuclear reactions [1], driven by accelerators in the energy range below 50 MeV, called High Brilliance Source (HBS). The operation of such accelerators is more flexible compared to high energy accelerators used for spallation sources. In particular different source repetition rates can be realized, tailored to the needs of an individual instrument. The low particle energy allows a more compact target-moderator–reflector assembly, bringing a larger fraction of the produced neutrons to thermal or cold energies. Using low dimensional neutron moderators [2], the moderator geometry can also be optimized to emit preferentially into a narrow solid angle, thus increasing the brightness along these directions. Last but not least, the lower nuclear energies involved require significantly less bulky shielding, not only saving cost, but also allowing optical components such as guides or choppers to be located closer to the moderator so that larger phase space volumes can be extracted.

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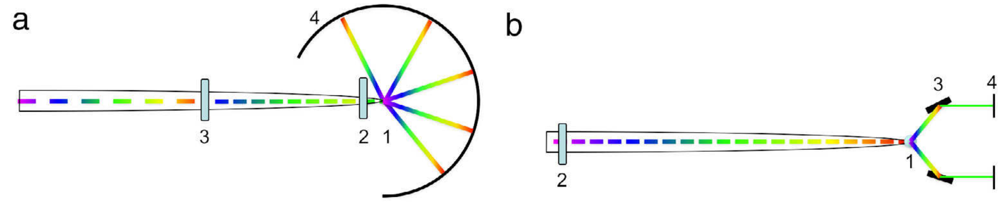


Fig. 1. Sketch to elucidate the working principle of direct (a) and indirect (b) time-of-flight spectrometers. The instrument components are (1) sample, (2) chopper, (3) initial (direct) or final (indirect) energy filter, (4) detector.

Here we will discuss the potential for time-of-flight spectrometers at such sources. We will show that despite the less efficient neutron production the special features, namely the optimization of the instrument from the neutron source on, enable instrument performance that is comparable or even superior to existing instruments focusing the same science.

We distinguish between the two cases of direct and indirect time-of-flight spectrometers, which are sketched in Fig. 1. In the direct geometry, the sample is illuminated by a short monochromatic pulse. A broad range of final neutron energies arrives a different times at the detector and the neutron energy resolution is then determined by the length of the illuminating pulse. The initial neutron energy can be defined in two ways. Using the time-of-flight between a pulsed source or an additional chopper, the pulse length of the source/choppers controls the initial neutron energy resolution. Alternatively, Bragg scattering from a single crystal can be used to select a narrow band of initial energies from the source spectrum.

The indirect spectrometer filters a narrow spectral range of final neutron energies by means of e.g. a monochromatic analyser or a Be transmission filter. The initial neutron beam, which has a broad spectral range, is pulsed at a rather large distance from the sample, so initial neutron energy is distinguished by the arrival time at the detector.

2. Dynamic range requirements

The dynamic range probed by a spectrometer is related to the repetition rate of the instrument and the geometry. For the direct geometry instrument, the range of scattered neutron wavelengths that can be recorded without frame overlap is given by

$$0\ \text{Å} < \lambda' < \frac{h}{m_n}\left(L_{\text{SD}} f_{\text{rep}}\right)^{-1} = \lambda'_{\text{max}} \tag{1}$$

and the corresponding dynamic range

$$-\infty < \hbar\omega = E_i - E_f < \frac{h^2}{2m_n}\left(\lambda^{-2} - \lambda'^{-2}_{\text{max}}\right) \tag{2}$$

assuming a monochromatic sample illumination with the repetition rate f_{rep} and a detector at a distance L_{SD} from the sample. To give an example, a repetition rate of 100 Hz and $L_{\text{SD}} = 3$ m yields $\lambda'_{\text{max}} = 13.2$ Å. The dynamic range is then set by the choice of the initial neutron wavelength λ. For thermal neutrons one can still cover a large energy transfer range at high repetition rate yielding a rather small λ'_{max}, while for long wavelength neutrons the repetition rate is limited to cover a sufficiently large range in energy transfer.

For an inverse instrument, the bandwidth for the initial neutron wavelength $\Delta\lambda$ is defined by the distance of the sample from the moderator or in the case of pulse shaping from the resolution defining chopper L_{S}:

$$\Delta\lambda = \frac{h}{m_n}\left(L_{\text{S}} f_{\text{rep}}\right)^{-1}, \tag{3}$$

giving a continuous range of the initial neutron energy. The final neutron energy after scattering from the sample is fixed by a suitable analyzer, e.g. a monochromator crystal or a Be filter. With these, the energy transfer range can be calculated from the initial band and the analyzer wavelength λ'_{Bragg} for an inverted geometry instrument. The inverse instrument has typically a fixed dynamic range, e.g. several hundred μeV for time-of-flight backscattering instruments or several hundred meV for vibrational spectrometers. Fig. 2 shows the repetition rate, which provides a given dynamic range centered around the wavelength fixed by the backscattering condition for the (002) reflection of pyrolitic graphite. It is clear, that for this narrow dynamic range a repetition rate well above 100 Hz is suitable for a moderate instrument length between 15 and 30 m.

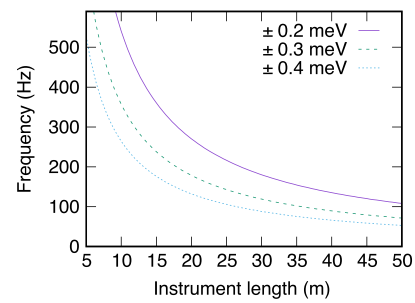


Fig. 2. Repetition rate as function of the instrument length to cover a given dynamical range using backscattering from pyrolitic graphite (002) reflection as analyzer.

3. Energy resolution requirements

Considering the different pulsed sources existing or in construction today, different routes have been exploited to optimize the energy resolution of a spectrometer. At short pulse spallation sources moderators have been designed with very short emission times by decoupling of the moderator from the reflector and poisoning of the moderator, which provide an extremely good energy resolution already for rather compact instruments [3]. Such 'poisoning' requires on the other hand, that neutron absorbers inside the moderator reduce the overall number of free neutrons.

For the long pulse source ESS, the energy resolution is controlled by choppers for most instruments. The accelerator pulse length provides an initial wavelength λ resolution, which is not sufficient to resolve the energy transfer $\hbar\omega$ with the required precision for many applications. Therefore choppers are employed to vary the pulse length by the chopper speed or the use of different windows to trade resolution for flux or in other words to enlarge or reduce the phase space volume of the neutrons probing the excitations of the sample. As they have certain technical limitations in particular for large beams, the instruments are typically longer than their counterparts at short pulse sources.

For the HBS, it is envisioned to match the neutron production time, i.e. the accelerator pulse length, with the moderation time of the spectral transformer, which ranges from several ten μs to a few hundred μs for thermal or cold moderators, respectively. For most spectrometer applications using cold and thermal neutrons, the phase space can be constrained sufficiently by choppers also for a modest instrument length, see Fig. 3. So the moderator pulse lengths should be long enough to allow the relaxation of the resolution by the choppers within a range defined by a specific instrument design.

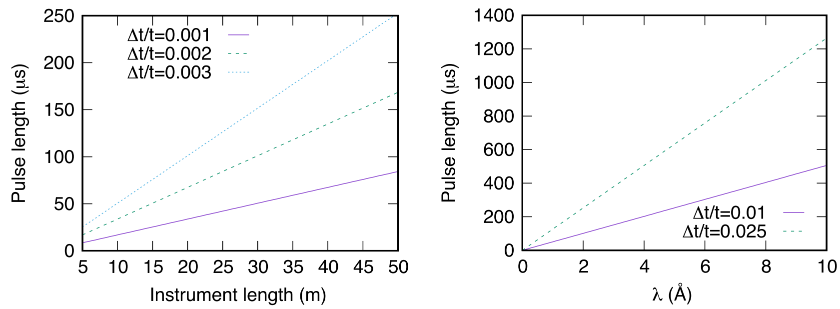


Fig. 3. Left: Pulse length requirements to realize a relative time-of-flight resolution for pyrolitic graphite (002) backscattering conditions as a function of the instrument length. Right: Pulse length requirements to realize 1% and 2.5% time-of-flight/wavelength resolution for 20 m primary flight path as a function of wavelength for a direct geometry spectrometer.

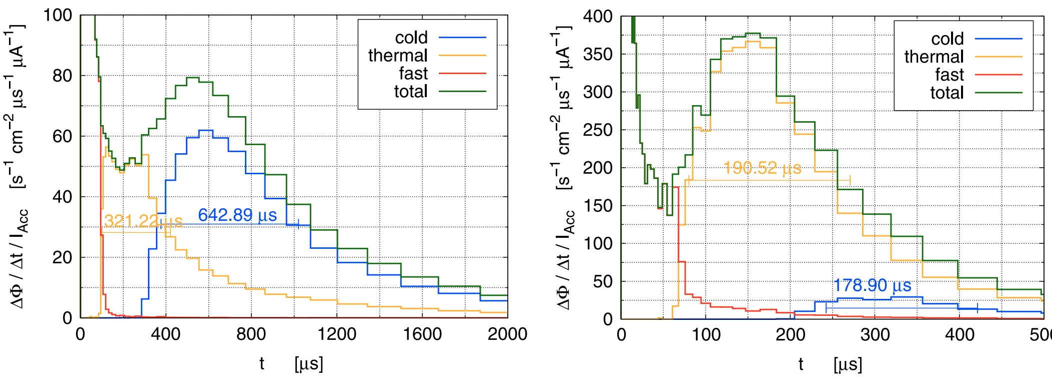


Fig. 4. Time distribution of the neutron emission from a cold (left) and a thermal (right) moderator for the different spectral ranges.

For the case of a high resolution instrument such as a backscattering spectrometer, we have investigated, for which instrument length a certain time-of-flight resolution can be realized within state-of-the-art chopper technology. We calculate the time-of-flight for the wavelength of a pyrolitic graphite analyser in backscattering condition ($E = 1.84$ meV)

$$t = \frac{m_n}{h} \times \lambda \times L \tag{4}$$

and plot the requested pulse length to yield a time-of-flight resolution of $\frac{\Delta t}{t} = 1, 2, 3 \times 10^{-3}$.

From Fig. 3 it is clear that very high resolution is accessible for instruments longer than 15 m if the choppers provide a pulse length of ≈20 µs. Also it becomes clear, that instruments longer than 50 m will run out of pulse, if the pulse length is limited by the moderation time for relaxed resolution settings. We conclude, that a backscattering instrument on an HBS should adapt a length of 15 to 30 m, depending on the optimization towards high resolution vs. high flux.

The pulse length requirements for the direct geometry instruments are fairly different and variable as the scattered neutron wavelength λ' covers a wide range. Matching primary and secondary resolution contributions might be varied between the two extremes of short illumination time and relaxed λ resolution if the final neutron energy is much larger than the initial, or long illumination times and tight λ resolution if the neutrons are slowed down strongly in the scattering process [4,5]. Therefore we compare in Fig. 3 the required pulse length for a 20 m long spectrometer to realize a narrow or a relaxed initial wavelength λ resolution.

In order to control the resolution by choppers, the moderator pulse most be long enough to allow the most relaxed resolution that may be requested by the user. For a 20 m long primary spectrometer, this requires already a pulse length larger than 500 µs to allow an incoming energy resolution of 5% at $E_i = 3$ meV, which is similar to the moderation time in low dimensional moderators, compare Figs. 3 and 4. It is also evident that a pulse length shorter than 100 µs will already constrain the incoming energy resolution to 2% for thermal neutrons with a wavelength $\lambda = 1.8$ Å. From that it is clear that chopper spectrometers at HBS can and must be compact to enable a tunable energy resolution, but that the requirements are well within the boundary of today's technology. For such compact instruments, the emission times of the moderators are also very well matched to allow the resolution tuning in a reasonable range.

4. Phase space requirements

Spectrometers are often flux-limited. Therefore the accepted divergence is increased on the cost of momentum transfer resolution. This is of course absolutely valid for any local excitation, which has no other momentum resolution dependency than a slowly varying form factor or the Q^2 dependence of vibrational motions. For these cases the divergence is limited by the achievable coating of the neutron guide and by the phase space volume of the source, which can be seen from the neutron guide entrance.

Low dimensional moderators such as the 'Pancake' or the 'Butterfly' moderators developed for the ESS feature a height of only 30 mm. Taking into account the minimum distance of ca. 2 m between moderator surface and the first optical element and constraints to the height can therefore limit the phase space volume fed into the neutron guide.

For the HBS the reduction of the moderator size is driven to an extreme to increase the brightness. In particular for the cold moderators it is realized by a reduction of two moderator dimensions resulting in a 'finger' shape and the use of para-hydrogen with a reduced scattering cross section for low energy neutrons and therefore a high escape probability. The moderator geometries used for the simulations in this paper have a diameter between 2 and 6 cm, resulting in a highly directed emission of thermal and in particular cold neutrons, see Fig. 5. For a compact moderator a large distance to the guide system would prevent any instrument that relies on a large phase space volume such as a spectrometer.

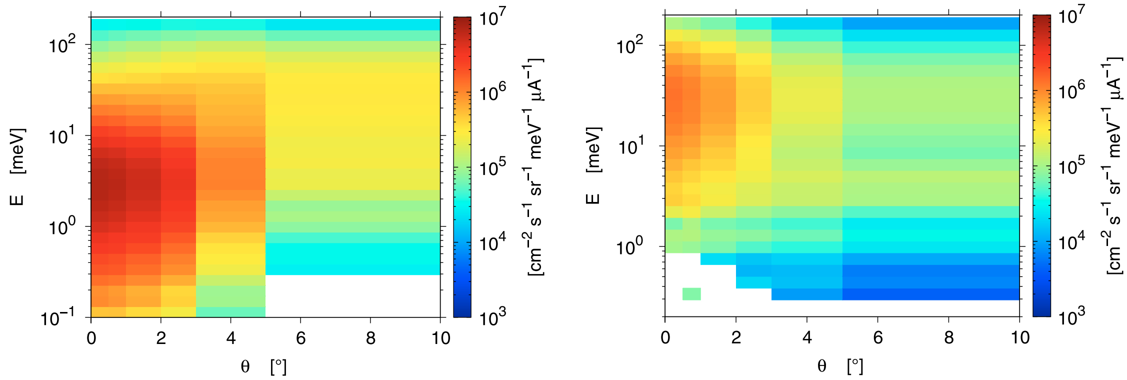
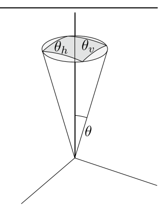


Fig. 5. Moderator peak brightness as function of neutron energy and emission polar angle in front of the cold (left) and the thermal (right) beam tubes.

Table 1
Parameters and performance for selected spectrometer types compared to reference instruments [9–11]. For the ease of comparison we give the resolution parameters in full width half maximum (FWHM), while the standard deviation $\sigma = \mathrm{FWHM}/(2\sqrt{2\ln 2})$ is used in the intensity calculations. The schematic shows the relation between the emission angle θ and the collimation of the neutron guide system.

	Backscattering	Cold ToF	Thermal ToF
$E_{i,f}$ (meV)	1.84	5	45
$\frac{\mathrm{FWHM}\,E_i}{E_i}$ (%)	1	2	5
FWHM $\theta_h \times \theta_v (° \times °)$	4×4	2×2	0.5×0.5
FWHM t(μs)	120	50	18
Rep. rate (Hz)	200	100	400
Flux (cm^{-2}s^{-1})	2.5×10^7	1.3×10^5	1×10^5
Reference instrument	OSIRIS	LET	MERLIN
Flux reference (cm^{-2}s^{-1})	2.7×10^7	5×10^4	6×10^4



It is therefore crucial that the production of rather low energy products by the nuclear reaction enables optical elements to be located in close proximity to the moderator.

The geometry of the moderator and the finger was chosen to enable the extraction of low collimation for cold instruments ($< 5°$) and an already fairly collimated thermal beam (collimation $< 1°$), reflecting the lower critical angle of neutron guides for higher energy neutrons.

Assuming for simplicity a straight m=4 supermirror coating for the neutron guide system, most of the divergence provided at the exit of each beam tube can be transported to the sample position. Applying modern concepts such as the Selene concept or focusing neutron guides with adapted coating [6–8], it will also be possible to make most of the neutrons 'produced' within the moderator useful at the sample. As these concepts do not require huge coated areas or allow the reduction of the maximum m-coating, they should also follow the request for reasonably low instrument cost.

5. Instrument realization

From the above it is clear that in particular narrow bandwidth instruments can profit from the HBS as it offers an order of magnitude higher repetition rate than today's pulsed sources. Therefore we have estimated the performance for three different instruments, namely a medium resolution backscattering instrument similar to OSIRIS at ISIS and a thermal and a cold direct geometry chopper spectrometer. We estimate the sample flux from the MCNP simulated brightness Φ, which are the basis of Fig. 5, performing the integration

$$I = \int_{\Delta\Omega}\int_{\Delta E_i}\int_{\Delta t} \Phi d\Omega dE_i dt, \tag{5}$$

or in other words we integrate the phase space density in the phase space volume defined by the resolution requirements. Here $\Delta\Omega$ represents the two dimensional collimation transmitted through the neutron guide system, which can be easily estimated from the supermirror coating of the top/bottom and left/right mirrors. E_i refers to the initial neutron energy. As seen from Fig. 1 the limits of the time integration are set by the chopper directly upstream the sample for the direct geometry instrument, which controls the illumination time of the sample. The limits of the energy integration are controlled either by the width of the that chopper and the second chopper further upstream or by the Bragg angle and the mosaicity of the monochromator crystal.

For the inverse instrument the integration limits are given by the pulse length of the chopper (or the moderator pulse), which then broadens along the flight path and defines the primary resolution, and the bandwidth of the instrument given by Eq. (3).

In case of the direct geometry instruments we assume Gaussian distributions for all variables of the integration, which is a simplified assumption for the transmission of the neutron guides, choppers and monochromators. For the inverse instrument we perform a trapezoidal integration of the moderator brightness across the dynamical range in energy. So we approximate the flux on sample by the following expressions:

$$I \approx (2\pi)^2 \sigma_{\theta_h}\sigma_{\theta_v}\sigma_E\sigma_t \Phi(\theta = 0, E = E_0, t = t_0), \tag{6}$$

or

$$I \approx (2\pi)^{3/2} \sigma_{\theta_h}\sigma_{\theta_v}\sigma_t \int_{E_{min}}^{E_{max}} \Phi(\theta = 0, E, t = t_0) dE \tag{7}$$

for direct and indirect instruments, respectively. θ_h and θ_v refers here to the horizontal and vertical collimation of the neutron guide system.

For the backscattering and the cold direct geometry instrument we balance the primary and secondary energy resolution for elastic scattering. For the thermal instrument, we optimize for a large energy transfer of 50% to the sample, i.e. the scattered neutrons are substantially slower than the initial neutrons. This defines the lengths of the chopper pulses (FWHM), which are given in Table 1.

To scale from the simulations, which have been normalized per μA beam power, we envision, that a medium flux type source will be operated at a beam power of about 100 kW and achieve a peak current of 100 mA. For 50 MeV proton or deuteron energy the duty cycle $\tau_{\mathrm{src}} \times f_{\mathrm{src}}$

should then be 1:50, τ_{src}, f_{src} denoting pulse length and frequency. A higher repetition rate results hence in a shorter pulse and vice versa.

For the spectrometer types discussed here, the duty cycle of 1:50 provides a pulse long enough not to constrain a tight energy resolution, but a repetition rate that provides a reasonable dynamic range. Therefore the ratio of produced neutrons to used neutrons is very favorable for high to moderate frequency sources such as the HBS.

Table 1 summarizes the parameters and the expected sample fluxes for an ideal brilliance transfer. Considering that today's instruments typically yield 50 to 90% brilliance transfer for the chosen collimation, this assumption allows to judge whether instruments at such a source have the potential to substitute the instrumentation at nowadays medium flux sources. The flux numbers are comparable to similar instruments at spallation sources at sub MW power or at modern research reactors. We compare them here to ISIS instruments of the same class using the flux and resolution values given on the instrument web sites [9–11]. Considering realistic conditions we can conclude that one can expect a similar monochromatic flux as on a medium power spallation source. Despite the fact that the number of neutrons produced in low-energy nuclear reactions is much lower, the compactness of the source enables the optimization of the instruments already from the neutron source. The reduced dimensions of the target/moderator assembly improve the coupling between them and increase the brilliance within a collimation suitable for neutron spectrometers. The short distance to the extraction system is a key feature to extract the rather large phase space volume needed for typical spectrometer applications. Finally, the adapted repetition rate compensates the lower neutron production to yield a similar flux on sample.

6. Conclusion

We have analyzed the performance of inverse and direct geometry time-of-flight spectrometers at low-energy accelerator driven neutron sources such as the HBS concept. We show that the provision of higher source repetition rates will be beneficial for any narrow band application since spallation sources typically run at repetition rates about 1 order of magnitude lower than requested by the dynamic range of the experiment. Compact target/moderator assemblies are feasible, which results in a larger fraction of the produced neutrons to be moderated to cold or thermal energies. Finally the comparably low energy of the underlying nuclear reaction and the smaller target/moderator assembly will enable neutron optics, that begin in close proximity to the neutron emission surface. Therefore, especially instruments requiring a large phase space volume will benefit from the particular features of a compact HBS. The compactness allows a more efficient use of the produced neutrons and hence we can expect a performance very competitive to today's medium flux sources.

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