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Performances of Neutron Scattering Spectrometers on a Compact Neutron Source

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Abstract. There is currently a big effort put into the operation and construction of world class neutron scattering facilities (SNS and SNS-TS2 in the US, J-PARC in Japan, ESS in Europe, CSS in China, PIK in Russia). On the other hand, there exists a network of smaller neutron scattering facilities which play a key role in creating a large neutron scattering community who is able to efficiently use the existing facilities. With the foreseen closure of the ageing nuclear research reactors, especially in Europe, there is a risk of seeing a shrinking of the community able to use efficiently the world class facilities. There is thus a reflection being conducted in several countries for the replacement of smaller research reactors with low energy accelerator based sources. We consider here a reference design for a compact neutron source based on existing accelerator components. We estimate the performances of various types of neutron scattering instruments built around such a source. The results suggest that nowadays state of the art neutron scattering experiments could be successfully performed on such a compact source and that it is thus a viable replacement solution for neutron research reactors.

1. Introduction

Considering the political situation in Europe, it is very unlikely that new nuclear research reactors will be built in replacement of the old ones. However, currently aging facilities are providing a broad user base to the most performing ones. It is thus necessary to try to find a solution to ensure that the broad user base (6000 users [1]) can be maintained in Europe in order to make the best use of the most powerful sources. Any possibility to build neutron scattering facilities which could replace existing nuclear reactors would be welcome provided the investment is in the 100-200 M€ range which would make it affordable to a single country on par with a synchrotron or a power laser facility. During the last decade a number of groups have independently considered the possibility of operating a high current / low energy proton accelerator to produce thermal and cold neutrons [2-7]. A few facilities have actually been built and are operating scattering instruments [8]. A UCANS network gathering these groups has been created [9].

In this communication we consider the design of a compact source based on existing components (proton source, accelerator, target, moderator, neutron optics) and evaluate the performances of a range of neutron scattering instruments which could operate on such a source. We focus mainly on elastic scattering instruments since the flux requirements are less stringent and the modelling of elastic instruments is significantly simpler than inelastic instruments.

As a starting point we consider a source design based on existing components: a proton source (100 keV, 100mA), a RFQ accelerator able to operate at proton currents up to 100mA bringing the proton energy to 3.6 MeV and a DTL section boosting the proton energy to 20 MeV. We also consider a pulsed operation (coupled with Time-of-Flight spectrometers) since this operation mode allows optimizing the (neutron production / energy input) ratio. For the pulsed operation we consider a duty cycle of 4% which corresponds to a beam energy on the target of 80kW and an average proton current of 4 mA. We do not make any assumption about the repetition rate and pulse length. We consider Beryllium as the target material.

Monte-Carlo simulations as well as a few experimental data show that rather simple moderator combining polyethylene and a beryllium reflector can allows to achieve a thermal neutron brilliance on the order of $3x10^7$ n/s/cm²/sr/µA at the exit of the moderator. Note that these values are coherent with the values which can be extrapolated from the measurements of Allen et al [10] at 10 MeV – 30µA on the Birmingham Nuffield Cyclotron using a PE moderator. Assuming an average proton current of 4 mA this leads to a source brilliance of $1.2x10^{11}$ n/s/cm²/sr. A source which the above brilliance was used as an input for the simulation of instruments using the McStas software [11] which is a tool dedicated to the modelling of neutron scattering instruments.

2. Instruments designs

For each class of instruments we assume that the repetition rate and the pulse length can be freely optimized (within the 4% duty cycle power envelope). We consider that this makes sense since we are trying to evaluate the optimal performances of different types of instruments.

2.1. Reflectivity

It can be considered that wavelength resolutions $\delta\lambda/\lambda$ up to 10% are perfectly usable for reflectivity. Let us assume a source operating with pulses of length 2 ms and with an operation frequency of 20 Hz. This corresponds to a duty cycle of 4% and is very close to the ESS neutron pulse structure. On a pulsed source, the wavelength resolution degrades very quickly for short wavelengths. For pulse widths of w=2 ms and a flight path L=16m, the usable wavelength band ranges from 3 to 12 Å which matches a cold neutron spectrum, with a wavelength resolution of 12% at the peak flux (4 Å). The resolution improves quickly to 7% at 8 Å. A shorter instrument would degrade the wavelength resolution but would also increase the cut-off wavelength to 16Å which might be usable in reflectivity experiments. A longer instrument (24 m) would provide a better wavelength resolution at the expense of a narrower wavelength bandwidth (λ_{max} = 8 Å). While it seems acceptable to work in the (L=16 m, w=2 ms) configuration even though the resolution is as low as 15% at 3 Å, there are a number of situations where there is an interest in improving the resolution. Besides it is somewhat unsatisfactory to have a resolution varying from 15% to 4% over the bandwidth. A simple improvement such as a double disk-chopper [12] right at the moderator exit would (i) improve the wavelength resolution at short wavelengths (2) cut-off neutron pulse tails. Note that if the double disk chopper solution is used, due to the versatility of the system, a shorter instrument could be built (typically 12m) so that the resolution could be set at 10% below 6Å with the double disk chopper and improved down to 5% at 13Å. This would roughly match the POLREF@ISIS settings [13]. In order to avoid a direct view from the moderator, since the instrument would be very short, a neutron mirror (e.g. m=6, length 500mm, height 20mm) could be used. The detector position (12m from the source) would be offset by more than 40cm from the direct view of the moderator.

We performed Monte Carlo simulations using McStas and the following design. From the moderator: straight guide of length 8m with m = 4, cross section 100x50mm²; a 2 m long collimator with F1 = 2 mm and F2 = 2 mm and a side guide with m = 4; a detector at 2 m from the sample position. The neutron flux at the sample position is $6x10^6$ n/cm²/s which is on the order of CRISP@ISIS and HERMES@LLB. Hence it should be possible to operate a reflectometer with sufficient flux to perform useful science on the reference source design.

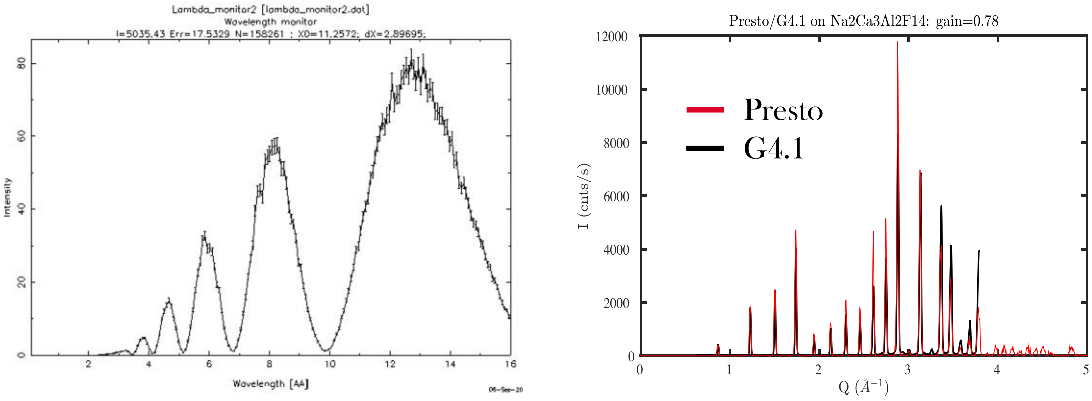

Figure 1: (a) McStas simulation of a 12m neutron reflectometer with a 10x5 cm² sample (Ni 20nm//Si) at an incidence angle of 3°. Wavelength spectrum measured in the specular reflectivity direction. (b) Comparison of the diffraction spectra measured on G41@LLB (λ = 2.43Å) and PRESTO (ToF). A wider Q range is accessible in ToF (above 4Å^{-1}).

2.2. *Small Angle Scattering*

SANS scattering instruments are workhouse instruments for neutron scattering in soft matter and metallurgy. Considering the implementation of a SANS instrument on a CNS, we may use as a starting point the fact that SANS instruments are low resolution instruments which can be nicely operated with a wavelength resolution δλ/λ ranging from 10 up to 20%. For SANS measurements, a wide lambda range is desirable to cover a Q range as large as possible. Hence a source with long pulses and a slow repetition rate is the most efficient way to operate. Let us again assume a source operating with pulses of length 2ms and with an operation frequency of 20 Hz (4% duty cycle). The wavelength resolution function is identical to the case of the reflectometer. Again, the configuration (L=12 m, w=2 ms) is rather favorable: (i) The wavelength band ranges from 3 to 16Å and matches perfectly a cold neutron spectrum with a wavelength resolution of 16% at the peak flux (4Å). The resolution improves quickly to 8% at 8 Å; (ii) for metallurgical studies, which require wavelengths above 5Å, the resolution is below 12% which is optimal. A shorter instrument would degrade the wavelength resolution and the wavelength band extension beyond 16 Å is realistically not usable. A longer instrument would provide a better wavelength resolution at the expense of a narrower wavelength bandwidth. Note that in general the total length of a SANS instrument can be varied by moving the detector closer or further from the sample position.

We suggest that an instrument with the following specifications would be perfectly suitable for SANS studies: (i) cold source; (ii) Source-Sample distance of 8 m. Sample – detector distance variable from 1 to 7m, total flight path from 9 to 15m; (iii) useful bandwidth from 3 Å to 16 Å. If one compares with the SANS2D@ISIS (f = 10 Hz, Source-sample = 19 m, Total length = 21 – 31m / Q_{min}~0.002 Å^{-1}, Q_{max}~3 Å^{-1}), the above specifications scale exactly as the operating frequency. At 20 Hz, an instrument should be twice as short as an instrument operating at 10 Hz for the same Q range. Monte-Carlo simulations for various configurations were performed. The results are summarized in Table 1. The flux are also on par with the PAXE instrument at the LLB [14]. The calculated flux are also on the order of the flux expected on SANS2D at ISIS TS2 (~10^6 cm^{-2} s^{-1}) [15].

Configuration	**L_g (m)**	**L_1 (m)**	**L_2 (m)**	**L_{tot} (m)**	**D_1 (mm)**	**D_2 (mm)**	**Flux (n/cm²/s)**
Small Q	1	7	7	15	20	16	0.7x10^6
Medium Q	4	4	4	12	20	16	2.2x10^6
High Q	6	2	1	9	20	16	6.7x10^6
PAXE [36]	6	2.5	2.5	11	12	8	0.7x10^6

Table 1: Flux at the sample position for various SANS configurations (small, medium, high Q). L_g being the length of the guide from the source to the first pin-hole, L_1 being the length of the collimation and L_2 being the sample-detector distance. D_1 and D_2 are the sizes of the holes at the entrance and exit of the collimator.

2.3. Powder diffraction

Power diffraction instruments are also workhorses in neutron diffraction. High resolution instruments are used for structure determination. High flux instruments are used to study phase transitions. Efficient powder diffraction in Time-of-Flight mode requires a large coverage of the space with detectors which turns into a rather expensive instrument (contrary to monochromatic instruments).

We consider a design for a powder spectrometer aiming at replacing G41@LLB (low resolution - high flux). The G41 instrument [16] is operating with a graphite monochromator on a cold neutron guide. The horizontal divergence is 0.3° and the vertical divergence is 3°. The detector is covering a solid angle of 80° x 3°. The neutron flux at λ = 2.43 Å is 4x10^6 n/cm²/s at the sample position. We consider the following design for a powder diffractometer: (i) cold source, (ii) pulse width w = 250µs, f = 40 Hz (1% duty cycle), (iii) Source-sample distance 52m, (iv) sample-detector distance of 1m, total flight path of 53m. This leads to a usable bandwidth ranging from 1.4Å to 3.3Å with $\Delta\lambda/\lambda$ ranging from 1.3% to 0.5%. The horizontal and vertical divergence are set to 0.6°. The flux on the sample would be 1.5x10^6 n/cm²/s (~70% of G41. By using the 7C2@LLB detector which is covering a solid angle of 120°x20° with a detection efficiency of 90% a gain of a factor 20 would be obtained. This shows that a powder instrument on a CNS can easily outperform existing very productive instruments at neutron reactor facilities.

3. Discussion

From our simulations, we think that it should be possible to build a compact neutron source with performances in the range of ORPHEE / ISIS TS2. While the performances of such a source would not match the performances of ESS, it could still serve the need of about 50-75% of the users who do not need extreme neutron flux. Such sources could successfully replace aging neutron reactors as well as lower the barrier for new entrant countries in the field of neutron scattering.

Technique	**Flux on sample**	**Reference spectrometer**	**Potential gains**
SANS	1x10^6 n/s/cm² (low Q) 3x10^6 n/s/cm² (med Q) 9x10^6 n/s/cm² (high Q)	PAXE@LLB (low Q) 0.7x10^6 n/s/cm² SANS2D@ISIS 1x10^6 n/s/cm²	Slit setup x10 Focusing optics for VSANS (small Q) x10
Reflectivity	6x10^6 n/s/cm²	HERMES@LLB 8x10^6 n/s/cm² POLREF@ISIS ~1x10^7 n/s/cm²	SELENE concept x10 [17] Advanced Deconvolution x3
Low resolution powder diffraction	1.5x10^6 n/s/cm²	G41@LLB 2x10^6 n/s/cm²	Large solid angle detector (7C2 type) x20

Table 2: Comparison of the performances of various types of instruments on a compact source with existing instruments.

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