Polarisation Analysis Neutron Spectrometer, POLANO, at J-PARC - Concept and Magnetic Field Optimisation

K. Ohoyama¹,²*, T. Yokoo³,⁴, S. Itoh³,⁴, M. Nanbu², K. Iwasa⁵, M. Ohkawara², N. Kaneko³,⁴, T. Ino³,⁴, H. Hayashida⁶,⁷, T. Oku⁴,⁷, H. Kira⁸, S. Tasaki⁸, M. Takeda⁶,⁷, H. Kimura⁹ and T. J. Sato⁹

¹Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan
²Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan
³Neutron Science Division, High Energy Accelerator Research Organization, Tsukuba, 305-0801, Japan
⁴J-PARC Center, Tokai, 319-1195, Japan
⁵Department of Physics, Tohoku University, Sendai 980-8578, Japan
⁶Comprehensive Research Organization for Science and Society, Tokai, 319-1106, Japan
⁷Japan Atomic Energy Agency, Tokai, 319-1195, Japan
⁸Department of Nuclear Engineering, Kyoto University, Kyoto, 615-8530, Japan
⁹Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, 980-8577, Japan

E-mail: kenji.ohoyama.vs@vc.ibaraki.ac.jp

Abstract. The status of the polarised neutron spectrometer constructed at the Japan Proton Accelerator Research Complex through a collaboration between Tohoku University and KEK will be reported. In particular, the optimisation of magnetic fields to minimise neutron-beam depolarisation using the finite element method will be discussed on the basis of several simulations using the finite element method.

1. Introduction
Tohoku University and the High Energy Accelerator Research Organization (KEK) are jointly constructing a polarisation analysis neutron spectrometer, POLANO, at beam line 23 (BL23: a decoupled H₂ moderator) in the second experimental hall of the Materials and Life Science Experimental Facility (MLF) at the Japan Proton Accelerator Research Complex (J-PARC) [1, 2]. POLANO will be the first dedicated polarised neutron spectrometer at MLF with polarisation analysis capability for spin dynamics investigation. The polarised neutron scattering technique is indispensable for novel materials science; it is an important and direct probe for observation of pure magnetic responses, nuclear-magnetic interference scattering, and spin chirality states. As a scientific target, for instance, POLANO aims at observing characteristic spin excitations, so-called hour-glass type magnetic excitations in some of high-$T_c$ superconductors [3]. It is thought that understandings of the characteristic magnetic excitations

* Present address: Graduate School of Science and Engineering, Ibaraki University, Nakanarusawa 4-12-1, Hitachi, 316-8511, Japan
are necessary to clarify the role of spin interactions in the superconductivity mechanism. For such investigations, the usable energy region around and above 50 meV is necessary. Another scientific target is electronic and magnetic multipole physics. For 4f-electron systems, multipolar degrees of freedom, such as in the case of quadrupolar and octupolar moments, are the main topics of interest. Although inter-multipolar interactions are thought to be responsible for determining properties of 4f systems, the current understanding of this subject is quite limited because the relevant dynamics are often hidden by magnetic excitations and lattice dynamics. Thus, observations of multipolar excitations are a research target of POLANO. A characteristic of scattering by octupolar moments is Q dependence; the octupolar form factor has a maximum at a higher Q region (Q ≈ 8 Å⁻¹), while magnetic form factors decrease with increasing Q [4]. Thus, POLANO will be used for observation in the high-Q (Q ≥ 8 Å⁻¹) region to detect octupolar excitations. To achieve this high-Q region, a scattering angle up to 130° will be covered with position-sensitive detectors with a diameter of 20 mm in the first stage, and an incident energy, $E_i$, of over 80 meV will be used. We choose polarised neutron devices, as described later, because of such a demand for the neutron energy range.

The proposal of POLANO project was accepted by the J-PARC Center in 2011. The construction of the radiation shields was completed in 2013 and the vacuum chamber was installed on January 15th, 2015. The first beam is expected in 2016.

2. Flux and Polarisation Devices

To obtain high beam flux for polarised analysis experiments, focusing guide tubes with 4Qc, supermirrors, where Qc is the critical momentum transfer of Ni mirror, are installed; details of the focusing guide are reported in Ref. 2. Figure 1 shows the calculated results of the neutron beam flux at the sample position given by the focusing guide tubes, calculated by the Monte Carlo simulation using a program McStas. A cylindrical 3He spin filter polarised by the on-beam spin exchange optical pumping (SEOP) technique will be installed at POLANO as a polariser. Because of the scientific targets briefly mentioned above, the SEOP-type 3He spin filter is the best choice for the required energy region at the moment. The SEOP-type 3He polariser is to be put on an elevator table so that the 3He spin filter height can be controlled for optimisation and for operation in the unpolarised mode. Details of the SEOP technique and the design of POLANO polariser are being reported by Ino et al. [6].

For 3He spin filters, the neutron polarisation and transmission are expressed as:

$$T_n = e^{-\sigma_n(\lambda)d} \cosh(P_{He}\sigma_a(\lambda)d)$$  \hspace{1cm} (1)

$$P_n = \tanh(P_{He}\sigma_a(\lambda)d)$$  \hspace{1cm} (2)
In this equation, $\sigma_a(\lambda)$ is the absorption cross section (cm$^2$) for the neutron wavelength, $\lambda$, while $d$ is a parameter corresponding to the number of $^3$He atoms in the spin filter cell. This is defined as $d = P \times l \times 2.414 \times 10^{20}$, where $P$ and $l$ are the $^3$He gas pressure (MPa) at room temperature and the length of the cell (cm), respectively. The blue line in Fig.1 indicates the flux of polarised neutrons using a $^3$He spin filter with $P_{^3\text{He}} = 0.73$, $P = 0.203$ MPa, and $l = 10$ cm; Note that $P_{^3\text{He}} = 0.73$ is the highest value in Japan [5]. A polarised beam flux of $\sim 3.6 \times 10^5$ s$^{-1}$/cm$^2$/meV can be expected to be obtained at $E = 60$ meV when the source power reaches 1 MW. On the other hand, Eqs.(1) and (2) indicate that higher neutron polarisation yields lower neutron transmission inevitably. Thus, for practical experiments, optimisation is important. An estimation of the optimisation of the parameters for $^3$He spin filters was discussed elsewhere [1].

Polarisation analysers are an important technical issue to resolve the magnetic scattering component from the nuclear scattering one. For high-energy regions, spin filter analysers are a reasonable choice, but there are many technical difficulties that should be overcome in order to realise a spin filter analyser covering a large solid angle. Thus, as a practical choice, in the first stage of the project, a polarisation analyser composed of a set of Fe/Si supermirror benders will be installed; the bender blade is a $5.5Q_c$ mirror on the convex surface, and $1.5Q_c$ mirror on the concave surface. The analyser covers a $2\theta$ range of approximately 16°, and will be installed on a table that rotates around the sample position in the vacuum chamber. The slit-width between the supermirror bender blades is 0.6 mm. The transmission of the supermirror analyser depends on the angular divergency of the incident neutron at the analyser entrance and the energy-dependent reflection angle on the supermirror surface. Figure 2 shows the energy dependence of calculated transmission which was defined as the ratio between the intensity at the entrance and exit positions of one supermirror slit set. The calculations were done under the planned POLANO configuration including the focusing guide tubes, and a standard vanadium cylinder (outer diameter: 25 mm, inner diameter: 24 mm, height: 40 mm) is set at the sample position; for the calculations, the McStas component, Pol_Bender, in which the mirrors were set to parallel, was used. As shown in Fig. 2, a transmission of $\sim 0.18$ can be expected at 20 meV, which is basically consistent with the data from the supermirror manufacturer.

We have confirmed the required angular accuracy of the analyser. Figure 3 shows the integrated intensity for $E = 20$ meV at a detector from the standard vanadium cylinder. The horizontal axis is the angle of the analyser optical axis. Figure 3 means that an angular accuracy of approximately $\pm 0.2^\circ$ is required in order to set the optical axis of the analyser to the maximum position. This condition is fulfilled by adopting the analyser table around the sample position that allows us to adjust the optical direction of the mirrors with an accuracy of 0.01° or less.
3. Magnetic Field Devices

Needless to say, the careful control of the magnetic fields around the beam is quite important for polarised neutron experiments. In this section, some results of estimation of magnetic fields are given. Firstly, we consider the magnetic field environment around POLANO. Only the minimum amount of iron is used in the radiation shield and vacuum chamber, but some iron materials are still present around POLANO; for instance, there are carbon steel nets under the floor of the experimental hall, and there is iron as part of the Fermi chopper pit, and as part of the radiation shields. Note that a side wall of the chopper pit which is nearest to the sample position is made of stainless steel to minimise the magnetisation effect. The effect of magnetisation of such iron materials on the polarised neutron beam should be estimated. Thus, as a worst case scenario, we considered the effects of 7 T magnetic fields generated by a MLF superconducting magnet on the iron materials using a finite element method program, ANSYS Maxwell.

Figure 4 shows the calculation model incorporating the structures containing iron materials in POLANO. The inset indicates the magnetic devices on the beam path, specifically: a solenoid coil for the SEOP-type $^3$He spin filter, magnetic guides, a Helmholtz coil for samples, and a magnetic housing for the supermirror analyser. Figure 5 shows the magnitude of total magnetic fields along the beam path under the planned standard alignment of magnetic devices. The red line indicates the initial condition of POLANO calculated before application of the magnetic field of 7 T. After the calculation of the initial condition, the magnetic field of 7 T was applied at the sample position by a superconducting magnet, so that the iron around POLANO was magnetised by leaked magnetic fields from the superconducting magnet. The blue line indicates that calculated magnetic fields following application of the magnetic field of 7 T, which includes magnetic fields from the magnetised materials. Note that the 7T superconducting magnet itself was not included in the calculations. The difference between the data before and after application of the magnetic field is less than 1.5 G, which is much smaller than the typical guide fields ($\approx$20 G) along the beam path. This means that magnetisation effects of the iron parts around POLANO are negligible even though the iron is magnetised by the 7 T superconducting magnet. The nearest iron part to the sample position is a wall of a radiation shield, which is at a distance of approximately 140 cm or more. This indicates that the distance of $\approx$140 cm is sufficiently large to prevent serious magnetisation effects caused by leaked magnetic fields from a 7 T superconducting magnet.

Secondly, we optimised the magnetic-field devices to minimise the depolarisation between the $^3$He spin filter and the analyser. When neutrons with finite velocity enter in a magnetic field, the neutron spin is rotated due to Larmor precession. The final spin wave function, $\psi_f$, due to
Figure 4. Model of estimation of magnetic fields, indicating iron parts around POLANO. The iron in radiation shields, the floor of the experimental hall which includes iron steel net 10 cm below the floor surface, some of the chopper pit walls, etc are included. Standard magnetic devices such as a solenoid coil for the SEOP-type 3He spin filter, magnetic guides, the Helmholtz coil for samples, and a magnetic housing for the supermirror analyser, as shown in the inset, are also included in the calculations. The 7 T superconducting magnet is set at the sample position and generates a magnetic field of 7 T.

Larmor precession can be represented using the initial spin wave function, $\psi_i$, as

$$\psi_f = \exp \left( -i \frac{S \cdot n}{\hbar} \frac{2 \omega l}{v} \right) \psi_i$$  \hspace{1cm} (3)
where \( \omega \), \( l \), and \( v \) are Larmor frequency, the length of the flight path under the magnetic field, and neutron velocity, respectively, and \( \mathbf{S} \) is the neutron spin. \( \mathbf{n} \) is the unit vector of the magnetic field, \( \mathbf{B} \), at \( l \). The average value of each spin component in \( \psi_f \) is obtained as \( \langle S_\alpha \rangle = \hbar / 2 \psi^*_f \sigma_\alpha \psi_f \) \((\alpha = x, y, z)\), where \( \sigma_\alpha \) is the Pauli matrix. From the average spin components, the neutron polarisation, \( P_n \), of the final state can be defined as

\[
P_n = \frac{\langle S_z \rangle B_z + \langle S_y \rangle B_y + \langle S_x \rangle B_z}{|\mathbf{S}| |\mathbf{B}|} \tag{4}
\]

Thus, when \( \psi_f \) and the magnetic field distribution with an interval of \( l \) are provided, the value of \( P_n \) at each point can be estimated. For these calculations, the \( z \)-axis is parallel to the beam direction, the \( y \)-axis is in the vertical direction, and the \( x \)-axis is perpendicular to the \( y \)- and \( z \)-axes. Since the magnetic field at the \( ^3 \text{He} \) spin filter is parallel to the beam direction, the initial neutron spin is parallel to the \( z \)-axis. Note that \( l \) must be sufficiently short to allow the magnetic field to be treated as a constant. In the calculations below, we calculated \( P_n \) with \( l = 1 \) mm condition because we confirmed that the typical results of magnetic field distribution with \( l = 1 \) mm and 0.1 mm gave the same \( P_n \) at each position.

We calculated the magnetic field distribution along the beam path within the area of \( x, y = \pm 3 \text{cm} \) with magnetic devices of a solenoid coil for the SEOP-type \(^3 \text{He} \) spin filter (current: 2 A), magnetic guides, a Helmholtz coil for samples, and a magnetic housing for the supermirror analyser. The SEOP-type \(^3 \text{He} \) spin filter is the same one as in Ref.6. Figures 6(a) and (c) show the total magnitude (\( B \)) of the magnetic field at the beam centre (a) and the \( y = -3 \text{cm} \) (c) position below the beam centre. These calculations were done using ANSYS in SR16000 supercomputing resources at the Center for Computational Materials Science of the Institute for Materials Research, Tohoku University. From the magnetic field distributions in Fig. 6, \( \langle S_\alpha \rangle \) and \( P_n \) can be obtained from Eqs. (3) and (4). We calculated \( P_n \) in the energy region between 10 and 100 meV in the beam area of \( -3 \text{cm} \leq x, y \leq 3 \text{cm} \). As typical results, Figs. 6(b) and (d) indicate the change in \( P_n \) for \( E = 80 \text{ meV} \) along the beam path at \( x = 0 \text{ cm} \). At the beam centre \( (y = 0 \text{ cm}) \) (Fig. 6(b)), \( P_n \) is almost constant except the slight depolarisation at \( z \sim 0.2 \text{ m} \) (blue triangle), and the final \( P_n \) at the analyser \((z \sim 1.7 \text{ m})\) is 0.96, which is satisfactory for practical experiments. On the other hand, for \( y = -3 \text{ cm}, \ P_n \) decreases drastically after the exit of the SEOP solenoid coil at \( z \sim 0.2 \text{ m} \). The obvious depolarisation is caused by the suppressed magnetic fields (blue triangle), where the magnetic fields generated by the SEOP solenoid coil and vertical guide magnet are almost cancelled; the suppressed magnetic field is at \( \sim 6 \text{ G} \), and the final \( P_n \) is \( \sim 0.14 \). To prevent the depolarisation found in Figs. 6(b) and (d), an additional solenoid guide coil with a length of 3 cm at \( z \sim 0.27 \text{ cm} \) is effective to cover the bottom of the magnetic field. The dashed red lines in Figs. 6(b) and (d) shows \( P_n \) when the 3 cm coil is used (current: 1.5 A), which increases the bottom of \( B \) around \( z = 0.2 \text{ m} \) above 20 G; the depolarisation in Fig. 6(d) is drastically improved, and the final \( P_n \) is almost 0.99. Note that the slight depolarisation in Fig. 6(b) around \( z = 0.2 \text{ m} \) also disappears. Based on systematic calculations of depolarisation, we found empirical criteria of the magnetic field that can prevent depolarisation; when \( B \) is 20 G or larger, depolarisation can be neglected even in the energy range between 10 and 100 meV in the alignment of POLANO.

On the other hand, there is a possibility that additional coils near the SEOP solenoid coil deteriorate the homogeneity of the magnetic field in the SEOP solenoid coil, which affects the relaxation time of the \(^3 \text{He} \) spin, and thus, \( P_{\text{He}} \) [6]. We calculated the effect of the 3 cm coil and other devices to the homogeneity of the magnetic field in the SEOP solenoid coil based on Ref.6. The required homogeneity of the magnetic field at the \(^3 \text{He} \) spin filter is expressed as

\[
\frac{dB_z}{dr} \frac{1}{B_z} < 0.0008 \tag{5}
\]
where $B_r$ and $B_z$ are the radial and longitudinal direction components of the magnetic field in the SEOP solenoid coil, respectively, at the radial position $r$ (cm), and at the longitudinal direction position, $z$ (cm). We confirmed that the homogeneity of the magnetic field in the SEOP solenoid coil in the alignment with the 3 cm coil satisfies the requirement of Eq. (5) in the area of the $^3$He spin filter, meaning that the alignment of the magnetic devices including the 3 cm coil found in the present calculations does not affect the $P_{He}$.

For the calculations mentioned above, the magnetic field applied by the Helmholtz coil is vertical at the sample position. We also confirmed that the same alignment of magnetic devices maintains $P_n$ larger than 0.95 in the energy range between 10 and 100 meV, even for application of a horizontal magnetic fields at the sample position. Thus, the alignment found in the present work makes both the $P_n//Q$ and $P_n\perp Q$ experimental conditions possible; these conditions are indispensable for the separation of pure magnetic and nuclear scattering components.

Figure 6. Results of estimation of depolarisation along the beam path for $E = 80 \text{ meV}$. The horizontal axis is the distance along the beam direction from the centre of the SEOP solenoid coil. (a) and (c) show the total magnetic field at each point at the beam centre ($x = 0 \text{ cm}$, $y = 0 \text{ cm}$) and the $x = 0 \text{ cm}$, $y = -3 \text{ cm}$ position. Note that the Helmholtz coil for the sample applies a vertical magnetic field at the sample position in this calculation. (b) and (d) show the neutron polarisation expressed according to Eq. 4, and the angle, $\theta_B$, between the spin and magnetic field at each point. The vertical lines indicate the edges of each magnetic device. Note that the scales of the vertical axis of (b) and (d) are different. The red solid and dashed lines in (b) and (d) indicate $P_n$ when the 3 cm coil at $z \sim 0.27 \text{ cm}$ is not used and is used (current: 1.5 A).
4. Summary
The first dedicated polarised neutron spectrometer, POLANO, at J-PARC is under construction through a collaboration between Tohoku University and KEK. The first beam is expected in the autumn of 2015. To obtain higher neutron flux, the $4Q_c$ supermirror guide tubes are installed; a polarised beam flux of $\sim 3.6 \times 10^5 / \text{s/cm}^2/\text{meV}$ at $E = 60 \text{ meV}$ can be expected when the source power reaches 1 MW, with a cylindrical $^3\text{He}$ spin filter polarised by the SEOP technique. The transmission of the supermirror analyser is estimated to be 0.18 at $E = 20 \text{ meV}$. We investigate the effect of magnetisation of iron around the beam line on the polarised neutron transportation. The iron in the radiation shields and the carbon steel net in the floor were taken into account, and magnetisation of these materials induced by a magnetic field of 7 T applied by a superconductor magnet was calculated. Using the finite element method, we confirmed that the effect of the magnetic fields from the magnetised iron on the polarised neutron beam is negligible. The alignment of magnetic devices on the beam path was optimised using a quantum physics treatment of spin transportation. From the calculations, we succeeded in finding an alignment of magnetic devices which gives satisfactory $P_n$ in the energy range between 10 and 100 meV for both the $P_n//Q$ and $P_n\perp Q$ conditions.

Acknowledgments
The calculations in Fig. 6 has been performed under the inter-university cooperative research program of the Center for Computational Materials Science, Institute for Materials Research, Tohoku University (Proposal No.: 13S0416, 14S0413). This work was partly supported by the S-type project of KEK (2009S09, 2014S09) and a Grant-in-Aid for Challenging Exploratory Research (24656004), Scientific Research (A)/(23244068), (S)/(23224009).

References
[1] K. Ohoyama, T. Yokoo, S. Itoh, J. Suzuki, K. Iwasa, T.J. Sato, H. Kira, Y. Sakaguchi, T. Ino, T. Oku, K. Tomiyasu, M. Matsunaga, H. Hiraka, M. Fujita, H. Kimura, T. Sato, J. Suzuki, H. Shimizu, T. Arima, M. Takeda, K. Kaneko, M. Hino, S. Muto, H. Nojiri, C.H. Lee, J.G. Park, and S. Choi, J. Phys. Soc. Jpn. 82 (2013) SA035.
[2] T. Yokoo, K. Ohoyama, S. Itoh, J. Suzuki, K. Iwasa, T. J. Sato, H. Kimura, N. Kaneko, and M. Ohkawara, J. Phys.: Conf. Ser. 502 (2014) 012046.
[3] For instance, J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu, G. Xu, M. Fujita, and K. Yamada, Nature 429 (2004) 534.
[4] R. Shina, O. Sakai, and H. Shiba, J. Phys. Soc. Jpn., 76 (2007) 094702.
[5] H. Kira, Y. Sakaguchi, T. Oku, J. Suzuki, M. Nakamura, M. Arai, K. Kakurai, Y. Endo, Y. Arimoto, T. Ino, H.M. Shimizu, T. Kamiyama, K. Tsutsumi, K. Ohoyama, H. Hiraka, K. Yamada, and L.J. Chang, Physica B 406 (2011) 2433.
[6] T. Ino, K. Ohoyama, T. Yokoo, S. Itoh, M. Ohkawara, H. Kira, H. Hayashida, K. Sakai, K. Hiroi, T. Oku, K. Kakurai, and L. J. Chang, Proceedings of Polarised Neutrons for Condensed-Matter Investigations 2014.