Magic-PASTIS for XYZ polarization analysis using SEOP polarized ^{3}He gas

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Abstract.   We present progress towards a complete system for neutron polarization analysis on a time-of-flight (TOF) neutron spectrometer with a large area/angle detector array. Finite element calculations have been used to model the field gradients of a newly proposed PASTIS coil set, which uses a wide-angle banana shaped ³He Neutron Spin Filter cell (NSF) to cover a large neutron scattering solid angle. The final goal of this insert is to enable X-Y-Z polarization analysis to be installed on the future hot/thermal time-of flight spectrometers, although the method is also applicable to thermal/cold spectrometers as well. The components of this system, such as the magnetic field coils and design are applicable to neutron spectroscopy with wide angle detector arrays in general, and the ³He wide angle cell developments for polarized inelastic neutron scattering are independent from the methods used to polarize the gas as well.

1. Introduction

Neutron polarization analysis, PA, is a powerful tool for separation of nuclear spin-incoherent background, analysis of complex magnetic structures and the study of magnetic excitations [1]. Several wide angle spectrometers with polarization analysis exist or are under construction [2, 3, 4, 5]. The PA can be performed in a variety of ways depending on the instrument's parameters and energy range using either supermirror analyzer arrays [2], or ³He neutron spin filters as described in this paper and in the references [5, 6, 7, 8]. The performance of the super mirror-based systems, is normally limited by the analyzer height and integration over the height of the detectors, as well as the maximum analyzable energy which is normally about 20 meV or less [9].

For ³He based systems, a sufficiently low magnetic field gradient must be maintained over the volume of the neutron spin filter cell in order to obtain ³He polarization lifetimes of a practical and useful level (see section 2). Further for any method to obtain information on the $Q_{\perp}$ and $Q_{\parallel}$ of the momentum transfer vector Q over a large solid angle detector, the sample field must be changeable between the three orthogonal X-Y-Z directions [10]. In the case of the ³He NSF, since the cell occupies the same field volume as the sample, the large volume highly uniform ³He holding field used to maintain long ³He NSF lifetimes, must also be able to be changed between the X,Y and Z directions. We present a design study with finite element magnetic field (FEM) calculations of possible X-Y-Z field configurations suitable for maintaining the polarization of the ³He and is adapted to the TOPAS instrument geometry. Two clear options exist, a magnetized

mu-metal geometry, similar to reference [7], or a resistive coil set similar to reference [6], however in our proposed designs, certain key differences exist which build on the experiences from prior devices. First we provide the reader with a review of the sources of ^{3}He relaxation, and how they should be optimized for effective neutron spin filter use.

2. ^{3}He relaxation time

Here to ease the discussion for the reader we provide a short review of ^{3}He nuclear spin relaxation in a closed volume. The ^{3}He polarization in NSF cell decays to thermal equilibrium with a characteristic time constant T_1. The longitudinal relaxation rate, $\Gamma_{\mathrm{He}} = T_1^{-1}$ consists of three main mechanisms for relaxations of spins and is characterized by:

$$\Gamma_1 = \frac{1}{T_1} = \frac{1}{T_1^{dipole}} + \frac{1}{T_1^{gradient}} + \frac{1}{T_1^{wall}} \tag{1}$$

T_1^{dipole} is the dipole-dipole relaxation time due to interaction between colliding ^{3}He atoms [11]. The magnetic dipole coupling of atoms during a binary collision results in the loss of nuclear polarization. This rate is well known and described by:

$$\frac{1}{T_1^{dipole}} = \frac{p}{817}, \tag{2}$$

where p is given the pressure in bar and 817 is the dipole-dipole relaxation rate constant in hours. This dipole relaxation effect is practically relevant at the one to several-bar pressures used for neutron spin filter cells and forms the upper limit to the maximum on beam storage times as the other two terms can theoretically approach 0 in ideal cases. For example at p=2.7 bar the maximum possible storage time constant is $T_1^{dipole} \simeq 300$ h.

In the presence of magnetic field gradient, a diffusing atom will transition through field gradients orthogonal to the B_0 magnetic holding field [12]. If the motion through these field gradients creates an effective field change with a rate close to or exceeding the Larmour frequency of the atoms, then spin flips can be inducted causing a loss of magnetization. $T_1^{gradient}$ is the relaxation due to diffusive motion through orthogonal field gradients and given by:

$$\frac{1}{T_1^{gradient}} = \frac{7000}{p} \left(\left(\frac{\Delta B_x}{B_0} \right)^2 + \left(\frac{\Delta B_y}{B_0} \right)^2 \right), \tag{3}$$

where ΔB_x and ΔB_y are the orthogonal gradients of the static holding field B_0. For example, to maintain reasonable neutron spin filter performance over time while refreshing the polarized ^{3}He gas or cell less than once once per day[8] for a cell of $p = 2.7$ bar,

$$\left(\left(\frac{\Delta B_x}{B_0} \right)^2 + \left(\frac{\Delta B_y}{B_0} \right)^2 \right)^{1/2} \leq 10^{-3} \mathrm{cm}^{-1} \rightarrow T_1^{gradient} \geq 100\mathrm{h}, \tag{4}$$

here the 2-2.7 bar pressure is chosen to reduce relaxation due to field gradients, while still allowing for a long T_1^{dipole}.

The final term T_1^{wall} in equation 1 is the relaxation time due to the interactions with the cell wall and is the least understood ^{3}He relaxation mechanism. This relaxation depends purely on the characteristics of the container which can contain magnetic impurities like magnetite (the most common impurity in glasses). The diffusion of helium into the glass may also cause relaxation by precession of the helium moment about the net local gradient field caused by the magnetic impurities. Many references have been written as to possible origins and characterizations of this relaxation and how it can be changed through application of external fields [13, 14, 15].
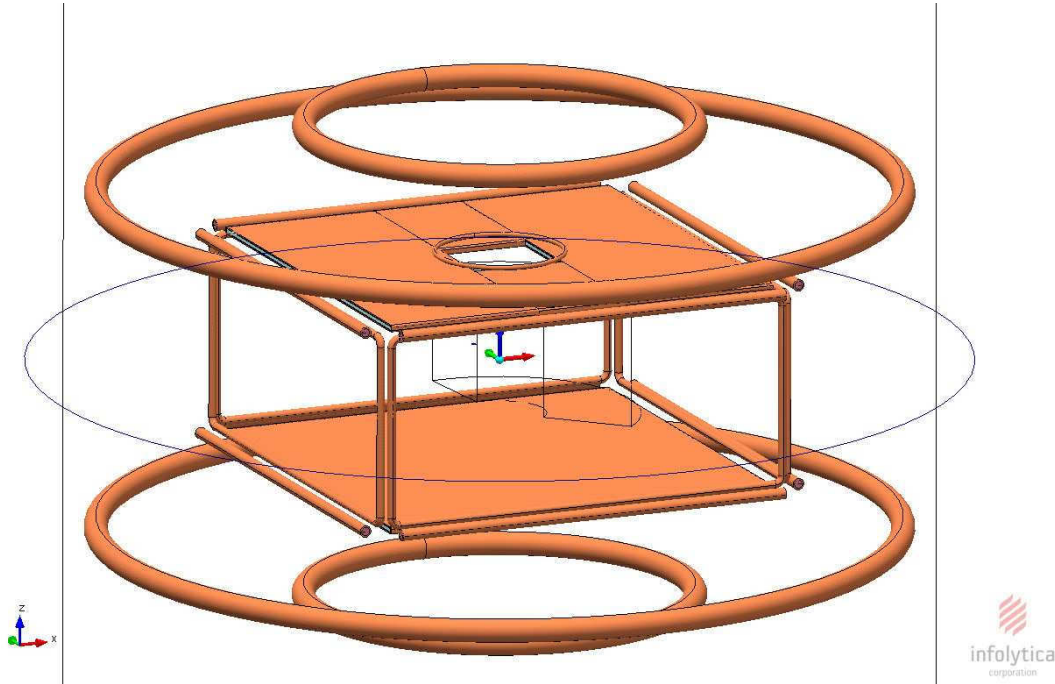
Figure 1. The model written in 3D finite element magnetic modelling software [16], showing the geometry of our concept. The square plates are 35 cm by 35 cm and the largest circular coils are D = 70 cm. (Color online)

3. Magnetic system design

Several steps have been made in the design of wide angle polarization analysis using polarized ^{3}He for analysis of $Q_\parallel$ and $Q_\perp$ magnetic scattering, i.e. X-Y-Z polarization analysis [10]. Previously a wide angle polarization analysis prototype called PASTIS was developed at the Institut Laue Langevin, where a set comprised of compensated X, Y and Z coils were used to create a homogeneous magnetic field in three orthogonal directions in a compact format suitable to known neutron instrumentation with acceptable ^{3}He relation times [6]. The idea has been further explored in the ILL and ISIS with a more exotic magnetized μ-metal configuration and a further minimization of dead areas with the original compensated coils geometry respectively [5, 7].

Our so called Magic-PASTIS design is based on an open μ-metal geometry. The design used for finite element calculations using commercially available software [16] is shown in figure 1. By introducing μ-metal sheets we aim to produce an improved homogeneous magnetic field in a large region while reducing the blind areas due to the coil frames of the more conventional compensated square/circular coils of the original, and optimized resistive coil PASTIS systems [5, 6]. Those systems for example have eight vertical dead areas (in the horizontal plane) of approximately $\geq 5°$ at $\pm18°, \pm71°$ and $\pm109°$ whereas the design presented here has a $> 40°$ opening in the vertical plane and only four small $3°$ dead angles, one every $90°$, in the horizontal plane. For either system these dead angles can be rotated arbitrarily with respect to the incident beam. The center of the configuration is the sample, placing the ^{3}He cell significantly off center, but this is largely defined by the typical sample environment geometry of any real neutron spectrometer that is designed to accept sample magnets and cryostat, which also place the sample at the center.
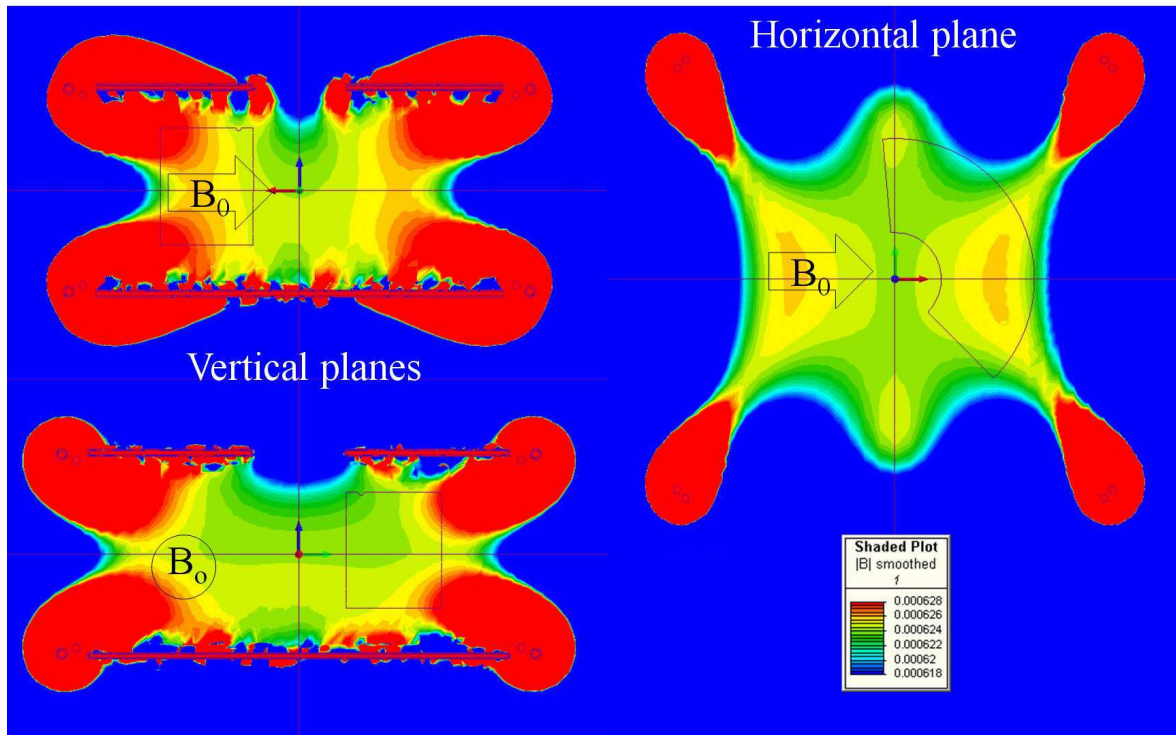
Figure 2. A color-shaded plot of the calculated Magnetic field distribution for the three planes of the x or y direction from FEM simulations. Each color gradient is a relative change of 8.33×10^{-4}. The size of the square plates is 35 cm x 35 cm.
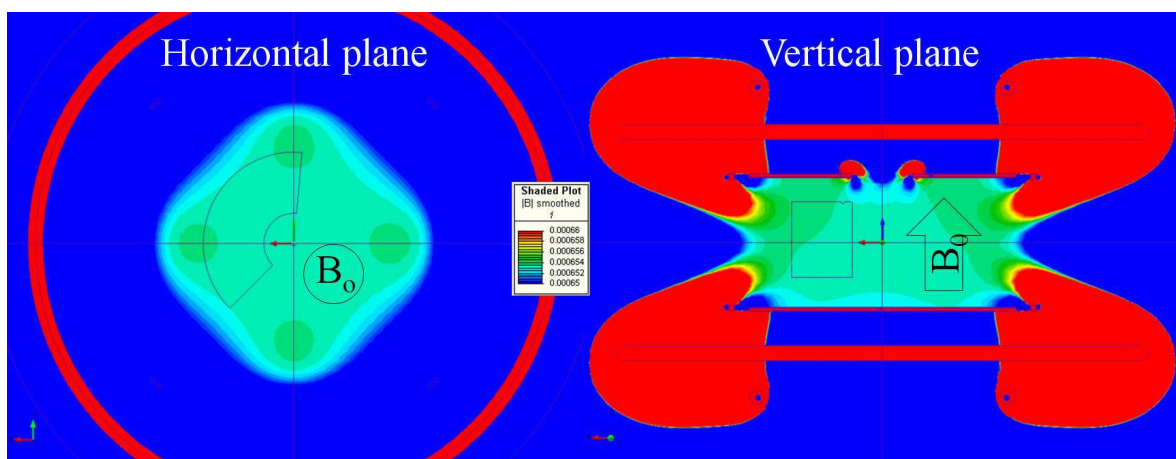

Figure 3. A color-shaded plot of the calculated Magnetic field distribution for the two planes of the z direction field from FEM simulations. Each color gradient is a relative change of 7.57×10^{-4}. The diameter or the main circular coils is 70 cm.
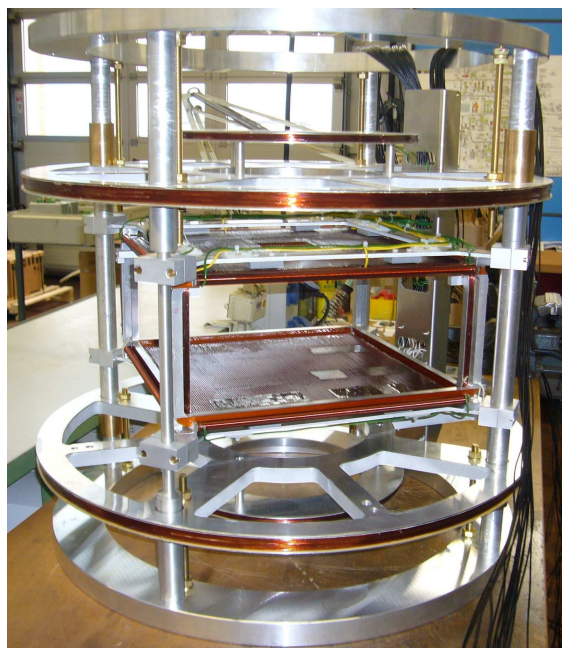
Figure 4. The current status of the magic PASTIS system. The system is now being optimized for the values of currents and fine positioning of coils. (Color online)

As discussed in the Section 2, in order to keep the depolarization of the polarized ^{3}He sufficiently low it is necessary that the field gradient is below about 10^{-3}cm^{-1} over the volume of a large neutron spin filter cell, see Equation 4. This level would allow the cells to remain on the instrument long enough to make experiments feasible by reducing the time spent refilling, calibrating and transporting polarized cells/gas to the beamline to once per day or less.

Figure 2 shows finite element calculations of the created magnetic field in the X or Y direction, and figure 3 is the same for the Z direction. It is clear that the inner part is highly homogeneous, including also up to the radius of the ^{3}He cell. As seen in figure 1, the coil setup fulfils the requirement of a large solid-angle opening with minimal dead area, allowing the polarization analysis over our large solid angle detectors. We have constructed a prototype of this new setup which will now be optimized experimentally for current values and optimal positioning of the coils starting with the ideal geometry from the FEM model. A picture of the completed prototype can be seen in figure 4. In parallel, the construction of the incident beam polarizer based on the design of the MARIA reflectometer in-situ SEOP analyzer is continuing [17]. Once TOPAS is brought into operation it will provide polarization analysis covering a wide angular range from day 1.

4. Development of wide angle GE180 cells for SEOP or MEOP polarized gas

The use of sealed ^{3}He cells made of GE180 glass could vastly simplify the equipment required for wide angle PA as they would allow direct polarization of the cell using the SEOP method [18]. Furthermore, an all blown glass construction using GE180 may indeed have practical advantages such as pressure resistance and durability compared to other proposed routes, such as attempts from other groups to form cells from bonded, or glued-together, flat and curved plates of crystal silicon, quartz, or even GE180 [5, 18]. Presumably such cells if made of GE180 could be used as sealed cells and be polarized directly by a SEOP polarizer system as in [18] or be used as valved

Figure 5. A first doughnut shaped cell for magic PASTIS testing called Homer. This cell is filled with 0.5 bar of ^{3}He to make it sensitive to magnetic field gradients. The T_1 lifetime of this cell is 1074 ± 20 hours. (Color online)

cells which are filled with pre-polarized ^{3}He gas from a large scale ^{3}He polarizer employing either the MEOP or SEOP technique [5, 7, 19].

Consequentially, the route towards suitable wide angle ^{3}He spin-filter cells we have been pursuing is that of an all-blown GE180 construction. Such cells are unique firsts, and results of the work in the Jülich glass workshop who have been developing the techniques. GE180 is chosen because of its suitability for good ^{3}He T_1 relaxation times, neutron compatibility, and the fact it is the best know material for use in SEOP polarization of the ^{3}He gas [20]. First doughnut shaped cells are formed by making a hole through the center of a large cell.

In figure 5 we show a picture of a very large, D =22 cm doughnut-shaped cell called Homer which was prepared with a Rb/K hybrid mixture [21], 0.07 bar N_2 and 0.5 bar of ^{3}He. This cell was made for tests of ^{3}He relaxation times in the new magic-PASTIS coil system from figure 4. As was shown in equation 3, the low ^{3}He pressure will make the cell sensitive to magnetic field gradient relaxation and a good probe to optimize the performance of the magic PASTIS magnetic cavity. Aided by the low ^{3}He pressure, good glass handling and cell preparation techniques, Homer was measured to have a 1074 hour T_1 in what we presume to be an nearly "ideal" magnetic holing field which has a relative field gradient better than 1×10^{-4} cm^{-1}. C-shaped cells optimized for spectroscopy applications are then made by sealing off sections of the doughnuts to obtain the desired angular acceptance.

5. Inelastic scattering test from GE180

The inelastic neutron scattering properties of GE180 glass was not known. Therefore we characterized the inelastic neutron scattering properties on TOFTOF [22], to determine if such cells can eventually be used for spectroscopy applications and/or under what conditions. Shown in figures 6 and 7 are the results of this test.

A sample of the glass was prepared in the same way as a ^{3}He spin filter cell is prepared [23]. The inelastic neutron spectrum for these samples was then measured of a broad range of resolutions and incident neutron wavelengths. The broad dynamic range, high incident energy measurement using 1.6 Å neutrons was performed at 70 °K and 298 °K where no difference
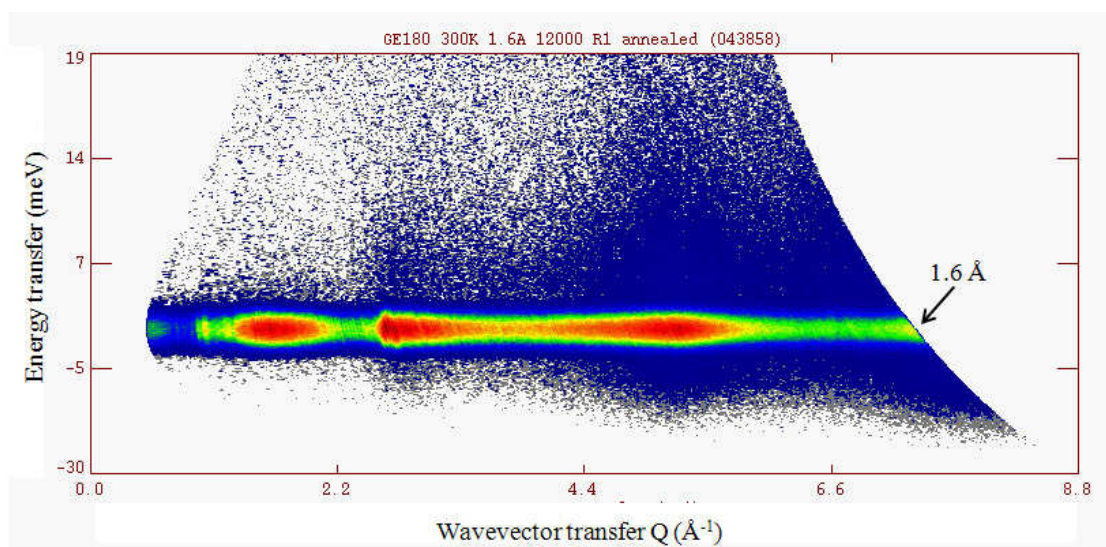
Figure 6. Wide dynamic range plot of E (meV) vs. Q (Å^{-1}) taking with an incident neutron wavelength of 1.6 Åat 298 °K. One can see a diffraction pattern which largely resembles the main component of the glass, SiO_2. Since this diffraction is at relatively high Q, it could be largely reduce with coarse collimation after the ^{3}He cell. Furthermore, this diffraction is nearly purely elastic in nature. (Color online)
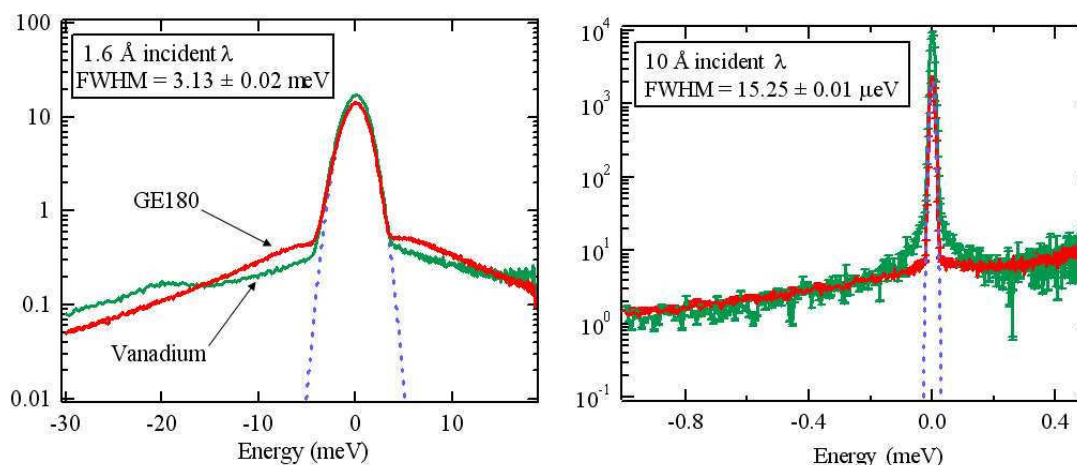

Figure 7. An example spectrum from GE180 (red) on TOFTOF spectrometer at MLZ. Left is a broad dynamic range/ low resolution scan which shows little inelastic contributions at large energy transfer. Right is a high resolution scan which shows that to the highest available resolution of TOFTOF, using GE180 one recovers the pure instrumental resolution. For comparison on both graphs a Vanadium sample (green) is also ploted, in the high enegy resolution graph to the right, GE180 is the lower curve. Neither data set has been scaled. (Color online)

in the spectra could be observed. Furthermore no appreciable structure or excitations from the glass were observed as can be seen in the the 1.6 Å spectrum at 298 °K shown in figure 6. By looking at the energy slices of this data for the two extreme incident energies, corresponding to 1.6 Å (left), and 10 Å (right) in figure 7, one sees that the GE180 scattering is largely elastic, and the pure instrument resolution of TOFTOF down to the minimum value of 15 μeV is readily recoverable as seen by the comparison to a vanadium sample. Future tests will compare the absolute levels of scattering from other possible wide angle ^{3}He cell materials, namely pure quartz and single crystal silicon to that of GE180.

6. Conclusions

Work is steadily progressing towards the realization of complete Magic-PASTIS wide angle polarization analysis system for neutron spectroscopy. The Magic-PASTIS magnetic cavity will be tested and optimized and the GE180 cells will be prototyped and prepared. Once the critical mass of components is available we will proceed with neutron sample measurements and data collection and analysis techniques.

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