Workshop on Neutron Focusing Optics – NFO

Thursday, 2 March 2023 - Friday, 3 March 2023
Paul Scherrer Institute, Villigen, CH

NFO

HighNess

SwissNeutronics

PAUL SCHERRER INSTITUT

PSI

Organizing Team

Dr. Stavros Samothrakitis, PSI

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Dr. Valentina Santoro, ESS

Sponsor

Swiss Neutronics

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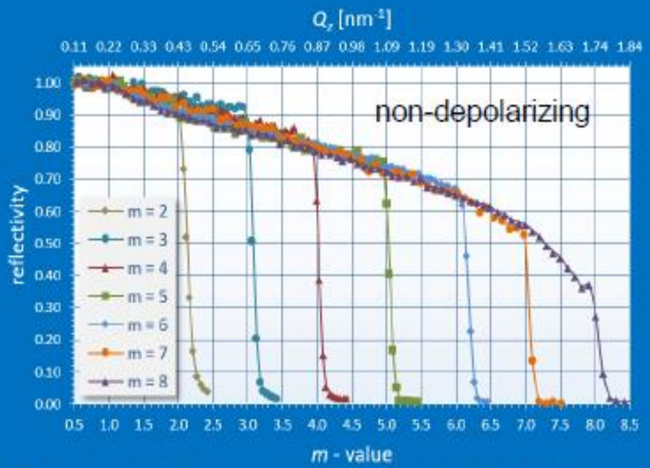
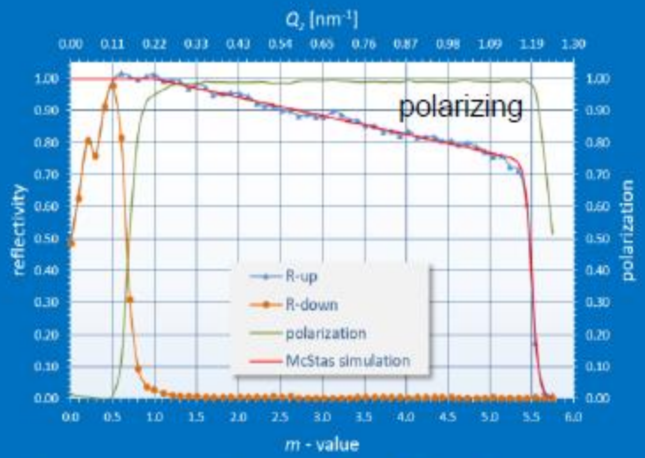
Neutron Optical Components and Instruments





Supermirror at its best: high reflectivity – large angles of reflection


POWTEX @ FRM II

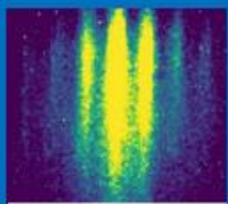

Insert @ ANSTO


BWFA for ODIN @ ESS

Complex elliptic guides made from glass, Al, or Cu


Nested mirror optics (not to scale)

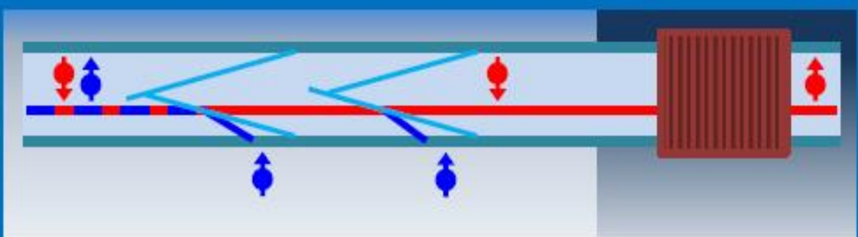

Object



Image


Photo of device

Neutron transport with nested mirror optics


Schematic spin selector


Spin selector @ CSNS

Spin selection: 2V-cavity combined with RF spin flipper

Swiss *Quality* for Excellence in Neutron Science

Contents

ESS - HighNESS

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European Spallation Source ERIC

HighNESS (development of High intensity Neutron source at the European Spallation Source) is a three-year EU-funded project aiming at designing a second neutron source at ESS, taking advantage of the upgrade possibilities offered by the facility. The main source, which will serve all the ESS instruments in the initial suite, consists of a high-brightness bi-spectral (thermal-cold) moderator. The second source focuses on delivering high intensity neutron beams of longer wavelengths, in the cold (2-20 Å), very cold (10-120 Å) and ultra-cold (>500 Å) regions. By using liquid deuterium instead of parahydrogen, it is possible to achieve a cold neutron intensity an order of magnitude higher than for the upper moderator. Very cold neutron beams of unprecedented intensity can be produced using advanced moderators and reflector materials, such as solid deuterium, nanodiamonds, and deuterated clathrate hydrates, which are all studied within the project. High intensity neutron beams will offer new possibilities in neutron scattering, in particular for spin echo, imaging, and SANS and world-leading experiments in fundamental physics like the search for neutron-antineutron oscillation. I will present the main features of the ESS second source, and give an overview of the possible applications.

Considering Instrumentation for a High Intensity moderator at the European Spallation source

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The European Spallation Source, currently under construction in Lund, Sweden, will originally make available a suite of 15 state-of-the-art neutron scattering instruments, which will be served by a high-brightness moderator placed above the spallation target. The current infrastructure of ESS, however, allows for a second, alternative moderator to be constructed and positioned below the spallation target. The second moderator is currently considered to have a larger viewable area, offering higher total cold neutron flux and higher intensities at longer wavelengths, potentially spanning a range from Cold (4 – 10 Å) to Ultra Cold (> 100 Å) neutrons. It is assumed that several areas of condensed matter research profit from such second moderator concept, including small-angle neutron scattering, spin-echo spectroscopy, and neutron imaging.

Here, we present the conceptual designs of potential instruments, giving focus to small-angle neutron scattering instrumentation. We make comparison of two conceptual designs, one having a conventional pin-hole geometry, optimized for the lower moderator, and the other making use of novel Wolter optics.

McStas Simulation Tools for Neutron Focusing Optics and Virtual Experiments

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The McStas[1-3] neutron ray-tracing simulation package is a versatile tool for producing accurate simulations of neutron optical systems and neutron scattering instruments at reactors, short- and long-pulsed spallation sources. McStas is extensively used for design and optimization of instruments, virtual experiments, data analysis and user training. McStas was founded as a scientific, open-source collaborative code in 1997.

This contribution presents the project at its current state and further gives an overview into the specific options for simulation of neutron-optical devices for beam focusing.

References:

1. K. Lefmann and K. Nielsen, Neutron News 10, 20, (1999).

2. P. Willendrup, and K. Lefmann, Journal of Neutron Research, vol. 22, no. 1, pp. 1-16, 2020

3. P. Willendrup, and K. Lefmann, Journal of Neutron Research, vol. 23, no. 1, pp. 7-27, 2021

A McStas Simulation Framework for Nested Mirror Optics - Method and Applications

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The transport of neutrons from the region where they have been generated (e.g. a moderator) to the a sample or detector are a crucial part of neutronic experiments and instruments.

In course of the currently running EU project HighNESS a particular kind of these transport systems is being studied: nested mirror optics. These devices are assembled from several layers of neutron mirrors that are arranged in an elliptical or a Wolter optic geometry. The nested arrangement makes highly efficient and compact components possible. To run Monte Carlo simulations that quantify the performance as well as to find the best geometries of such devices a collection of Python methods was developed. With its help McStas components for the simulations can be generated automatically from a couple of input parameters.

I will present the capabilities of the library and the simulation framework used and show two application examples: i.e. the NNBAR experiment and an in-beam ultracold neutron (UCN) source.

Conceptual design of a reflective focusing system for a SANS instrument

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European Spallation Source ERIC

The focusing devices used in small angle scattering have a completely different purpose comparing with other neutron techniques. In other methods, like diffraction or spectroscopy, focusing devices are used in order to increase the amount of neutrons going through the sample, at the cost of increasing the divergence of the beam and therefore, causing a decrease in the angular resolution of the measurement. On the other hand, in small angle scattering, focusing optics cannot be used with the same purpose due to the need of collimated beams. The focusing devices in SANS are designed to focus at the detector, not at the sample, in order to increase the momentum transfer (Q) range of the measurement and its resolution.

This work proposes a design of a reflective focusing system that would avoid the chromatic aberrations found in MgF_2 lenses and could be used in integrated in existing TOF-SANS instruments. Its performance is found to be good and it is possible to focus at the required distances. The limitations of this device are analyzed and engineering requirements as alignment and surface quality are also discussed in detail.

Neutron beam focusing in SANS experiments

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Since the 1960s, with the advent of the SANS technique, there were also ideas to enhance the resolution at lowest q-values by the application of beam focusing. Alongside with mirror focusing as it found its early adaptation to the KWS-3 beamline in Jülich and later in Garching, there are lenses, magnetic arrays and collimation systems that are more and more applied to complement standard SANS pinhole principles, in order to bridge the regime of measurable momentum transfers towards what is accessible with USANS. These principles are in the meantime referred to as VSANS. Higher brilliance neutron sources of our time are a chance to make VSANS a more common user application to investigate additional information on mesoscopic structures. We look back on developments as well as to the perspectives in the field.

Towards a Novel Focusing SANS at the MIT Nuclear Reactor for Materials, Energy, and Biology Research

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We propose to build a SANS diffractometer at the MIT Nuclear Reactor (MITR). SANS is a very popular technique for studies of materials with characteristic length scales in the range of 10 - 1000 nm. Unfortunately, all six US SANS diffractometers at national neutron research facilities (at Oak Ridge National Lab and NIST) are severely oversubscribed and require months of waiting time. The beamtime competition will become much worse in the next five years with planned (and possibly unplanned) long outages at both Oak Ridge and NIST facilities, thus crippling projects and making it nearly impossible for graduate students to substantially include SANS methods in their thesis research. Therefore, there is a pressing need for increased SANS capacity.

The 6 MW MITR has been in service since 1958 and has a long and proud tradition of carrying out education and research in the areas of fission engineering, materials, neutron physics, etc. Currently, a primarily neutron-irradiation facility with small confinement building a no cold source, MITR is not ideally suited for hosting SANS. However, there is an opportunity to build a novel SANS instrument at the MITR. Our detailed ray-tracing work points out that the best option is focusing SANS, which is much shorter and faster than traditional SANS. It will use neutron Wolter mirrors developed at MIT. If successful, it will be the first-of-its-kind instrument, potentially leading the way for more compact SANS facilities. Detailed estimates showed the achievable resolution of $Q_{min} \approx 4\times10^{-3}$ Å^{-1} and the flux on the sample of 2×10^{4} n/cm^{2}/s. This resolution will enable studies of structures with length scales below about 150 nm with typical measurement times of several hours. While this is longer than at national neutron research facilities at ORNL or NIST, such longer measurements are preferable to months of waiting for the beamtime at ORNL or NIST or giving up on critical information that requires SANS.

From focusing monochromators to nested mirror optics

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Neutron scattering is a well-established technique for the investigation of the static and dynamic properties of materials over a wide range of spatial and temporal scales. Many studies of high interest, however, can only be performed on small samples and typically require elaborate extreme environments. To improve the signal-to-noise ratio, various focusing techniques have been developed during the last 50 years such as focusing monochromators or focusing neutron guides. Indeed, impressive gains in flux of more than two orders of magnitude have been achieved.

In this contribution I will give an overview about various concepts for beam focusing, the efficient transport of neutrons, and the selection of their phase space, i.e. beam size and divergence. In combination with highly-brilliant neutron sources, the flux and the cleanleness of the beams can be improved tremendeously thus allowing conducting experiments that were thought to be not feasible many years ago.

Simulation of Neutron Focusing Optics using the Simulation Package VITESS

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Though focusing neutrons is by far more difficult than focusing charged particles or photons, several optical devices for this purposes have been developed over the last decades: focusing guides and benders, lenses and prisms, focusing mirrors and mirror assemblies as well as hexapole magnets. Except for the latter ones, they can all be simulated using the neutron instrument simulation package VITESS. In this talk, we present the VITESS modules repesenting these devices and show how they are used. In most cases, examples of applications are also given.

The NIST Wolter optic neutron microscope

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Wolter optics - axisymmetric, nested mirrors comprised of two conic sections - hold great promise for use in neutron imaging and other neutron transport and scattering applications. M. Gubarev at NASA introduced the idea of using Wolter optics for neutron scattering in 2007 [1]. It took a couple years, and the added enthusiasm of B. Khaykovich [2] for the first tests as a microscope objective lens at NIST in 2011 [3]. Including a condensing optic was demonstrated by measuring the semi-metal to ferromagnet transition temperature in $HgCr_2Se_4$ [4]. This lead to a final optical system design composed of a Wolter type-I telescope as the condenser and a hyperbola-elliptical objective with magnification 10. The ray tracing results suggest this optical system will yield a 104 gain over a conventional pinhole imaging setup. Or, a single projection image with 3 μm resolution in about 1 s with a maximum field of view of 10 mm [5]. The design and sources of inspiration for this optical system will be reviewed as will thoughts on how to create a user instrument.

References

1. https://doi.org/10.1016/j.nimb.2007.09.041

2. https://doi.org/10.1016/j.nima.2010.11.110

3. https://doi.org/10.1063/1.4804178

4. https://doi.org/10.1016/j.jmmm.2018.11.086

5. https://doi.org/10.1016/j.nima.2020.164813

Current guide design ideas at Oak Ridge National Laboratory

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ORNL is home to two of the most powerful neutron sources in the world (SNS and HFIR) and is currently in the design phase for a third one (STS). Each one of these has their unique moderator design and therefore guide design challenges. Over the past several years and under the initial guidance of Alexandru 'Ducu' Stoica, several predominant ideas have evolved on how to best deal with each of them.

In this talk, I will discuss some of these concepts, for example beam focusing from large moderators, phase space matching using secondary sources for small moderators, the benefits of octagonal guides for tube moderators, and phase space smoothing after curved guides.

Mirror focusing VSANS: Q-range extension option for an existing pinhole SANS and default configuration for a new VSANS instrument, based on experience the user operation of the focusing instrument KWS-3 operated by JCNS at MLZ

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Since 2011, the mirror-focusing small-angle scattering diffractometer KWS-3 has been open for user operation in the standard configuration with Q-range between Q_{min} = 0.0001 and Q_{max} = 0.003 Å^{-1}. Several options have been implemented over the past decade to extend the Q-range and functionality of the instrument. The implementation of the second (very high-resolution) detector with three times smaller pixel size (about 0.1 mm) allowed to achieve a minimum wavevector under Q_{min} = 0.00003 Å^{-1} with a standard wavelength of 12.8 Å and the sample-to-detector-distance SDD=9.5 m. The second vacuum/air sample position at SDD = 1.5 m extended the maximum Q value to Q_{max} = 0.02 Å^{-1}, a wide Q-overlap with most of existing pinhole SANS diffractometers is available now. Polarized neutron and polarization-analysis options, the full suite of SANS sample environments can be used to analyze structures within the characteristic length scale of 30nm to 20 µm.

This presentation will discuss the possibility of using a focusing mirror as a VSANS option for existing SANS instruments on a reactor or TOF source. Vertical and horizontal layouts of a dedicated VSANS diffractometer are compared.

Phase correction by ellipsoidal focusing mirrors for a high-resolution neutron resonance spin echo spectrometer

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Neutron focusing mirrors can increase the signal-to-noise ratio of neutron scattering experiments by concentrating neutrons with a large divergence angle and controlling the beam trajectory. In addition to this advantage, elliptical focusing mirrors can be useful for phase correction for higher resolution neutron spin echo instruments [1].

Neutron resonance spin echo spectrometers aiming a high SN ratio and high-resolution are being developed at the pulsed neutron source of Materials and Life Science Experimental Facility (MLF) of J-PARC [2, 3]. The conventional solenoid coils upstream and downstream of the sample are replaced by two resonance spin flippers (RSF) and a zero-field space between the flippers. By inserting a pair of ellipsoidal focusing mirror between RSFs, the neutron flight path lengths between RSFs can be kept constant, thereby making neutron phases uniform. We develop 900 mm long ellipsoidal focusing supermirrors with metal substrate with semi-major axis of 1250 mm and semi-minor axis of 65.4 mm. The ellipsoidal mirror is divided into several segments considering the uniformity of supermirror deposition and the size limitation of the polishing equipment. The segments are assembled in a cage-like mirror holder designed to ensure precise positioning [2].

In the presentation we will describe the fabrication of the ellipsoidal focusing mirror and performance evaluation, and discuss experiments and simulations [4] for phase correction by a focusing mirror in a high-resolution neutron resonance spin echo spectrometer.

References:

[1] F. Mezei et al., Eds., “Neutron Spin Echo Spectroscopy”, Lecture Notes in Physics 601, Springer, 176–200 (2002).

[2] T. Hosobata et al., JPS Conf. Proc. 22, 011010 (2018)

[3] H. Endo et al., Physica B 564, 91-93 (2019)

[4] F. Funama et al., Nucl. Instrum. Methods A 1010, 165480-165480 (2021)

Nanofabrication of diffractive X-ray optics – opportunities for neutron imaging?

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X-rays are used in a wide range of scientific experiments to investigate the structure of matter. They have the ability to penetrate thick samples, and provide information on the elemental and even chemical composition. Moreover, their short wavelength enable excellent spatial resolution down to the atomic scale. In practice, the spatial resolution of x-ray probes and x-ray microscopes are limited by the quality of the available x-ray optics.

We report on the development of diffractive X-ray optics for imaging applications at synchrotron sources. In order to obtain good resolution and efficiency, diffractive structures with dimensions ranging from microns down to the nanoscale have to be produced by lithography techniques. Examples for the fabrication and application of such optics will be presented.

The presented technological concepts and developments also have potential for neutron imaging. Already more than 15 years ago, the concept of grating based phase contrast and dark field imaging has been successfully transferred from X-rays to neutron radiation. Presently we are investigating the concept of achromatic X-ray lenses for applications in neutron microscopy.

Focusing Strategies at SINQ Beamlines

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The development and use of focusing optics to improve signal is long-established at SINQ. In particular, the development of adaptive optics and Coron optics inside the sample environment was the core area of improvements over the last 10 years. Furthermore, during the 2019 guide upgrade, guide geometries designed for the specific instrument needs were installed, resulting in a significant performance increase. The three different types of focusing guide systems now in place are presented in this talk. In addition to gaining signal via focusing, we improved the shielding in the hall to reduce the neutronic background originating from the neutron source.

Despite bespoke neutron guides, secondary focusing (close to sample) is still needed at the instruments, as sample sizes can vary from few cm^3 to few mm^3 in volume. Our solutions of adaptive and Coron optics can be used as an add-on to the guide system when very small samples are the target of investigations. For these particular samples, we have in recent years made several efforts to also decrease the noise from the sample environment. We present our approach and investigated possibilities, e.g., radial collimation, aperture systems and systematic study via simulation.

Performance of the Selene guide of Amor and related optics

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Starting with the idea, that the ideal neutron guide is one which delivers as much useful neutrons to the sample as possible, but not more, led to the development of what I called 'Selene optics'. Later it turned out that it was already suggested in 1963 by Maier-Leibntiz - and it is based on the same principles as many synchrotron beam lines. Also, there is not one ideal guide design for all applications.

In short, the Selene optics consists of two subsequent elliptic reflectors, sharing the long axis and a focal point. This set-up forms an imaging optics, mapping some luminescent area (the ' virtual source') to the sample (or detector) position. Two reflectors are necessary to correct to first order for coma aberration.

During the SINQ upgrade program in 2019 a Selene guide was installed for the neutron reflectometer Amor. And even though the secondary instrument is not yet ready for user operation, we managed to perform several measurements to characterize the guide's performance and the instrument's capabilities.

I will present the concept and design of the Selene guide, the actual realisation including the compromises and the mentioned first measurements. This includes the new polariser which is optimally adapted to the beam converging to or emerging from a small spot, respectively.

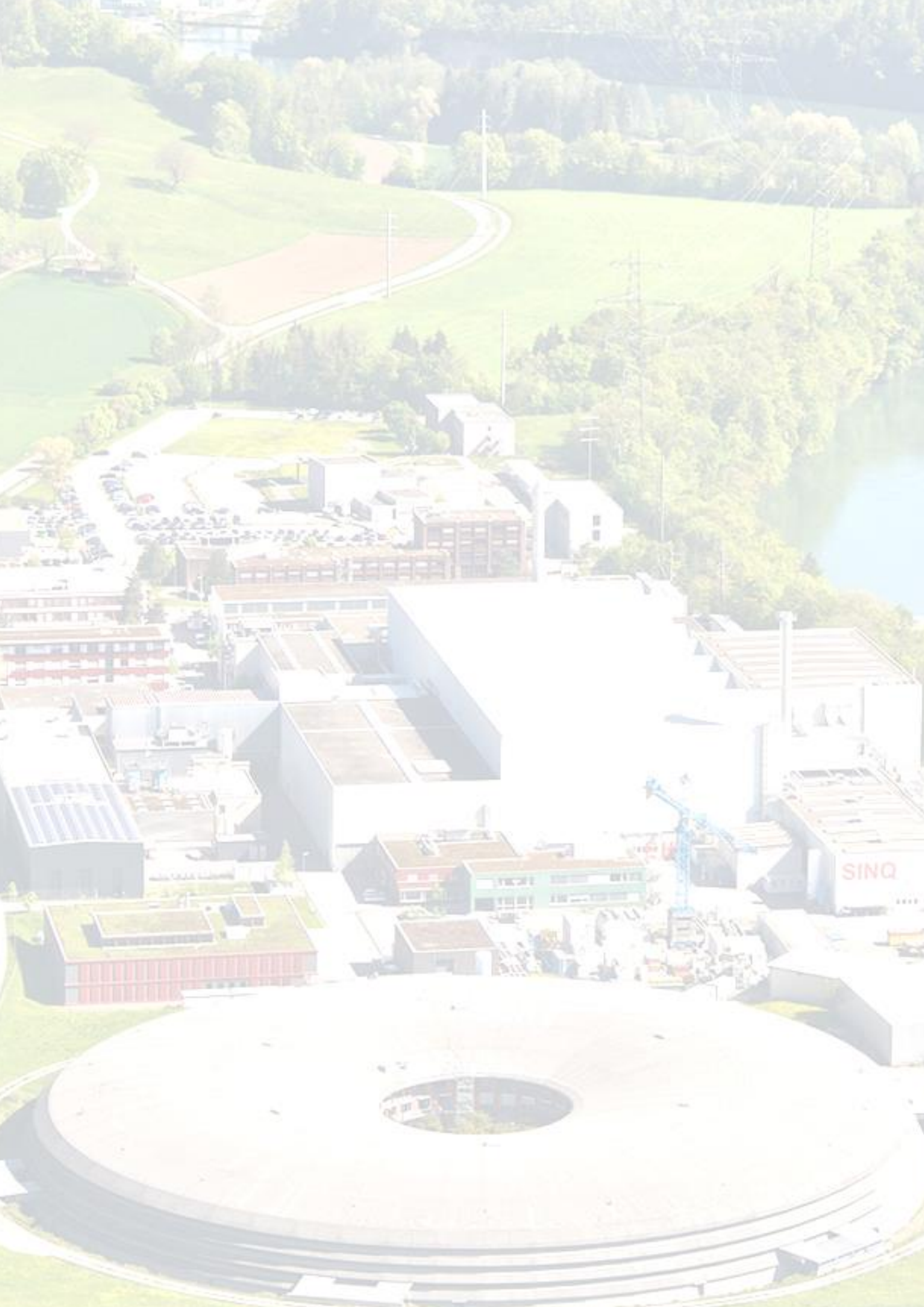
Timetable

Thu 02/03

12:00	Registration and Lunch		WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	12:00 - 13:00
13:00	Welcome	*Markus Strobl*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	13:00 - 13:10
	ESS - HighNESS	*Valentina Santoro*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	13:10 - 13:30
	Considering Instrumentation for a High Intensity Moderator at the European Spallation Source	*Stavros Samothrakitis*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	13:30 - 14:00
14:00	McStas Simulation Tools for Neutron Focusing Optics and Virtual Experiments	*Peter Willendrup*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	14:00 - 14:30
	A McStas Simulation Framework for Nested Mirror Optics - Method and Applications	*Richard Wagner*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	14:30 - 15:00
15:00	Coffee Break		WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	15:00 - 15:30
	Conceptual design of a reflective focusing system for a SANS instrument	*Dr Damian Martin Rodriguez*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	15:30 - 16:00
16:00	Neutron beam focusing in SANS experiments	*Dr Daniel Clemens*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	16:00 - 16:30
	Towards a Novel Focusing SANS at the MIT Nuclear Reactor for Materials, Energy, and Biology Research	*Boris Khaykovich*		
17:00	From focusing monochromators to nested mirror optics	*Peter Böni*	WHGA/001/Auditorium (PSI), Paul Scherrer Institute, Villigen, CH	17:00 - 17:30

Fri 03/03

09:00	**Simulation of Neutron Focusing Optics using the Simulation Package VITESS** *OGSA/EG06, Paul Scherrer Institute, Villigen, CH*	*Klaus Lieutenant* 09:00 - 09:30
	The NIST Wolter optic neutron microscope *OGSA/EG06, Paul Scherrer Institute, Villigen, CH*	*Daniel Hussey* 09:30 - 10:00
10:00	**Current guide design ideas at Oak Ridge National Laboratory** *OGSA/EG06, Paul Scherrer Institute, Villigen, CH*	*Thomas Huegle* 10:00 - 10:30
	Coffee Break *OSGA/EG06, Paul Scherrer Institute, Villigen, CH*	10:30 - 11:00
11:00	**Mirror focusing VSANS: Q-range extension option for an existing pinhole SANS and default configuration for a new VSANS instrument, based on experience the user operation of the focusing instrument KWS-3 operated by JCNS at MLZ** *Vitaly Pipich*	
	Phase correction by ellipsoidal focusing mirrors for a high-resolution neutron resonance spin echo spectrometer *Tatsuro Oda*	
12:00	**Nanofabrication of diffractive X-ray optics – opportunities for neutron imaging?** *OGSA/EG06, Paul Scherrer Institute, Villigen, CH*	*Christian David* 12:00 - 12:30
13:00	**Lunch** *OASE Restaurant, Paul Scherrer Institute, Villigen, CH*	12:30 - 14:00
14:00	**Focusing Strategies at SINQ Beamlines** *OGSA/EG06, Paul Scherrer Institute, Villigen, CH*	*Christine Klauser* 14:00 - 14:30
	Performance of the Selene guide of Amor and related optics *OGSA/EG06, Paul Scherrer Institute, Villigen, CH*	*Jochen Stahn* 14:30 - 15:00
15:00	**Discussion, Networking, and Goodbye** *OSGA/EG06, Paul Scherrer Institute, Villigen, CH*	15:00 - 16:00


SINQ