A scientific wingman: AI co-pilot for triple-axis users at the NCNR

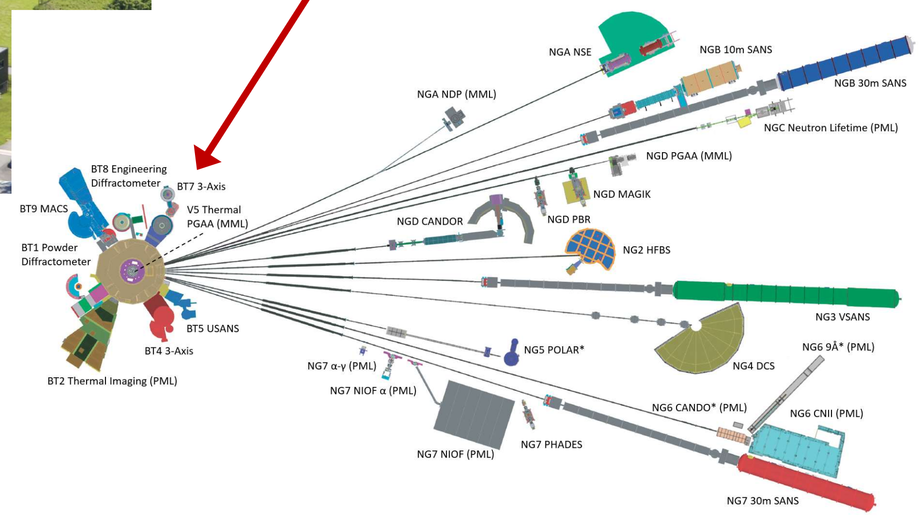
Carina Jacobson

Purdue University

Mentor: Dr. William Ratcliff

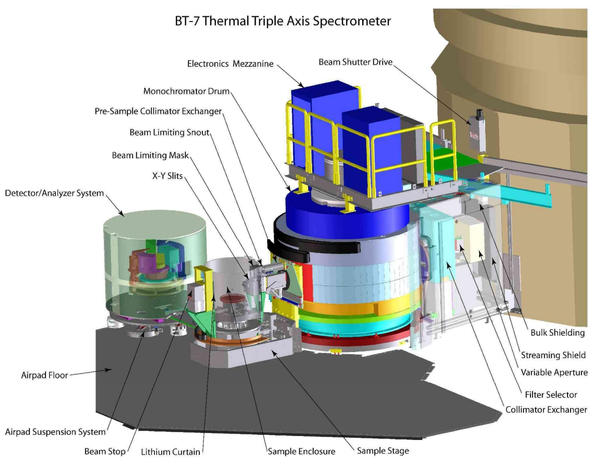
NIST Center for Neutron Research (NCNR)

BT-7 triple-axis spectrometer

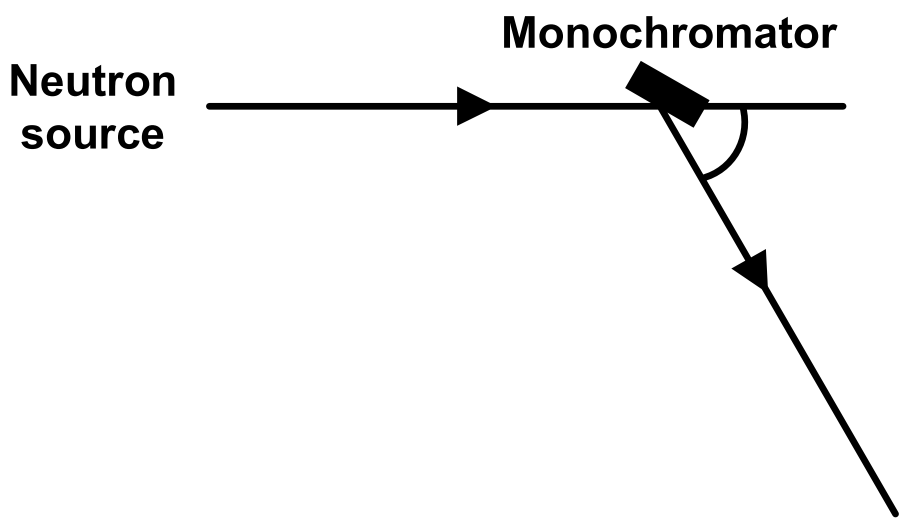


Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample

Neutron source



Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample



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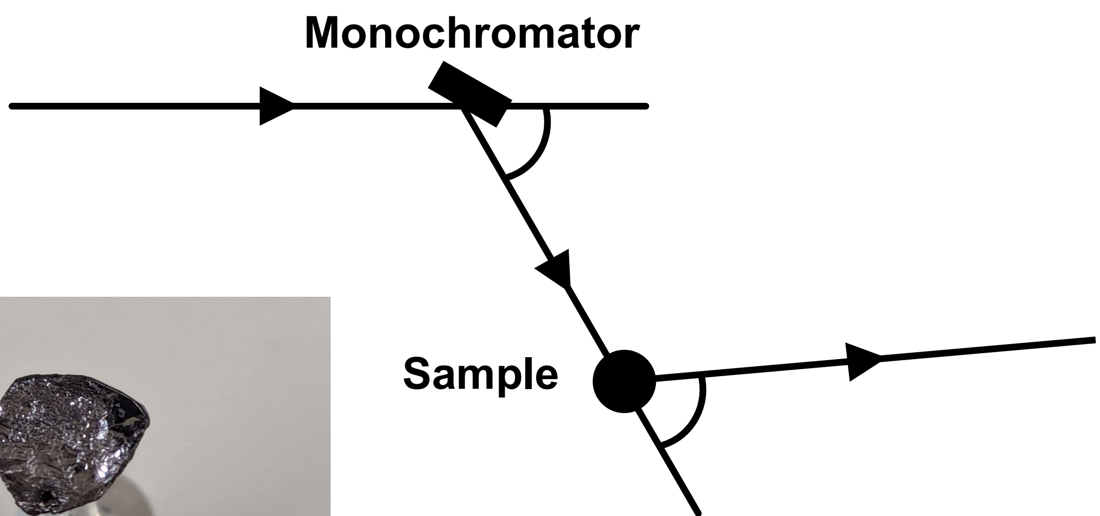

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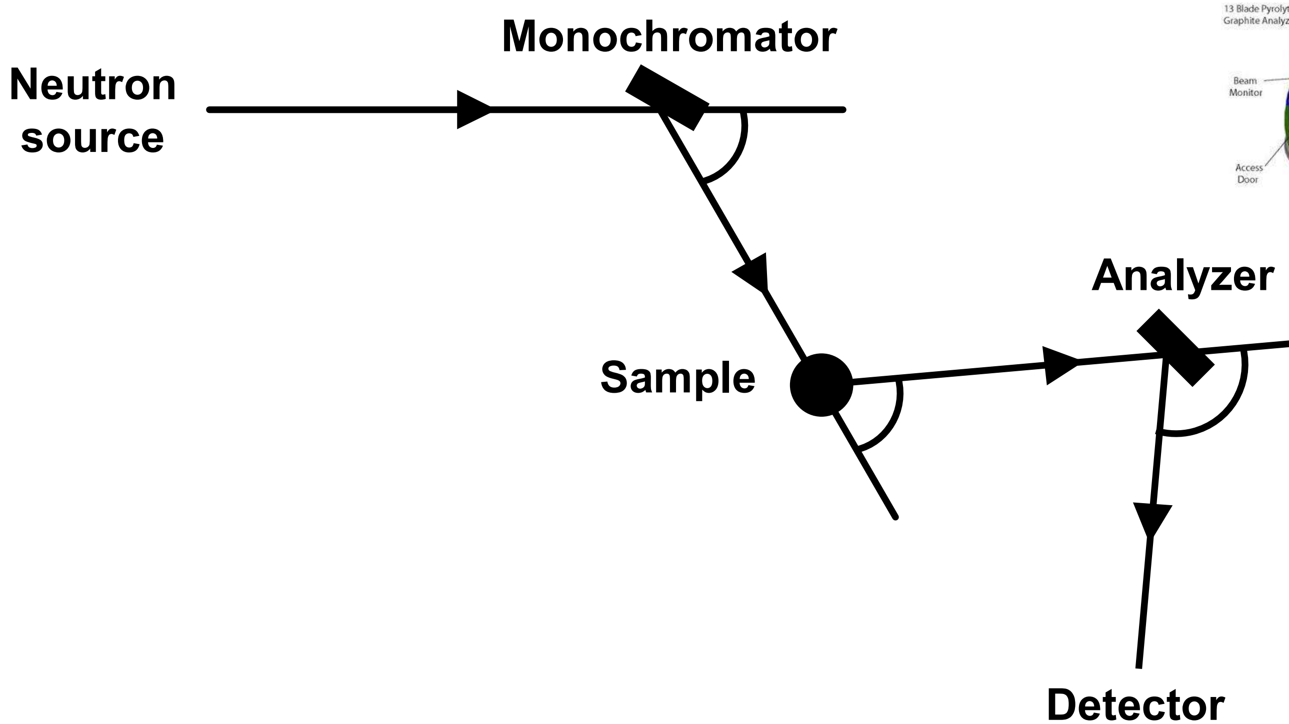
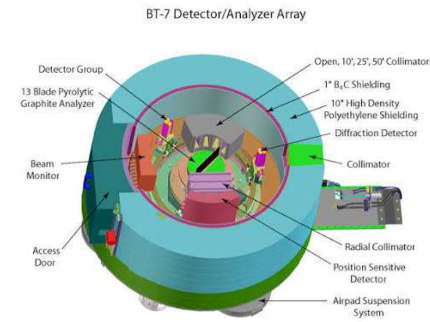
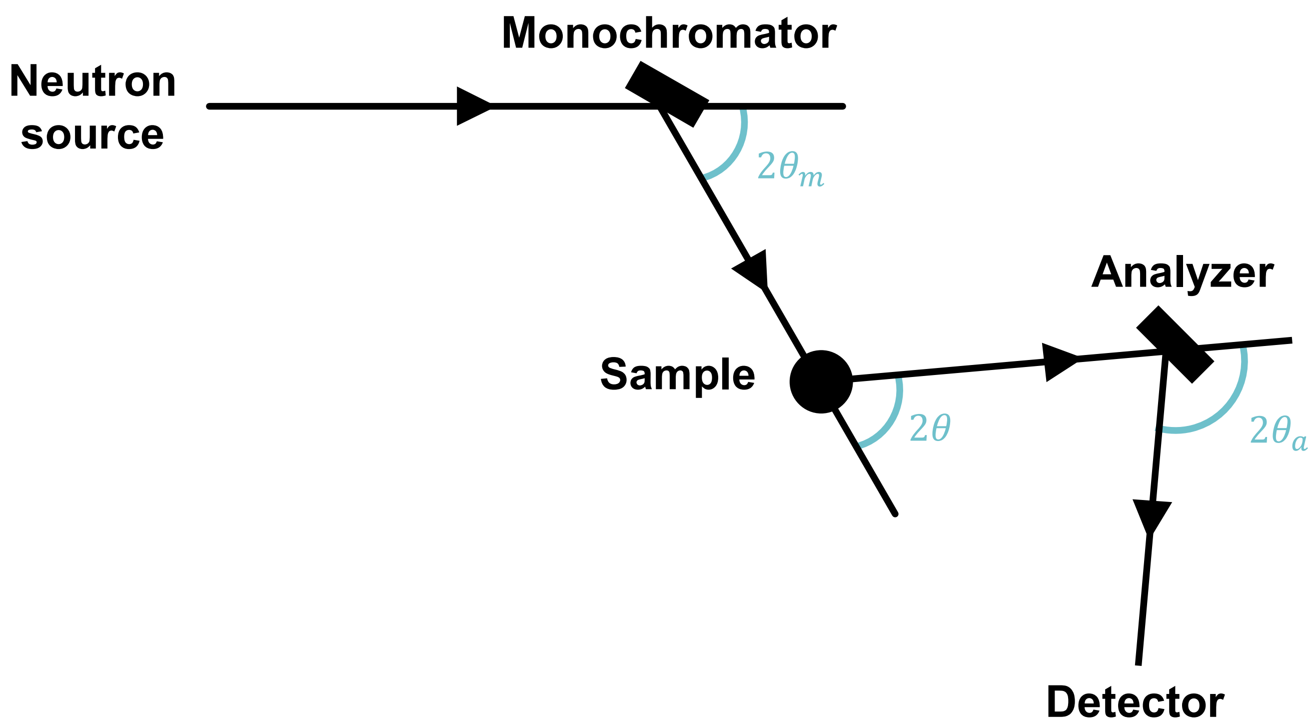
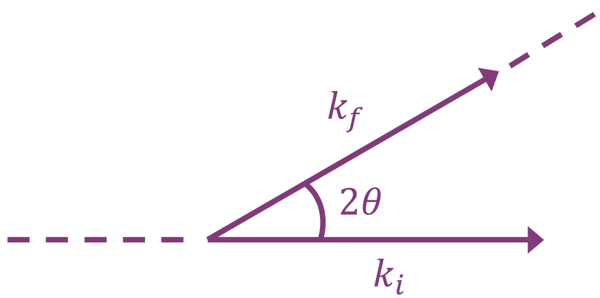




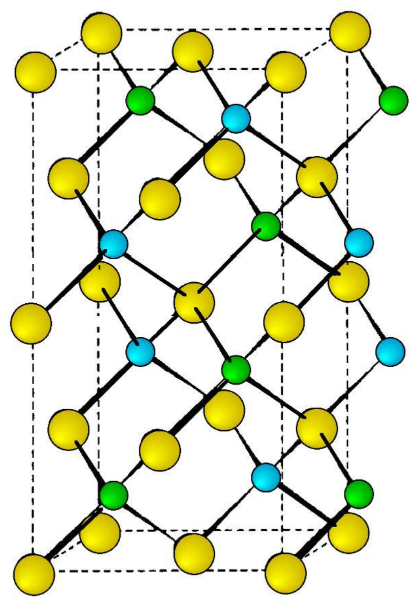
Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample



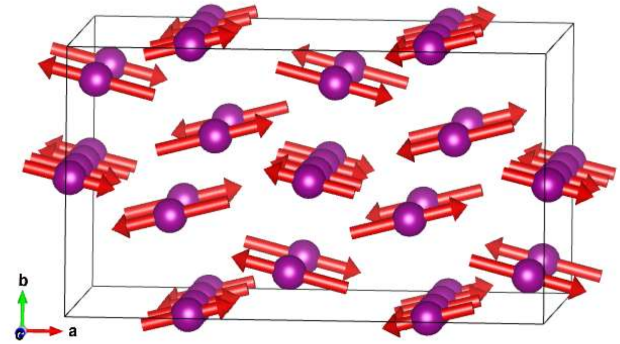
Elastic neutron scattering measures static properties



$$\boldsymbol{k_f} = \boldsymbol{k_i}$$

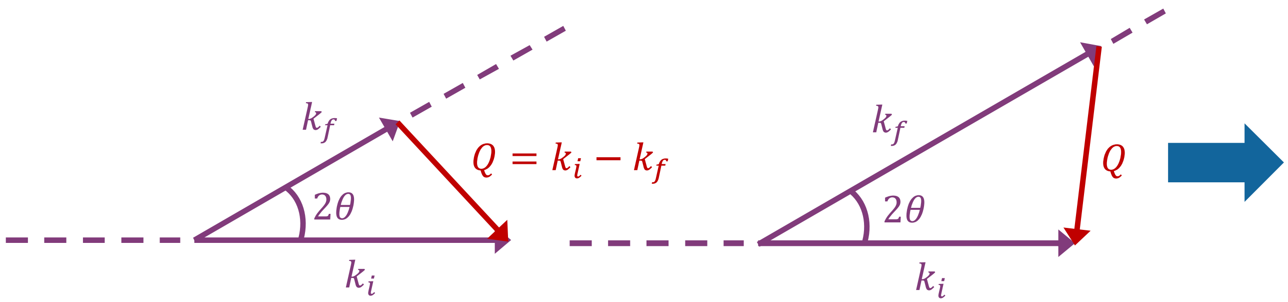


Atomic structure



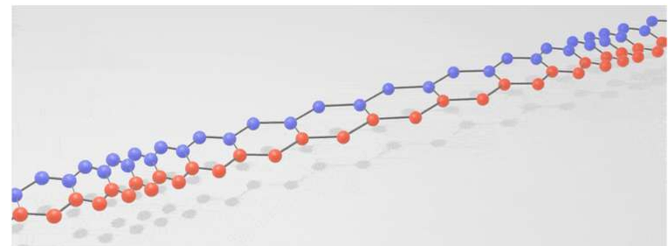
Magnetic ordering

Inelastic neutron scattering measures dynamic properties

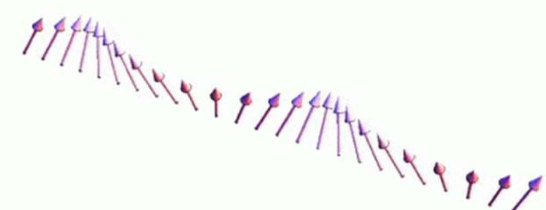


$$\boldsymbol{k_f} \neq \boldsymbol{k_i}$$

Neutrons exchange energy with the sample



Phonons



Spin waves

How do you begin a TAS experiment?

Magnetic structures of rare earth intermetallic compounds $RCuAs_2$ (R = Pr, Nd, Tb, Dy, Ho, and Yb)

Y Zhao [a, b, *], J W Lynn [a], G S Thakur [c,1], Z Haque [c], L C Gupta [c,2] and A K Ganguli [c,d]

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Broadband critical dynamics in disordered lead-based perovskites

C. Stock, M. Songvilay
School of Physics and Astronomy, University of Edinburgh, Edinburgh

P. M. Gehring, Guangyong Xu

Acoustic Phonon Lifetimes Limit Thermal Transport in Methylammonium Lead Iodide

Aryeh Gold-Parker[a,b], Peter M. Gehring[c], Jonathan M. Skelton[d], Ian C. Smith[a], Dan Parshall[c], Jarvist M. Frost[e], Hemamala I. Karunadasa[a], Aron Walsh[f,g], Michael F. Toney[b,1]

Neutron spin resonance as a probe of superconducting gap anisotropy in partially detwinned electron underdoped $NaFe_{0.985}Co_{0.015}As$

Chenglin Zhang,[1] J. T. Park,[2] Xingye Lu,[1,3] Rong Yu,[4,5] Yu Li,[1] Wenliang Zhang,[3] Yang Zhao,[6,7] J. W. Lynn,[6]

Magnetic Structure of Hexagonal Mn-doped $LuFeO_3$

Steven M. Disseler[1], Xuan Luo[2], Yoon Seok Oh[3], Rongwei Hu[3], Dylan Quintana[4], Alexander Zhang[1,*], Jeffrey W. Lynn[1], Sang-Wook Cheong[2,3], William Ratcliff II[1]

Large anomalous Hall effect in a half-Heusler antiferromagnet

T. Suzuki[1], R. Chisnell[2], A. Devarakonda[1], Y.-T. Liu[1], W. Feng[3], D. Xiao[4], J. W. Lynn[2] and J. G. Checkelsky[1★]

Nonreciprocal Magnons and Symmetry-Breaking in the Noncentrosymmetric Antiferromagnet

G. Gitgeatpong,[1,2,3] Y. Zhao,[4,5] P. Piyawongwatthana,[1] Y. Qiu,[5] L. W. Harriger,[5] N. P. Butch,[5] T. J. Sato,[6] and K. Matan[1,2,*]
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[2]*ThEP, Commission of Higher Education, Bangkok 10400, Thailand*
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ment of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA
NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA
[6]*IMRAM, Tohoku University, Sendai, Miyagi 980-8577, Japan*
(Received 27 February 2017; published 24 July 2017)

Symmetry and correlations underlying hidden order in URu_2Si_2

Nicholas P. Butch,[1,2,3,*] Michael E. Manley,[4] Jason R. Jeffries,[3] Marc Janoschek,[5,6] Kevin Huang,[6] M. Brian Maple,[6] Ayman H. Said,[7] Bogdan M. Leu,[7] and Jeffrey W. Lynn[2]

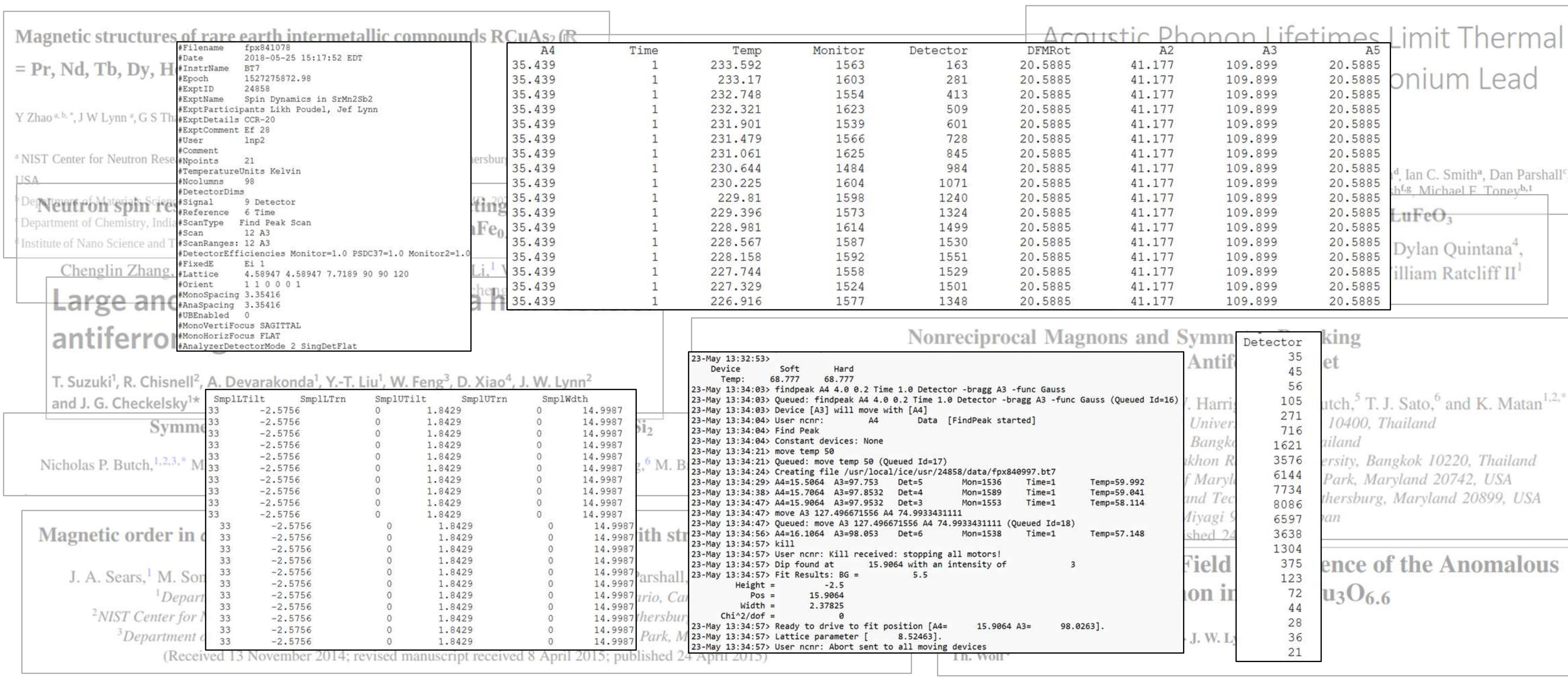
Magnetic order in α-$RuCl_3$: A honeycomb-lattice quantum magnet with strong spin-orbit coupling

J. A. Sears,[1] M. Songvilay,[1] K. W. Plumb,[1] J. P. Clancy,[1] Y. Qiu,[2,3] Y. Zhao,[2,3] D. Parshall,[2] and Young-June Kim[1,*]
[1]*Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario, Canada M5S 1A7*
[2]*NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*
[3]*Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA*
(Received 13 November 2014; revised manuscript received 8 April 2015; published 24 April 2015)

Absence of Magnetic Field Dependence of the Anomalous Bond-Stretching Phonon in $YBa_2Cu_3O_{6.6}$

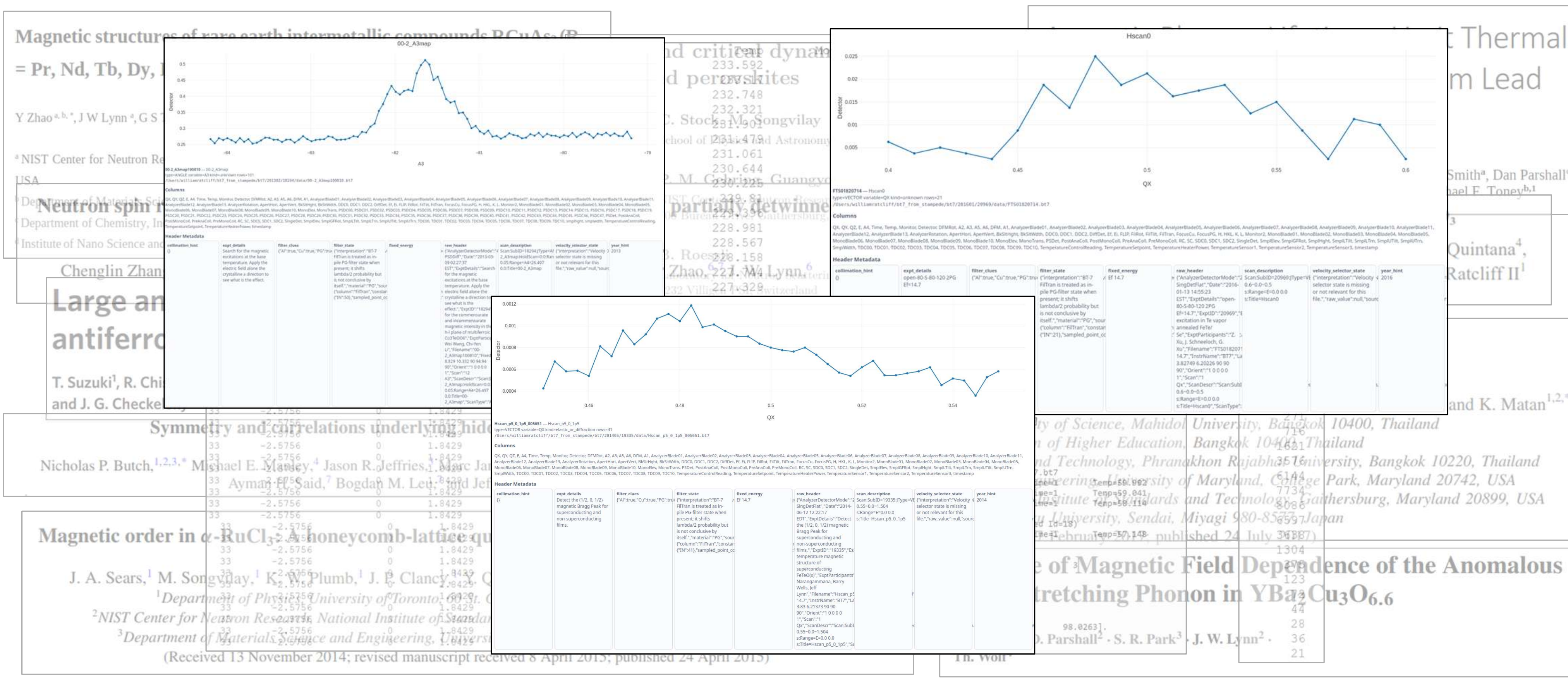
D. Reznik[1] · D. Parshall[2] · S. R. Park[3] · J. W. Lynn[2] · Th. Wolf[4]

How do you begin a TAS experiment?



NIST NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY U.S. DEPARTMENT OF COMMERCE

How do you begin a TAS experiment?



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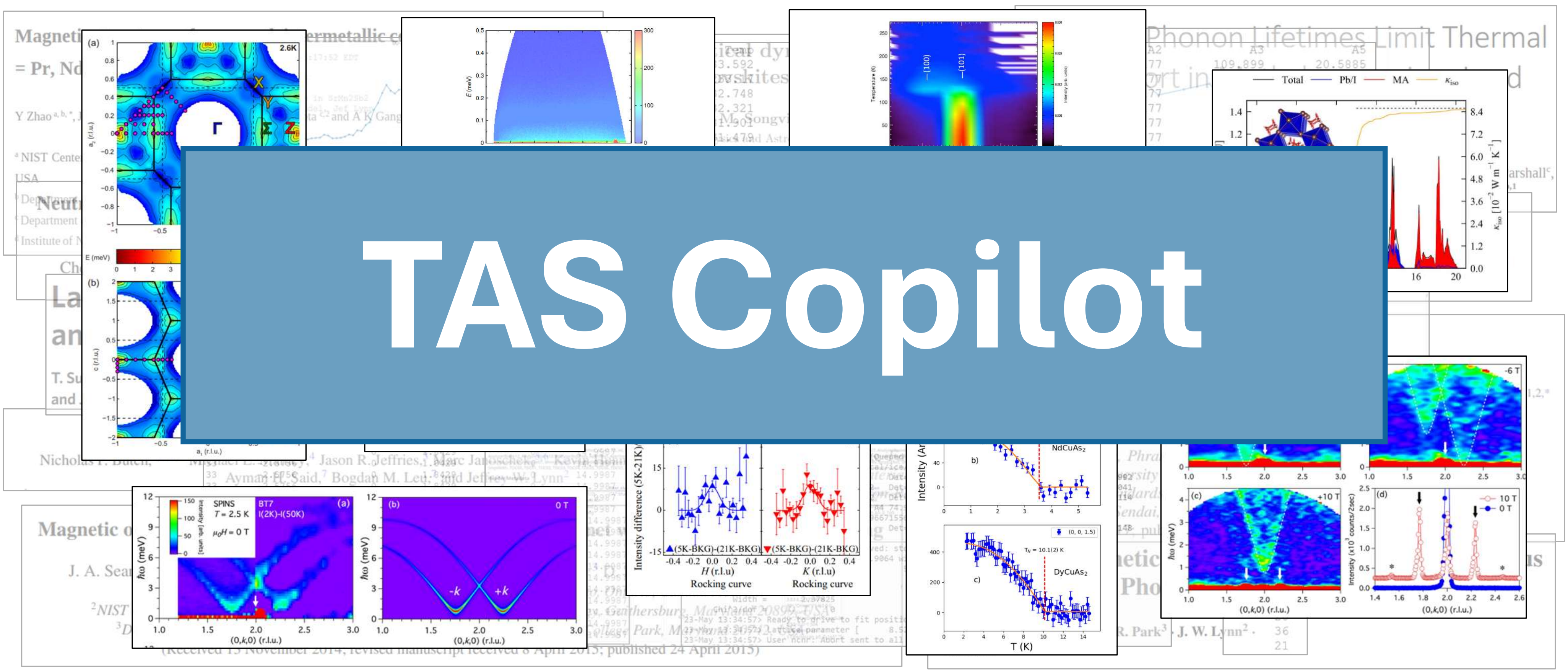
How do you begin a TAS experiment?



TAS Copilot centralizes evidence and calls tools for more efficient experiments

Search corpus

Inspect scans

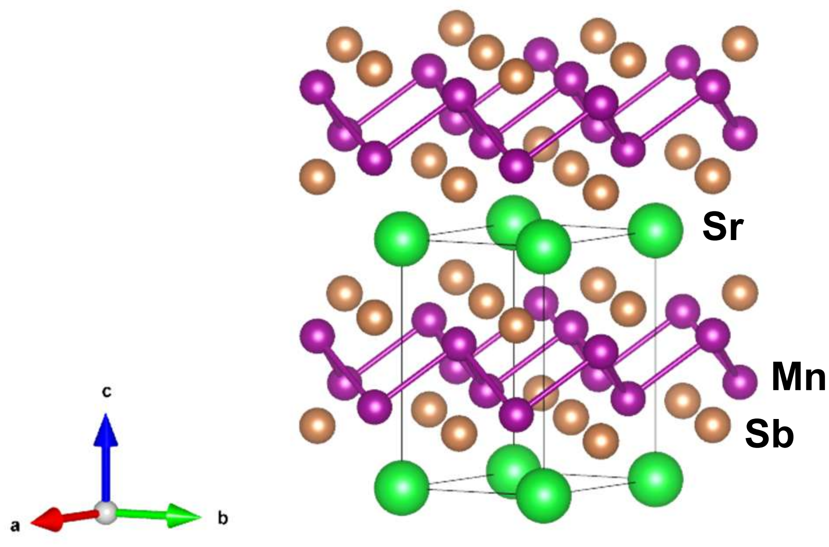
Build dashboards

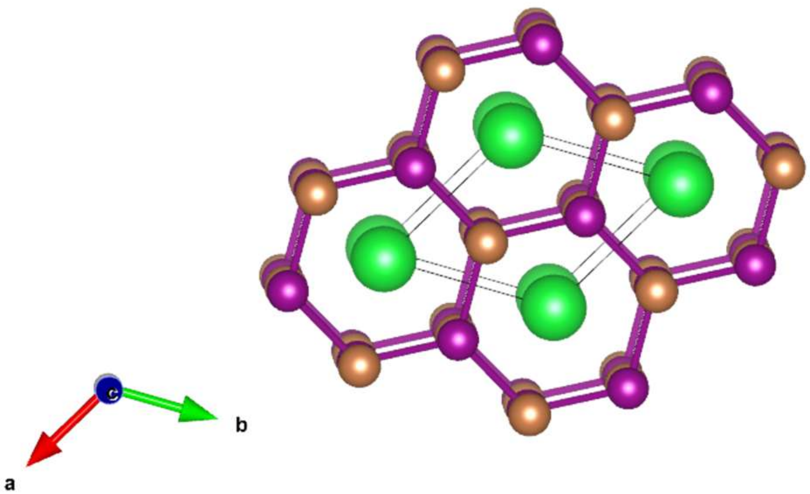
What can you do?

Plan experiment

Summarize overnight data

Case study for TAS Copilot workflow



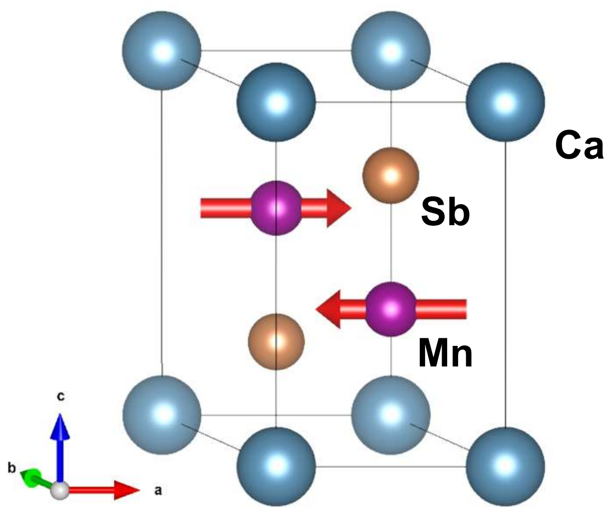


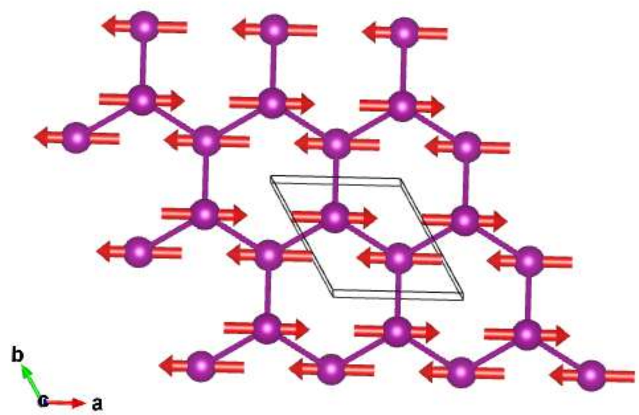
$SrMn_2Sb_2$

Use extracted facts from a similar material

- Magnetic structure
- Propagation vector
- Spin direction
- Ordered moment
- Exchange interaction

Use $CaMn_2Sb_2$ as a model for $SrMn_2Sb_2$



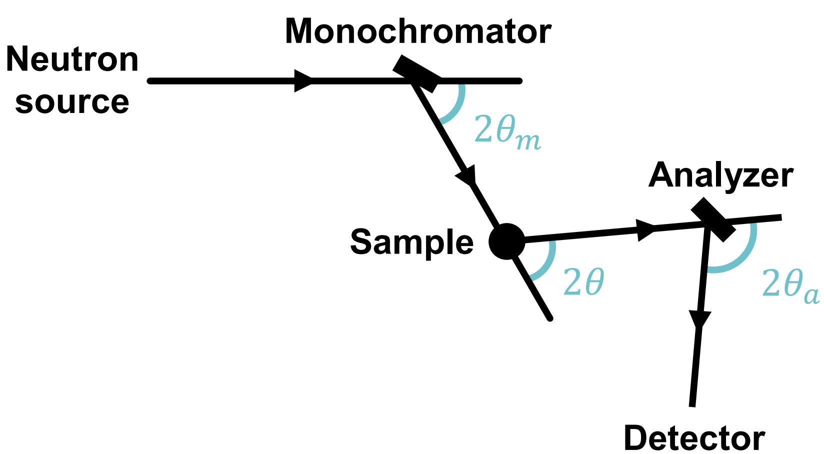


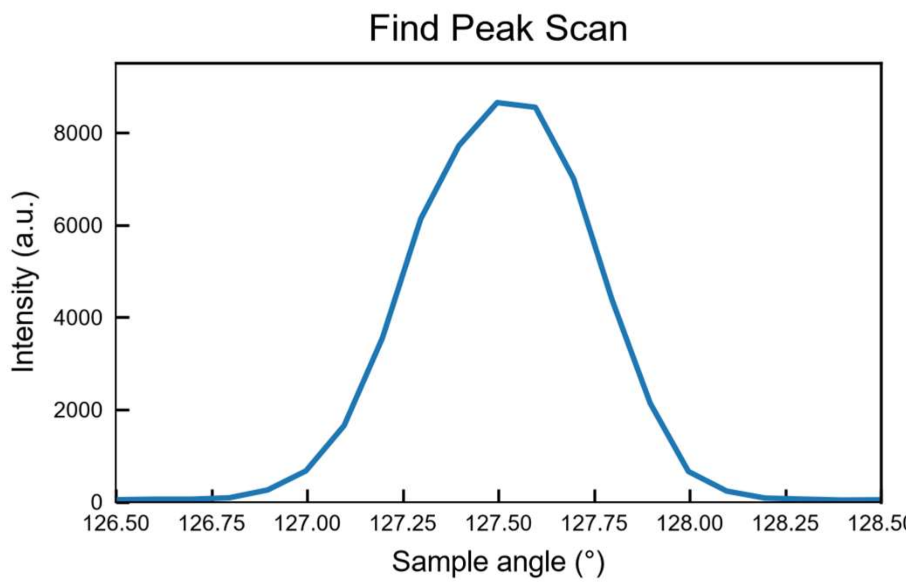
Align TAS via Bragg peaks

Bragg's Law: $\boldsymbol{n\lambda = 2d\sin\theta}$

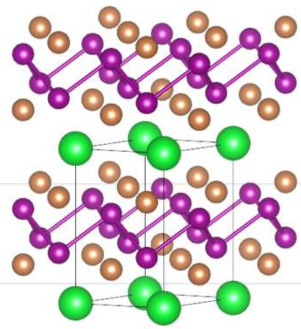
Bragg angle θ

Scattering angle 2θ





Choose peaks based on structure and instrument configurations



1. Structure (CIF)

Choose File SrMn2Sb2.cif

Sr(MnSb)2 | P-3m1 (#164, trigonal) | a=4.5888 b=4.5888 c=7.7529 alpha=90.00 beta=90.00 gamma=120.00 | 3 asymmetric sites

Final energy

2. Plane, Energy, Environment

Sample environment

Orient 1 (H K L)			Orient 2 (H K L)			Ef (meV)
1	1	0	0	0	1	14.7

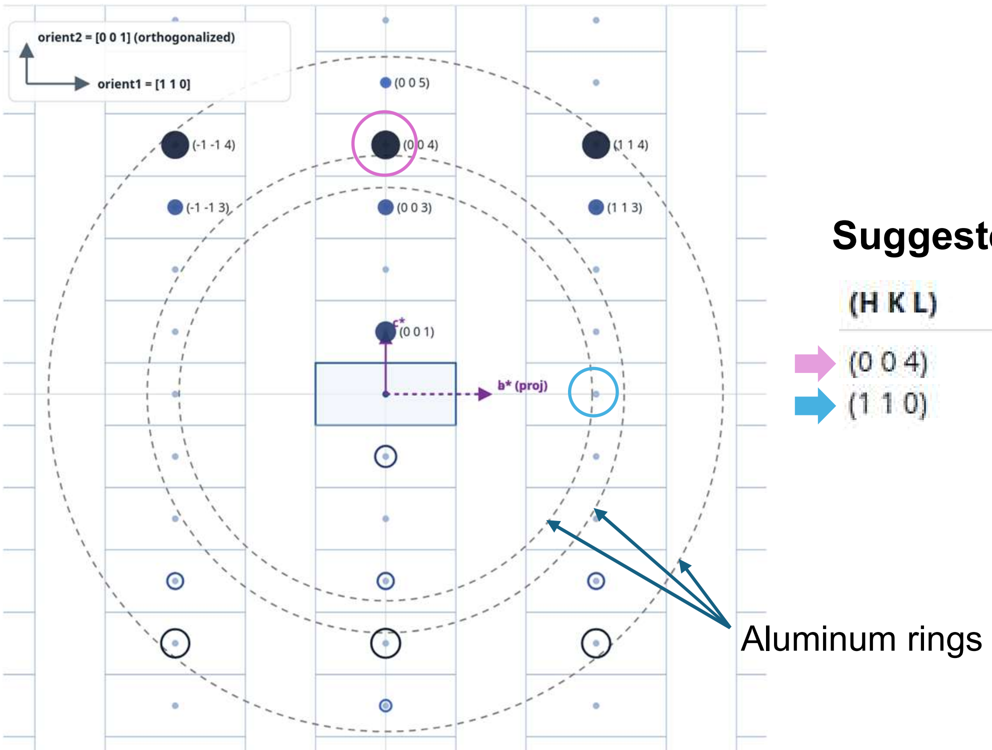
Environment

☑ Aluminum ☐ Copper

Calculate

Scattering plane

Suggested reciprocal lattice vectors describe scattering angles



Suggested peaks

(H K L)	d (Å)	|Q| ($Å^{-1}$)	2θ	mult	F^2 (max=100)
(0 0 4)	1.9382	3.2417	74.97	2	100.00
(1 1 0)	2.2944	2.7385	61.87	6	31.07

Suggested scan plans improve alignment efficiency

Scan plan suggestions:
- A3 – sample rotation
- A4 – scattering angle
- Tilt
- Translation

Experimental alignment corresponds with suggested alignment

Scattering angle (2θ) — A4

Sample rotation angle — A3

Scan	Ei	Ef	Orientation	A4	A3
A3	14.7	14.7	1 1 0 0 0 1	35.5374	107.628-110.628
A4	14.7	14.7	1 1 0 0 0 1	33.5374-35.7374	108.948-110.048
SmplLTilt	14.7	14.7	1 1 0 0 0 1	35.439	109.899
SmplUTilt	14.7	14.7	1 1 0 0 0 1	35.439	109.899
A3	14.7	14.7	1 1 0 0 0 1	35.439	108.899-110.899
A3	14.7	14.7	1 1 0 0 0 1	62.0038	30.002-31.902
SmplLTilt	14.7	14.7	1 1 0 0 0 1	62.0038	30.9813
SmplWdth	14.7	14.7	1 1 0 0 0 1	62.0038	30.9813
SmplHght	14.7	14.7	1 1 0 0 0 1	62.0038	30.9813
BkSltWdth	14.7	14.7	1 1 0 0 0 1	62.0038	30.9813
A3	14.7	14.7	1 1 0 0 0 1	74.9934	126.497-128.497
SmplUTilt	14.7	14.7	1 1 0 0 0 1	74.9934	127.511
SmplWdth	14.7	14.7	1 1 0 0 0 1	74.9934	127.511
SmplHght	14.7	14.7	1 1 0 0 0 1	74.9934	127.511
BkSltWdth	14.7	14.7	1 1 0 0 0 1	74.9934	127.511
A3	14.7	14.7	1 1 0 0 0 1	74.9934	126.511-128.511

(002)

(110)

(004)

Started with (002) using $\frac{\lambda}{2}$ to reduce sensitivity to tilt

(004) and (110) define plane

Summarize measurements and locate important features

What was measured overnight and what should I review next?

Overnight Scan Summary

Status: ok Data root: `raw_data/bt7/201804/24858/data` Scans summarized: 251 Series groups: 12

Summary

The overnight files form 12 scan-family group(s). The strongest report suggestion is `inelastic_dispersion_or_lineshape_report` with probability 0.843; this is a triage prior, not a completed reduction.

Summary

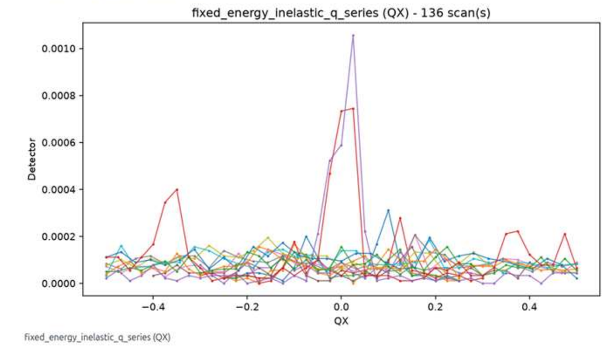
Suggestions

TAS Copilot outlines results clearly

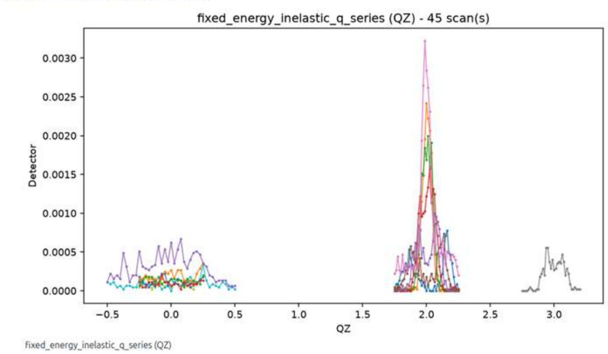
Plots for each scan family

Scan Family Plots

24858-fixed_energy_inelastic_q_series-qx



24858-fixed_energy_inelastic_q_series-qz



Type of scan

Ranges measured

Scan Families

- `fixed_energy_inelastic_q_series` scans=136 points=3701 confidence=high report=inelastic_dispersion_or_lineshape_report (E=2.0-35.0 meV; T=2.9557-50.002 K)
- `fixed_energy_inelastic_q_series` scans=45 points=1319 confidence=high report=inelastic_dispersion_or_lineshape_report (E=1.0-33.0 meV; T=2.9585-2.9888 K)
- `constant_q_inelastic_energy_series` scans=38 points=901 confidence=high report=inelastic_dispersion_or_lineshape_report (E=-1.0-42.0 meV; T=2.956-2.9883 K)
- `alignment_or_rocking_scan` scans=13 points=318 confidence=high report=alignment_progress_report (T=2.9601-255.123 K)
- `alignment_or_rocking_scan` scans=4 points=58 confidence=high report=alignment_progress_report (T=49.705-247.0 K)
- `elastic_q_scan_or_reciprocal_space_map` scans=3 points=83 confidence=high report=reciprocal_space_or_detector_map_report (E=0.0-0.0 meV; T=2.9608-2.9886 K)
- `elastic_q_scan_or_reciprocal_space_map` scans=2 points=62 confidence=medium report=reciprocal_space_or_detector_map_report (E=0.0-0.0 meV; T=2.9603-2.9883 K)
- `alignment_tilt_scan` scans=2 points=34 confidence=medium report=alignment_progress_report (T=164.046-233.592 K)
- `alignment_slit_or_translation_scan` scans=2 points=33 confidence=medium report=alignment_progress_report (T=155.645-192.312 K)
- `alignment_slit_or_translation_scan` scans=2 points=26 confidence=medium report=alignment_progress_report (T=160.286-197.193 K)
- `alignment_slit_or_translation_scan` scans=2 points=20 confidence=medium report=alignment_progress_report (T=152.059-185.979 K)
- `alignment_tilt_scan` scans=2 points=17 confidence=medium report=alignment_progress_report (T=199.375-238.041 K)

Next steps are suggested based on previous measurements

What to do next

Next Actions

- [high] Draft a `inelastic_dispersion_or_lineshape_report` from the grouped scan families before sending a user update. p=0.843

  Basis: Uses the highest-probability report type inferred from scan-family counts.
- [medium] Overlay fixed-energy Q scans and check whether peak positions agree with constant-Q E scans. p=0.86

  Basis: Based on family `fixed_energy_inelastic_q_series` , confidence `high` , 136 scan(s), and 3701 parsed point(s).
- [medium] Overlay fixed-energy Q scans and check whether peak positions agree with constant-Q E scans. p=0.86

  Basis: Based on family `fixed_energy_inelastic_q_series` , confidence `high` , 45 scan(s), and 1319 parsed point(s).
- [high] Overlay E scans by Q point and temperature; extract tentative peak positions only after background and repeatability checks. p=0.94

  Basis: Based on family `constant_q_inelastic_energy_series` , confidence `high` , 38 scan(s), and 901 parsed point(s).
- [medium] Summarize peak centers, widths, and instrument/sample moves to decide if alignment is stable. p=0.86

  Basis: Based on family `alignment_or_rocking_scan` , confidence `high` , 13 scan(s), and 318 parsed point(s).
- [medium] Summarize peak centers, widths, and instrument/sample moves to decide if alignment is stable. p=0.82

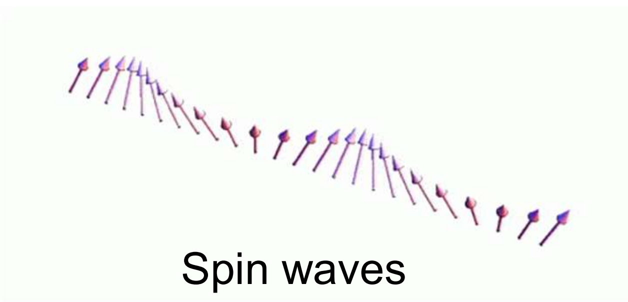
  Basis: Based on family `alignment_or_rocking_scan` , confidence `high` , 4 scan(s), and 58 parsed point(s).
- [medium] Check Q/angle coverage, detector mode, calibration requirements, and whether a map can be reconstructed without guessing. p=0.78

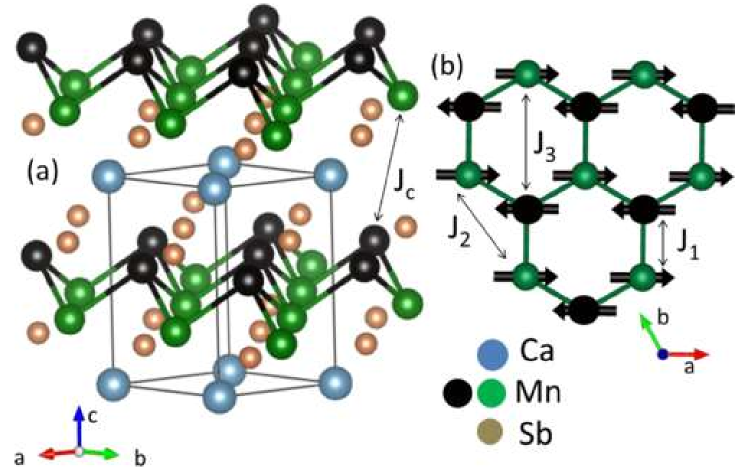
  Basis: Based on family `elastic_q_scan_or_reciprocal_space_map` , confidence `high` , 3 scan(s), and 83 parsed point(s).

Basis of suggestion

Priority

Calculate spin waves using known $CaMn_2Sb_2$ Hamiltonian

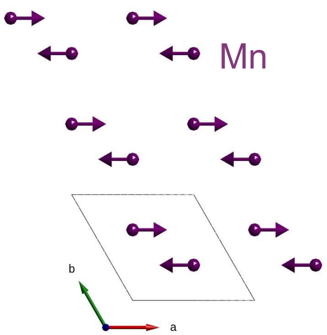




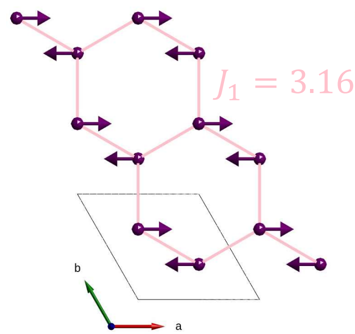
$$\mathcal{H} = \sum_{1NN} J_1 S_i \cdot S_j + \sum_{2NN} J_2 S_i \cdot S_j + \sum_{CNN} J_c S_i \cdot S_j$$

McNally et al., Phys. Rev. B 91, 180407(R), 2015.

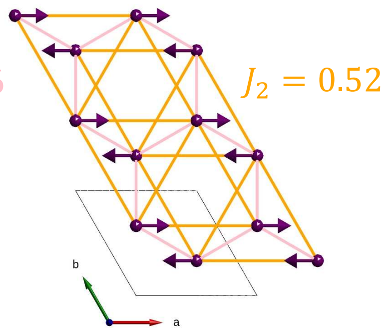
Magnetic interactions produce magnon dispersion



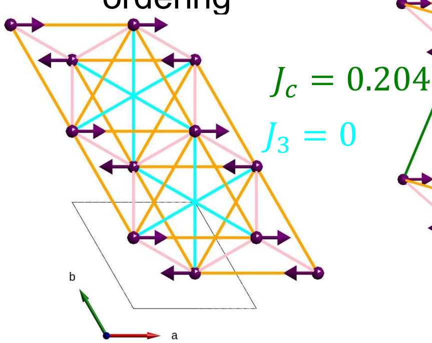
Néel antiferromagnetic ordering



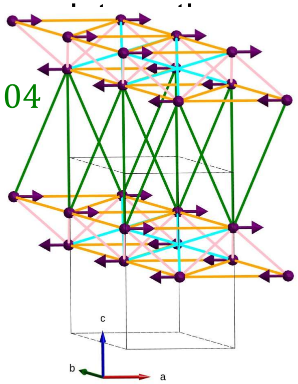
First nearest neighbor



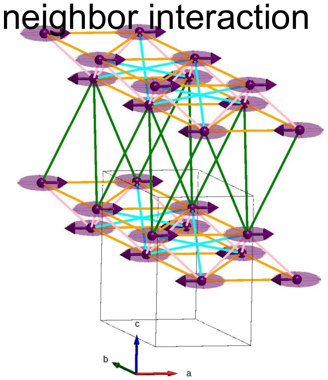
Second nearest neighbor interaction



Third nearest neighbor interaction



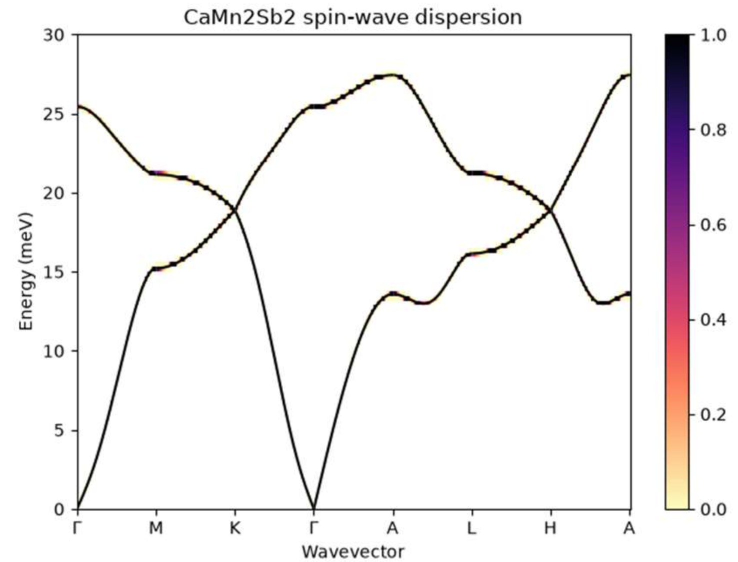
Out-of-plane nearest neighbor interaction



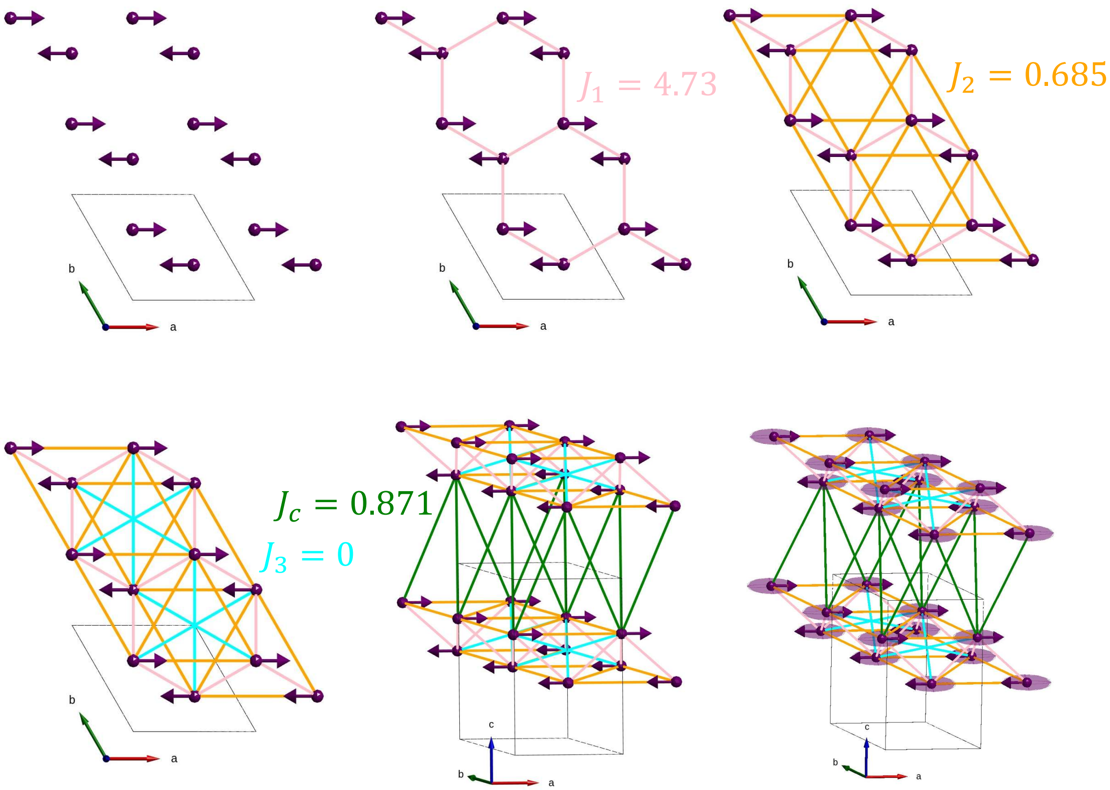
Easy-plane anisotropy

Hamiltonian describes total energy

$$\mathcal{H} = \sum_{1NN} J_1 S_i \cdot S_j + \sum_{2NN} J_2 S_i \cdot S_j + \sum_{CNN} J_c S_i \cdot S_j$$

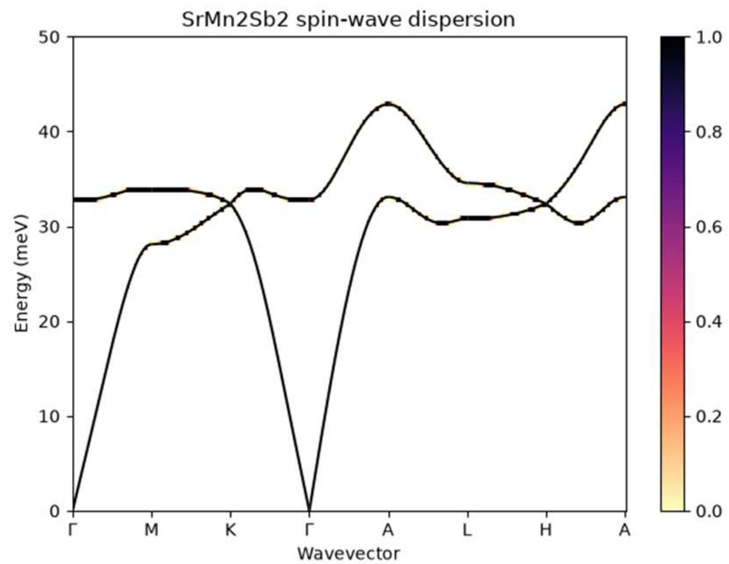


$SrMn_2Sb_2$ has similar magnetic interactions

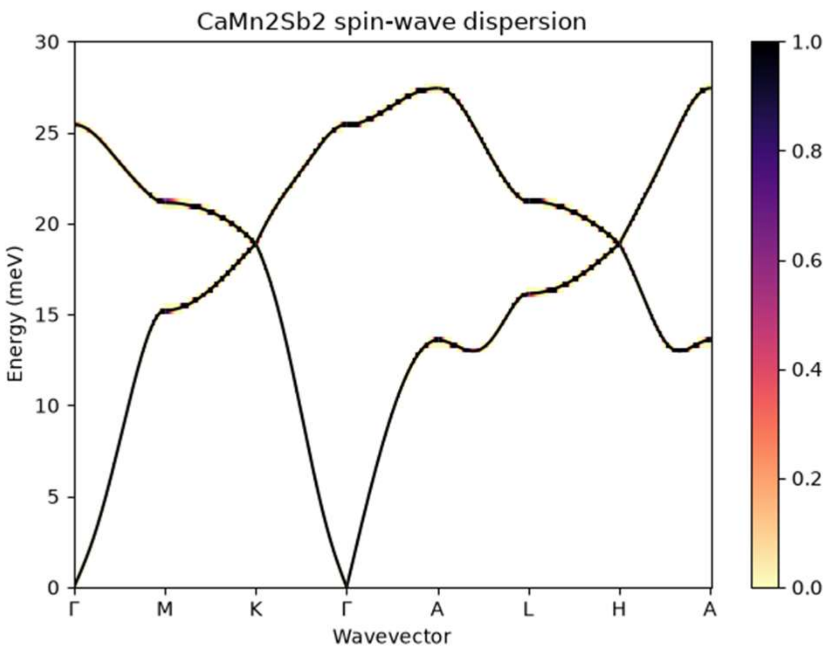


Hamiltonian describes total energy

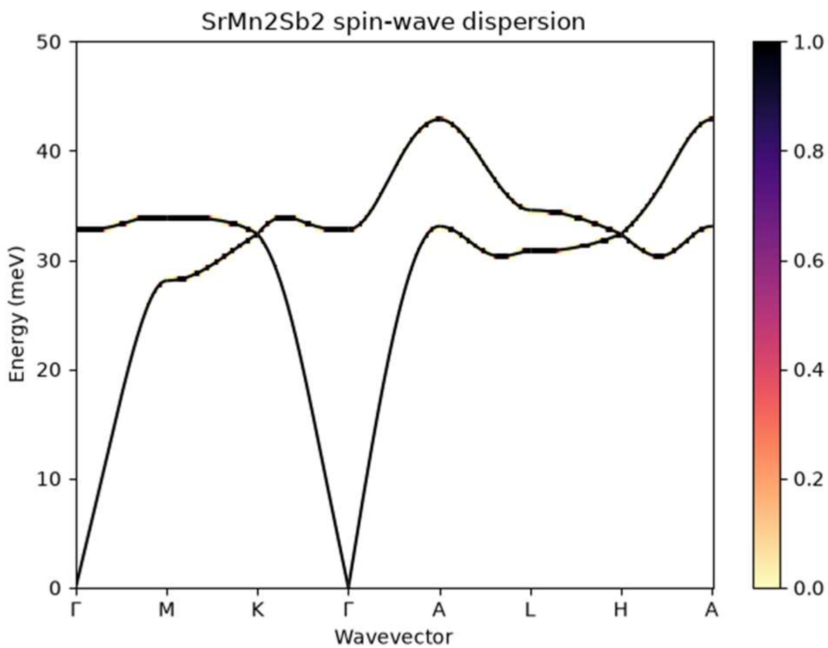
$$\mathcal{H} = \sum_{1NN} J_1 S_i \cdot S_j + \sum_{2NN} J_2 S_i \cdot S_j + \sum_{CNN} J_c S_i \cdot S_j$$



Distance and angle between magnetic atoms determine strengths of interactions



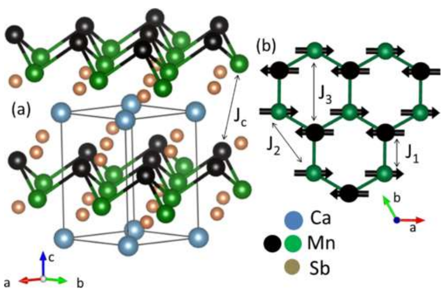
a = 4.5285(4) Å α = 90°
b = 4.5285(4) Å β = 90°
c = 7.4453(7) Å γ = 120°



a = 4.5888(2) Å α = 90°
b = 4.5888(2) Å β = 90°
c = 7.7529(4) Å γ = 120°

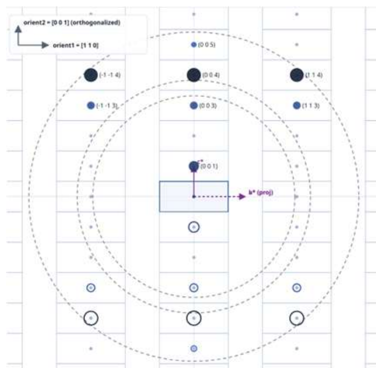
TAS Copilot assists users with experiment planning and experiment analysis

Evidence

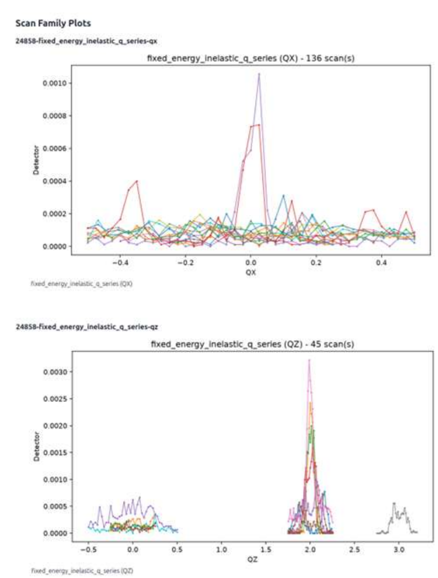


$$\mathcal{H} = \sum_{1NN} J_1 S_i \cdot S_j + \sum_{2N} J_2 S_i \cdot S_j + \sum_{CNN} J_c S_i \cdot S_j$$

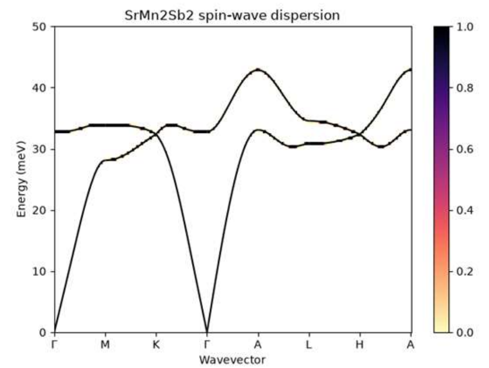
Alignment



Measurement summaries and suggestions



Analysis



Future directions

Publish paper outlining TAS Copilot

↓

Visiting researchers use TAS Copilot at the NCNR!

↓

Expand to other instruments/facilities

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The Fishbowl™ and Shark Tank

Thank you!

Photo by Yiming Qiu

(002) alignment

$$\boldsymbol{n\lambda = 2d\sin\theta}$$

Primary scattering: $n = 1$

Pyrolytic graphite (PG) filter removes higher order wavelength contamination

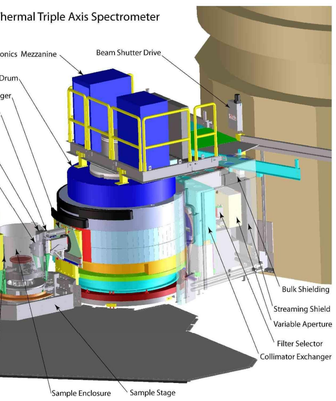
$$\boldsymbol{n\lambda = 2d\sin\theta}$$

Higher order Bragg peaks observed: $n = 2, 3, \ldots$

Removing the PG filter allows for neutrons with $\frac{\lambda}{2}$

Measure at a lower 2θ, which makes the measurement less sensitive to tilt

Triple-axis spectrometer (TAS)



Neutron source