Magnetic field optimization and design of a superconducting neutron Wollaston prism

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Abstract. We present finite element simulations of a superconducting magnetic Wollaston prism (WP) for neutron scattering with high encoding efficiency and low Larmor phase aberrations. To achieve this, we develop and quantify the design criteria. The validation of simulation tools used for this work are investigated by using two software packages: RADIA and MagNet\textsuperscript{\textregistered}. Based on the optimization criteria, various possible configurations of WP are explored with MagNet, from which the best configuration is chosen for further optimization. To optimize the best configuration, the influence of various physical parameters is investigated, including the dimensions, shapes and arrangements of components of the device. The optimum WP was built and measured at both pulsed and constant wavelength neutron sources. In flipping mode, a neutron spin flipping efficiency of \textasciitilde98.5\% was measured independent of neutron wavelength and applied current. In a precession mode, measurements showed a highly linear Larmor phase variation along the horizontal direction with low depolarization. Simulations of the device agree well with the experimental measurements. Possible applications of the device are also discussed.

1. Introduction

In optics, a Wollaston Prism (WP) consisting of two triangular calcite prisms with orthogonal optic axes can split unpolarized light into two spatially separated, linearly-polarized, in-phase beams with orthogonal polarizations. For neutrons, a magnetic WP with an inclined interface separating oppositely directed magnetic fields can produce a spatial separation between the two different neutron spin states [1]. Based on the interference of these two spin states, one can construct a spin echo small angle neutron scattering (SESANS) [2-4] or spin echo modulated small angle neutron scattering (SEMSANS)[5-7] instrument, consisting of four and two such magnetic WPs respectively, which allows the measurement of the density correlations in a scattering object [8]. Classically the change of the neutron beam trajectory due to scattering can be encoded into a net neutron spin Larmor phase by

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the magnetic fields [4, 9]. Consequently SESANS resolves the neutron scattering angle independently of the neutron beam collimation and extends the accessible length scale up to several μm [4].

Various types of devices have been employed to implement SESANS, including room temperature WPs [1, 4], permalloy foils [10] and radio frequency (RF) flippers [11]. As discussed in ref. [9], each of these devices has its own shortcomings for measuring long length scales with low aberrations, which requires a high magnetic field intensity to create a large magnetic field integral gradient along the hypotenuse in a single WP. To overcome several of the limitations of the devices described above, we have developed a magnetic WP [9] using high temperature superconducting (HTS) materials. We use HTS tape for current carrying and HTS films for magnetic field confinement. The WP consists of two neighboring triangular field regions sharing the same 45°-inclined HTS film at the common hypotenuse of the two regions. The magnetic field in each region is provided by coils wound on soft iron pole pieces and all the field regions then are surrounded by four HTS films that ensure magnetic field uniformity. The whole assembly is then enclosed by a Mu metal box which has a dual purpose, allowing for flux return and shielding from external fields. The HTS tape and soft iron pole pieces allow high field intensity to be achieved while the HTS films can confine the magnetic flux and thus allow us to create a large, uniform field-integral gradient. The optimized WP was built and measured at both pulsed and constant wavelength neutron sources. In flipping mode, a neutron spin flipping efficiency of ~98.5% was measured independent of neutron wavelength and applied current above 2A at a pulsed neutron source [12] (LENS). In the precession mode, a highly linear Larmor phase variation along the encoding direction with low depolarization was measured using a thin monochromatic neutron beam on the MAGIK instrument [13] at NCNR (NIST Center for Neutron Research). The simulation results of the device agree well with the measurement.

To simulate the device, the validity of two simulation packages was investigated, these were RADIA [14] and MagNet© (Infolytica, Canada). These codes are based on boundary integral and finite element methods respectively. We concluded that RADIA is unable to model superconducting materials with sufficient quality and can produce magnetic field artifacts depending on the meshing size of the components in the region close the superconducting material. Because of its ability to handle the HTS materials involved, MagNet was used in all the simulations and optimization of the device. The criterion for optimization of the WP is introduced below and the critical parameters to build a HTS WP with high encoding efficiency and low phase aberrations are presented. To reduce the thermal load and the risk of quenching the HTS films, a series of simulations are also presented.

2. Model selection

For a neutron traveling in a magnetic field oriented perpendicular to the neutron spin, the spin precesses around the magnetic field vector in a motion called Larmor precession [15]. The accumulated Larmor phase of the neutron spin is proportional to the neutron wavelength and the magnetic field integral along the neutron trajectory.

Figure 1 Schematic of a WP where \( k \) is the neutron wave vector and the Larmor precession is indicated. The neutron trajectory has a divergence angle of \( \psi \) with respect to the \( x \) axis in the \( xy \) plane. The divergence angle of \( \psi \) in the \( xz \) plane is not shown.
A single magnetic WP composed of two neighboring triangular field regions is shown in Error! Reference source not found. with the Larmor precession indicated. Based on the geometrical symmetry of the device, for a neutron wave vector with divergence angles $\phi$ and $\psi$ in the $xy$ plane and the $xz$ plane respectively, the magnetic field integral $FI$ can be expanded to the lowest order as [9].

$$FI = ay + b\phi + cz\psi + dyz^2 + O(\phi^2, y^3)$$

where $z$ denotes the direction of the main field and $y$ is the gradient direction of the field integral as shown in Error! Reference source not found., which denotes the encoding direction of the WP. As ref. [9] makes clear, to build a WP with high encoding efficiency and low Larmor phase aberration, the magnitude of $a$ needs to maximized, while minimizing the magnitude of $d$.

Since most available HTS tapes either contain gadolinium, which is a strong neutron absorber, or are too rigid to wind a well-defined triangular solenoid, the WP is defined by two pairs of gapped solenoids through which neutrons pass. As shown in Figure 2, possible configurations of the WP were simulated using MagNet by manipulating the positions of the HTS films and soft iron pole pieces. For all the configurations, the inclination angle of the boundary between the triangular coils was kept at 45°. The materials used in the simulation were HyMu 80 0.014, Hiperco 50A 0.014 and Copper 5.77e7 Siemens/meter for the Mu metal, pole pieces and coils respectively. The HTS films are defined by a flux tangential boundary condition due to the Meissner effect.

Figure 2. The models we have investigated. Gray with black stripes: HTS film; purple: Mu metal yoke; dark red: soft iron pole pieces; brown: coils wound on pole pieces

Model (a): Hollow triangular coil with HTS film at hypotenuse only
Model (b): Triangular coil filled with pole pieces, HTS film at hypotenuse only
Model (c): Triangular coil filled with pole pieces, HTS films on the side and hypotenuse
Model (d): Triangular coil filled with pole pieces, HTS films on all sides

For each model shown in Figure 2, the corresponding $z$ dependence of the magnetic field is shown in Figure 3, which makes clear that model (c) and model (d) generate the largest field with the best uniformity. Also the term $a$ and $d$ in the field integral expansion are summarized in Figure 4 showing that model (d), which employs soft iron pole pieces and HTS films on all sides, gives the largest linear term $a$ and the lowest aberration term $d$ due to the better field confinement and coupling efficiency between the upper and lower pole pieces. Thus model (d) is the best configuration of the WP and is further optimized in the following sections.
Field intensity of various models along the z direction at the center (y=0) of the triangular-cross section of various models. The gap between the upper and lower coils is 30mm. Model (a) uses the right axis and model (b), (c) and (d) use the left axis.

The simulated $a$ and term $d$ for various model configurations. Meshed and blank bars are for term $a$ (upper axis) and $d$ (lower axis) respectively with their values indicated on the right.

3. Optimization of the geometry

In the following section, a WP with soft iron pole pieces and HTS film on each side will be optimized by investigating the dependence of the terms $a$ and $d$ on various physical parameters of the device. Parameters that were varied include the coil height along field direction, coil size, coil arrangement, gap between pole pieces and gaps between coil and HTS films.

3.1. Variation of the coil height
Figure 5. The variation of the terms $a$ and $d$ as a function of coil height. The gap between upper and lower coils is fixed to be 40mm. The current density in the coils was 4 A/mm. Black hollow points are for term $a$ (left axis) and blue solid points are for term $d$ (right axis).

The contribution of the coil height is investigated and shown in Figure 5 and the term $a$ and $d$ both scale linearly with the height of the coils, the ratio of these terms is constant and there is no particular optimum height for the coils. However the maximum height of the coil is limited by the available size of the HTS film.

3.2. Variation of the size and arrangement of coils

Since each triangular-cross section coil has three round corners, they can be configured in at least two possible ways, as shown in Figure 6 (a) and (b). In Figure 6 (a), the two triangular coils are symmetric about the HTS film at the hypotenuse, while for Figure 6 (b), these two triangular coils are configured such that their circumcenters are aligned parallel to the beam direction. The consequent variations of the terms $a$ and $d$ as a function of the size of the coils for both configurations are shown in Figure 6 (c). It is clear that increasing the size of the coil decreases the $d$ term dramatically while the linear term $a$ remains constant. Figure 6 (c) also shows that the arrangement of the two triangles is important, with the triangles arranged as shown in Figure 6 (b) being the optimum arrangement. Again, the maximum size of the coil is mainly restricted by the largest HTS film available from the manufacturer.

Figure 6. (a) and (b): top view of two possible arrangements of the triangular coils. Purple: Mu metal, brown: pole pieces and black stripe: HTS films. (c): The variation of term $a$ and $d$ term when changing the hypotenuse length of the coil. Solid points are for model (a) while open points are for model (b). The scale for black points is the left axis while the scale for blue points is the right axis.
3.3. Variation of the gap between the pole pieces

To calculate the maximum obtainable beam size, the influence of the gap between the upper and lower coils upon the terms \( a \) and \( d \) was simulated. As shown in Figure 7, when increasing the gap, due to the decrease of the coupling efficiency between these two coils, the magnetic field intensity will decrease whilst the field homogeneity increases. Consequently, term \( a \) will decrease while term \( d \) will increase, which means the gap should be kept as small as the maximum beam size allows.

![Figure 7](image_url)

Figure 7. The variation of the terms \( a \) and \( d \) as a function of the gap between upper and lower coils.

Black hollow points (left axis) are for term \( a \) and blue solid points (right axis) are for term \( d \).

A series of calculations were carried out to determine the effects upon magnetic field-integral homogeneity for gaps between HTS films in the various designs. This was done because it is clearly easier to manufacture designs in which the tolerance on film positions is relaxed. The general finding from these calculations was that gaps between films need to be avoided where possible to confine the magnetic flux.

3.4. Design of the pole pieces

In all the calculations described above, solid triangular-cross-section soft-iron pole pieces with a high permeability were used inside the coils to confine and guide magnetic fields. However these can create an unnecessary thermal load at low temperature and constrain the cooling speed and base temperature. Thus the effect of hollow pole pieces on the field integral expansion was calculated, which shows that a soft iron core with a finite wall thickness is sufficient to guide and confine the magnetic flux between the upper and lower pole pieces provided they are not saturated. The calculation of the field-integral expansion shows no effect on either the term \( a \) or \( d \) compared with the model with solid pole pieces.

A key parameter to constrain the maximum current which can be applied is the critical field of the HTS film. Since the edge of the pole piece is close to the HTS films the gradient of the magnetic scalar potential around a sharp corner can be higher than the lower critical magnetic field of the HTS films, which are type-2 superconductors [16]. To minimize the local magnetic field perpendicular to the HTS films and avoid the mixed state in the HTS films, the local field intensity for various types of pole pieces was calculated and is shown in Figure 8, where (b), (c), (d) and (e) demonstrate a corner of the WP indicated by the yellow box in Figure 8 (a). The magnetic field intensity hot spot usually happens where the edge of the pole pieces and coils meet. Figure 8 shows that the minimum local field can only be obtained when the sharp edges on both the HTS coils and the pole pieces can be avoided. The configuration shown in Figure 8 (e) is used in the actual design of the WP.
3.5. Design conclusions
To summarize these simulation results, for a WP with a large linear term $a$ and a small aberration term $d$, the transverse ($y$) dimension of the coil needs to be maximized with a particular arrangement while the gap in between the upper and lower coils needs to be no larger than the maximum beam size required. To confine the main magnetic field region and keep the field uniform, gaps between the HTS films need to be avoided where possible. To reduce the thermal mass of the device, hollow pole pieces need to be employed and sharp corners of either the coils or the pole pieces have to be avoided to protect the HTS films from being quenched.

4. Construction of the WP
Based on the optimization criteria described above and the size of the HTS films commercially available [17], the optimized WP configuration is as shown in Figure 9 (a). It consists of 2 pairs of triangular-cross section solenoids, which generate opposite fields on two sides of the shared hypotenuse. All the coils are then yoked in a Mu metal enclosure to ensure magnetic flux return. To reduce the remnant field produced by the soft iron, material with low magnetic coercivity is preferred. Soft iron A1018 is used in the fabrication of the WP due to its availability, although Hiperco 50A 0.014 with lower coercivity is used in the simulation. The complete assembly of the WP is shown in Figure 9 (b). The whole device is sealed inside a helium gas exchange can and can be cooled down to ~30K within 12 hours by a close-cycle refrigerator with a cooling power of 6.7W at a temperature of 20K.
5. Characterization of the WP

The magnetic field integral expansion describes the Larmor precession efficiency of the device, which gives the encoding efficiency and phase aberration of a SESANS instrument. Besides the phase aberration in Larmor precession, the spin transport efficiency of the device is also determined by the magnetic field transitions at the HTS films. For the HTS films, the field transition efficiency is mainly determined by the coupling efficiency between the magnetic fields generated by the device itself and the external guide field. The average angular deviation of the magnetic field inside the device from the $z$ direction is calculated to be $0.004^\circ$ and $0.014^\circ$ for $10 \times 10 \text{mm}^2$ and $20 \times 20 \text{mm}^2$ beam sizes respectively. Considering the HTS film at the hypotenuse, again, the calculated average misalignment of the magnetic field vectors from the $z$ direction is $0.004^\circ$ and $0.01^\circ$ for $10 \times 10 \text{mm}^2$ and $20 \times 20 \text{mm}^2$ beam sizes respectively. The highly aligned magnetic field vectors contribute to a highly efficient spin transport from external guide field to the WP. The spin transport efficiency of the triangular region is determined by the adiabaticity of the magnetic field [18]. According to the calculation, the minimum adiabaticity parameter is larger than 100, which is $>>1$ and means the precession can perfectly follow this geometrical rotation of field in the WP and conserve polarization [18].

Various coefficients in the field expansion in equation (1) can be calculated, $a=3.045 \text{mT/A}$, $b=3.033 \text{mT/(A-rad)}$, $c=0.045 \text{mT/(A-rad)}$ and $d=-1.3 \times 10^{-5} \text{ mT/(A-mm}^2)$. As discussed earlier in ref. [9], for a neutron beam of $10 \AA$ wavelength with divergence angle $\pm 0.5^\circ$ in all directions, the integrated polarization efficiency over the whole beam height as a function of spin echo length takes the values shown in Figure 10 for three different beam heights. According to the simulations, a spin echo polarization of 90% can be obtained at a spin echo length of $5 \mu\text{m}$ using a 30mm beam height.
Figure 10. The polarization efficiency integrated over the whole beam height for various beam sizes in the $z$ direction as a function of spin echo length. The applied currents for various spin echo lengths are indicated on the top axis. For this calculation, the spin echo length was calculated using a separation distance of 30cm between the WP centers and neutron wavelength of 10Å.

The field intensity of the assembled device was measured using a 1-D hall probe and the performance of the device with polarized neutrons was also measured at both pulsed and constant wavelength neutron sources. All these results are presented in more detail in ref. [9]. In flipping mode, a neutron spin flipping efficiency of ~98.5% was measured independent of neutron wavelength and applied current. In the precession mode, a highly linear variation of the Larmor phase along the horizontal direction was measured with low depolarization. The simulation results of the device agree well with the measurement.

6. Discussion
We have presented our simulations of an HTS magnetic WP. The criteria used for the optimization are introduced and the contributions of the critical parameters of the WP for a high encoding efficiency with low phase aberrations are evaluated. As an example, the expected performance of a SESANS instrument is presented with a high polarization at long spin echo length. The simulations using MagNet© indicate its capability for defining the HTS materials. Also our neutron measurements of the WP make it clear that the HTS films can be employed to split two neighboring magnetic field regions with high spin transport efficiency. Thus both the simulation package and the HTS films may have potential applications to facilitate the design of neutron spin-manipulation devices.

To further simplify the maintenance of the device and extend the achievable magnetic field intensity, a second generation of the device has been constructed with optimized thermal and electrical conductivity, which can possibly allow at least 50mT to be achieved without the gas exchange can, and decreases the coupling distance to the external guide field. Thus, a larger encoding efficiency with higher magnetic coupling efficiency can be achieved.

Besides the application in SESANS, the separated two spin states can record the phase change introduced by a scattering object, thus the gradient of the phase distribution of the object along the hypotenuse of the device can be measured by the interference of these two spin states, which can be used to implement neutron differential interference contrast (DIC) radiography. The same setup of the DIC radiography can also be employed to do spin-echo modulation small angle neutron scattering. The implementation of SEMSANS using two of such WPs has been achieved at a reactor source[7].
Recently we also proposed a new neutron spin echo method to measure the phonon excitation life time using two of such WPs with a rectangular magnetic field region between them on both the incident and scattered neutron beams on a triple-axis spectrometer [19]. By introducing well-defined magnetic field regions with triangular and rectangular cross sections, the lines of constant spin echo phase can be tuned electromagnetically to a wide range of phonon energies and group velocities simply by changing currents. By introducing electromagnetic tuning and allowing higher current to be applied, the new method may accommodate a wider range of phonon energies and group velocities than the traditional resonant spin echo technique.

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References

[1] Pynn R, Fitzsimmons M R, Lee W T, Stonaha P, Shah V R, Washington A L, Kirby B J, Majkrzak C F and Maranville B B 2009 *Physica B* 404 2582-2584
[2] Uca O, Spin-Echo Small-Angle Neutron Scattering Development, in, Delft University Press, 2003.
[3] Rekveldt M T, Plomp J, Bouwman W G, Kraan W H, Grigoriev S and Blaauw M 2005 *Rev. Sci. Instrum.* 76 033901
[4] Pynn R, Lee W T, Stonaha P, Shah V R, Washington A L, Kirby B J, Majkrzak C F and Maranville B B 2008 *Rev. Sci. Instrum.* 79 063901
[5] Strobl M, Tremsin A S, Hilger A, Wieder F, Kardjilov N, Manke I, Bouwman W G and Plomp J 2012 *J. Appl. Phys.* 112 014503
[6] Strobl M, Wieder F, Duif C P, Hilger A, Kardjilov N, Manke I and Bouwman W G 2012 *Physica B* 407 4132-4135
[7] Li F, Parnell S R, Bai H, Yang W, Hamilton W A, Maranville B B, Ashkar R, Baxter D V, Cremer J T and Pynn R 2016 *J. Appl. Crystallogr.* 49 55-63
[8] Andersson R, van Heijkamp L F, de Schepper I M and Bouwman W G 2008 *J. Appl. Crystallogr.* 41 868-885
[9] Li F, Parnell S R, Hamilton W A, Maranville B B, Wang T, Semerad R, Baxter D V, Cremer J T and Pynn R 2014 *Rev. Sci. Instrum.* 85 053303
[10] Rekveldt M T, Duif C P, Kraan W H, Plomp J and Bouwman W G 2008 *Rev. Sci. Instrum.* 79 015113
[11] Plomp J, Spin-echo development for a time of flight neutron reflectometer, in, Delft University of Technology, South Holland, Netherlands, 2009.
[12] Baxter D V, Cameron J M, Derenchuk V P, Lavelle C M, Leuschner M B, Lone M A, Meyer H O, Rinckel T and Snow W M 2005 *Nucl. Instrum. Methods Phys. Res., Sect. B* 241 209-212
[13] Dura J A, Pierce D J, Majkrzak C F, Maliszewskyj N C, McGillivray D J, Löschke M, O’Donovan K V, Mihailescu M, Perez-Salas U, Worcester D L and White S H 2006 *Rev. Sci. Instrum.* 77 074301
[14] Elleaume P, Chubar O and Chavanne J, Computing 3D magnetic fields from insertion devices, in: Particle Accelerator Conference, 1997. Proceedings of the 1997, 1997, pp. 3509-3511 vol.3503.
[15] Bloch F 1946 *Phys. Rev.* 70 460-474
[16] Böhmer C, Brandstätter G and Weber H W 1997 *Supercond. Sci. Technol.* 10 A1
[17] ceraco ceramic coating GmbH http://www.ceraco.de/hts-films/
[18] Seeger P A and Daemen L L 2001 Nucl. Instrum. Methods Phys. Res., Sect. A 457 338-346
[19] Li F and Pynn R 2014 J. Appl. Crystallogr. 47 1849-1854