

# ESTIA Polariseres and Analyser

## 1 Introduction

This document discusses the design of the polariseres and the analyser for the ESTIA instrument. The Virtual Source (VS), a system of 2 L-shaped slits, defines the beam image to be projected onto the sample by the Selene guide system, consisting of two guides with opposite elliptical shape. The first Selene guide, Selene 1, has VS and the Middle Focus (MF) as focal points, whereas the second Selene guide, Selene 2, has MF and the sample as focal points.

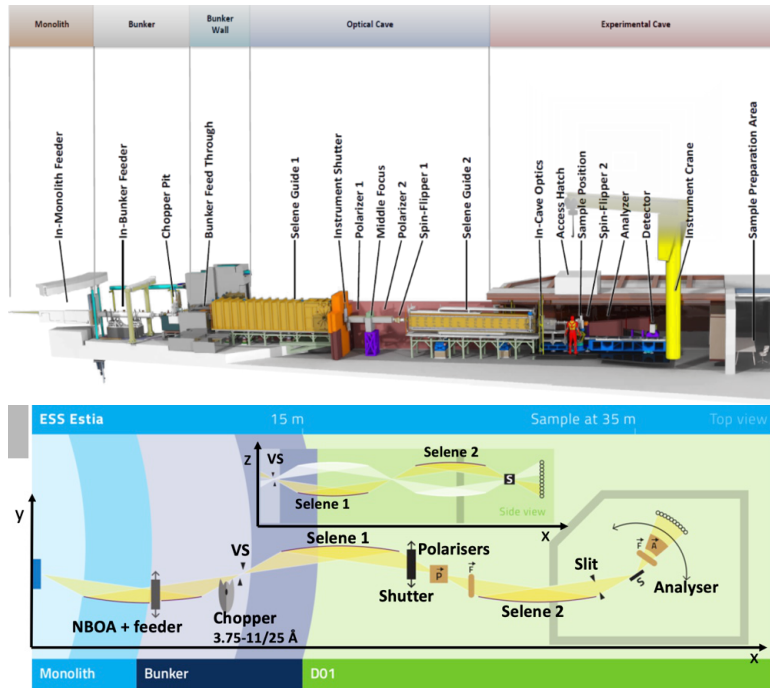


Figure 1: Overview of the ESTIA instrument (top). Projection of the beam path across the instrument in the y-x plan and z-x plan (bottom).

ESTIA can be operated with or without a polarised neutron beam. MF is the most convenient location for the polarisers as i) sufficient space is available; ii) it is located after the instrument shutter, and, therefore, is accessible for maintenance even when the proton beam is on. Each polariser is a Si-wafer with Fe/Si coating ( $m=5/m=5.5$ ). Transmission of the beam through two consecutive polarisers produces a beam polarisation  $> 98\%$  (according to data provided by Swiss Neutronics AG). In order for the beam to be spin-polarised, a vertical (along z-direction) magnetic field is required. This will be provided by a guide field mounted around the polarisers. The beam transmitted by the polarisers will have spin-polarisation "down" with respect to the vertical direction of the magnetic field. A spin-flipper located before the entrance of Selene 2 will enable the option of using spin-polarisation "up" or "down". A guide field is mounted inside the Selene 2 and until the sample to preserve the beam polarisation. Finally, after the sample an analyser is mounted inside the detector arm to enable the analysis of the spin-component of the beam reflected by the sample. The analyser is also a Si-wafer with Fe/Si coating ( $m=5/m=5.5$ ).

Both the polarisers and the analysers are mounted on a motorised support which enables alignment with respect to the beam and their positing in or outside of the beam. This way, the option for polarised neutrons and spin-analysis can easily be selected.

The polarisers not only produce a spin-polarised beam but act also as frame overlap mirrors. When the polarised beam is not required, a frame overlap mirror mounted on the same motorised support as the polarisers is placed in the beam. The frame overlap is a Ni-coated Si wafer. Details on the design of the frame overlap shape are described in this document as well.

Two different scenarios are described and compared for the polarisers: 1) the polarisers are symmetrically located before and after the MF point; 2) the polarisers are both located before the MF point. Scenario 1 is the design originally proposed, whereas Scenario 2 is an alternative solution offering comparable performances, but much simpler mechanical design, easier use during instrument operation (the two polarisers have a fixed position with respect to each other and are simultaneously moved with respect to the beam), as well as lower costs.

The results discussed in this document are based on calculation of the path of rays generated at VS, reflected on the Selene guides, and transmitted/reflected first at the polarisers and later at the analyser. Such calculations allow a fast comparison between different location and shape of the polarisers and analyser. The shape and location of the polarisers is optimised for two different horizontal opening of VS, i.e. 1.5 mm and 5 mm.

VS=1.5 mm is the largest opening relevant for standard polarised neutron reflectometry (PNR) experiments on ESTIA, where the sample area to be illuminated is expected to be  $1\text{cm}^2$ . VS=5 mm could be relevant for experiments where it is required to illuminate a larger sample area. This latter is expected to be a less used instrument configuration for PNR measurements with high beam polarisation compared to VS=1.5mm.

McStas simulations, currently in progress, will provide additional information on the performances of the optimised design of the polarisers/analyser described here.

## 2 Abbreviations

VS= Virtual Source

MF=Middle Focus

$\gamma$ = ideal angle of incidence on the polarisers/analyser

$\Delta\gamma$ = deviation of actual angle of incidence from  $\gamma$

pol1=polariser 1

pol2=polariser 2

FOM=frame overlap mirror

## 3 Fixed parameters

VS-MF distance = 12 m

Ellipse parameters:  $b=104.7$  and  $c=6000.9134$  (both Selene 1 and Selene 2)

VS horizontal opening = [5mm, 1.5 mm]

VS vertical opening = [10 mm]

wavelength range = 3.75-20 Å;

coating  $m=5$

$q_{cmax}=0.109 \text{ \AA}^{-1}$  (according to Swiss Neutronics AG reference plot)  $q_{cmin}=0.0165 \text{ \AA}^{-1}$  (according to Swiss Neutronics reference plot)

## 4 Polarisers and FOM

### 4.1 Scenario 1: polarisers separated at MF

Figure 2 (top) shows the y-x projection of the beam: i) generated at VS=5mm (x=0) ii) reflected by the elliptical Selene 1, iii) transmitted by the first polariser (Pol1), iv) refocused at MF, transmitted by the second polariser (Pol2), v) reflected by the elliptical Selene 2; vi) refocused at the sample; vii); hitting the detector. The location of the polarisers (Figure 2, bottom) is such to maximise their distance from MF without exceeding the space available.

Both Pol1 and Pol2 have the same logarithmic spiral shape calculated according to equation 1 and 2 with  $b = 1/\tan(\gamma)$  and  $\gamma = 1.65^\circ$ . The parameters for Pol1 and Pol2 shape/location are summarised in Table 1.

$$x = ae^{(-b\Theta_2)}\cos(\Theta_2) \quad (1)$$

$$y = ae^{(-b\Theta_2)}\sin(\Theta_2) \quad (2)$$

$$b = \frac{1}{\gamma} \quad (3)$$

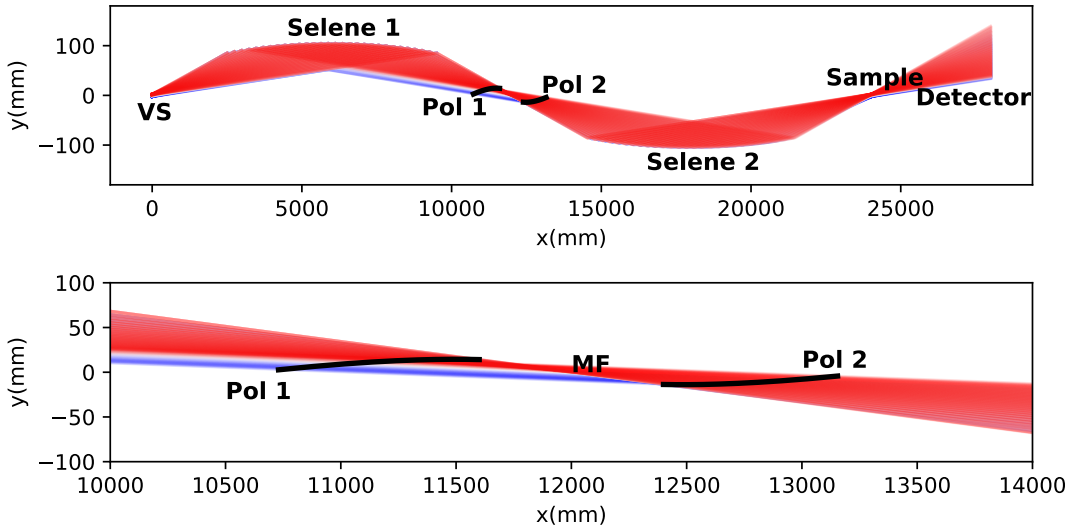


Figure 2: Projection in the x-y plane of the beam path (top). Neutrons generated at VS (horizontal opening = 5mm) are i) reflected by Selene 1; ii) transmitted by Pol 1; iii) refocused at MF, iv) transmitted by Pol 2; v) reflected by Selene 2; vi) refocused at the sample position, vii) revealed by the detector. Zoom on the polarisers and MF (bottom). The rays are coloured from blue to red starting from the bottom to the top of VS.

Table 1: Polariseres separated at MF. Pol1 and Pol2 both have logarithmic spiral shape. Their location along x is expressed as distance from the MF. The reported interval corresponds to the space occupied by the polariseres along x.

Parameters	Pol 1	Pol2
$\gamma$	1.65	1.65
length (mm)	870	870
x-position with respect to MF (mm)	365-1198	365-1158

In an ideal case, i.e. the virtual source is a point source, all neutrons would have an angle of incidence at the polariseres equal to  $\gamma$ . On the other hand, the horizontal opening of VS produces a range of angles of incidence at the polariseres that is reported as  $\Delta\gamma$ , i.e. the difference between the actual angle of incidence and  $\gamma$ . Given the  $m=5$  coating of both polariseres,  $\Delta\gamma$  cannot exceed  $0.3^\circ$ , as larger  $\Delta\gamma$  would reduce the overall beam polarisation.

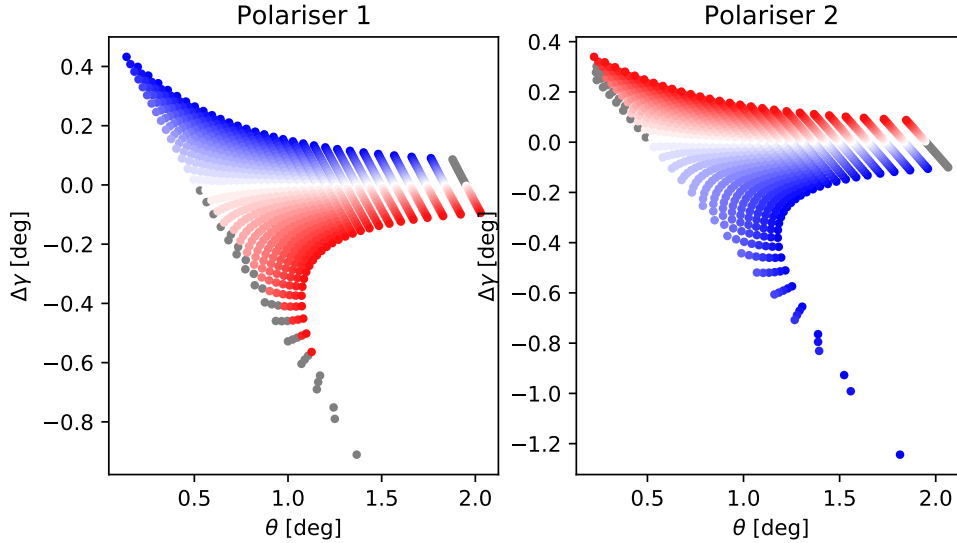


Figure 3:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ). Datapoints coloured from blue to red indicate the rays starting from bottom to top of the VS (5 mm). Datapoints in grey represent rays that are not going to enter the Selene 2 and therefore will not reach the sample position.

In principle, by increasing the distance between MF and the polariseres, the corresponding  $\Delta\gamma$  values can be minimised. However, because of space limitations imposed by the

other instrument components, Pol1 cannot be placed further away from MF. Pol2 was placed at the same distance from MF as Pol1.

Figure 3 shows the calculated  $\Delta\gamma$  for Pol 1 and Pol2, respectively, as a function of the azimuth angle ( $\Theta$ ). The largest  $\Delta\gamma$  for both Pol1 and Pol2 is larger than  $0.3^\circ$  and therefore a polarisation  $< 98\%$  is expected when VS= 5 mm.

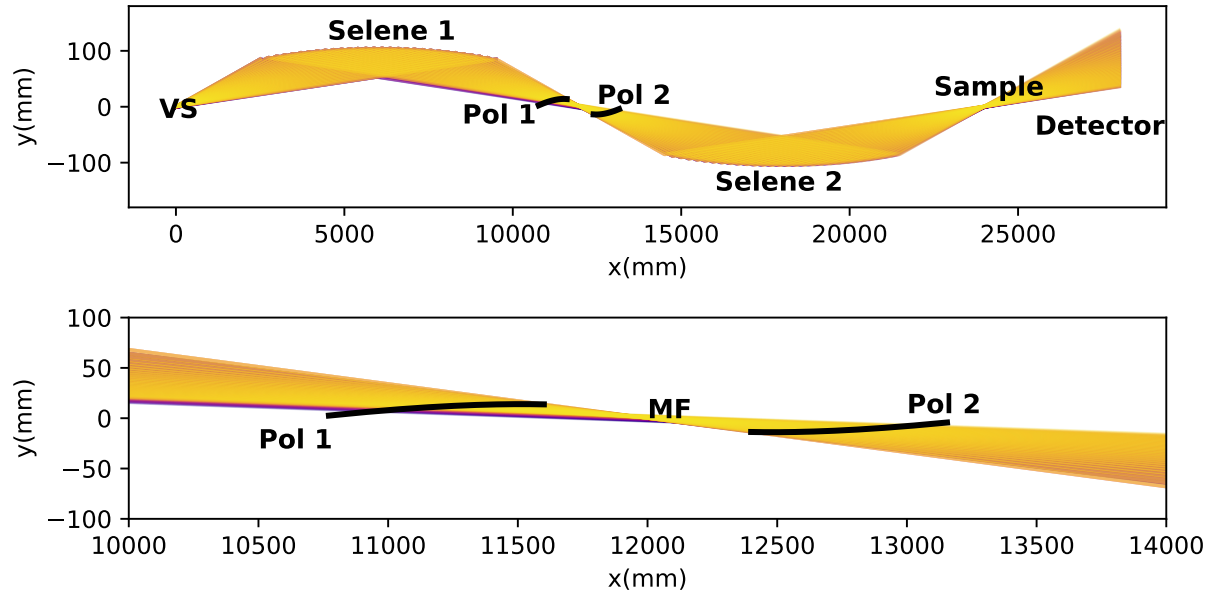


Figure 4: Projection in the x-y plane of the beam path (top). Neutrons generated at VS (horizontal opening = 1.5 mm) are i) reflected by Selene 1; ii) transmitted by Pol 1; iii) refocused at MF, iv) transmitted by Pol 2; v) reflected by Selene 2; vi) refocused at the sample position, vii) revealed by the detector. Zoom on the polarisers and MF (bottom). The rays are coloured from purple to yellow starting from the bottom to the top of VS.

Figure 4 and 5 show the same plots as in Figure 2 and 3, but for VS = 1.5 mm. In this case, only the top part of the Pol 1 and the bottom part of Pol 2 are illuminated by the beam and in both cases the corresponding  $\Delta\gamma$  values are within the maximum limit.

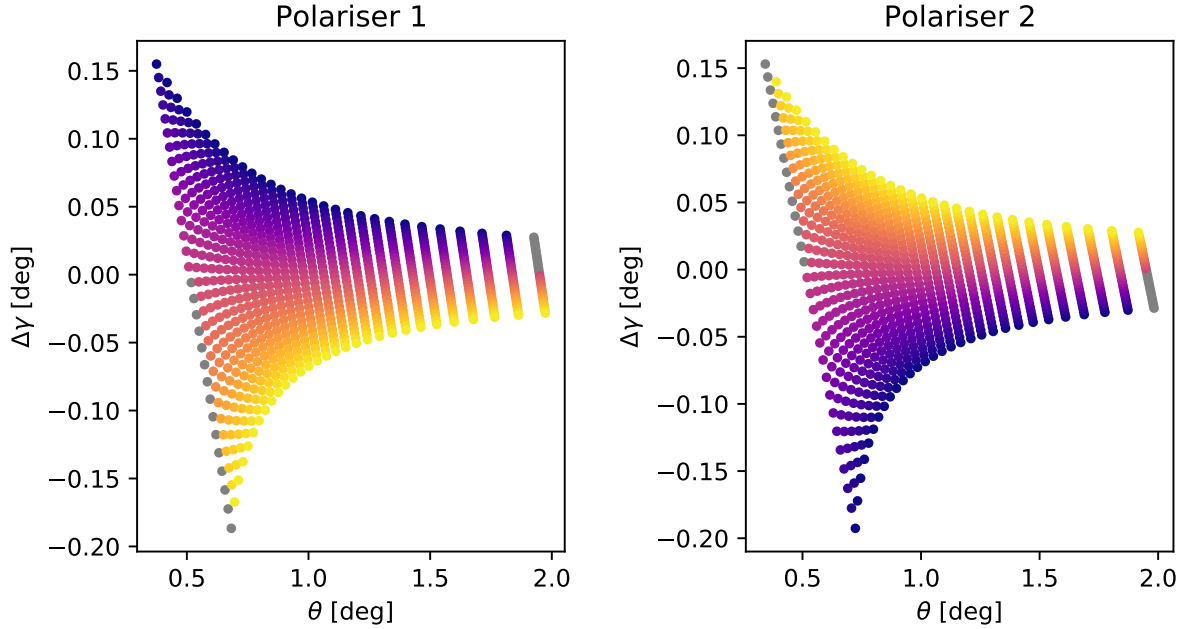


Figure 5:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ). Datapoints coloured from purple to yellow indicate the rays starting from bottom to top of the VS (1.5 mm). Datapoints in grey represent rays that are not going to enter the Selene guide 2 and therefore will not reach the sample position.

Figure 6 shows the plots corresponding to Pol 1 with V-shape and Pol 2 with logarithmic spiral shape. The V-shape of Pol1 enables to reduce the overall polariser size, which consequently can be placed further away from MF. The V-shape involves a top segment with logarithmic spiral shape followed by a linear segment (Table 2). Pol 2 has the same shape as the top part of Pol 1 (i.e. logarithmic spiral with  $\gamma = 1.65^\circ$ ). A V-shape also in case of Pol 2 is not optimal as multiple reflections between the spiral and linear segment will reduce the beam polarisation and potentially attenuate the beam. On the other hand, in case of Pol 1, no multiple reflections are expected.

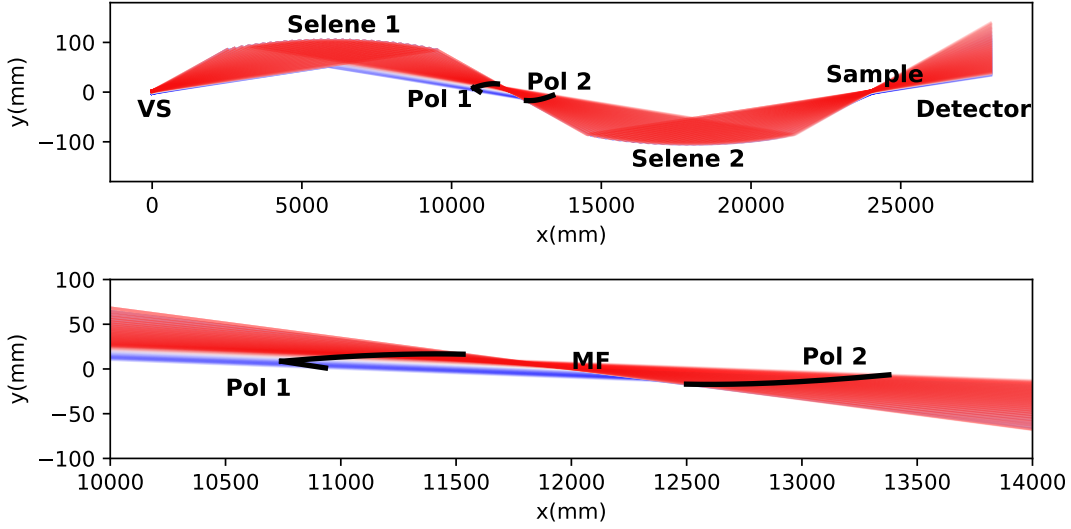


Figure 6: Projection in the x-y plane of the beam path (top). Neutrons generated at VS (horizontal opening = 5mm) are i) reflected by Selene 1; ii) transmitted by Pol 1 (V-shape); iii) refocused at MF, iv) transmitted by Pol 2; v) reflected by Selene 2; vi) refocused at the sample position, vii) revealed by the detector. Zoom on the polarisers and MF (bottom). The rays are coloured from blue to red starting from the bottom to the top of VS

Table 2: Polarisers separated at MF. Pol1 (V-shape) and Pol2 (logarithmic spiral shape) location along x is expressed as distance from the MF. The reported interval corresponds to the space occupied by the polarisers along x.

Parameters	Pol 1	Pol2
$\gamma$	1.65	1.65
length (mm)	788(spiral); 191(linear)	878
x-position spiral (mm)	469-1257	499-1377
x-position linear (mm)	1257-1066	–

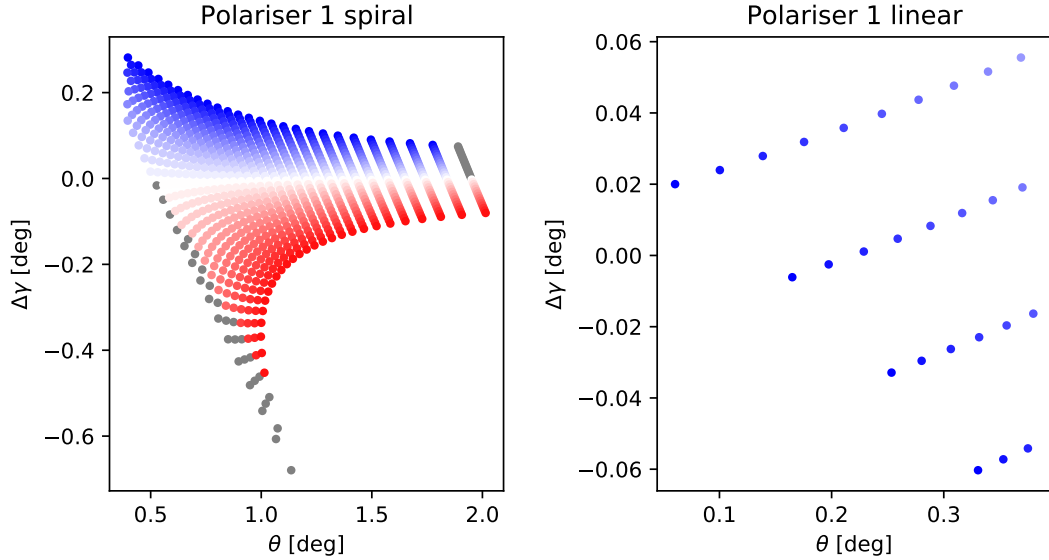


Figure 7:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ). Datapoints coloured from blue to red indicate the rays starting from bottom to top of the VS (5 mm). Datapoints in grey represent rays that are not going to enter the Selene guide 2 and therefore will not reach the sample position.

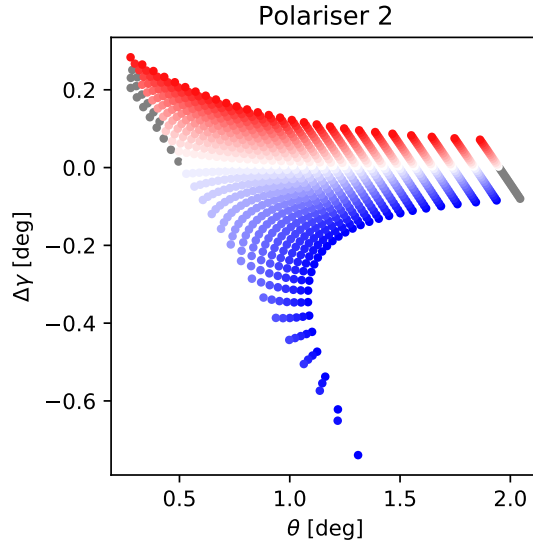


Figure 8:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ). Datapoints coloured from blue to red indicate the rays starting from bottom to top of the VS (5 mm), respectively. Datapoints in grey represent rays that are not going to enter the Selene guide 2 and therefore will not reach the sample position.

Figure 7 shows the  $\Delta\gamma$  values calculated for the logarithmic spiral (left) and linear (right) segment of Pol 1, when  $VS = 5\text{mm}$ . Placing Pol 1 at 469 mm from MF reduced the largest  $\Delta\gamma$ . However, being the  $\Delta\gamma$  approximately  $0.28^\circ$ , only very limited mechanical tolerance is left for the actual construction and assembly of the polariser, i.e. approximately  $0.01^\circ$ . On the other hand, the  $\Delta\gamma$  for the linear section of Pol 1 is well within the maximum  $\Delta\gamma$  of  $0.3^\circ$ . As for Pol 1, very limited tolerance is left for the actual construction and assembly of Pol2, i.e. approximately  $0.01^\circ$  (Figure 8). Altogether, the largest  $\Delta\gamma$  for Pol1 and Pol2 are too close the maximum limit to expect a beam polarisation  $> 98\%$  from the finally assembled system when  $VS= 5\text{mm}$ .

As shown in Figure 9, with  $VS = 1.5\text{ mm}$  only the logarithmic spiral segment of Pol 1 is illuminated by the beam. Figure 10 shows the  $\Delta\gamma$  values for Pol 1 and Pol 2 with  $VS = 1.5$ , which are considerably reduced compared to  $VS = 5\text{ mm}$  and well within the maximum  $\Delta\gamma$  value.

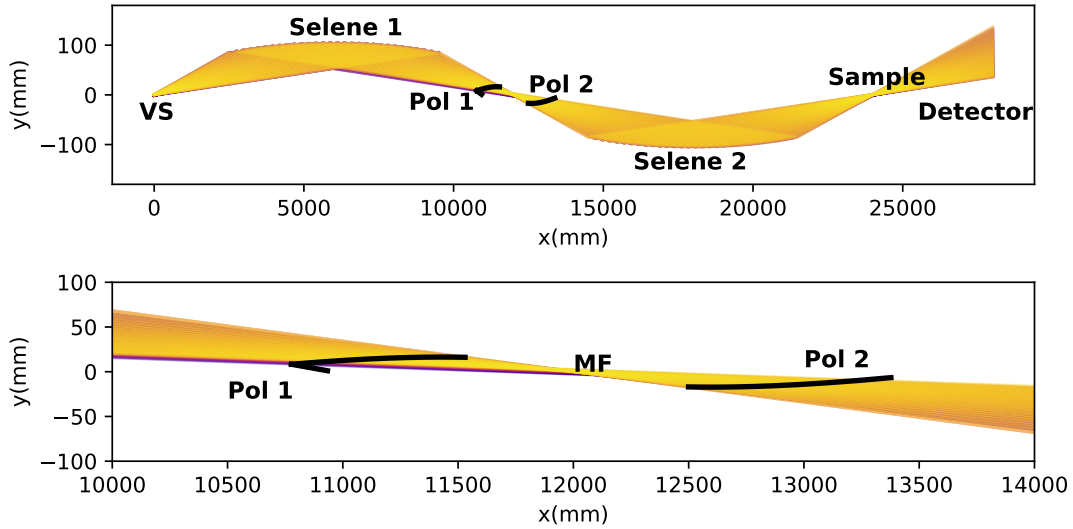


Figure 9: Projection in the x-y plane of the beam path (top). Neutrons generated at VS (horizontal opening = 1.5 mm) are i) reflected by Selene 1; ii) transmitted by Pol 1 (V-shape); iii) refocused at MF, iv) transmitted by Pol 2; v) reflected by Selene 2; vi) refocused at the sample position, vii) revealed by the detector. Zoom on the polarisers and MF (bottom). The rays are coloured from purple to yellow starting from the bottom to the top of VS.

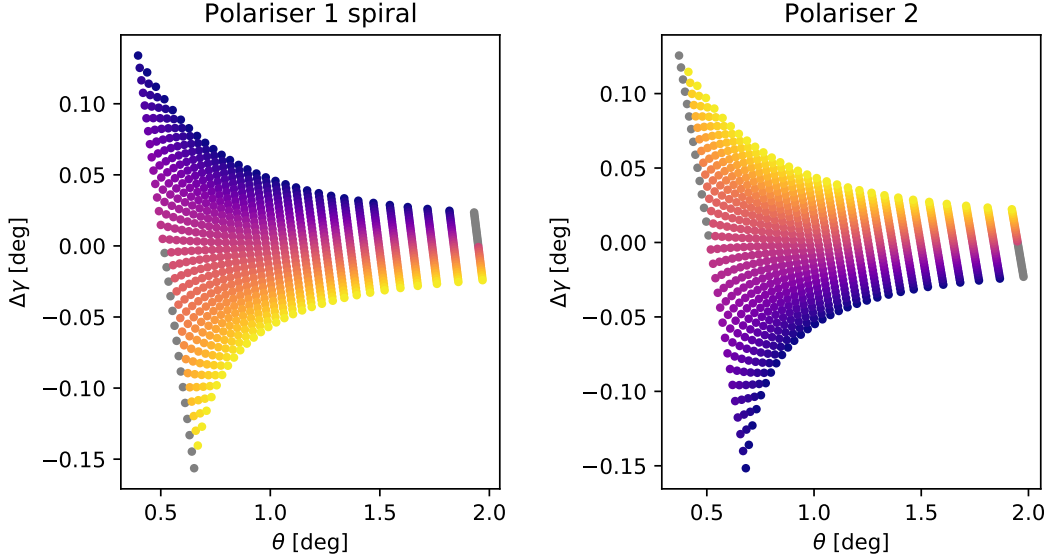


Figure 10:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ). Datapoints coloured from purple to yellow indicate the rays starting from bottom to top of the VS (5 mm). Datapoints in grey represent rays that are not going to enter the Selene guide 2 and therefore will not reach the sample position.

## 4.2 Scenario 2: Polarisers with V-shape and before the MF

Figure 11 shows Pol 1 and Pol 2 both with V-shape, i.e. logarithmic spiral segment followed by a linear segment with negative slope, and both placed before the MF. The proposed location (Figure 11 and Table 3) of Pol1 and Pol2 was designed to use all the available space between the MF and Selene 1, and at the same time to maximise the distance between Pol1 and MF, which reduces the  $\Delta\gamma$ .

Table 3: Polarisers before MF. Pol1 and Pol2 both have V-shape. Their location along x is expressed as distance from the MF. The reported interval corresponds to the space occupied by the polarisers along x.

Parameters	Pol 1	Pol2
$\gamma$	1.65	1.7
length (mm)	642(spiral); 195(linear)	785(spiral); 192(linear)
x-position spiral (mm)	365-1007	500-1285
x-position linear (mm)	1007-812	1285-1093

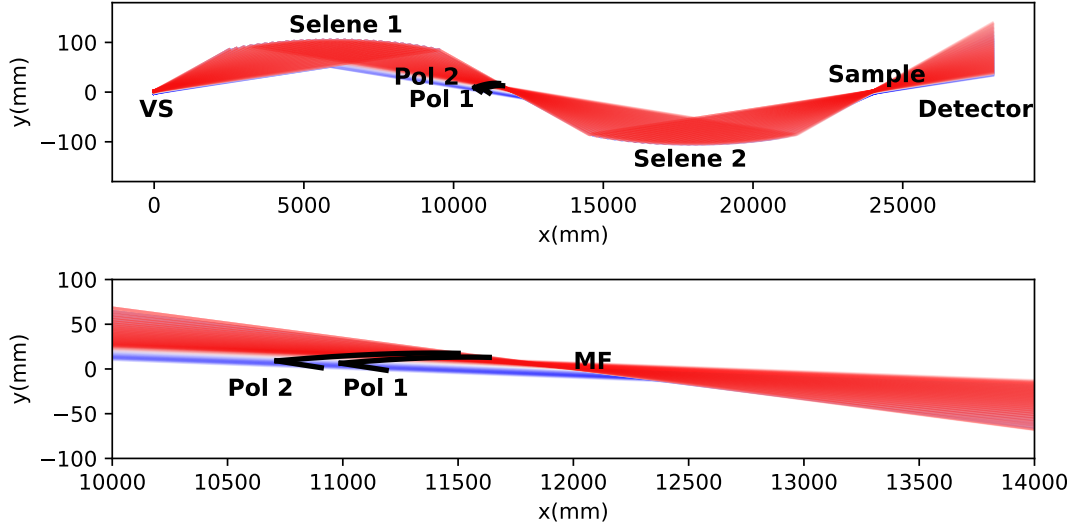


Figure 11: Projection in the x-y plane of the beam path (top). Neutrons generated at VS (horizontal opening = 5 mm) are i) reflected by Selene 1; ii) transmitted by Pol 2 (V-shape); iii) transmitted by Pol 1 (V-shape); iv) refocused at MF ; v) reflected by Selene 2; vi) refocused at the sample position, vii) revealed by the detector. Zoom on the polarisers and MF (bottom). The rays are coloured from blue to red starting from the bottom to the top of VS.

Figure 12 and 13, show the  $\Delta\gamma$  values for Pol 1 and Pol 2. The largest  $\Delta\gamma$  is approximately  $0.31^\circ$  for Pol 1 and  $0.26^\circ$  for Pol 2. For Pol 1 this is slightly above the maximum limit value of  $0.3^\circ$ . Therefore, as for scenario 1, when VS = 5 mm the polarisation of the beam is expected to be lower than for VS = 1.5 mm.

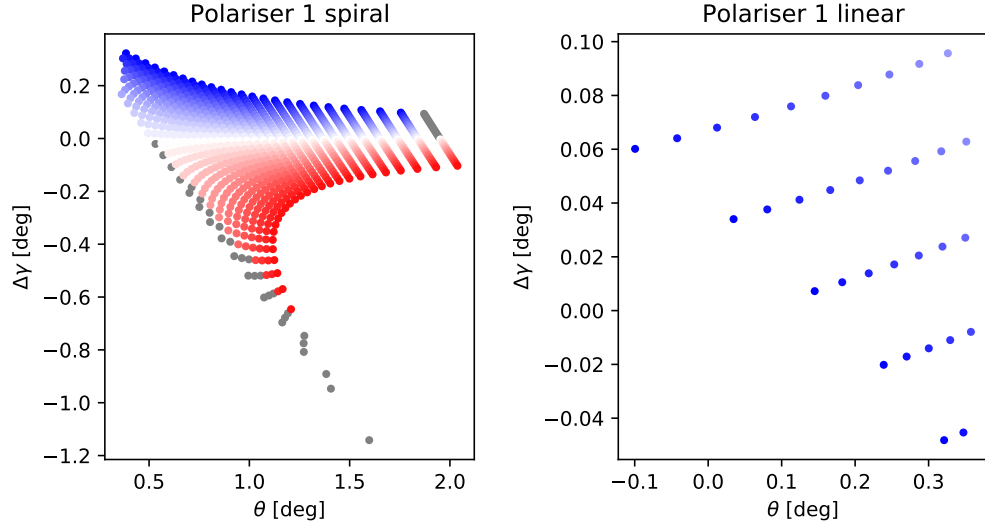


Figure 12:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ) for Pol 1. Datapoints coloured from blue to red indicate the rays starting from bottom to top of the VS (5 mm). Datapoints in grey represent rays not entering the Selene 2 and therefore will not reach the sample position.

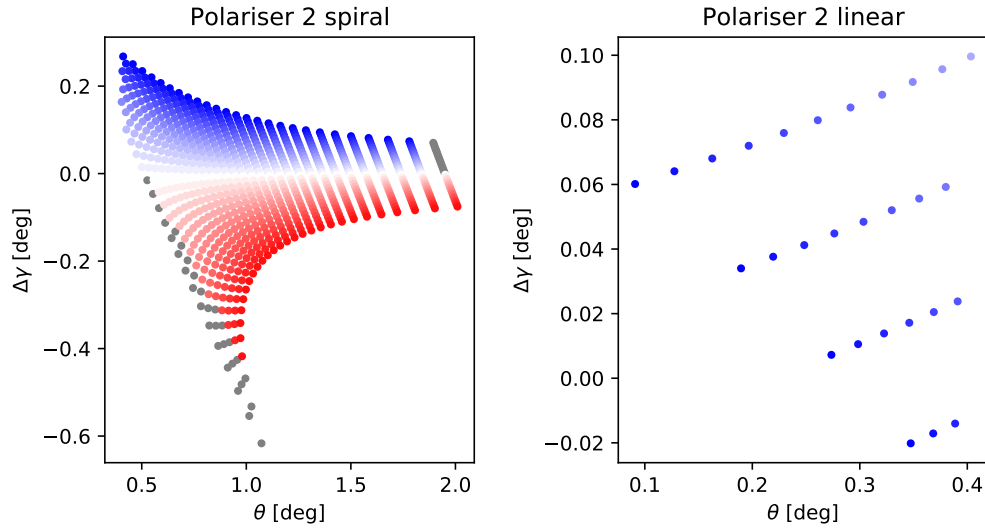


Figure 13:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ) for Pol 2. Datapoints coloured from blue to red indicate the rays starting from bottom to top of the VS (5 mm). Datapoints in grey represent rays not entering the Selene 2 and therefore will not reach the sample position.

Figure 14 and 15 shows the results for  $VS = 1.5$  mm. In this configuration only the top section of the polarisers, with logarithmic spiral shape, is illuminated by the beam. The  $\Delta\gamma$  values are similar to those reported for scenario 1 with  $VS = 1.5$  mm, i.e. the values are within the maximum  $\Delta\gamma$  of  $0.3^\circ$  and leave about  $0.15^\circ$  of tolerance for the construction and assembly of the polarisers.

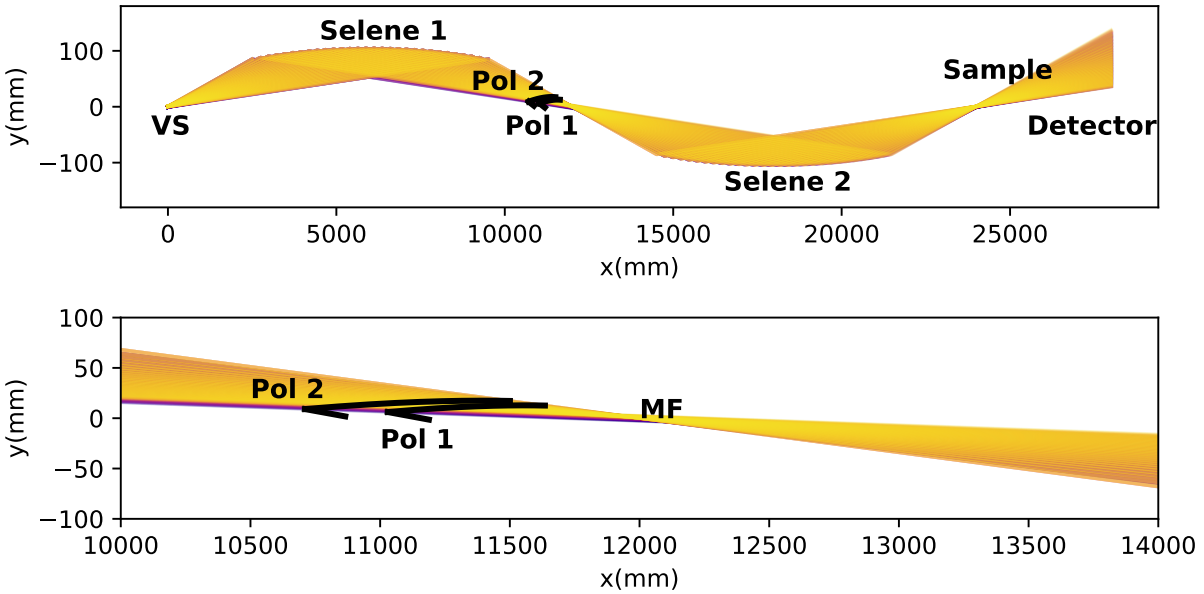


Figure 14: Projection in the x-y plane of the beam path (top). Neutrons generated at VS (horizontal opening = 1.5 mm) are i) reflected by Selene 1; ii) transmitted by Pol 2 (V-shape); iii) transmitted by Pol 1 (V-shape); iv) refocused at MF ; v) reflected by Selene 2; vi) refocused at the sample position, vii) revealed by the detector. Zoom on the polarisers and MF (bottom). The rays are coloured from purple to yellow starting from the bottom to the top of VS.

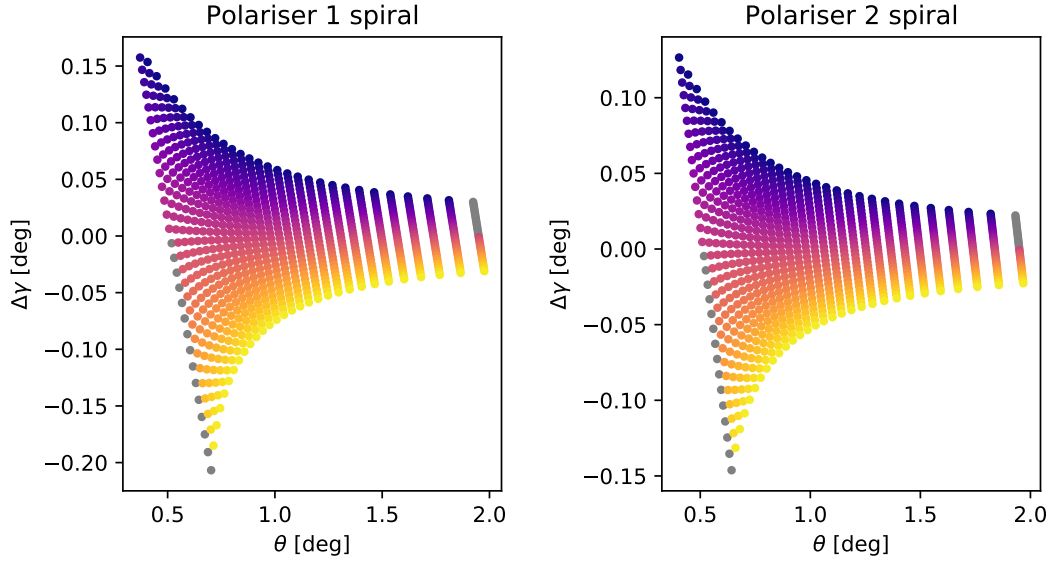


Figure 15:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ) for Pol 1 (left) and Pol 2 (right). Datapoints coloured from purple to yellow indicate the rays starting from bottom to top of the VS (1.5 mm). Datapoints in grey represent rays not entering the Selene 2 and therefore will not reach the sample position.

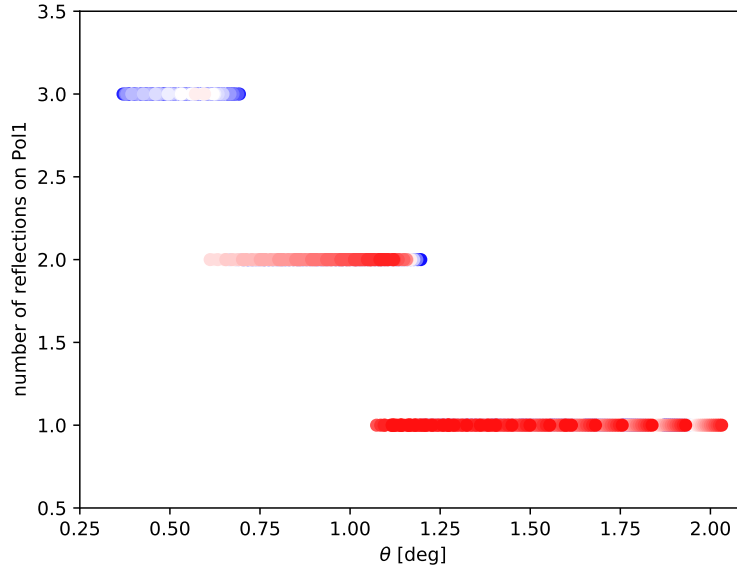


Figure 16: Number of reflections on Pol 1 as a function of the azimuth angle  $\theta$ . Numbers larger than 1 correspond to multiple reflections.

In this configuration Pol 1 and Pol 2 are relatively close to each other, and therefore

multiple reflections can occur between the two polarisers, e.g. the beam is reflected on Pol 1 and reflected back from Pol 2 towards Pol 1. At each reflection, part of the spin-up neutrons can be transmitted, therefore reducing the overall beam polarisation.

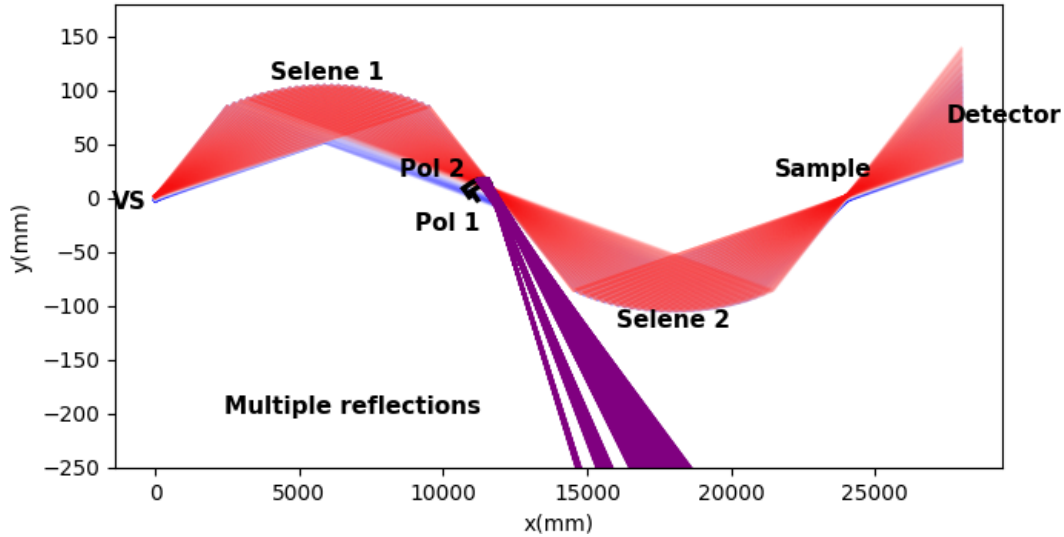


Figure 17: Projection in the x-y plane of the beam path. Neutrons generated at VS (horizontal opening = 5 mm) are i) reflected by Selene 1; ii) transmitted by Pol 2 (V-shape); iii) transmitted by Pol 1 (V-shape); iv) refocused at MF ; v) reflected by Selene 2; vi) refocused at the sample position, vi) revealed by the detector. Rays coloured in purple are those transmitted by Pol1 upon multiple reflections between Pol1 and Pol2

Figure 16 shows how the number of reflections varies along Pol 1. Numbers larger than 1 correspond to multiple reflections. The calculation for the multiple reflections was performed with  $VS = 5\text{mm}$ . As multiple reflections only occur in the top spiral section of the polarisers, the number multiple reflections does not change significantly when the  $VS = 1.5\text{mm}$ . According to this calculation, approximately 57% of the simulated rays is reflected more than once on Pol 1. Nevertheless, Figure 17 shows that the rays reflected more than once on Pol1 have propagation direction such that they do not enter in the Selene 2 and therefore will not reach the sample. As a conclusion, multiple reflections should not affect the beam polarisation.

Altogether, scenario 2 is a convenient solution for the shape/location of the polarisers as beam polarisation performances are expected to be comparable to scenario 1 (with Pol1 V-shape), but design and operation are simpler and the associated costs are lower.

### 4.3 Frame overlap mirror (FOM)

Slow neutrons (wavelength  $\geq 30\text{\AA}$ ) can create overlap between different pulses reaching the detector (Figure 17). The polarisers have a cut-off at  $26\text{\AA}$  and therefore no frame overlap will occur during PNR experiments. However, when the experiment does not require a polarised neutron beam, a FOM is needed to remove the overlap between different pulses.

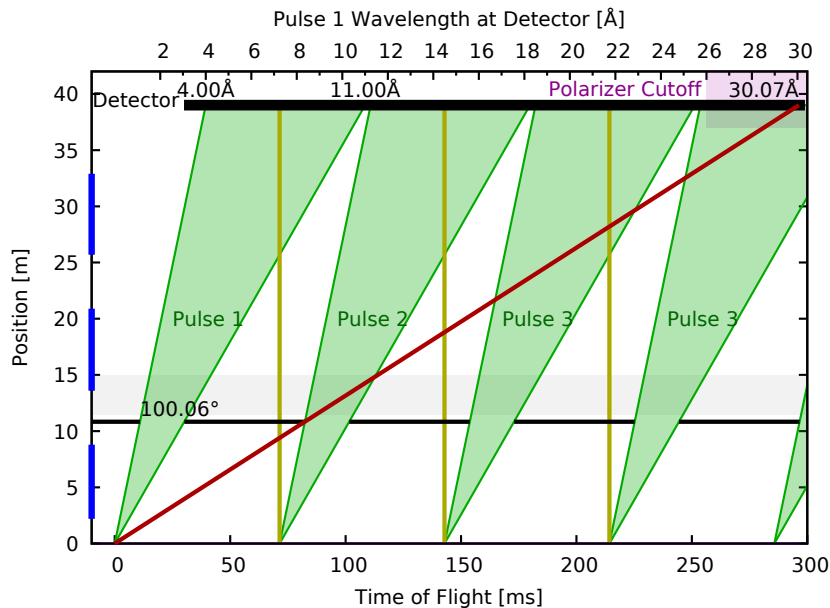


Figure 18: Schematic representation of the position of the neutron pulses travelling from the ESS source to the ESTIA detector as a function of the time of flight.

The FOM is designed to be a simple Si wafer with Ni coating layer ( $300\text{\AA}$ ). The shape is a logarithmic spiral with  $\gamma = 2^\circ$  (table 4). The corresponding  $\Delta\gamma$  is reported in Figure 19 for  $VS = 5\text{ mm}$ . Theoretical maximum and minimum  $\Delta\gamma$  values, to keep the cutoff above  $30\text{\AA}$  and below  $12\text{\AA}$ , are  $\pm 0.7^\circ$ , respectively. Therefore the described design allows to have approx.  $0.3^\circ$  tolerance for the positioning and actual construction of the FOM (Figure 19).

Table 4: Frame overlap mirror

Parameters	FOM
$\gamma$	$2^\circ$
length (mm)	771
x-position with respect to MF (mm)	500-1271

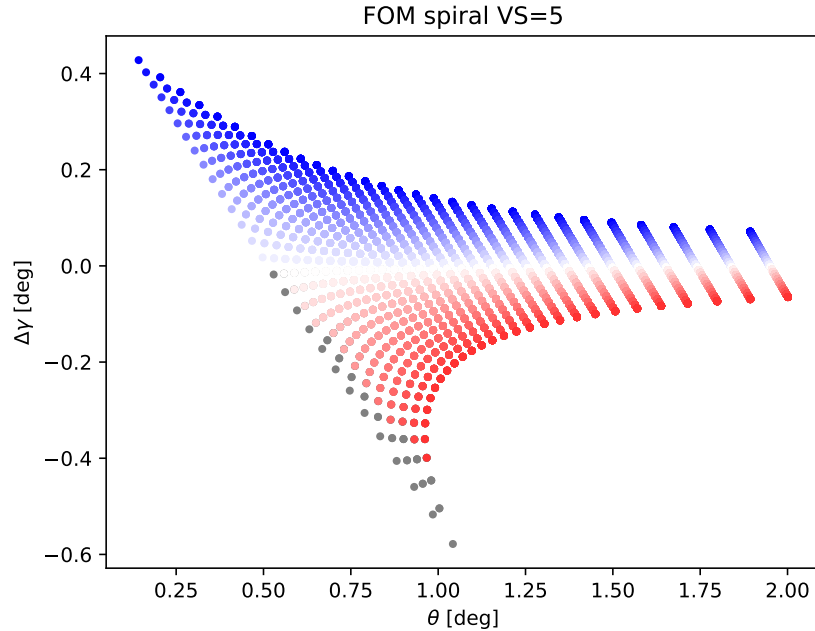


Figure 19:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ) for FOM. Datapoints are coloured from blue to red to represent the neutrons starting from bottom to top of the VS (5 mm), respectively.

Altogether the FOM allows to use the wavelength range 3.75-12Å without pulse overlap. To extend the wavelength range the chopper rotation speed can be reduced from 14Hz (same frequency as the proton source) to , e.g., 7Hz. This instrument configuration, named pulse-skipping mode, enables to almost double the largest wavelength available. During operation with pulse skipping mode, the FOM is no longer required and will be removed from the beam (Figure 17).

## 5 Analyser

The analyser is located after the sample and before the detector. It is designed to be a Si-wafer with Si/Fe supermirror coating ( $m=5/5.5$ ) with logarithmic spiral shape as the polarisers (Table 5). In order to simultaneously analyse at the detector both the beam transmitted (spin-polarisation down) and reflected (spin-polarisation up) the orientation of the analyser is rotated by 90° with respect to the polarisers (Figure 20). Therefore the logarithmic spiral shape is now laying in the z-x plane instead of the x-y plane.

Table 5: Analyser

Parameters	FOM
$\gamma$	1.65°
length (mm)	2115
x-position with respect to sample (mm)	885-3000

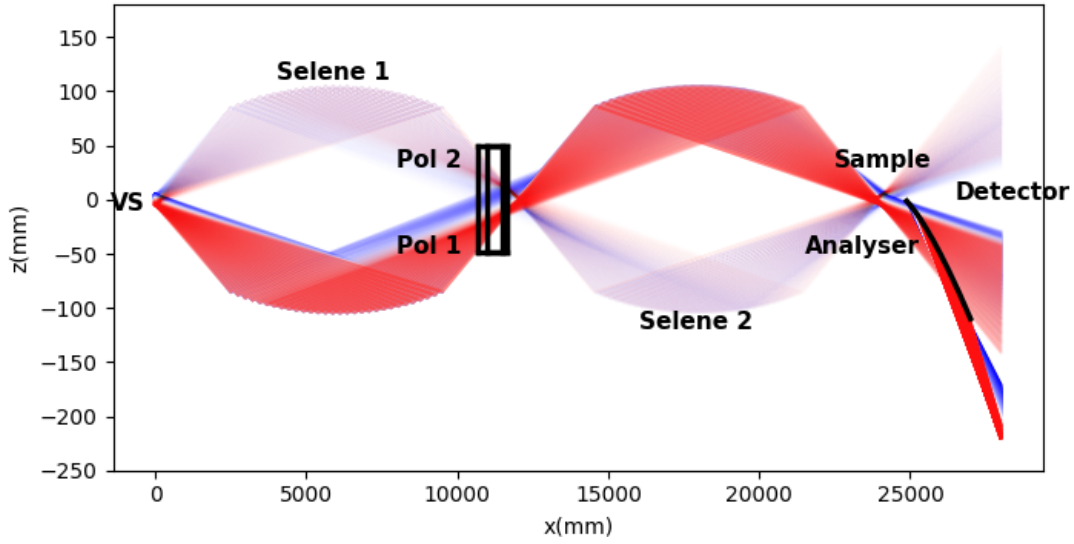


Figure 20: Projection in the z-x plane of the beam path. Neutrons generated at VS (vertical opening = 10 mm) are i) reflected by Selene 1; ii) transmitted by Pol 2 (V-shape); iii) transmitted by Pol 1 (V-shape); iv) refocused at MF ; v) reflected by Selene 2; vi) refocused at the sample position, vii) transmitted/reflected by the analyser; viii) revealed by the detector. The rays are coloured from blue to red starting from the bottom to the top of VS. The transparent beam path represents the second beam that will be available at the instrument after the upgrade of the Selene guides.

Figure 21 shows the  $\Delta\gamma$  plot for the VS vertical opening 10 mm. As for the polarisers the maximum  $\Delta\gamma$  is 0.3° and the estimated  $\Delta\gamma$  values are well within this limit.

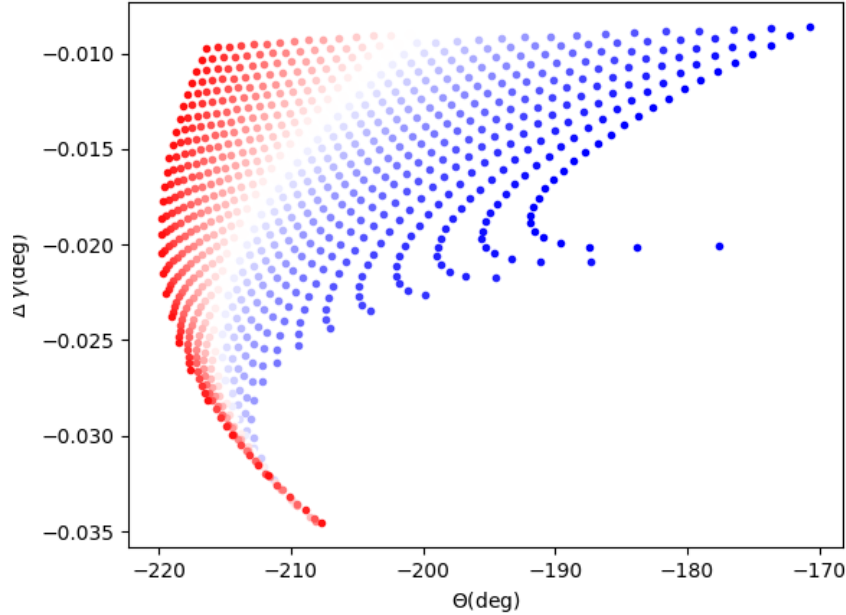


Figure 21:  $\Delta\gamma$  values as function of the azimuth angle ( $\theta$ ) for the analyser. Datapoints coloured from blue to red indicate the rays starting from bottom to top of the VS (10 mm vertical opening).

Figure 20 shows that the polarisers will have a rectangular shape in the z-x plane so that they cover the two beams, which will be available on ESTIA upon future upgrading of the selene guide system. On the other hand, Figure 22 shows again the beam path in the x-y plane, but with also the analyser. Because of the highly variable size of the beam along x at the location of the analyser, the analyser is designed with a trapezoidal shape as reported in Figure 21. A second analyser will be installed to cover the second beam during the upgrade of the instrument.

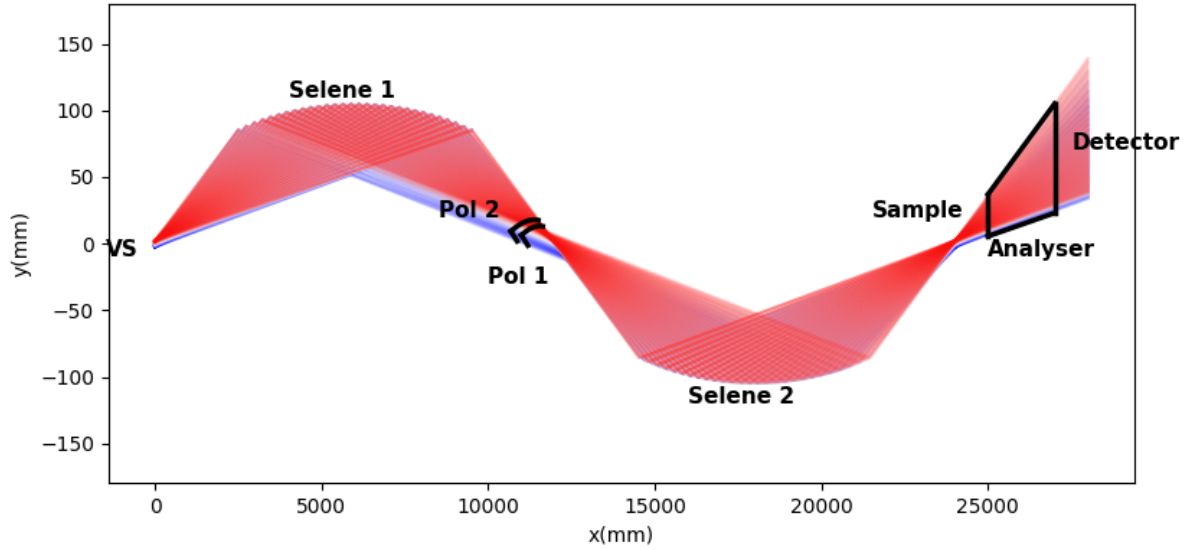


Figure 22: Projection in the  $y$ - $x$  plane of the beam path. Neutrons generated at VS (horizontal opening = 5 mm) are i) reflected by Selene 1; ii) transmitted by Pol 2 (V-shape); iii) transmitted by Pol 1 (V-shape); iv) refocused at MF ; v) reflected by Selene 2; vi) refocused at the sample position, vii) transmitted by the analyser; viii) revealed by the detector. The rays are coloured from blue to red starting from the bottom to the top of VS, respectively.