ZEEMANS - a new facility to probe matter at high magnetic field through neutron scattering

A. T. Savici$^{1,2}$, G. E. Granroth$^2$, C. Broholm$^1$, Y. S. Lee$^3$ and M. D. Bird$^4$

$^1$Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, USA
$^2$Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA
$^3$Department of Physics, MIT, Boston, MA, USA
$^4$National High Magnetic Field Laboratory, Tallahassee, FL, USA

E-mail: savici@pha.jhu.edu

Abstract. We describe ZEEMANS, a new instrument proposed for the Spallation Neutron Source (SNS) to probe matter at extremely high magnetic fields. The complexity of the high field magnet demands a versatile neutron scattering instrument, capable of performing diffraction (powder and single crystal), SANS, reflectometry, and inelastic spectrometry, with minimal modifications between configurations. In this paper we present a conceptual design for neutron scattering instrumentation to be built around the horizontal conical high field magnet. Monte Carlo simulations and analytical calculations indicate performance on a par with other SNS instrumentation despite limited access to the sample.

1. Introduction

High magnetic fields can perturb condensed matter to reveal or alter properties while neutrons can provide detailed information about nano-scale structure and dynamics. As recommended in a recent NRC report,[1] a world class facility is under development to combine these techniques and create a powerful new tool for a wide range of materials science.

Two recent technological advances enable this new instrument that we call ZEEMANS, in honor of Pieter Zeeman. (1) The increased brightness of the Spallation Neutron Source (SNS) enables experiments on small samples under extreme thermodynamic conditions and (2) NSF investment to develop a new hybrid high field technology at the National Magnetic field Laboratory makes it feasible to bring a neutron beam into a >25 Tesla DC magnet and operate it cost effectively at the duty cycle of a neutron source.

The ZEEMANS facility will provide unique materials research capabilities in areas including quantum magnetism, correlated metals, molecular magnetism, nano-structured magnets, superconductivity, metallurgy, macro molecular crystallography, hydride structure determination.[2, 3, 4] This basic research has the potential to impact technological areas such as high-density magnetic information storage, quantum computing, superconducting power transmission, steel processing, pharmacology, and hydrogen based energy distribution.

The central component of ZEEMANS is an all superconducting electro-magnet capable of reaching 25 T. Designed at the National High Magnetic Field Laboratory,[5] it is a horizontal solenoid with a conical bore to provide access for the sample environment system and neutron scattering. The full conical opening angle will be 30 degree total at either end.
To make best possible use of the unique high field conditions, the neutron scattering instrument will be capable of all major neutron scattering techniques: powder and single crystal diffraction, small angle scattering, reflectometry, and inelastic scattering.

For versatility and high intensity in the relevant energy range, the instrument will view the coupled liquid H\(_2\) moderator, from beamline 14A at SNS. The magnet is large, has considerable utility requirements, and must be sufficiently removed from other instruments to avoid fringe field interference problems. Consequently ZEEMANS will be outside the target building, with a sample to moderator distance \(L_{m-s}\) of 70 m. The magnet will be able to rotate about a vertical axis, to vary the angle between the incident beam and the field axis from 0 degrees for SANS to 15 degrees for access to scattering angles of thirty degrees. Detectors at \(L_{s-d}=5\) m will be placed in both the forward and backward scattering directions. Fixed detectors, a rotating magnet, and a common detector-magnet vacuum space is the chosen configuration for flexibility in scattering, operational convenience, and engineering feasibility. A conceptual drawing of the instrument is shown in Fig1(a).

2. Projected performance for Neutron Scattering

ZEEMANS will accommodate up to a 2 cm by 2 cm sample located 70 m from the 10 cm wide, 12 cm tall liquid H\(_2\) moderator. To compensate for the limited angular access, a wide incident energy (wavelength) range \(E_i = 1-150\) meV (\(\lambda = 0.8-10\) Å) will be employed.

Monte Carlo optimizations for different guide configurations were performed using McStas.[6] Independent optimizations were performed for the horizontal and vertical profiles. An \(m=3.6\) guide coating was used in the simulations. The horizontal profile of the guide will consist of a curved section, 15 m in length, with a 8200 m radius of curvature, followed by an 8 channel bender, with the same length, and a 726 m radius of curvature. Close to the sample position, the end of the guide has a parabolic profile. The elliptical ballistic guide concept[7] was used for the vertical profile, and placement of the focal points was optimized for the finite sized source and sample. The maximum height of the guide is 15 cm.

Figure 1. (a) Conceptual design for ZEEMANS. Neutron flux on sample for ZEEMANS in different experimental configurations: (b) diffractometer mode with and without apertures 5 m before the sample, and comparison to TOPAZ; (c) spectrometer mode. Note it will also be possible to run the instrument in rep-rate multiplication mode where several discrete incident energies appear at the sample during a single frame.
Four bandwidth choppers and at least two high speed choppers will be required for the various experimental configurations. For the elastic scattering configurations, the maximum bandwidth without frame overlap is $\Delta \lambda = 0.876 \text{ Å}$. An aperture can be introduced 5 m before the sample, to control beam divergence. Alternatively, to maximize flux, a focusing guide section can be used. The wavelength dependent flux on sample is shown in Fig. 1(b), for various configurations. Also shown is a simulation for Topaz,[8] a single crystal diffractometer at SNS. The higher flux at shorter wave lengths on Topaz is due to a bender configuration optimized for diffraction alone. For the direct geometry spectroscopy, high speed choppers are used. The energy dependent flux is shown in Fig. 1(c) for typical experimental setups, corresponding to different chopper transmission times, and therefore different energy resolutions.

The conical bore allows scattered neutrons to emerge from the magnet in both the forward and backward directions. To increase the maximum accessible momentum transfer, $Q$, for a fixed $E_i$, the magnet can rotate as described earlier. Rotation of the sample around the magnet axis will further extend momentum space coverage.

For elastic scattering, the $Q$ space available is shown in Fig. 2(a). Forward scattering (detailed in Fig. 2(b)) can be used for both nuclear and magnetic scattering, and will probe scattering with wave vector transfer roughly perpendicular to the field direction. Due to the form factor, magnetic scattering in the backward direction will be reduced in strength but importantly will probe scattering with wave vector transfer approximately parallel to the field. The energy-$Q$ range of ZEEMANS is shown in Fig. 2(c)-(e) for several values of $E_i$, and for magnet orientations at 0° and 15° with respect to the incident beam. The corresponding range of energy transfer is indicated by the color scheme in Fig. 2(f). The lack of overlap for accessible $Q_{\perp}$ regions at the highest energy transfers in Fig. 2(c)-(e) indicates that it is necessary to be able to rotate the magnet to non-extremal positions.

**Figure 2.** Momentum range for elastic scattering (a) with detail for the forward detectors (b). $E$-$Q_{\perp}$ ranges for different incident energies (c)-(e), at the values of energy transfer indicated by (f). As only $Q_{\parallel}$ depends on forward or backward scattering, these figures apply for both cases.

For momentum resolution calculations, we considered geometrical factors, beam divergencies, and the neutron emission time uncertainty from the moderator.[9, 10] Results are shown in Fig. 3(a)-(b). The resolution in the forward direction is dominated by geometrical factors, while in the backscattering detectors moderator contributions are most important. For energy resolution, McStas simulations for different running conditions are shown in Fig. 3(c).
3. Conclusions

Built around a unique all superconducting magnet that will be able to reach at least 25 Tesla, the ZEEMANS instrument will be extremely versatile. It will be capable of performing diffraction, reflectometry, and spectroscopy, with minimal configurational changes. The expected flux and resolution of the instrument are comparable to state of the art instrumentation at the SNS. ZEEMANS will thus provide a first view of structure from nano-meters to angstrom and dynamics from nano to pico-seconds in materials perturbed by fields beyond 25 Tesla.

Acknowledgments

We acknowledge fruitful discussions with F. Mezei, P. Smeibidl, M. Steiner, and others from Helmholtz Zentrum Berlin, where a similar instrument is under development. We thank SNS instrument scientists, for providing information on their instruments. The National Science Foundation funded this work under DMR-0603126. GEG is funded by the US DOE contract DE-AC05-00OR22725.

References

[1] Committee on Opportunities in High Magnetic Field Science 2005 Opportunities in High Magnetic Field Science (The national Academies Press), http://www.nap.edu/openbook.php?isbn=0309095824.
[2] Yoshii S, Yamamoto T, Hagiwara M, Takeuchi T, Shigekawa A, Michimura S, Iga F, Takabatake T and Kindo K 2007 J. Magn. Magn. Mater. 310 1282.
[3] Jo Y J, Balicas L, Capan C, Behnia K, Lejay P, Flouquet J, Mydosh J A and Schlottmann P 2007 Phys. Rev. Lett. 98 166404.
[4] Zhao J K 2005 Physica B 356 168.
[5] Bird M D, Bole S, Gundlach S and Toth J 2006 IEEE Trans. Appl. Supercond., 16 957.
[6] Willendrup P, Farhi E and Lefmann K 2004 Physica B 350 735.
[7] Schanzer C, Boni P, Filges U and Hils T 2004 Nucl. Instr. Meth. A 529 63
[8] Hoffmann C, Stoica A, Lee H, Wang X -L, Schultz A, Piccoli P B, Koetle T, Bau R, Thomison J and Davis L http://neutrons.ornl.gov/instrument_systems/beamlne_12_topaz/pdf/poster-1105-advances-1.pdf
[9] Windsor C G 1981 Pulsed Neutron Scattering (London: Taylor and Frances); Crawford R K 1978 in IPNS a National Facility for Condensed Matter Research Argonne National Laboratory Report ANL 78-88 206; Carlile C J, Taylor A D, and Williams W G 1985 Neutron Scattering in the 90s IAEA-CN.46/SP 421
[10] Iverson E B, Ferguson P D, Gallmeier F X, and Popova I I 2002 Detailed SNS Neutronics Calculations for Scattering Instrument Design: SCT Configuration, Spallation Neutron Source Report SNS 110040300-DA0001-R00, http://neutrons.ornl.gov/instrument_systems/components/moderator/110040300-DA0001-R00.pdf