Polarized inelastic neutron scattering on HYSPEC HYbrid SPECtrometer at SNS

Igor Zaliznyak
Condensed Matter Physics and Materials Science Division
PNCMI, July 6, 2016
Related presentations

- At PNCMI 2016
  - B. Winn: “3D Polarization Analysis with a Polarizing Supermirror Array Analyzer at HYSPEC” – Session 9
  - A. Savici: “Data processing workflow for time of flight polarized neutrons inelastic measurement” – Session 3

- At ACNS 2016
  - O. Garlea: “The first results from the HYSPEC polarization analysis capability”
History: HYSPEC timeline

2000
- The Concept of the Hybrid Spectrometer proposed at BNL

2001
- Direct Geometry Hybrid Spectrometer presented to SNS EFAC
- HYSPEC Instrument Development Team (IDT) formed

2002
- HYSPEC IDT filed Letter of Intent with SNS
- HYSPEC proposal submitted to DOE

2003
- DOE CD0, HYSPEC is approved as part of the SING project

2004
- HYSPEC’s placement approved on BL14B; Design & Engineering begins

2005
- DOE CD2, HYSPEC’s performance baseline approved

2006
- DOE CD3, construction begins

2011
- DOE CD4, HYSPEC commissioning & operation begins

2013
- HYSPEC enters SNS User Program

2015
- Polarized beam operation on HYSPEC is commissioned

http://neutrons.phy.bnl.gov/HYSPEC

PNCMI 2016
4-7 July 2016, Munich (Freising), Germany
HYbrid SPECtrometer, HYSPEC: BNL Instrument Design Group

Igor Zaliznyak, PI

Steve Shapiro, co-PI

Larry Passell, advisor

Bill Leonhardt, engineer

Vinita Ghosh, scientist – MC simulations

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HYbrid SPECtrometer, HYSPEC – ORNL Instrument Team

HYSPEC: SNS Instrument Construction Team (… - 2013)

HYSPEC SNS Instrument Team now

Mark Hagen  Barry Winn  Tony Tong  David Anderson
Lead Scientist  Scientist  Scientist  Engineer

Melissa Graves-Brook
Science Associate

Ovidiu Garlea, Scientist
Joined in May, 2013

Barry Winn, Scientist

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**HYSPEC Team - 2002**

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<td>Ames/Iowa St.</td>
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<tr>
<td>A. Zheludev</td>
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**Instrument design team**

- I. Zaliznyak (BNL)
- S. M. Shapiro (BNL)
- L. Passell (BNL)
- V. J. Ghosh (BNL) Monte-Carlo simulations
- S. Doran (SNS/ANL) Engineering design concept
HYSPEC Team - 2015

**Instrument Development Team**

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**IDT Executive Committee**

- I. A. Zaliznyak, PI (BNL)
- S. M. Shapiro, PI (BNL)
- M. Kenzelmann (PSI)
- A. Goldman (Ames/Iowa State)
- T. Sato (Tohoku)
- J. Tranquada (BNL)
HYSPEC science case: polarization first

- Characterization of spin-dependent cross-sections by means of polarization analysis
- Coherent collective excitations in single crystals:
  - lattice dynamics (phonons)
  - spin dynamics (magnons, critical scattering)
- Structure and dynamics of partially ordered and glassy phases
  - spin glasses
  - charge glasses
  - correlated amorphous phases
  - small angle
- Study of the microscopic physical properties of samples in extreme environments:
  - temperature
  - pressure
  - magnetic field

http://neutrons.phy.bnl.gov/HYSPEC
HYSPEC place among the SNS inelastic instruments.

**High energy transfer**
10-1000 meV Fermi Chopper Spectrometer
- $E = 10 - 1000$ meV
- $Q = 0.1 - 22$ Å$^{-1}$

**High intensity at moderate resolution and medium energy transfer + polarized beam**
Crystal-Focussing Hybrid Spectrometer
- $E = 3.8 - 90$ meV
- $Q = 0.1 - 8$ Å$^{-1}$

**High resolution and low energy transfer**
10-100 μeV Multichopper Spectrometer
- $E = 2 - 20$ meV
- $Q = 0.1 - 4$ Å$^{-1}$

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HYSPEC conceptual design - 2003

- $T_0$ Chopper
- Disc Chopper
- Monochromator
- Goniometer
- Radial Collimator, or Bender
- Polarizers
- Flight Chamber (evacuated or Ar/He filled)
- Detectors

http://neutrons.phy.bnl.gov/HYSPEC
Short straight blade Fermi chopper at $L_1=37.2$ m to select $E_i$: trade off between $E$ resolution and flux via frequency range 60-420 Hz

Measures variable $E_f$ of scattered neutrons using ToF $L_2=3.6$ m, $L_3=4.5$ m
HYSPEC in operation - 2012

Commissioning Experiments, D. Fobes and I. Zaliznyak (2012)

http://neutrons.phy.bnl.gov/HYSPEC
HYSPEC in operation - 2013

Tune-up complete: apertures, beam stop, shielding, shielding
HYSPEC in operation - 2013

Tune-up complete: apertures, beam stop, shielding, shielding

http://neutrons.phy.bnl.gov/HYSPEC
Initial HYSPEC concept for polarized beam measurement with a Position Sensitive Detector (PSD)


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Initial concept for HYSPEC polarization analysis: experimental demonstration with PSD on SPINS

Nuclear and magnetic scattering intensities in \( \text{La}_{5/3}\text{Sr}_{1/3}\text{NiO}_4 \)

Polarized incident beam is supplied by reflection from the vertically focusing Cu$_2$MnAl (Heusler alloy) crystal monochromator.

10 meV < $E_{i\text{pol}}$ < 90 meV

Polarization analysis of the scattered neutrons is performed by a set of 18-22 supermirror-bender transmission polarizers, each 2 cm wide, 5 cm thick and 15 cm high,

3.7 meV < $E_{f\text{pol}}$ < 15-25 meV

A supermirror-bender transmission polarizer setup for HYSPEC (2002)

A very compact device (but needs a saturating magnetic field)

An array of 20 benders covers 60 deg. acceptance of the detector bank.


http://neutrons.phy.bnl.gov/HYSPEC
MC simulation (NISP) of HYSPEC operation in the polarized beam mode: beam separation

Simulation for the bender geometry optimized for $E=14.7$ meV (C. Majkrzak, 1995)
Sample-to-detector distance $L_{SD}$ is 4.5 m

Opportunistic change of plan: PSI Supermirror Polarization Analyzer

Supermirror analyzer assembled with around 200 supermirrors

Prototype I (1.8 deg)  Prototype II (4.0 deg)

2011 status:

- 780 out of 960 polarizers produced
- ~100 polarizers per month
- 200 polarizers installed in housing & tested on BOA (optics beamline at SINQ, PSI)
- Anticipated completion in March 2011, followed by tests at SINQ

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Polarized beam setup with the PSI Polarizing Supermirror Array (B. Winn)

Remove radial collimator

Switch to Heusler

Put polarizing supermirror
Intensity at sample, V scatterer

- 15 cm high beam from guide vertically focused to sample
  ~2.5 cm x 2.5 cm FWHM
- 4.2E5 n/s/MW/cm²: Gold foil measurement at sample position, PG focus
  array to sample 1.8 m, Ei=15 meV, Fermi 180 Hz
- Plot: Vanadium incoherent isotropic scatter integrated over detector
  array at 40° < 2Θ < 100°, PG & Heusler

3.8 meV < Ei < 50 meV

Common Ei’s: 3.8, 7, 15, 20, 27, 35 meV
Rare Ei: 50 meV
Performance of the Polarizer

960 supermirrors, 60°
U. Filges
BOA beamline at SINQ
Ready to ship

Magnetization unit at HYSPEC

supermirror analyzer - effective polarization $P_{\text{eff}} < 95\%$

supermirror analyzer - transmission $I_{\text{ana,up}} / I_{\text{beam,up}}$

Transmission $_{\text{max}} = 67\%$

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More Power to HYSPEC

November 11, 2015

After installing the new wide-angle super mirror array at SNS’s hybrid spectrometer, beam line 14B, HYSPEC is ready to tackle new problems using fully polarized neutron scattering.
HYSPEC polarized beam setup in operation
First test: antiferromagnetic structure of the layered semimetal YbMnBi$_2$

YbMnBi$_2$ (~0.5g) single crystal
Polarized diffraction measurement of YbMnBi$_2$: one night on HYSPEC
Polarized diffraction scans on YbMnBi$_2$ Bragg peaks
HYSPEC is not a diffractometer, but... can do diffraction, if needed

The refinement compares favorably to HB3 diffractometer

Fit of the 4K – 300 K data with P || Q. AFM model with spins along c axis gives ordered moment amplitude of $4.37(18) \mu_B$

Fit of the 4K – 300 K data with P vertical (┴Q). AFM model with spins along c axis gives ordered moment amplitude of $4.52(17) \mu_B$

RF-factor: 25.9, $\chi^2$(Intensity): 0.72

RF-factor: 17, $\chi^2$(Intensity): 0.46
Magnetic dynamics in FeTe$_{0.45}$Se$_{0.55}$ superconductor: sample geometry

Large (~ 23g) bulk single crystal, irregularly mounted on Al plate
Beam depolarization in superconducting FeTe$_{0.45}$Se$_{0.55}$

Sample is cooled in guide field $\sim 10\sim 20\text{G} \Rightarrow$ the beam is fully depolarized at $T<T_c$!

Flipping Ratio ($T>T_c$) = 13(1)
Zero field cooling: FR = 5 ~ 8

• Cooled in a mu-metal shield from 16 K to 5 K
• Cooled on the instrument sample table, in a compensating guide field providing zero field environment
• Effect is similar: flipping ratio improved.
• FR varies from 5 to 8, depending on the sample rotation angle
“P||Q” setup: align polarization with the middle of detector at E=0

Change of the mutual alignment of P and Q with energy transfer

E=0 meV

E=8.0(9) meV

SNS @ 1 MW. Ei = 20 meV. Each dataset is approximately 24 hours on HYSPEC: 6-8 min for each of the 191 angular positions of the sample.

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SF and NSF at 5 K
SF and NSF at 5 K
SF and NSF at 300 K
SF and NSF at 300 K
Magnetic and non-magnetic excitations in FeTe<sub>0.55</sub>Se<sub>0.45</sub> by polarized neutron scattering on HYSPEC


Comparison of the equivalent slices from the Spin-Flip (left) and the Non-Spin-Flip (right) data sets

Spin-Flip Scattering (magnetic)
\[ I_{SF}(Q,E) \] at \( T = 300 \) K

Non-Spin-Flip Scattering (phonon)
\[ I_{NSF}(Q,E) \] at \( T = 300 \) K

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FeTe$_{0.55}$Se$_{0.45}$ $\chi_{SF}(5K)$, [0,0,L]=[-0.25,0.25], E=[7.1,FeTe$_{0.55}$Se$_{0.45}$ $\chi_{NSF}(5K)$, [0,0,L]=[-0.25,0.25], E=[7.1,8.9] meV

Non-Spin-Flip Scattering (phonon)
$I_{NSF}(Q,E)$ at $T = 5$ K

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FeTe$_{0.55}$Se$_{0.45}$ $\chi_{SF}(300K)$, $[0,0,L]=[-0.25,0.25]$, $[H,0,0]=FeTe_{0.55}$Se$_{0.45}$ $\chi_{NSF}(300K)$, $[0,0,L]=[-0.25,0.25]$, $[H,0,0]=[0.4,0.6]$
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Non-Spin-Flip Scattering (phonon)

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Temperature-induced dynamical magnetism in Fe$_{1.1}$Te

FeTe on ARCS, $E_i = 100$ meV
Zaliznyak, et. al., arXiv:1103.5073

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Temperature induced magnetism in Fe$_{1.1}$Te

Sum rule defines the effective fluctuating magnetic moment

$$\left[ \mu_{\text{eff}} / (g \mu_B) \right]^2 =$$

$$= \int S(Q, E) d^3 Q dE = S(S + 1)$$

Zaliznyak, et. al.,
PRL 107 216403 (2011);
PRB 85, 085105 (2012).
Dynamical spin response in FeTe$_{1-x}$S$_x$.

FeTe$_{1-x}$S$_x$ (x $\approx$ 0.13) on HB3.


Fe$_{1.1}$Te, ARCS (E = 6 meV).

Brookhaven National Laboratory
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Non-Spin-Flip Scattering (phonon)
$I_{NSF}(Q,E)$ at $T = 300$ K

SNS @ 1.3MW. $E_i = 20$ meV. Each dataset is approximately 20 hours on HYSPEC: 6 min for each of the 191 angular positions of the sample.

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$I_{SF}(Q,E)$ at $T = 300$ K

Non-Spin-Flip Scattering (phonon) 
$I_{NSF}(Q,E)$ at $T = 300$ K

SNS @ 1.3MW. $E_i = 20$ meV. Each dataset is approximately 20 hours on HYSPEC: 6 min for each of the 191 angular positions of the sample.

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[Slice images]

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Summary

- Polarized neutron surveys of a large volume of the sample’s phase space are possible despite
  - Factor 20 to 80 transmission losses in the polarized setup
  - Restricted field of view at the focus of the radial supermirror array
  - Large number of corrections for transmission and deflection in the polarized setup (talks by A. Savici and B. Winn)

- It’s a miracle?
  - Careful experiment planning and execution
  - Precise instrument and sample alignment
  - Steady and maintenance-free setup

- It’s a miracle!