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Workhorse scattering instruments for low power compact accelerator driven neutron sources

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We investigate the potential of neutron scattering instrumentation fed by a compact accelerator driven neutron source. Such a source can be built and operated easily at any large university. Reference designs of typical workhorse scattering instruments for small-angle neutron scattering, powder diffractometry and reflectometry are presented. The neutron flux at sample position and the instrument resolution have been calculated from the parameter design of a pulsed neutron source with 400 W average accelerator power. Instrument performances allow for reasonable scientific use even at this low power level.

KEYWORDS: CANS, neutron production, instrumentation, neutron scattering

1. Introduction

Beam time at neutron scattering facilities is accessed through a complex and time consuming proposal system. Normal neutron scattering instruments are heavily overbooked resulting in long waiting times until the beam time is granted. This system is not suitable for a fast feedback during the sample preparation. Therefore, we are presenting the design for a novel neutron scattering facility called NOVA ERA "Neutrons Obtained Via Accelerator for Education and Research Activities" [1], which can be built and operated at any large university or medium sized company. This allows the setup of a network of small neutron scattering facilities establishing neutron scattering as a method for laboratory sample characterization, routine experiments, education and instrument development. Exemplary such a network is being set up in Japan: the Japanese Collaboration on Accelerator driven Neutron Sources (JCANS) [2].

The NOVA ERA is a compact accelerator driven neutron source (CANS) [3, 4] utilizing the nuclear reaction of protons in the low MeV range in a light target material like beryllium [3] for neutron production. Beryllium has a relatively high neutron production cross section [5] in the low MeV range so that neutrons can be produced in a small volume. Together with a flexible pulsed proton accelerator and a dedicated moderator / reflector system producing thermal and cold neutrons, one can design neutron scattering instruments that offer experimental opportunities already at an average accelerator power level of 400 W.

In this paper we report on the design of a neutron scattering facility based on a pulsed neutron source. The main components of NOVA ERA for neutron production are presented and the performance of instruments designed for small-angle neutron scattering, powder diffractometry and reflectometry are estimated.

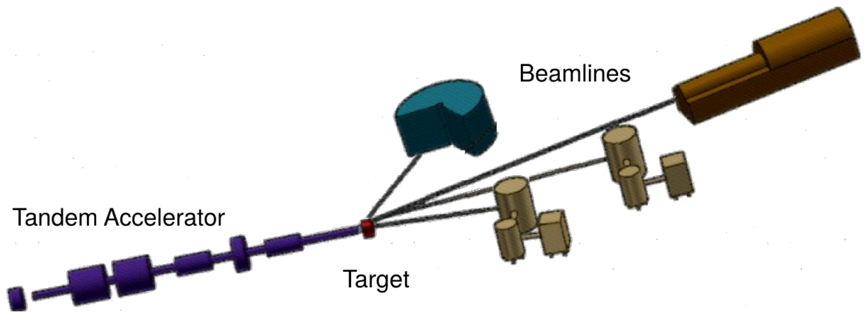

Fig. 1. NOVA ERA (Neutrons Obtained Via Accelerator for Education and Research Activities) concept for neutron scattering experiments.

2. Compact accelerator driven neutron source

A small compact accelerator driven neutron source aimed to be built at universities consists of an ion accelerator, a target, thermal and cryogenic moderators, neutron delivery optics and a few instruments as can be seen in Figure 1.

Normally, neutrons produced in research reactors or spallation sources are extracted from a moderator and delivered to the instruments. The instruments can be optimized starting from the extraction point up to the instrument with fixed operation parameters of the reactor or the accelerator. At a CANS a holistic approach is possible, the whole facility including accelerator timing and cryogenic moderators can be optimized according to the needs of each instrument.

2.1 Accelerator

For low power CANS aimed to be built at universities, the accelerator has to be reliable and commercially available with a reasonable price. Furthermore, the tritium production in the beryllium target should be avoided for radiation safety requirements. Therefore, proton accelerators working at energies below 13 MeV are preferable. A commercially available tandem accelerator is a good choice because it can produce ion currents up to 1 mA with changeable pulse lengths. A big advantage of such an accelerator system is the possibility to perform time-of-flight (TOF) measurements using a broad fraction of the neutron spectrum produced. The ion pulse has to be for this type of measurement in the range of the neutron moderation time ranging between 100 μs and 1 ms. With desired frequencies between 20 Hz for a large wavelength band and 300 Hz for a high resolution, the duty cycle of the accelerator can be in the range of 1% to 5%. A higher duty cycle results in reduced wavelengths resolution while a lower duty cycle reduces the overall neutron flux. A summary of useful parameters for a low power CANS is presented in Table I. The intensity calculations presented in this paper are based on a 4% duty cycle, i.e. 400 W average accelerator power.

Table I. Parameter set of the accelerator.

Ion type	Protons
Energy	10 MeV
Frequency	20 to 300 Hz
Current	1 mA
Duty cycle	1 to 5 %
Peak power	10 kW
Average power	100 to 500 W

2.2 Target / moderator assembly

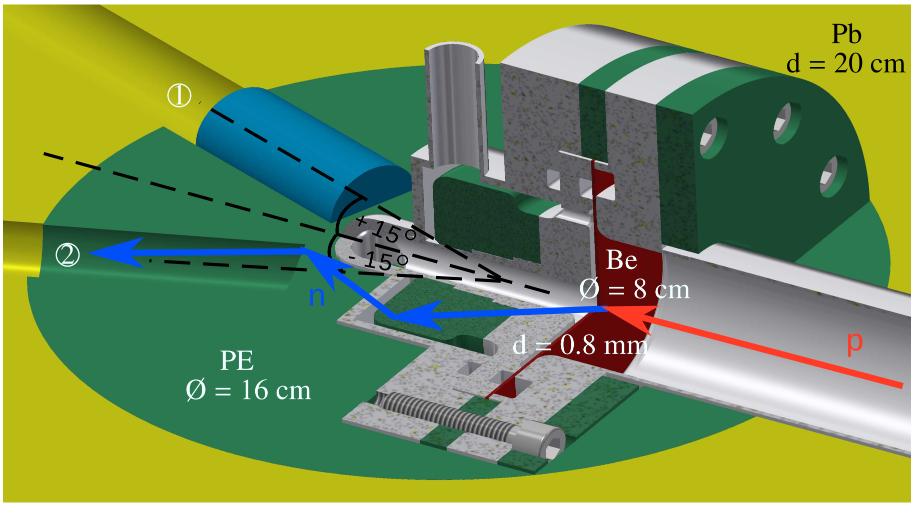

Fig. 2. Target / moderator assembly with a thermal extraction channel labeled ② and a cold extraction channels labeled ①. The red disc is the beryllium target, the green volume is the PE moderator and the yellow part is the Pb reflector.

The target / moderator assembly is shown in Figure 2 which was investigated with the ANSYS toolkit for mechanical stability. The target consists of a 0.8 mm thick beryllium disc with a diameter of 80 mm held by an aluminum housing. The target thickness was adjusted to the ion stopping range to avoid hydrogen implantation inside the beryllium target and its embrittlement [6]. A polyethylene (PE) moderator with a radius of 8 cm surrounding the beryllium target moderates the neutrons to thermal energies and a Pb reflector with a thickness of 20 cm increases the thermal neutron density inside the PE moderator. Low dimensional extraction channels [7, 8] inside the moderator / reflector assembly direct the thermalized neutrons to the instruments. They have an inclination of ±15° with respect to the proton beam. Cryogenic moderators can be inserted in the extraction channels moderating the thermal neutrons to energies in the low meV range. Some materials like methane, mesitylene or para-/orthohydrogen show good performances for a cryogenic moderator. We decided for a parahydrogen moderator because of the useful cold energy spectrum and optimal moderator dimensions due to preferable mean free paths for thermal and cold neutrons with λ = 1 cm and λ = 10 cm, respectively.

2.3 Simulations

The brilliance at the extraction channels for the above mentioned target / moderator assembly was investigated with Monte Carlo simulation using the MCNP6 toolkit with the ENDF/B-VII.1 database for neutron production [5]. In Figure 3 a)-b), the brilliance at the extraction point of the target / moderator assembly for a 100 μs ion pulse are presented for the thermal extraction channel ② and the extraction channel filled with parahydrogen ①, respectively. They show the brilliance depending on the neutron energy and the inclination to the extraction channel axis. The instrument performances can be estimated by integrating over the energy spectrum and the divergence for the individual instrument acceptance.

The time structure for the thermal and cold extraction channel is important for the estimation of the neutron pulse length. Therefore, we looked at the moderation time at the exit of the extraction channels for thermal neutrons of 13.1 meV to 127 meV and cold neutrons of 0 meV to 13.1 meV for a 100 μs proton pulse. As shown in Figure 3 c - d), the moderated neutron pulse length is 160 μs for thermal neutrons at the exit of the extraction channel ② and 280 μs for cold neutrons at the exit of the extraction channel ①.

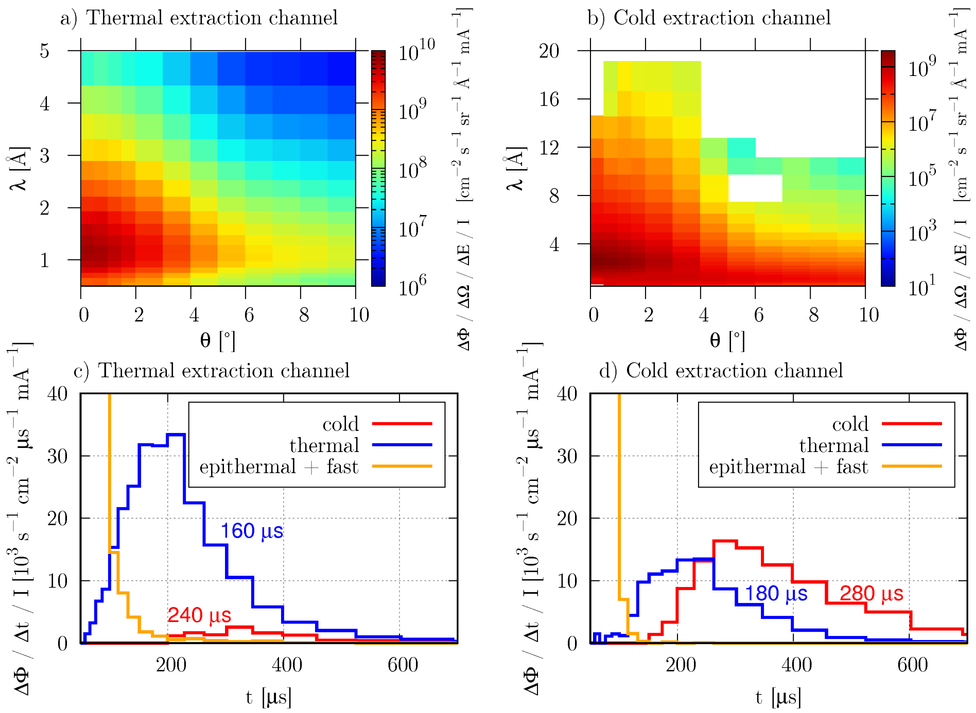

Fig. 3. a - b) Maps showing the brilliance as a function of the wavelength and the angle with respect to the extraction channel axis. c - d) Time structure for a 100 μs ion pulse at the exit of the extraction channels.

3. Instruments

Low power CANS are intended to be built close to standard laboratory facilities where they can support the characterization of materials quickly after sample preparation. This enables a fast feedback of the sample quality to the synthesis methods allowing an improved sample preparation. For the instrumentation of such a source, we have chosen instruments used by many scientist which can still give important information when being operated at low fluxes. The wavelength band and divergence acceptance is defined and the neutron flux at sample position is estimated for a typical reflectometer, a powder diffractometer and a small-angle scattering instrument, each in a TOF setup.

Table II. Resulting ion pulse length and neutron pulse length after the moderation to thermal and cold energies for typical frequencies and a duty cycle of 4%.

Frequency [Hz]	Frame length [ms]	Ion pulse length [μs]	Neutron pulse length [μs]	
			Thermal	Cold
48	20.8	833	840	870
144	6.9	278	300	380
192	5.2	208	240	330
288	3.5	139	190	290

As already mentioned, the advantage of a CANS is the possibility to optimize the whole setup to the needs of the instruments. Especially, the accelerator timing, i.e. the repetition rate and length of the ion pulses can be adjusted to the requirements of the instruments. Typical frequencies range from 20 Hz resulting in a large wavelength band up to 300 Hz for high resolution. Table II presents the ion pulse length and the neutron pulse length for thermal or cryogenic moderators for some example frequencies at a duty cycle of 4%.

3.1 Reflectometer

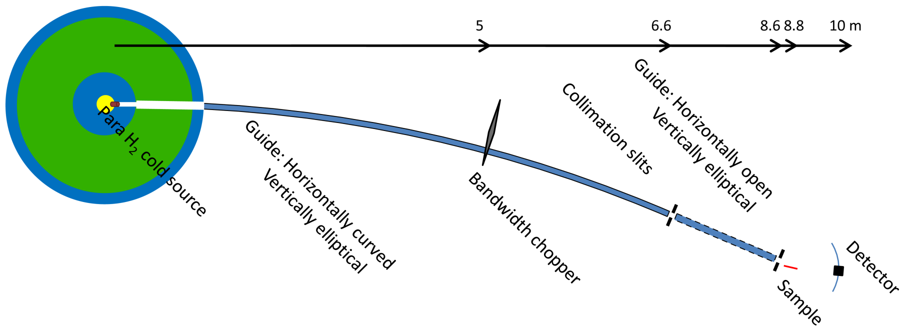

Fig. 4. A reflectometer in time-of-flight setup.

A typical neutron reflectometer is presented in Figure 4. This type of instrument is very well suited to be built at a pulsed source due to the large wavelength band acceptance. As the reflectivity increases strongly with decreasing scattering vector Q, the drop in spectral density towards long wavelengths is compensated well. A suitable source for a reflectometer is a cold source filled with liquid parahydrogen. We adjust the instrument parameters in such a way that the wavelength band used ($\approx$ 2 Å (20 meV) – 10 Å (0.8 meV)) covers the maximum intensity visible in the maps shown in Figure 3b). A 10 m long instrument with 48 Hz accelerator frequency will have a wavelength band of 7.5 Å covering the wavelengths from 2 Å up to 9.5 Å selected by a bandwidth chopper in a distance of 5 m from the source. A neutron pulse length of 0.87 ms and a instrument length of 10 m results in a wavelength uncertainty of $\Delta\lambda = 0.34$ Å resulting in $\Delta\lambda/\lambda = 17\%$ at 2 Å decreasing to 4% at 9.5 Å.

The neutron guide is curved in the horizontal plane to avoid direct view to the source minimizing the background. A double slit system is mounted directly in front of the sample position with a collimation length of 2 m. The divergence in the horizontal plane can be adjusted with the slit system defining the angular resolution of the reflectometer. In the vertical direction, the slit system is used to reduce the background. In this direction, the reflectometer can accept a large divergence without losing resolution. Therefore, the vertical shape of the guide will be elliptical.

In order to transport a sufficient number of neutrons also at low wavelength, the upper and lower surface of the focusing section of the ellipse will be equipped with an m = 3 supermirrors. For the curved section, the outer side of the neutron guide will be equipped with an m = 2 supermirror and the inner part with m = 1.

In order to estimate the flux at the sample position, we assume a collimation with slit widths set at S_1 = 10 mm and S_2 = 10 mm, resulting in a divergence of $\Delta\Theta = 0.3°$ in the horizontal plane. Integrating over the brilliance for the solid angle used and a 2 Å – 9.5 Å bandwidth at the extraction channel, yields a neutron flux of $5 \cdot 10^4\ \mathrm{s^{-1}cm^{-2}}$ at the sample position.

3.2 Small-Angle Scattering

The proposed small-angle neutron scattering instrument (SANS) is shown in Figure 5. Similar to the reflectometer, SANS can use a broad wavelength band and will be built at an extraction channel with a cryogenic moderator. In difference to the reflectometer, a symmetric divergence, a movable 2-dimensional position sensitive detector and an adjustable collimation length will be employed. The movable detector is necessary to cover the Q-range from medium to high resolution. The collimation section with a neutron guide changer enables to use a long collimation length for high resolution experiments as well as a short collimation length for high flux experiments. The total length of the instrument defines the usable wavelength band. Together with the longest collimation and the largest detector distance, we do not want to afford a long curved neutron guide

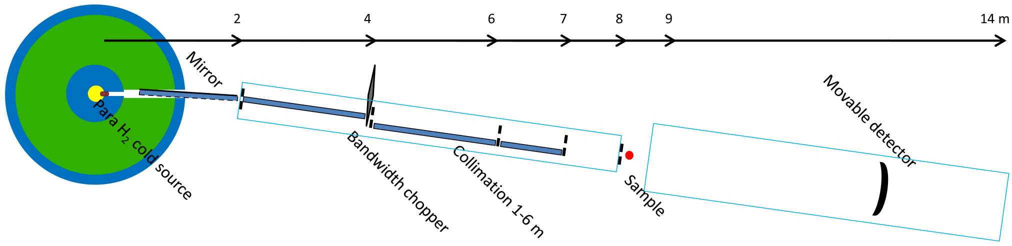

Fig. 5. A Small-Angle Neutron Scattering instrument (SANS) in time-of-flight setup.

in front of the collimation further reducing the wavelength band. As a compromise, we propose to use a 2 m long mirror between cold source and the beginning of the collimation to eliminate the direct sight to the target.

A bandwidth chopper in a distance of 4 m from the source has to be tuned to the requirements of the proposed experiment by defining the wavelength band and Q_{min}. Some examples for wavelength band, the divergence, the slit width and the estimated flux at the sample position are presented in Table III.

Table III. Estimated neutron flux at the sample position for different collimation lengths and detector distances with resulting wavelength bands.

Collimation [m]	Detector [m]	S_1 [mm]	S_2 [mm]	Divergence [°]	Solid angle [μsr]	Wavelength band [Å]	Q_{min} [$Å^{-1}$]	Flux [$s^{-1}cm^{-2}$]
1	1	20	10	0.86	225	2 – 10.3	$1.8 \cdot 10^{-2}$	$7 \cdot 10^4$
2	2	20	10	0.43	56	2 – 9.5	$1.0 \cdot 10^{-2}$	$2 \cdot 10^4$
4	4	20	10	0.21	14	2 – 8, 3	$5.5 \cdot 10^{-3}$	$4 \cdot 10^3$
6	6	20	10	0.14	6.3	2 – 7.4	$4.1 \cdot 10^{-3}$	$1.5 \cdot 10^3$
6	6	10	10	0.1	2.8	2 – 7.4	$3.0 \cdot 10^{-3}$	$6.7 \cdot 10^2$

3.3 Powder diffractometer

The powder diffractometer presented in Figure 6 differs from the reflectometer and the small-angle scattering instrument described above as to resolve atomic structures thermal neutrons are required. Therefore, the powder diffractometer will be built at a thermal extraction channel. A fast rotating double chopper defines the neutron pulse length and the wavelength resolution as well. Between the chopper and the sample position an elliptical neutron guide is used to focus the neutron beam onto the sample. To be able to use a wavelength band as wide as possible and also to avoid the wavelength dispersion before the neutron pulse passes the chopper, the double chopper is positioned as close to the source as possible. Therefore, the beamline cannot be shielded against the fast neutron background coming from the source. Consequently, the detector acquisition is closed during the ion pulse defining hereby the limits of the natural wavelength band. Changing the frequency of the accelerator allows to tune the wavelength band to the experimental requirements.

Table IV shows a selection of useful frequencies, the associated wavelength bands, the resolution and the resulting flux at the sample position for a 25 μs neutron pulse length defined by the double chopper. The flux and the resolution scale linearly with the neutron pulse length allowing to chose the wavelength band freely. For the flux estimation at the sample position, we chose an elliptical neutron guide with $m = 3$ supermirror coating in the focusing section optimized for small samples. With a divergence changer, the focusing section of the neutron guide can be replaced with a straight guide useful to homogeneously illuminate larger samples or for measurements at low Q-values where a small angular divergence is needed.

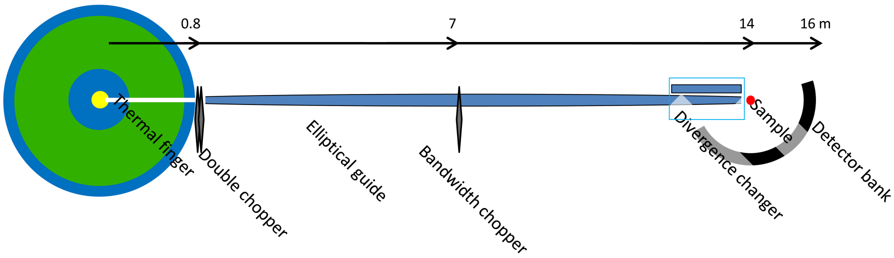

Fig. 6. A powder diffractometer in time-of-flight setup.

Table IV. Estimated neutron fluxes at the sample position for different accelerator frequencies and resulting wavelength bands. The operation parameters of the bandwidth chopper are defining λ_{min} so that the fast neutrons from the next frame are not overlapping with the used wavelength band and λ_{max} is defined by the instrument length and the frame length.

Frequency [Hz]	λ_{min} [Å]	λ_{max} [Å]	$\Delta t/t$ in backscattering	Flux [$s^{-1}cm^{-2}$]
144	1.78	3.42	$2.5 \cdot 10^{-3}$	$2.8 \cdot 10^{3}$
192	1.34	2.57	$3.2 \cdot 10^{-3}$	$4.3 \cdot 10^{3}$
192	2.63	3.86	$2.0 \cdot 10^{-3}$	$1.9 \cdot 10^{3}$
288	0.90	1.73	$5.0 \cdot 10^{-3}$	$5.3 \cdot 10^{3}$

4. Results and Discussion

Table V shows the summary of the instrument performances at a low power CANS as well as a comparison to present neutron scattering instruments at BER-II [9]. The summary shows that a reflectometer and a powder diffractometer are very well competitive to the instruments operated at a medium flux research reactor like BER-II. The lower flux can be overcompensated with the easy access to a CANS laboratory source. A measurement over night at NOVA ERA will have the same scientific outcome as a few hours of beamtime at the reactor. In the case of SANS, the situation looks worse because the strength of the compact source i.e. high brilliance neutron beam being fed into adapted neutron optics could not be offered because of the strict collimation requirements. Still, the SANS instrument proposed is a reasonable workhorse for a soft matter laboratory.

Table V. Results of the instrument performance investigation as well as a comparison with working scattering instruments at todays research reactors.

Source	Instrument	Collimation	Flux [$s^{-1}cm^{-2}$]
NOVA ERA	Reflectometer	5 mrad	$5 \cdot 10^{4}$
BER-II	V6	1 mrad	$3 \cdot 10^{4}$
NOVA ERA	SANS (low resolution)	15 mrad	$7 \cdot 10^{4}$
BER-II	V4	10 mrad	$2 \cdot 10^{7}$
NOVA ERA	Powder diffractometer	20 mrad	$4.3 \cdot 10^{3}$
BER-II	E9	5 mrad	10^{5}

Future developments will improve the moderator spectrum and moderator brilliance especially for the cryogenic moderators. Specially adapted neutron optics will further improve the neutron transport to the sample and the instrument performance. Additionally, novel techniques can be investigated like a TOF-PGNAA. Last, new concepts can be implemented like an improved data reduction allowing the relaxation of the divergence in the horizontal plane for a reflectometer [10].

5. Conclusion

With the NOVA ERA concept for a CANS, universities and also industry can afford to built and to maintain a neutron source. We presented here the target / moderator concept and showed the estimated brilliance at the extraction channels. With this, the instrument performances of typical elastic scattering instruments have been investigated. We showed that the neutron flux at sample position is lower then the neutron flux at today's research reactors but that it is still large enough to perform elastic neutron scattering experiments. Especially the instruments with a high divergence acceptance like a reflectometer show a comparable neutron flux. The operation of elastic neutron scattering instruments like a reflectometer, a powder diffractometer and a SANS at a NOVA ERA source build at large universities enables an easier and faster access, a fast feedback during sample preparation and also a reasonable scientific output.

After the analytical investigation of typical scattering instruments, we plan to simulate these instruments using a ray tracing code like McStas [11] or Vitess [12]. This would give more reliable values for the neutron flux at the sample position. Simultaneously, we are planning to investigate the target / moderator geometry for each individual instrument with MCNP6 simulations. With this approach, we will be able to present optimized instrument designs within near future.

References

[1] E. Mauerhofer, U. Rücker, T. Cronert, P. Zakalek, J. Baggemann, P.-E. Doege, J. Li, S. Böhm, H. Kleines, T. Gutberlet, T. Brückel, Conceptual Design Report - NOVA ERA (Neutrons Obtained Via Accelerator for Education and Research Activities) - A Jülich High Brilliance Neutron Source project, Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag Jülich (2017)

[2] Y. Kiyanagi, JCANS network of compact neutron facilities in Japan, Eur. Phys. J. Plus **131**, 132 (2016)

[3] U. Rücker, T. Cronert, J. Voigt, J. P. Dabruck, P. E. Doege, J. Ulrich, R. Nabbi, Y. Beler, M. Butzek, M. Büscher, C. Lange, M. Klaus, T. Gutberlet, Th. Brückel, The Jülich high-brilliance neutron source project, The European Physical Journal Plus, **131**, 19 (2016)

[4] A. Menelle, F. Ott, B. Homatter, B. Annighöfer, F. Porcher, C. Alba-Simionesco, N. Chauvin, J. Schwindling, N. Tran, A. Letourneau, A. Marchix, Neutrons production on the IPHI accelerator for the validation of the design of the compact neutron source SONATE, arXiv:1612.00237

[5] M.B. Chadwick, et al., ENDF/B-VII.1: Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data, Nucl. Data Sheets **112**, 2887 (2011)

[6] T. Rinckel, D. Baxter, J. Doskow, P. Sokol, T. Todd, Target Performance at the Low Energy Neutron Source Physics Procedia, **26**, 168 - 177 (2012)

[7] F. Mezei, L. Zanini, A. Takibayev, K. Batkov, E. Klinkby, E. Pitcher, T. Schönfeldt, Low dimensional neutron moderators for enhanced source brightness, arXiv:1311.2474 (2013)

[8] T. Cronert, J. P. Dabruck, P.-E. Doege, Y. Bessler, M. Klaus, M. Hofmann, P. Zakalek, U. Rücker, C. Lange, M. Butzek, High brilliant thermal and cold moderator for the HBS neutron source project Jülich, Journal of Physics Conference Series **746**, 012036 (2016)

[9] M. Tovar, H. A. Graf (Editors), Neutron Scattering Instrumentation at the Research Reactor BER II, Berlin Neutron Scattering Center (2007)

[10] R. Cubitt, T. Saerbeck, R. A. Campbell, R. Barker and P. Gutfreund, An improved algorithm for reducing reflectometry data involving divergent beams or non-flat samples, J. Appl. Cryst. **48**, 2006 (2015)

[11] K. Lefmann, K. Nielsen, McStas, a general software package for neutron ray-tracing simulations, Neutron News **10 (3)**, 20-23 (1999)

[12] C. Zendler, K. Lieutenant, D. Nekrassov, M. Fromme, VITESS 3 Virtual Instrumentation Tool for the European Spallation Source, Journal of Physics: Conference Series, **528**, 012036 (2014)