MUSHROOM Detailed Technical Case

Technical case

Indirect geometry spectrometers such as TOSCA or IRIS are more efficient than direct geometry machines such as LET or MAPS, because for the same energy resolution they 'extract' much more flux from the neutron source (moderator). This is because their resolution is determined by the full instrument length rather than just sample to detector distance. However, direct geometry machines such as LET have arrays of position sensitive detectors (PSDs) covering a large solid angle, unlike the small non-PSD coverage of traditional indirect machines. The large PSD coverage is useful both for single crystal measurements, mapping out reciprocal space using crystal rotation scans, and powder measurements for accessing a wide range in |Q|. MUSHROOM will use a unique geometry, with an array of pyrolytic graphite (PG) analyser crystals focusing through a rotating "order selector" (to cut out higher order reflections from the analysers) and PSD detectors underneath. By judicious choice of final energy for each analyser element, the prismatic effect may be utilised to allow analyser crystals with a relatively broad mosaic to be used without compromising the energy or wavevector resolution. The energy resolution of MUSHROOM will be approx. 75 μeV. The count rate expected on MUSHROOM will be between 18 and 75 times higher than on LET in its most commonly used multirep setting[1], with superior energy resolution for most of the incident energy reps in that setting, and a count rate 65 times higher for a setting with the same resolution. Unlike the other cold neutron spectrometers at ISIS, LET and OSIRIS, MUSHROOM would not offer a capability to do QENS measurements, since the energy resolution is insufficient.

In the following sections we will describe the components of the instrument starting from the source and working downstream. We will discuss individual instrument components, as well as the principles of operation of the instrument.

Overview description

MUSHROOM would go on TS2 port W8, viewing the hydrogen moderator, and would have a primary (source to sample) length of 40m. This primary part of MUSHROOM is fairly standard: a WISH style elliptical guide focusing on to a 1cm^2 sample, and two slow (10 Hz) bandwidth choppers 7 m and 10 m from the source to prevent frame overlap. Calculations, without further optimisation of the guide configuration[2], show that MUSHROOM would have between 18 and 75 times the count-rate of LET for a 1cm^2 sample, with LET running in its most commonly used configurations. Surrounding the sample position on both sides, and up to 8 degrees out of plane, there is a large array of PG analysers arranged on the inner surface of a section of toroid. Each analyser element focuses through a slot directly below and on to a plane of position sensitive detectors – see fig 1. The sample, analysers and PSDs are all positioned such that each analyser element focuses on to a specific detector pixel. By judicious alignment of the analyser elements the prismatic effect may be exploited to achieve the quoted large gains in count rate over LET, since the information about the variation in final energy selected by the analyser crystal as a result of its mosaic is encoded in the detector pixels the neutron arrive at on the PSD. This allows broad mosaic analyser crystals to be used, which then "extract" much more flux from the moderator. A rotating curved collimator is placed between the analysers and detectors and allows selection of the PG002 reflection without contamination of the measured signal by higher order reflections. The PSD detectors would be WISH-style 8mm tubes. Because the resolution is set by the total instrument length, rather than the secondary flight path, the instrument can be quite compact.

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[1] That is to say the gain over the highest flux rep of the "standard" LET configuration will be 18, and the gain over the lowest flux rep for this standard setup will be 75.

[2] i.e. putting MUSHROOM on the end of a guide that has the same characteristics as the one currently employed on LET

This in turn means that the detector array will be much smaller than those employed on direct geometry machines and in consequence, ^{3}He-based detectors can be used without being prohibitively expensive. Indeed, the detector tank would have a volume of just 6 m^3 (in contrast to 70 m^3 on LET) and the area of detectors would be approx. 1.3 m^2 using 25 cm long, 8 mm diameter PSDs (in contrast to 4 m long PSDs covering 44 m^2 on LET). If the detectors use ^{3}He, then MUSHROOM would use 94 litres compared to 8000 litres on LET.

Table 1 Technical summary

Incident/final energy	Ei=1 – 25 meV , Ef=3.8 – 4.7 meV
Energy resolution	75 μeV @ elastic, 1% $\Delta E/E_{trans}$
Q range	Q_{min}=0.07 Q_{max}=2Å^{-1}
Primary/secondary flight path	40m / ≈2m
Beam size at sample	1 x 1 cm
Sample environment	All standard + extreme (large magnets, pressure cells, etc.)

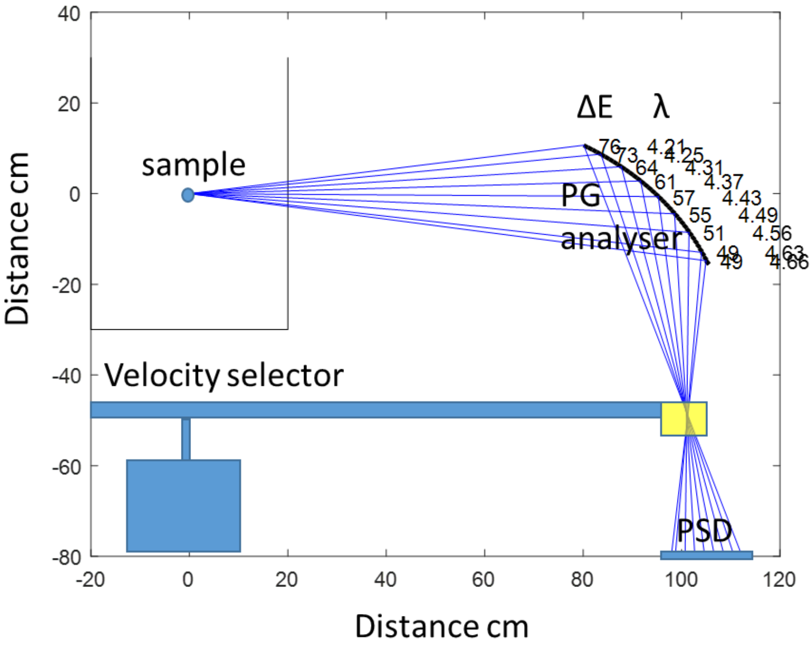

Figure 1: Cross-sectional view of MUSHROOM, viewed along the incident beam direction. Each analyser element is labelled according the energy resolution, ΔE, that it offers, together with the final wavelength of neutrons selected, λ

Instrument operating principles

In this section we provide a detailed description of the underlying concepts for how the instrument will work.

A pseudo-white beam is incident on the sample and a fixed final energy is selected by an analyser crystal. With a pulsed neutron source energy transfer is thus determined using time of flight. The energy resolution of such an instrument is given, in general, by

$$\Delta E = 2\sqrt{E_i^2\left(\frac{\Delta t_{mod}}{t}\right)^2 + E_f^2[\left(\frac{\Delta t_f}{t}\right)^2 + (cot\theta\Delta\theta)^2]}$$

From left to right these components arise from the moderator pulse width, time errors due to distance and the magnitude E_f, and angular uncertainty in reflections from the analyser (i.e. mosaic spread). Each can be minimised to improve energy resolution. The first term can be minimised by increasing the overall time-of-flight, i.e. making the instrument longer. The second can be minimised by using the Johann / Rowland geometry [1], whereby sample, detector and curved analyser all lie on a sphere such that the path from sample to detector is identical for all scattering angles. The final term is traditionally minimised by approaching backscattering (i.e. $\cot\theta \rightarrow 0$) and/or the mosaic spread of the analyser, $\Delta\theta$, is minimised. However, this final approach also reduces the eventual count rate, because the flux extracted from the moderator is also directly proportional to the mosaic spread. However, this can be overcome by using the prismatic effect whereby the mosaic of the analyser is relaxed to increase count rates, and the neutron wavelength is instead encoded onto an individual detector pixel on a PSD (see fig. 2).

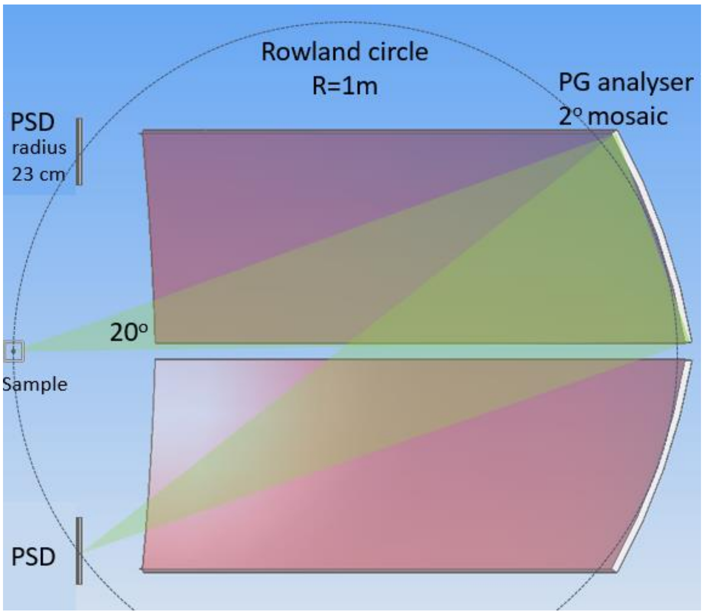

Figure 2: Schematic of the prismatic effect obtained using the Rowland circle geometry

Unfortunately, the prismatic concept as described above suffers from several shortcomings. The first is that the signal from all out-of-plane scattering is integrated, giving rise to very poor out-of-plane resolution. The second is that each detector pixel “sees” the full solid angle of the analyser, and thus is likely to suffer from high background due to thermal diffuse scattering from the analyser. Finally, with such a setup it is not possible to use a velocity selector to separate cleanly higher order reflections from the analyser, since the neutrons only converge at the point of detection.

MUSHROOM is designed to use a novel variant of the prismatic effect to overcome the above shortcomings. Multiple small analyser crystals with orientations chosen to select slightly different final neutron energies are arranged on the inner surface of a toroid. The angular height of this when viewed from the sample is ±8°. The neutrons are scattered from the analyser elements to a PSD array below the sample / beam. Each analyser crystal is oriented such that it scatters the same wavelength of neutrons down on to the same detector pixel as all of the other analysers (see fig. 3). By judicious choice of geometry, the paths from the scattered neutrons pass through almost a focal point below the analyser position. At this position, a rotating neutron velocity selector is placed, allowing isolation of a single order of Bragg reflection from the analysers. It can therefore be seen that each of the shortcomings of the traditional prismatic effect are overcome with this arrangement, allowing the instrument to have both high resolution and a high count rate.

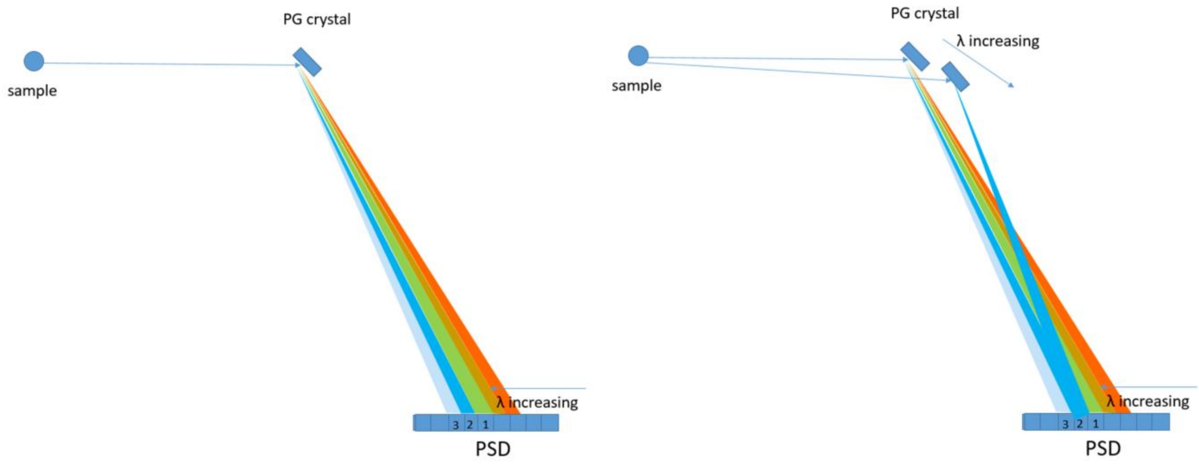

Figure 3: Left - single analyser prismatically focusing on to a PSD. Right - addition of a second analyser whose Ef is offset from the first to focus the same wavelengths onto the same pixels as the first analyser (in this case pixel no. 2 is shown)

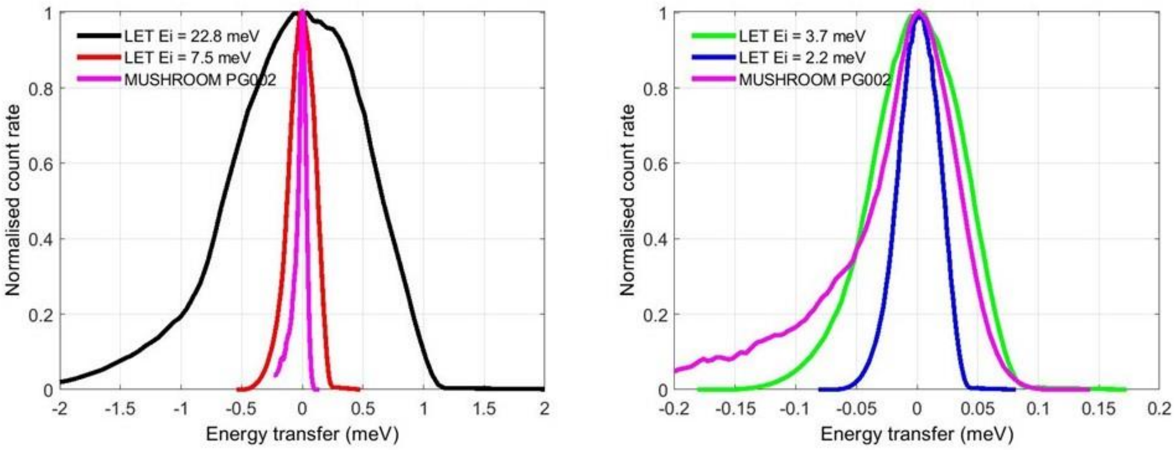

Figure 4: Comparison of lineshape in energy transfer of MUSHROOM (magenta line in both panels) with the most commonly used LET multirep configuration, viz. Ei = 22.8 and 7.5meV (left panel); Ei = 3.7 and 2.2meV (right panel).

In order to quantify the instrument's characteristics, McStas simulations have been performed. By placing the instrument on the same source and guide as LET currently occupies, and assuming a 1x1 cm^2 cross-section beam, MUSHROOM would have a resolution at the elastic line (FWHM) of approx. 75 μeV (see fig. 4), albeit with a rather asymmetric lineshape due to the intrinsic moderator characteristics. Similar resolution can be achieved with LET, with an incident energy of 3.8 meV and the final chopper spinning at 240 Hz (a commonly-used setup on LET). However, for such a configuration the count rate on each detector is approx. a factor of 55 higher on MUSHROOM than it is on LET. Because of the use of choppers on LET, the tails of the moderator lineshape can be cut, giving a more symmetric resolution function. With the analysers on MUSHROOM arranged in almost a complete torus, i.e. covering scattering equally on both sides of the incident beam, unlike LET, in some circumstances (e.g. powders at low scattering angle, crystals in symmetric orientations) a further factor of two can be gained in the number of measured neutrons.

A reasonable point to make at this stage would be that LET can be run in a configuration with higher flux, albeit at the expense of worse energy resolution. However for many experiments this is perfectly acceptable. One of its chief advantages of LET is the ability to cover a wide dynamic range using repetition rate multiplication, with the different reps giving access to different energy scales with different resolution. For the standard configuration described above, of E_i = 3.7 meV and the final chopper at 240 Hz focusing on the high flux slot, repetition rate multiplication offers incident energies of 22.8, 7.5, 3.7 and 2.2 meV. The first two of these settings have lower resolution than that available with MUSHROOM, and the gains in count rate of MUSHROOM over LET are 52, 18, 26 and 77 respectively. Thus the gains are still transformative compared to a best-in-class instrument such as LET. Indeed MUSHROOM will enjoy count rates significantly higher than all cold neutron direct geometry instruments operating in the world today.

For completeness we have also calculated the gain in flux of MUSHROOM over OSIRIS using its analyser in the PG004 setting, for similar resolution. In this case the flux gain of MUSHROOM is expected to be approx. a factor 35 for similar resolution[3]. We note that the PG004 setting is rarely used on OSIRIS anyway, due to issues with background and limited dynamic range.

Turning to the resolution as a function of energy transfer, E, (see fig. 5), as with any indirect geometry instrument the energy resolution of MUSHROOM is better at low energy transfer, opposite to the trend on direct geometry instruments. At any given energy transfer the resolution is superior to that of the frequently used LET setup described. Indeed, the fractional resolution (ΔE / E) on MUSHROOM is almost flat as a function of energy transfer, at approx. 1%.

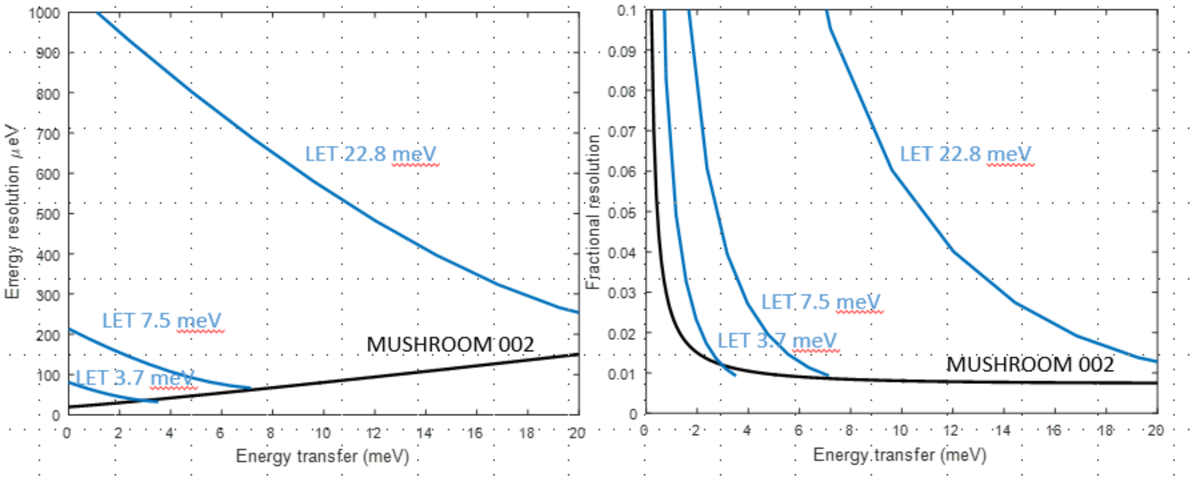

Figure 5: Left – energy resolution vs energy transfer for MUSHROOM compared to the commonly used multirep setting on LET. Right - as left, showing resolution expressed as a fraction of energy transfer.

We now consider wavevector resolution. This can be divided up approximately into two contributions, the first as a result of divergence in the incident beam due to the guide (primary spectrometer), and the second due to the arrangement of the analyser crystals and PSDs (secondary spectrometer). Assuming a guide with characteristics similar to that used on LET, the two contributions for the *x*-, *y*-, and *z*-directions (perpendicular to the beam in the horizontal plane, vertically upwards, and along the beam respectively) are shown in fig 6. This indicates that the resolution for the *x*-component is dominated by the primary spectrometer, the z-component is independent of the primary spectrometer but is much less than the *x*- and *y*-components, and only the *y*-component gets a sizeable contribution from both primary and secondary spectrometers. We would therefore expect the Q_y resolution to be approximately a factor 2 worse on MUSHROOM than on LET.

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[3] We do not compare to OSIRIS in its more commonly used PG004 setup, since this gives superior resolution to MUSHROOM and is used for different kinds of science

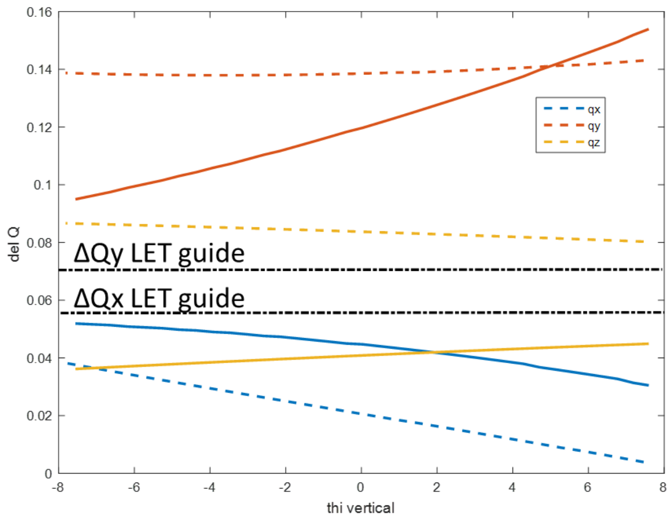

Figure 6: Individual components of the Q-resolution on MUSHROOM. Solid lines are the terms from the secondary spectrometer, dashed lines are the terms from the primary spectrometer. The total resolution is approximately these added in quadrature

In fig. 7 we show simulated spectra for LET in two of the commonly used configurations (7.5 and 3.7 meV incident energy reps) compared to spectra over the same range of energy transfer simulated on MUSHROOM with the PG002 analyser setting. Simulations were performed for a two-dimensional dispersive excitation, with a bandwidth of 4 meV and a cubic lattice of 6.28 Å. This is representative of a typical experiment performed on a magnetic material on LET at present. It can be seen that the Q resolution is superior on LET for E_i = 3.7 meV, however the difference is not especially pronounced, indeed the Q resolution of MUSHROOM is very similar to that of LET operating with E_i = 7.5 meV. The one-dimensional cuts shown in the bottom right figure (integrating in energy in the range 1 < E < 1.2 meV) bear out this impression, and illustrate that for practical purposes the Q resolution of MUSHROOM is perfectly adequate for the measurement of typical dispersive excitations.

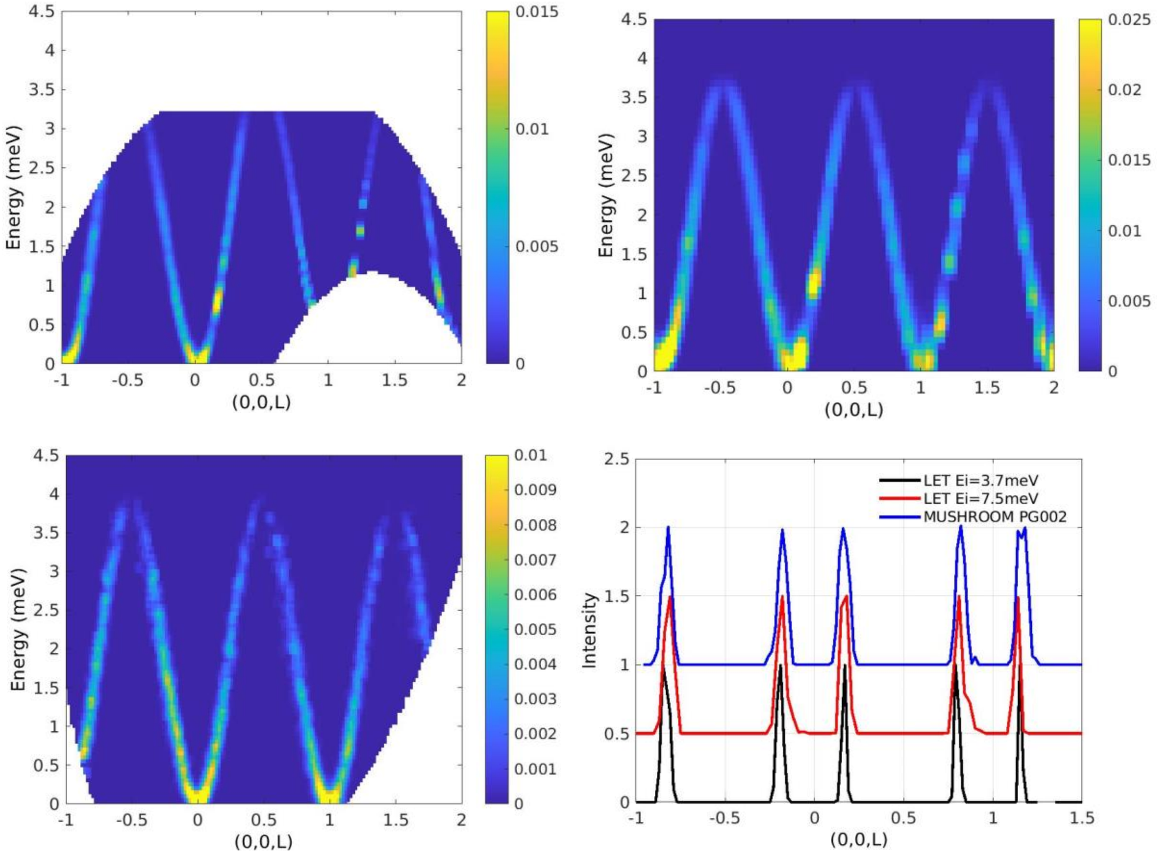

Figure 7: Simulated data from LET and MUSHROOM. Top left - dispersion on LET with Ei=3.7meV; top right - dispersion on LET with Ei=7.5meV; bottom left - dispersion on MUSHROOM; bottom right - comparison cuts along Q for all three

In fig. 8 we show the reciprocal space coverage as |**Q**| vs energy transfer on MUSHROOM compared to that available in the commonly-used LET setup. The coverage is comparable at the lowest energies for the PG002 analyser reflection but is narrower for higher energy transfers. In particular, the coverage at larger |**Q**| is smaller on MUSHROOM. It is anticipated that for experiments involving magnetic scattering, which is strongest at small |**Q**|, no problems will be posed. There will be a compromise compared to LET for studies of lattice dynamics, for which the strength of the signal scales approximately as $|\mathbf{Q}|^2$, though it should be noted that the gain in count rate compensate for any loss here. What will be lost compared to LET is the number of accessible Brillouin zones, so it is expected that the majority of lattice dynamics experiments on materials with complex unit cells, for which measuring in a large number of zones is important, will be conducted on LET.

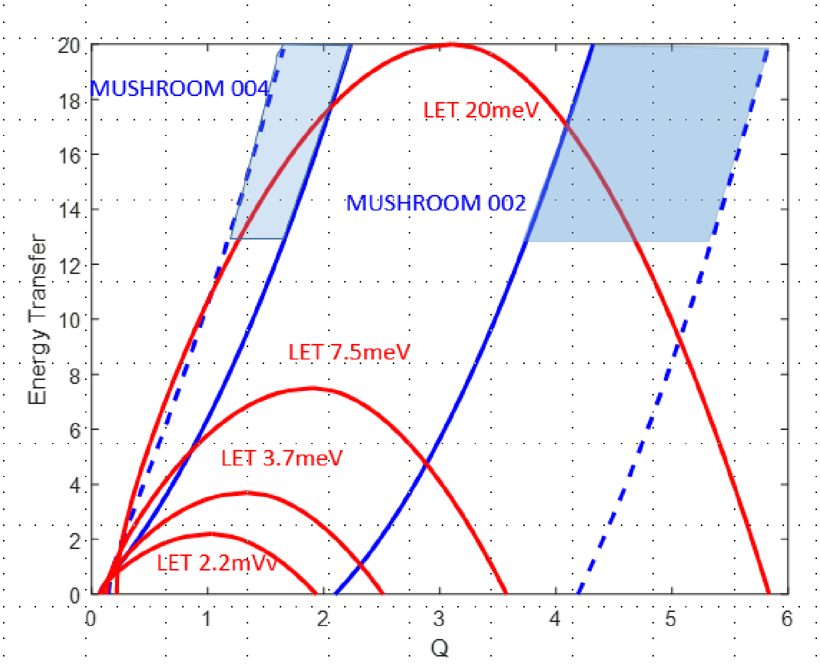

Figure 8: Reciprocal space coverage of MUSHROOM (blue) vs LET (red) for different analyser reflections and incident energies respectively. In practice the 004 analyser setup is highly unlikely to be used, but is shown for reference.

We will describe individual instrument components in the following sections. We will begin with the most complex and novel of these, that is responsible for the transformative capabilities already described, namely the secondary spectrometer.

Secondary spectrometer

The analyser crystals will be mounted on a borated aluminium surface. This will have to be accurately-machined, but its physical scale is not large compared to direct geometry instruments, being only 2.5 metres in diameter. A known challenge will be to ensure that the crystals can be robustly mounted and correctly aligned on the accurately-machined surface. The issue of analyser crystal alignment has been addressed on other instruments already such as CAMEA at PSI and VISION at SNS, and can be done using lasers.

A further challenge is to ensure that background scattering / spurious scattering from components other than the analyser crystals is minimised. This will be addressed in a number ways. Around the sample space there will be sample environment, and as has been used already on numerous beamlines, an oscillating radial collimator can be employed to ensure that scattering from material not in the central section does not reach the analysers at all. The substrate that holds the analysers themselves might also be an unwanted source of scattering. This can be eliminated by the application of a highly absorbing backing material to each of the analyser crystals. Experiments have been performed to determine the optimal backing material [32], and ^{10}B spray coating will be used. To further reduced background the analyser crystals will be attached to the substrate using glue impregnated with a strong neutron absorber, an approach that was used on VISION is also being used on the VESPA instrument at ESS. Finally, the substrate itself can be made from borated aluminium, to reduce the unwanted scattering from it. This approach has been successfully adopted on VISION.

It is not yet clear whether the analyser crystals will need to be cooled. We note that neither VISION nor CAMEA employ cooled analysers, and the CAMEA team in particular studied in detail whether to do so [33]. The effect of cooling the analysers is largely suppression of background at the lowest energies, and is hence most relevant for QENS, which MUSHROOM will not do. For inelastic scattering above ~0.3 meV the CAMEA team found little performance benefit from cooling the analysers. This is somewhat sensitive to the details of the analyser geometry, so to understand the issues for MUSHROOM specifically we were due to have neutron beamtime in February 2021 on LET to test a PG crystal in the right geometry. The delay of the ISIS beam cycle to April 2021 has correspondingly delayed this test.

Finally, the rotating order selector below the plane of the sample and analysers is a key component. This will not have to rotate especially quickly, but it will nevertheless be subject to some mechanical strain due to its horizontal plane of rotation. The wheel will be made from carbon fibre, with carbon fibre blades impregnated with ^{10}B for the order selection[4]. FEA calculations are in progress to confirm that the system will be mechanically stable at the expected frequency of operation, though initial expert opinion from Airbus is that the design should be achievable [32].

Beam port

MUSHROOM is envisaged to us port W8 of TS-2, next to NIMROD. This allows it to view the hydrogen moderator which has peak flux in a suitable neutron energy range, and would be the same view as is used by LET now. We have considered the alternative, of viewing the solid methane moderator on TS-2, however this moderator has lower flux over the bandwidth desired for MUSHROOM, with a much more dramatic high-energy cutoff that occurs at lower energies. We have also considered whether MUSHROOM could be situated on TS-1. In that case there would be significant problems with frame overlap unless the instrument was shortened significantly (worsening resolution) or a pulse removal chopper was used (reducing the incident number of pulses, and hence flux) by a factor of 2 or more. Furthermore, the cold moderators on TS-1 are less well-optimised than those on TS-2.

Guide

As stated above, the guide system will be comparatively straightforward. A straight 40 m guide like that used on LET already has good brilliance transfer for the wavelength range of interest, i.e. about 80% for 1^{o} divergence at long wavelengths, so further optimisation will deliver only modest gains. Nevertheless, we have also performed simulations with a WISH-style elliptical guide with m = 4, and this is our preferred configuration. Like on WISH, we would deploy beam scrapers along the length of the guide in order to offer some control of the beam divergence if necessary. What is certain is that the guide will use standard technology, and will not be challenging to manufacture.

Choppers

MUSHROOM requires only a pair of slow bandwidth disk choppers approx. 7 m and 10 m from the source and running at 10 Hz to limit the wavelength range incident on the sample, to avoid very long wavelength neutrons coming across multiple frames and showing up as spurions. Such a specification is very similar to a very large number of disk choppers already employed on many ISIS instruments, so there will be no technical challenges in delivering choppers of the necessary specification for MUSHROOM.

Polarised neutron option

The recent addition of a polarisation analysis option on LET, after many years of effort, has proven to be a tremendous asset, opening several new scientific opportunities. Lessons learned from the implementation of polarised neutrons on LET can be taken over to MUSHROOM. The use of an interchangeable final guide section, either polarising V-cavity or standard guide, would be immediately

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[4] ^{10}B-impregnated carbon fibre is used for disk choppers on LET, so is proven technology

applicable to MUSHROOM. For polarisation analysis the preferred technical solution would be to use an array of polarising S-bender mirrors just above the rotating order selector, to analysis the polarisation of the scattered beam. By placing such a device above the order selector, any neutrons with the “wrong” polarisation would be absorbed by the order selector and would not scatter to the detectors as spurions. A similar system is being considered for another Endeavour instrument, WISH-2, so the development work for one need not be repeated for the other. We note that a supermirror polariser like this is likely to be quite expensive up-front (~£1m), but it will require essentially zero operational support, unlike the ^{3}He polarisers on LET that require ongoing staff effort to operate and maintain them. Notwithstanding this, our preference is to build the instrument without polarised neutron capabilities initially, but to design it in such a way that this offers a simple upgrade path for the future if it becomes apparent that there is a strong scientific and business case for doing so after more experience of running LET with polarisation has been gained.

Sample environment

The MUSHROOM design is such that a wide range of different sample environment from the current central pool of ISIS equipment could be used. Aside from the standard options of a cryostat and CCR, and ultra-low temperature options such as dilution fridges, the 9 T cryomagnet would work well on MUSHROOM since the vertical opening angle does not restrict the view of the analysers / detectors out of plane like it does on LET. However that magnet has only a 90 degree opening in-plane, so a significant fraction of the MUSHROOM analysers / detectors would be shadowed. The ISIS strategy for future cryomagnets should bear this in mind and consider magnets with a wider horizontal opening. With the high count rate we expect the small samples that can typically be accommodated in pressure cells to be more easily measurable than they are on LET. Existing ISIS pressure cells would be used in the first instance, though there is clearly scope for development of new dedicated equipment later, e. g. Paris-Edinburgh cells. More non-standard tuning parameters might also be explored as future sample environment developments after the instrument has commenced operations. For example, uniaxial strain has been used successfully on small single crystalline samples on WISH so a natural extension of this work would be to use it in conjunction with inelastic scattering. Similarly, applied electric fields have been used on ISIS diffraction instruments, where again small samples are necessary to achieve relevant electric fields without breakdown inside the sample cell. Such apparatus might then be repurposed or redesigned for use on MUSHROOM.

With the high count rates available on MUSHROOM there is a high likelihood that the rate-limiting factor for some measurements will be cool-down and warm-up times when changing samples. To mitigate against this development work should commence in parallel with the instrument build on a multi-sample changer capable of operating in cryogenic conditions. Such a device, for three samples, has recently entered user operation on MARI and has already proven invaluable. Something similar with capacity for a great many more samples would be required for MUSHROOM.

Data analysis

We explicitly consider data analysis provision, development of suitable software, and hardware infrastructure to support the operation of MUSHROOM, to be part of the instrument project. MUSHROOM will be a very different kind of instrument compared to the existing suite of chopper spectrometers at ISIS, and will therefore require some development work to be done to existing software tools so that they can be used to visualise and analyse data from MUSHROOM. Commonalities with data analysis tools will exist with the BIFROST instrument at ESS, and the ESS DMSC and the PACE team at ISIS already collaborate, making the developments needed for MUSHROOM easier to achieve. Particular focus is needed on how to account for resolution effects when modelling data, as these will be very different to those implemented for direct geometry instruments. We expect that in the time between a decision to proceed with building MUSHROOM and it entering the user programme, existing scientific computing effort will be utilised to develop the necessary analysis capabilities.

Very high count rates are expected on MUSHROOM, and even though there will not be a large out-of-plane detector like on LET there will be a wider in-plane angular range such that the total number of detector pixels will be similar. We therefore anticipate the individual data file sizes will be about the same size as those from LET, but that these files will be generated at a much faster rate. Careful attention needs to be paid to the computing hardware to cope with this high data rate so that users are able to monitor their experiments in real time. This should be achievable, since existing hardware can already cope with the data rates from WISH, which will be very similar. Notwithstanding, work already done for the ESS on streaming data direct from instruments as it arrives, which is a UK-based work package being undertaken at ISIS, could be utilised. In general, some development of the computing infrastructure will be needed for MUSHROOM to be exploited successfully. Work should start on this infrastructure as soon as approval to build the instrument is given.

Risks and mitigations

A number of technical risks have already been described in the preceding sections, together with their mitigations. More detail is also provided in the MUSHROOM feasibility report [REF]. A short summary of the technical risks at mitigations is as follows:

Technical Risk	Mitigation
Mechanical stability of velocity selector	Expert opinion is that this should be possible to design out, with FEA calculations pending to confirm.
Impact on neutronic performance of analyser misalignment	±0.2° misalignment has negligible effect. Alignment can be done with lasers, as on VISION
Background from scattering by materials near the analyser crystals	^{10}B backing on crystals, borated aluminium substrate (as on VISION), borated glue to attach crystals (as on VISION and VESPA)
Background from diffuse scattering from PG crystals	Order selector arranged so that each detector only sees a small part of the analyser array
Magnetisation of instrument tank or surroundings prohibits the use of high field magnets and / or neutron polarisation	Great care to be taken. This was an issue on MERLIN, but lessons were learned for LET. Those same lessons must be applied again.
Data analysis provision is insufficient for users to analyse their data	Build in computing requirements from the very start of the project. Liaise closely with instrument teams and DMSC at ESS to learn lessons from their experience of similar issues arising from high count rate instruments

References

[1] https://space.mit.edu/home/guenther/Lynx/RowlandGeometry.html
[32] MUSHROOM feasibility report, R. Ewings, R. Bewley and P. Galsworthy (2021)
[33] J. Larsen, https://infoscience.epfl.ch/record/190504?ln=en