Beam transport and polarization at TOPAS, the thermal time-of-flight spectrometer with polarization analysis

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Abstract. We present the design for the polarization analysis of the future thermal time-of-flight spectrometer at the Juelich Centre for Neutron Science (JCNS) at the FRM II. TOPAS is a time-of-flight spectrometer covering a range of incident energies $20 \text{ meV} < E_i < 160 \text{ meV}$ and an angular range $-3^\circ < 2\theta < 150^\circ$. A set of Fermi choppers selects the incoming energy $E_i$ with a resolution up to 3%. The instrument is optimized for a high flux on small samples using an elliptical neutron guide. The special feature of TOPAS is the polarization analysis. The incident polarization will be realized by means of a $^3\text{He}$ continuously pumped polarizer, which is a downscaled version of the device developed for small angle applications at JCNS. The polarization analysis over a wide angular range demands either short distances between the sample and the analyzer or a large volume of polarized $^3\text{He}$. Here we propose the latter alternative to allow the study of magnetic samples and modest magnetic fields at the sample position.

1. Introduction
Time-of-flight spectrometers have traditionally been used to study incoherent and/or dispersionless scattering processes, such as vibrational density of states (VDOS), crystal field excitations or molecular dynamics. However, with the advent of Megawatt spallation sources and large pixelized detectors, they provide an excellent tool to map coherent excitation in novel single crystalline materials with a modest momentum resolution. TOPAS will be a reactor-based TOF spectrometer that runs at high repetition rates to compensate for the lower pulsed flux at continuous sources compared to the high peak flux of spallation instruments. Particularly for thermal neutrons with comparatively large velocities, the time frames can be rather short. Accordingly all distances have been chosen: The sample to detector distance will be to 2.5m. A system of two Fermi Choppers FC1 and FC2, placed at a distance of 5 m, will select the incoming energies. Unwanted energies will be removed by a higher order removal chopper. The chopper FC2 will spin with up to 36000 revolutions per minute (rpm). Due to a larger neutron window, the chopper FC1 will be limited to a speed of 27000 rpm which determines the maximum repetition rate $\nu_{\text{max}} = 900 \text{ Hz}$. Frame overlap that might be significant particularly for low incoming energies can be avoided running FC1 at half the frequency of FC2. The rather short distances between the monochromatizing choppers and the detector bank yield an energy resolution that can be tuned from 3 % to 10%. The distance between the sample position and
the biological shielding of the FRM II and hence the neutron guide length will be approximately 49 m. An elliptical neutron guide will focus neutrons into a small beam spot, giving a high flux over an area 1x4 cm$^2$.

So far polarization analysis has been applied in inelastic experiments nearly exclusively on triple axis spectrometers. Thinking of coherent magnetic excitations in particular in correlated electron systems, polarization analysis comes also in the focus of ToF spectrometers. The application requires once more a high flux, as the polarization devices reduce the flux at least by a factor 2.

2. Neutron guide design
The neutron guide design is guided by three requirements

(i) Focus a high intensity onto a small sample spot.
(ii) Generate a uniform divergence distribution.
(iii) Prevent the direct sight onto the reactor core.

Following the proposal of Schanzer et al. [1], we have investigated different guide geometries. It turns out, that an elliptic guide becomes a better choice than parabolic or linearly tapered guides, when the length of the neutron guide becomes larger than 40 m. This can be understood considering that in geometric optics the ellipse images the source into the image by only one reflection. However, in the case of a neutron guide, one does not image a point source. Therefore the elliptical guide shape is not obvious. Numerical optimization of different guide shapes (including a free variation of guide segments optimizing the flux) yielded the highest flux for the ‘free’ guide. However, the elliptical shape with virtual foci that are slightly different from the flux maximum and the sample position, gives nearly the same flux and a more homogeneous divergence distribution. In particular, closing the entrance and exit windows of the neutron guide improves the divergence distribution. The shape of the resulting guide is given in Fig. 1 showing the horizontal and vertical direction, respectively. The entrance and exit window cover only $\frac{1}{3}$ of the area in the center of the guide. Hence the direct sight onto the reactor core can be prevented easily by placing a beamstop there as indicated in Fig. 1. Fig. 2 a) shows, that the flux at the sample position is reduced by 5% only with the addition of the beamstop. The design of such a beamstop is guided by the requirements to moderate fast neutrons, to absorb the neutrons and to absorb the gamma radiation. Finally we discuss the divergence distribution at the sample position. Fig. 2 b) shows the homogeneous distribution. It has a single maximum and a trapezoidal shape. The width of 1.0 to 1.5° (FWHM) depending on the wavelength matches the contributions from the sample size and detector pixel size to the angular resolution. It provides also short opening and closing times of the wavelength selecting Fermi choppers.

3. Polarizer
To polarize the thermal neutrons we have chosen polarized $^3$He neutron spin filter (NSF) cells. The use of 140 meV neutrons ($\lambda = 0.76$ Å) along with other factors including beam divergence demands the utilization of NSF over supermirror polarizers or Heussler crystals especially given the current attainable levels of $^3$He polarization of 70% or more. A discussion of the factors involved in such a comparison are given in ref [2].

The polarizer concept for TOPAS is based on the polarization analyzers for the small angle applications at instruments KWS1 and MARIA from JCNS. The demands for the different applications share major components and designs. The analyzer applications on MARIA and KWS1 will require very large cells optimized for comparatively low neutron energy from the cold moderator. For TOPAS the beam dimension at the end of the elliptical neutron guide requires an 8 cm diameter cell, whereas the analyzer systems are being designed to accept cells of 14-16
Figure 1. 3d model of the primary and secondary spectrometer. The neutron energy is selected by the phase between the Fermi choppers FC1 and FC2. The disc chopper suppresses neutron velocities that could also pass through the Fermi choppers.

Figure 2. Horizontal and vertical guide shape. At the centre of the ellipse (Position = 25 m) an 1.8x4.5 cm$^2$ beamstop will block the direct sight.

cm in total height. Therefore TOPAS will use a downsized version of the continuously optically pumped analyzer being prototyped and tested for those applications. It will have a very similar format to the polarizer of\cite{3, 4} with somewhat smaller dimensions. A scheme of the polarizer concept is shown in Fig. 4. However the high energy of the TOPAS beam will require the cells to contain 20-30 bar cm of $^3$He leading to a cell of 10 to 15 cm long at 2 bar (absolute) pressure.
Figure 3. Comparison of flux a) and divergence b) at sample position with and without beamstop at the centre of the double elliptic neutron guide.

Figure 4. a) Block diagram of configuration of the SEOP system for online polarization.

We note these estimates of required cell opacity \( (i.e. {^3}\text{He pressure times neutron wavelength times cell length}) \) are based on the analysis given in [5].

The cell will be polarized \textit{in situ} because this will provide a higher time averaged figure of merit compared to \(^3\text{He} \) gas polarized remotely. Off-line polarized gas undergoes \( T_1 \) nuclear spin relaxation, and thus loss of polarizing efficiency and neutron transmission over time. Consequently the cell must be replaced leading to an interruption of measurement time for the procedure and the required instrument calibration for the new cell filling. Fig. 5 shows \( \Theta(t) \), the square root of the time integrated figure of merit, or \( P^2 T \) for three conditions, steady \(^3\text{He} \) polarization of 70\%, a cell with 70\% initial polarization decaying with a 100 hour polarization decay time constant, and a cell with 70\% initial polarization and a 100 hour polarization decay time constant refilled or replaced each day. \( \Theta(t) \) is the obtained data quality where the figure of merit can be thought of as the number of usable neutrons, thus \( \Theta(t)^{-1} \) would be proportional to the measurement error assuming counting statistics. To obtain a given level of data quality for
Figure 5. Comparison of three cases for use of $^3$He NSF as a polarizer. The value plotted is the data quality $\Theta(t)$. We defined $\Theta(t)$ as the square root of the time integrated figure-of-merit or $P^2T$ of the $^3$He polarizer cell ($P$: Polarisation, $T$: transmission of the cell). $\Theta(t)^{-1}$ is hence proportional to the measurement error assuming counting statistics. The grey line indicates the obtained quality vs time for a cell initially polarized to 70% and allowed to decay assuming a typical 100 hour on-beam relaxation time for the NSF. The blue line shows the improvement obtained by refreshing the polarization daily accounting for a pause of one hour to change the cell and perform a calibration. The red line indicates the performance for constant $^3$He polarization of 70% maintained by in situ polarization.

a device using an in-situ polarized NSF with equal initial values of $^3$He polarization, 70% in this case, about 20-25% less counting time is required for a continuously polarized NSF compared to an off line polarized cell undergoing $T_1$ polarization decay for an experiment with a 1-2 day measuring time where we have assumed an on beam $T_1 = 100$ h.

The device will be placed just upstream the second Fermi chopper; as it is expected polarization can be maintained through the Fermi chopper if care is taken to insure an adequate guide field inside the device and eliminate sources of neutron depolarizing eddy currents [6]. Another feature of NSF is the ability to reverse the $^3$He neutron polarizing power through adiabatic fast passage (AFP), thus no extra flipper will be required [7].

4. Analyzer

The polarization analyzer will have much more rigorous demands as it will require a similar thickness of $^3$He, but over at least a significant fraction of the TOPAS detectors. The $^3$He is foreseen to be polarized off-line because of these challenges. Novel techniques for in-situ polarization are being considered but will not be discussed here. It is also foreseen that prototyping/testing of systems similar in philosophy to the “PASTIS” concept [8] will be conducted at DNS at the JCNS [9] as an intermediate stage for a full scale TOPAS analyzer.

Here we will consider simply the ‘brute force’ method to obtain polarization analysis for TOPAS. For the brute-force method to cover the entire detector with a large container, or array of containers is not out of the question. This container would need approximately 100 bar L of polarized $^3$He per day. While this number is beyond the production capacity of systems currently available to neutron research centers, researchers are prototyping systems with this daily capacity [10]. Further single MEOP systems have capacities of 20 bar L per day [11] and single SEOP systems similar to the ones we are using in the in-situ polarizers, have been shown to produce over 2.5 bar liter per day when used in the laboratory [12]. Thus it is possible to obtain partial coverage starting with one or several of these smaller systems and scale up to full detector coverage via additional systems. AFP inversion of the $^3$He gas can be performed in the polarizers to reverse the analyzing efficiency of the NSF eliminating the need to develop a wide angle, large area spin flipper.
5. Conclusion
We have presented the neutron guide and polarization analysis concept for TOPAS. A high flux, which is a pre-requisite for single crystal studies or application of polarization analysis, is realized by a focusing neutron guide. A continuously pumped $^3$He polarizer provides the best performance for experiment lasting for several days, as it is anticipated for inelastic experiments. For the polarization analysis it is crucial to have $^3$He system with a large capacity $\approx 100$ bar L per day, if the polarization analysis has to be spatially displaced from the sample position and covers still a large fraction of the solid angle.

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