Polarized neutron scattering on the triple-axis spectrometer PANDA: first results

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Abstract. PANDA is a triple-axis spectrometer utilizing the cold neutron source of the German research reactor FRM II in Garching. Its typical applications comprise studies of spin dynamics and lattice dynamics, magnetic excitations and magnetic structures. In the past years, PANDA has earned its reputation by excellent performance in these fields operating in conventional, unpolarized mode. To complement this normal mode of operation, a full polarization analysis of the scattered neutrons was highly desired and, therefore, was recently implemented. First tests to characterize the different spectrometer components for the polarization analysis mode were performed with neutron spin directions perpendicular to the scattering plane, utilizing static vertical guide fields between sample, Heusler monochromator, spin flipper and Heusler analyzer. Finally, a fully automated setup of split coils around the sample space was implemented to allow for longitudinal polarization analysis for arbitrary configurations. Different neutron spin polarization directions were successfully investigated, showing polarizations of 92\% or higher.

1. Introduction

Because of its high flux, unique large dynamic range and optional flexibility PANDA acquired a position among the leading cold TAS instruments. Typical applications comprise studies of magnetic excitations, spin and lattice dynamics as well as the investigation of magnetic structures. Up to now, PG monochromator and analyzer were used for Beryllium filter wavelengths \( k_f \leq 1.55 \text{ Å}^{-1} \) or for PG filter wavelengths at \( k_f = 2.557 \text{ Å}^{-1} \) or \( k_f = 2.662 \text{ Å}^{-1} \). The best energy resolution observed in an user experiment is \( \Delta E = 37 \mu\text{eV} \) at \( k_f < 1.078 \text{ Å}^{-1} \). The momentum transfer can vary from 0.1 up to 6 \( \text{Å}^{-1} \), with energy transfers up to 23 meV.

The sample environment available on PANDA allows temperatures from from 50 mK up to 2100 K and for temperatures below 100 K magnetic fields fields up to 14.5 T. The combination of very low temperatures, high magnetic fields and cold neutrons matches perfectly the energy scales in typical magnetic samples.

To complement this normal, unpolarized mode of operation of PANDA, the instrument was equipped with Heusler type monochromator and analyzer. As the polarized operation was planned from the beginning, some guide-field elements were already included during the construction of the instrument.
2. Mode of Operation
The neutrons leave the Heusler type monochromator (variable vertical, fixed horizontal focusing) with a horizontal polarization. A vertical guide field then turns the spins adiabatically to a vertical polarization. A spin flipper (sf1) can be activated to flip the spin orientation around. A vertical magnetic field at the sample position (basic setup) or a magnetic vector field around the sample (3-directional setup) might either keep the vertical direction of the spins \( P \parallel z \) or turn them into the scattering plane parallel \( P \parallel Q \) or perpendicular \( P \perp Q \) to the scattering vector \( Q \). The polarization of the scattered neutrons is then turned vertical again. A second spin flipper (sf2) can invert the polarization direction. The Heusler analyzer (fixed vertical and variable horizontal focusing) finally accepts only neutrons with a vertical polarization pointing up and allows the energy selection required for operation as triple axis instrument. All field gradients of the guide fields along the neutron path are low enough to allow for adiabatic changes of spatial directions of the neutron polarization.

3. Basic setup
As a first step an instrumental setup with a vertical guide field around the sample position was tested and found operational [1]. The elements providing the static magnetic guide field were arranged close to the sample, avoiding a depolarization of the beam near the sample. This setup exclusively provides a vertical guide field and therefore supports only vertical polarizations. Utilizing some attenuation to safeguard the detector, only minor depolarization of the primary beam was found, as illustrated in figure 1 showing the observed neutron counts versus the flipping current at optimal field compensation. Using a single crystal of Lead, a flipping ratio of up to 40 was found in a rocking scan across the \((200)\) Bragg reflection, as shown in figure 2(a). An energy scan across the elastic incoherent line of Vanadium shows the expected intensity ratio of 1:2 for non spin flip (nsf) vs. spin flip (sf) scattering (see figure 2(b)). Compared to the completely unpolarized setup with PG monochromator/analyser, the polarized mode provides a factor of 20 less neutrons in the detector.

To test the setup under realistic conditions, an experiment on a single crystal of \( \text{Er}_2\text{PdSi}_3 \) was performed in the basic setup at low temperatures. The hexagonal compound \( \text{Er}_2\text{PdSi}_3 \) shows a strong crystal electric field (CEF) transition from the ground state doublet to the first excited state (also a doublet) around an energy transfer of 3.5 meV. Despite good crystal quality...
and heating treatment, superstructure peaks are observable in the hole series of $R_2PdSi_3$. The corresponding superstructure is formed by an ordering of the Pd and Si atoms [2, 3, 4] which leads to distinct Er site environments. This gives raise to (slightly) different CEF schemes. Calculations indicate the occurrence of two distinct CEF excitation energies [2]: One resulting from a Er site with local hexagonal symmetry and one with reduced local symmetry. Since the matrix elements for inelastic neutron scattering do not vanish, both transitions should be observable. In fact, in an unpolarized inelastic neutron scattering experiment instead of one transition at around 3.5 meV, two transitions at 3.3 and at 3.6 meV, were observed. In addition, both transitions differ in their directional dependence of the CEF matrix elements and hence in their intensity [4]. To proof the magnetic origin of these two signals, we performed the first polarized experiment on PANDA.

Since $Er_2PdSi_3$ displays an antiferromagnetic order below $T_N \approx 7K$ [5], the measurements were done at 10 K to avoid the magnetic order modifying the CEF scheme. The sample was mounted in a (HK0) scattering plane with a vertical polarization of the incoming neutrons. After careful alignment of both the instrument and the sample, the overall polarization was determined on the (010) Bragg reflection. This is illustrated in figure 3, where the intensity of the Bragg peak versus the flipping current of the spin flipper at optimal compensation current is displayed. From the raw data one finds a flipping ratio of $R = 35$, a sine fit to the data points results in a more realistic value of $R = 31$ yielding an overall polarization of $P \geq 93.75\%$.

![Intensity of the (010) Bragg reflection of Er$_2$PdSi$_3$ versus flipping current at optimum compensation field. (raw data: black, sine fit: red)](image)

**Figure 3.** Intensity of the (010) Bragg reflection of Er$_2$PdSi$_3$ versus flipping current at optimum compensation field. (raw data: black, sine fit: red)

After this encouraging result, inelastic scans were measured at two perpendicular $Q$-positions (0T0) and (1.050), having a comparable $|Q|$ value. Figure 4 shows the obtained neutron counts for sf (blue curve, sf2:on) and nsf channels (green curve, sf2:off), respectively. At both $Q$ positions the two inelastic CEF excitations were found in the sf channel, whereas (within the error bars) no signal was found in the nsf channels. The latter finding indicates a negligible $J_z$ matrix element for both CEF transitions. Furthermore, the intensity of the low-energy transition at

![Inelastic signal in Er$_2$PdSi$_3$ at two perpendicular $Q$ positions (0T0) and (1.050). (sf channel: blue, nsf channel: green) Blue lines indicate two-peak Gaussian fits to the data.](image)

**Figure 4.** Inelastic signal in Er$_2$PdSi$_3$ at two perpendicular $Q$ positions (0T0) and (1.050). (sf channel: blue, nsf channel: green) Blue lines indicate two-peak Gaussian fits to the data.
3.3 meV shows a strong directional dependence while the behavior of the high-energy transition at 3.6 meV is isotropic in the basal plane (see upper and lower panel in figure 4). These findings correlate well with the unpolarized results [4]. From these facts we can conclude that the isotropic (i.e. 3.6 meV) excitation belongs to Er-sites with higher symmetry, whereas the Er-sites with lower symmetry show a slightly smaller excitation energy. A site occurrence of 1:1 is calculated from the averaged intensities, fitting very well to recent calculations [2].

4. 3-directional Polarization Analysis
To give access to additional polarization channels, a coil system around the sample position was implemented1. It allows to use any field direction for the neutron guide field at the sample position. In the experiment, the field is applied by these coils along the $P \parallel Q$ and $P \perp Q$ directions with $Q$ within the scattering plane. Figure 5 shows a view of the setup as mounted on the sample table of PANDA. The construction allows to use most of the sample environment, except the 14.5 T cryomagnet. Due to the split design, no beam blockage occurs. Nevertheless, this design can be improved further: (i) At some point between the upper and lower coils the dipole field vanishes leading to a strong beam depolarization. The problem is fixed by an additional static vertical field next to the coils which shifts this point out of the scattering plane. (ii) The outside stray field of the vector coils influences the compensation current of the spin flippers. Therefore, the flippers need to have a certain distance from the coils.

1 The original design of the coil system was made by Peter Böni. It was manufactured by Swiss Neutronics, Switzerland.

Figure 5. View of the coil setup as mounted on PANDA.
To test the device and the controlling software, we performed an inelastic neutron scattering experiment on the magnons of a single crystal of the magnetic salt RbMnF$_3$ [6]. Although the instrument was aligned very well, we found a flipping ratio of only$^2$ $R = 3.5$ corresponding to a polarization of $P = (R - 1)/(R + 1) = 55.6\%$. We found that magnetic parts of the closed-cycle refrigerator add an additional $z$-component to the guide field at the sample position, thus effectively depolarizing the beam. In this setup we performed longitudinal $Q$-scans at selected energies between 1 and 5 meV across the antiferromagnetic Bragg peak at $(-0.5 - 0.5 - 0.5)$ at $T = 60\, K < T_N = 83\, K$. Figure 6 shows the polarization corrected intensities$^3$ for an energy transfer of 2 meV for all six accessible scattering channels. As expected, the sum of nsf and sf channels is the same for the polarization directions $P \parallel z$, $P \parallel Q$ and $P \perp Q$. The sum of all nsf channels is half of all sf channels. And, most important, there is (almost) no signal in the nsf channel for $P \parallel Q$, as expected from scattering theory (see for example [7]). The coupling and magnon stiffness constants obtained from our dataset are comparable to the results given in [6] (see formulas and text therein). The finite intensity at positions between the magnon peaks can be attributed to longitudinal moment fluctuations occurring close to $T_N$ [8, 9]. The occurrence of domains results in an even distribution of the scattering intensity over the allowed channels.

$^2$ Values without this cryostat are above 25.

$^3$ The polarisation was determined in the elastic condition on the Bragg Peak and this value was used to correct the measured inelastic signal according to: $\left(\frac{I_{\text{sf}}}{I_{\text{nsf}}}\right)_{\text{corr.}} = \frac{1}{2\pi} : \left(\frac{P_{+1}}{P_{-1}}\right)_{\text{meas.}} \cdot \left(\frac{I_{\text{sf}}}{I_{\text{nsf}}}\right).$
This experiment shows that despite unexpected problems a successful measurement could be performed.

5. Conclusion
The polarization option of the cold-triple axis spectrometer PANDA has been successfully commissioned. The specifically crafted vector guide field allows to access almost all possible spin related scattering channels. Due to the chosen construction, no beam blockade occurs.

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References
[1] Link P 2007 Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Annual Report pp 46-47
[2] Tang F, Link P, Frontzek M, Mignot J M, Hoffmann J U, Löser W and Loewenhaupt M 2009 Proc. Int. Conf. on Neutron Scattering (Knoxville) accepted for publication in Journal of Physics: Conference Series
[3] Frontzek M, Kreyssig A, Doerr M, Hoffmann J U, Hohlwein D, Bitterlich H, Behr G and Loewenhaupt M 2004 Physica B 350 E187
[4] Tang F, Link P, Frontzek M, Schneidewind A, Löser W and Loewenhaupt M 2009 Proc. Int. Conf. on Neutron Scattering (Knoxville) accepted for publication in Journal of Physics: Conference Series
[5] Frontzek M, Tang F, Link P, Schneidewind A, Mignot J M, Hoffmann J U and Loewenhaupt M 2009 Proc. Int. Conf. on Neutron Scattering (Knoxville) accepted for publication in Journal of Physics: Conference Series
[6] Windsor C G and Stevenson R W H 1966 Proc. Phys. Soc. 87 501-4
[7] Shirane G, Shapiro S M and Tranquada J M 2002 Neutron Scattering with a Triple-Axis Spectrometer (Cambridge University press)
[8] Cox U J, Cowley R A, Bates S and Cussen L D 1989 J. Phys.: Condens. Matter 1 3031-5
[9] Coldea R, Cowley R A, Perring T G, McMorrow D F and Roessli B 1998 Phys. Rev. B 57 5281-90