Nuclear Instruments and Methods in Physics Research A 764 (2014) 30–41

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Probing static and dynamic correlations in matter under extreme conditions: Concept of multi-purpose instrument at the European Spallation Source

O. Prokhnenko [a,b,*], K. Lieutenant [a,b], L.D. Cussen [a,b], W.-D. Stein [a,b], C. Zendler [a,b], K. Prokeš [a,b]

[a] Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany
[b] ESS Design Update Programme, Germany

ARTICLE INFO

Article history:
Received 29 January 2014
Received in revised form
2 July 2014
Accepted 6 July 2014
Available online 15 July 2014

Keywords:
European Spallation Source
Neutron scattering instrumentation
Time-of-flight technique
Extreme sample environment
Monte-Carlo simulations
VITESS

ABSTRACT

Properties of neutrons, in particular high penetration depth for most materials, make them very powerful for studying matter under extreme conditions, e.g. high pressures or magnetic fields. A new generation of high power spallation neutron sources, such as the existing SNS and J-Parc and the coming ESS, brings neutron scattering in extreme environments to a completely new level. Indeed, measurements of smaller samples, use of more complex equipment and neutron instruments optimized for operation with extreme sample environment become readily available. The latter is actually one of the most important factors contributing to the field. In this paper a novel concept of an instrument for extreme environments at the ESS is presented. The main feature of the Extreme Conditions Instrument is its multi-purpose nature. It is not optimized for a single scattering technique but combines in a balanced way elastic (Diffraction and Small Angle Neutron Scattering) and inelastic capabilities. Such a concept enables effective combination of neutron scattering with a state-of-the-art sample environment independent of the complexity, dimensions and transportability of the latter. In addition, all available types of neutron experiments can be performed at the same thermodynamic conditions. The instrument concept has been verified by Monte-Carlo ray-tracing simulations and the results for instrument operation modes are compared with world-class instruments.

1. Introduction

The European Spallation Source (ESS) is going to be a 5 MW long pulse neutron spallation source driven by a superconducting proton linac [1]. Operating at 14 Hz with 2.86 ms pulse length, its time-averaged flux will be comparable to the flux of the most powerful continuous neutron sources. A challenging task for the neutron scattering community now is to multiply the increased peak flux by the corresponding gain from the neutron instrumentation tailored for the above source parameters.

Clearly, the unprecedented brightness of the ESS opens new opportunities for many areas of modern research including the so-called science at extreme conditions. The latter could mean either traditional extremes for thermodynamical variables, such as temperature, pressure, magnetic field, or could be extended to other types of complex (e.g. in situ) chemical or engineering equipment.

Experience from the existing neutron sources shows that a dedicated instrumentation for extreme sample environments makes a real scientific impact as compared to general purpose instruments. Many neutron facilities have special instruments optimized for sample size or particular scattering geometry imposed by high pressure or high magnetic field equipment [2–5]. For some types of such equipment, e.g. multianvil presses or high field (>20 T) steady state magnets, any combination with general purpose instruments becomes in principle impossible as a result of their dimensions and complexity [10,11]. One can generally conclude that a commonly accepted way of exchanging sample environment between different instruments becomes inefficient or even impossible when going to extreme conditions. Other weighty arguments are costs of the equipment, its running costs and lifetime. Extreme environments by definition are associated with approaching the limits in current sample environment technologies. This often results in a *unique* equipment at the price of high development costs or limited lifetime.

A way out of these problems is to consider a stationary sample environment. Its main drawback is inability to be used with

* Corresponding author at: Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany.
E-mail address: prokhnenko@helmholtz-berlin.de (O. Prokhnenko).

http://dx.doi.org/10.1016/j.nima.2014.07.013
0168-9002/

different scattering techniques that is crucial for solving modern scientific tasks. In order to address this, we propose a novel multi-purpose instrument concept. The latter is not optimized for a single class of measurements but is capable of doing multi-techniques, e.g. diffraction and spectroscopy. Obviously, combining different techniques results in lower individual performance than can be achieved for each measurement type on a dedicated specialist instrument. This is, however, compensated by the capability to carry out unique experimental series that are not limited by sample environment complexity, geometry and dimensions or reproducibility of experimental conditions. The major remaining challenge is to combine the scattering techniques of interest in an optimal way in a single instrument.

In this paper we report on the development of a multi-purpose instrument concept capable of performing large dynamic *Q*-range elastic (covering Diffraction (DIF) and Small Angle Neutron Scattering (SANS)) and inelastic (Spectroscopy (SPEC)) experiments. A diagram of the instrument is shown in Fig. 1. Its main characteristics are (i) access to a broad wavelength range realized by a compact bispectral (thermal and cold moderators) extraction system; (ii) intense neutron beam transported over 150 m distance by means of a specially developed supermirror neutron guide with built-in collimation system; (iii) enormous flexibility in terms of wavelength/energy resolution and choice of wavelength band provided by an advanced chopper system; and (iv) a single detector system matching a special sample environment around which the instrument is built. With respect to the last, the chosen scattering methods would be perfectly suited for (i) high (30 T) steady state magnets combined with (ultra) low temperatures and high pressures (Fig. 1) and (ii) high (30 GPa) pressure apparatuses, such as multi-anvil presses, combined with high and low temperatures.

2. Instrument design

2.1. Main criteria

If the instrument performance is not a limiting factor, the thermodynamic parameter space accessible in neutron scattering experiments becomes a defining parameter for the type of science that can be addressed by a given instrument. Expanding it will impact many areas of applied and fundamental science. Examples are magnetism and superconductivity, planetary sciences and geosciences, energy- and materials-research. Generally, to address all of them, a coverage of a broad $(Q, \hbar\omega)$-range is necessary, where Q and $\hbar\omega$ are momentum and energy transfers, respectively. Taking high magnetic fields as an example, momentum transfer range from <0.01 up to >15 Å^{-1} and energy transfer over 1–100 meV are typically required. The former covers both the elastic magnetic scattering and the lattice response to the external perturbation [6]. The latter is necessary for studying low and high energy phenomena, such as softening of finite energy gaps in frustrated and quantum systems as a function of field or mapping magnetic excitations in unconventional superconductors [7,8]. Speaking the language of modern neutron instrumentation it would imply building several specialized instruments. Indeed, the existing instruments are optimized for narrow *Q*- or $\hbar\omega$–ranges, e.g. conventional, biological (medium *Q*-range) and SANS diffractometers or thermal and cold spectrometers, respectively (see, e.g. [9]). This approach is well-grounded as it allows maximizing the instrument performance. On the other hand, it is based on a standard sample environment model that breaks down when expanding the existing borders of the thermodynamic parameter space. For instance, modern DC high field hybrid magnets are quite massive (size scales with the field) and require a complex infrastructure for their operation [10]. To cool down the 16 Tesla magnet Fat Sam at SNS, the largest existing split-pair superconducting magnet, about 1000 l of liquid He are required [12]. Multianvil presses that allow larger sample volumes are large and bulky [4,11]. To achieve the highest pressures, one has to use diamond anvil cells that make the experiments rather expensive.

As a result, to allow an effective use of extreme sample environment and, simultaneously, cover the required *Q*- and $\hbar\omega$–ranges, a novel instrument concept that combines the relevant scattering techniques has been developed. Elastic, covering DIF and SANS, and inelastic, SPEC, have been defined as main operation modes of the instrument.

2.2. Operation modes

As a starting point for the instrument design, an optimum configuration for each of the operation modes has been identified. Special attention has been paid to wavelength resolution needed for the chosen techniques and its compatibility with using the full ESS pulse, the ways to fill the 1/14 s time frame available, phase space requirements and wavelength operation ranges. For that,

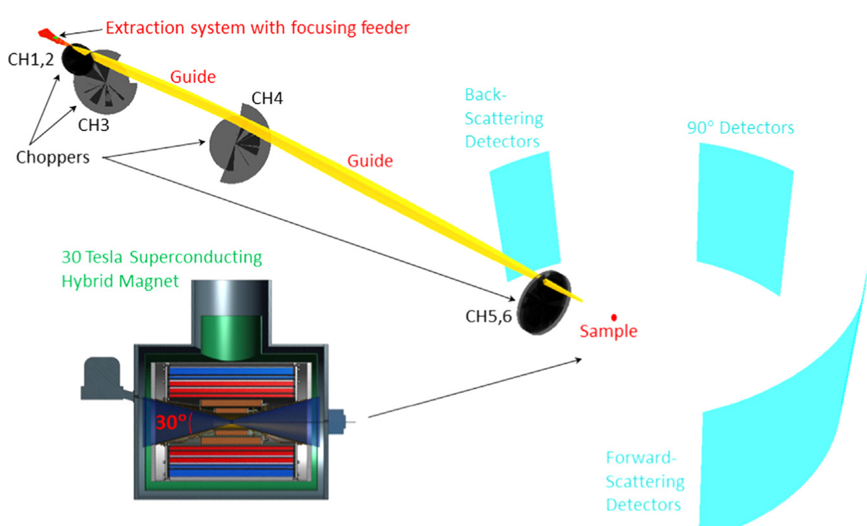

Fig. 1. (Not to scale) Schematic instrument layout displaying main instrument components: extraction system with focusing feeder, neutron guide, chopper cascade, and sample surrounded by detector banks (only those located on one semicircle are shown). One of the possible sample environments – a dedicated high field hybrid superconducting magnet with 30° conical openings – is also shown.