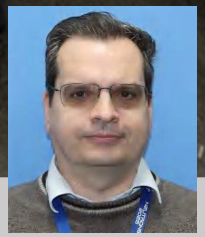
OAK RIDGE National Laboratory

HYSPEC, 2017-2020

B. Winn (point of contact)
O. Garlea (neutron scattering scientist)
M. Graves-Brook (scientific associate)
A. Savici (computational instrument scientist)

2020 Review of the Instrument Suites for Spectroscopy, Sept 17, 10:50 AM
Direct Geometry Suite



U.S. DEPARTMENT OF ENERGY

watch for Easter eggs,
responses to 2017 review (Slide 22)

Niche

- Polarization analysis option
  - 44% of beamtime
- Large configurable horizontal angle detector acceptance
- Vertical focusing for good statistics
  - small single crystals
  - extreme conditions
- Cold neutrons
  - 3.8 meV < E_i < 60 meV unpolarized
  - 3.8 meV < E_i < 25 meV polarized
- Moderate energy resolution 3-5% E_i

Moderator	Coupled cryogenic hydrogen
Source – Fermi chopper distance	37.2 m
Chopper – sample distance	3.2 m
Sample – detector distance	4.5 m
Focusing crystals to sample distance	1.8 m
Incident energy range	3.8 — 60 meV
Resolution (elastic scattering)	3 — 5% E_i
Detector coverage horizontal	2° — 120° (60° at one time)
Detector coverage vertical	-7.5° — 7.5°
Minimum detector angle	2°
Beam Size	3 cm x 3 cm focused

Topics of study

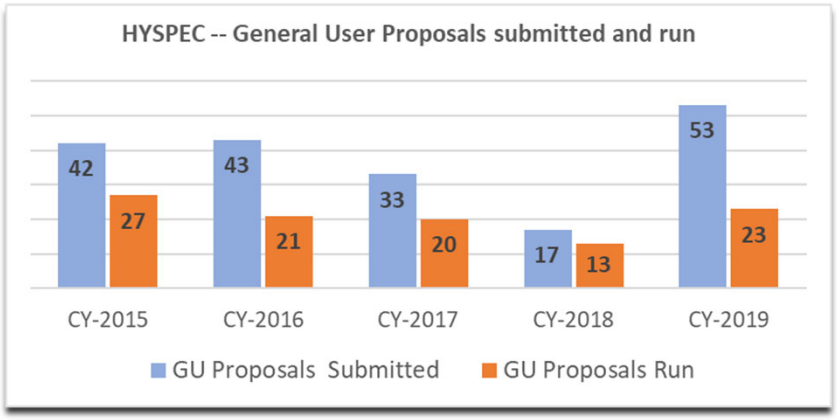
- exotic ground states in quantum magnets and quantum critical phenomena
- unconventional superconductors
- lattice and magnetic dynamics in functional materials including ferroelectrics
- magnetoresistive and magnetocaloric materials
- excitations in geometrically frustrated magnets
- itinerant magnets

Program & User Community Development

- Half Polarized
- XYZ Polarization Analysis

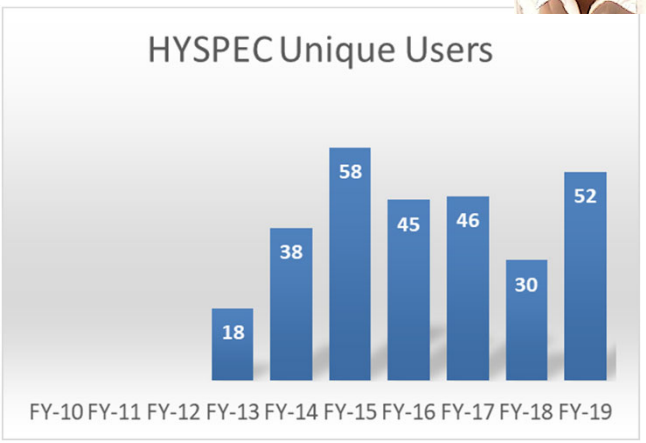
3. General user program and beam time usage

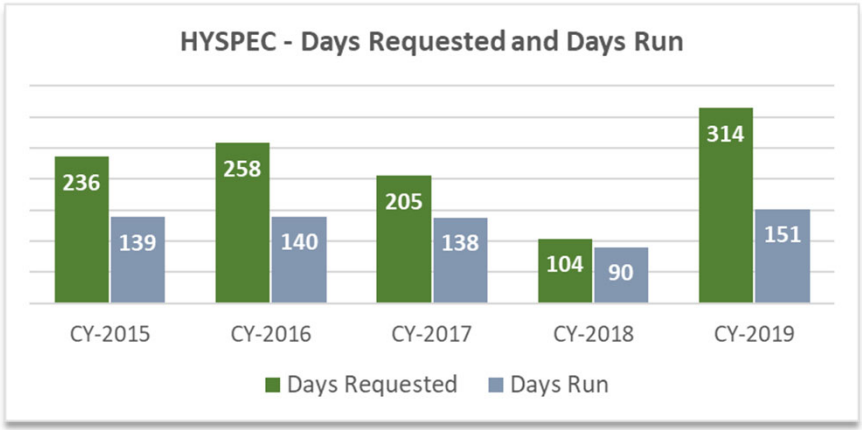
Gabrielle D. Boudreau
User Facilities Analyst

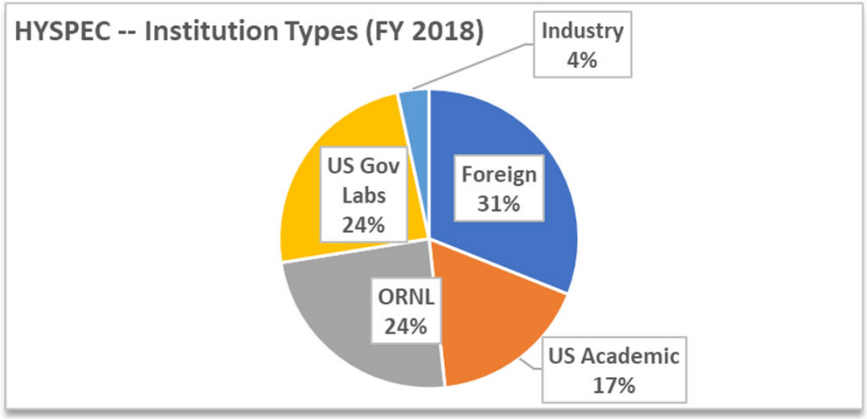


TOP EXTERNAL INSTITUTIONS USING HYSPEC (FY 2019)

BROOKHAVEN NATIONAL LABORATORY
DUKE UNIVERSITY
STANFORD UNIVERSITY
FLORIDA STATE UNIVERSITY
COLORADO STATE UNIVERSITY
MCMASTER UNIVERSITY
GEORGIA INSTITUTE OF TECHNOLOGY
TOHOKU UNIVERSITY
OCHANOMIZU UNIVERSITY







OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

3. Discretionary Time Usage

Instrument Development Team

- Most discretionary beamtime before December 2018
- 8 publications since 2017
- This final IDT was disbanded September 2018
- PSI loan agreement replaced by purchase, wide-angle polarizing supermirror array
- Colleagues from Brookhaven National Laboratory remain strong users and partner in commissioning new techniques

Quantum Materials Initiative

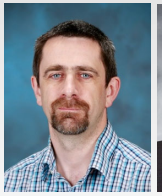
- QMI established 2018
- Starting Fall 2019, 50% of Discretionary Beamtime goes through QMI Science Review
- 2 completed experiments. Analysis ongoing

C. dela Cruz
Quantum Materials Initiative

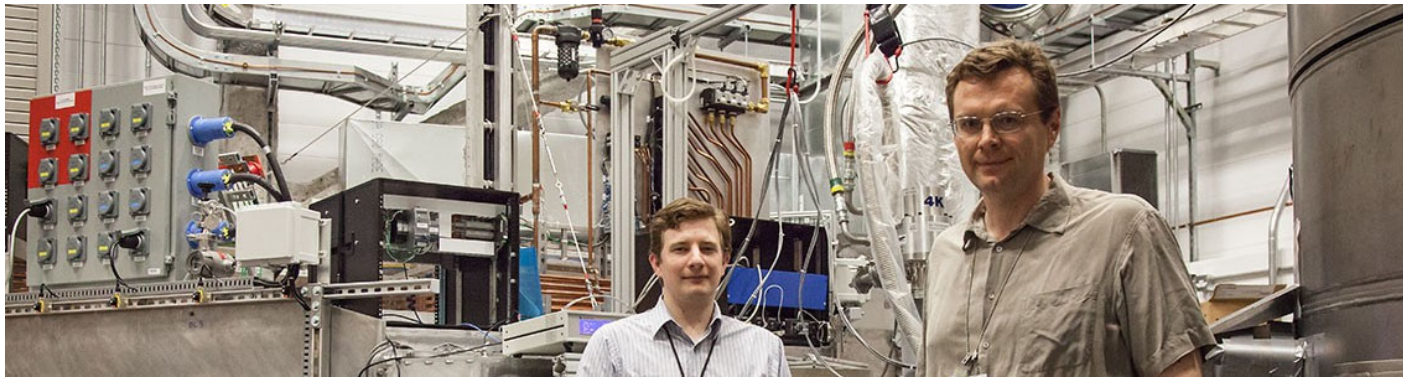
Other Discretionary

- Getting that last data for publication
- Fostering inter-ORNL collaborations
- Fostering Florida State University collaboration

R. Hermann ORNL **M. Manley**



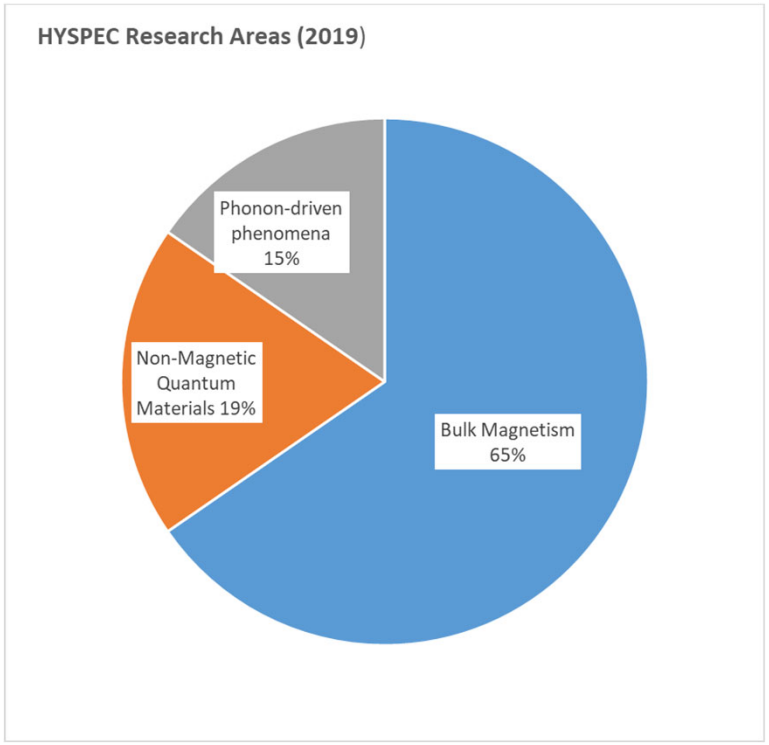
M. Shatruk
FSU

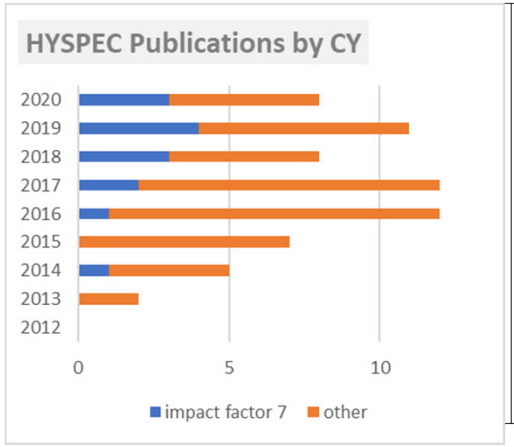


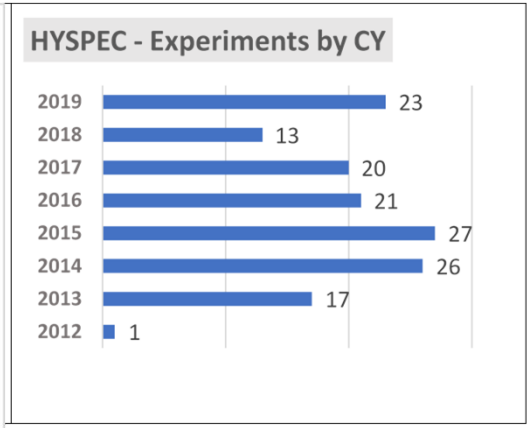
D. Fobes **I. Zaliznyak**, BNL

4. Beamline Productivity

Gabrielle D. Boudreau
User Facilities Analyst







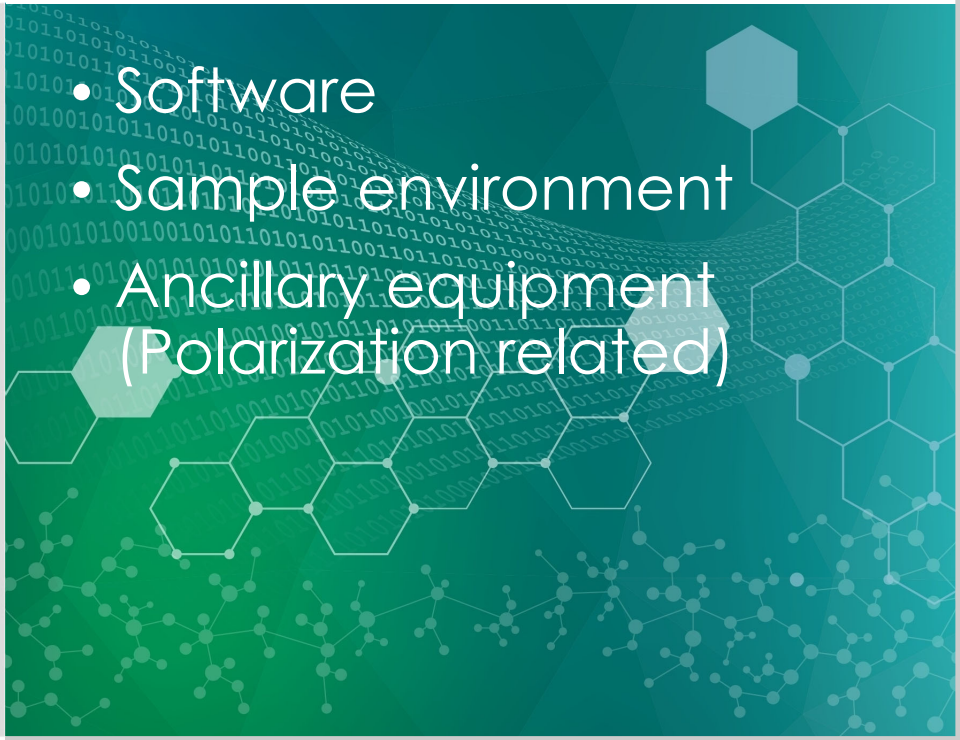
Exciting growth in increasing publications with high impact factor!

Possible new user community would leverage removal of spin-incoherent scattering as advocated at ISIS' LET[1] and NCNR's MACS[2]

[1]G. Cassella et al, *Jour. Phys.: Conf. Ser.* **1316**, 012007 (2019)
[2]W. Chen et al, *Physica B: Cond. Matt.* **564**, 166 (2019)

OAK RIDGE National Laboratory

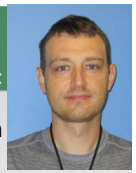
5. Adequacy and Reliability of



OAK RIDGE National Laboratory

5. Software

Acquire



Klemen Vodopivec
Instrument
Data Acquisition

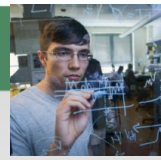
- Since 2017
  - EPICS process variables communication protocol
  - ADARA neutron and fast metadata event protocol
  - CSS graphical user interface
    - Scan and table scan GUI's
- In development
  - (DGS) Supported script interface for automated scans
  - (DGS) Features facilitate remote participation
  - (DGS) Standardize
- How HYSPEC team operates
  - Very involved in alignment and overnight planning due to moving components

Reduce

Andrei Savici
Computational
Instrument
Scientist

- Autoreduction
  - (DGS) Slice generation combines data from different sample orientations
- Set of reduction scripts
  - (DGS) Works. Proper noise handling. Several tutorials
  - (HYSPEC) spin flip correction
- In development
  - (DGS) MSLICE GUI leveraging reduction script workflow
  - (DGS) Time independent background, lower noise subtraction method
  - (HYSPEC) Additional polarization reduction features for 3D Schärpf angle correction

Analyze & Model



Marcus Daum
Georgia Tech

- MCVINE*
  - (DGS) only way to account for resolution for now
- Spin wave analysis
  - Database begun by HERE student
- Ugly Data Challenge (2018)
  - Regularization to address low statistics data
  - An effort to foster interaction with ORNL's computing group 'Math for Deep Learning'
  - Benefits await publication
- ICEMAN (not yet tried @ HYSPEC)
  - Modular, flexible platform
  - Integrated phonon modeling OCLIMAX

*J.Y.Lin et al, *NIM A* **810**, 86–99 (2016)

5. Sample Environment

- HYSPEC solicits experiment proposals for
  - 14 tesla vertical bore split coil
  - Down to 300 mK
  - Unpolarized
- Preserve access to magnets
  - New path?
- When to try Longitudinal polarization analysis with magnet?
  - 5 tesla compensated: Await approved GU or DT proposal
  - 14 tesla uncompensated: Await modeling and testing, forces on wide-angle polarizing supermirror array

OAK RIDGE National Laboratory

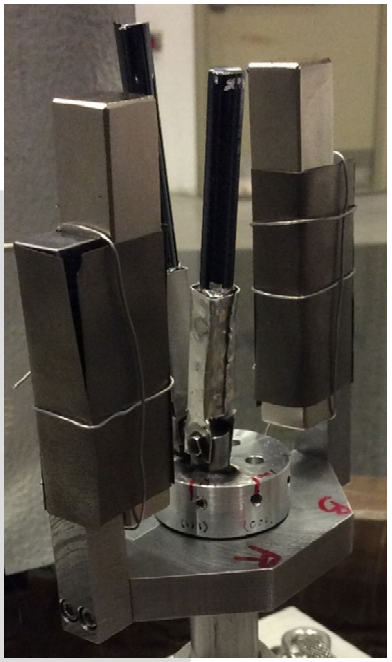


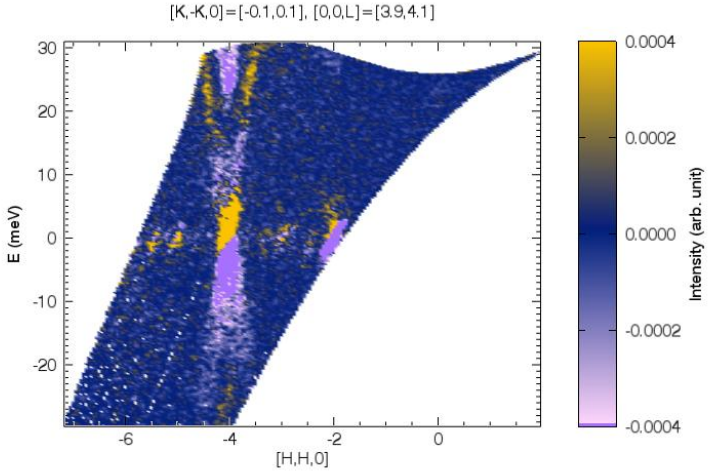
Y. Nambu Tohoku U
K. Kakurai CROSS, CEMS
D. Conner ORNL

5. Lesson learned for half-polarized / horizontal field

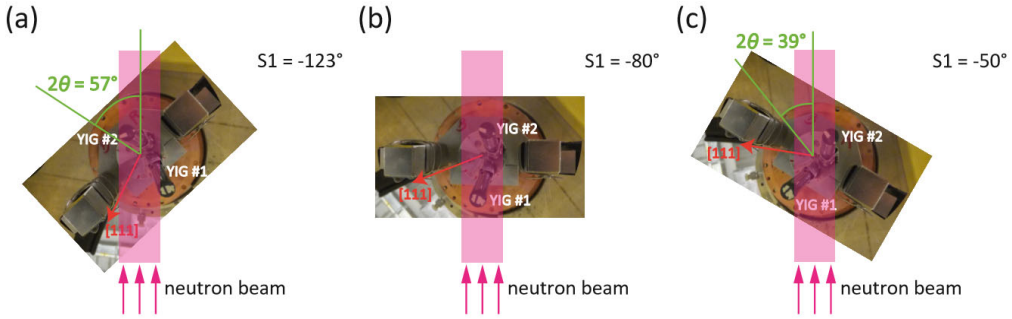
- Horizontal Yoke, permanent magnet + steel
- Careful single crystal orientation
- Polarization inversion near poles
- Learned afterwards to employ vertical guide field
- Motivates future investment in multipole horizontal field magnet
- Technique for both ferromagnets and ferrimagnets

Y. Nambu et. al., *Physical Review Letters,* **125,** 2, 027201 (2020)



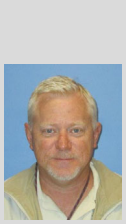


Flipper ON - OFF



5. Polarization Upgrade: Elevator & Alignment

- Elevator
  - User desire for unpolarized in same experiment
  - Better statistics
  - Better energy resolution
    - We insist on sloppy energy resolution for polarized experiments…
- Alignment for supermirror array
  - From maximum polarization to maximum intensity position



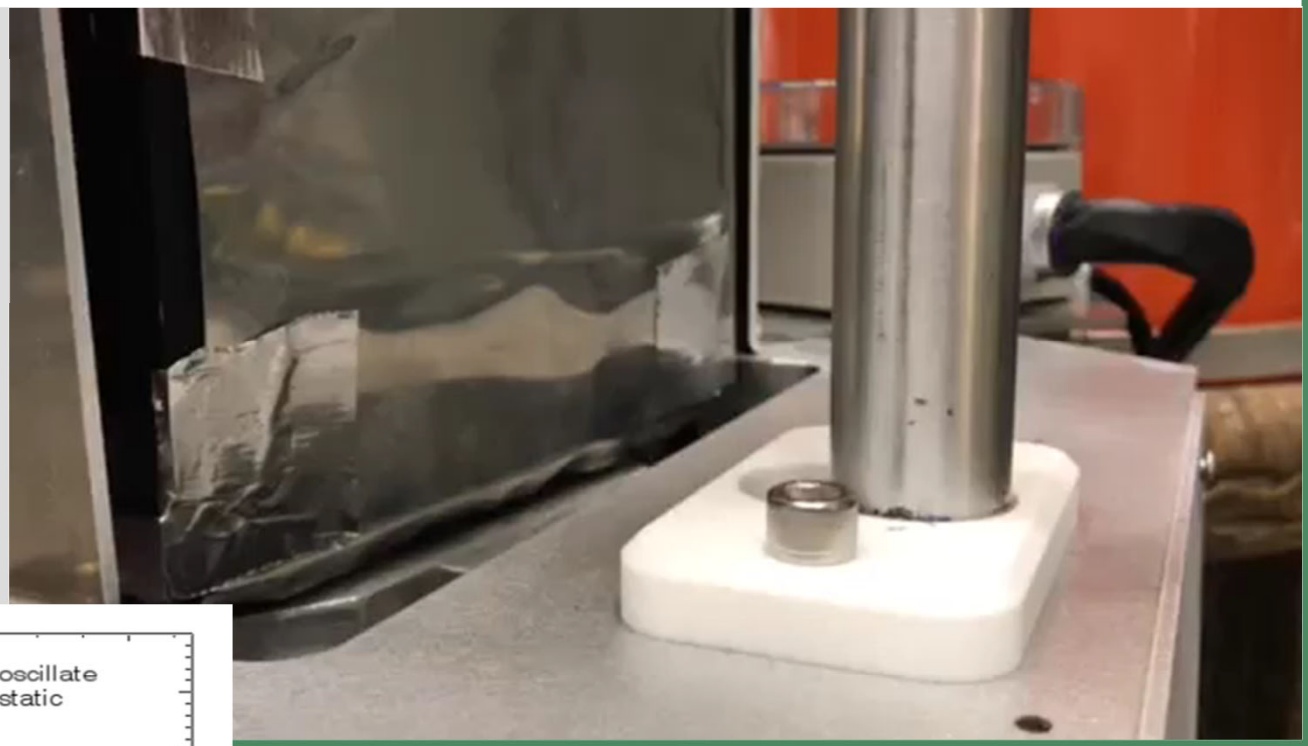
David Conner
Engineer
Neutron Technologies Division

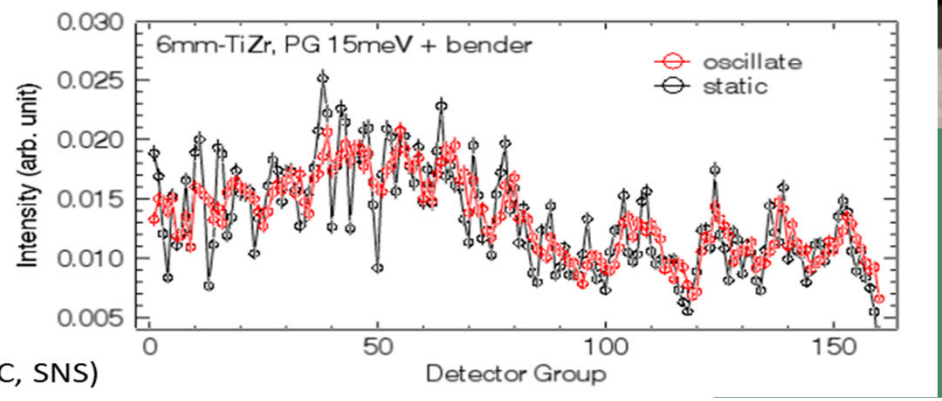
OAK RIDGE National Laboratory

David Conner
Engineer
Neutron Technologies Division

5. Polarization upgrade: Oscillator

- Improve data quality with more uniform normalization





Transmission per tube, both stationary and oscillating

OAK RIDGE National Laboratory

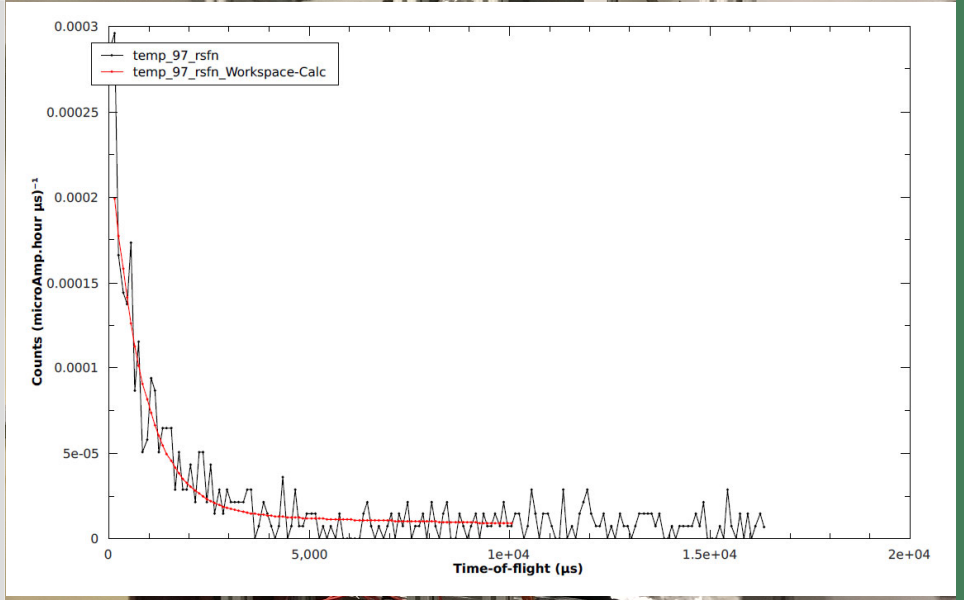




M. Graves-Brook HYSPEC | **K. Berry** Detectors | **E. Iverson** Neutronics | **S. Hicks** Instrument-Data-Acqisition | **K. Vodopivec**

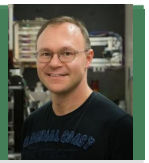
5. Polarization Epiphany: reduce time-independent background

- Some low-moment systems have proved problematic to characterize
- Motivated concerted effort to characterize time independent background
- Portable detector station
  - Different locations in HYSPEC experiment room
  - Different shielding materials
- Request investment in flexible borated shielding product for 4x reduction
- <u>Approved to purchase new shielding</u>!



5. Ongoing Polarization Upgrades

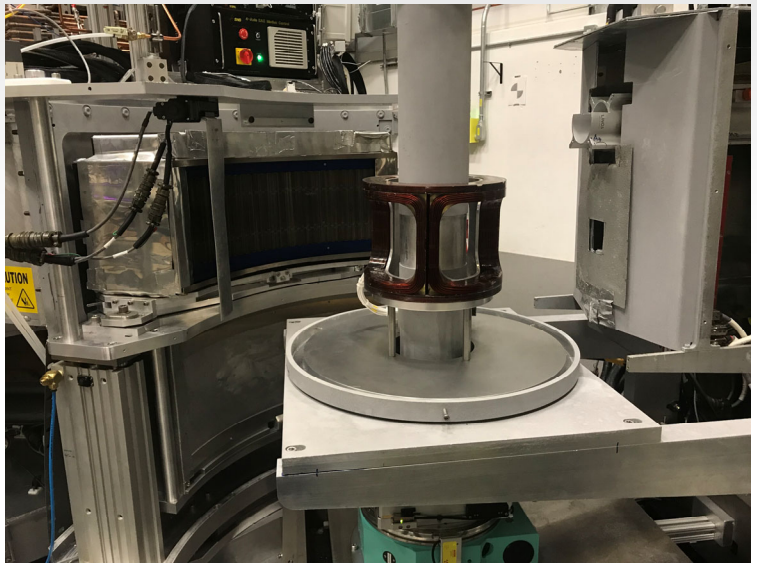
RF Flipper, pre-sample

Y. Kang **A. Parizzi**
Linac RF Engineer, RAD
Scientific Associate Lead

Compact 3D coils


R. Morgan **D. Conner**
Instrument Development, RAD
Engineer, NTD



8. Extra space afforded by Compact 3D coils for planned wide-angle scattered-beam flipper

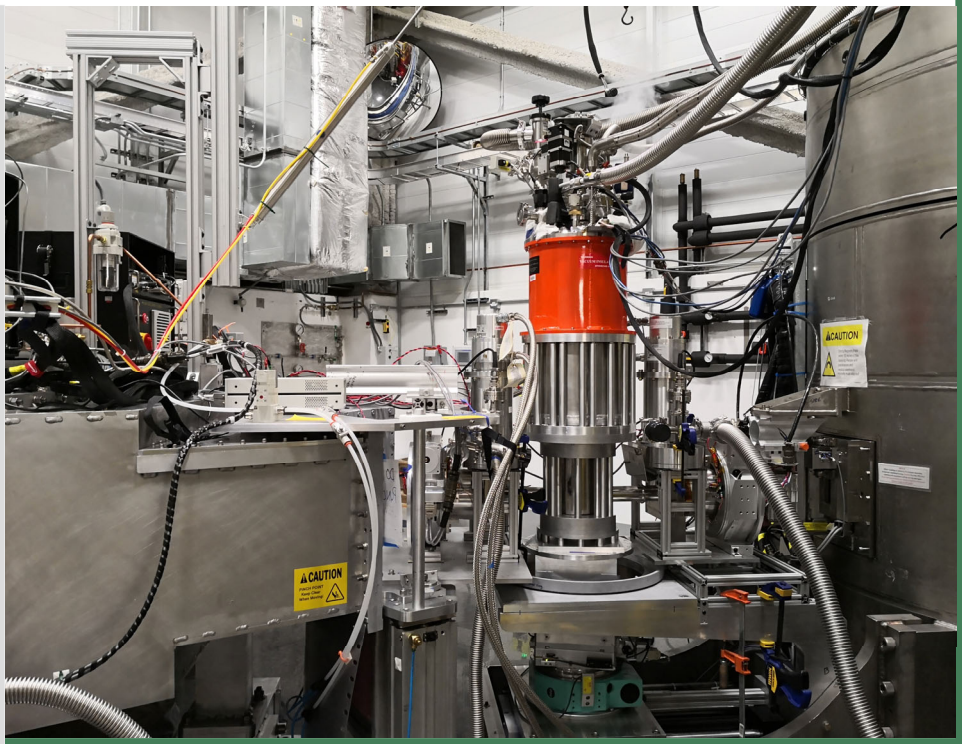
OAK RIDGE National Laboratory



N. Silva **R. Wang*** **P. Jiang**
Instrument and Polarization Development
Neutron Technology Division
*Now at Chinese Spallation Source

5. Spherical Neutron Polarimetry

- Intended for HFIR
  - PTAX and GP-SANS
- Active project, Lab Directed Research and Development
- Direct beam test at MURR
- HFIR down most of CY2019
- So HYSPEC tested it out
  - First test with scattered beam
  - First test with orange cryostat
- HYSPEC Wide Angle variant in design concept stage
  - Part of Early Career Project for P. Jiang



Trend towards narrow tail cryostats to accommodate polarization optics

5. Polarization overview

Developments

- Elevator / Oscillator
- Reduce time-independent background (ongoing)
- RF flipper and compact coils (ongoing)
- Spherical Neutron Polarimetry (TAX mode only)
- Software
  - Customizable Python scripts enable per-pixel normalization and flip ratio corrections

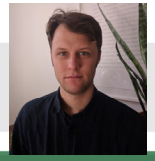
3. Science & User Program

- 44% of beamtime, 2017-2020
- Long experiments
  - Limited efficiency optics
  - Multiple measurements
- Education
  - (OG) Polarization tutorial workshop 2019
  - (OG) Magnetic structure determination tutorial workshop every-other year
  - NXS 2017, polarized mode
  - (OG) HERE & GO students

8. New Directions

- Wide-angle scattered beam flipper
- Wide-angle spherical neutron polarimetry
- Horizontal field quadrupole magnet
- Possible extension into soft matter studies
  - Spin-incoherent removal with Longitudinal polarization analysis
  - Similar to MACS & LET
- Tutorial every-other year
- Press forward for new optics & techniques

6. Science highlights, polarization



K. Plumb
Brown U

M. Shatruk
Florida State U

Continuum of quantum fluctuations in a three-dimensional S = 1 Heisenberg magnet

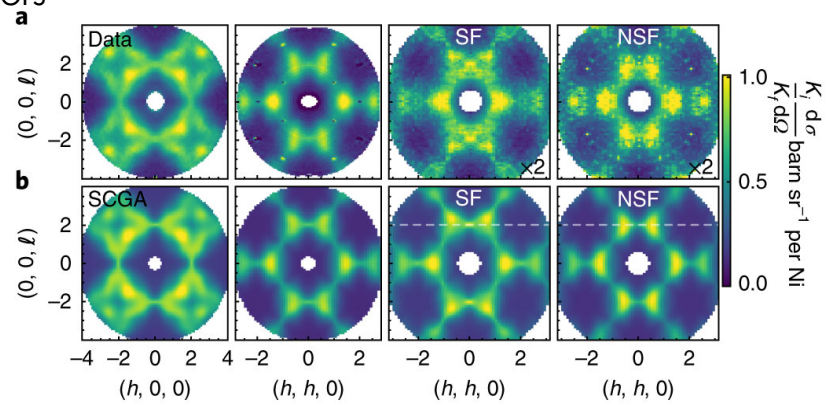
K.W. Plumb et al., *Nature Physics* **15**, 54-59, 2019

Achievement Comparison of polarized result to SCGA model provided solid numbers for Hamiltonian

Impact Measured excitations consistent with fractionalized excitations, so $NaCaNi_2F_7$ must be a 3D S=1 Heisenberg antiferromagnet

Details 1D polarization analysis, integrated signal over 0 < E < 14 meV

Why HYSPEC? Diffuse. Inelastic. Polarized. Broader kinematic range required than available at MACS. Simultaneous measurement of continuous range of energy transfers



Reentrant spin glass state induced by structural phase transition in $La_{0.4}Ce_{0.6}Co_2P_2$

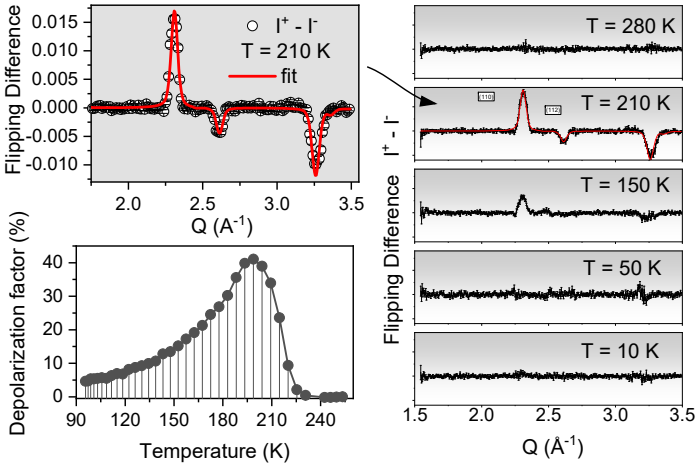
J. K. Clark et al., *Phys. Rev. Matt* (2020) -in press

Achievement measure incredibly weak 0.15(1) μ_B per Co atom and negligible –0.01(1) μ_B per Ce atom

Impact gradual dissipation of a weak ferromagnetic ordering and onset of a glassy state

Details Depolarization is an underutilized, highly effective order parameter probe

Why HYSPEC? Half polarized, full polarized, and depolarization. Low detection limit of ordered moment only possible via nuclear-magnetic interference term



OAK RIDGE National Laboratory

6. Science highlights

Exotic Magnetic Field-Induced Spin-Superstructures in a Mixed Honeycomb-Triangular Lattice System

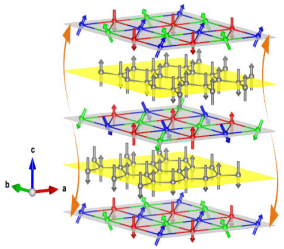
V.O. Garlea et al., *Physical Review X* **9**, 011038, 2019

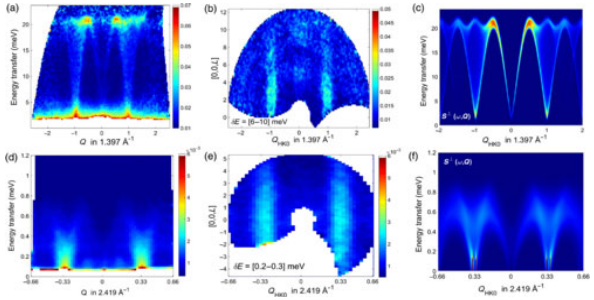
Achievement observations suggest subtle thermal and quantum fluctuations generate effective interlayer tunneling

Impact new and unexpected magnetic arrangements could not be explained via quasi-classical theory. Required innovative modeling

Details unconventional strategy: 2D powder measurement reveals intricate features which were effectively modeled and compared

Why HYSPEC? versatility: measure two different energy and momentum scales. Near other neutron scattering instruments to enable comprehensive study





Excitations in the field-induced quantum spin liquid state of α-$RuCl_3$

A. Banerjee
Purdue U

A. Banerjee et al., *npj Quantum Materials* **3**, 8, 2018

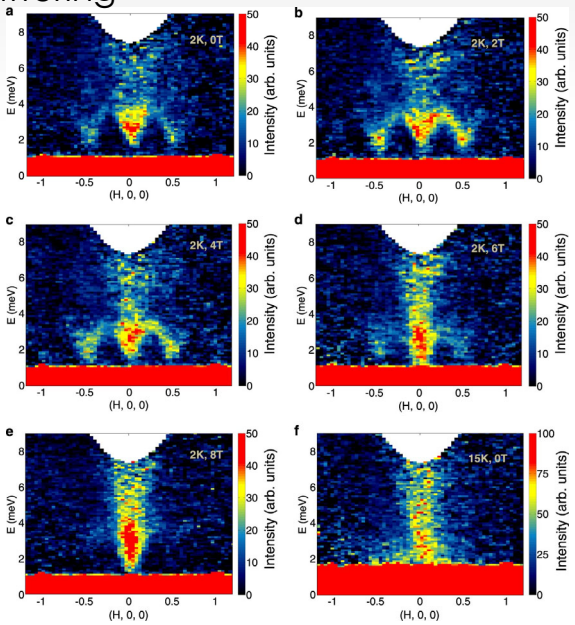
Achievement suppressed conventional spin waves with magnetic field, in order to reveal excitations consistent with Kitaev quantum spin liquid

Impact broader quantum computing community finally wakes up to neutron scattering

Details weak 1D signal integrated over large region of reciprocal space

Why HYSPEC? sufficiently clean background using this magnet
(tightest radial collimator in ORNL DGS suite, and possibly worldwide)

S. Nagler ORNL **A. Tennant**



6. Science Highlights, phonons

Intrinsic anharmonic localization in thermoelectric PbSe

M. Manley ORNL

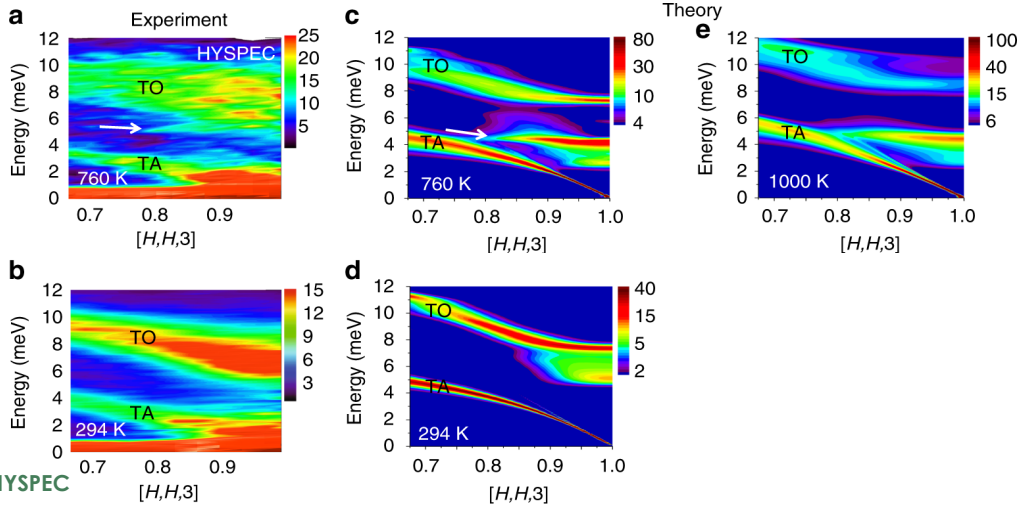
M.E. Manley et al., *Nature Communications* **10**, 1928, 2019

Achievement nonlinear localization of a large fraction of an entire phonon revealed for first time

Impact nonlinear localization plays important role in transport properties

Details fruits of growing collaboration

Why HYSPEC? Failed to resolve feature with TAX



Anharmonic Eigenvectors and Acoustic Phonon Disappearance in Quantum Paraelectric $SrTiO_3$

O. Delaire Duke U

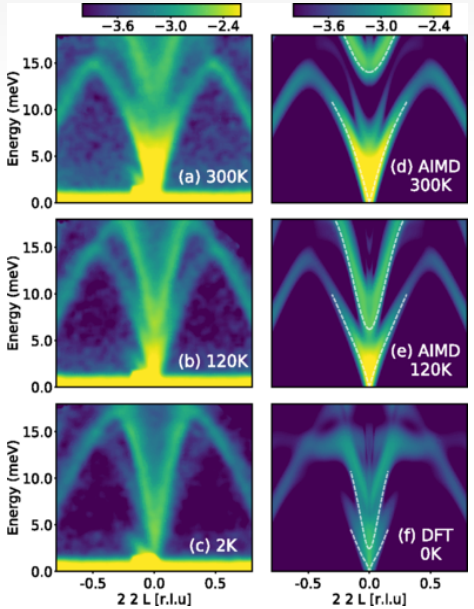
X. He et al., *Phys Rev Lett* **124**, 145901, 2020

Achievement compared observations to first-principles simulations including anharmonic effects

Impact anharmonic renormalization of eigenvectors for Ti and O motions drives unusual thermal transport

Details HB3 TAX provided critical complementary information at more temperature points

Why HYSPEC? extended Q-E teased out effects first hinted at in TAX measurements. Perfect energy range



7. Risks

- Future higher field, uncompensated magnets
  - Impact on wide-angle polarizing supermirror array
  - No neutron scattering instrument in US accounts for stray field in design
  - Straddled by neutron spin echo and fundamental physics…
- Moderator transition away from cold coupled
  - Part of long-term 3-source strategy
- Sample size more limited for polarization analysis
  - Less a risk than an intrinsic limitation, but with limited efficiency polarization optics already, this just adds insult to injury…

8. Future instrument science and development plan

Near-term vision (1-3 years)

- Lower background
- Wide-angle scattered-beam spin flipper
- hybridized magneto-elastic excitations
- Wide-angle spherical neutron polarimetry
- Longitudinal polarization with vertical field magnet
- New users remove spin-incoherent via Longitudinal polarization analysis
- Preserve magnet access during construction
- Remote participant user model during pandemic
- Top loading dry cryostat
- Polarized Post-Doc!

Strategic vision (3-10 years)

- Polarization tutorial workshop every other year
- Horizontal field magnet
- Socialize spin-wave database
  - Extend HERE project to complete database
- Unpolarized INS remains central
- HTS magnets >14 tesla
- Part of 3-source strategy
  - HYSPEC remains unique using polarization analysis with wide-angle supermirror array
  - DGS of choice for testing new optics, sample environments, and new techniques

9. Response to instrument specific recommendations from last review

Recommendations	What we've done
1. Increase efforts on software-data reduction and modelling with resolution	1. Progress. Slide 8
2. Investigate and understand the main barriers to publication from HYSPEC experiments	2. Impact. Slide 6
3. Go ahead with the project to install analyzer changer/oscillator	3. Done. Slides 11-12
4. Go ahead with the commissioning of z-only PA in field	4. Positioning. Slide 9
5. Launch a project to look at implementation of a secondary spectrometer wide-Angle flipper	5. Preparing. Slide 14.

Remember these?

10. Summary

Polarization driving progress at HYSPEC

- No more "*polarization analysis is just one technique*"
  - Select from growing suite of techniques and optics to target experiment demands
- Improvements are a rising tide lifting all 'boats'
  - Lower time independent background
  - Elevator provides flexibility for scheduling and individual experiments
  - New sample environment strategy
    - Narrow tail / modular top-loading system
    - Horizontal field magnets
  - Potential new science / user community with incoherent removal
- The next generation will embrace polarization and will fully leverage its scientific potential
  - Training and mentoring

Mature operations, Productive science

- Strong collaborations
- Repeat users
- High impact publications
- No longer the easiest DGS to win time on
- The go-to place for
  - Low energy phonons
  - Isolating magnetism in itinerant magnets and spin liquid systems (polarization)
  - 14 tesla magnets
  - Cleanest background with complex sample environments
  - Capable instrument team that gets your science and is committed to your success
- Integral part, powerful suite of polarized instruments at HFIR & SNS