MUSHROOM Detailed Science Case

Summary

MUSHROOM (Multi-Use Spectrometer for High Rate Observations of Ordered Materials) is a new type of neutron spectrometer taking the best of direct and indirect geometry machines. As an indirect geometry instrument utilising the prismatic effect it will extract much more flux from the moderator than a direct geometry instrument for the same energy resolution. It will have a large solid angle analyser and detector array that will cover ±10-170^o in-plane and ±8^o out of plane, allowing reciprocal space mapping such as is commonly performed using modern direct geometry machines. Compared to many other indirect geometry instruments around the world, MUSHROOM will offer much better out-of-plane resolution, on accounted of the pixelated analyser array. By combining these advantages it will offer up to 50 times the count rate of LET in commonly-used settings (FWHM ~70 μeV) with a similar reciprocal space coverage, and 20 – 70 times the count rate of LET for the other "reps". Indeed, MUSHROOM will have an order of magnitude higher count rate than any other cold time-of-flight neutron spectrometer operating in the world today. The instrument will be designed to allow the inclusion of a polarised neutron option later. As polarised neutron spectroscopy is the archetypal flux-limited technique, the high count rates will allow a step change in what it can be used for. Taken together, these features will allow a host of new scientific opportunities to be exploited.

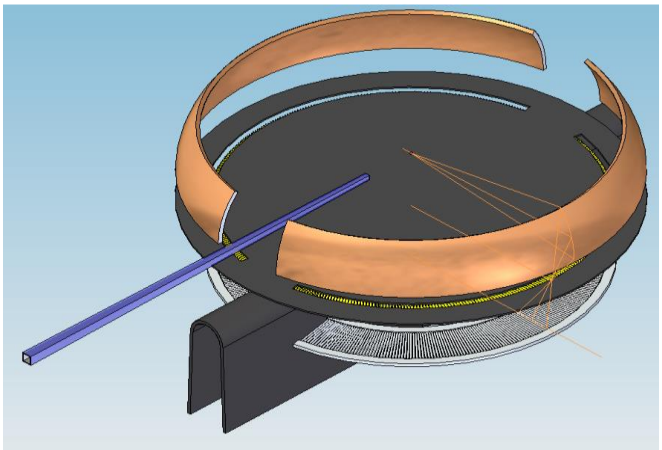
Figure 1: Artistic impression of the MUSHROOM instrument, with incident beam travelling from the bottom left. Thin lines indicate the trajectories of neutrons scattered from the sample, to analysers, down through a velocity selector and on to detectors.

Central among these new opportunities is the ability to perform inelastic neutron scattering reciprocal space survey experiments on the small sizes of samples more normally associated with neutron diffraction experiments, i.e. tens of milligrams. This is not currently attempted on any time-of-flight neutron spectrometer in the world. Aside from small samples being more readily available for more users, the most topical materials tend only to exist as small crystals until time-consuming optimisation of growth conditions has taken place, which can take years or might even be impossible. Furthermore, small samples (whether single crystals or not) are typically necessary when conducting experiments using more complex sample environment such as high magnetic field, applied electric field, high pressure or uniaxial strain, which allow more sophisticated tuning of desirable properties in the materials being studied. In addition to small samples, newly discovered materials in any scientific field tend first to be available only as powders. With high count rates and good reciprocal space coverage in a single shot, MUSHROOM will afford the opportunity to perform high throughput neutron spectroscopy studies on powders with varying composition and/or other tuning parameters. This will then allow the unique insights that can be gained from neutron spectroscopy to become available much earlier in the materials design – synthesis – characterisation – modelling chain.

MUSHROOM would not be a replacement for LET or OSIRIS, rather complementary to them. LET would be used for inelastic neutron scattering studies that require better Q resolution, or need a wider reciprocal space coverage out of plane when the location of signals of interest are unknown, and for which sample size is not such a constraint[1]. LET would also continue to be used for experiments using polarised neutrons, as we envisage MUSHROOM initially not having this capability though being designed to accommodate it later should the need arise. OSIRIS, IRIS and LET would remain the workhorse QENS spectrometers.

Instrument description in brief

MUSHROOM will be an indirect geometry spectrometer, situated on port W8 of TS-2. A white beam of cold neutrons is incident on the sample, which is surrounded by an array of analyser crystals covering 320^o in-plane and ±8^o out of plane. Each analyser element Bragg-reflects neutrons with a specific final energy on to a specific element of a position sensitive detector in a plane below (see fig. 2 below). By analysing the position and time-of-flight of neutrons arriving at the detectors, and then scanning the sample orientation, the 4-dimensional hypervolume of reciprocal space (three components of wavevector, and energy transfer as the fourth component) can be reconstructed. A similar method is routinely employed on direct geometry time-of-flight spectrometers, except with fixed incident energy.

Between the analysers and detectors, close to a focal point, there is a neutron velocity selector. This serves to prevent higher order reflections from the analysers reaching the detectors, which is a common source of background in indirect geometry instruments. Furthermore, the velocity selector has a narrow beam aperture so only allows a line of sight between specific analysers and specific detectors, rather than each detector pixel having a line of sight to the entire analyser array. This latter case can give rise to significantly elevated background levels on indirect geometry instruments due to diffuse scattering from the analysers and is avoided here. Thus, the background is minimised both spatially and temporally by the velocity selector and leads us to believe that the kinds of background issues that have bedevilled indirect geometry spectrometers in the past will be significantly reduced on MUSHROOM. Additional background reduction measures include the use of an oscillating radial collimator between the sample environment and the analysers, spray coating the backs of the analyser crystals with neutron-absorbing ^{10}B, and making the surface to which the analysers are attached from neutron-absorbing borated aluminium.

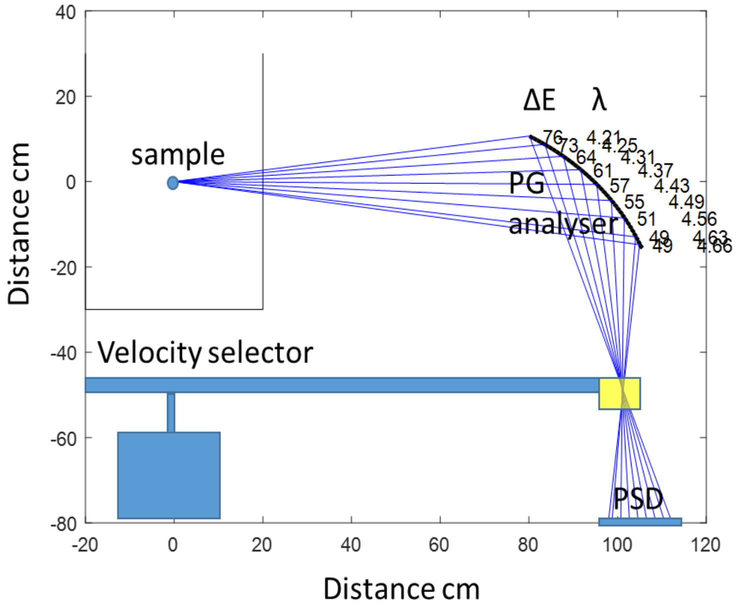

Figure 2:Cross-sectional view of MUSHROOM, viewed along the incident beam direction. Each analyser element is labelled according the energy resolution, ΔE, that it offers, together with the final wavelength of neutrons selected, λ

The gain in count rate of an indirect geometry instrument over its direct geometry counterpart comes from the finite mosaic of the analyser crystals, allowing a range of final energies to be accepted at the

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[1] If the sample is very small then MUSHROOM would be the only option, since there is little benefit in good Q resolution if the signal is too weak to be seen

cost of degraded energy resolution compared to the ideal case[2]. A significant recent innovation, now employed on the CAMEA spectrometer at PSI and which will also be used on BIFROST at ESS, is to utilise the prismatic effect to improve the energy resolution without paying such a large cost in count rate. The effect is explained in greater detail in the accompanying technical case, but in essence it involves encoding the spread in final energies due to the analyser mosaic on to different detector pixels, i.e. treating each analyser like a prism. A key insight that led to the development of MUSHROOM is to realise that by employing slightly different final energies on each analyser element in the vertical scattering plane, each detector pixel can be arranged to accept only neutrons with a much narrower range of final energies. Continuing the analogy with a prism, each detector element "sees" the same "colour" of neutrons from different analyser elements. By doing this the energy resolution penalty associated with a broader mosaic on the analyser crystals is significantly reduced, without losing any of the gain in count rate.

MUSHROOM will be designed from the outset to allow neutron polarisation analysis as an option, most likely as a later upgrade. The polarised setup would have a moveable section of polarising supermirror guide upstream of the sample position to polarise the incident beam. This is a concept which has been proven in user operation on LET and on other instruments around the world. Polarisation analysis would be achieved using a supermiror array, similar to that being developed for the WISH-II concept, between the sample position and the analyser. This can be optimised for the final energies that would be used on MUSHROOM, and is more suited to a planar geometry instrument with limited out-of-plane coverage than the ^{3}He spin-filter analyser cells used on LET.

It is worth emphasising that although MUSHROOM is a new kind of neutron spectrometer, few components require anything fundamentally new in terms of beamline engineering. The main exception to this in the velocity selector, for which detailed feasibility studies are in progress. The rest of the instrument brings together known components (guide, disk choppers, crystal analysers, PSDs,…) in a novel combination. Because the secondary spectrometer is very compact, with a sample tank just 6 m^3 in volume and a detector area of 1.3 m^2 (in contrast to the LET tank which is 70 m^3 with a detector area of 44 m^2) it will be a very cost-effective beamline to build. Indeed, just in terms of (expensive) ^{3}He in the detectors alone only 94 litres will be used in contrast to the 8000 litres required for LET.

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[2] The broader the analyser crystals' mosaic, the greater the count rate measured on the detectors, but the worse the energy resolution.

Science case

MUSHROOM will allow us to explore the complex physics that arises from atomic scale interactions. Such interactions govern a whole host of phenomena, from materials that are being used in applications now or will be in the future such as the next generation of battery materials, photovoltaics, ferroelectrics, thermoelectrics, multiferroics, magneto-resistive materials, and many more; to fundamental quantum effects in strongly correlated electron systems. Neutron spectroscopy is an exquisite probe of the strength, symmetry and nature of atomic scale interactions. With the unprecedented count-rates at high resolution, and the reciprocal space mapping that MUSHROOM will afford, whole new fields will be opened up to the powerful tool of neutron spectroscopy. At the same time, new opportunities for previously impossible experiments on tiny samples and/or involving complex sample environments will become possible, offering the chance of new insights in both new and in more established fields.

Introduction

The study of excitations in solids is the key to understanding the fundamental interactions between atoms, and their connection to emergent physical properties of materials. These studies fulfil two important roles: to characterise and inform the design of functional materials, and to test the predictions of current many-body theories of solids. For many years, inelastic neutron scattering (INS) has proved to be highly effective in probing excitations in solids. It has proved invaluable in studies of applied materials such as thermoelectrics, magneto-resistive materials, ionic conductors, and permanent magnets to name but a few. It also has a long and successful track-record of giving key insights in studies of the fundamental physics in strongly correlated electron systems, such as in frustrated magnets, quantum spin liquids, and superconductors. At the same time, quasi-elastic neutron scattering (QENS) has a similarly strong track record in providing insights into the nature of diffusive processes and correlated atomic motions relevant in a whole host of materials.

Cold neutrons are especially valuable because their energy scale, 0.1 meV – 20 meV, corresponds quite closely to the energy scales of many of the phenomena described above. This is closely analogous to the argument of why neutrons are such a valuable experimental probe for diffraction, i.e. that the neutron wavelength is closely matched to the interatomic spacings that are of interest in most systems. Systems that exist in a delicate balance between competing interactions are very commonly where interesting functionality and phases emerge. Because of this delicate balance the net energy scale is often rather low, hence the need for cold neutrons to probe the dynamics. A good example would be systems for which the spin quantum number $S=1/2$, that can be tuned between phases by the application of magnetic fields of the order 10 Tesla, which is a field accessible with current sample environment at ISIS. The energy scale associated with such a field is about 1 meV, so shifts in the spectra are likely to be of similar energy scale. Furthermore, in magnetic materials the energy scale roughly follows the magnitude of the spin, which means that cold neutrons are especially useful for $S=1/2$ systems. These are precisely the systems that exhibit exotic quantum phenomena due to the fluctuations of these spins, and are of the most interest in fundamental studies of emergent behaviour. Finally, the energy resolution available in a neutron spectroscopy experiment scales approximately as the energy of the neutrons themselves. Thus the best resolution, used for looking at the most subtle effects, is available on cold neutron instruments.

Over the past decade and a half, a new generation of direct geometry chopper spectrometers at facilities around the world (including MERLIN and LET at ISIS) has been developed, allowing for massive reciprocal space and dynamic range studies of excitations. Together with step-change improvements in data reduction and analysis software, as well as very low background levels, these instruments have led to an entirely new method of performing inelastic neutron scattering (INS) studies of single crystals. However, these instruments suffer from relatively low flux compared to their three-axis counterparts at reactor neutron sources - therefore demanding large single crystals, or arrays of crystals, or large volumes of powder / liquid samples; and long periods of time (of order days) to complete a single scan. Compared to high-flux three-axis instruments they offer a simple single-shot survey capability, which contrasts with the single-point-by-single-point measurement method of the three-axis[3].

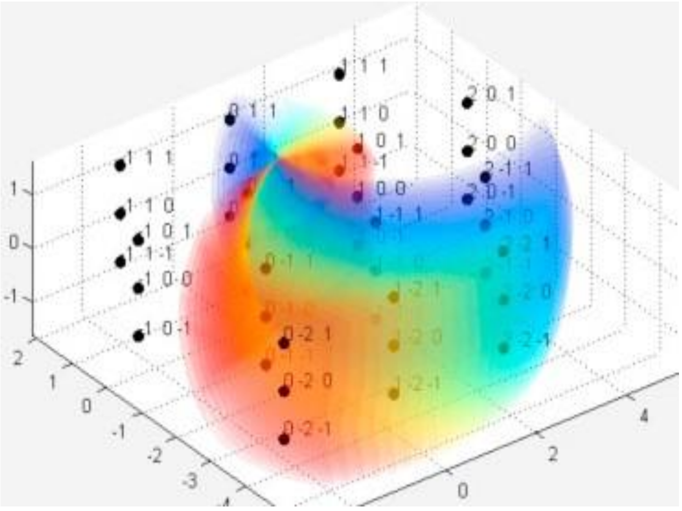

Figure 3: Schematic of reciprocal space volume coverage at constant energy of a time-of-flight chopper spectrometer. The shading indicates which sample orientation samples that part of reciprocal space. A similar scan on a triple axis would measure a single line through this volume.

The MUSHROOM concept bridges this gap between the two existing techniques, taking the best from both direct geometry instruments (reciprocal space coverage in a single shot) and indirect geometry / three axis instruments (high count rate). MUSHROOM will, in consequence, revolutionise neutron spectroscopy studies in a number of areas. The large increase in count rate compared to the current state of the art cold neutron spectrometer at ISIS (LET), will lead to several new or improved capabilities. Specifically, these are: Building on the success of direct geometry spectrometers, **broad single-shot reciprocal space coverage** will be a key feature of MUSHROOM allowing diffuse and weak features of the response to be identified readily from only a few measurements. When combined with a significantly higher count rate, we will gain the **ability to perform high-resolution measurements on tiny (~10 mg) single crystal samples**, previously beyond the reach of survey methods in neutron spectroscopy. Related to this, we will also gain the **ability to perform measurements with new tuning parameters**, such as high pressure, uniaxial strain or applied electric fields. Finally, we will gain the **ability to perform much more rapid surveys of excitations**, thus allowing parametric studies of not just simple characteristics of materials such as energy gaps, but the whole excitation spectrum. All of these factors together will open up a host of **new scientific opportunities for inelastic neutron scattering**, beyond its traditional core fields, opportunities that will be explored in more detail in the following sections.

The rest of this document is organised into four sections, each exploring the key capabilities of MUSHROOM, as described above. Related scientific opportunities will be discussed in general terms in the main text. Accompanying this document there are three sets of case studies. These are grouped by those for which MUSHROOM will have immediate impact, those that present medium term development opportunities for ISIS, and those that are more challenging but point the way towards future directions.

Case study 1 considers the immediate impact MUSHROOM would have in the field of magnetochemistry, for studies of magnetic metal organic frameworks. Here the immediate impact arises because MUSHROOM will be capable of measuring tiny samples from day 1. Case study 2 concerns development opportunities presented by studies of the dynamics of functional materials under applied pressure. High pressure apparatus very often necessitates small samples. Optimised pressure cells (with low background) together with the high count rate of MUSHROOM would allow a host of new opportunities to be explored in the near future. Case study 3 concerns the most

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[3] Triple-axis spectrometers can in principle be used to build up reciprocal space surveys, but in practice this is very rare since their strength lies in focusing the high count rate on a limited region of interest.

ambitious longer term trajectory, that of measuring nanostructured functional materials. This arises because we note that measurements of samples of thickness ~0.2 mm are already routine on LET, so with the increased count rate of MUSHROOM this would correspond to a thickness of just 10 µm. Several examples, of phononic and magnonic materials that are nanostructured on these length scales, may one day be feasible on MUSHROOM.

Key capabilities of MUSHROOM

1. Broad single-shot reciprocal space coverage

As described already, a key strength of direct geometry time-of-flight neutron spectrometers is their capability of providing a complete map of the dynamic response function S(Q,ω) that can then be directly computed from a host of different kinds of theoretical model. Increasingly it is the case that measurements of coherent excitations are focused not on a single branch of a dispersive excitation such as a phonon or a magnon. Rather, many such branches need to be mapped out across multiple Brillouin zones in order to obtain a more complete picture, which can then be modelled in a more comprehensive and sophisticated way. A good recent example of this is a study using ISIS' MAPS spectrometer of yttrium iron garnet (YIG) [1], see fig. 4, which is used as the material of choice for magnon spintronic (or "magnonic") devices[4]. Another example, described in **case study 2**, is the study of phonons throughout the Brillouin zone in adamantane, a barocaloric that is a potential material for environmentally friendly refrigeration applications. This points to the fact that often the most technologically relevant materials are far from being model systems, and instead have many-atom unit cells and/or large numbers of inter-atomic interactions. The survey capability, combined with good resolution, is crucial to disentangle all of the different modes of excitation (lattice or magnetic) that are then present.

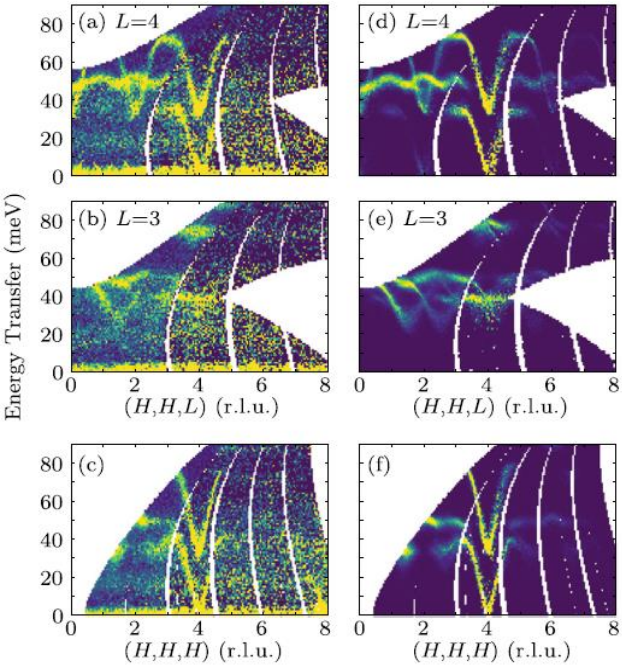

Figure 4: Data (left column) and simulations (right column) of magnon spectrum in yttrium iron garnet (YIG), taken on MAPS. Measurements in many Brillouin zones were required to disentangle all of the modes

Another advantage of the INS survey capability is that it allows features of the excitation spectrum that are broad and/or weak to be discerned from the background. In many systems of interest, especially those in which quantum effects are significant such as quantum spin liquids, but many others besides, all of the signal of interest is found in such broad or diffuse features of continuum scattering. The survey capability is crucial for being able to observe this, and to characterise it in detail. Here, MUSHROOM would offer transformative capability, because the signal from such samples is often very weak as well as being broad. The high count rate would allow data of materially better quality to be collected, with the opportunity to measure under a greater range of conditions of temperature, magnetic field, etc. This would result in a change from multiple sets of ~1 week long experiments conducted over several years,

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[4] Magnonic devices offer the possibility of performing logic operations, as are required in a CPU, without generating the large quantities of waste heat through Joule heating that existing electronic devices do. This makes them potentially much more energy efficient.

to a single experiment in which data of overall better quality is collected in all of the relevant experimental conditions.

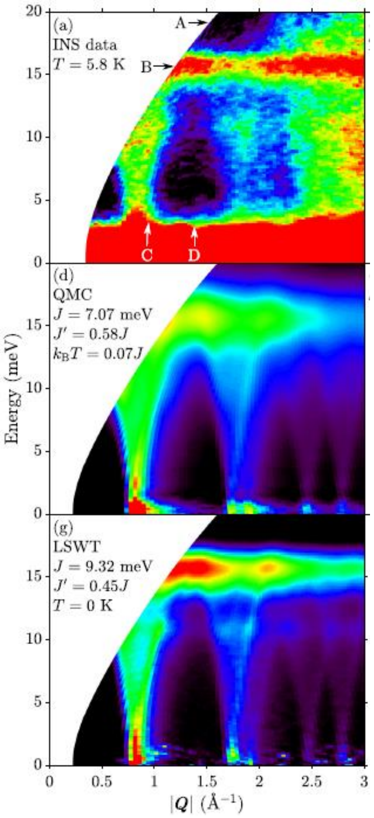

Figure 5: Powder spectrum in the spin ladder Ba2CuTeO6 (top) with QMC (middle) and linear spin wave theory (bottom) simulations

One of the great successes of direct geometry spectrometers over the years, and an area that is seeing a resurgence at the moment [2], is the ability to map the dynamic response function in powders[5]. Even before tiny crystals are first synthesised (see next section), newly discovered materials usually first emerge as powders. Being able to measure the spherically averaged excitations in such compounds can be very valuable, and with recent advances in data modelling software [3,4] much more quantitative information can be extracted from such measurements. Much as for the previous example of continuum scattering in crystals, the relevant information is distributed across a large area, making the survey capability crucial in isolating it from the background so that it can then be characterised and modelled. A characteristic example is shown in fig. 5, with data measured on MERLIN of Ba2CuTeO6, a model spin ladder system [5].

The MUSHROOM spectrometer has an out of plane coverage of ±8°, which is less than the ±30° available on LET. However, the experience of a decade's operation of LET shows that not all experiments exploit the full out of plane detector coverage, with many groups aligning their samples such that the expected regions of interest are close to the scattering plane. Indeed, the often-used 9 T cryomagnet restricts the vertical view of the detectors to ±15° in any case[6]. What MUSHROOM does offer beyond LET is much greater detector coverage in-plane, spanning 320° (two banks of analysers with 10° < 2θ < 170°) compared to 180° (asymmetrically distributed between -45° < 2θ < 135°) on LET. This means that LET and MUSHROOM would be very much complementary. The choice between LET and MUSHROOM will be multi-faceted and will depend on factors such as the amount of out-of-plane coverage required, the necessary resolution, whether polarisation analysis is required, and so on.

2. *Tiny samples*

Progress in materials research, from the magnonic materials that could be in the next generation of computer CPUs (see case study 3) to fundamental studies of strongly correlated electron systems, has at its cornerstone a constant stream of new materials. These will have been designed or discovered to have desirable properties that need to be investigated experimentally. New materials are often grown using synthesis methods that produce small samples, however. It can take years to optimise the growth of large samples and some samples can never be grown as large crystals. MUSHROOM will permit time-of-flight INS studies of samples that are currently too small to attempt to measure. This in turn will permit the usefulness of the technique to be brought to bear on the materials characterisation process much sooner in the design – synthesis – characterisation – modelling – design cycle, accelerating the development of the next wave of new materials. It will obviate the need for tedious co-alignment of

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[5] MUSHROOM will have ±8 degrees out of plane detector coverage, which is much less than LET. This means that MUSRHOOM will be able to integrate far fewer detectors around Debye-Scherrer rings. Despite this, because of the much higher count rate, we still expect MUSHROOM to offer faster measurements of powder samples than LET.

[6] It also limits the in-plane coverage to a 90 degree wedge

many crystals, which can be a barrier to some groups attempting experiments, and through imperfect co-alignment can result in broadened signals and lost information for those groups who do pursue this approach. **Case studies 1, 2 and 3 are all relevant here.**

Examples of functional materials that might benefit from this include thermoelectrics, ferroelectrics, battery materials and calorics [6-10], to name but a few. Thermoelectric materials allow conversion of heat into electrical current, and can hence be used for a host of applications such as using waste heat in exhaust systems to power car electrical systems, or on space probes as a vibration-free long-lived power source. The newest materials developed during the design / optimisation process are often small so at present it is impossible for INS surveying capabilities to be brought to bear on problems early in the material design cycle. MUSHROOM would change this. Surveying the excitations, in this case the low energy phonons (see fig. 6 for an example), in these materials is important because it allows a direct, unique and comprehensive validation of first-principles calculations that are then used to predict other properties of the material. Often of greatest interest is finding when DFT fails to predict the phonon spectrum, with resulting anomalous material properties (e.g. anomalous dielectric response in ferroelectrics, useful for ultrasound transducers), for which reciprocal space surveying is required. A similar example already noted in the previous section is that of barocaloric materials, **explored in greater depth in case study 2**.

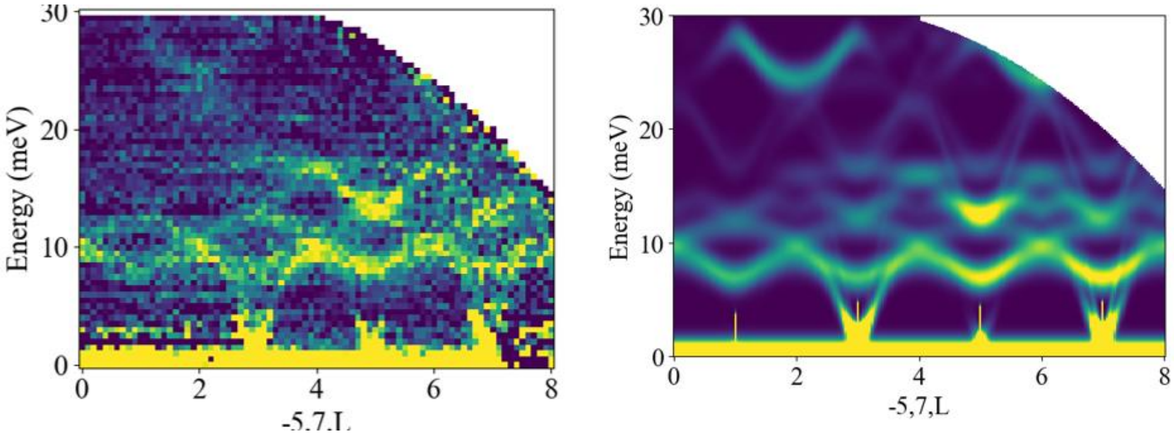

Figure 6: Phonon spectrum of La2Zr2O7 measured (left) and simulated using density functional theory (right). Images courtesy of D. J. Voneshen

Examples of materials from the strongly correlated electron field that would become feasible to measure in crystalline form using time-of-flight INS surveying for the first time on MUSHROOM might include metal-organic-framework magnets or molecular magnets made via hydrothermal / solvathermal methods [11]. Such systems offer a degree of flexibility and designability of desirable characteristics (both magnetic and functional in other ways) not available in more established alternatives such as transition metal oxides. This is, in part, because the latter have been comparatively easier to grow in large crystalline form and have hence been studied more. Furthermore, MOFs often contain hydrogen so to produce samples suitable for neutron scattering they must be deuterated, which is difficult and expensive. By being able to measure smaller samples it would make growth of suitable samples cheaper and hence accessible to more groups and potentially new user groups. **This is explored in more detail in case study 1.**

A very important theme in modern condensed matter physics is that of topology, which might be harnessed in the future for the next generation of electronic devices or quantum computers. Such effects are frequently explored in materials that exhibit strong spin-orbit coupling. A prominent example is the work that has gone into realizing model systems such as the Kitaev quantum spin liquid [12]. Much effort in this area has been focused on 4d and 5d transition metal oxides, however only a few of these systems have been amenable to the growth of large crystals. Furthermore, several of the most interesting of these systems contain components that are strong neutron absorbers, meaning that successful studies necessarily require thin / small samples. Studying the magnetic excitations of such compounds is useful because they often do not order magnetically so are less amenable to study by diffraction, whereas the dynamics discriminates between different physical models. At the same time, the signals are often broad / diffuse, so MUSHROOM will be the ideal instrument for such studies.

3. New tuning parameters

Studies of materials as a function of pressure, strain, magnetic or electric field are, or are now becoming, routine with neutron diffraction (e.g. strain studies of electronic nematic phases, pressure-driven phase transitions in quantum magnets, phase diagram studies in skyrmionic materials, highly entropic phase transitions in caloric materials used for solid state refrigeration, and many more besides). Particularly in the case of pressure and strain studies the samples are often small by necessity due to the nature of the sample environment required to reach such extreme conditions. This factor alone poses a significant challenge for neutron spectroscopy to deploy similar extreme sample environments, since the count rate acts as the limiting factor. When such experiments are attempted, they are typically limited in the number of pressure settings and maximum applied pressure that can be used, and are fraught with technical challenges [13]. By combining the possibility of measuring small samples (due to its high flux at high resolution) with the capability of surveying large swathes of reciprocal space in a single shot to discern broad features more readily, MUSHROOM will enable a whole new range of experiments to become possible with neutron spectroscopy. Measurement of excitations at high pressure with existing cells (normally only used for diffraction measurements) will become routine. As the instrument matures it may eventually be possible to consider experiments with Paris-Edinburgh type pressure cells, using pressures up to 70 kbar. **This is explored in more detail in case study 2.**

Recent experiments on the WISH diffractometer have showcased uniaxial strain as a valuable but relatively under-utilised tuning parameter [14]. The samples for such experiments are necessarily very small (see fig. 7). MUSHROOM would be capable of measuring similar samples under strain, opening up new possibilities to study effects such as electronic nematicity, which has for example been posited

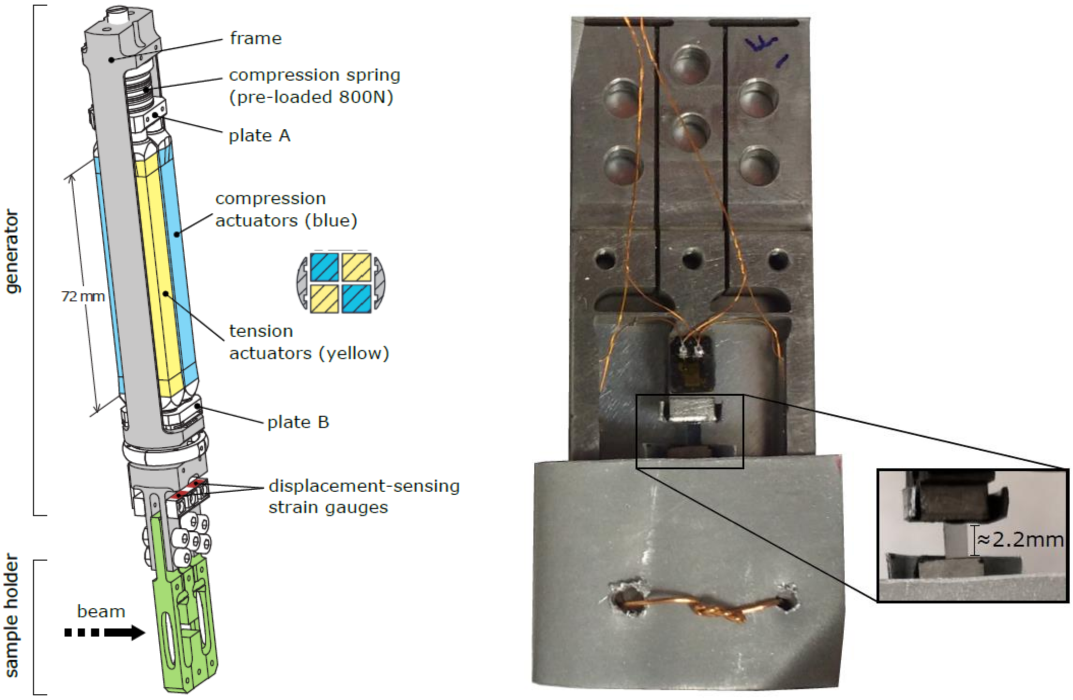

Figure 7: Schematic of the uniaxial pressure apparatus used for recent WISH experiments to study CeAuSb2 (left); photograph of the apparatus, with image of the sample inset (right). All images courtesy of R. Waite and C. Hicks

to underpin superconductivity in iron pnictides and to explain the decades-old puzzle of "hidden order" in the heavy fermion compound URu_2Si_2.

Reciprocal space survey experiments with applied electric field will also become feasible for the first time. In order to access fields of interest in materials such as multiferroics or ferroelectrics, either unfeasibly high voltages or very small samples are required. By measuring the latter, MUSHROOM will allow experiments in which the excitations (phonons, magnons, or hybrid excitations) can be monitored while the order parameter is switched using an electric field. This could then afford new insights into the microscopic mechanisms responsible, and as in other examples already discussed then feed into the materials design process more readily.

4. Rapid surveying and parametric studies

On direct geometry spectrometers the mode of operation that has seen widespread adoption over the past decade is one in which the sample's orientation is incrementally scanned to build up a dataset that covers a large volume in reciprocal (Q,E)-space [3]. With current instruments, the time required to complete such a scan can be prohibitive, resulting in compromised experiments with lower than desired statistical quality, fewer temperatures / magnetic fields / samples measured, and lower than desired numbers of experiments run in a cycle. In the context of the large oversubscription on LET, it is clear that demand for similar capabilities is already very high. MUSHROOM, with its huge gain in count rate, will massively increase our capacity to perform INS single crystal experiments quickly, and result in much higher experimental throughput. At the same time, rapid scanning will allow careful tracking of phase diagrams - invaluable in following soft modes and critical scattering phenomena. Indeed, being able to follow the evolution of all of the modes of excitation (when there are many) with some tuning parameter, which is currently too slow to be realistic with existing instruments, becomes possible with MUSHROOM. This might be brought to bear, for example, on the problem of negative thermal expansion (in which a material contracts as it is warmed, the opposite to what usually happens). It is well-established that the phonon modes are the key to unlocking this unusual behaviour, however it has recently been suggested that it is actually large numbers of modes which contribute, rather than a single one that softens or hardens with temperature [15], see fig. 8 for an example calculation for ZrW2O8. Being able to map this, and then follow with temperature or pressure, would be well within the capability of MUSHROOM, but beyond current instrumentation due to flux limitations. As mentioned above, broad continuum scattering can be of crucial importance in certain systems. The high count rate and broad reciprocal space coverage means that MUSHROOM would then offer the hope that the continuum itself could be monitored as a function of an external tuning parameter. This might then allow scaling relations, which are often key predictions of analytical theories, to be explored more readily [16].

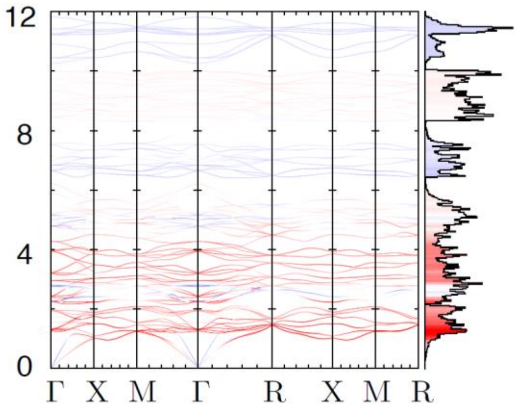

Figure 8: Mode Grueneisen parameters of phonon modes in ZrW2O8, with blue (red) colouring indicating positive (negative) values. The Gruneisen parameters are directly related to the negative thermal expansion effect.

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