MUSHROOM Business Case

Strategic Aims

MUSHROOM will enable new science on small samples

The most exciting experiments attempted on LET, and on other comparable cold neutron spectrometers elsewhere, are those to study newly-discovered materials and / or those employing extreme sample environments such as high magnetic field or high pressure. These range from materials exhibiting topological effects that might become the basis of electronic devices in decades to come, to caloric materials which undergo large entropy changes under external stimulus (magnetic field for magnetocalorics, pressure for barocalorics) and hence could be used for environmentally-friendly solid-state refrigeration. Inelastic neutron scattering provides information that cannot be gained from other analytical methods about the underpinning microscopic mechanisms, and hence is a crucial part of the materials design - discovery – characterization – modelling – design chain.

Inelastic neutron scattering is, at its core, a flux limited technique. New instruments being designed for next generation neutron sources (e.g. at the ESS or the SNS-STS) will provide gains in flux of the order of the *source gain* – likely to be around one order of magnitude. However much larger (and much more cost-effective) gains are possible with innovative instrument design. The factor-of-50 increase in effective flux (count-rate per unit detector solid angle) on MUSHROOM compared to LET will be transformative.

- Sample masses of order 1g commonly studied on LET can be reduced to ~20 mg
- This will enable experiments on new materials and high quality (therefore small) crystals
- High field (~ 15 T) and high pressure (100 kbar) INS measurements become possible

MUSHROOM will provide opportunities for the existing user base

MUSHROOM comes in to its own when measuring single crystals of magnetic materials. This is due to:

- A horizontal planar (flat-cone) scattering geometry
- A relaxed energy resolution

Currently, on LET, experiments on single crystals of magnetic materials make up around 60% of the user program. Most often these experiments are attempted with relaxed energy resolution of around 80-100 μeV in order to maximise flux on the sample and hence count rate on the detectors. Very often, experiments are attempted on co-aligned crystal arrays (ranging from 2 to 100s of individual crystals) with resultant alignment errors leading to large effective crystal mosaics and poor Q-resolution. MUSHROOM will remove the need for crystal co-alignment. This in turn will result in much higher quality samples and will drastically reduce the time and effort required to prepare samples for measurement – resulting in faster turnaround.

MUSHROOM will attract new users

The current requirement of ~1 g samples for time-of-flight inelastic neutron scattering experiments acts as a significant barrier to entry to many user groups. Many labs are not (indeed should not be) designed to produce such large samples or quantities of samples. This is particularly true of groups working in university chemistry departments engaged in novel materials synthesis. A good example, which emerged from our engagement with such stakeholders, is in the broad field of coordination frameworks (a.k.a. MOFs). Such materials only grow as small crystals, and furthermore often have to be made using expensive deuteration processes to make them suitable for neutron scattering. However, their chemical flexibility makes them an exciting prospect for engineering a whole host of desirable properties in both fundamental and applied science. The unique insights that can be gained from inelastic neutron scattering are very rarely exploited in this context, but could add tremendous value with an instrument like MUSHROOM opening up so many new possibilities.

The aforementioned requirement of ~1g samples for time-of-flight inelastic neutron scattering experiments (worldwide) effectively rules out studies of protein crystals and ”true” low-dimensional (multi-layer) materials. With the flux gains enabled by MUSHROOM, we will – for the first time – be in a position to consider experiments on these materials with time-of-flight inelastic neutron scattering.

The transformative nature and uniqueness of MUSHROOM in the world neutron landscape will mean that a high number of international users will apply for beamtime. The evidence for this is clear – LET was a similarly ground breaking instrument when it was built, and it has had a strong international user base ever since it entered operation.

User Engagement

Key to the success of the MUSHROOM project, and future science opportunities, is the early engagement of the international user community. Prof. Andrew Goodwin of the University of Oxford has agreed to act as Science Champion for MUSHROOM. With his help, we are engaging with the community at this early stage in order to both consult their views and ideas, and inform them of progress and developments.

We will engage our users *via*

- Regular meetings and workshops held to discuss scientific themes appropriate to MUSHROOM
- Presentation of MUSHROOM to university research groups and departments

- Involvement of our current LET user group in formulating near-term scientific challenges for MUSHROOM to ensure early scientific success

Since the main thrust of our proposal is concerned with opening up inelastic neutron scattering to much smaller samples it is important that we make contact with materials synthesis groups for which inelastic neutron scattering would not normally be considered as a viable technique.

MUSHROOM at ISIS and beyond

Capabilities

MUSHROOM is a low-energy, medium resolution inelastic neutron spectrometer. Experimental proposals to ISIS calling for low energy transfers and medium resolutions would currently apply for beamtime on either OSIRIS (using the PG004 analyser setting) or LET. A comparative table of MUSHROOM with OSIRIS and LET is shown below. In practice, the OSIRIS (004) option is rarely used due to low resolution with low energy transfer range and high background.

Table 1: Comparison of the ISIS medium resolution, low-energy spectrometers with MUSHROOM

	LET	OSIRIS(004)	MUSHROOM
Energy transfer range	0.05 – 20 meV	0.2 – 4 meV	0.15 – 15 meV
(elastic) Q-range	$0.07\sqrt{E_i} - 1.3\sqrt{E_i}$ Å^{-1}	0.4 - 3.6 Å^{-1}	0.25 – 2.8 Å^{-1}
Energy resolution	10 – 1000 μeV	100 μeV	70 μeV
Q-resolution	Good – in and out of plane	Poor in plane, zero out of plane	Good in plane, medium out of plane
Beam size at sample	40(h) x 20(w) mm	40(h) x 20(w) mm	10(h) x 10(w) mm
Maximum sample pressure	10-20 kbar	10-20 kbar	>50 kbar
Maximum sample field	8.8 T	7 T	> 14 T
Approx. "equal resolution" count-rate (w.r.t. LET)	-	x1 (@ 100μeV)	x50

Comparing LET with MUSHROOM we see that:

- For small samples (~ 1 cm^2) MUSHROOM is 50 x LET at equal resolution
- For samples large enough to fill the LET beam (e.g. powders), MUSHROOM is still 6 x LET equal resolution
- Experiments which require good energy resolution (e.g. quasi-elastic neutron scattering – QENS) are not suitable for MUSHROOM – and will continue to be well served by LET, OSIRIS(002) and IRIS
- Experiments which require good out-of-plane Q-resolution will continue to use LET
- MUSHROOM will expand the available magnetic field and pressure range on ISIS spectrometers

Capacity

LET is commonly one of the most oversubscribed instruments at ISIS. This is partly due to the high regard for LET in the user community as a world-leading cold neutron spectrometer. It is also due to the fact that ISIS hosts only one low-energy spectrometer optimized for measurement of coherent excitations (i.e. with good Q-resolution).

For comparison, the low-energy good Q-resolution spectrometers at other major facilities are listed below. This list does not include low Q-resolution instruments commonly used for QENS (e.g. backscattering and neutron spin-echo instruments).

Table 2: Low energy good Q-resolution neutron spectrometers at major facilities. Time-of-flight spectrometers are shown in bold type.

Facility	Low-energy spectrometers
ILL	ThALES, IN12, **IN5** and **SHARP**
SNS/HFIR	**CNCS**, **Hyspec**, CTAX
J-PARC	**AMATERAS**
MLZ	PANDA, **TOFTOF**, MIRA
SINQ	**Focus**, TASP, CAMEA
NCNR	**DCS**, MACS, SPINS

Clearly, with only one low-energy spectrometer, ISIS (along with J-Parc) is an outlier in comparison to other major neutron facilities. Therefore, an increase in the capacity of ISIS for low-energy spectroscopy experiments – provided by MUSHROOM – would certainly better serve the community. Crucially it will also provide users with an alternative to three-axis spectroscopy[1] for small-samples.

International position

MUSHROOM has a higher count-rate than **all** of the time-of-flight spectrometers listed in table 2. Of the time-of-flight spectrometers shown, only IN5, Amateras, CNCS, and Hyspec have a higher flux than LET – and then only by around a factor of up to 4.

There will be two cold neutron spectrometers built at the European Spallation Source, C-Spec[2] and BIFROST[3]. C-Spec is a conventional cold time-of-flight direct geometry spectrometer, which due to increases in source flux will provide roughly a factor of 10 increase in flux over LET / CNCS, and which will have variable energy resolution – much like LET. BIFROST – like MUSHROOM – will be an inverse geometry time-of-flight cold neutron spectrometer with relaxed energy resolution. It will have an enormous flux, probably exceeding that of MUSHROOM. However, unlike MUSHROOM, BIFROST uses the conventional "prismatic effect" technique when selecting the final energy whereby a range of final energies is discriminated by position sensitive detectors. This means that on BIFROST there will be no out of plane Q-resolution, and the analyser solid angle will be much reduced compared to MUSHROOM.

ISIS Options for low-energy coherent spectroscopy

Do nothing

If MUSHROOM is not built at ISIS, then LET will continue to be the sole instrument capable of low-energy coherent spectroscopy at ISIS. The existing and increasing demands for low-energy neutron spectroscopy at ISIS would therefore continue not to be met at an appropriate level. There is scope for some improvement in LET performance, perhaps via a modernized guide design. This, however, would not lead to more than a factor of 2 or 3 in flux on LET. LET will continue to perform excellent science in many fields of study, indeed it is expected that polarized neutron spectroscopy on LET will become increasingly popular. This will open up further scientific opportunities to a wider community on LET, but will result in relatively less time available for conventional low-energy spectroscopy. This is, by definition, the cheapest option.

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[1] Three-axis spectrometers can achieve high flux / count rate, but only for a single (or small number) of points in reciprocal space at a time. They lack the broad snapshot overview that time-of-flight spectrometers provide. Furthermore, they are highly specialised tools and difficult for inexperienced groups to use.
[2] https://europeanspallationsource.se/instruments/cspec
[3] https://europeanspallationsource.se/instruments/bifrost

Build a second LET

To address the lack of capacity for low-energy spectroscopy at ISIS, we could consider building a second version of LET. Such an instrument might initially seem like a good option, based on in-house expertise and trusted technology with low levels of technical risk. However, given the impossibility of using ^{3}He detector technology (due to cost), a new version of LET would have to use ^{10}B-based detectors which represent a significant technical risk – one which is now being tackled by the C-Spec instrument team at the ESS. Whichever detector technology were to be used for a second LET at ISIS, the instrument would likely be prohibitively expensive, or would be compromised by having a much lower detector coverage than LET.

Build MUSHROOM

MUSHROOM will both address increasing demand for low-energy spectroscopy at ISIS but will also extend our capability to measure milligram-sized samples (for the first time), and extend our available magnetic field and pressure range. Compared to a second LET, MUSHROOM presents much less risk. The MUSHROOM guide, detector array and analyser arrays are all based on tried and tested technologies. A factor of 50 increase compared to LET will inevitably lead to new scientific opportunities at ISIS. Additionally MUSHROOM will leave space on LET for lower energy spectroscopy (including QENS), experiments for which the out-of-plane detector coverage and/or resolution is essential, and polarized neutron experiments. The residual risk of building MUSHROOM lies in the construction of the velocity selector, which can be mitigated by design of the instrument geometry (already performed) and by early engagement with suitable external expertise (underway).

Build MUSHROOM XYZ

It would be technically feasible to install 3-directional (XYZ) polarization analysis devices on MUSHROOM (unlike the uniaxial polarization analysis option on LET). This would extend MUSHROOM's capability very significantly – with the ability to perform magnetic diffuse scattering measurements on disordered magnetic materials, and to understand magneto-structural coupling in materials such as conductive magnets. To date, there are only two instruments worldwide able to perform polarized neutron diffuse scattering: D7 at the ILL and DNS at MLZ. XYZ polarization analysis for studying other effects is available on several three-axis spectrometers around the world, though this is subject to the shortcomings of three-axis spectroscopy already described. The Hyspec instrument at ORNL has a polarized option, but this is still some way from being optimized for routine use. The XYZ polarization option on MUSHROOM has an associated extra cost of ~£1m and a degree of extra technical complexity (though well within the capabilities of external suppliers of the relevant equipment).

Preferred option

We propose in the first instance to build MUSHROOM without XYZ polarization analysis. However, we should leave sufficient space and use appropriate (non-magnetic) construction materials so that the addition of polarized neutron devices to MUSHROOM is possible at a later date – should a compelling science case arise.

Project considerations

Top five risks and mitigations

1) Project cost outside funding envelope – risk that the project has to be de-scoped to accommodate fixed funding and therefore does not meet the full specification. Mitigated through strong project management controls.
2) Procurement – STFC / UKRI procurement mechanisms mean that compromises on quality have to be made that result in the instrument not meeting the full specification. Mitigated by early engagement with local procurement teams and external suppliers.
3) Project delays – financial risks with suppliers, costs of delay in terms of installation manpower and disruption to ISIS operations. Mitigated through strong project management controls.
4) Design or manufacturing error – leads to instrument not meeting the full specification. Mitigated through external scrutiny of final physics and engineering designs.
5) Computing hardware / software – risk that data rates are so high that computing infrastructure cannot cope, users cannot analyze their data, and hence benefits are not realized; extra financial commitment required to fix computing issues after the fact. Mitigated by engaging early with scientific computing colleagues, and making data analysis part of the project.

Monitoring and evaluation

During project: follow standard ISIS and STFC project management controls; oversight board with external stakeholder involvement.

At project completion: review of schedule and budget, and whether engineering specification has been met.

After commissioning: detailed report from science team outlining instrument performance against metrics pre-agreed with the external advisory board. Measurements of standard samples measured on other instruments to enable benchmarking.

After first year of operation: follow up report from science team, interviews with early users, feedback to project team for snagging.

After first five years of operation: publications monitored, surveying the capabilities of MUSHROOM that were used compared to those outlined in the business case. Metrics of average sample size, sample environment, experiment duration, time to publication, publication rate, journal impact factor all collated.

Deliverability

1. *Supply chain capability*
   Many beamline components are "standard" (e.g. shielding, DAE, etc.) and existing supply chains are well established. The guide is relatively standard too, so multiple suppliers are capable of delivering it. The analyser crystals cover approx. 2 m^2, with pricing from at least one company per square meter indicating no difficulties. There are several possible suppliers of the order selector (existing supply chains for choppers).
2. *Accessible expertise*
   The lead scientist (Rob Bewley) has built two beamlines in the past, and is a world expert in time of flight spectroscopy instrumentation. Engineering expertise in house is experienced with the large majority of beamline components from previous builds at ISIS and ESS.