

## New POLDI – project of reincarnation of a polarized neutron diffractometer at the reactor PIK

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**Abstract.** The project of a considerable modernization of the polarized neutron diffractometer POLDI is discussed. It assumes the adoption of POLDI to a broader range of magnetic investigations such as determination of magnetic structures, detailed investigation of complex magnetic structures, studies of magnetic domains, study of the magnetization density maps, magnetic form-factor particularities, local susceptibility, etc. The flexible construction should permit to use either spherical neutron polarimetry technique or flipping ratio technique. Different types of polarization system were analyzed. Original focusing fan-like bender is proposed as polarizer unit. Our simulations give evidence that for the wavelength range 1.3 - 3 Å and with suitable size, such a device can give much better efficiency than <sup>3</sup>He cells, which are often in use. The higher flux at the sample position of a factor of at least 3.3, with lower divergence and good polarization degree from 98% (1.3 Å) to above 94% (3 Å) makes the bender set-up favorable over the layout with a <sup>3</sup>He-cell.

### 1. Introduction.

The polarized neutron diffractometer POLDI was built by the Physikalisch-Technische Bundesanstalt (PTB), Braunschweig. Initially it was installed and operated at the 1 MW PTB research reactor. It was adapted to studies of ferromagnetic domain structures and ferromagnetic correlations in the range from 20 nm to several mm. POLDI was equipped with a set-up for full 3-dimensional depolarization analysis of the beam transmitted by the sample. In magnetized media, the neutron polarization changes during the passage through the sample, and this information can be obtained from the depolarization matrix **D**. This latter relates the initial polarization **P**<sub>0</sub> to the final polarization **P**' = **D****P**<sub>0</sub>. In this way, the mean domain size  $\delta$  and the magnetic texture  $\gamma$  in multi-domain samples could be extracted.

After the PTB reactor shutdown, POLDI was set up on the 5MW FRG-1 reactor at GKSS, where it continued to operate thanks to team from PTB under the guidance of Dr. Volker Wagner.

After that reactor was shut down, POLDI was delivered to PNPI (Gatchina), where it will be installed at new high-flux reactor PIK. The current plan of placement of POLDI on PIK is the 5<sup>th</sup> thermal channel in the main reactor hall (Fig.1), where it will be the first instrument on the channel, and the second will be another instrument, probably a polarized triple axes spectrometer.

Since we expect to have high intensity of polarized neutrons, it is natural to adapt POLDI to the broader range of magnetic investigations such as determination of magnetic structures, sound investigation of complex magnetic structures, studies of magnetic domains, study of magnetization density maps, magnetic form-factor particularities, local susceptibility, etc. Thorough magnetic investigations with polarized neutrons become more demanded as in recent years increasing attention is paid to magnetic materials with strong interacting order parameters. These include multiferroics



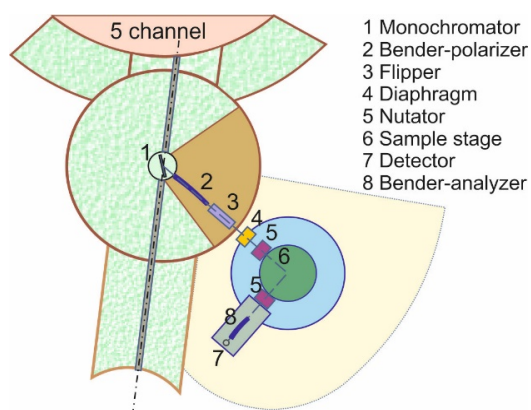
which have some magnetic subsystems, compounds with colossal magnetoresistance and giant magnetocaloric effect, high temperature superconductors etc. The study of microscopic mechanisms responsible for interaction in such materials can ensure progress in the area of study and creation of new materials.

For the implementation of these possibilities, two main different working modes should be realized: spherical neutron polarimetry technique (SNP) [1,2] and flipping ratio technique (FRT) [3]. In both of these techniques, diffraction of polarized neutrons is used. In SNP the polarization matrix  $\mathbf{P}(hkl)$  is measured for selected Bragg reflections. This matrix relates the change of neutron polarization in diffraction  $\mathbf{P}'(hkl) = \mathbf{P}(hkl)\mathbf{P}_0$ . In this case, the change of the polarization can take place due to a rotation of polarization and/or to the appearance of additional polarization in the diffraction process. The coefficients of the polarization matrix depend strongly on the particular type of magnetic scattering [2] and this permits to make unique investigations of complex magnetic structures. FRT in turn, uses the exceptional sensibility of polarized neutron scattering to weak magnetic responses. In this method, flipping ratios  $R(hkl) = I^+(hkl)/I^-(hkl)$  for all possible Bragg reflections should be collected, where  $I^+(hkl)$  is the reflection intensity with incident neutron spin “up” and  $I^-(hkl)$  is the intensity with spin “down”. In this way, one can obtain magnetization density maps, anisotropy of magnetic form-factors, etc. The essential difference between these two experimental methods is the completely opposite requirements for the magnetic field on the sample stage: for SNP there should be zero field on the sample position, which could be implemented with a zero-field device like CryoPAD [1], and for FRT there should be a very high magnetic field, which could be implemented with a cryomagnet. In order to satisfy these requirements the flexible construction of some stages is considered.

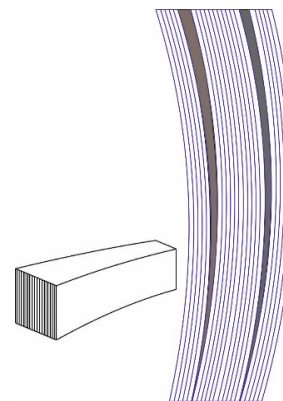
The important parts of the polarized diffractometer are polarizer and analyzer units. In order to choose the most effective way for realization of polarized neutron diffraction methods we performed a number of simulations in which we considered some different variants for the polarizer unit.

## 2. Simulations.

The numerical simulations were performed using the McStas software [4]. For the simulation of the PIK reactor source the following parameters have been used: temperature  $T=300$  K and the estimation value of the brilliance for 5<sup>th</sup> PIK channel was given by  $I_0 = 1.432 \cdot 10^{13}$  n/cm<sup>2</sup>sec·st.rad·Å, which is close the flux of thermal H2 channel of HFR ILL.



**Figure 1.** Placement of the diffractometer POLDI in the PIK main reactor hall on the 5<sup>th</sup> channel. Next to POLDI is supposed to be one more instrument.



**Figure 2.** Three-section fan-like polarizing bender.

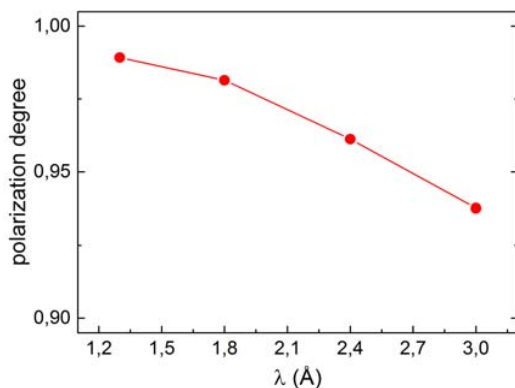
First, we made estimations of the use of a polarizing double focusing monochromator. Since the diffractometer POLDI will not be the only instrument installed on the channel, the most effective decision based on polarizing Heusler crystals  $\text{Cu}_2\text{MnAl}$  (111) is not suitable. As the main working wavelength  $\lambda$  should be  $\sim 1.3$  Å, the take-off angle for  $\text{Cu}_2\text{MnAl}$  ( $d_{111}=3.362$  Å) is very small and it will not be possible to place another instrument on the same beam. Therefore we considered polarizing focusing monochromator using FeCo single crystals ( $d = 1.771$  Å). This leads to the appropriate take-

off angle ( $\sim 43^\circ$ ), though reflection efficiency is very small – about 4%. For the calculations the following parameters of the monochromator unit were chosen:  $28 \times 6$  FeCo plates with  $10 \times 10$  mm dimensions and mosaicity  $30'$ ; vertical focusing radius – 2202 mm, horizontal one – 16348 mm. These parameters yield a flux value  $\Phi$  on the sample position equal to  $\sim 3.76 \cdot 10^5$  n/cm<sup>2</sup>sec.

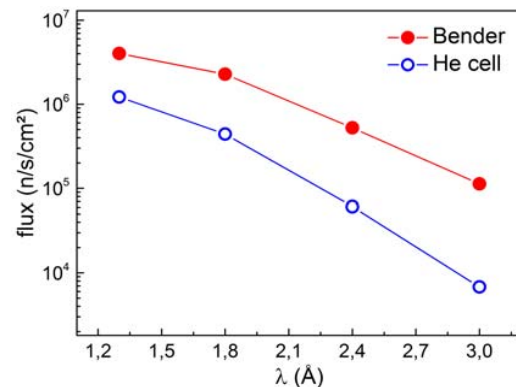
A helium cell was chosen as polarizing unit for the next step of the simulation. In this variant we use monochromator model on the base of Cu single crystals with  $d_{200}=1.807$  Å. The reflection efficiency of Cu (200) is  $\sim 50\%$ . The number of crystals and their dimensions were taken as in the previous case. Vertical focusing radius here was 3052 mm, horizontal one – 16680 mm. The parameters of the helium cell were the following: height and radius were 100 mm, helium pressure – 2.75 bar and a polarization degree of about 70%. This configuration leads for neutrons with a wavelength of 1.3 Å to a polarization degree of about 96%. In these conditions the neutron flux on the sample position was calculated to be  $\sim 12.2 \cdot 10^5$  n/cm<sup>2</sup>sec, i.e. about 3 times higher, than in the case of a FeCo monochromator. The variant with FeCo polarizer was excluded from subsequent analysis. In addition, high activation of Co gives one more drawback of this monochromator.

As an alternative decision for a  $^3\text{He}$  polarizer, we develop an idea of a compact focusing bender. The optimized construction of fan-like bender looks like the following. The bender consists of 3 sections as shown in Figure 2. The central section is divided into 26 channels. The width of each channel is 1.4 mm. The glass substrates have a thickness of about 0.3 mm and are coated with  $m=4$ . The outer sections consist of 9 channels and they are tilted about  $\pm 0.0167$  rad with respect to the central section. The curvature of each section has a radius of 54012 mm leading to a characteristic wavelength of 1.04 Å. The length of 800 mm together with the curvature of the bender guarantees that the direct flight is blocked and that the neutrons are scattered at least once in the bender.

For the simulations, the same Cu double focused monochromator was used as for the helium cell set-up. The polarization degree for 1.3 Å has a value of  $> 98\%$  and the intensity at the sample position has a value of about  $4 \times 10^6$  n/cm<sup>2</sup>sec  $\pm 1 \times 10^5$  n/cm<sup>2</sup>sec which is a factor of about 40 higher than at the FRG-1. In Figure 3 it can be seen that the polarization degree of the bender set-up is wavelength dependent. At 2.4 Å the polarization degree has a value of about 98% and drops to 94% for 3 Å. At the same time the flux decreases to  $\sim 1 \times 10^5$  n/cm<sup>2</sup>sec  $\pm 3 \times 10^3$  n/cm<sup>2</sup>sec at 3 Å, which is a result of the Gaussian distribution of the thermal flux from the source, as can be seen in figure 4.



**Figure 3.** Polarization efficiency of a fan-like polarizing bender.



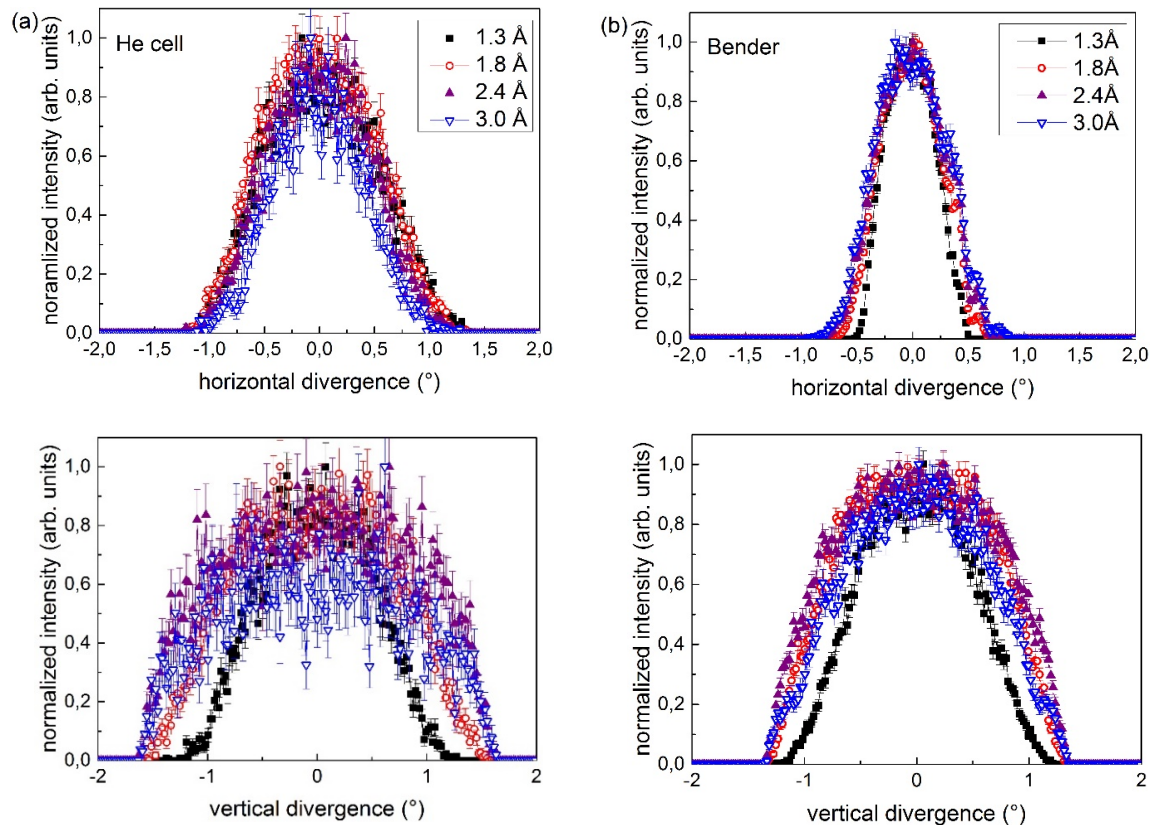
**Figure 4.** Neutron flux on the sample position for a fan-like polarizing bender and a helium cell.

Contrary to the bender set-up the polarization degree for the He-cell shows only a slight decrease of the polarization for higher wavelengths. For 3 Å the polarization degree decreases from 96% at 1.3 Å to a value of about 93%. On the another hand the intensity on the sample position at He cell set-up is  $1.22 \times 10^6$  n/cm<sup>2</sup>sec  $\pm 4 \times 10^4$  n/cm<sup>2</sup>sec at 1.3 Å, which is almost a factor 3.3 lower compared to the bender set up (see figure 4). For 3 Å, the flux decreases to  $6.79 \times 10^3$  n/cm<sup>2</sup>sec  $\pm 5 \times 10^2$  n/cm<sup>2</sup>sec, thus the ratio between intensities for the bender set-up and the helium cell increases considerably for longer wavelengths. The vertical divergences for both the He cell and the bender set-ups are approximately the same at 1.3 Å:  $\pm 0.65^\circ$ , while at higher wavelengths it grows in different ways – up to  $\pm 1.3^\circ$  at 3 Å for the He cell and to  $\pm 0.9^\circ$  for the bender. Horizontal divergence for the bender set-up

significantly better than for the He-cell beginning from 1.3 Å, where it has a value of  $\pm 0.32^\circ$  against  $\pm 0.44^\circ$  (Figure 5).

### 3. Conclusion

The instrument layout of POLDI at the PIK reactor with a polarizing bender was compared to that of a He cell. The simulation demonstrates that bender set-up has higher flux at the sample position for a wavelength range from 1.3 Å to 3 Å and lower divergence distribution. For the bender set-up, is found that the polarization degree depends on the wavelength. For short wavelengths a polarization degree better than



**Figure 5.** Horizontal and vertical divergences for different wavelengths for (a) helium cell set-up and (b) fan-like polarizing bender set-up.

98% can be reached, which drops for longer wavelengths down to about 94% for 3 Å. The polarizing He-cell on the other hand shows only a slight change of the polarization with the wavelength, here, the polarization degree decreases from 96% to only 93% for 1.3 Å and 3 Å, respectively. The higher flux at the sample position, a factor of at least 3.3, with lower divergence and still good polarization degree of above 93% makes the bender set-up favorable over the layout with the He-cell. The He-gas has to be polarized from time to time; consequently, the polarization degree is time dependent. It should be emphasized also that a bender acts as a  $\lambda/2$  filter which gives one more benefit. Finally yet importantly, it can be noted that the bender set-up needs less service efforts.

### Acknowledgment

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