Nuclear Instruments and Methods in Physics Research A 828 (2016) 229–241

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

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

HEIMDAL: A thermal neutron powder diffractometer with high and flexible resolution combined with SANS and neutron imaging – Designed for materials science studies at the European Spallation Source

Sonja L. Holm [a,*], Kim Lefmann [a], Paul F. Henry [b], Mads Bertelsen [a,b], Jürg Schefer [c], Mogens Christensen [d]

[a] Nano-Science Center, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen Ø, Denmark
[b] European Spallation Source ERIC, 22100 Lund, Sweden
[c] Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, 5232 Villigen, Switzerland
[d] Department of Chemistry & Interdisciplinary Nanoscience Center (iNANO), Langelandsgade 140, 8000 Aarhus C, Denmark

ARTICLE INFO

Article history:
Received 12 February 2016
Received in revised form
10 May 2016
Accepted 10 May 2016
Available online 13 May 2016

Keywords:
ESS
Neutron instrumentation
McStas
Powder diffraction
SANS
Imaging
Materials science
In situ

ABSTRACT

HEIMDAL will be a multi length scale neutron scattering instrument for the study of structures covering almost nine orders of magnitude from 0.01 nm to 50 mm. The instrument is accepted for construction at the European Spallation Source (ESS) and features a variable resolution thermal neutron powder diffractometer (TNPD), combined with small angle neutron scattering (SANS) and neutron imaging (NI). The instrument uses a novel combination of a cold and a thermal guide to fulfill the diverse requirements for diffraction and SANS. With an instrument length of 170 m, HEIMDAL will take advantage of the high neutron flux of the long pulse at ESS, whilst maintaining a high q-resolution due to the long flight path. The q-range coverage is up to 20 Å^{-1} allowing low-resolution PDF analysis. With the addition of SANS, HEIMDAL will be able to cover a uniquely broad length scale within a single instrumental set-up. HEIMDAL will be able to accommodate modern materials research in a broad variety of fields, and the task of the instrument will be to study advanced functional materials in action, as *in situ* and *in operandi* at multiple length scales (0.01–100 nm) quasi simultaneously. The instrument combines state-of-the-art neutron scattering techniques (TNPD, SANS, and NI) with the goal of studying real materials, in real time, under real conditions. This article describes the instrument design ideas, calculations and results of simulations and virtual experiments.

1. Introduction

Advances in materials science come through an in-depth understanding of the relationships between structure and properties. Profound insights into these relationships are a common goal across condensed matter science, from high precision crystallography to fast kinetics studies, and are a prerequisite for the rational design of new and improved materials. Traditionally, materials have been studied at equilibrium, far from operating conditions, but growing efforts seeks to investigate materials under more realistic conditions and on multiple length scales, a trend pioneered by developments at synchrotron sources [1–4].

The intention with HEIMDAL is to build a neutron instrument able to access a wide length scale provided by the combination of thermal neutron powder diffraction (TNPD), small angle neutron scattering (SANS), and neutron imaging (NI). Multiple length scales are crucial to expand the understanding of advanced functional materials under external stimuli such as gas flow, pressure, or temperature, which can be difficult to recreate exactly in subsequent experiments. A classic example is heterogeneous catalysis, which depends on the atomic structure of catalytic nanocrystallites in a microporous matrix. All length scales are relevant for the efficiency of the catalytic process; therefore, in-depth knowledge into the structure and functionality requires multiple length scale coverage with sufficiently good time resolution. In these types of systems HEIMDAL will be a game-changer in neutron scattering, because it will provide new capabilities for investigating multiple dimensions at fast time scales. Topics of particular interest are materials containing light elements, related to energy, composites, matrix embedded systems, phase transition and nucleation, and magnetic materials.

* Corresponding author.

http://dx.doi.org/10.1016/j.nima.2016.05.046
0168-9002/

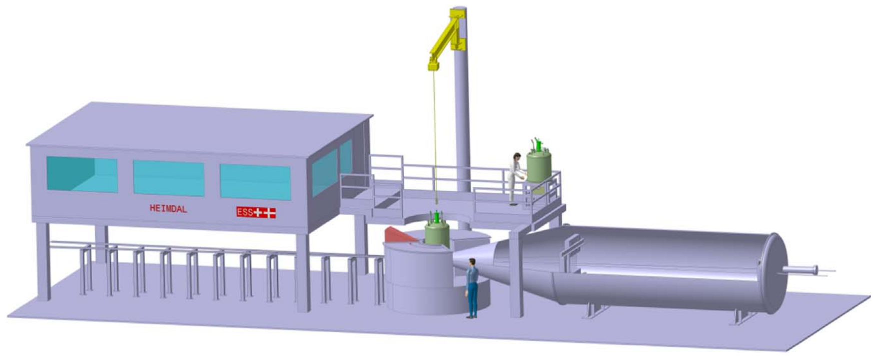

Fig. 1. Illustration of the HEIMDAL experimental station. Drawn in collaboration with Peter Keller, Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institut, Switzerland.

Neutrons are an ideal probe for *in situ* and *in operandi* studies inside bulky sample environments. However, only few neutron instruments existing today are capable of covering multiple length scale in real time as the experimental techniques of TNPD, SANS, and NI have highly different requirements to the incoming neutron beam. Therefore, all existing instruments covering broad length scales are focused towards either SANS or TNPD (*e.g.*, NOVA, i-Materia at J-Parc [5,6] or NIMROD at ISIS [7]). The HEIMDAL design uses an entirely novel concept, where two independent guides view the cold and thermal moderators independently. The two beams are extracted from the same beam port, and can be individually optimized without compromising the capability of either technique. This unique combination of three different neutron scattering techniques in a single setup will enable HEIMDAL to cover the atomic regime (0.01–5 nm) with TNPD, the nanometer regime (2–100 nm) with SANS, and structural features in direct space from 0.05 to 50 mm with NI. The total length scale coverage thus spans nine orders of magnitude, with minor gaps in the μm range.

The name HEIMDAL originates from the Norse Mythology. In Asgard, the home of the gods, HEIMDAL is the guardian of the rainbow bridge Bifrost that spans the worlds of gods and men. He has the most keen senses among gods, a vision so powerful that he can see and hear the grass grow in real time [8].

In the following sections we shall go though the design considerations, calculations, and simulations done in order to propose this instrument for construction at the ESS, starting with the instrument concept. After that we present the unique guide system and the chopper set-up of the instrument, before going into details with first the powder diffractometer, then the SANS set-up, and finally the imaging insert. Finally full virtual experiments, performed using the Monte Carlo ray tracing software McStas [9,10], will be presented for the TNPD and SANS set-up along with a discussion of the software needs associated with the data analysis.

2. The instrument concept

The powder diffraction part of the instrument is by far the most demanding due to the high resolution requirements. Therefore, the instrument design is based around an optimized, high performance thermal powder diffractometer, modified in order to also accommodate SANS and NI around a single sample position.

The source at ESS will run with a pulse period of $T = 71$ ms and a pulse length $\tau = 2.86$ ms. The benefits and challenges of such a time structure are described in [11–13], and the long pulse at ESS is, at first glance, not ideal when building high resolution powder diffraction instruments; As such an instrument requires a combination of good resolution ($\sigma d/d \approx 0.1\%$), wide reciprocal space coverage, and access to as high a q as possible (at least 15 Å^{-1}). However, a long pulse source combined with a pulse shaping (PS) chopper close to the source and a long flight path between the moderator and the sample provides a tailored, well-defined pulse with high time-resolution (and thereby a good q-resolution) for the instrument. The q_{max} of the instrument is determined by the moderator configuration and the efficiency of the beam transport system. The design results in a relatively narrow wavelength band ($\Delta\lambda = 1.74$ Å) that can be matched to the q-range of interest with regard to the sample.

The major advantage of the long-pulse spallation source/PS chopper combination is that the pulse length can be matched to the requirements of the material. Therefore, the instrument configuration can be changed from high-resolution (short pulse with lower intensity) to high count-rate (long pulse with lower resolution) simply through chopper rephasing, adding a degree of operational flexibility not possible using current generation time-of-flight diffractometers.

A significant benefit of the HEIMDAL design is that a simple analytical two dimensional peak profile function can describe the raw data, due to the relatively simple chopper system and the cylindrical detector geometry. The wide detector angular coverage (10–170°), coupled with the instrument wavelength band (see next section) allows a q-range of 0.73–19.87 Å^{-1} to be covered, ideal for most aspects of chemical crystallography while also suitable for some low resolution pair distribution function (PDF) analysis. Additional backscattering detectors (highlighted in red in Fig. 1) are placed above and below the incoming guide to provide improved counting statistics for data collected at high q, critical to high-resolution chemical crystallography and PDF.

For SANS, a separate guide delivers cold neutrons to the sample position, where the angle between the incoming thermal and cold beams is 3.5°. This ensures that the direct beam from the thermal guide will not contaminate the SANS signal on the detector, while retaining sufficient space upstream of the sample for incident beam tailoring using apertures and minimizing the curvature of the cold guide. The main SANS detector (1×1 m^2) is situated 10 m from the sample position, giving a q_{min} limit of 8.6×10^{-4} Å^{-1} using 11 Å wavelength neutrons and a 15 mm radius beamstop 0.2 m from the detector. Additional detector panels are placed in the vacuum tank 4 m from the sample position to cover the q-range between that accessible by the main SANS detector and the wide angle diffraction detectors.

A model drawing of the experimental area of HEIMDAL is presented in Fig. 1.

2.1. Instrument length and wavelength band

To obtain high resolution TNPD at a long pulsed source, it is necessary to build a very long instrument or make drastic modifications to the pulse shape after the source. We have chosen to