TAX (HB3) Triple Axis Spectrometer

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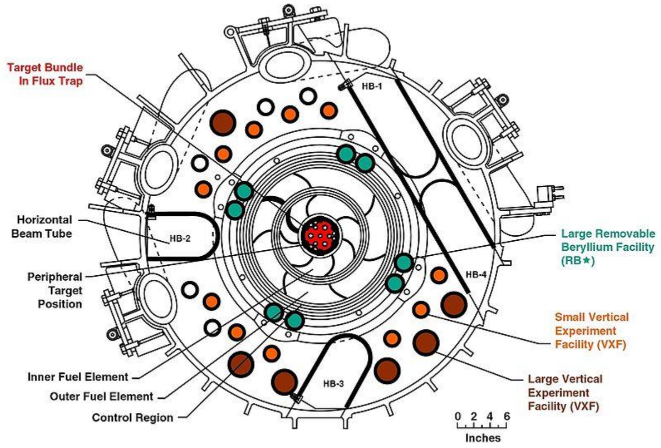
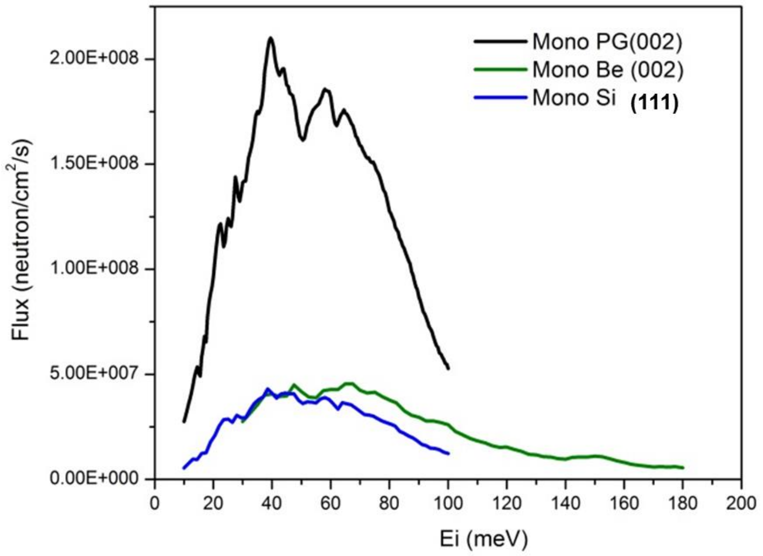
Beamline Review Checklist

1. TAX (HB3) overview
2. Scientific Mission and Impact
3. Beamline Productivity
4. General user program and beam time usage
5. Adequacy and reliability of software, sample environment and ancillary equipment
6. Science Highlights
7. Future instrument science and development plan
8. Risks
9. Summary

Overview



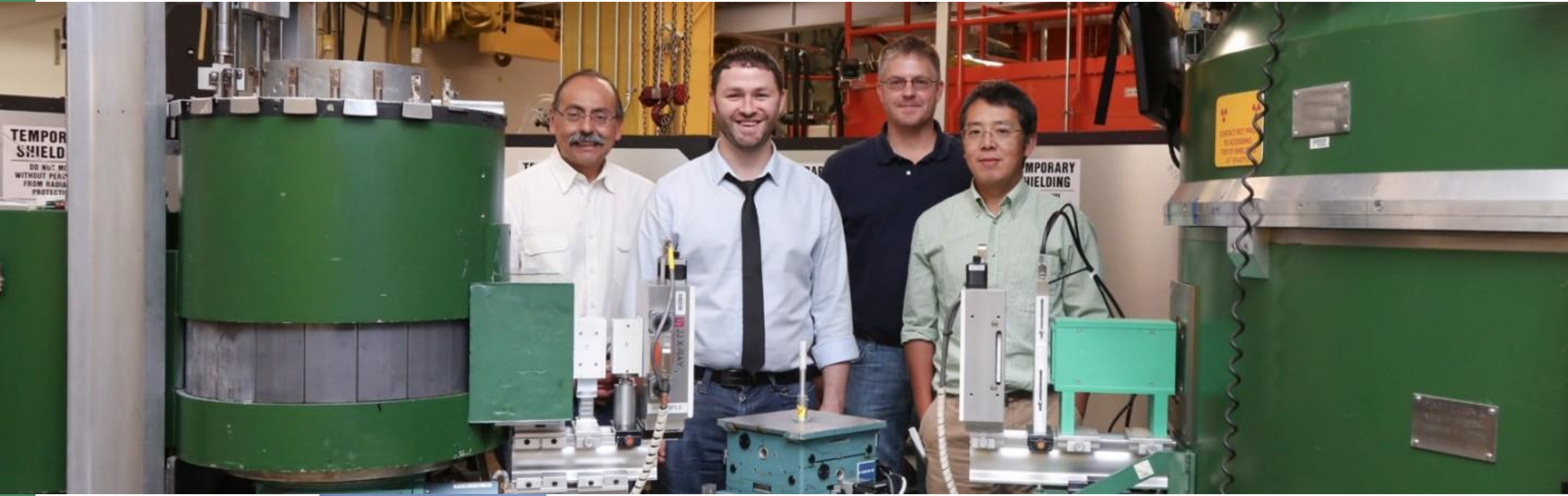


- ❑ Beam tube angle provides high flux
- ❑ In-pile sapphire filter for the white beam before the monochromator.
- ❑ Choices of 3 vertically focused monochromators.
- ❖ PG(002) optimized high flux at each energy
- ❖ Be(002) allows good energy resolution at high E transfer
- ❖ Si(111) provides 2nd-order-free clean beam
- ❑ Wide range of momentum transfers
- ❑ Availability of various Söller collimators provides flexibility.

Instrument Specifications

Beam Spectrum	Thermal
Monochromators	Variable vertical focusing PG (0 0 2) Be (0 0 2) Si (1 1 1)
flux	$2x10^8 n/cm^2/s$ PG (0 0 2) E_i=40 meV
Analyzer	Fixed vertical focusing PG (0 0 2)
Monochromator takeoff angle	12° - 88°
Sample angle	±180°
Scattering angle	-90°-130°
Analyzer angle	-40°–90°
Detector	Single ^{3}He gas counter
Resolution (elastic)	5-10% E_i (adjustable with collimators)
Collimations (FWHM)	Premonochromator: 30', 48' Monochromator– sample: 20', 40', 60', 80' Sample– analyzer: 20', 40', 60', 80' Analyzer– detector: 30', 70', 90', 120', 210', 240'

HB3 Instrument Team



CIS:
Andrei Savic

Instrument team (left to right):

- Jaime Fernandez-Baca (33%)
- Travis Williams (33%)
- Michael Cox   (50%)
- Songxue Chi (100%)

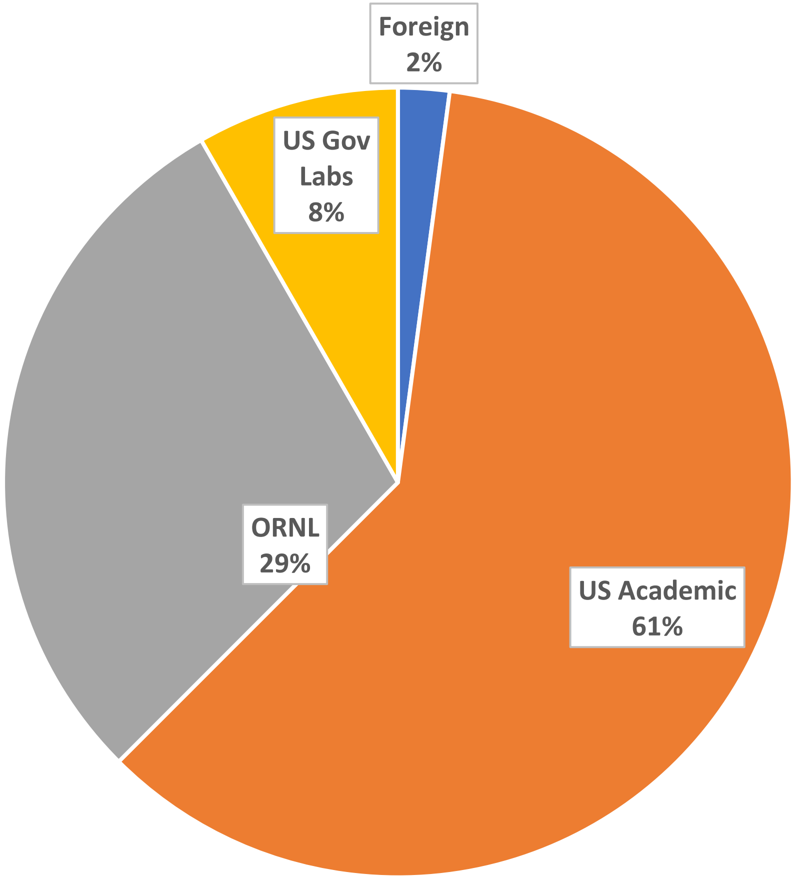
Scientific Mission and Impact

HB3 focuses on inelastic neutron scattering in Hard Condensed Matter physics

- Spin and lattice dynamics in high-temperature superconductors and related compounds;
- Low-dimensional magnetic model systems;
- Magnetic excitations in colossal magnetoresistive materials, multiferroics, semiconductors, paraelectric; and other magnetically ordered materials.
- Phonons in Weyl semimetals, thermoelectrics, ferroelectric/multiferroics,disordered and mixed valence materials

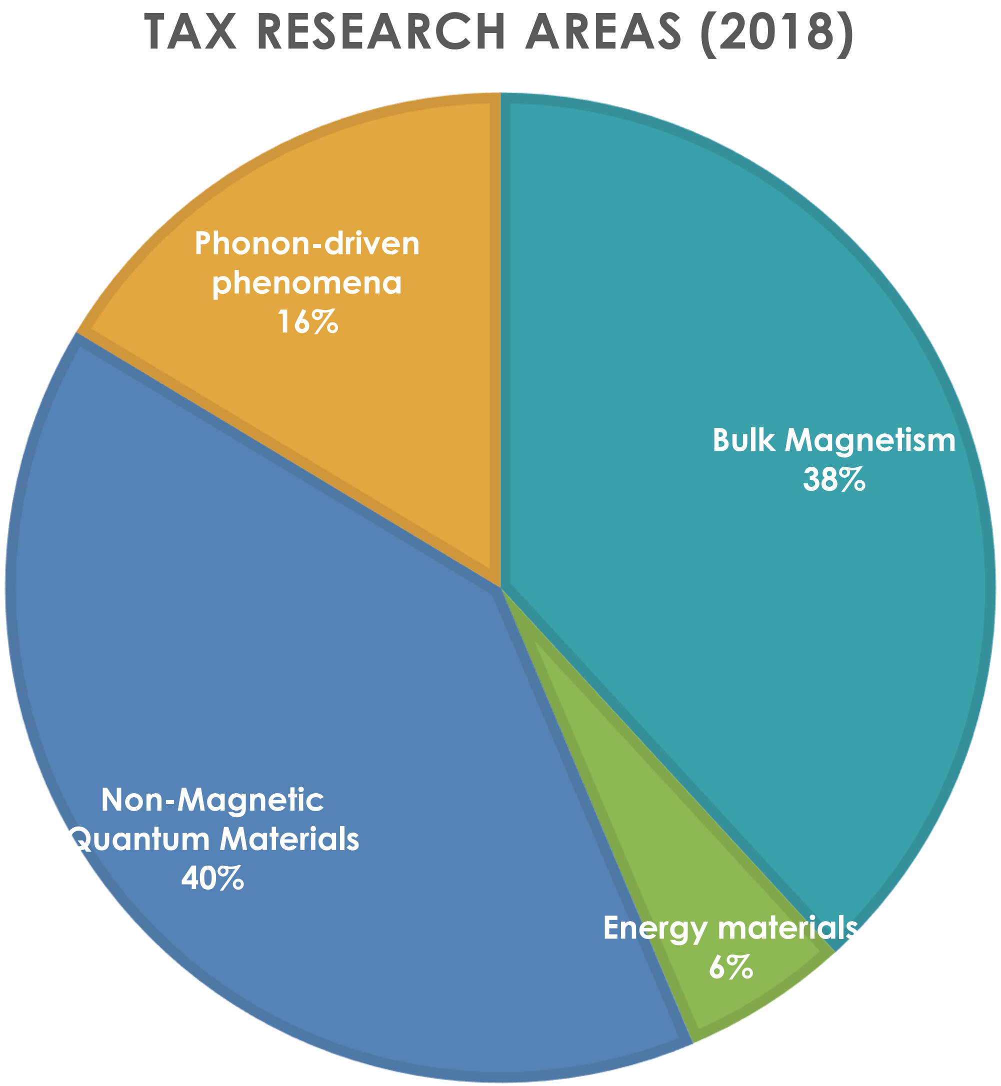
Institution Types FY-2018

Top Author Institutions (2017-2019)
Rice University
Duke University
Chinese Academy of Sciences
Beijing Normal University
University of Tennessee
Meggitt Sensing Systems
Max Planck Institute for Solid State Research



- 19 Unique institutions represented
- US Academic increased from 39% to 61%
- *Foreign institution falls from 18% to 2%*

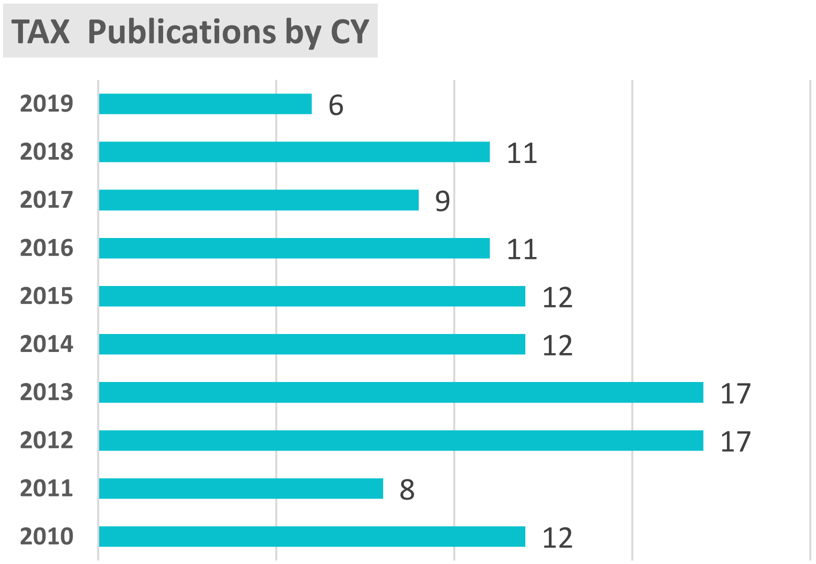
User Community

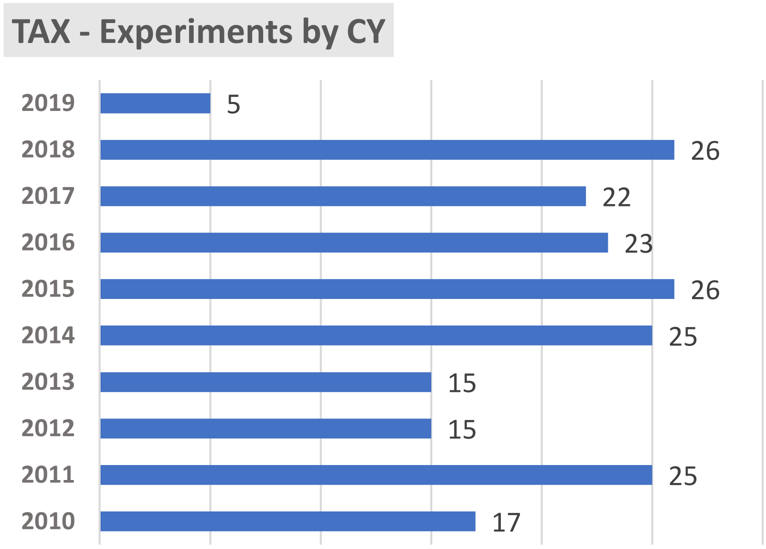


Compare to 2017:

The distribution of research areas remains consistent between 2017 and 2018.

Beamline Productivity





*Total Publications: **139***
*Instrument H-Index: **32***
*Publication Impact: **23%** publications with a high impact factor (recent 3 years)*
*Results from use of both facilities: **32%***
*Results from use of multiple instruments: **64%***
*Unique authors 2017-2019: **156***

Software

Data Acquisition

- **SPICE**

  Controlling motors, sample environments, and accessories as well as data acquisition

Experiment Planning

- **Virtual SPICE**

  Simulating scans and checking angle accessability to select the best configuration of scattering plane and neutron energy

- **TAS Tools (DAVE)**

  Developed at NCNR/NIST for resolution calculation

Data Analysis

- **Graffiti**
  Peak fitting with Gaussian, Lorentzian and squared Lorentzian
- **Mfit**
- **Reslib for Matlab**

  Resolution deconvolution

Modeling

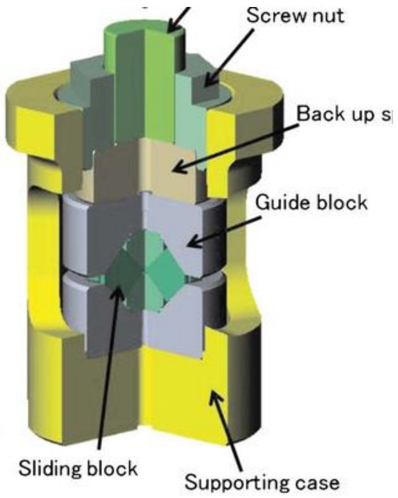
- **spinW**
- **MCViNE**

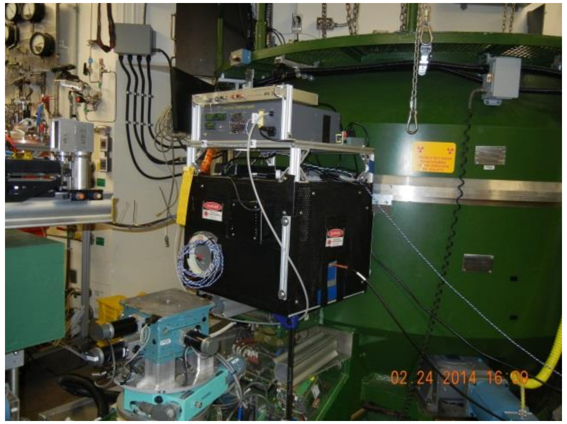
Future Plan

More user-friendly software for resolution convolution calculation

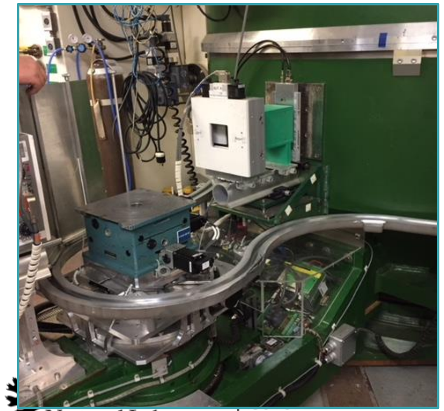
Sample Environments

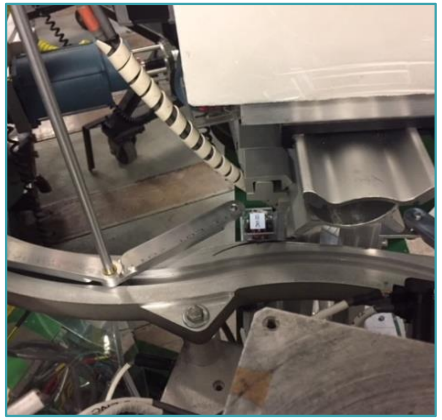
- Bottom loading CCR (4-300 K)
- Top loading orange cryostat (1.4-300 K)
- ^{3}He and dilution refrigeration inserts for cryostats
- High temperature CCR (30-800 K)
- Furnace (30-1600°C) including Controlled Atmosphere Furnace
- Magnet vertical bore
  - 5 T & 8 T compensated
  - Dilution refrigeration insert
- Static electric field up to 5 kV
- High Pressure (hydrostatic, clamp, anvil cells)
- compact *in situ* polarized ^{3}He neutron spin filter





Ongoing Upgrade





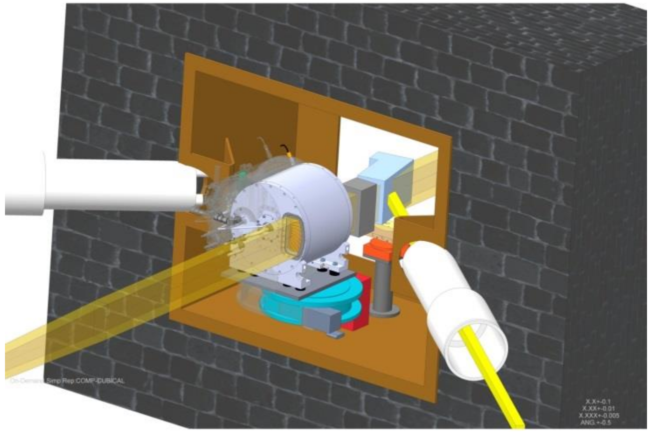
Sample area shielding on HB3

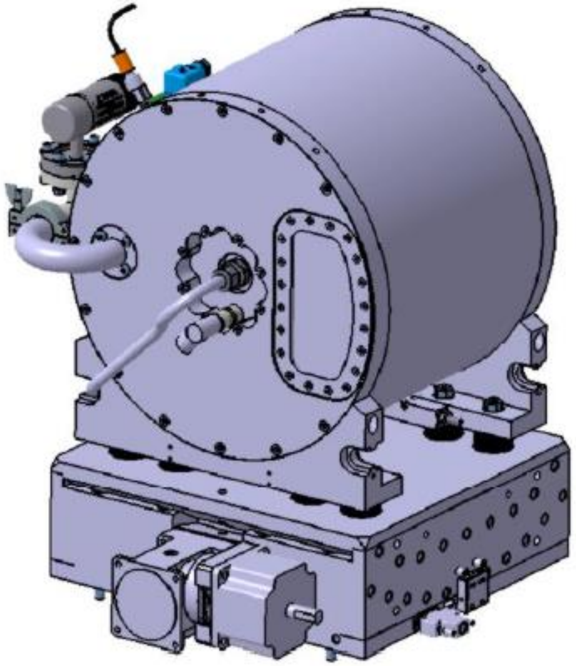
- It doesn't form a closed circle.
- Shielding panels are removable.
- A window is fixed to the analyzer arm to follow the beam path downstream the sample.
- The linkage between the shielding pieces are easily unlocked for sample loading or high-Q measurements.

		Without the shielding	With the shielding
North side (HB2B side)	Neutron (millirem)	20	10
	Gamma (millirem)	100	45
South side (HB3A side)	Neutron (millirem)	14	5
	Gamma (millirem)	60	34
HB2B detector			50% reduction in erroneous counts

Ongoing Upgrade

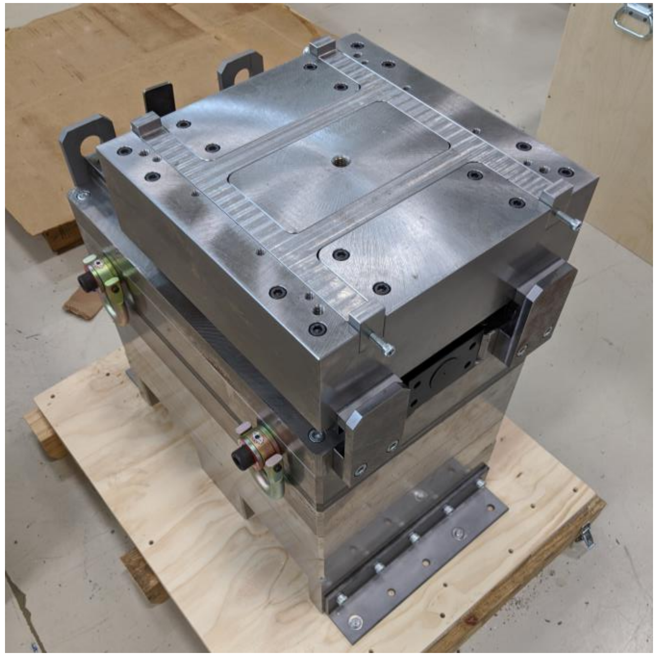
Neutron Velocity Selector





Requirements for VS installation

- ❑ Replace existing shutter,
- ❑ rebuild the cubicle to isolate vibration,
- ❑ shift mono drum downstream,
- ❑ reconfigure the saddle shield
- ❑ Manual override to move the NVS out of beam



Significance and Impact:

- ❑ **VS reduces neutronic background** by cutting neutrons of higher order harmonics. Better signal/noise ratio makes it possible to study the magnetic excitations in samples with small volume or reduced magnetic moment.
- ❑ **VS reduces radiological background**. Clean incident beam reduces the chance of radiological events and allows users to take full advantage of the high flux and big beam size of HB3.
- ❑ Clean beam would **eliminate spurious scatterings** resulting from incident higher wavelength contamination.

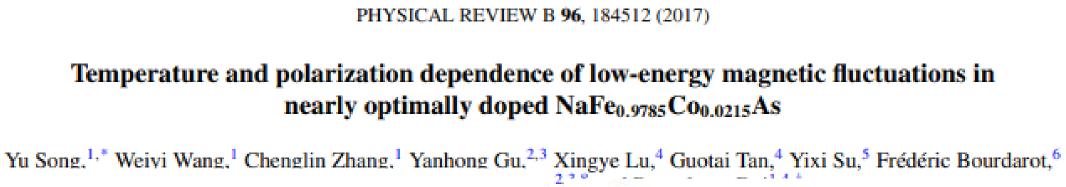
Schedule:

- ❑ **Engineering effort underway**
- ❑ **Procurement: FDR signed, Delivery 2020**
- ❑ **Installation: after the beryllium change-out**

Research highlights

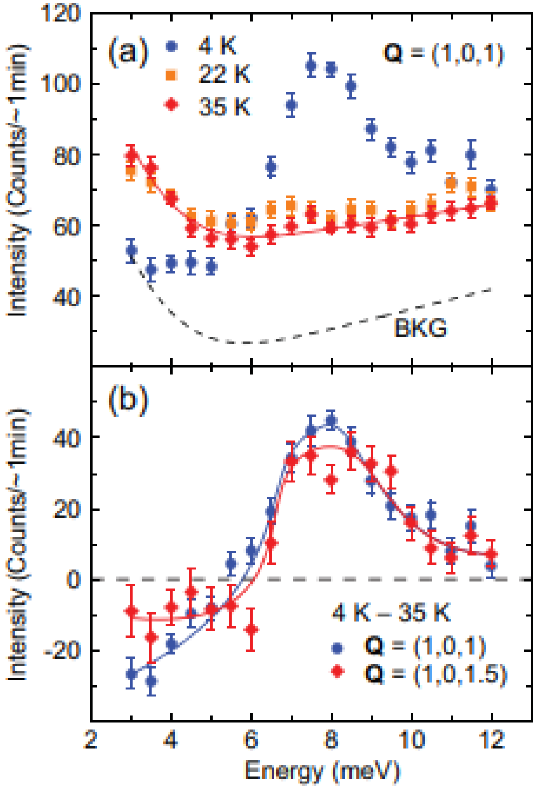
- ***Temperature and polarization dependence of low-E magnetic fluctuations in iron-based superconductor***
- ***CEF scheme in $PrPd_5Al_2$***
- ***Supersonic propagation of lattice energy by phasons in fresnoite***
- ***Anharmonic Eigenvectors and Acoustic phonon Disappearance in Quantum Paraelectric $SrTiO_3$***

Temperature and polarization dependence of low-E magnetic fluctuations in $NaFe_{0.9785}Co_{0.0215}As$

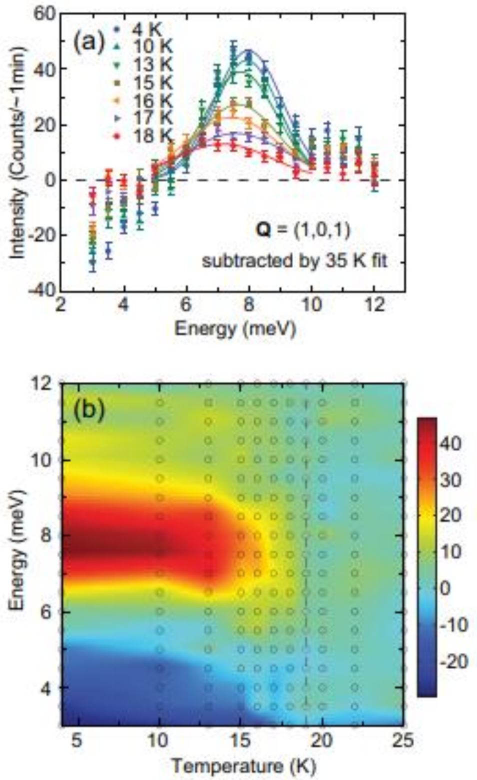

PHYSICAL REVIEW B **96**, 184512 (2017)

Temperature and polarization dependence of low-energy magnetic fluctuations in nearly optimally doped $NaFe_{0.9785}Co_{0.0215}As$

Yu Song,[1,*] Weiyi Wang,[1] Chenglin Zhang,[1] Yanhong Gu,[2,3] Xingye Lu,[4] Guotai Tan,[4] Yixi Su,[5] Frédéric Bourdarot,[6]



Constant-Q scans that shows spin resonance.



Spin resonance at different temperatures.

Yu Song et al., Physical Review B, **96,** 184512 (2017).

Scientific Achievement

A single spin resonance mode with intensity tracking the superconducting order parameter is observed in nearly optimally Co-doped NaFeAs, although energy of the mode only softens slightly upon approaching Tc. Polarized neutron scattering reveals that the single resonance is mostly isotropic in spin space, similar to overdoped NaFeAs but different from optimal electron-, hole-, and isovalently doped $BaFe_2As_2$ compounds, all featuring an additional prominent anisotropic component. Spin anisotropy in $NaFe_{0.9785}Co_{0.0215}As$ is instead present at energies below the resonance, which becomes partially gapped below Tc, similar to the situation in optimally doped $YBa_2Cu_3O_{6.9}$.

Significance and Impact

These results indicate that anisotropic spin fluctuations in $NaFe_{1-x}Co_xAs$ appear in the form of a resonance in the underdoped regime, become partially gapped below Tc near optimal doping, and disappear in overdoped compounds.

Research Details

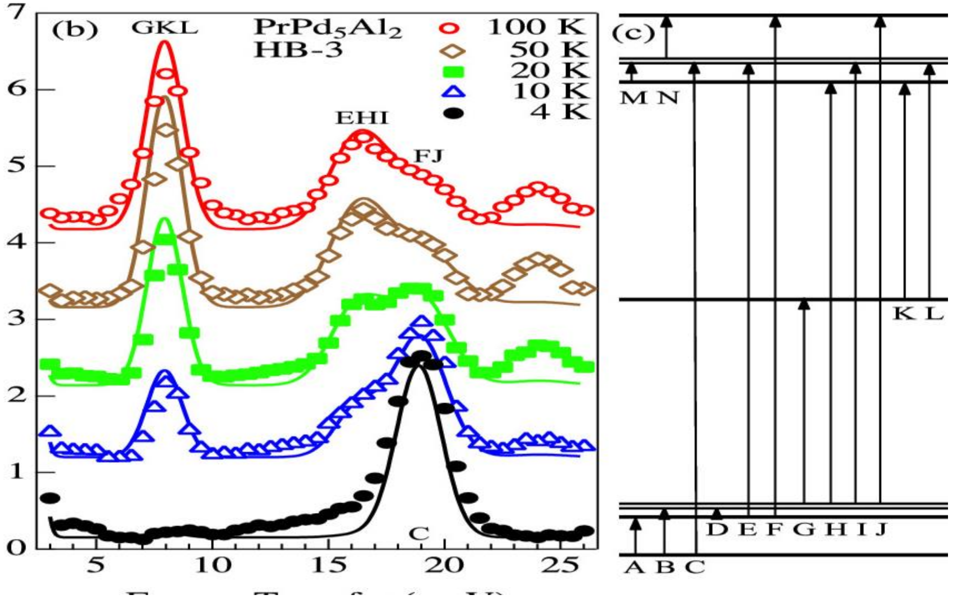
Unpolarized inelastic neutron scattering measurements in this study were carried out on HB3. The sample is the early optimally Co-doped NaFeAs, with coexisting superconductivity (Tc ≈ 19 K) and weak antiferromagnetic order (T_N ≈ 30 K, ordered moment ≈0.02 μB/Fe).

f-Electron States in $PrPd_5Al_2$

Journal of the Physical Society of Japan **87**, 094704 (2018)
https://doi.org/10.7566/JPSJ.87.094704

f-Electron States in $PrPd_5Al_2$

Naoto Metoki[1,2*], Hiroki Yamauchi[1], Hiroyuki S. Suzuki[3], Hideaki Kitazawa[3], Masato Hagihara[4], Takatsugu Masuda[4], Adam A. Aczel[5], Songxue Chi[5], Tao Hong[5], Masaaki Matsuda[5], Daniel Pajerowski[5], and Jaime A. Fernandez-Baca[5]



Neutron inelastic scattering spectra of $PrPd_5Al_2$ measured using HB3. The solid lines are the model calculation based on HCEFHCEF. The CEF scheme is shown on the right

Scientific Achievement

The CEF Hamiltonian of the Pr^{3+} ion ($^3H_4$) under tetragonal point symmetry was orthogonalized analytically and the CEF parameters were determined from the excitation energies. The *f*-electron states reproduce the distinctive temperature dependence of the magnetic excitation spectra as well as the macroscopic properties. A point charge model is effective for understanding the systematic change in the *f*-electron states in RPd_5Al_2. The Ising anisotropy in $CePd_5Al_2$, $PrPd_5Al_2$, and $NdPd_5Al_2$ originates from the flat orbitals with large J_z due to the CEF potential developed in the crystal structure.

Significance and Impact

The temperature dependence of the magnetic susceptibility in $NpPd_5Al_2$ can be explained qualitatively on the basis of the identical charge distribution in RPd_5Al_2. *XY*-type anisotropy is expected from the positive Stevens factors α_l for the Np^{3+} ion. Thus, the conclusion is that the local property is important in $NpPd_5Al_2$, whose origin is common in the RPd_5Al_2 isostructural family.

Research Details

The crystalline electric field (CEF) excitation spectra of $PrPd_5Al_2$ have been studied using HB3 and CTAX in order to reveal the *f*-electron states, where $PrPd_5Al_2$ is a Pr-based isostructural compound of the heavy-fermion superconductor $NpPd_5Al_2$.

N. Metoki et al., J. Phys. Soc. Jpn. **87**, 094704 (2018)

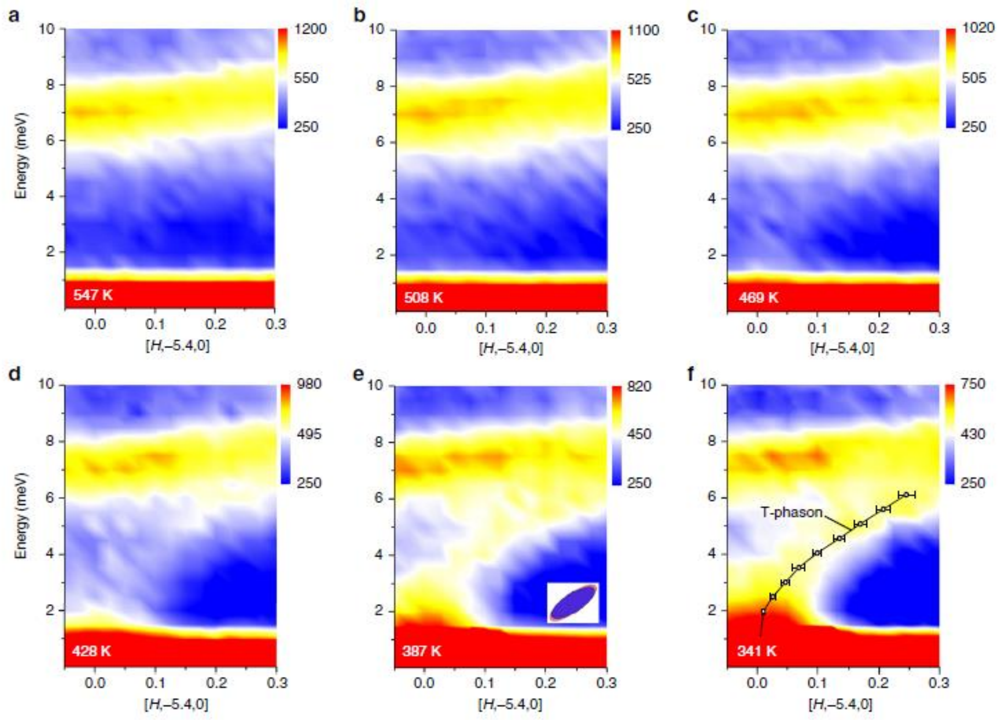
Supersonic propagation of lattice energy by phasons in fresnoite

ARTICLE

DOI: 10.1038/s41467-018-04229-1 OPEN

Supersonic propagation of lattice energy by phasons in fresnoite

M.E. Manley[1], P.J. Stonaha[1], D.L. Abernathy[2], S. Chi[2], R. Sahul[3], R.P. Hermann[1] & J.D. Budai[1]



Phason formation measured on HB3.

Significance and Impact

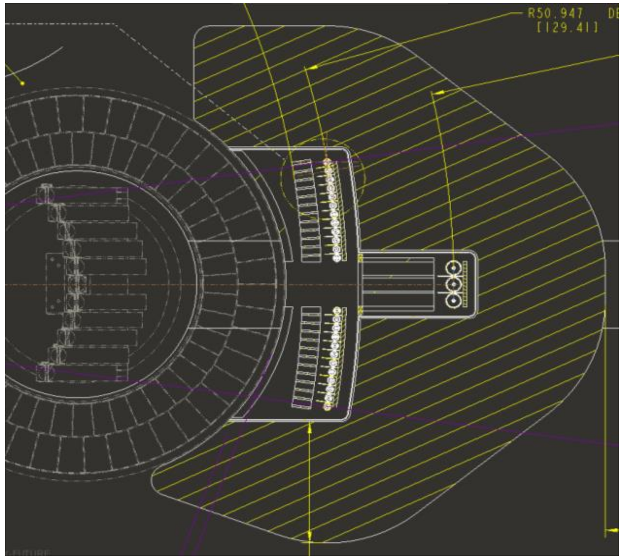
To remove heat without shorting electrical connections, heat must be carried in the lattice of electrical insulators. Phonons are limited to the speed of sound, which, compared to the speed of electronic processes, puts a fundamental constraint on thermal management. This study reports a supersonic channel for the propagation of lattice energy in fresnoite ($Ba_2TiSi_2O_8$) using neutron scattering. Lattice energy propagates 2.8−4.3 times the speed of sound in the form of phasons, which are caused by an incommensurate modulation in the flexible framework structure of fresnoite. The phasons enhance the thermal conductivity by 20% at room temperature and carry lattice-energy signals at speeds beyond the limits of phonons.

Scientific Achievement

Highly supersonic propagation of pure lattice energy in fresnoite in thermal equilibrium, breaking the conventional limit set by the speed of sound. The supersonic phasons carrying this thermal energy are exposed in our neutron scattering measurements by a wave vector rotation that moves the phason dispersion cones away from interference from the soft phonon mode. This rotation challenges established ideas on how incommensurate structural modulations develop from soft phonon modes and suggests unexpected phason reorientation instability. Taken together these remarkable findings open a new venue for understanding and controlling heat transport.

M. E. Manley et al., *Nature Communications*, 9, 1823 (2018).

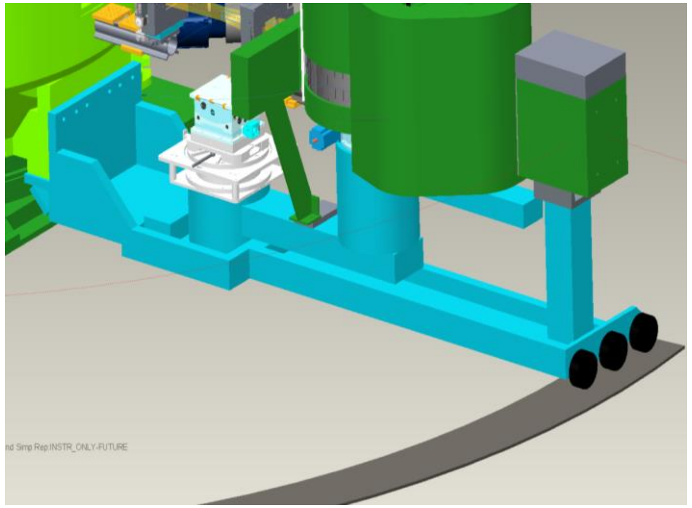
Future Upgrades: Backend

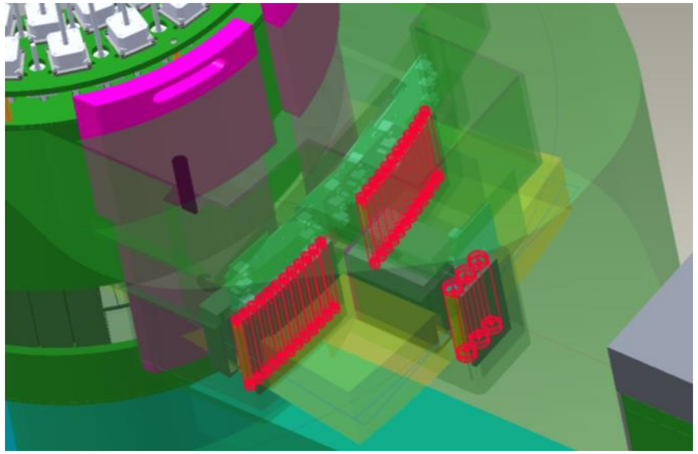


- **Improve signal/BKGD ratio**
  - Analyzer/detector 2-tank
  - Better shielding

- **Improve data acquisition rate**
  - Multiplex analyzer system
  - Multi-detector
  - Single detector group

- **Increased tolerance with sample environments**
  - M2 arm is supported at its far end
  - Increased sample table to beam distance
  - Possible adjustable sample to analyzer distance





Risks

- **The instrument floor doesn’t allow air pad. This means the low data collection efficiency will be a long-term problem.**
- **The low ceiling also limits our future plan for sample environments.**
- **The long term performance of the NVS in the high radiation environment**
- **The space is limited for low energy range.**
- **A variety of x-ray inelastic scattering techniques have been advancing and competing with inelastic neutron scattering.**

Overall Summary

- Flux is HB3's greatest strength.
- Scientific output has been stable.
- The ongoing upgrade will greatly improve its performance.
- Long term plan for the backend upgrade.