Mushroom

Multi-Use Spectrometer for High Rate Observation Of Materials

A cold neutron spectrometer with a difference

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FRMII
31/1/18
ISIS Facility

TS1
32 years

Diamond Light source

TS2
10 years
• Have built two direct geometry spectrometers at ISIS

• Would like to build one more in-direct spectrometer - MUSHROOM

**MERLIN (TS1)**
Hot-thermal neutrons

**LET (TS2)**
Cold-thermal neutrons
The talk

1. The TOF direct geometry technique
2. Problems with the TOF technique and 3D systems
3. A potential solution - The MUSHROOM spectrometer
4. Properties of the MUSHROOM spectrometer
Comparison of triple-axis and time-of-flight technique

**Triple axis spectrometer**
- Supreme workhorse spectrometer for measuring $S(Q,\varepsilon)$ in single crystals
- Every reactor has a suite optimised for different energy ranges and resolution

**Why successful?**
- Go anywhere in $(Q,\varepsilon)$
- Constant-$\varepsilon$ or constant-$Q$ according to requirement
- Focus on a single point at chosen $(Q,\varepsilon)$
  - Focussing monochromator, analysers
  - Tune resolution (collimation)

$\Rightarrow$ if one knows where want to study: ultimate
Comparison of triple-axis and time-of-flight technique

Time-of-flight chopper instruments
• Equivalent workhorse spectrometer

Why successful?
• Comprehensive measurement of $S(Q, \varepsilon)$
  - Intrinsically parallel
  - Large solid angle and bandwidth
  - Full tests of models for $S(Q, \varepsilon)$
• Negligible background
• Complementary to triple axis

Time of flight $\rightarrow \varepsilon$

$\varepsilon$

$Q_{\parallel}$

$Q_{\perp}$
Position sensitive detector array:

Three degrees of freedom (two scattering angles, time-of-flight)

1D system: $S=\frac{1}{2}$ chain

2D system: $S=\frac{1}{2}$ square lattice

• Highly successful in 1D and 2D systems
  $S=1/2$ chain, square lattice, high-$T_c$, ...

Rubbish for 3D systems!!!

\[ Q_{z} \]
\[ Q_{\perp} \]
\[ Q_{\parallel} \]
Measuring Excitations - 3D

Three degrees of freedom

Four independent coordinates:
\((Q_{\parallel}, Q_{\perp}, Q_z, \varepsilon)\)

Need fourth degree of freedom:
\(E_i\) or crystal rotation

These days with large banks of PSDs and new software ‘HORACE’ 3D systems are possible
Measuring Excitations

Scan crystal angle

\[ \varepsilon = 0 \]

\[ \varepsilon > 0 \]
Measuring Excitations

Scan crystal angle

\[ Q_z \]

\[ Q_{\parallel} \]

\[ Q_{\perp} \]
Measuring Excitations

Scan crystal angle
Measuring Excitations

Scan crystal angle

Need 100-200 scans

• Can make short runs (15 mins typically on LET)

• Finish with large data file now ~100GB!
3D Heisenberg antiferromagnet – RbMnF$_3$

$-0.05 \leq Q_{kk}\leq 0.05 \text{ in } [Q_{kk}, Q_{kk}, 0]$, $0.45 \leq Q_{hh}\leq 0.55 \text{ in } [Q_{hh}, Q_{hh}, 0]$

$Q_I=1:0.01:2 \text{ in } [0.5, 0.5, Q_I]$, $E=-2.25:0.25:12.25$
3D Heisenberg antiferromagnet – RbMnF$_3$

-0.05 \leq Q_{\|} \leq 0.05$ in $[Q_{\|}, Q_{\perp}, 0]$, $0.45 \leq Q_{\perp} \leq 0.55$ in $[Q_{\perp}, Q_{\perp}]$, $Q_{\perp} = 1:0.01:2$ in $[0.5, 0.5, Q_{\perp}]$, $E = -2.25:0.25:12.25$

Constant energy cuts
3D Heisenberg antiferromagnet – RbMnF$_3$

-0.05 \leq Q_{kk} \leq 0.05 in [Q_{kk}, -Q_{kk}, 0], 0.45 \leq Q_{hh} \leq 0.55 in [Q_{hh}, \ldots, Q_{hh}], Q_I=-1:0.01:2 in [0.5, 0.5, Q_I], E=-2.25:0.25:12.25

Constant Q cuts
Most experiments on LET/MERLIN want to do HORACE scans (measure the full 4D $Q_x$, $Q_y$, $Q_z$, $E$ data set). Very time consuming taking around 1-2 days for one scan.

Samples getting smaller as systems become more complex/more complex sample environments

Want parametric HORACE scans as function of pressure/field and temperature

He3 costs have made these instruments too expensive

To build up 4D $S(Q,w)$
Solution – an In-Direct Geometry (crystal) spectrometer

- IG spectrometers are much more efficient than DG

\[ \Delta E \propto \frac{\Delta t_{Det}}{L_2} \]

Same resolution and solid angle

count rate \( \frac{IG}{DG} \approx \frac{L_{tot}}{L_2} \)
Problem- No TOF IG machines for 4D mapping

Backscattering spectrometers
In plane, quasi elastic instruments

Molecular spectroscopy – for hydrogenous materials, almost no Q info
Solution – The MUSHROOM

- There is no reason why you cannot have a large position sensitive coverage using a crystal analyser and position sensitive detectors.

The MUSHROOM

- PG analyser
- Sample
- Guide
- PSD detectors

6 Steradians PSD coverage
45 ueV resolution at elastic

PG analyser

0.8° mosaic

30°

-30°

ΔE

Ef

2.19
2.18
2.17
2.15
2.12
2.08

sample

PSD detectors
• Used Mcstas simulations to compare
• Put Mushroom on end of LET guide
• $E_i=2.2\text{ meV}$ for LET, $E_f=2.2\text{ meV}$ for Mushroom
• Both simulated for 45 $\mu$eV elastic resolution
• Both scatter $1\text{ cm}^3$ vanadium to same solid angle
Performance - Count rate

MUSHROOM has 12 x count rate of LET for same resolution and solid angle.

Mcstas simulation of elastic line

Peaks scaled

45 µeV

………but this can easily be doubled………
• \( \Delta E/E \) depends on TOTAL flightpath

• 8mm 6 atm He3 tubes
• 1.5 m long @ 0.5m radius
• 80 \% efficient at \( E_f = 2.2 \) meV

• \( \Delta E/E \) depends on secondary flightpath

• 25 mm 10 atm He3 tubes
• 4m long @ 3.5m radius
• Efficiency dependent on \( E_f \)

Count Rate is
\[ 2 \times 12 = 24 \times \text{LET} \]

Solid angle x Inverse geometry

Detectors $ 530 \text{ k}
Analyser \approx $ 5 M

Detectors $ 20 \text{ M}
Performance - Energy resolution

1% $\Delta E/E_{\text{trans}}$
Performance - Q resolution

- **Mushroom full beam divergence**
- **LET**
- **Mushroom divergence as LET**
- **Mushroom with detectors at 1m**
MUSHROOM needs PG004 as well as PG002 to get enough Q range.
Performance - Q range

MUSHROOM needs PG004 as well as PG002 to get enough Q range.
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How do we cleanly select PG004 or PG002?
How do we cleanly select PG004 or PG002?

Focussing the neutrons through a point allows one to build a realistic ‘order selector’.
The ‘order selector’

- A velocity selector with Aluminium blades coated in Gadolinium (electroplating)

- Rotates @ 120 Hz
- Blades set at two different angles ($\theta$)
  - Top blades for PG004 $\theta=10^0$
  - Bottom blades PG002 $\theta=20^0$
- Initial FEA analysis shows its OK
- Hoping to 3D print in Aluminium
Performance of order selector

Transmission vs wavelength

Bottom blades $\theta=20^0$

Top blades for $\theta=10^0$
Performance - background

- **Diffuse thermal scattering (particularly from PG crystals)**

- Detectors view analysers through a narrow 3cm slit. Should substantially reduce Diffuse thermal contribution to background

- Detectors in a well shielded box well away from sample, whitebeam and analysers

- Order selector stops contamination from different orders plus will reduce possible spurions from bragg scattering from sample

- Will never be as quiet as Direct geometry
Summary

Presented a new style of cold in–direct geometry spectrometer capable of rapid 4D $S(Q,w)$ mapping of crystals or for studying small samples.

Advantages

• High count rates $>20 \times$ direct geometry instruments like LET.

• Easy to cleanly select PG002 or PG004 for 1% or 3% $\Delta E/E_{\text{trans}}$ and different $Q$ ranges.

• Massive $2\pi$ steradians of position sensitive detector coverage.

• MUCH cheaper and smaller than a direct geometry machine.

Dis-advantages

• Likely to have worse background/spurions.

• $Q$ resolution is slightly worse.
Thanks for your attention
MUSHROOM on a reactor

Could work;
• Would scan Ei and sample rotation
• Would effectively be a super flatcone
Be transmission
Bifrost Bragg peaks

Bragg peak distribution for a standard cubic sample with lattice parameter 4π for high and low wavelengths
Shoulder Bragg peaks
\[ \Delta E \propto \frac{\Delta t_{IG}}{L_1} \]
Indirect Geometry is much more efficient

\[ \frac{\Delta \lambda_{\text{in}}}{\Delta \lambda_{\text{d}}} = \frac{L_{\text{tot}}^d}{L_f^d} \approx 8 \text{ for LET or 11 for CNCS} \]