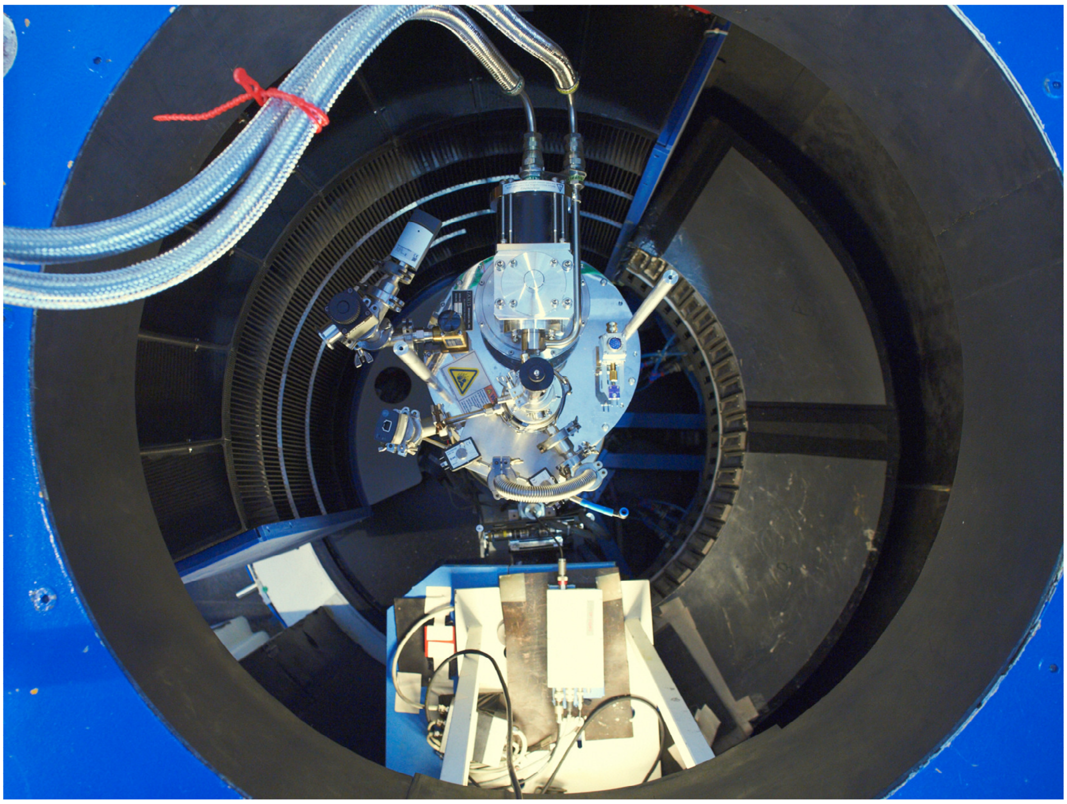
DNS

Neutron Polarization Analysis

Y. Su

Jülich Centre for Neutron Science
Forschungszentrum Jülich



Manual of the JCNS Laboratory Course Neutron Scattering

Contents

1 Introduction

Polarized neutron scattering and polarization analysis represents a powerful technique for the studies of complex ordering phenomena and dynamics of condensed matters. The elements of this technique and its advanced applications in particular in magnetism have been comprehensively covered in a number of recent lecture notes [1-4] and several seminal papers [5-7]. The aim of this exercise on *Neutron Polarization Analysis* is to provide you with some hands-on experience on the practical aspects of polarized neutron scattering based on the multi-detector time-of-flight spectrometer DNS at FRM II. The details on the handling of polarized neutrons and the fundamentals of polarization analysis will be demonstrated from a range of carefully designed experiments and exercises.

In Section 2 of this manual, an overview of the instrument DNS as well as its unique capabilities will be given. Section 3 consists of necessary preparatory exercises and questions which can be studied before the experiment. Section 4 describes the details of the experiment procedure and provides the experiment-related exercises.

2 Overview of the DNS instrument

DNS is a versatile diffuse scattering cold neutron time-of-flight spectrometer with polarization analysis at the neutron guide NL6a, FRM II. DNS has the capability to allow unambiguous separations of nuclear coherent, spin incoherent and magnetic scattering contributions simultaneously over a large range of scattering vector **Q** and energy transfer E. A schematic layout of DNS is shown in Fig. 1.

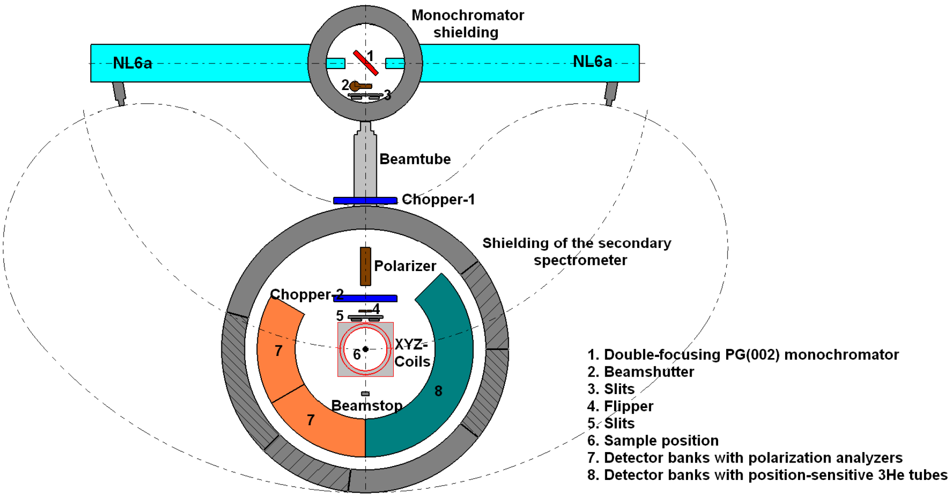


Fig. 1 The schematic layout of DNS

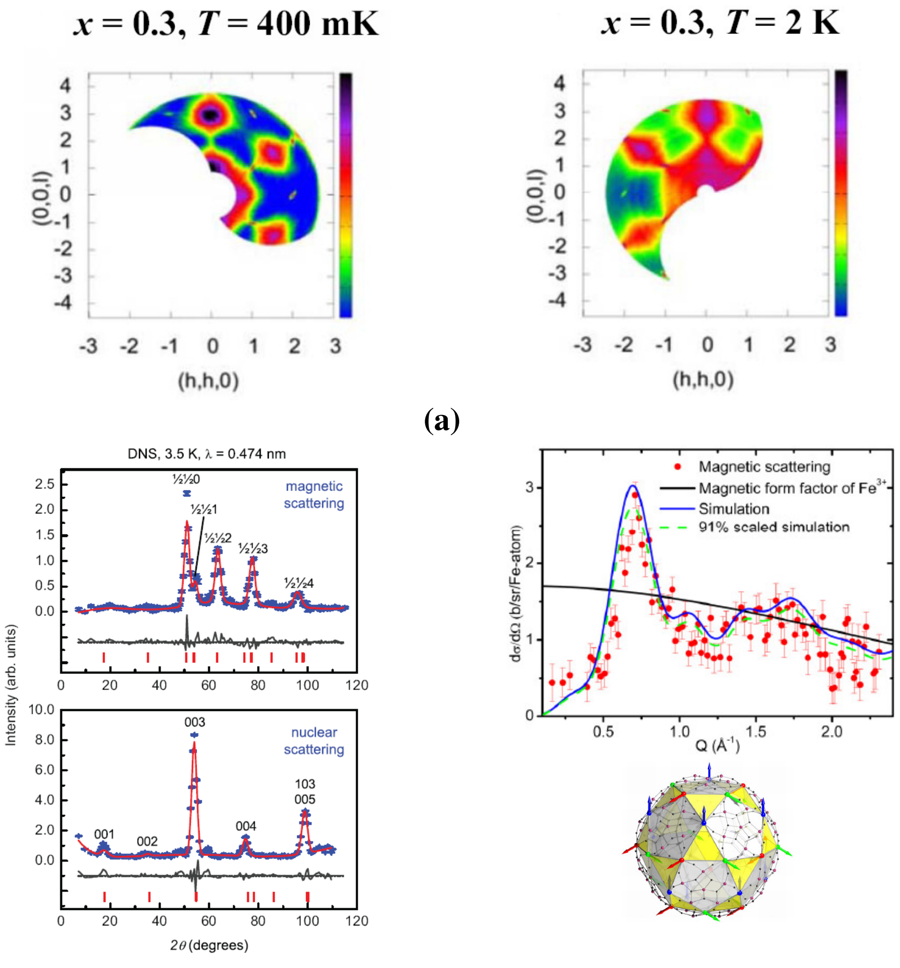
DNS has a number of unique features such as wide-angle polarization analysis, a large position-sensitive detector array and a high frequency double disc chopper system. With its compact design and the powerful double-focusing PG(002) monochromator, DNS is optimized as a high intensity instrument with medium resolution. The monochromatic neutron beams with the wavelength ranging from 2.4 to 6 Å are available at DNS. Newly constructed polarizer and polarization analyzers, both using m = 3 Schärpf bender-type focusing supermirrors, perform very well. A polarized neutron flux as high as 5×10^6 n/(s·cm^2) has been achieved at 4.74 Å. The polarization rate of the incident neutron beams is nearly 96%. The wide-angle polarization analysis in the horizontal scattering plane is achieved via using 24 units of polarization analyzers simultaneously. The neutron spins are manipulated using a Mezei-type π-flipper, followed by a set of orthogonal XYZ-coils situated around the sample position for providing guide fields. In addition to high polarized flux, the unique strength of DNS lies on its extreme versatility. DNS can be operated in a number of modes for a wide range of samples. There are three polarization analysis (PA) modes at DNS: uniaxial-PA for separation of coherent and spin-incoherent scattering in non-magnetic samples; longitudinal-PA for separation of magnetic scattering in paramagnetic and antiferromagnetic samples; vector-PA for the determination of complex magnetic structures.

Time-of-flight spectroscopy is another important application at DNS. The installation of 128 position-sensitive ^{3}He tubes of 1m height and half inch diameter has just been completed at DNS, and the commissioning is expected soon. This will increase the covered solid angle up to 1.9 sr. DNS will be running with a double disc chopper system with the frequency up to 300 Hz. The setup with two phase-controlled choppers would allow to eliminate high-order (e.g. λ/2) background or to select only high orders. DNS is targeted as a high count-rate cold neutron time-of-flight spectrometer with medium resolution. DNS is thus ideal for the studies of spin dynamics in many novel magnetic materials. The technical details of DNS are shown in Table 1.

Monochromator	horizontal- and vertically adjustable double-focusing	PG(002), d = 3.355 Å (at NL6a)
	crystal dimensions	2.5×2.5 cm^2 (5×7 crystals)
	wavelengths	2.4 Å $\leq \lambda \leq 6$ Å
Double-chopper system	chopper frequency	≤ 300 Hz
	repetition rate	≤ 900 Hz
	chopper disks	Titanium, 3 slits, $\phi = 420$ mm
Expected flux at sample (n/cm^{2}s)	Non-polarized	$\sim 10^8$
	Polarized (polarizer: $m = 3$ supermirror benders)	$\sim 5\times10^6$–10^7
Detector banks for non-polarized neutrons	position sensitive ^{3}He detector tubes	128 units, $\phi = 1.27$ cm, height ~100 cm
	total solid angle covered	1.9 sr
	covered scattering angles in the horizontal plane	$0° < 2\theta \leq 135°$
Detector banks for polarized neutrons	polarization analyzers	24 units, $m = 3$ supermirror
	^{3}He detector tubes	24 units, $\phi = 2.54$ cm, height 15 cm
	covered scattering angles in the horizontal plane	$0° < 2\theta \leq 150°$
Q_{max}	$\lambda_i = 2.4$ Å ($E_i = 14.2$ meV)	4.84 Å^{-1}
	$\lambda_i = 6$ Å ($E_i = 2.28$ meV)	1.93 Å^{-1}
Expected energy resolution	$\lambda_i = 2.4$ Å ($E_i = 14.2$ meV)	~ 1 meV
	$\lambda_i = 6$ Å ($E_i = 2.28$ meV)	~ 0.1 meV
Suitable samples	single crystals, powders, soft matters (e.g. polymer, liquid etc.)	
Sample environments	top-loading CCR, closed-cycle cold head, orange cryostat, cryo-furnace, ^{3}He/^{4}He dilution cryostat (~20mK), cryomagnet (self-shielding, vertical field up to 5T)	

Table 1 The technical details of the DNS instrument

Typical scientific applications at DNS are the studies of complex magnetic correlations, such as in highly frustrated magnets and strongly correlated electrons, as well as the structures of soft condensed matter systems, such as the nanoscale confined polymers and proteins, via polarization analysis. The exploration of unusual magnetic properties can also be efficiently undertaken on single-crystal samples by reciprocal space mapping. Fig. 2(a) shows an example of the measured magnetic diffuse scattering patterns in frustrated spin-ice pyrochlore compound $(Ho_{1-x}Y_x)_2Ti_2O_7$, due to in-plane magnetic correlations as determined by the spin-flip scattering of the initial P_z polarization [8]. In addition to the separation of magnetic cross section from nuclear and spin-incoherent ones, polarization analysis can also be used to explore possible anisotropy of spin correlations in complex materials. Polarized powder diffraction carried out at DNS is complementary to standard neutron powder diffraction and may be extremely useful for magnetic structure refinements, particularly in case of small magnetic moments by improving the signal to background ratio. Fig. 2(b) shows the magnetic and nuclear scattering of iron-based superconductor Sr_2CrO_3FeAs measured at DNS via polarization analysis and the corresponding Rietveld refinements [9]. Fig. 2(c) shows the magnetic diffuse scattering derived with the same approach on the $\{Mo_{72}Fe_{30}\}$ molecule magnet [10]. DNS also represents a powerful instrument for the soft condensed matter community for the separation of nuclear coherent scattering from often dominating spin incoherent scattering background in hydrogenous materials.



(a)

(b)

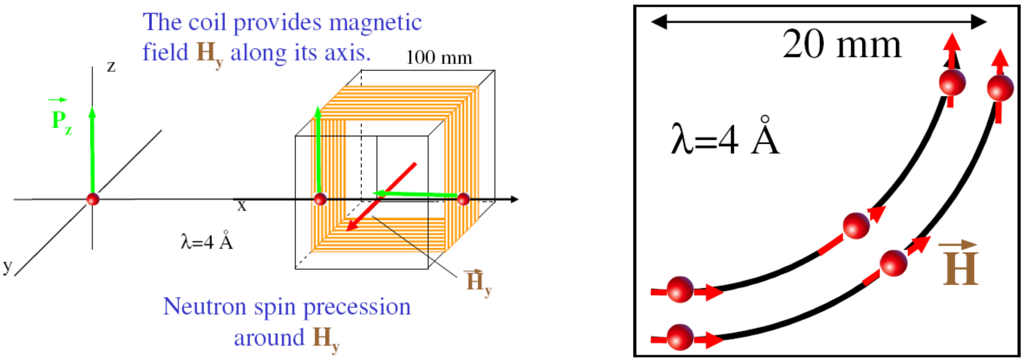
(c)

Fig. 2 Examples of the scientific applications at DNS: (a) peculiar magnetic diffuse scattering patterns observed on the frustrated spin-ice pyrochlore compound $(Ho_{1-x}Y_x)_2Ti_2O_7$ *via polarization analysis [8]; (b) magnetic and nuclear scattering of iron-based superconductor* Sr_2CrO_3FeAs *at 3.5 K as measured (blue) at DNS via polarization analysis and the Rietveld refinements (red) [9]; (c) differential magnetic scattering cross section measured at 1.5 K and the theoretical simulation with the three-sublattice spin model of the* $\{Mo_{72}Fe_{30}\}$ *molecule magnet [10].*

3 Preparatory Exercises

The practical aspects and the experimental setup of DNS with respect to polarization analysis have been addressed and discussed in great details in the lecture [1]. Therefore, it is strongly recommended to go through the relevant sections of the lecture notes thoroughly before the exercises. Try to answer the following general questions would greatly improve your understandings:

1. What is the Larmor precession? How to calculate the Larmor frequency (ω_L)?
2. How neutron spins would respond to changing magnetic fields? What are adiabatic and non-adiabatic behaviour?
3. How to produce polarized neutrons and how to analyze the spin state of the neutrons after the scattering process?
4. What is the spin flipper? How does it work?
5. What is the flipping ratio? What is the polarization rate of the neutron beams?
6. What are nuclear coherent, spin incoherent, isotopic incoherent and magnetic scattering processes? Whether and how the spin states of the scattered neutrons would be changed in those scattering processes?



(a) **(b)**

Fig. 3 Preparatory exercises

In addition to these general questions, the following exercises are provided:

1. How strong the magnetic fields $\mathbf{H_y}$ should be provided in the coil of length L = 100 mm to perform 90° turn for neutrons with λ=4 Å? (see Fig. 3(a))
2. A magnetic field **H** changes its space direction by 90° over a distance of L = 20 mm (as shown in Fig. 3(b)). How strong **H** should be to provide adiabatic evolution of the neutron spins guided by such fields? The neutrons wavelength is λ=4 Å.

4 Experiment Procedure and Experiment-related Exercises

4.1 Manipulating neutron spins

After the DNS instrument and its major instrument components are briefly introduced by the tutor, the first task for students is to learn how to manipulate neutrons spins via the Larmor precession and properly set guide fields. The following experiments are planned:

- Alignment of the π-flipper and z-compensation field coils for the incident neutrons with λ=4.74 Å
- Alignment of the magnetic guide fields at the sample position along three orthogonal directions via XYZ-coils
- Measurement of the flipping ratio and the polarization rate of the incident neutron beams at DNS

In addition, the following exercises are provided:

1. For neutrons with a wavelength λ=4.74 Å and a flight path of 10 mm through the flipper coil, how strong the flipping field would be required to achieve a π-flip?
2. The measured flipping ratio (R) is 25, what is the polarization rate (P) of the incident neutron beams?

4.2 Demonstration of the principle of neutron polarization analysis

The principle of neutron polarization analysis will be demonstrated here by the measurement of various standard samples. The following samples are planned,

- (002) Bragg reflection of pyrolytic graphite: nuclear coherent scattering
- Vanadium hollow-cylinder: nuclear spin-incoherent scattering
- Non-magnetic alloy $Ni_{0.89}Cr_{0.11}$: isotopic incoherent scattering
- A prototypical antiferromagnet: magnetic scattering

The students are expected to perform the experiment to measure the spin-flip and non-spin-flip scattering intensities of each sample via wide-angle polarization analyzers at DNS. The basic rules for the separation of different scattering cross-sections can thus be derived. The students will be encouraged to compare the results obtained at DNS to those reported in the seminal work by R.M. Moon [5].

The polarization efficiency can never achieve 100% due to polarization losses by depolarizations in the polarizer, the analyzer and the guide fields and the imperfections of the polarizer, the analyzer and the flipper. This would always lead to a finite flipping ratio even for an ideal non-spin-flip scatter. The correction for finite flipping ratio thus becomes an important and always necessary practical issue in order to obtain a precise separation. Therefore, the following exercise related to the flipping ratio correction is provided,

1. The measured flipping ratio from an ideal isotopic incoherent scatter $Ni_{0.89}Cr_{0.11}$ is 20, the spin-flip scattering intensity is $I_{\uparrow\uparrow}$ and the non-spin-flip scattering intensity is $I_{\uparrow\downarrow}$, how to calculated the corrected intensities for $I_{\uparrow\uparrow}$ and $I_{\uparrow\downarrow}$ by taking into account the finite flipping ratio?

4.3 Case studies

In the final part, two case studies will be provided for students to maser neutron polarization analysis via the measurements on two real samples. The first one is the separation of nuclear coherent scattering from incoherent scattering in heavy water D_2O [11]. The second case study is the measurement of magnetic ordering in the novel superconducting compound via the XYZ-method [9]. The following exercises are provided,

1. How to separate nuclear coherent scattering from spin-incoherent scattering in soft condensed matter?
2. How to obtain the magnetic scattering cross section via the XYZ-method? Which necessary corrections need to be done for a precise separation?

References

[1] W. Schweika, *Polarized Neutron Scattering and Polarization Analysis,* in *Lecture Notes on Laboratory Course Neutron Scattering,* Eds. Th. Brückel, G. Heger, D. Richter, G. Roth and R. Zorn (Forschungszentrum Jülich, 2010)

[2] J. Schweiza, *Polarized Neutron and Polarization Analysis*, in *Neutron Scattering from Magnetic Materials*, Ed. T. Chatterji (Elsevier, Amsterdam, 2006)

[3] P.J. Brown, *Spherical Neutron Polarimetry*, in *Neutron Scattering from Magnetic Materials*, Ed. T. Chatterji (Elsevier, Amsterdam, 2006)

[4] L.P. Regnault, *Inelastic Neutron Polarization Analysis*, in *Neutron Scattering from Magnetic Materials*, Ed. T. Chatterji (Elsevier, Amsterdam, 2006)

[5] R.M. Moon, T. Riste, W.C. Koehler, Phys. Rev. **181**, 920 (1969)

[6] O. Schärpf, H. Capellmann, Phys. Stat. Sol. (a) **135**, 359 (1993)

[7] J.R. Stewart *et al.*, J. Appl. Cryst. **42**, 69 (2009)

[8] L.J. Chang *et al.*, Phys. Rev. B **82**, 172403 (2010)

[9] M. Tegel *et al.*, EPL **89**, 37006 (2010)

[10] Z.D. Fu *et al.*, New Journal of Physics **12**, 083044 (2010)

[11] L. Temleitner *et al.*, J. Phys.: Condens. Matter **19**, 335207 (2007)

Contact

DNS

Phone: `089/289-14339`
Web: `http://www.frm2.tum.de/wissenschaftliche-nutzung/spektrometrie/dns/index.html`

Dr. Yixi Su

Juelich Centre for Neutron Science JCNS-FRM II
Forschungszentrum Juelich GmbH
Outstation at FRM II

Phone: `089/289-10714`
e-Mail: `Y.Su@fz-juelich.de`
Web: `http://www.fz-juelich.de/SharedDocs/Personen/JCNS/EN/Su_Y`

Dr. Kirill Nemkovskiy

Juelich Centre for Neutron Science JCNS-FRM II
Forschungszentrum Juelich GmbH
Outstation at FRM II

Phone: `089/289-10779`
e-Mail: `k.nemkovskiy@fz-juelich.de`