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The Nanoscale Ordered MAterials Diffractometer NOMAD at the Spallation Neutron Source SNS

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ABSTRACT

The Nanoscale Ordered MAterials Diffractometer (NOMAD) is neutron time-of-flight diffractometer designed to determine pair distribution functions of a wide range of materials ranging from short range ordered liquids to long range ordered crystals. Due to a large neutron flux provided by the Spallation Neutron Source SNS and a large detector coverage neutron count-rates exceed comparable instruments by one to two orders of magnitude. This is achieved while maintaining a relatively high momentum transfer resolution of a $\delta Q/Q \sim 0.8\%$ FWHM (typical), and a possible $\delta Q/Q$ of 0.24% FWHM (best). The real space resolution is related to the maximum momentum transfer; a maximum momentum transfer of 50 $Å^{-1}$ can be obtained routinely and the maximum momentum transfer given by the detector configuration and the incident neutron spectrum is 125 $Å^{-1}$. High stability of the source and the detector allow small contrast isotope experiments to be performed. A detailed description of the instrument is given and the results of experiments with standard samples are discussed.

1. Introduction

The Nanoscale Ordered MAterials Diffractometer NOMAD is a diffractometer for the determination of pair distribution functions (PDF) [1–3]. Determination of the PDF by diffraction experiments involves the determination of the scattered intensity as a function of momentum transfer Q – ideally from zero to infinity – which is then related by a Fourier transform to the pair distribution function. High intensity, a large accessible momentum transfer range, high stability and a reasonably good momentum transfer resolution are requirements for this type of experiment. Although most samples studied at NOMAD are expected to be isotropic – in which case the PDF depends only on the absolute value of the distance r – it is conceivable that samples with preferred orientation [4–6] may play a more important role in the future. In that case the PDF depends not only on r but also on the angle with respect to a preferred axis. The almost complete detector coverage in the final build-out stage allows for preferred orientation studies.

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory provides intense short-pulsed neutron beams at 60 Hz repetition rate [7,8]. High intensity is thus an obvious feature setting NOMAD apart from neutron diffractometers with similar mission currently existing at pulsed and reactor sources. A rough figure of merit for a powder diffractometer is the product of neutron flux on the sample and the solid angle seen by the detector [9]. NOMAD combines large detector coverage with a high incident flux, thus making efficient use of the source. A comparison with similar instruments has been given previously [10].

In what follows, we will describe the features of NOMAD, demonstrate the beam characteristics, and present early experimental results obtained with the instrument.

2. Instrument description

A general overview of the instrument is shown in Fig. 1.

2.1. Incident beam path

NOMAD is located at beamline 1B facing the poisoned decoupled hydrogen moderator [11]. It shares a main shutter with beamline 1 A, which will host an ultra small angle neutron scattering instrument scheduled for completion in 2014. The moderator has an active surface of 10 cm (h) × 12 cm (v) and the beam is transported over the first 7 m via a system of fixed tapered BN apertures. From 7 to 18.5 m neutrons are transported through an $m = 3$ super-mirror guide system, the last 2 m of which are mounted in an optics carousel and are hence removable. The guide system is designed to increase the flux of neutrons at the sample position for wavelength above 0.5 Å at the expense of additional

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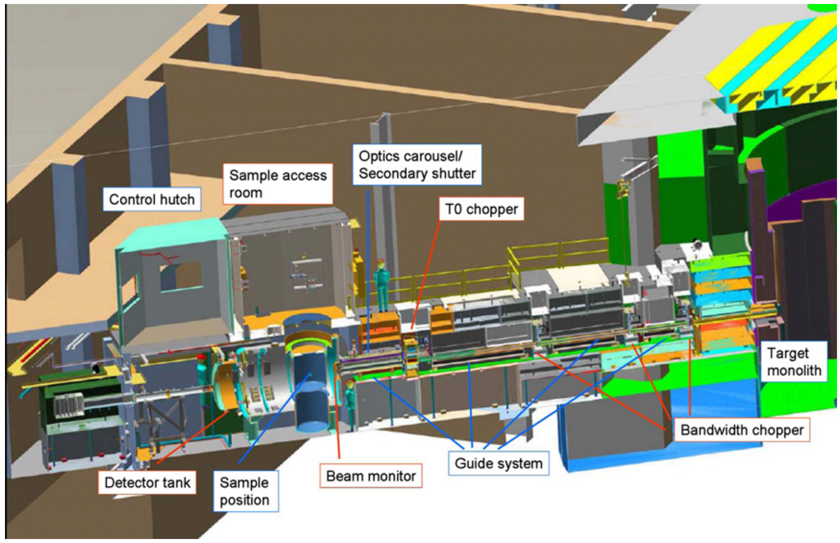

Fig. 1. Cut-away overview of the NOMAD beam layout. A person standing on the top of the shielding gives an idea of the scale. The distance from the moderator inside the target monolith to the sample position is 19.5 m.

divergence on the sample. The guide is sectioned to provide room for the bandwidth (BW) choppers. Each guide section is terminated at both ends with a BN aperture to minimize streaming alongside the guide and radiation damage to the guides optical glass. The optics carousel also doubles as a secondary beam-shutter which allows access to the instrument while beamline 1 A is operating.

The system of BW choppers largely eliminates frame overlap that would cause slow, long wavelength neutrons from a previous pulse to be detected at the same time as faster short wavelength neutrons and would make a unique wavelength assignment impossible. The standard set-up is illustrated in Fig. 2. It allows for 3 Å neutrons to reach the detector at 22 m from the moderator before fast neutrons from the next pulse arrive at the detector. It is possible to run the choppers at reduced speed, which allows accessing a wider wavelength bandwidth at the expense of intensity. For example, with the choppers running at 30 Hz, every second accelerator pulse is blocked. Therefore, at high Q the intensity is reduced by a factor of 2, the break even point is at about $Q = 2.5\ \text{Å}^{-1}$ and below that value intensity is gained from longer wavelength neutrons. A T_0 chopper upstream of the optics carousel at 16.5 m blocks the prompt pulse of high energy neutrons and γ- rays generated when the proton beam hits the target. The T_0 chopper is located as far downstream as possible – while still providing adequate shielding between it and the detectors – permitting transmittance of fast 0.1 Å neutrons needed at the sample. A system of three motorized adjustable apertures allows modification of the optical system in the incident beam path. One meter upstream of the sample position a ^{3}He transmission

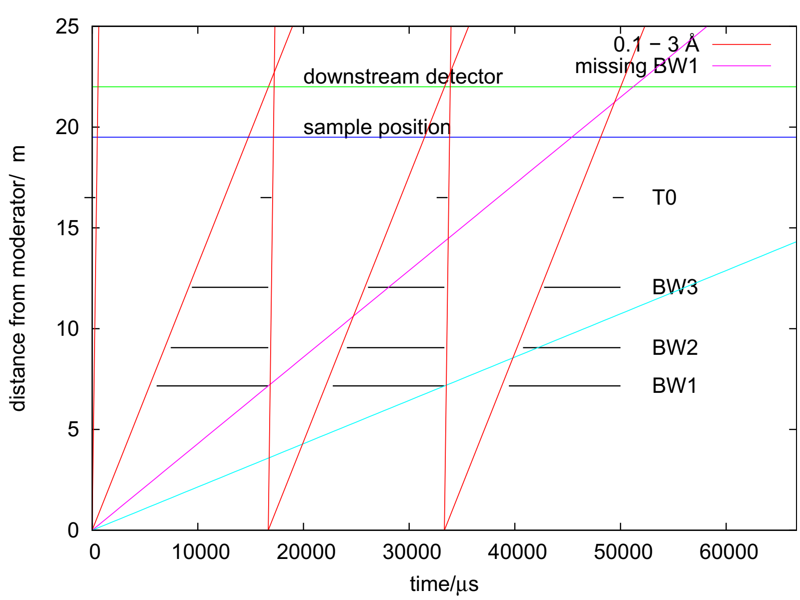

Fig. 2. Time path diagram of the standard chopper setting. Horizontal black lines indicate the time that the choppers block the neutron path. The BW chopper system passes a wavelength band from 0.1 to 3 Å indicated by red lines. Neutrons from a previous pulse missing the trailing edge of BW chopper 1 (in purple corresponding to about $\lambda = 9$ Å and blue corresponding to about $\lambda = 18$ Å) are absorbed in BW chopper 2 and 3. The position of the most downstream detector and the sample position are indicated with horizontal lines. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)