ICANS XIX,
19th meeting on Collaboration of Advanced Neutron Sources
March 8 – 12, 2010
Grindelwald, Switzerland

SPIN-ECHO INSTRUMENT CONCEPTS FOR THE ESS-LUND

MICHAEL MONKENBUSCH
IFF, Forschungszentrum Jülich
Jülich, 52425, Germany

ABSTRACT

Considerations concerning the choice and layout of possible neutron spin-echo instruments for the long pulse spallation source, which is expected to be build in Lund, are reported. The selection of one or two instruments that would serve as workhorses for very high resolution spectroscopy has been prepared in a recent (august 09) workshop on long pulse instrumentation in Frascati. The implications of the source characteristics on the optimization of these instruments as well as the requirements of these instruments to the source will be discussed and a tentative comparison of the expected performance with that of existing NSE instruments will be made.

1. Introduction

1.1. Motivation

In order to find optimized instrumentation for the planned MW long-pulse spallation sources in Europe, ESS with 5MW and in USA, SNS second target station with 1MW, instrument concepts were discussed that are best suited to become "flagship" installations in their class. In this short report the considerations and conclusions on the optimal combination of Larmor precession instruments with the characteristics of the upcoming long-pulse sources are communicated. At this stage of the source development it is still possible to feed back the requirements of the optimal instruments to the moderator selection and design by defining the best suited source parameters. The general challenges for the instrumentation at a new facility may be described by the following keywords: Smaller samples (access to new materials existing only in small quantities), faster measurements (kinetic processes, non-equilibrium systems, parametric processes), larger length scales (biology, soft-matter chemistry, aggregation, self-assembly, vortex lattices) and longer time scales (big floppy systems). Especially the latter pertains Neutron Spin-Echo spectroscopy as one of the most prominet examples of Larmor techniques. In combination with performance optimization the instrument design concepts should also take into account practical factors such as instrument cost, practicality of very long beamlines, limitations due to beamline crowding close to the moderators, radiation shielding, correlations of spectral features, pulse lengths and inentsity of possible moderators, etc..

Larmor techniques in the instrumentation suite of a future long-pulse spallation source have been discussed in a workshop on long pulse spallation source instrumentation in Aug. 09 in Frascati [1]. Here a report is given on the general conclusions.

2. Larmor devices and Spin-echo

2.1. Considered Larmor methods

Concerning the variety of Larmor precession devices, it turned out the focus here will be on high resolution spectroscopy. A number of other ingenious and useful Larmor techniques have been identified as add-ons for SANS instruments and reflectometers. The following techniques have been considered: high resolution NSE spectroscopy (using precession magnets) [2], wide angle NSE spectroscopy (using precession magnets) [3], Resonance NSE, MIEZE etc. (using zero field and RF-flippers) [4], New approaches, like NSE with time varying flippers [5], high resolution SANS with NSE (SESANS) [6], grazing incidence: SERGIS, GINSE [7], 3D polarimetry (in combination with NSE) [8], beam modulators (Drabkin filters, choppers).

As genuine full instruments at a new long-pulse spallation source only the first two items have the potential to become state-of-the-art workhorses for the community. Among the others, angle encoding by Larmor precession are well developed methods that are recommended as (optional) add-ons for the corresponding basic instruments, i.e. SESANS[6] for SANS and SERGIS[7] as SESANS on a polarized reflectometer as it is already realized at OFFSPEC[9] at ISIS-TS2. GINSE (spectroscopic NSE at grazing incidence) and polarimetry are to be considered as options for the spectroscopic high resolution or wide angle NSE. Instruments with time varying flipper or Drabkin beam modulators are still experimental so in the near future they will not justify the assignment of a high intensity beamport. However, they may be further developed using some time at a general purpose test beamline.

Finally resonance or zero field NSE was identified as a method that offers unique possibilities if installed on a three axis type spectrometer in order to measure the widths of dispersion surfaces[10] or for ultrahigh resolution diffraction [11]. Resonance NSE for spectroscopy and MIEZE are due to the technical limitation imposed by the RF-flippers and the non-availability of correction elements that enable larger beam divergence and high resolution not in a state to serve as competitive ultra-high resolution spectroscopic instruments.

Therefore we focus the further considerations on the instruments of the first type, analog to (IN11, IN15[12], J-NSE[13], NSE@SNS[14], ….) and to those of the second type (SPAN[3], WASP[15]). There are several properties and conditions that are common to these instruments.

2.2. Resolution of NSE

The main resolution parameter of spectroscopic NSE instruments is the maximum Fourier-time, t. It is completely decoupled from any time structure of the neutron pulse and depends solely on the shaping and control of the instruments spin-encoding magnetic fields. This decoupling of wavelength width and resolution is one of the main features of NSE and ensures sufficient neutron intensity. At reactor instruments the FWHM wavelength spread of the incoming neutrons typically is between 10% to 15%. The resolution on the other hand depends on the magnetic fields of the instrument that serve to realize the spin precession analysis. By this means minimal velocity changes of neutrons upon scattering at the sample can be detected and lead to a change in final poarization. The resulting polarization at the detector is proportional to the Fourier transform of the spectrum. The relevant resolution parameter is the maximum Fourier time. For a given magnetic field integral along the neutron flight path from, e.g. sample to analyzer (π to π/2 –flipper), $J = \int |B| dl$, the Fourier-time is $t = \alpha J \lambda^3$ with $\alpha \approx$ 0.2nsT^{-1}m^{-1}Å^{-3}. Since the state-of-the art magnets and auxiliary elements allow for J≈1Tm, the only efficient way to reach Fourier-times in the several 100ns to µs region is the use of (very) long wavelength neutrons. E.g. a wavelength of 16Å would be required to obtain t=0.8 µs with J=1Tm. This observation leads to the first request on the moderator type and layout, i.e. high intensity at very long wavelength is essential. Also the next property will add input to the moderator design.

2.3. Pulse gain factor

All reactor based instruments accepts a wavelength band of 10-15% of the incoming neutrons, which is well adapted to most of the soft-matter-problems. The envisaged proton pulse length of the source is 2ms. We assume that resulting effective neutron pulse length is in the range of 3ms. Thus the wavelength uncertainty of intensity reaching the detector with distance L from the moderator is a any time given by $\delta\lambda \cong 4 \times 10^{-7}\,\mathrm{m^2 s^{-2}}\,\Delta t / L$. For an instrument with detector distance L=50m this yields $\delta\lambda$=0.24Å which corresponds to 10% width at λ=2.4 Å becoming worse for shorter wavelength, however, much better for longer ones, i.e. 2% at 12Å.

Since intensity is one of the most important limitation factors for all present NSE spectrometers –in view of the above mentioned “natural” wavelength spreads— the best choice is to refrain from any (intensity eating) pulse shaping and restrict the chopper system to frame selection only.

The wavelength range covered by one frame between chopper pulses is again independent of wavelength and is $\Delta\lambda \cong 4 \times 10^{-7}\,\mathrm{m^2 s^{-2}}\,(1/f)/L$. With a repetition frequency f=16.66Hz we obtain $\Delta\lambda \cong$5Å at a detector distance of L=50m.

The gain factors due to the pulsed operation compared to a continuous source of the same average flux may be computed by a naively unbiased comparison of the same sequence of experiments done at a continuous source with wavelength width W=δλ/λ and the pulse source $g = \ln[(\lambda + \Delta\lambda/2)/(\lambda - \Delta\lambda/2)]/W$ with W=0.1, $\Delta\lambda \cong$5Å and a central wavelength λ we get λ=5 (g=11), λ=10 (g=5), λ=16 (g=3). However, the experiment at the pulsed source imposes the same counting times for all partial experiments, which in many cases would be conducted with different, optimized times at a continuous source. Thus the above gain factors are upper limits.

2.4 Space requirement

If a sector of 12° is available at a beamline this would imply a lateral space of 8-10m for an instrument with L=50m. For a generic IN11 type instrument which is designed without restrictions to space, however, with scattering angle limited to one side one would like to have a 0.5m for shielding and >1.5m distance of the beam axis and the inner (magnetic) shielding wall. At the scattering side the secondary arm should be able to swing to 90° or more, a total length of 5m plus 0.5m for shielding then implies a total width of 7.5m at the sample distance. In the above example 9m would be available, but the described scenario is not symmetric with respect to the beam. In the latter case 4.5m would be available also on the scattering arm side whereas 5.5m would be desirable. Detailed design has to show how much deviation from symmetry may be available and how the extraction of two beams from one beam port can be made compatible with these conditions. Shorter distances down to L=30m can certainly be realized –in particular if asymmetric configurations are allowed. They would yield wider frame width (8Å) but may already require compromises with respect to the magnetic design due to arm length restriction.

For a wide angle instrument of the SPAN type one may consider the WASP design [15] as a reference. The diameter of this instrument is ~7m if analyzers, detector and detector shielding is included with some space on both sides for shielding and bypass a minimum of L=50m results.

A large distance (even beyond 50m) has additional advantage that the background is low and direct sight to the moderator may be easily avoided by curved (prepolarizing) guides. For NSE instruments it is also of genuine importance to have a clean magnetic environment with field variation of less than some mGauss during a scan. On the other hand the instruments themselves generate magnetic fields that contribute to fraction of a Gauss outside the own sector for a compensated IN11 type instruments and of several Gauss for a WASP type instrument. A large L helps to cope with the magnetic interference problem by increasing the distance between instruments. It also yields enough space to install a magnetic shielding if required.

2.5. Source

Source parameters and moderators that meet the requirements of the instruments described above are discussed here. The pulse length of 2ms is compatible with the majority of applications for the NSE spectrometers. In particular high intensity in terms of number of neutrons in the pulse is the most important criterion. On the other hand there is no special advantage to have long pulses. Some experimental problems that need better Q-resolution (e.g. samples with sharp structures in S(Q) like oriented lamellar microemulsions) would benefit from the lower wavelength spread due to shorter pulses. The envisaged repetition rate of 16.66Hz for ESS is acceptable but going to a somewhat lower frequency (10Hz) would still increase the overall performance of the NSE instruments, provided that the average power stays unchanged.

Since the challenge for NSE spectroscopy specifically lies in the ultra high resolution sector it is essential to have high neutron flux at long wavelengths up to 20Å or more. This requires in any case a cold coupled moderator. In addition optimization for the best available long wavelength neutron flux is requested. In the course of such an optimization –for NSE instruments—it is acceptable that the pulse length is increased by an extended moderation time.

2.6. Conclusion

As flagship instruments from the Larmor/Spin-echo class a high intensity, high resolution IN11 type spectrometer and/or a wide angle NSE spectrometer of the SPAN/WASP type are recommended. If there is room to modify the accelerator parameters, a slight reduction of repetition frequency (without reduction of average power) would be beneficial. The pulse width of 2ms is acceptable but if technology allows shorter pulses could improve experiments on samples with sharp structures in S(Q). But, intensity –particularly at long wavelengths—is of paramount importance even if it is achieved by measures that extend the neutron pulse width.

3. References

1. Long-Pulse Instrumentation Workshop, August 26-28, 2009, Villa Mondragone, Italy, members of the Larmor group were: G. Ehlers, R.M. Dagleish, B. Farago, A. Ioffe, G. Kali, F. Mezei, M. Monkenbusch.

2. F. Mezei, editor. *Neutron Spin Echo*, in *Lecture Notes in Physics* **Vol. 128**, Springer, Berlin, Heidelberg, New York, (1980).

3. C. Pappas, G. Kali, T. Krist, P. Boni, and F. Mezei, *Physica B-condensed Matter* **283** (2000) 365–371.

4. R. Golub and R. Gahler, *Physics Letters* **A 123** (1987) 43–48; R. Gahler, R. Golub, and T. Keller, *Physica* **B 180** (1992) 899–902; P. Hank, W. Besenbock, R. Gahler, and M. Koppe, *Physica* **B 234** (1997) 1130–1132.

5. A. Ioffe, *Nuclear Instruments and Methods in Physics Research* **A 586** (2008) 31–35.

6. J. Major, H. Dosch, G.P. Felcher, K. Habicht, T. Keller, S.G.E. te Velthuis, A. Vorobiev, M. Wahl, *Physica* **B 336** (2003) 8–15.

7. M.T. Rekveldt, J. Plomp, W.G. Bouwman, W.H. Kraan, S. Grigoriev, and M. Blaauw, *Review Of Scientific Instruments* (2005) 76.

8. C. Pappas, E. Lelievre-Berna, P. Bentley, E. Bourgeat-Lami, E. Moskvin, M. Thomas, S. Grigoriev, V. Dyadkin, *Nuclear Instruments and Methods in Physics Research* **A 592** (2008) 420– 427.

9. J. Plomp, V.O. de Haan, R.M. Dalgliesh, S. Langridge, A.A. van Well, *Thin Solid Films* **515** (2007) 5732-5735.

10. K. Habicht, T. Keller, and R. Golub, *Journal Of Applied Crystallography* **36** (2003) 1307–1318; S.P. Bayrakci, T. Keller, K. Habicht, and B. Keimer, *Science* **312** (2006) 1926–1929.

11. M. Jernenkov, H. Lauter, V. Lauter-Pasyuk, B. Toperverg, S. Klimko, and R. Gahler. Angular encoding with Larmor precession. Physica B-condensed Matter 357, 94–97, 2005.

12. P. Schleger, B. Alefeld, J.F. Barthelemy, G. Ehlers, B. Farago, P. Giraud, C. Hayes, A. Kollmar, C. Lartigue, F. Mezei, and D. Richter, *Physica* **B 241** (1997) 164–165; B. Farago, *Physica* **B 268** (1999) 270–276.

13. M. Monkenbusch, R. Schatzler, and D. Richter, *Nuclear Instruments & Methods In Physics Research* **A399** (1997) 301–323.

14. M. Ohl. M. Monkenbusch, D. Richter, C. Pappas, K. Lieutenant, T. Krist, G. Zsigmond and F. Mezei, *Physica B-Condensed Matter* **350** (2004) 147-150.

15. R. Holzel, P.M. Bentley. P. Fouquet, *Review Of Scientific Instruments* **77** (2006) 105107.

ICANS XIX,
19th meeting on Collaboration of Advanced Neutron Sources
March 8 – 12, 2010
Grindelwald, Switzerland