OAK RIDGE National Laboratory

Triple Axis Spectroscopy Team Overview

Jaime Fernandez-Baca
TAS team Leader
Neutron Scattering Division

2020 Review of the Instrument Suites for Spectroscopy
September 17–18, 2020

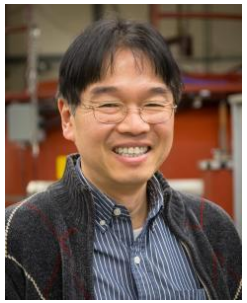
ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

Triple Axis Spectroscopy Team

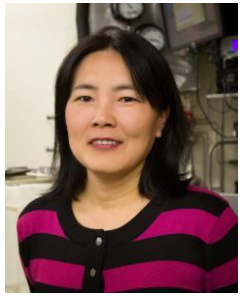
Jaime Fernandez-Baca
Team Leader

Instrument Scientists

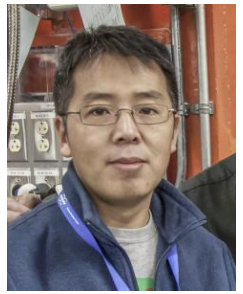


Masa Matsuda

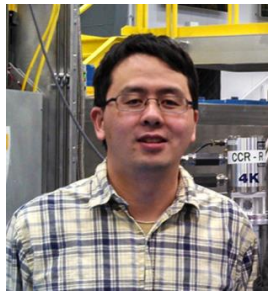
Adam Aczel



Wei Tian



Songxue Chi



Tao Hong

Travis Williams

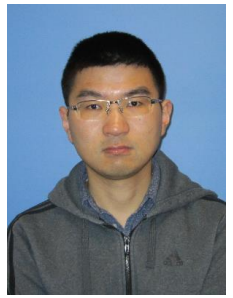
Scientific Associates

Shirley Xu

Mike Cox

Post Docs Associates

Fei Li



Depei Zhang

Computational Instrument Scientist

Andrei Savici

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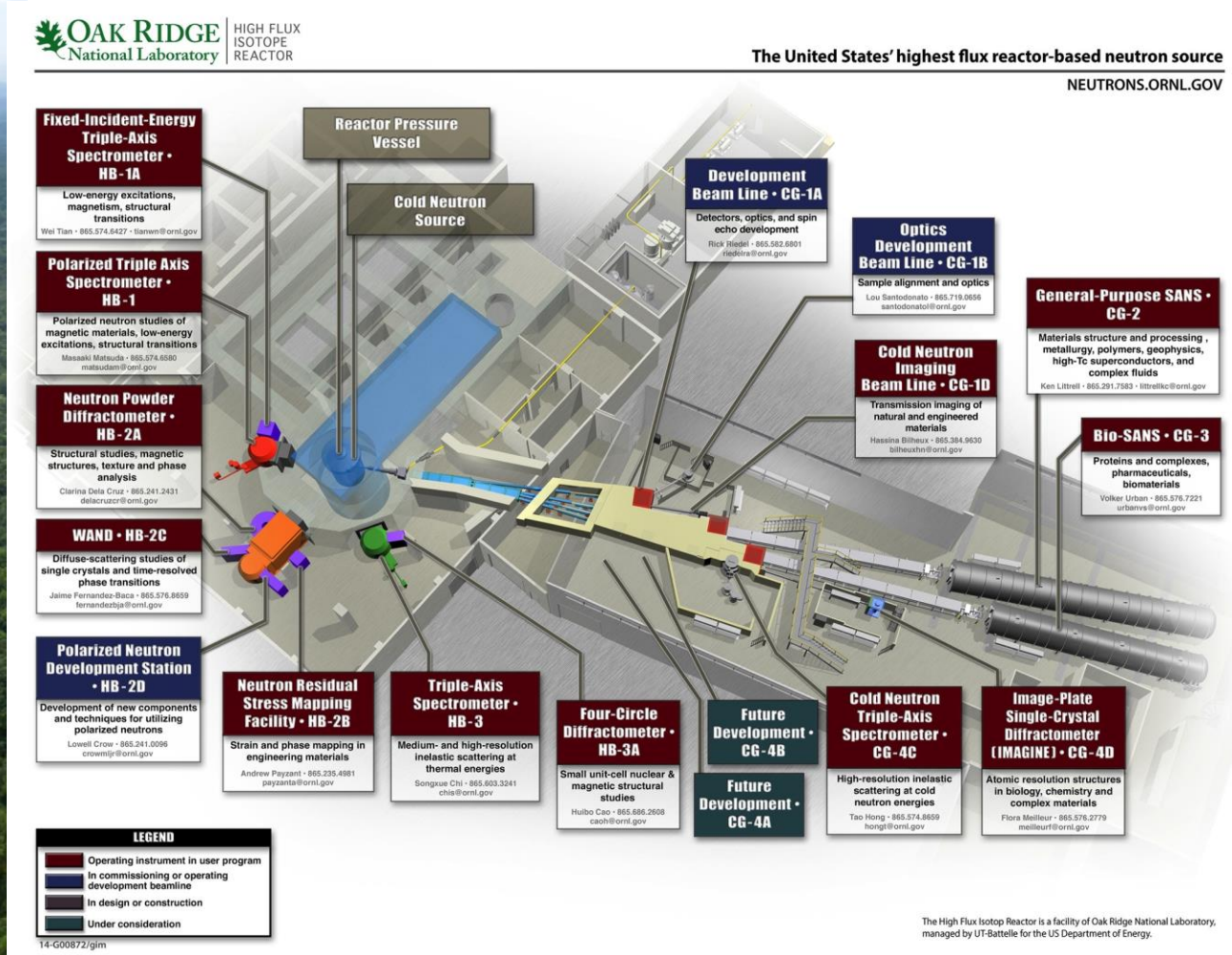
Scientific output comparable with other facilities

Publications

Year	IN8-ILL	BT-4+BT-7	PUMA-FRMII	TAIPAN	HB1A	HB3	IN20-ILL	HB1	SPINS	MACS	CTAX
2019	6	23	6	3	17	6	3	16	8	14	11
2018	4	14	5	9	23	11	5	14	10	11	12
2017	8	15	10	8	16	9	8	9	9	12	8
2016	4	16	13	10	23	11	4	14	11	11	4
2015	10	17	5	6	15	12	8	15	8	6	10
5-yr Average	6.4	17	7.8	7.2	18.8	9.8	5.6	13.6	9.2	10.8	9
Staffing											
Scientists	2	1+3	2	3	2	1.66	2	1.66	1	2	1.66
Techs/SAs	0.5				0.5	0.5	1	0.5			0.5

- Output due to dedication of staff
- Staffing levels lower than at other facilities
- HFIR TAS instruments among the oldest NS instruments in the US
- Need to upgrade TAS instruments to international standards

Triple Axis Spectrometers located at the High Flux Isotope Reactor (HFIR)

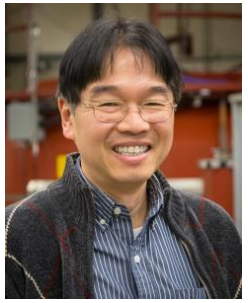


HB-1 PTAX Polarized Triple-Axis Spectrometer

Status: Operating in the User Program since 2003
Beamtime: 75% GUP, 20% PD, 5% IS
Description: Variable E_i TAS, polarized neutrons capability

Applications:
Spin waves in ordered magnetic materials
Excitations in low-dimensional, molecular, itinerate, and other "quantum" magnets
Spin and lattice excitations in HTCS, CMR materials, and multiferroic systems
Spin density distributions in magnetic compounds
Phonon dispersion curves and phonon-driven phase transitions

Developments and Upgrades:
Wollaston prisms for ultrahigh-resolution
Spherical Neutron Polarimetry (test in November 2020)
Pending upgrade of polarizing monochromator and analyzer

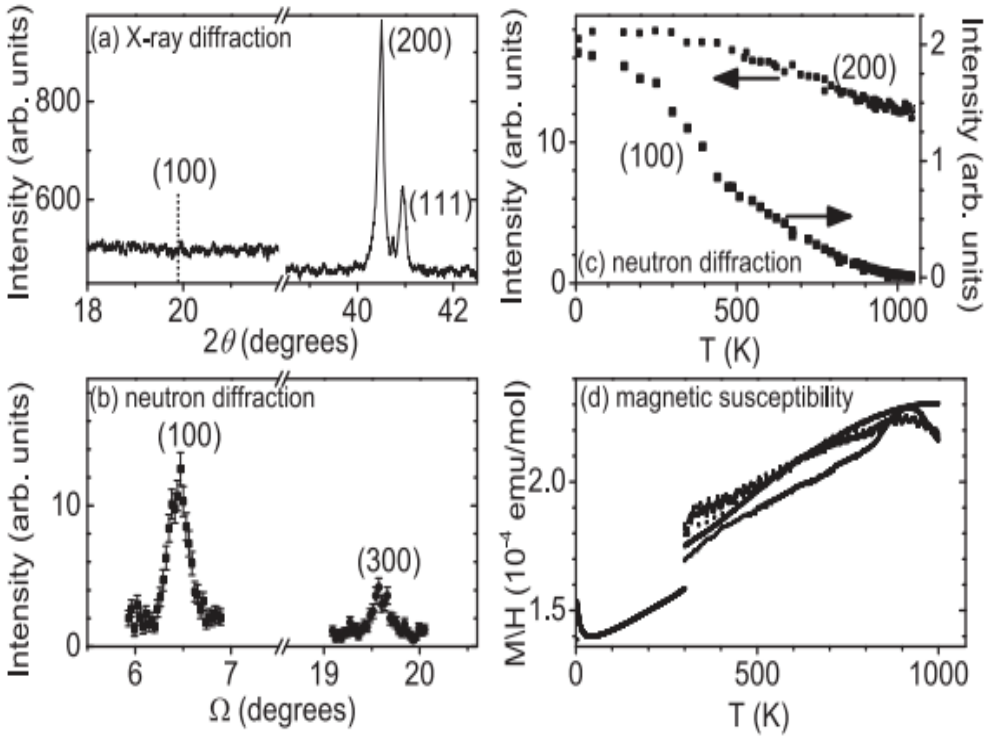

Masaaki Matsuda


Travis Williams


Jaime Fernandez-Baca

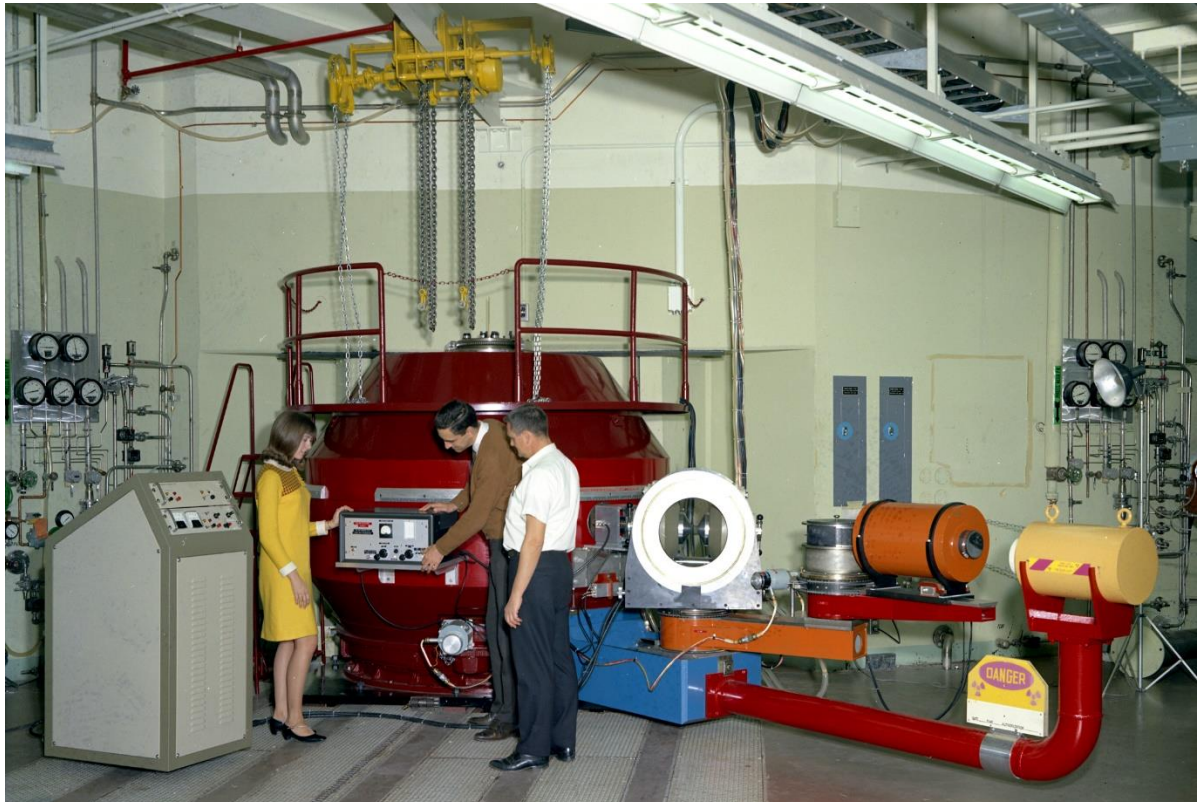

Shirley Xu


Andrei Savici



Berlijn T., Snijders P.C., Delaire O., Zhou H.D., Maier T.A., Cao H.B., Chi S.X., Matsuda M., Wang Y., Koehler M.R., Kent P.R., Weitering H.H., Itinerant antiferromagnetism in RuO_2. *Physical Review Letters* 118, 077201 (2017).

HB-1 in the 1960's



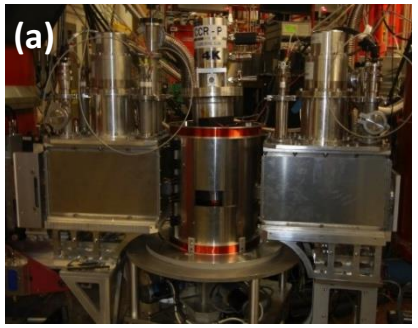
PHYSICAL REVIEW VOLUME 181, NUMBER 2 10 MAY 1969

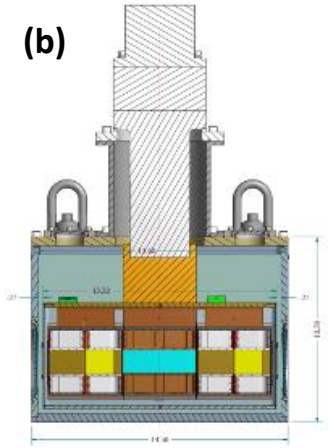
Polarization Analysis of Thermal-Neutron Scattering*

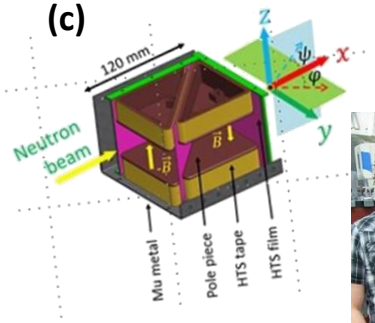
R. M. Moon, T. Riste,† and W. C. Koehler
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830
(Received 30 December 1968)

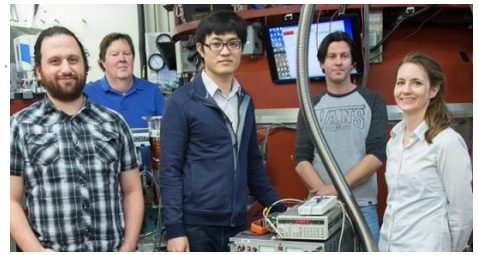
A triple-axis neutron spectrometer with polarization-sensitive crystals on both the first and third axes is described. The calculation of polarized-neutron scattering cross sections is presented in a form particularly suited to apply to this instrument. Experimental results on nuclear incoherent scattering, paramagnetic scattering, Bragg scattering, and spin-wave scattering are presented to illustrate the possible applications of neutron-polarization analysis.

Neutron Diffraction Resolution Improved by Orders of Magnitude by Using Superconducting Magnetic Wollaston Prisms









(a) Wollaston prisms setup at the HB1 triple axis spectrometer at HFIR. A Wollaston prism pair (WPP) is placed in the incident neutron beam and another in the scattered beam. The sample is at the middle, surrounded by a Mu-metal shield cylinder

(b) WPP schematic, two superconducting Wollaston prisms separated by a guide field all in a closed cycle refrigerator

(c) Schematics of a single superconducting Wollaston prism

Work performed at ORNL's HFIR triple axis spectrometer, a DOE Office of Science User Facility. This work was supported by the LDRD project "Development of novel neutron spin echo methods for ultra-high resolution spectroscopy".

Scientific Achievement

The ability to perform high-resolution Larmor diffraction using superconducting magnetic Wollaston prisms in a thermal neutron triple axis spectrometer has been demonstrated. The coefficient of thermal expansion of a single-crystal of copper was measured successfully, in agreement with dilatometry results. This result benchmarks the use of magnetic Wollaston prisms in Larmor diffraction experiments.

Significance and Impact

This work demonstrated that superconducting magnetic Wollaston prisms can be used to tilt magnetic field boundaries in a way that is equivalent to the Neutron Resonance Spin Echo (NRSE) setup. This setup can now be used routinely to perform high-resolution Larmor diffraction experiments and, in the near future, to perform measurements of excitations linewidth with μeV resolution to study quasiparticle lifetimes and mode softening in quantum materials, as well as quantum critical behavior and phonon signatures in quantum spin liquids.

Research Details

The achievable resolution of this technique with this setup is $\Delta d/d = 1.4 \times 10^{-5}$. The expected energy resolution for phonon focusing is of the order of μeV.

F. Li, H. Feng, A.N. Thaler, S.R. Parnell, W.A. Hamilton, L. Crow, W. Yang, A.B. Jones, H. Bai, M. Matsuda, D.V. Baxter, T. Keller, J.A. Fernandez-Baca, R. Pynn, *Scientific Reports,* **2017**.

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HB-1A FIE-TAX, Fixed Incident Energy Triple-Axis Spectrometer

Status: Operating in the User Program since 2003
Beamtime: 75% GUP, 25% DT
Description: Fixed E_i TAS (E_i=14.5 meV)

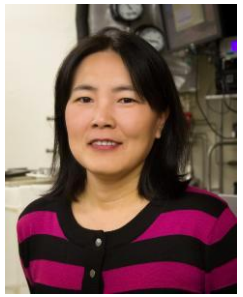
Applications

(1) Elastic studies of single crystals, powders, and thin films, to determine crystallographic and magnetic structures, phase transitions, and phase diagrams under various conditions (T, H, P, E)

(2) Studies of low-lying magnetic excitations up to ~ 9 meV using neutron energy loss and high-temperature phonons up to ~35 meV using neutron energy gain

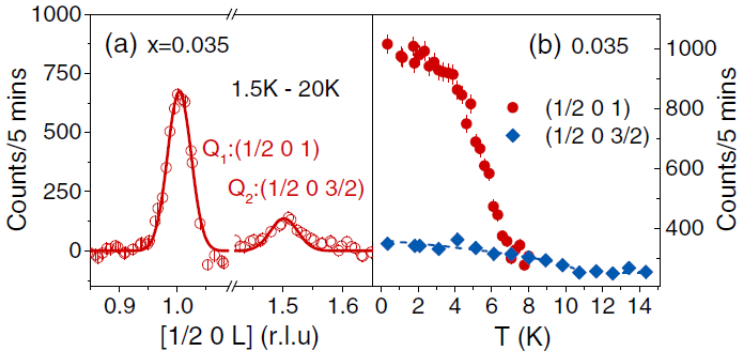
Developments and Upgrades:
Front-end upgrade completed
Back-end upgrade in progress

Adam Aczel



Wei Tian

Shirley Xu



Andrei Savici

Lampen-Kelley P., Banerjee A., Aczel A.A., Cao H.B., Stone M.B., Bridges C.A., Yan J.Q., Nagler S.E., Mandrus D., "Destabilization of Magnetic Order in a Dilute Kitaev Spin Liquid Candidate", *Physical Review Letters* **119**, 237203 (2017)

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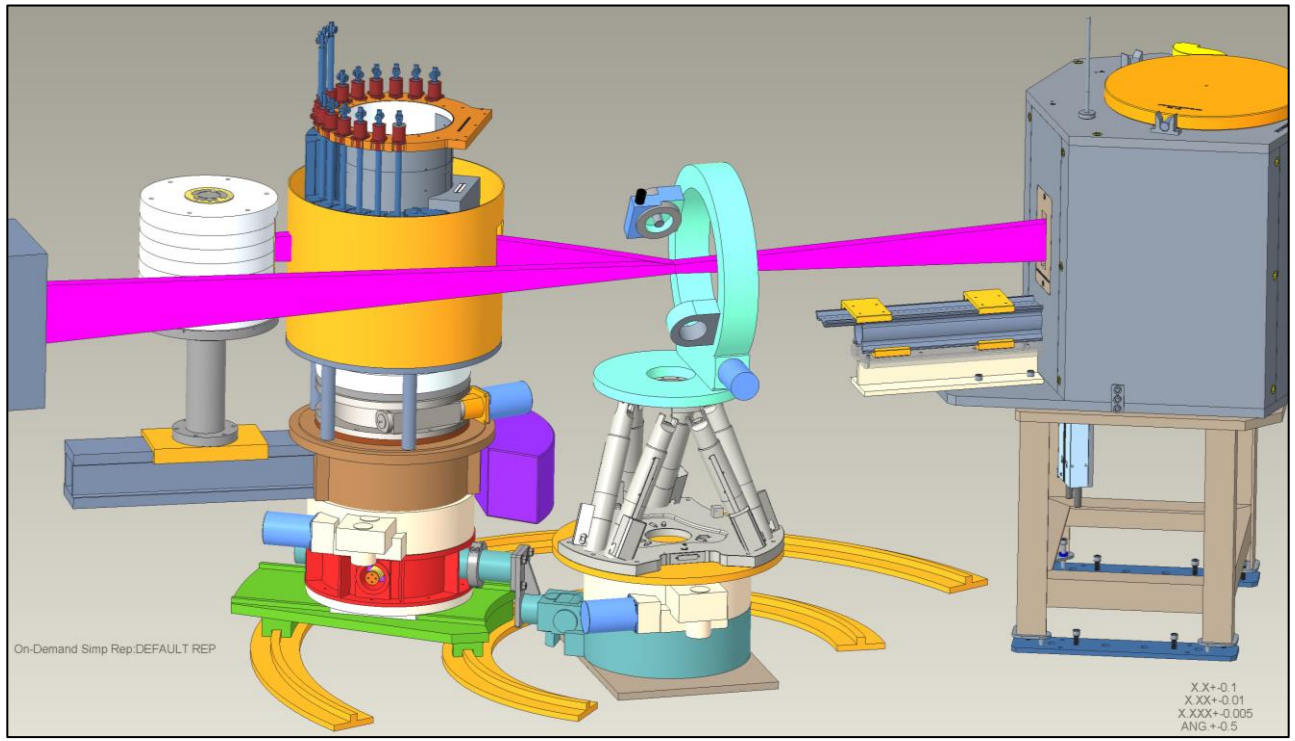
Back-end upgrade in progress



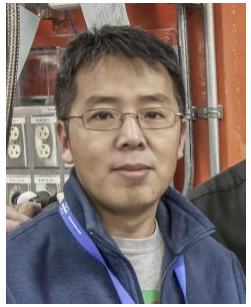
Overall view showing a 4-circle goniometer mounted on a hexapod that is under consideration for the sample table upgrade. The primary spectrometer represents the current set-up at the instrument and the secondary spectrometer represents the tentative new design.

New back-end features:

- Vertically-focused analyzer
- Single analyzer-detector design for most experiments to retain good signal-to-noise ratio
- Enables polarize beam
- Facilitates new types of experiments
  - A 4-circle goniometer option can be installed at the sample position to enhance reciprocal space coverage
  - The new analyzer can be swapped out for a 2D area detector to facilitate diffraction experiments

HB-3 TAX, Triple Axis Spectrometer

Status: Operating in the User Program since 2003
Beamtime: 75% GUP, 20% PD, 5% IS
Description: Triple Axis spectrometer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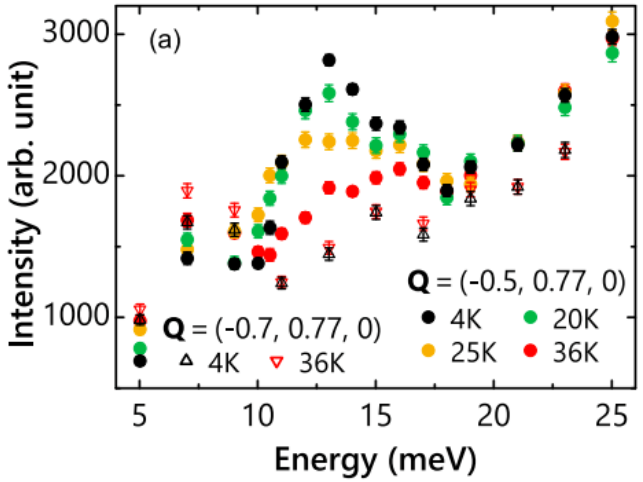
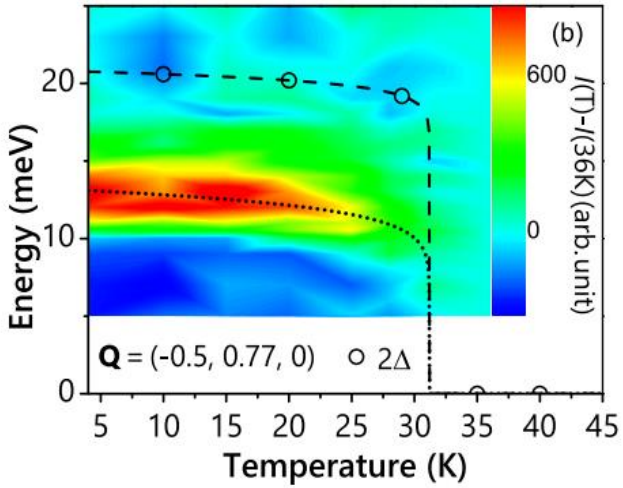
Mike Cox





Applications: Excitations in materials with energies ranging from 2 to 100 meV, including spin and lattice dynamics in high-temperature superconductors and related compounds, low-dimensional magnetic model systems, CMR materials, multiferroics, and ruthenates, and spin waves in magnetically ordered materials.

Developments and Upgrades:
Front end upgrade completed in 2003
Backend upgrade and velocity selector pending

Wang Q., Park J.T., Feng Y., Shen Y., Hao Y., Pan B., Lynn J.W., Ivanov A.S., Chi S.X., Matsuda M., Cao H.B. Birgeneau R.J., Efremov D.V., Zhao J., Transition from sign-reversed to sign-preserved Cooper-pairing symme in sulfur-doped iron selenide superconductors. *Physical Review Letters* 116, 197004 (2016).

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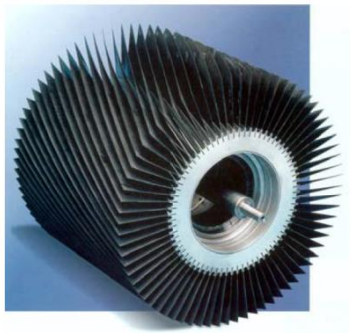
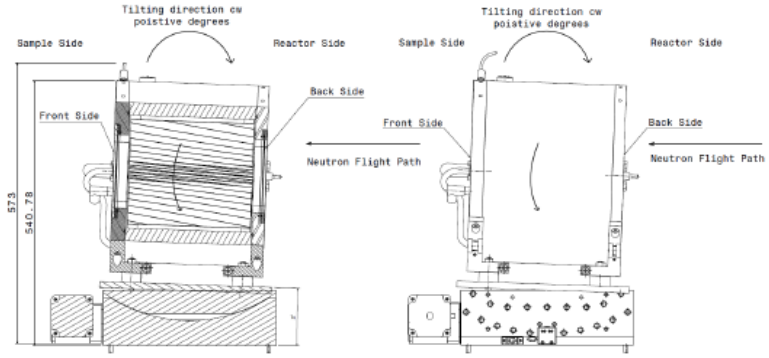
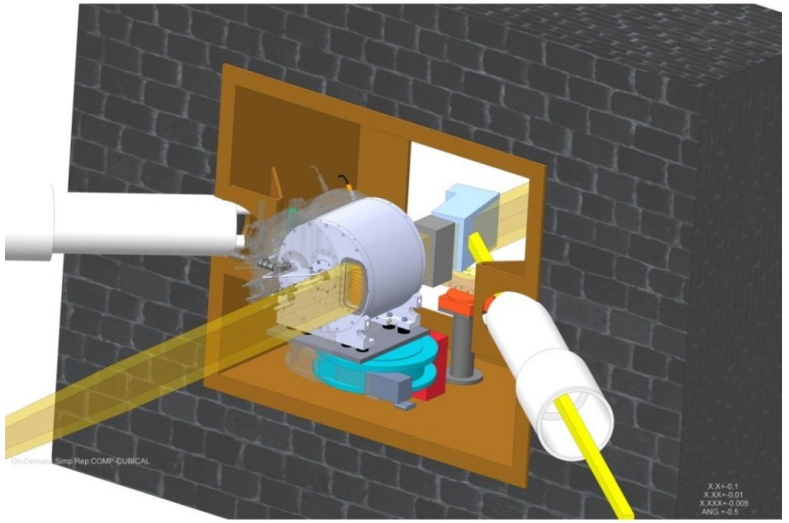
HB3 Velocity selector project







Scientific Benefits:

- **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.

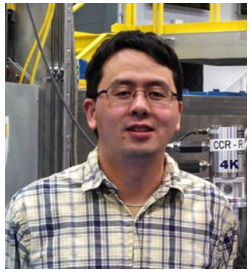
- Clean beam would **eliminate spurious scatterings** resulting from higher wavelength contamination.

CG-4C CTAX

Status: Operating in the User Program since 2011
Beamtime: 75% GUP, 20% IDT (US-Japan), 5% IS
Description: Triple-axis spectrometer

Applications:
High-resolution measurements of low-energy, atomic-scale dynamics of crystalline solids with high signal-to-noise ratios due to the low background.
Studies of magnetic phenomena exploiting the energy range that matches achievable applied fields

Developments and Upgrades:
Horizontally focusing analyzer, 2014



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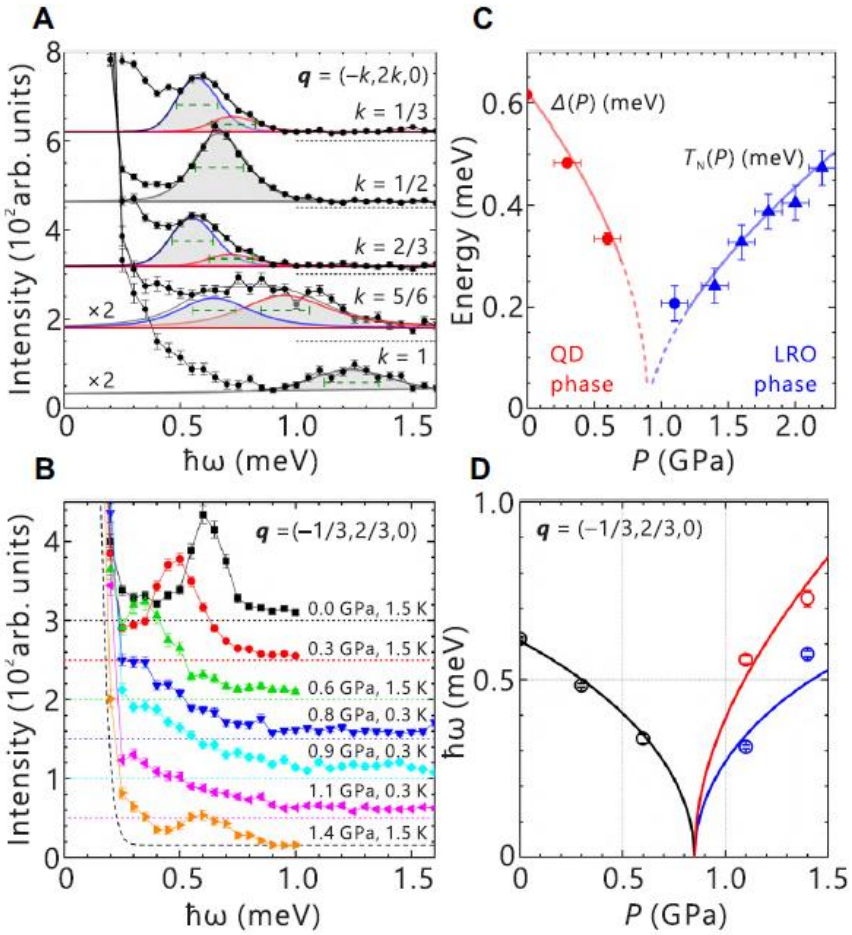


S. Hayashida, M. Matsumoto, M. Hagihala, N. Kurita, H. Tanaka, S. Itoh, T. Hong, M. Soda, Y. Uwatoko and T. Masuda, Novel excitations near quantum criticality in geometrically frustrated antiferromagnet $CsFeCl_3$. *Science Advances* ***5****, eaaw5639 (2019).*

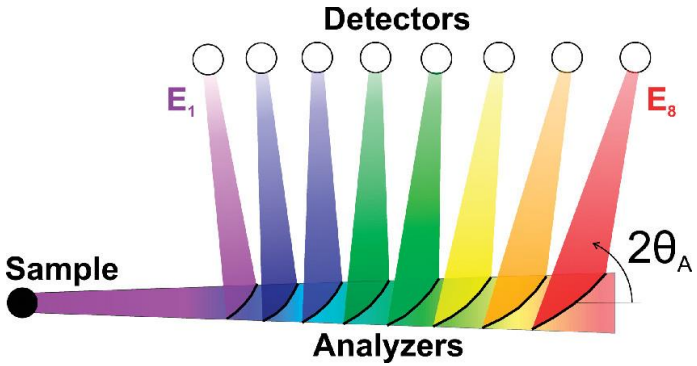
Overview of MANTA

❑ Phase 1, Features of "MANTA"

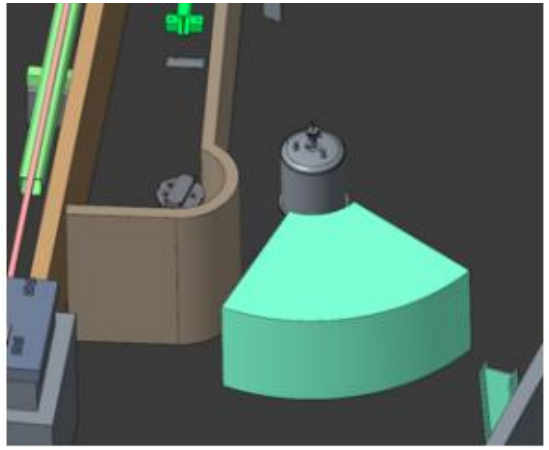
- ❑ New neutron guides optimized for cold neutrons
- ❑ Neutron velocity selector to cut out $\lambda/2$
- ❑ Rowland / Vertical Focusing Monochromator
- ❑ Large sample space for cryogenics and magnets
- ❑ Single-ANalyzer Triple Axis: SANTA
  - ❑ Use CTAX backend as the secondary spectrometer
  - ❑ Useful for high Q resolution measurements and eventually Spherical Neutron Polarimetry

❑ Phase 2, Features of MANTA

- ❑ Multi-ANalyzer Triple Axis: MANTA
  - ❑ CAMEA-like multi analyzer
- ❑ Polarization Capabilities
  - ❑ Although an integral part of the design for Phase 1, investment for polarization optics is planned for Phase 2



CAMEA back-end

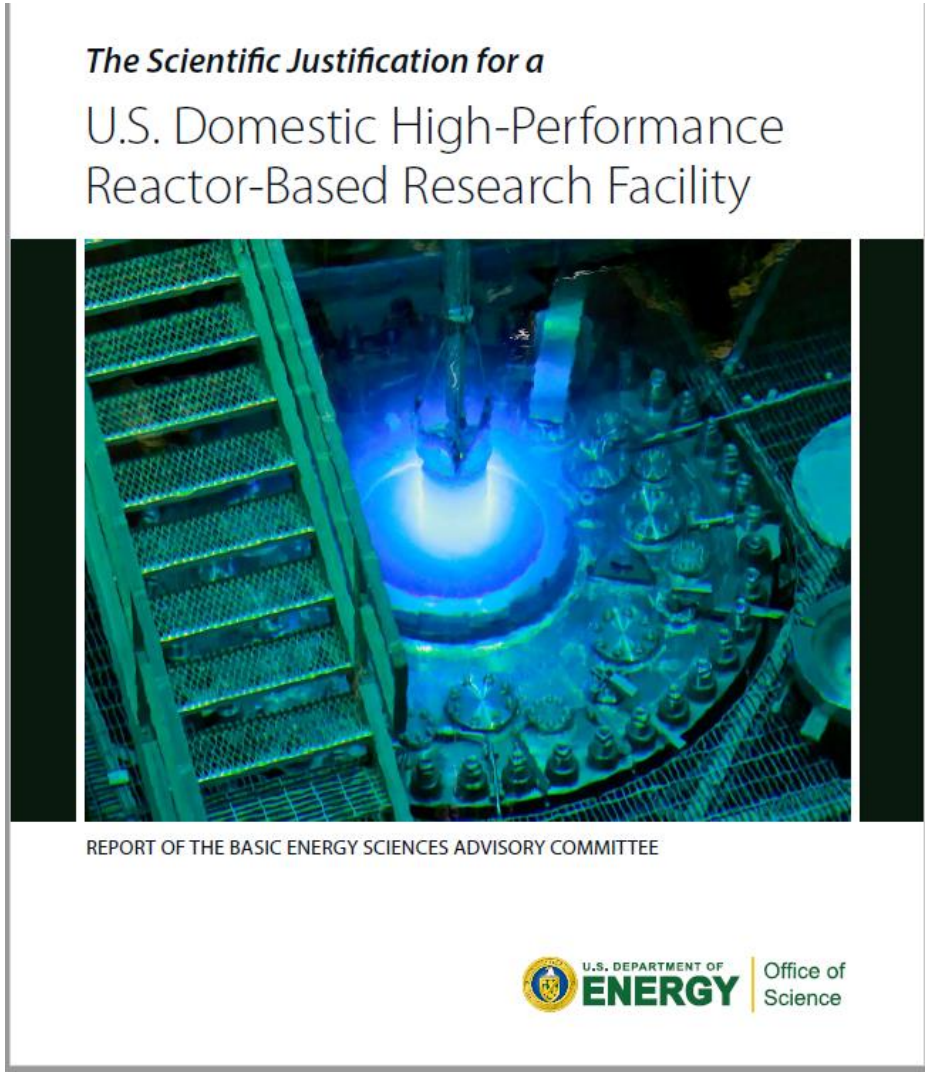


Review of Scientific Instruments **87**, 035109 (2016); https://doi.org/10.1063/1.4943208

HFIR Future Plans

- Beryllium reflector change-out 2024
- Beam room rearrangement
- Cold-neutron guides upgrade, guide hall reconfiguration
- **TAS priorities**
  - **Build MANTA**
  - **Complete all thermal TAS upgrades**

HFIR Future Plans – Beyond the 2024 Be-reflector changeout



- Recent BESAC subcommittee recommended the extension of the HFIR life
- Pressure vessel replacement
- Construction of a second, thermal neutron guide hall