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The Mushroom neutron spectrometer

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Abstract

This paper presents a concept for a new type of in-direct time of flight cold neutron spectrometer called Mushroom. Mushroom has a unique pyrolytic graphite (PG) analyser/position sensitive detector geometry enabling a massive 2π steradians of continuous position sensitive detector coverage, emulating some of its direct geometry counterparts such as IN5 or LET. It has many advantages over its direct geometry cousins though, being much more compact and much less expensive to build, but its biggest advantage is the order of magnitude larger count rates for the same resolution. It is envisaged it will be used to map out the 4 dimensional $S(Q,\omega)$ of single crystals in a matter of hours rather than days. Its design is aimed at minimising background and also uniquely allows easy selection of analyser reflection order PG002 or PG004. This paper presents details of the design along with full simulations of its potential performance using ray tracing software.

1. Introduction

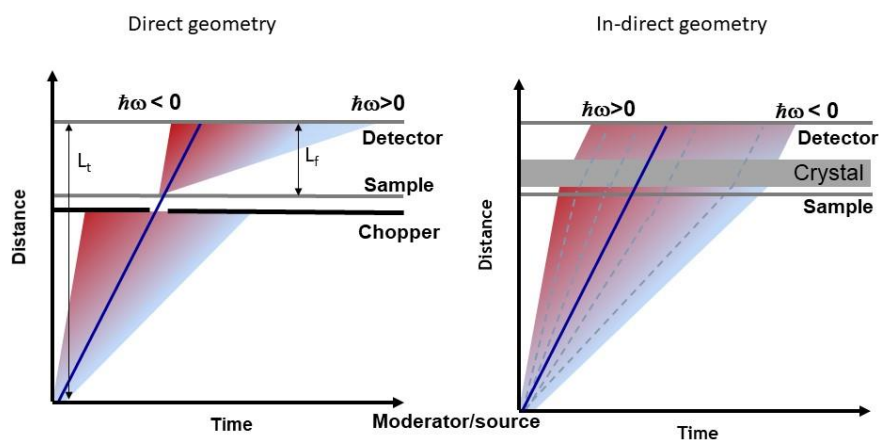
The cold neutron direct-geometry (see figure 1 for meaning) time-of-flight (TOF) spectrometer is seen as an essential neutron instrument existing at nearly every neutron facility (CNCS at SNS (1), IN5 at ILL (2), LET at ISIS (3), DCS at NIST (4), TOFTOF at FRM-II (5), AMATERAS at J-PARC (6)). One of the big advantages the Direct Geometry Spectrometer (DGS) is the ability to have a very large virtually continuous detector array, both in and out of plane often covering nearly π steradians of solid angle. This enables large swathes of $S(Q,\omega)$ space to be measured in one shot. A fairly recent capability of these instruments thanks to the development of software such as HORACE (7), is to map out the complete $S(Q,\omega)$ space for single crystals samples (at least for the latest generation using position sensitive detectors). This is achieved by making many measurements at different rotation angles of the crystal and then combining all these measurements into a single $S(Q,\omega)$ using the HORACE software. A typical experiment would make 90 measurements with the sample rotated by 1 degree around a vertical axis for each measurement. The resultant $S(Q,\omega)$ file (typically around 150 Gb) contains all the inelastic processes within the Brillouin zone and one can make 2 dimensional slices or 1 dimensional cuts in any direction from this data. There is increasing demand to do such measurements and instruments such as LET (3) and MERLIN (8) at the ISIS facility now spend the majority of beam time mapping $S(Q,\omega)$ for single crystals. However such measurements are very time consuming, typically taking a day or two to do a single scan, so it is not well suited for parametric studies.

39 Another issue with the DGS stems from the fact that energy resolution is predominantly
40 dependent on the sample to detector distance (9). Thus to achieve a reasonable resolution
41 the instruments are very large with massive detector tanks and corresponding ^3He detector
42 areas. For example the LET instrument has 40 m^2 of ^3He position sensitive detectors set 3.5
43 m away from the sample. Not only do they take up large areas of real estate which can be
44 problematic but since 2009 the cost of ^3He has sky rocketed (10) making them prohibitively
45 expensive. Even if one could get the money, simply getting hold of such large volumes of ^3He
46 is very difficult these days. This has been dubbed the 'Helium-3 crisis' and because of this
47 there has been a concerted effort to find new detector technologies, in particular ^{10}B thin film
48 technologies (11) which will be used for two new DGS at the ESS (12), called CSPEC (13) and
49 T-REX (14).

50 All of these DGS issues are circumvented with the new instrument concept presented in this
51 paper called the Mushroom shown in figure 2. The Mushroom is an In-direct Geometry
52 Spectrometer (IGS) (see figure 1 for meaning) utilising a large mushroom shaped pyrolytic
53 graphite (PG) analyser scattering to a relatively small position sensitive detector array.
54 Mushroom is designed to emulate a DGS like IN5 or LET in that it can detect neutrons
55 scattered over a large solid angle both in and out of plane with continuous position sensitive
56 coverage. It should be emphasised that in this aspect the Mushroom is very different from
57 multi analyser systems being used on triple axis instruments such as flatcone (15) (16) or the
58 new PUMA type multi analyser (17). These systems utilise multiple individual analysers in a
59 single scattering plane and cover a relatively small solid angle.

60 It will be shown that the Mushroom is very compact and cheap compared to its DGS
61 counterpart and in particular that it has an order of magnitude higher count rate for the same
62 energy resolution. This potentially means that a full $S(Q,\omega)$ scan could be done in hours rather
63 than days opening up the possibility of parametric studies and measurements on smaller
64 samples.

65 The rest of this paper gives details and performance of Mushroom including full Monte Carlo
66 simulations using the ray tracing software McStas (18).



67

68

69 Figure 1 Distance time diagrams showing direct geometry (left) with monochromatic incident neutron beam on
 70 sample (usually from mechanical choppers) and a spread of final energies on detector . In-direct geometry (right)
 71 with white beam on sample but monochromatic final energy neutrons on detectors determined by crystal
 72 analyser. Both techniques use time of flight (TOF) to determine energy transfer to sample.

73

74 2. The Mushroom instrument description

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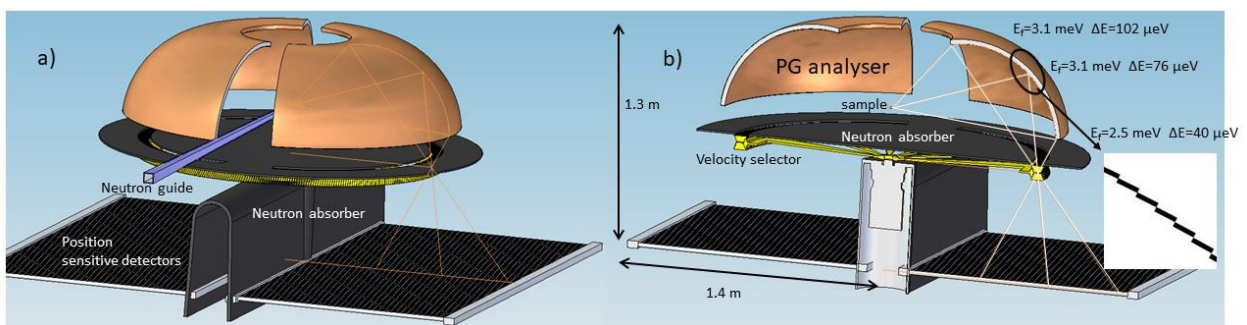
76 The interesting and unique part of the Mushroom spectrometer is the analyser/detector
 77 geometry. The primary part of the spectrometer such as guides and choppers (delivering
 78 neutrons to the sample) are standard and details are not presented in this paper as they are
 79 not important to the Mushroom concept. In the following description the parameters are just
 80 stated, the justification for them come later in the paper. Figure 2 shows the Mushroom
 81 instrument with two large PG analysers, one either side of the sample. Each PG analyser is
 82 made from individual flat PG crystals measuring $1 \times 1 \text{ cm}^2$ with a mosaic spread, μ . Two values
 83 μ are studied in this paper, either $\mu = 0.5^\circ$ or $\mu = 0.8^\circ$, both values readily available commercially.
 84 The analysers cover a continuous range of scattering angles $2\theta = 10^\circ - 170^\circ$ horizontally and
 85 $\phi = -5^\circ - 50^\circ$ vertically around the sample. Providing enough space for sample environment
 86 equipment limits the maximum vertical value of ϕ to around 50° , this allows for a standard
 87 40 cm diameter 'ISIS' flange.

88 Most importantly every point on the analyser will scatter to a unique point on the position
 89 sensitive detector which forms a horizontal sheet 90 cm below the sample position. The
 90 detectors are position sensitive ^3He tubes, 1.2 m long and 1 cm diameter. This simple
 91 arrangement allows for the first time a massive 2π steradians of continuous in and out of
 92 plane detector coverage in an IGS.

93 Figure 2b shows a vertical section through the sample, analyser and detector. This figure
 94 shows that all scattered neutrons from any vertical angle pass through a radial focal point 85
 95 cm from the sample origin and 28 cm below. There is a 4 cm wide radial opening in the
 96 neutron shielding centred on this focal radius through which the neutrons pass. The neutrons
 97 then pass through a rotating velocity selector before reaching the detector. The velocity
 98 selector is a large disk (85 cm radius) spinning around a vertical axis. At the edge of the disk
 99 there are many flat neutron absorbing blades set at an angle of 14° off vertical. When spinning
 100 at 30 Hz this velocity selector lets through only the PG002 order and at 60 Hz the PG004 is
 101 selected. Focusing all the neutrons through a small opening in the shielding and then passing
 102 through a velocity selector is a critical part of the design in reducing background and possible
 103 spurious signals as well as cleanly separating the different orders scattered from PG. More on
 104 this will be said later.

105 Initially one may think that the vertical loci of the analyser must be elliptical in shape as it
 106 focuses all neutrons from one point (the sample) to the focal point at the velocity selector.
 107 However, a truly elliptical shape is not desirable as it would cause a large variation in the
 108 analysed energy, E_f , and corresponding energy resolution in going from the lowest to highest
 109 vertical angle ϕ . Instead, specially written software starts laying down crystals vertically one
 110 at a time starting with the highest angle at $\phi=50^\circ$ which is set at 50 cm from the sample. The
 111 angle of each crystal is adjusted such that it reflects neutrons to the focal point, but a crystal
 112 can vary its position along the line bisecting the sample to crystal and crystal to the focal point.
 113 Each crystal is allowed to move by up to 3 mm relative to the crystal before it in order to try
 114 and keep the analysed energy constant. So moving a sample further away reduces E_f or
 115 moving it closer increases it. Using this method the spread of E_f is kept much smaller ranging
 116 from around 2.5 meV from the bottom of analyser ($\phi=-5^\circ$) to 3.1 meV at $\phi=50^\circ$ for the PG002
 117 reflection.

118



119

120

121 *Figure 2 Engineering drawing of the Mushroom showing the essentials of the instrument. A vertical slice through*
 122 *the instrument b) shows some neutron ray paths from sample to analyser to detector along with the analysed*
 123 *energy E_f and energy resolution of the elastic line ΔE . The inset in b) shows a close up of how the crystals are*
 124 *stepped relative to each other. Each crystal is 10 mm long and 2 mm thick.*

125

126 Other possible analyser/detector geometries of the instrument have been studied but the
127 one presented in figure 2 shows the most promise in terms of Q resolution, background and
128 simplicity.

129

130 3. Performance and instrument simulations

131

132 In the following the simulated performance of the energy resolution, Q resolution and count
133 rate of the Mushroom instrument is presented, along with a discussion of backgrounds. Full
134 simulations were performed using the ray tracing software McStas (18). A moderator to
135 sample distance of 25 m was chosen to be the same as the DGS LET (3) at ISIS to which
136 comparisons are made. The sample size chosen for the Mushroom is 1x1x1 cm³ matching the
137 1x1 cm² size of the individual PG crystals and similarly the detector pixels were chosen to be
138 1x1 cm² in size. There was no component in McStas for the large Mushroom analyser so a
139 new one was written which was a modification to the existing
140 'Monochromator_curved.comp' (19). The McStas simulations were output in a standard
141 nexus file format which can be directly loaded into the software Mantid (20) (21), which is
142 used by many neutron facilities for data reduction and analysis. Within Mantid a file is
143 uploaded giving the E_f and distance from sample to every detector pixel for the Mushroom
144 instrument. One can use then utilise all the standard routines in Mantid to reduce and
145 visualise data just as one does for the real spectrometers.

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147 3.1 Energy resolution

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149 Assuming the contributions are not correlated the energy resolution for an inverted TOF
150 spectrometer like the Mushroom can be written as (22),

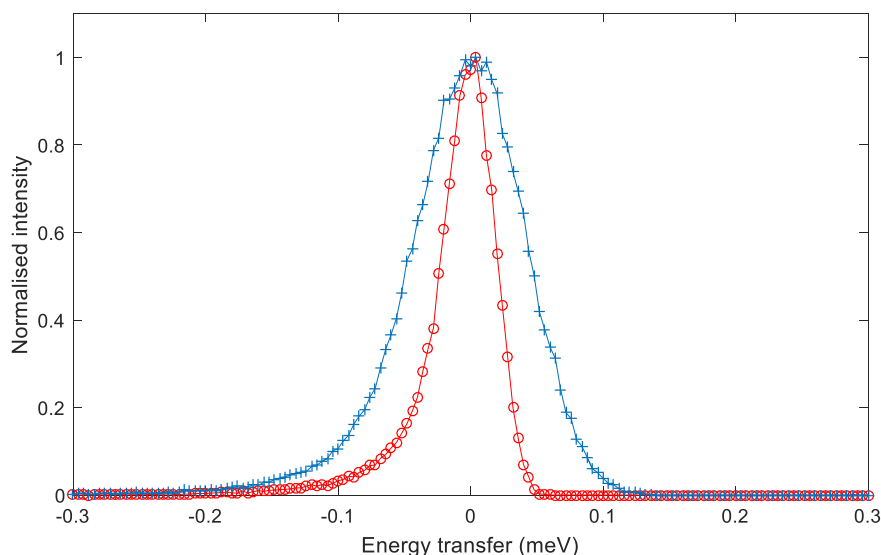
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$$152 \Delta E = 2 \sqrt{E_i^2 \left[\left(\frac{\Delta t_i}{t} \right)^2 + \left(\frac{\Delta L}{L} \right)^2 \right] + E_f^2 \left[\left(\frac{\Delta t_f}{t} \right)^2 + \left(\frac{\Delta d}{d} \right)^2 + (\cot \theta \Delta \theta)^2 \right]} \quad (1)$$

153 where Δt_i and ΔL are the time and distance uncertainties in the primary spectrometer. The
154 time uncertainty comes mainly from the moderator pulse width which is around 110 μ s for
155 the coupled hydrogen moderator at ISIS at 3 meV. ΔL comes mainly from path uncertainties
156 due to guide reflections and can be neglected (23). L is the total length of instrument from
157 the moderator to the detector (25 m from moderator to sample) and t is the tof of the
158 neutron. Δt_f is any time uncertainty in the secondary spectrometer from things such as sample
159 and detector size but is so small compared to the final term it can be ignored. $\Delta d/d = 6 \times 10^{-4}$
160 (24) is the lattice spacing uncertainty of the PG crystals and θ is the Bragg angle of the
161 analysed beam from the crystal which for the Mushroom varies from 55.0° in plane (giving
162 E_f=2.7meV) to 50.7° at $\phi=50^\circ$ the largest vertical scattering angle (giving E_f=3.1meV). The

163 uncertainty in the Bragg angle $\Delta\theta$ is from both the mosaic spread of the crystals, μ , and the
164 angular spread due to the sample size, $\Delta\theta_{\text{sam}}$, such that $\Delta\theta = \Delta\theta_{\text{sam}} * \mu$. Whilst the mosaic spread
165 is fixed the value of $\Delta\theta_{\text{sam}}$ changes with vertical angle ϕ due to the variation in the sample to
166 analyser distance (95 cm at $\phi=0^\circ$ to 50 cm at $\phi=50^\circ$). This is the reason for the worsening
167 energy resolution with increasing ϕ shown in figure 2b. Figure 3 shows McStas simulations of
168 the elastic line both in plane, $\phi=0$, and at a $\phi=45^\circ$ for a mosaic spread $\mu=0.5^\circ$ for the PG002
169 reflection giving full width half maximum (FWHM) resolutions of 46 μeV and 97 μeV
170 respectively, very close to the expected resolutions of 52 μeV and 97 μeV using equation 1.
171 The asymmetry in the elastic line shape shown in figure 3 is due to the moderator component
172 which is very asymmetric for the coupled hydrogen moderator used in the simulations.

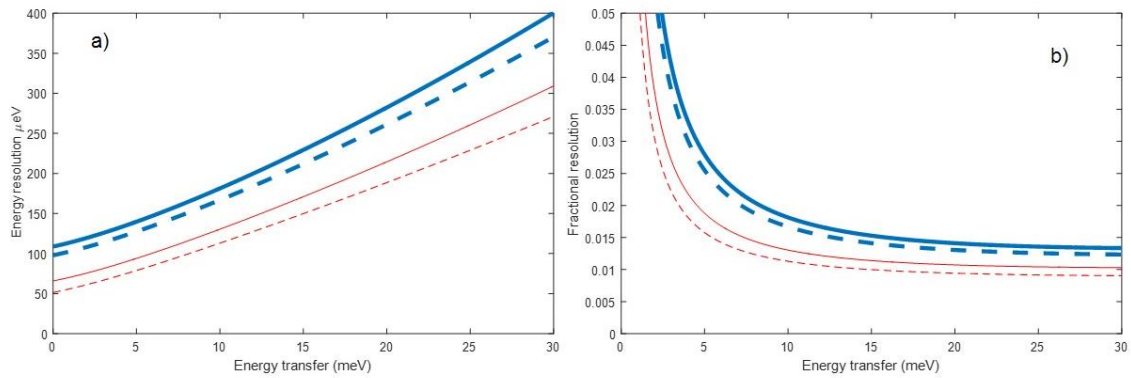
173 All the terms in equation 1 are important for high resolution backscattering spectrometers
174 such as IRIS (25) or OSIRIS (26) where the final term in equation 1 vanishes as θ goes to 90° .
175 The Mushroom is well away from backscattering and the final term dominates at the elastic
176 line. However, at higher energy transfers the first term in equation 1 starts to dominate.
177 Figure 4 shows the calculated energy resolution of the Mushroom versus energy transfer
178 (E_{tran}) for neutron energy loss.



179

180 Figure 3. Simulated elastic resolution for PG002 of Mushroom with $\mu=0.5^\circ$. The maximum intensity has been
181 normalised to 1. The circles show data in plane ($\phi=0^\circ$) with a 46 μeV resolution. Crosses show $\phi=45^\circ$ with a
182 resolution of 97 μeV .

183



184

185

186 Figure 4 Calculated energy resolution a) and fractional energy resolution $\Delta E/E_{\text{tran}}$ b). The solid lines represent
 187 $\mu=0.8^\circ$ and dashed $\mu=0.5^\circ$. Thick lines are at $\phi=45^\circ$ while thin lines are at $\phi=0^\circ$.

188 The energy resolution can be improved further at higher energy transfers by increasing the
 189 moderator to sample distance which reduces the first term in equation 1. This will have little
 190 effect on the sample flux as a good modern guide should transport it with only small losses.
 191 So ideally one should increase L to be as long as possible to fill the time frame, with the final
 192 length depending on the energy transfer range required and the repetition rate of the source.
 193 Figure 4b shows that even at a relatively short distance of 25 m the Mushroom has an
 194 excellent energy resolution, with a fractional energy resolution $\Delta E/E_{\text{tran}} \approx 1\%$ over much of its
 195 range.

196

197 3.2 Q Resolution

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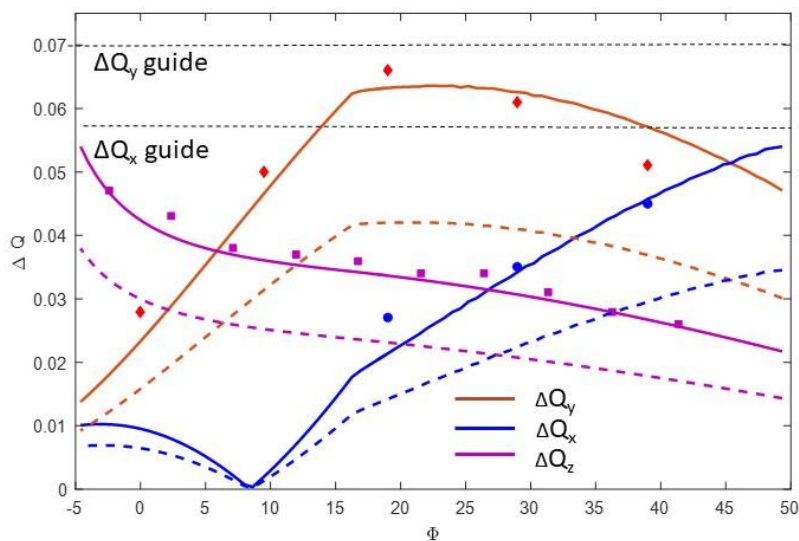
199 If the Mushroom is to fulfil its purpose of mapping out the 4D Brillouin zone for single crystals
 200 then it is crucial it has a reasonable Q resolution. Unlike a DGS where the neutrons scatter
 201 directly from the sample to the detector, for the Mushroom they reach the detector via the
 202 PG analyser which has a mosaic spread μ . For this reason the Q resolution of the Mushroom
 203 will not be as good as its DGS counterparts but with careful design respectable Q resolutions
 204 can be obtained as will be demonstrated. One could simply choose crystals with a very low
 205 mosaic spread but this reduces the spectrometers detector count rate as the wavelength
 206 spread 'analysed' by the PG crystals is given by $\Delta\lambda_{\text{PG}} = \lambda_{\text{PG}} \cot\theta \cdot \mu$. It's the usual case of
 207 resolution versus count rate. Also there is no point in making μ much smaller than $\Delta\theta_{\text{sam}}$ as
 208 this will then dominate the Q resolution. Ideally one matches them such that $\mu = \Delta\theta_{\text{sam}}$ but for
 209 the Mushroom $\Delta\theta_{\text{sam}}$ varies with vertical scattering angle from $\approx 0.5^\circ$ in-plane to $\approx 1^\circ$ at 50°
 210 scattering angle. In the simulations presented in this paper the values of μ are 0.5° and 0.8°
 211 as they are both commercially available and also approximately match $\Delta\theta_{\text{sam}}$.

212 The aim is to optimise the Q resolution of the secondary spectrometer so for now
 213 contributions from the primary are neglected. In the McStas simulations presented this is
 214 achieved by using a perfectly collimated incident beam. The three components of the Q
 215 resolution are the vertical component, ΔQ_y , the component along the incident beam, ΔQ_z , and
 216 the component perpendicular to the incident beam but in plane ΔQ_x (perpendicular to both

217 ΔQ_y and ΔQ_z). Each of these components is a function of both θ and ϕ , thus giving many
218 thousands of values in the highly pixelated detector. To simplify the optimisation all
219 simulations were performed at $2\theta=90^\circ$, representing a vertical strip in the middle of the
220 analyser/detector bank. There are 4 parameters to optimise in this instrument geometry, the
221 distance R to the first crystal ($\phi=50^\circ$), the value of E_f from this crystal which defines the line
222 on which the focal point, FP, will lie, the distance along this line to FP and finally the vertical
223 distance the detectors sit below FP is Y_{det} . Specially written software scans through this 4
224 dimensional phase space numerically calculating values of $\Delta Q_y(\phi)$, $\Delta Q_z(\phi)$ and $\Delta Q_x(\phi)$ at every
225 point along ϕ . The maximum values $\Delta Q_y(\phi)^{\text{max}}$, $\Delta Q_z(\phi)^{\text{max}}$ and $\Delta Q_x(\phi)^{\text{max}}$ are recorded at each
226 point in the 4D phase space and the best set of parameters was chosen as the set which
227 minimised the sum of the squares $\Delta Q_{\text{tot}}^2 = (\Delta Q_y^{\text{max}})^2 + (\Delta Q_x^{\text{max}})^2 + (\Delta Q_z^{\text{max}})^2$. The software
228 numerically calculating the three components by simply calculated the FWHM spread of the
229 neutron beam at the detector as a function of ϕ for each PG crystal, incorporating the effects
230 of mosaic spread, sample size and angle the beam hits the detector. The spread along the z
231 direction on the detector converts to ΔQ_z while the spread along x direction converts to ΔQ_x
232 and ΔQ_y . Although rather crude in that it does not account for possible correlations, it is very
233 fast and allows a rapid transit through the large phase space which would not be feasible in a
234 reasonable time frame with simulations. Justification for the simple technique is shown in
235 Figure 5 showing the numerical calculations for the optimised Mushroom along with full
236 McStas simulations of these components. It can be seen there is good agreement between
237 the two techniques. The McStas simulations used a virtual sample which creates perfect one
238 dimension rods in Q space, either vertically or horizontally. These rods are broadened due to
239 instrumental effects giving the Q resolution. The data was reduced in Mantid (described
240 earlier) and the width of the Q rods was then fitted with a Gaussian function and the FWHM
241 of this versus ϕ is presented in Figure 5.

242 It was found during the optimisation process that the Q resolution asymptotically improves
243 with R , which is to be expected as the effect of sample size gradually reduces with increasing
244 R . However, the cost of the analyser will go as R^2 so in the end R was fixed at 0.5 m giving a
245 contribution to the Q resolution less than that given by the guide divergence and a reasonable
246 cost and size for the Mushroom analyser. This is in much the same way that the energy
247 resolution improves with sample to detector distance in a DGS but cost and size limits the
248 distance chosen. The optimisation program always keeps FP close to the PG analyser which
249 reduces beam spreading from the PG mosaic thus improving Q resolution. At FP the vertical
250 beams all converge and a detector here, $Y_{\text{det}}=0$, would have no Q resolution. On increasing
251 Y_{det} then ΔQ_x and ΔQ_y improve with the increased resolving power as the beams diverge away
252 from FP. This also reaches an asymptotic limit due to the opposing effect of increased beam
253 spread with increasing Y_{det} . As Y_{det} increases scattering from the smallest ϕ reaches the
254 detector closer and closer to zero radius rapidly degrading ΔQ_z as can be seen in figure 5. A
255 reasonable balance between ΔQ_z increasing and ΔQ_x , ΔQ_y decreasing with increasing Y_{det}
256 occurs when $Y_{\text{det}} \approx 90$ cm. Similarly the program optimised E_f around 3 meV which creates an
257 analysed beam which on average is coming vertically down so hitting the flat horizontal
258 detector as perpendicular as possible. The Q resolution could in principle be further improved
259 if the detectors were not flat but on circular loci around FP. Then the beam would always hit
260 the detectors perpendicularly thus reducing beam spread and ΔQ_z would not degrade so

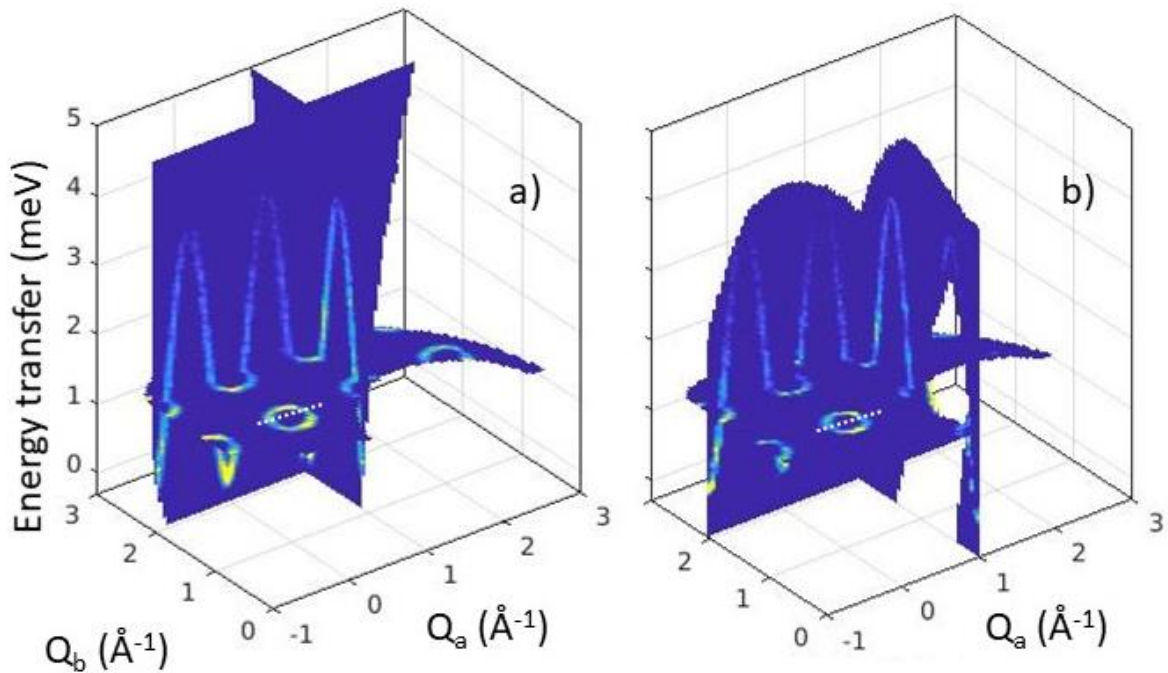
261 much at low ϕ . However, with the aim of trying to keep the instrument simple and reasonable
 262 we will stick to the simple flat detector array.
 263



264
 265
 266 Figure 5. The three components of the Mushroom Q resolution at $2\theta=90^\circ$ versus the vertical angle ϕ . Solid lines
 267 represent the simple numerical calculations for $\mu=0.8^\circ$ and dashed lines represent $\mu=0.5^\circ$. The square markers
 268 represent the results of full simulations at $\mu=0.8^\circ$. The thin dashed lines at the top show the uncertainty in ΔQ_x
 269 and ΔQ_y due to the incoming guide for 3 meV neutrons.
 270

271 To see how well the optimised version of the Mushroom instrument performs a full McStas
 272 simulation was done on a virtual crystal with a 2 dimensional (2D) spin wave in the x-z plane
 273 (dispersion less along y). The spin wave had a periodicity of 1\AA^{-1} in both x and z directions and
 274 had a band maximum of 4 meV. It is not possible to do a direct simulation comparison with a
 275 DGS like LET as they are very different instruments but simulation parameters for LET were
 276 chosen be reasonable values for such an experiment. So an incident energy of $E_i=5$ meV was
 277 picked, to just cover the 4 meV band maximum, and the final monochromating chopper spun
 278 at 300 Hz (maximum) giving an energy resolution at the elastic line of about 100 μeV
 279 compared to Mushrooms 46 μeV . The Mushroom was put on the end of the LET guide
 280 (choppers removed) which has a moderator to sample distance of 25 m. The simulations
 281 involved a HORACE scan of the virtual 2D crystal through 90° in 1° steps and then the
 282 simulated data was reduced and analysed in exactly the same way we would with
 283 experimental data from the real instruments.

284 Figure 6 shows the results of the Mushroom and LET simulations in 3 dimensions, with the
 285 momentum transfer in plane, Q_a and Q_b , and energy transfer. The simulations show that
 286 Mushroom performs well and gives similar results compared to LET.



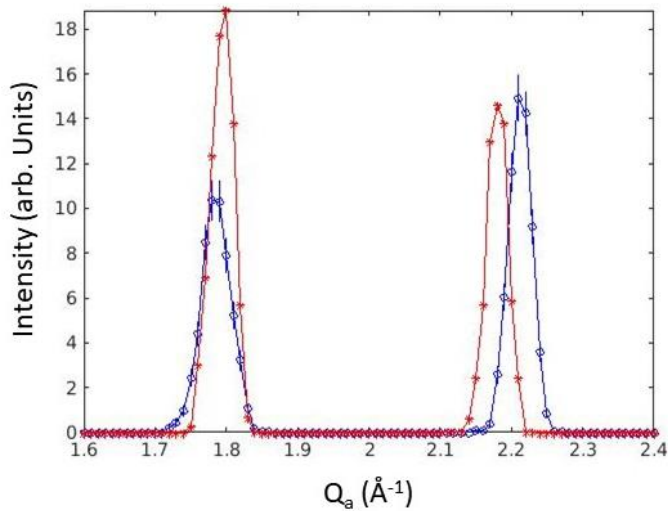
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289 *Figure 6. Full McStas simulations of 2D spin waves in a crystal with a periodicity of 1 \AA^{-1} along Q_a and Q_b and a 4*
290 *meV band maximum. The simulations are for a) Mushroom and b) LET. The white dashed line shows the cut*
291 *shown in figure 7.*

292

293 A more detailed comparison is presented in figure 7 showing simulated data along an identical
294 cut, indicated by the dashed line in figure 6. The cut has a width of 0.1 \AA^{-1} along Q_b and 0.1
295 meV in energy transfer. It can be seen that the Q resolution of Mushroom is only slightly
296 worse than LET. Like most inelastic spectrometers the LET guide has a large incident beam
297 divergence to increase sample flux. At 3meV the incoming momentum uncertainty due to the
298 incident divergence is $\Delta Q_x=0.058 \text{ \AA}^{-1}$ and $\Delta Q_y=0.07 \text{ \AA}^{-1}$ as shown by the dashed horizontal lines
299 on figure 5. These values are similar to the momentum uncertainties due to the Mushroom
300 secondary spectrometer and therefore it is not surprising that the Mushroom Q resolution is
301 only slightly worse than LET. It can be seen in figure 7 that there is a slight discrepancy in the
302 second peak position between LET and Mushroom. The Mushroom peak is in the correct
303 position but the reason for the slight discrepancy in the LET peak position is not understood.
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319 *Figure 7. A cut through the simulation shown in figure 6 as indicated by the dashed line at $Q_b=1$ and energy*
 320 *transfer of 1.5 meV. Mushroom data is represented with the circles and stars LET. The intensity is arbitrary and*
 321 *has been scaled so they are roughly the same height.*

322

3.3 Count rate

323

324 When comparing the performance of spectrometers the incident neutron flux on the sample is often
 325 given as one of the performance criteria. However, this is a useless measure when comparing
 326 Mushroom to a DGS with one having a monochromatic incident beam and the other a whitebeam.
 327 The important measure is the detector count rate for the same sample, resolution and solid angle. In
 328 this section it is shown that the Mushroom has much higher detector count rates than a DGS using the
 329 same neutron guide. This is because indirect geometry machines are much more efficient than direct
 330 geometry which stems from the fact that energy resolution of indirect instruments comes from the
 331 full instrument length whereas it's predominantly the much shorter length of the secondary
 332 spectrometer in DGS instruments.

333 A simple analytical argument is given below which is then backed with simulations. The energy
 334 resolution, ΔE , of an indirect and direct geometry instrument are given by equations 2 and 3
 335 respectively.

336

337 $\frac{\Delta E}{E_i} = \frac{2\Delta t^i}{t_t^i}$ 2) $\frac{\Delta E}{E_f} = \frac{2\Delta t^d}{t_f^d}$ 3)

338 The superscript 'i' and 'd' denotes in-direct and direct respectively. Δt^i and Δt^d is the total time
 339 spread/uncertainty at the detectors due to all the resolution components. E_i and E_f are the incident
 340 and final neutron energy and t_t^i is the total time of flight (moderator to detector) and t_f^d is the time of
 341 flight from sample to detector. At the elastic line such that $E_i = E_f$ and for equal energy resolutions
 342 equation 2 and 3 combine to give

343 $\frac{\Delta t^i}{\Delta t^d} = \frac{t_t^i}{t_f^d}$ 4)

344

345 The Mushrooms energy resolution is dominated by the mosaic spread of the PG crystals (shown in
346 section 3.1) which take a wavelength spread $\Delta\lambda^i$ from the scattered beam. One can express Δt^i in
347 equation 4) in terms of $\Delta\lambda^i$ such that

$$348 \quad \Delta t^i = t_t^i \Delta\lambda^i / \lambda \quad 5)$$

349

350 Similarly for a DGS spectrometer like LET one can express Δt^d in equation 4) in terms of the wavelength
351 spread $\Delta\lambda^d$ taken by the final monochromating chopper such that

$$352 \quad \Delta t^d = t_t^d \Delta\lambda^d / \lambda \quad 6)$$

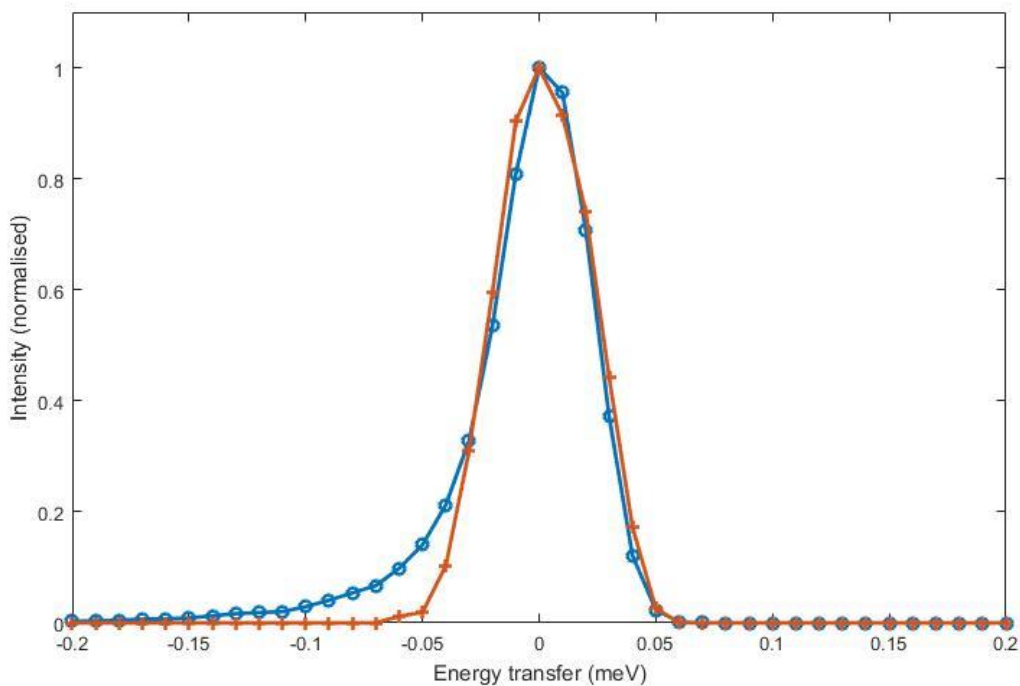
353 This assumes that the resolution is dominated by the final chopper term which is usually the case
354 although not at very high energy resolutions. Combining equations 4), 5) and 6) we get

355

$$356 \quad \frac{\Delta\lambda^i}{\Delta\lambda^d} = \frac{t_t^d}{t_f^d} = \frac{L_t^d}{L_f^d} \quad 7)$$

357 The ratio of the detector count rates for the indirect over the direct spectrometer is given by $\Delta\lambda^i/\Delta\lambda^d$
358 as this represents the wavelength spread taken from the moderator for each spectrometer for an
359 equivalent energy resolution. As $L_t^d \gg L_f^d$ we can immediately see that the indirect machine 'extracts'
360 far more flux for the same resolution as the direct machine. Typical $L_t^d / L_f^d \approx 10$ for cold neutron
361 spectrometers like LET, AMATERAS and CNCS. This does not take into account any losses due to
362 reflectivity of the crystals but for the Mushroom this loss is small as PG crystals have a high reflectivity
363 of $\approx 90\%$.

364 To check this result simulations have been performed comparing the detector count rates for
365 Mushroom and LET. In the simulations the Mushroom has again been put on the end of the LET
366 neutron guide and both instruments used a $1 \times 1 \times 1 \text{ cm}^3$ vanadium sample scattering to exactly the same
367 solid angle of $5 \times 5^\circ$ and both had the same resolution at the elastic line of $48 \mu\text{eV}$. To achieve this
368 resolution on LET the incident energy was set to $E_i = 2.8 \text{ meV}$ which is the same as the final energy of
369 the Mushroom (in plane) and the final chopper was run at 260 Hz with a 28 mm opening. This is an
370 optimal setup for LET. Figure 8 shows the simulation of the elastic line for both instruments and
371 demonstrates the same energy resolution. The intensities have been normalised to 1 for easy
372 comparison. It can be seen that Mushroom has a 'tail' on the neutron energy gain side which was
373 discussed in section 3.1 as being due to the asymmetric moderator component. The LET spectrometer
374 has a 'tail cutting' chopper at the start of the instrument which eliminates this feature. In the
375 simulations Mushroom had a count rate of 12.40 neutrons per second on the detector while LET had
376 1.52 neutrons per second. This means Mushroom had an increased count rate of $8 \times$ LET for exactly
377 the same sample, resolution and solid angle. Using equation 7 where $L_t^d = 28.5 \text{ m}$ and $L_f^d = 3.5 \text{ m}$ the
378 expected gain is also around 8 . It should be remembered that the Mushroom has $2 \times$ the solid angle of
379 LET with detectors on both sides so the real gain for most samples will be more like 16 . The overall
380 gain though must take into account losses from the velocity selector which is shown in the next
381 section. Taking these losses into account the overall gain of the Mushroom is closer to $\approx 10 \times$ LET.



382

383 *Figure 8. The elastic line for Mushroom (circles) and LET (crosses). The energy resolution of LET has been set equal*
 384 *to Mushroom and both have been normalised to a peak intensity of 1.*

385

386

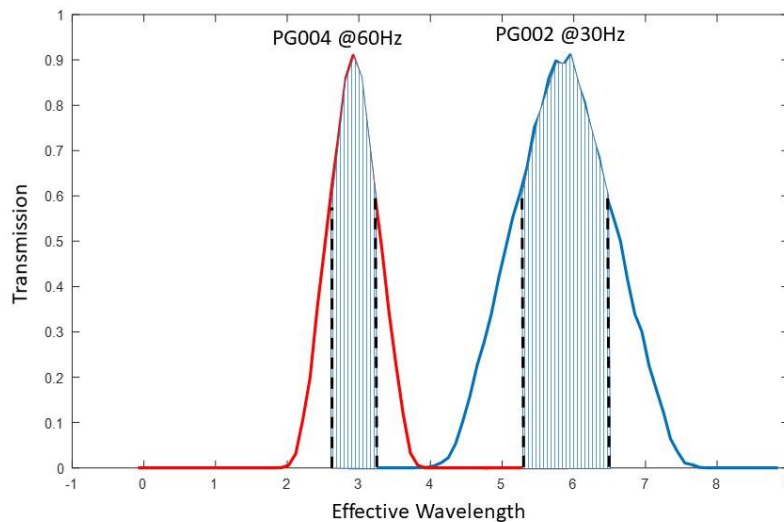
387 **3.4 Background and velocity selector**

388

389 Mushroom has been carefully designed such that the analysed neutrons are focussed through
 390 a small radial opening where it passes through a velocity selector. There are two reasons for
 391 this important design feature, the first being that passing the neutrons through a radial point
 392 enables the construction of a velocity selector as shown in figure 2. This velocity selector
 393 enables the clean selection of either the PG002 or PG004 reflection by running the velocity
 394 selector at 30 or 60 Hz respectively. The velocity selector does not need to be phased to any
 395 timing signal and even the frequency does not need great accuracy so it is simple to run. The
 396 neutron absorbing blades of the selector have a 5 mm pitch at their centres and are 8 cm long
 397 and set at an angle of 14° off vertical. On average the neutrons pass vertically down through
 398 the selector from the analyser but with a range of $\approx \pm 30^\circ$ off vertical for neutrons coming from
 399 the highest and lowest analyser angles. The off vertical angle lowers the vertical velocity
 400 component (increasing the effective vertical wavelength component) through the selector
 401 and reduces the probability of it being transmitted. The velocity selector was designed such
 402 that it is 'sloppy' enough to boost the transmission over the desired wavelength range but
 403 just 'tight' enough to stop the transmission of other orders. This can be seen in figure 9 which
 404 shows the transmission versus the vertical component wavelength for the velocity selector.
 405 The striped area represents the effective wavelength range from the Mushroom analyser
 406 showing that the transmission peaks at $\approx 90\%$ and drops to around 60% at the extremes. The

407 velocity selector has clear advantages over a Beryllium filter in that it can cleanly select PG002
408 or PG004 whereas the Beryllium filter can only select PG002. Also the velocity selector acts as
409 both a high and low pass filter compared to the low pass Beryllium filter, thus reducing
410 possible backgrounds.

411 The second important reason for this design is to minimise background and possible spurious
412 signals. The main contribution to the background from PG crystals comes from thermal diffuse
413 scattering (25). One way to reduce this effect is to cool the PG crystals as is done on the IRIS
414 and OSIRIS spectrometers and in principle could also be done with the Mushroom analyser.
415 Another way to reduce the diffuse scattering reaching the detectors is to minimise the solid
416 angle view of the analyser from the detector which is precisely what the Mushroom geometry
417 does very effectively. Each point on the detector can only see a very small section of the
418 analyser looking through both the collimator blades and the radial ring. The collimation is not
419 just spatial but also temporal as the velocity selector will reduce possible spurious signals
420 from neutrons with the wrong final energy. Although this design does as much as possible to
421 reduce backgrounds it should be noted that the Mushroom instrument like any indirect
422 instrument will still not have backgrounds as low as DGS instruments like LET which have
423 monochromatic incident beams and effects of scattering from analysing crystals.



424
425 *Figure 9. Transmission of the velocity selector versus the vertical component of the wavelength or 'effective'*
426 *wavelength. The striped regions represent the effective wavelength range from the Mushroom analyser. To select*
427 *the PG002 or PG004 reflection the velocity selector is run at a frequency of 30 or 60 Hz respectively.*

428
429 **4. Summary and discussion**

430
431 This paper has presented a concept for an in-direct tof spectrometer called Mushroom which
432 has a massive 2π steradians of continuous position sensitive detector coverage, emulating

433 some of its direct geometry counterparts such as IN5 or LET. It has advantages over its direct
434 geometry cousins, such as being much more compact with the Mushroom having a radius of
435 just 1.4 m. It is also much cheaper as massive areas of ^3He position sensitive detectors are not
436 needed. The Mushroom needs needs 1.7 m² of PG crystal analyser to cover π steradians of
437 solid angle (similar to LET) costing \$1.2 M to \$1.8 M depending on whether 0.8° or 0.5° mosaic
438 crystals are used respectively and another \$0.5 M for the detector array. For the same solid
439 angle coverage a direct geometry instrument like LET needs around 40 m² of ^3He detectors
440 costing around \$10 M (27) at the time of writing (assuming 2.5 cm diameter tubes with 6 atm
441 ^3He pressure) and at least another \$1 M is needed for the very large detector tank. However,
442 the main advantage is its much higher count rate for the same resolution. It was shown that
443 the Mushroom will have about an order of magnitude higher count rate than LET, thus
444 allowing much more rapid mapping of $S(Q,\omega)$ space for single crystals. This opens up the
445 opportunity to do parametric HORACE scans or just to measure smaller crystals.

446 Minimisation of background was at the forefront of considerations when designing
447 Mushroom, particularly from the thermal diffuse scattering of PG crystals. The focussing
448 design of the analyser through a point at the velocity selector tightly collimates the beam
449 both spatially and temporally to maximise background reduction. In addition this design
450 enables the use of a mechanical velocity selector to easily select the PG order to use. Although
451 it is envisaged that PG002 will be used predominantly, PG004 would be selected if a larger Q
452 range is necessary although this comes at the price of worse energy and Q resolution. This is
453 in much the same way as you would increase E_i on a direct geometry instrument to increase
454 Q range, also at the expense of energy and Q resolution.

455 Mushroom has some limitations compared to a DGS. The mosaic spread of the PG crystals
456 degrades the Q resolution but the effect is minimal as large incoming beam divergences from
457 the neutron guides, necessary to increase the count rate on low counting inelastic
458 spectrometers, tend to dominate the Q resolution. Sample size will affect the energy
459 resolution of the Mushroom, and therefore it is vital that beam slits are used just before the
460 sample to define a beam size on sample. Mushroom will not have the flexibility of a DGS
461 where one can choose any incident energy and resolution within the mechanical limits of the
462 choppers, although the upshot of this is the simplicity of operation with just two modes to
463 choose from (PG002 and PG004). If it was built on a reactor source or a long-pulse spallation
464 source like the ESS then there is the possibility to use a pulse shaping chopper to vary the
465 resolution of Mushroom. Although much effort has gone towards minimising Mushroom
466 background it is never going to be as good as a direct geometry instrument like LET.

467 Finally there is no reason why Mushroom could not go onto a reactor source. One could
468 employ choppers to pulse the beam and use it in a time of flight mode as in this paper, but a
469 more efficient mode would probably use a PG monochromator. Just like a triple axis
470 instrument the Mushroom analyser would rotate around the monochromator to scan through
471 E_i and hence the energy transfer. Colleagues at FRMII are studying this possibility at present
472 (28).

473

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477

478 1. **G. Ehlers, A. A. Podlesnyak, J. L. Niedziela, E. B. Iverson, and P. E. Sokol.** 2011, *Review of Scientific*
479 *Instruments*, Vol. 82 085108.

480 2. **J. Ollivier, H. Mutka and L. Didier.** 2, 2010, *Neutron news*, Vol. 21.

481 3. **R.I.Bewley, J.W.Taylor and S.M.Bennington.** 1, 2011, *Nuclear Instruments and Methods in Physics*
482 *A*, Vol. 637.

483 4. **J.R.D.Copley, J.C.Cook.** 2-3, 2003, *Chemical Physics*, Vol. 292.

484 5. **Tobias Unruh, Jurgen Neuhaus, Winfried Petry.** 3, 2007, *Nuclear Instruments and Methods in*
485 *Physics A*, Vol. 580.

486 6. **Kenji Nakajima, Seiko Ohira-Kawamura, Tatsuya Kikuchi, Mitsutaka Nakamura, Ryoichi**
487 **Kajimoto, Yasuhiro Inamura, Nobuaki Takahashi, Kazuya Aizawa, Kentaro Suzuya, Kaoru Shibata,**
488 **Takeshi Nakatani, Kazuhiko Soyama, Ryuji Maruyama, Hiromichi Tanak.** SB028, 2011, *J. Phys. Soc.*
489 *Jpn*, Vol. 80.

490 7. **R.A. Ewings, A. Buts, M.D. Lee, J. van Duijn, I. Bustinduy, T.G. Perring.** 2016, *Nuclear Instruments*
491 *and Methods in Physics Research A*, Vol. 834.

492 8. **R.I. Bewley, T. Guidi and S. Bennington.** 1, 2009, *Notiziario Neutroni e Luce di Sincrotrone*, Vol. 14.

493 9. **R. Bewley, R. Eccleston.** 2002, *Appl. Phys. A*, Vol. 74.

494 10. **The 3He Supply Problem. Kouzes, R. T.** 2011, *Technical Report 11-753, US Government*
495 *Accountability*.

496 11. **10B multi-grid proportional gas counters for large area thermal neutron detectors. T. Bigault, J.**
497 **Birch, J.C. Buffet, J. Correa, R. Hall-Wilton, L. Hultman, C. Hoglund, B. Guerard, A. Khaplanov, F.**
498 **Piscitelli , P. Van Esch.** 2012, *Scientific reviews*.

499 12. <http://www.esss.se>.

500 13. <https://europeanspallationsource.se/instruments/cspec>.

501 14. <https://europeanspallationsource.se/instruments/t-rex>.

502 15. **J.Kulda, M.Kempa B.Janousova J.Saroun P.Flores M.Boehm F.Demmel.** 2006, *Physica B:*
503 *Condensed Matter*, Vols. 385-3862.

504 16. **Kulda, J. 433, 2005, Nucl. Eng. Technol**, Vol. 38.

505 17. **Oleg Sobolev, Ron Hoffmann , HolgerGibhardt , Norbert Jünke , Andreas Knorr, Volker Meyer ,**
506 **Götz Eckold.** 2015, *Nuclear Instruments and Methods in Physics A*, Vol. 772.

507 18. **P. Willendrup, E. Farhi E. Knudsen, U. Filges and K. Lefmann.** 1, 2014, *Journal of neutron*
508 *research*, Vol. 17.

509 19. **Emmanuel Farhi, Kim, Lefmann, Peter Link.** <http://www.mcstas.org/download/components/>.

- 510 **20. J.Zikovsky, O.Arnold J.C.Bilheux J.M.Borreguero A.Buts S.I.Campbell L.Chapon M.Doucet**
511 **N.Draper R.Ferraz Le M.A.Gigg V.E.Lynch A.Markvardsen D.J.Mikkelson R.L.Mikkelson R.Miller**
512 **K.Palmen P.Parker G.Passosa. 11, 2014, Nuclear Instruments and Methods in Physics Research A,**
513 **Vol. 764.**
- 514 **21. https://www.mantidproject.org/Main_Page.**
- 515 **22. F. Demmel, K. H. Andersen. 2008, Measurement Science and Technology, Vol. 19, p. 034021.**
- 516 **23. Keener, K. W. Herwig W. S. Appl. Phys. A, Vol. 74.**
- 517 **24. Panasonic, Highly Orientated Graphite catalog 2015/04.**
- 518 **25. C. Carlile, M.A. Adams. 4, 1992, Physica B, Vol. 182.**
- 519 **26. D. Martín, y Marero and D.Engberg. 1999, Physica B, Vol. 268.**
- 520 **27. Private communication .**
- 521 **28. Private communication with Robert Georgii,Ran Tang and Peter Böni.**
- 522