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

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2020 Spectroscopy Suite Review

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

Talk outline

- HB-1A overview, science mission, and specs
- Beamtime statistics, productivity, and impact
- Data acquisition, reduction, visualization, and analysis
- Sample environment
- Science highlights
- Instrument vision
- Instrument needs

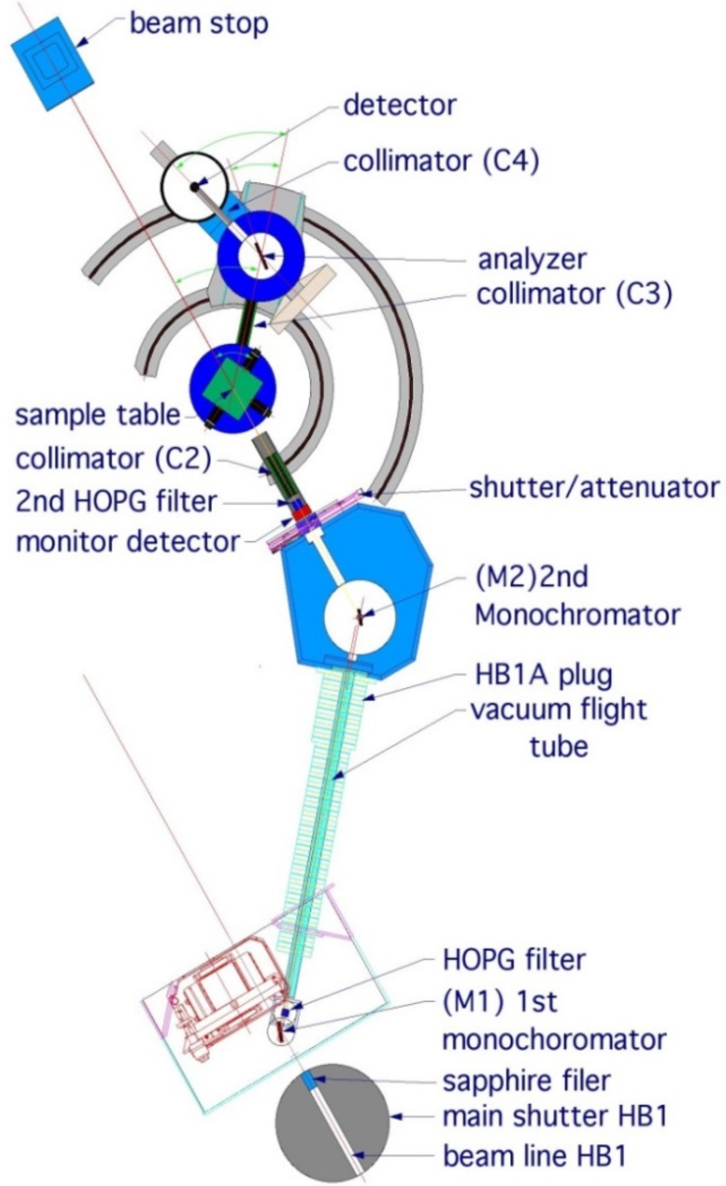
Main Conclusions: HB-1A is an outstanding instrument for measuring weak elastic scattering, and the ongoing backend upgrade will enhance this capability and increase instrument flexibility

HB-1A overview

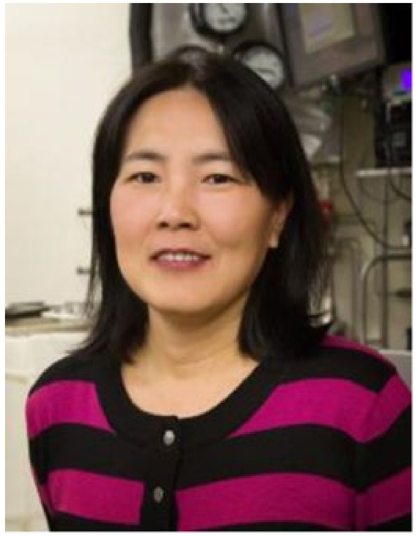
- HB-1A was designed, built, and installed at HFIR between 1988-90, originally owned by Ames Lab
- Double bounce monochromator system: Intense beam at fixed E_i = 14.5 meV with low background and low higher order contamination
- Front-end upgrade: completed Nov. 2019
- Back-end upgrade: in progress

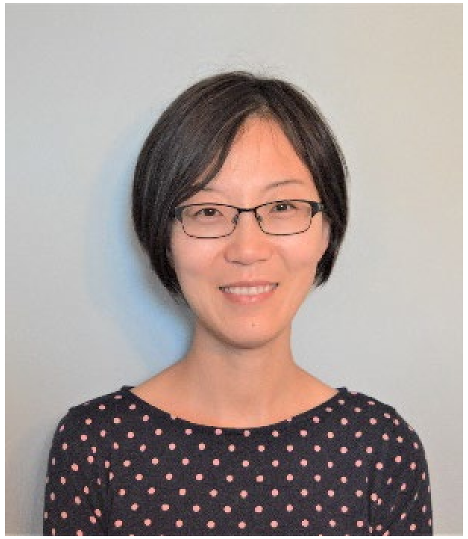
Before monochromator upgrade

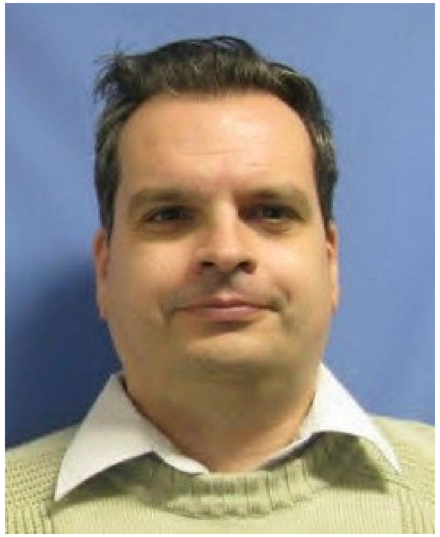
After monochromator upgrade



HB-1A instrument team







Instrument team (left to right):

- Adam Aczel (Instrument Scientist, POC)
- Wei Tian (Instrument Scientist)
- Shirley Xu (Scientific Associate, 50%)
- Andrei Savici
  (TAX and DGS Computational Instrument Scientist)

HB-1A science mission, capabilities and status

Science mission and capabilities

- *Elastic scattering* in single crystals, powders and thin films with an emphasis on magnetic quantum materials and structural phase transitions in single crystals
- *Inelastic scattering*: low-lying magnetic excitations (up to 9 meV) and high temperature phonons (up to 35 meV)
- Mostly **elastic scattering** experiments, often using samples with weak signals due to high signal-to-noise ratio
- A workhorse for parametric elastic scattering studies as a function of T and H, some E and P experiments are performed

Adam and Gabriele at HB-1A with MAG-E installed

Dilution fridge insert

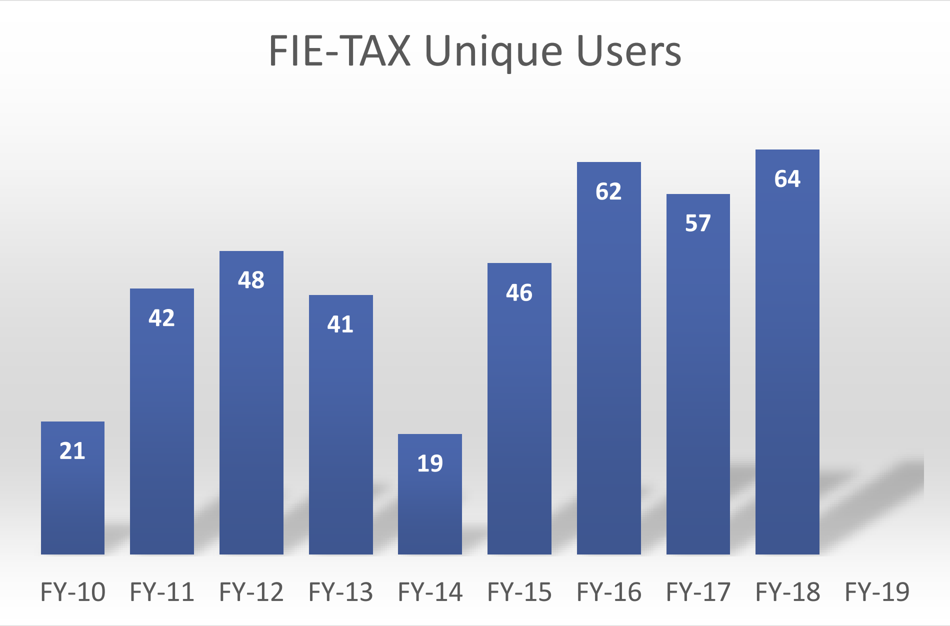
Current status

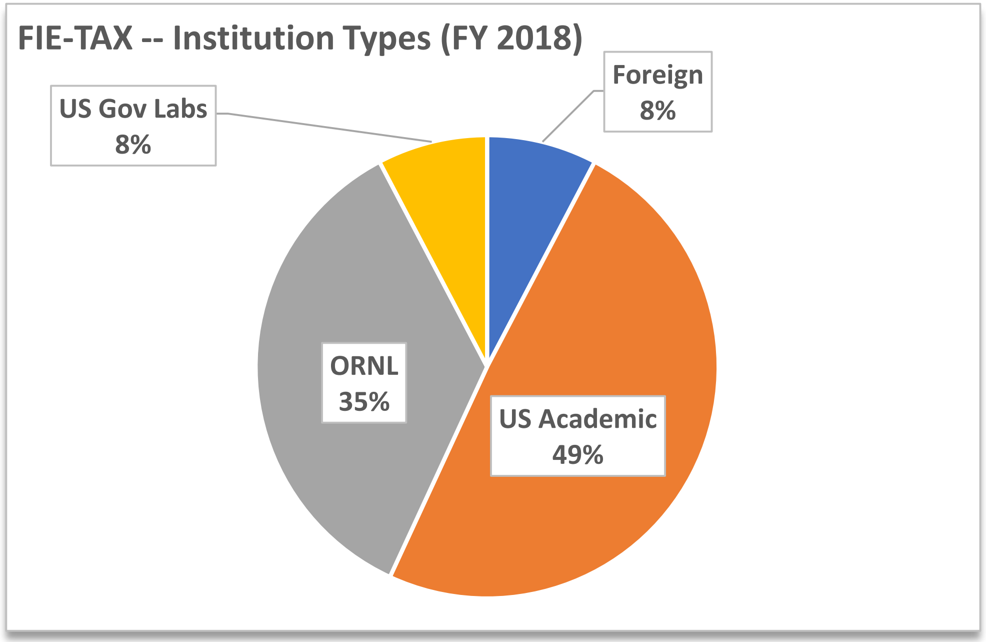
- In the user program (since 2007)
- Analyzer-detector assembly upgrade is well underway, and a new sample table is also being considered

HB-1A Instrument Specifications

Beam Spectrum:	Thermal
Incident neutron energy:	14.5 meV (fixed)
Monochromator system:	Double-bounce PG(002), fixed vertical focusing
Analyzer:	Workhorse PG(002); Be(101), Be(002), and Si(111) available
Analyzer range:	$-60° \leq 2\Theta \leq 120°$
Sample scattering angles:	$-5° \leq 2\Theta \leq 135°$
Collimation before sample:	(1) Pre-monochromator: 40’ (2) Monochromator – sample: 10’, 20’, or 40’
Collimation after sample:	(1) Sample – analyzer: 10’, 20’, 40’, 60’ and 80’ (2) Analyzer – detector: 20’, 40’, 60’, 80’, 140’, and 240’
Detector:	Single He^3 detector
Resolution:	1 meV (FWHM) resolution at the elastic line
Flux on sample (n cm^{-2} s^{-1})	$4.2*10^7$

HB-1A user community





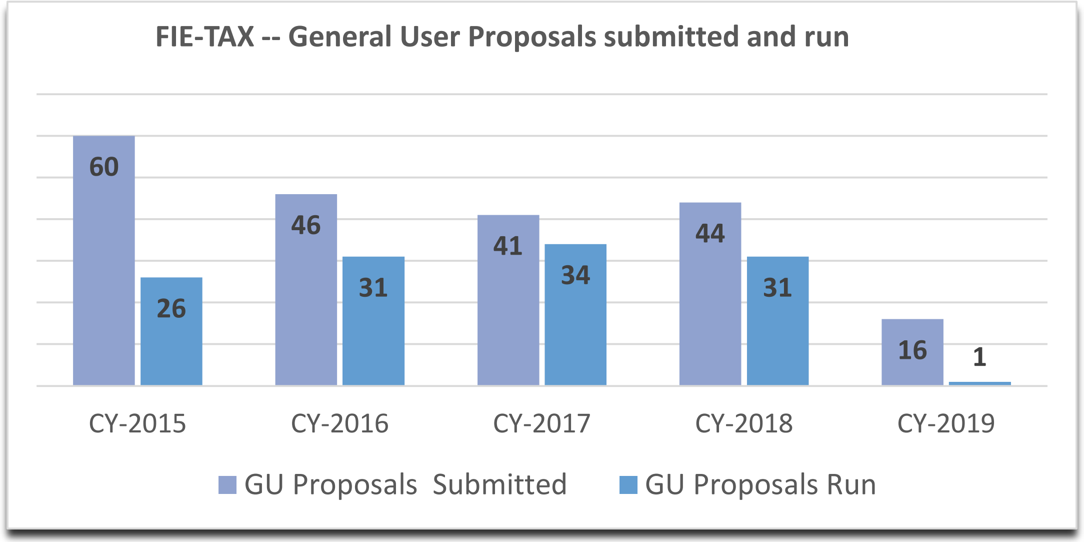
FY2017 - 2019:

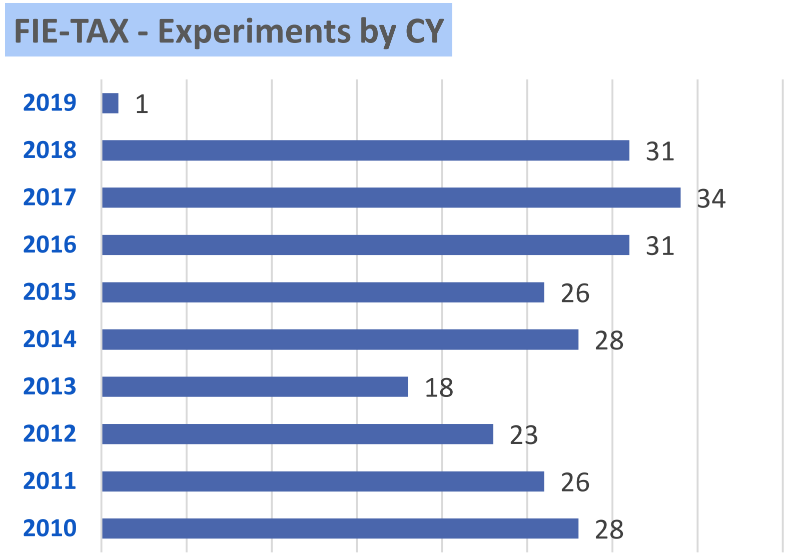
- 121 unique users
- No users in FY2019 due to long, unplanned HFIR outage
- Majority of users from US academic institutions and ORNL

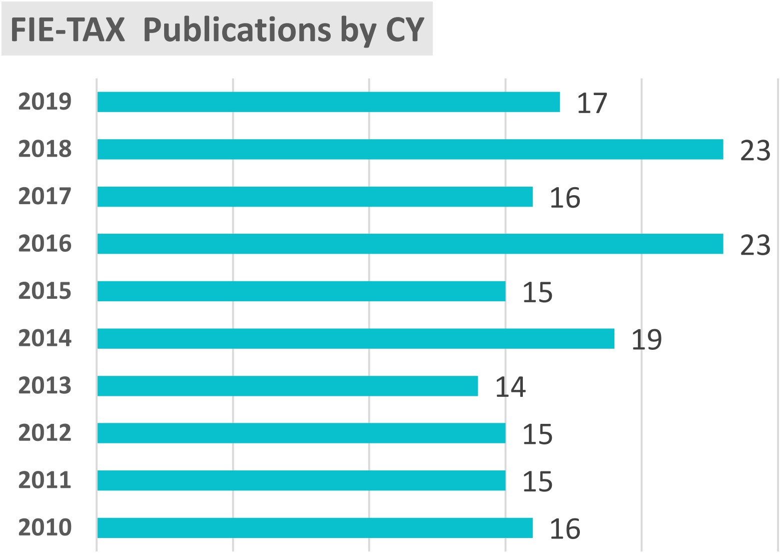
TOP EXTERNAL INSTITUTIONS USING FIE-TAX (FY 2018)

RICE UNIVERSITY
MCMASTER UNIVERSITY
AMES LABORATORY
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
STANFORD UNIVERSITY
UNIVERSITY OF TENNESSEE

HB-1A experiments and publications







CY2017 - 2019:

- 101 GU proposals submitted; 68 GU experiments run (67%)
- Subscription rate: 190%
- 56 publications (9 with IF >7)

Instrument stats (2008 – present):

- 208 publications, H-index: 36

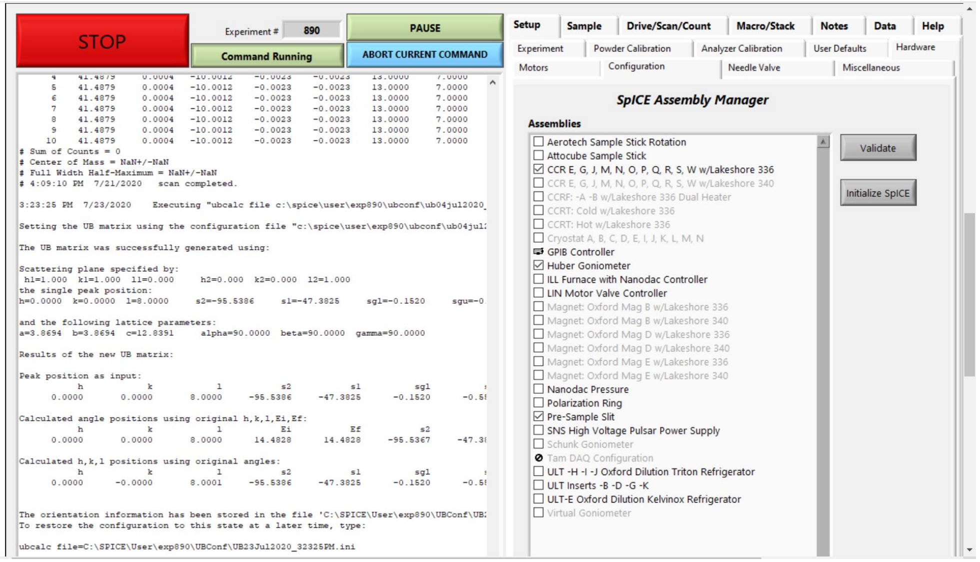
Data acquisition, reduction, visualization & analysis

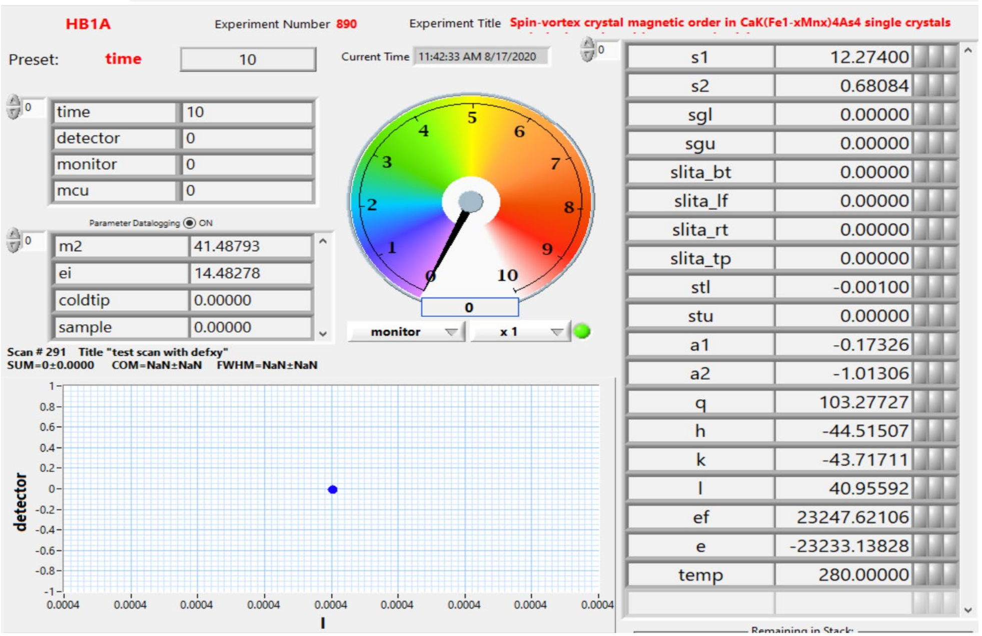
- **Data acquisition**: SPICE now, Epics in the future

- **Data reduction and visualization:** Graffiti (quick plotting and peak fitting) and DAVE now; Graffiti replacement in the future

- **Data analysis and modeling:** Matlab (Reslib) for resolution convolution and FullProf for magnetic structure refinements

- **Planning tools:** Virtual SPICE and TAS tools (DAVE)





Sample environment

Workhorses

- CCRs, cryostats, ultra-low temperature inserts (He-3 and dil fridges), vertical field cryomagnets (≤ 8 T)

Uncommon

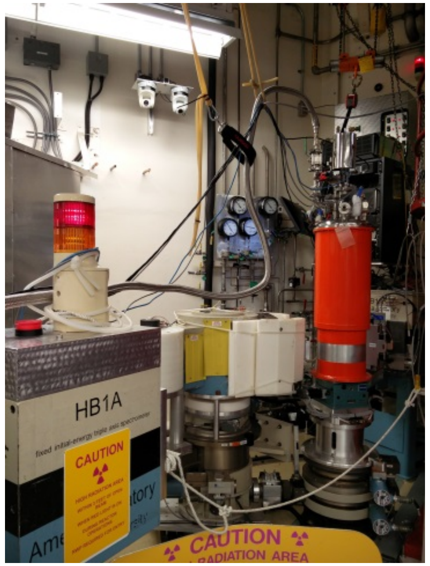
- Furnaces (≤ 1500°C), clamp & gas pressure cells (≤ 2 GPa), electric field (V ≤ 10 kV)

Recent Developments

- New sample sticks for cryostats and cryomagnets (in-situ operation)
  - sample tilt stick – change scattering plane
  - two single crystal sample changer
  - uniaxial pressure stick

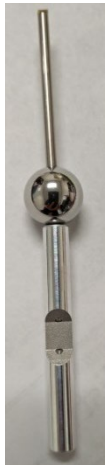
Desired

- Wide-angle horizontal field cryomagnet (≤ 4 T)



He-3 system on HB-1A


MAG-E on HB-1A

Clamp and gas pressure cells

Science highlights

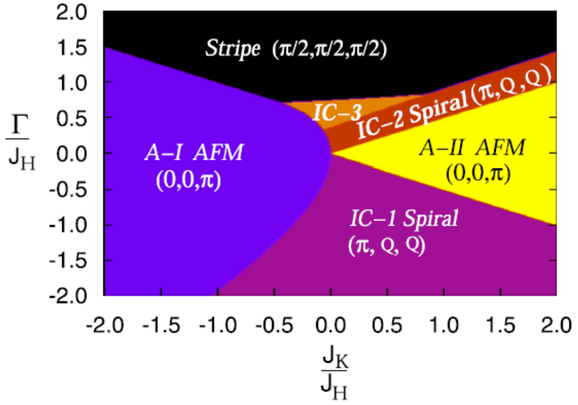
- Revisiting the Kitaev material candidacy of Ir^{4+} double perovskite iridates
  - Physical Review B **99**, 134417 (2019)
  - Polycrystalline measurement of a weak magnetic signal
- Spin canting and orbital order in spinel vanadate thin films
  - Physical Review Materials **2**, 104411 (2018)
  - Thin film measurement of a weak magnetic signal
- Destabilization of magnetic order in a dilute Kitaev spin liquid candidate
  - Physical Review Letters 119, 237203 (2017)
  - Diffraction measurement of a single crystal doping series
- Novel strongly spin-orbit coupled quantum dimer magnet: $Yb_2Si_2O_7$
  - Physical Review Letters 123, 027201 (2019)
  - Diffraction measurement of field-induced behavior in a single crystal

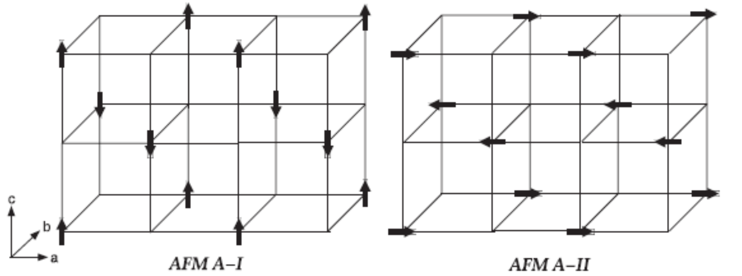
Revisiting the Kitaev material candidacy of Ir^{4+} double perovskite iridates

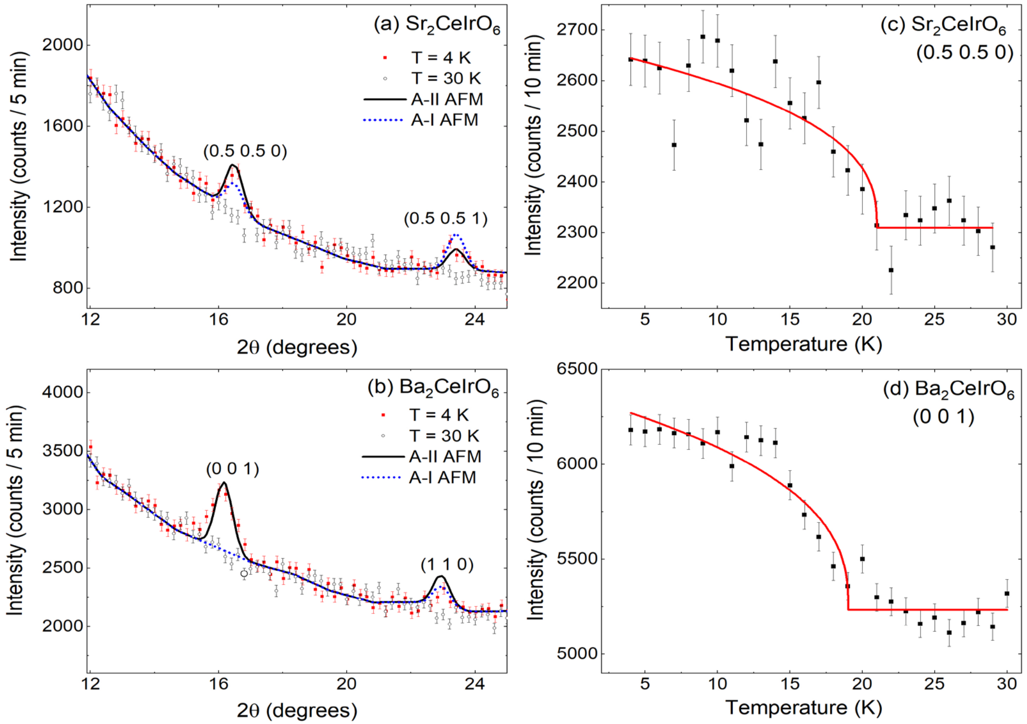
Key question: Does a Kitaev interaction play a role in magnetic ground state selection for double perovskite iridates?

- Theoretical phase diagram for fcc magnets shows Kitaev interactions drive A-I or A-II ordered states
- HB-1A data on polycrystalline samples identifies A-II ordered states, consistent with expectations for an AFM Kitaev interaction
- Results are consistent with exchange interactions determined by subsequent DFT calculations

Publication: PRB **99**, 134417 (2019)



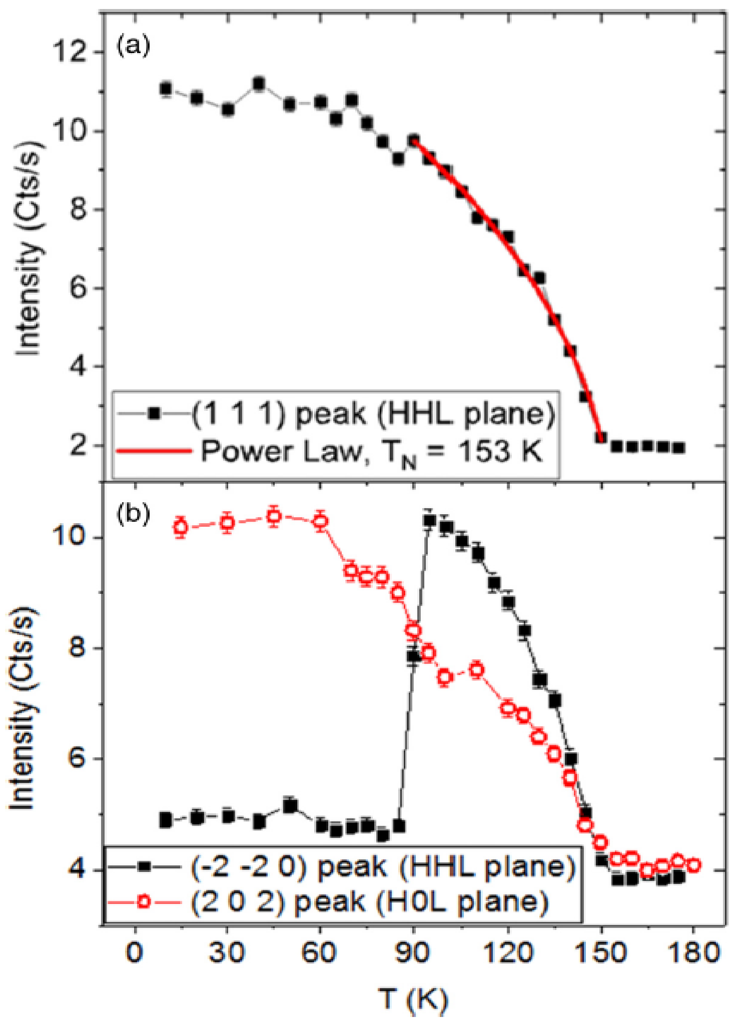




Spin canting and orbital order in spinel vanadate thin films

Key question: How does compressive strain modify the magnetic properties of CoV_2O_4?

- Bulk, cubic CoV_2O_4 exhibits ferrimagnetic order below T_N = 156 K and a weak first order structural transition with small V spin canting at T_{N2} = 90 K (i.e. orbital glass state). Very close to itinerant – localized transition due to short V-V distance.
- 300 nm films studied here are orthorhombic at room T and show very different magnetic behavior
- Ferrimagnetic transition unchanged, but lower T transition corresponds to spin reorientation of Co spins. V spins show larger canting away from Co spins as compared to bulk samples.
- Compressive strain pushes CoV_2O_4 deeper into the insulating state



Publication: PRB **99**, 134417 (2019)

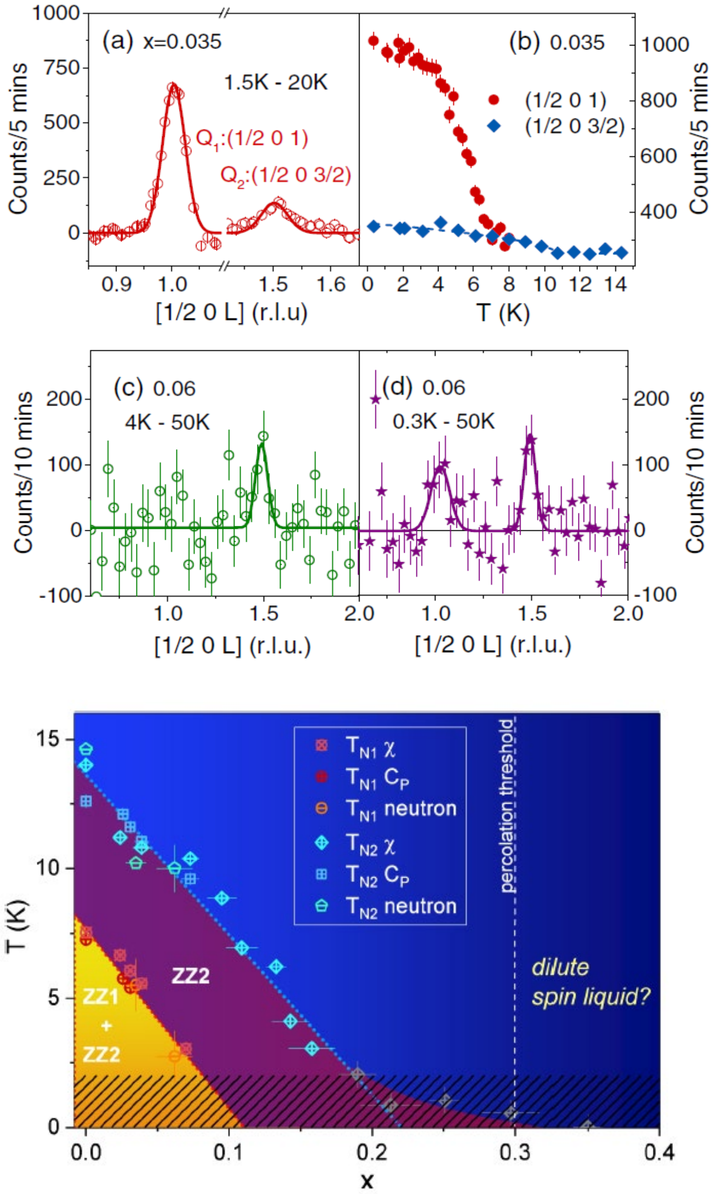
OAK RIDGE National Laboratory

Destabilization of magnetic order in a dilute spin liquid candidate

Key question: Does Ir doping suppress magnetic order in α-$RuCl_3$ and generate a spin liquid state?

- α-$RuCl_3$ is proximate to a spin liquid state, but orders into a zigzag spin configuration at low temperatures
- HB-1A and bulk characterization measurements on Ir-doped samples show that T_N of the zigzag order is suppressed to zero at x = 0.3
- Complementary SEQUOIA data shows that scattering continuum associated with spin liquid state persists up to x = 0.35, suggesting that Ir-doping produces spin liquid ground state

Publication: PRL 119, 237203 (2017)

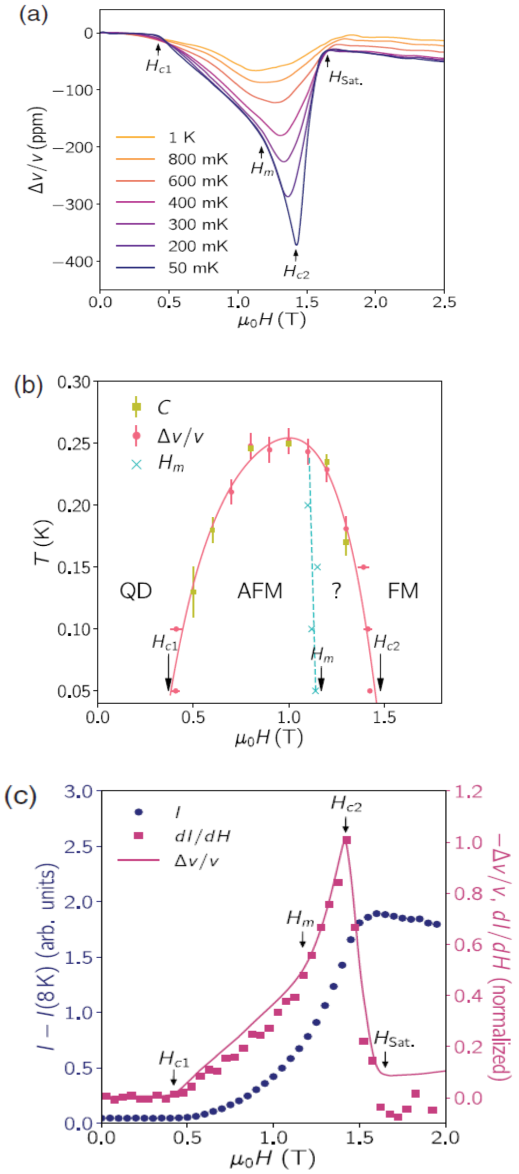


Oak Ridge National Laboratory

Novel strongly spin-orbit coupled dimer magnet: $Yb_2Si_2O_7$

Key question: Does $Yb_2Si_2O_7$ exhibit field-induced order that represents a magnetic BEC?

- Heat capacity and ultrasound velocity measurements were used to identify a non-magnetic ground state of interacting dimers in zero field and map out a phase diagram in an applied magnetic field
- HB-1A neutron diffraction data identified field-induced order and CNCS data found gapless magnon excitations, indicative of the U(1) symmetry required for a magnetic BEC phase
- A second phase may be present under the dome, but the nature of this state is not understood yet
- $Yb_2Si_2O_7$ represents the first example of a rare-earth-based magnetic BEC, with several transition metal counterparts identified previously



Publication: PRL 123, 027201 (2019)

OAK RIDGE National Laboratory

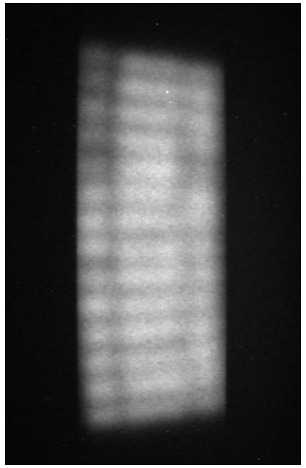
Instrument vision

Ensure that HB-1A becomes a world-leading instrument for single crystal, thin film, and powder studies of weak elastic scattering signals using a wide range of sample environments.

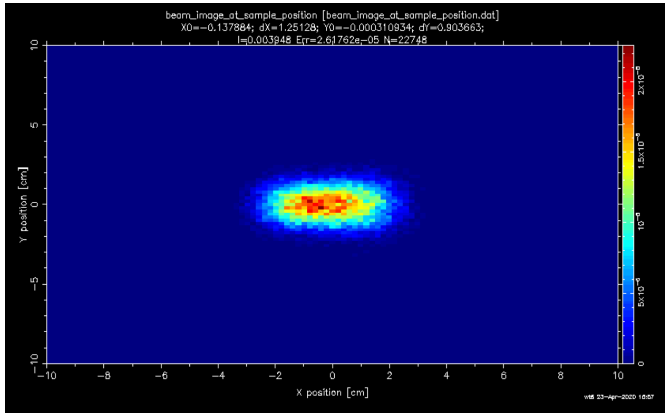
This vision will be achieved in three steps:

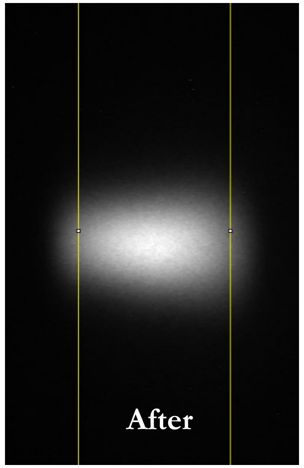
1) Optimize double-bounce monochromator system – completed Nov. 2019
2) Upgrade the sample table and secondary spectrometer – in progress
3) Purchase and/or design additional sample environment capabilities, including in-situ pressure capabilities and a wide-angle horizontal field magnet – rolling investments

HB-1A monochromator upgrade completed



Neutron camera image at M2 drum exit



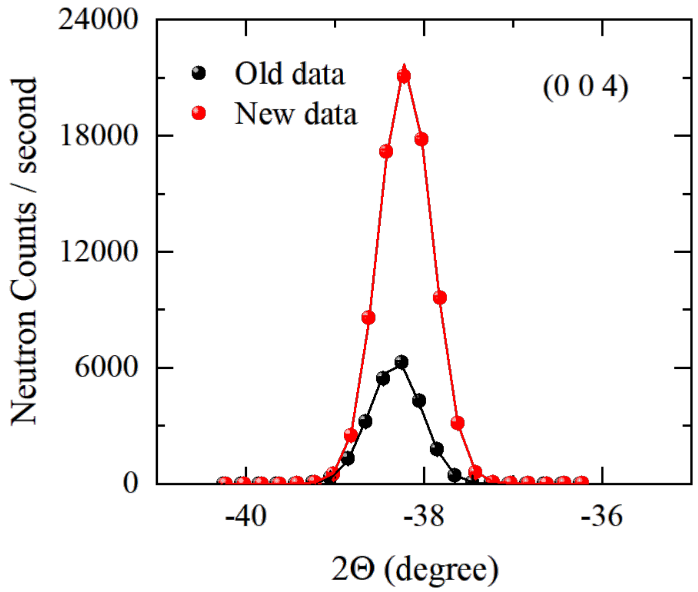


Beam size after the monochromator upgrade

Beam Size (FWHM) at sample position after upgrade:

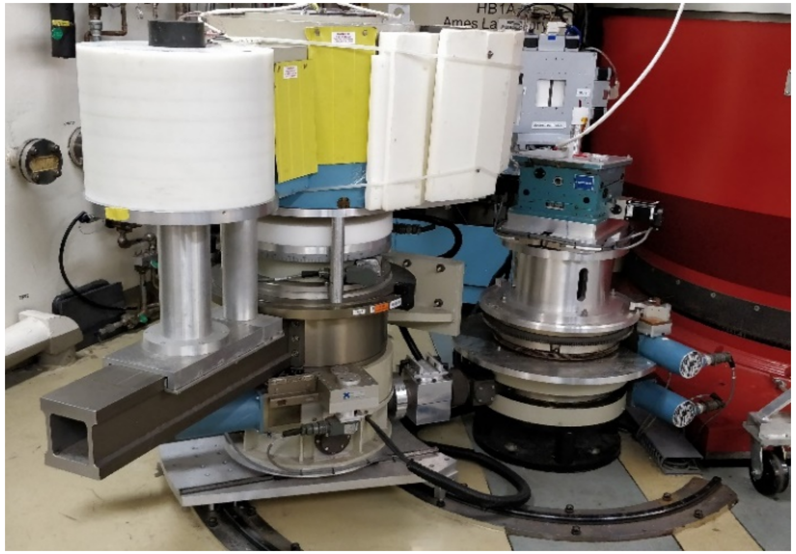
McStas simulation:
22.5 mm H x 35 mm W

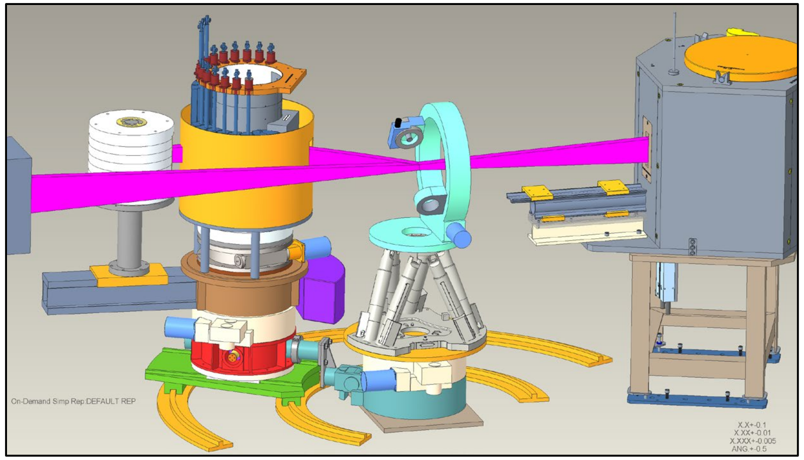
Measured:
24 mm H x 39 mm W



- ❑ Improved beam focus at sample position critical for HB-1A's current scientific mission
- ❑ The upgrade commissioning was successfully completed in cycle 484 (Nov. 2019)
- ❑ Data collected on a single crystal before and after the upgrade shows at least three times flux gain on sample
- ❑ Flux measurement using a calibrated monitor yields 4.17 x 10^7 n/cm^2 s flux at sample position vs. 1 x 10^7 n/cm^2 s flux before the upgrade.

Secondary spectrometer upgrade





Specifications:

- 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

Instrument needs

Near term

- Completion of secondary spectrometer project (already funded)
- A new sample table with an increased weight capacity and a z-stage. Pitch was made to Science Productivity committee; waiting on final decision.
- More vertical field cryomagnets to increase capacity at HFIR. Pitch was made to Science Productivity committee for a 6 T vertical field cryomagnet; waiting on final decision.
- In-situ pressure capabilities – uniaxial pressure stick just ordered from Rice University
- Expanded liquid cryogen autofill (LHeAF) capabilities at HFIR

Longer term

- New software for data reduction, visualization, and analysis
- Wide-angle horizontal field magnet
- Development and implementation of polarized beam capabilities, including single axis, XYZ, and spherical neutron polarimetry.
- New neutron alignment station with increased flux in the re-optimized cold guide hall

Summary

- HB-1A is an excellent instrument for elastic scattering studies of weak signals in polycrystalline, single crystal, and thin film samples
- Completed double-bounce monochromator upgrade provides 3x increased flux on sample
- Ongoing secondary spectrometer upgrade will improve the signal-to-noise ratio further and make the instrument more flexible
- Rolling investments in new sample environments, including cryomagnets and in-situ pressure capabilities, will enhance the HB-1A user program
- Addition of computational instrument scientist to the HB-1A team will lead to improved instrument software for data reduction, visualization, and analysis with new functionalities
- HB-1A is a highly productive instrument with complementary capabilities to ORNL's other diffractometers and spectrometers. The near- and long-term visions are clear and exciting.