

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

Carina Jacobson

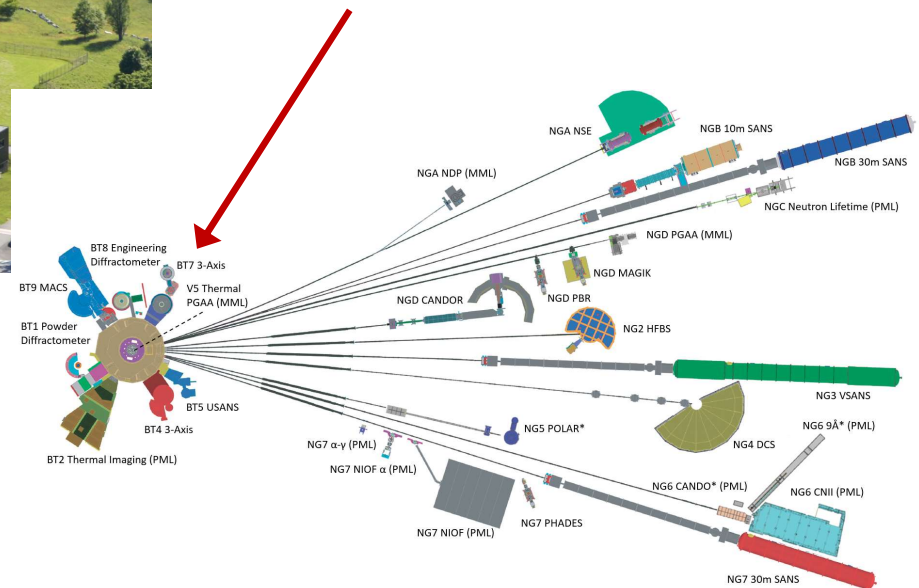
Purdue University

Mentor: Dr. William Ratcliff

NIST Center for Neutron Research (NCNR)

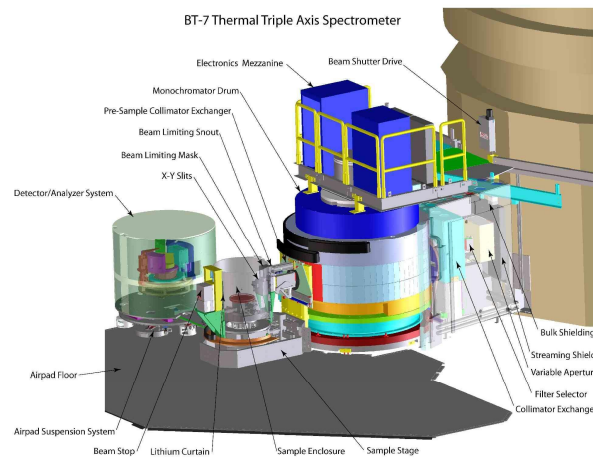


BT-7 triple-axis spectrometer

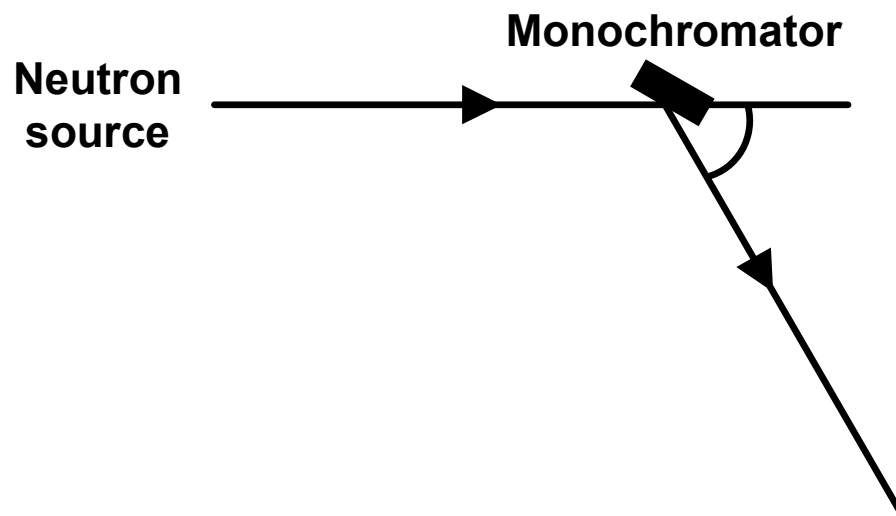


Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample

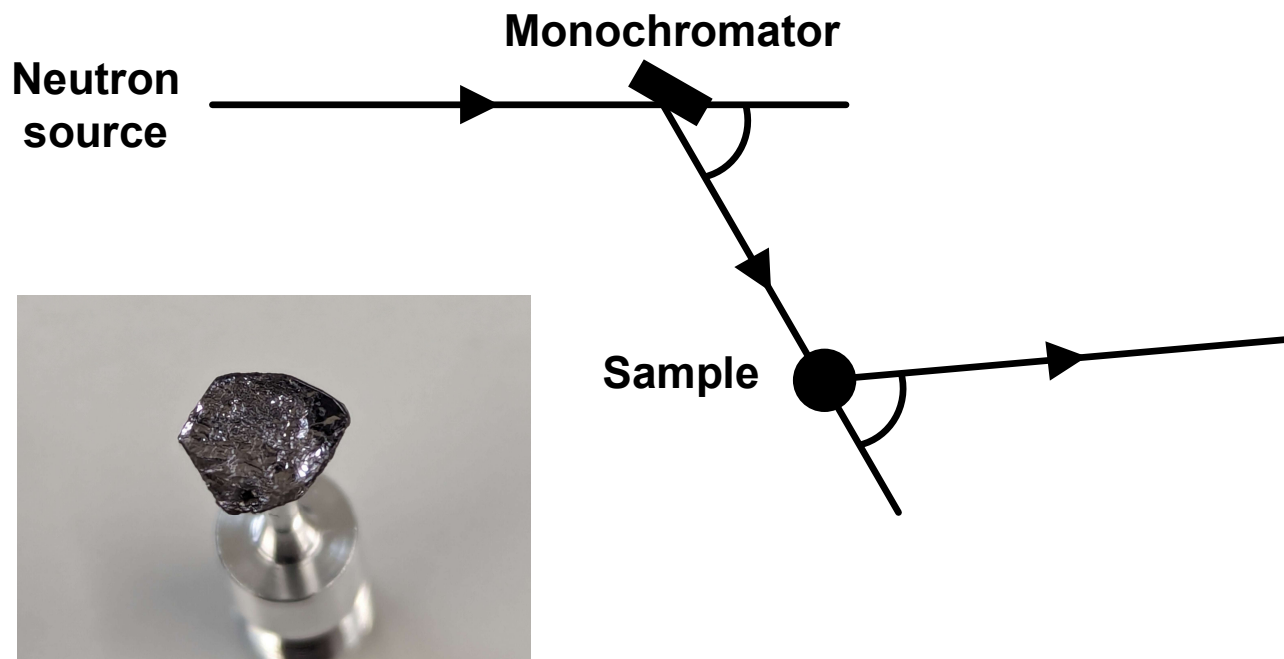
**Neutron
source**



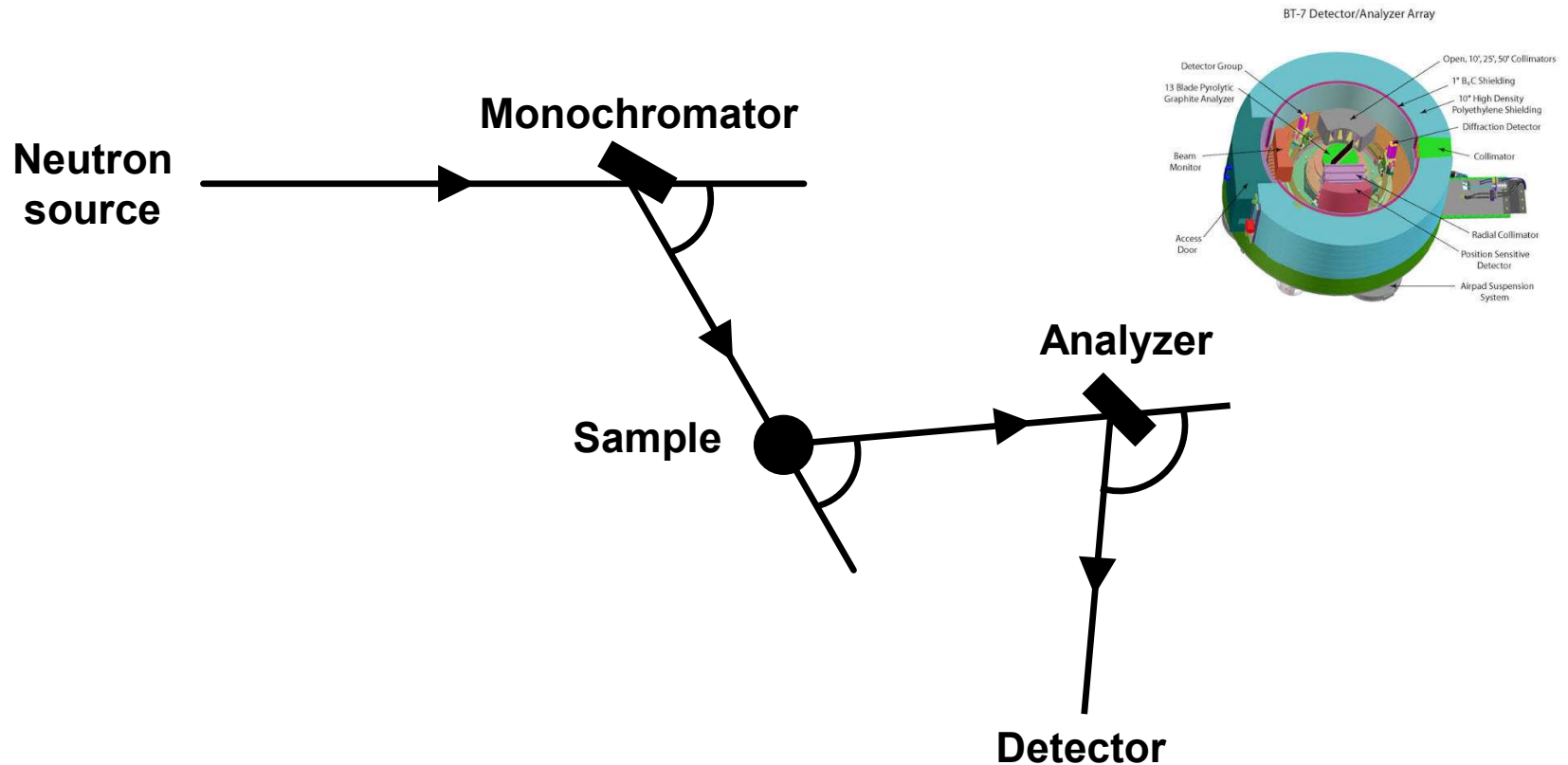
Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample



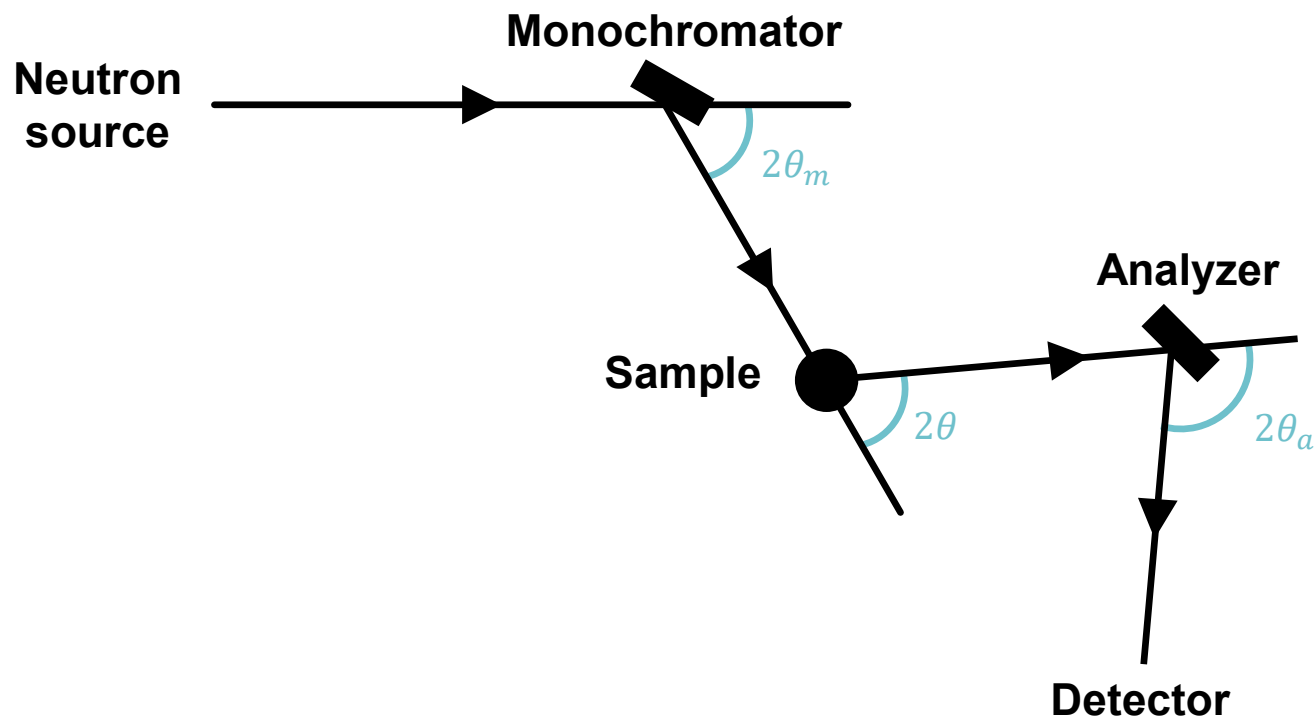
Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample



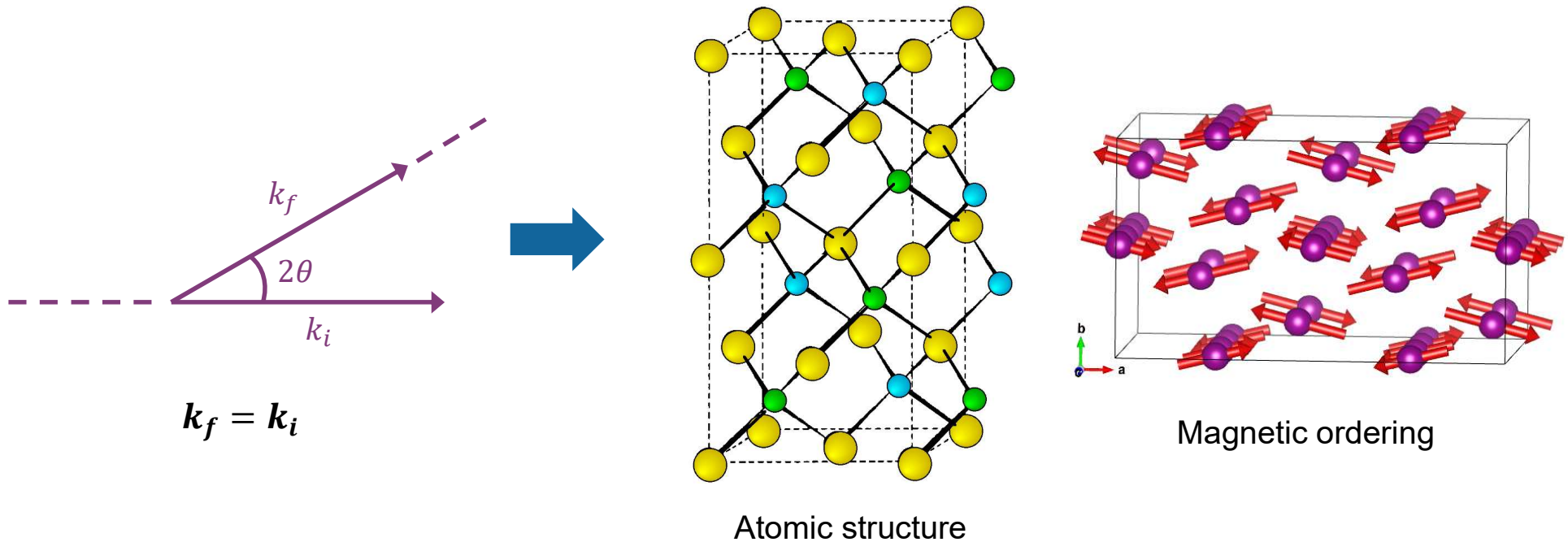
Triple-axis spectrometer (TAS) selects wavelengths of neutrons before and after the sample



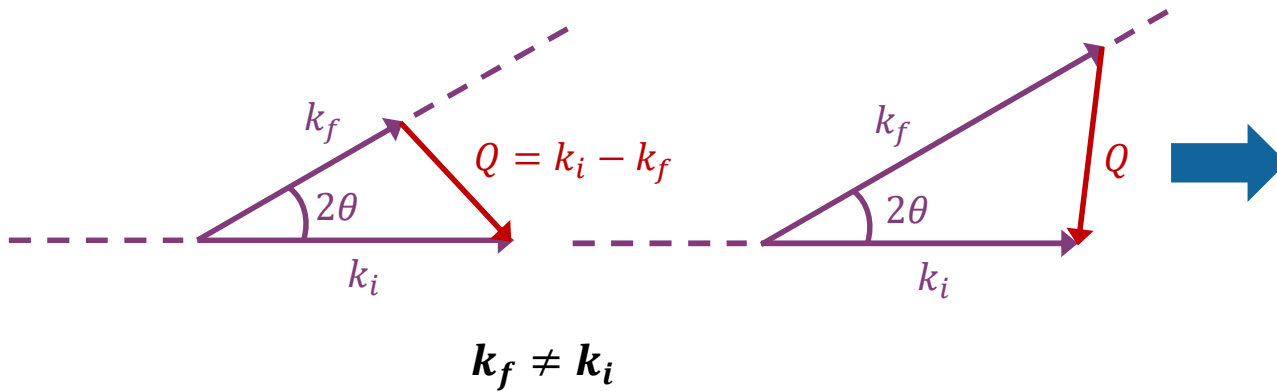
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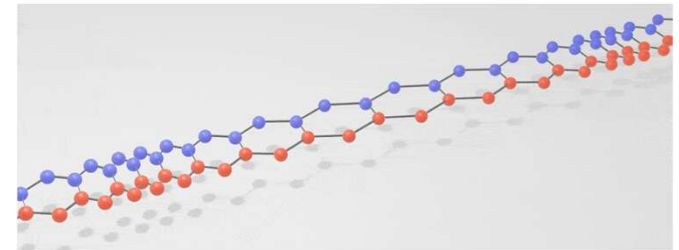
Elastic neutron scattering measures static properties



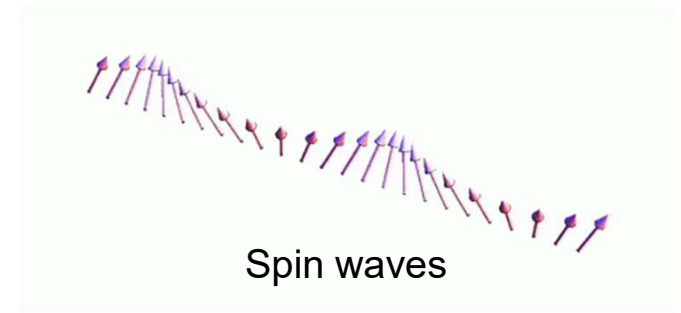
Inelastic neutron scattering measures dynamic properties



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 ($\text{R} = \text{Pr, Nd, Tb, Dy, Ho, and Yb}$)

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}

^a NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, 20899, USA

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^e, Jarvist M. Frost^e, Hemamala I. Karunadasa^a, Aron Walsh^{f,g}, Michael E. Toney^{b,h}

Neutron spin resonance as a probe of superconducting gap anisotropy in partially detwinned electron underdoped $\text{NaFe}_{0.985}\text{Co}_{0.015}\text{As}$

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

Large anomalous Hall effect in a half-Heusler antiferromagnet

T. Suzuki¹, R. Chisnell², A. Devarakonda¹, Y.-T. Liu¹, W. Feng³, D. Xiao⁴, J. W. Lynn² and J. G. Checkelsky^{1*}

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. Lynn²

Magnetic order in $\alpha\text{-RuCl}_3$: 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,*}

¹Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario, Canada M5S 1A7

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³Department 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)

Nonreciprocal Magnons and Symmetry-Breaking in the Noncentrosymmetric Antiferromagnet

G. Gietgeatpong,^{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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⁶IMRAM, Tohoku University, Sendai, Miyagi 980-8577, Japan

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Absence of Magnetic Field Dependence of the Anomalous Bond-Stretching Phonon in $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$

D. Reznik¹ · D. Parshall² · S. R. Park³ · J. W. Lynn² · Th. Wolf⁴

How do you begin a TAS experiment?

Magnetic structures of rare earth intermetallic compounds RCuAs_2 ($\text{R} = \text{Pr, Nd, Tb, Dy, Ho}$)

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^aNIST Center for Neutron Res

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Institute of Nano Science and T

Chenglin Zhang

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antiferro

T. Suzuki¹, R. Chisnell², A. Devarakonda¹, Y.-T. Liu¹, W. Feng³, D. Xiao⁴, J. W. Lynn²

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Symme

Nicholas P. Butch,^{1,2,3,*} M

Magnetic order in d

J. A. Sears,¹ M. Sor

¹Depart

²NIST Center for

³Department o

```
#Filename fpx841078
#Date 2018-05-25 15:17:52 EDT
#InstName BT7
#Epoch 1527275872.98
#ExptID 24858
#ExptName Spin Dynamics in SrMn2Sb2
#ExptParticipants Likh Poudel, Jef Lynn
#ExptDetails CCR-20
#ExptComment Ef 28
#User lnp2
#Comment
#Npoints 21
#TemperatureUnits Kelvin
#Ncolumns 98
#DetectorDims
#Signal 9 Detector
#Reference 6 Time
#ScanType Find Peak Scan
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#ScanRanges: 12 A3
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#FixedE E1 1
#Lattice 4.58947 4.58947 7.7189 90 90 120
#Orient 1 1 0 0 0 1
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#AnaSpacing 3.35416
#UBEnabled 0
#MonoVertiFocus SAGITTAL
#MonoHorizFocus FLAT
#AnalyzerDetectorMode 2 SingDetFlat
```

A4	Time	Temp	Monitor	Detector	DFMRot	A2	A3	A5
35.439	1	233.592	1563	163	20.5885	41.177	109.899	20.5885
35.439	1	233.17	1603	281	20.5885	41.177	109.899	20.5885
35.439	1	232.748	1554	413	20.5885	41.177	109.899	20.5885
35.439	1	232.321	1623	509	20.5885	41.177	109.899	20.5885
35.439	1	231.901	1539	601	20.5885	41.177	109.899	20.5885
35.439	1	231.479	1566	728	20.5885	41.177	109.899	20.5885
35.439	1	231.061	1625	845	20.5885	41.177	109.899	20.5885
35.439	1	230.644	1484	984	20.5885	41.177	109.899	20.5885
35.439	1	230.225	1604	1071	20.5885	41.177	109.899	20.5885
35.439	1	229.81	1598	1240	20.5885	41.177	109.899	20.5885
35.439	1	229.396	1573	1324	20.5885	41.177	109.899	20.5885
35.439	1	228.981	1614	1499	20.5885	41.177	109.899	20.5885
35.439	1	228.567	1587	1530	20.5885	41.177	109.899	20.5885
35.439	1	228.158	1592	1551	20.5885	41.177	109.899	20.5885
35.439	1	227.744	1558	1529	20.5885	41.177	109.899	20.5885
35.439	1	227.329	1524	1501	20.5885	41.177	109.899	20.5885
35.439	1	226.916	1577	1348	20.5885	41.177	109.899	20.5885

Acoustic Phonon Lifetimes Limit Thermal

onium Lead

^a, Ian C. Smith^a, Dan Parshall^c,

^b, Michael E. Toney^{b,1}

LuFeO_3

Dylan Quintana⁴,

William Ratcliff II¹

Nonreciprocal Magnons and Symm

Antif

```
23-May 13:32:53>
Device Soft Hard
Temp: 68.777 68.777
23-May 13:34:03> findpeak A4 4.0 0.2 Time 1.0 Detector -bragg A3 -func Gauss
23-May 13:34:03> Queued: findpeak A4 4.0 0.2 Time 1.0 Detector -bragg A3 -func Gauss (Queued Id=16)
23-May 13:34:03> Device [A3] will move with [A4]
23-May 13:34:04> User ncnr: A4 Data [FindPeak started]
23-May 13:34:04> Find Peak
23-May 13:34:04> Constant devices: None
23-May 13:34:21> move temp 50 (Queued Id=17)
23-May 13:34:21> Queued: move temp 50 (Queued Id=17)
23-May 13:34:24> Creating file /usr/local/ice/usr/24858/data/fpx840997.bt7
23-May 13:34:29> A4=15.9064 A3=97.753 Det=5 Mon=1536 Time=1 Temp=59.992
23-May 13:34:38> A4=15.7064 A3=97.8532 Det=4 Mon=1589 Time=1 Temp=59.041
23-May 13:34:47> A4=15.9064 A3=97.9532 Det=3 Mon=1553 Time=1 Temp=58.114
23-May 13:34:47> move A3 127.496671556 A4 74.9933431111 (Queued Id=18)
23-May 13:34:47> Queued: move A3 127.496671556 A4 74.9933431111 (Queued Id=18)
23-May 13:34:56> A4=16.1064 A3=98.053 Det=6 Mon=1538 Time=1 Temp=57.148
23-May 13:34:57> Kill
23-May 13:34:57> User ncnr: Kill received: stopping all motors!
23-May 13:34:57> Dip found at 15.9064 with an intensity of 3
23-May 13:34:57> Fit Results: BG = 5.5
Height = -2.5
Pos = 15.9064
Width = 2.37825
Chi^2/dof = 0
23-May 13:34:57> Ready to drive to fit position [A4= 15.9064 A3= 98.0263].
23-May 13:34:57> Lattice parameter [ 8.52463].
23-May 13:34:57> User ncnr: Abort sent to all moving devices
```

Detector
35
45
56
105
271
716
1621
3576
6144
7734
8086
6597
3638
1304
375
123
72
44
28
36
21

(Received 13 November 2014; revised manuscript received 8 April 2015; published 24 April 2015)

Th. Wolf

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Magnetic structures of rare earth intermetallic compounds RCuAs ($\text{R} = \text{Pr, Nd, Tb, Dy}$)

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^aNIST Center for Neutron Research, USA

^bDepartment of Chemistry, Institute of Nano Science and

Neutron spin Hall effect in antiferromagnetic Fe_2O_3

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Magnetic order in $\alpha\text{-RuCl}_3$: A honeycomb-lattice quantum spin liquid

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Thermal expansion of PbTe

Smith^a, Dan Parshall^a, Michael E. Toney^{a,b,1}

^aQuintana⁴, Ratcliff II¹

and K. Matan^{1,2,*}

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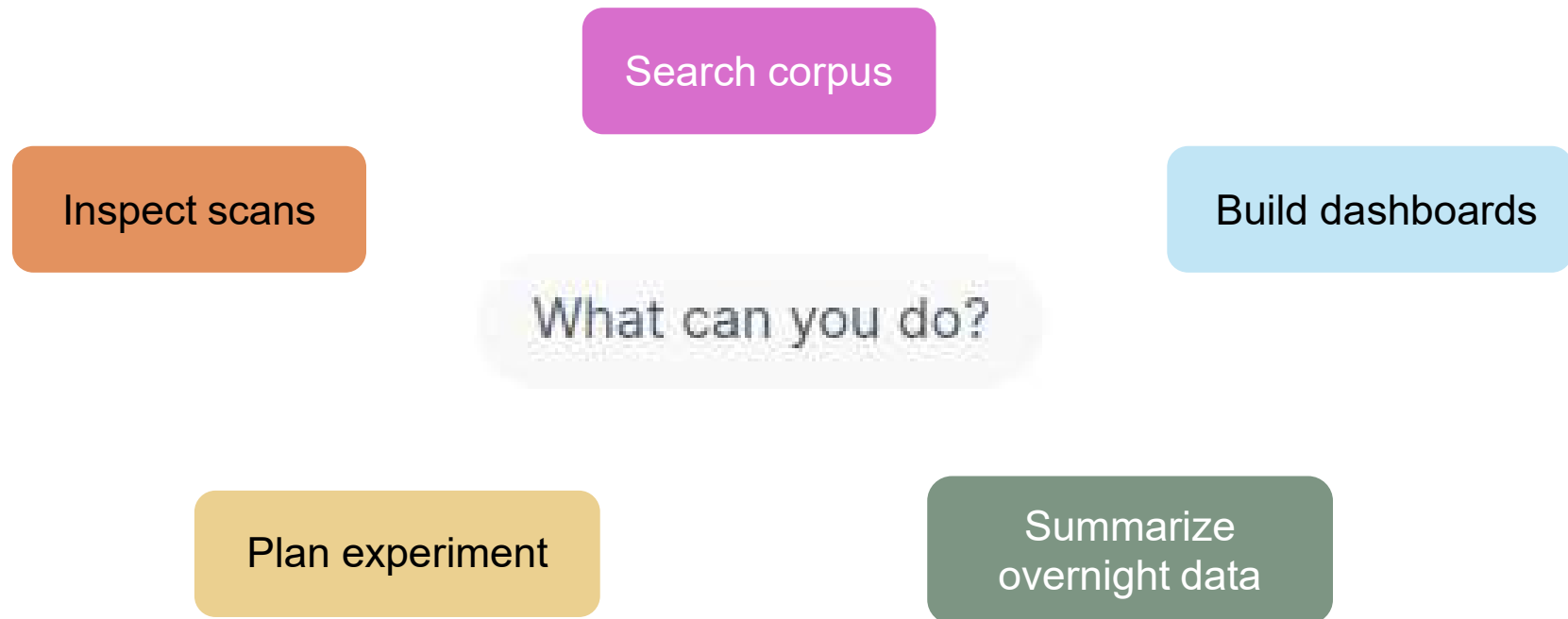
^aQuintana⁴, Ratcliff II¹

and K. Matan^{1,2,*}

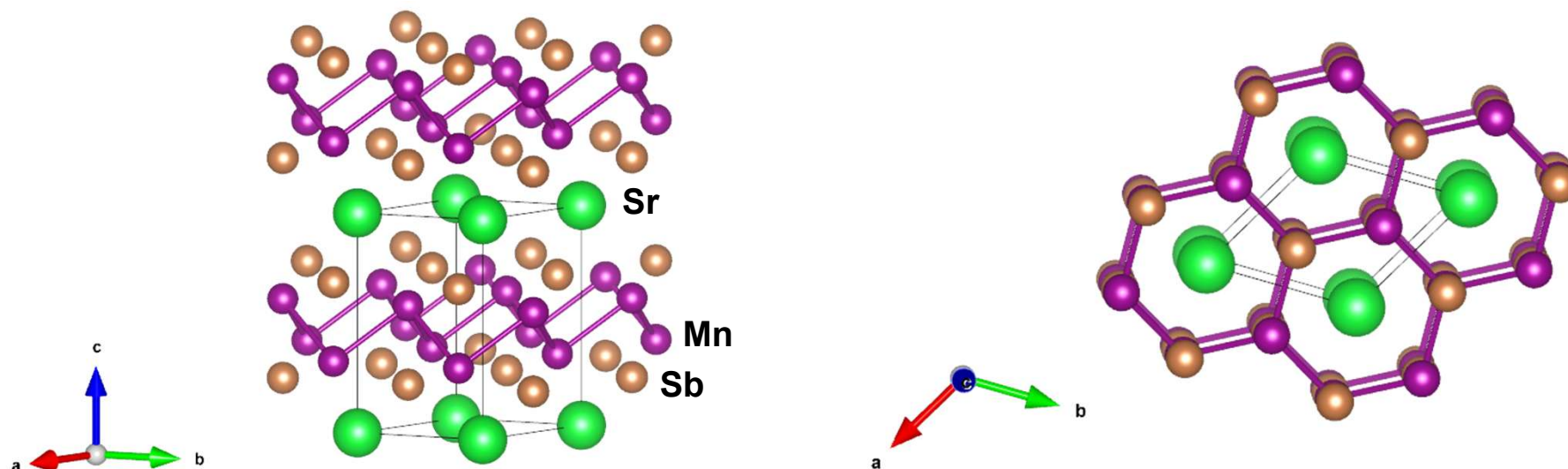
How do you begin a TAS experiment?

TAS Copilot

TAS Copilot centralizes evidence and calls tools for more efficient experiments



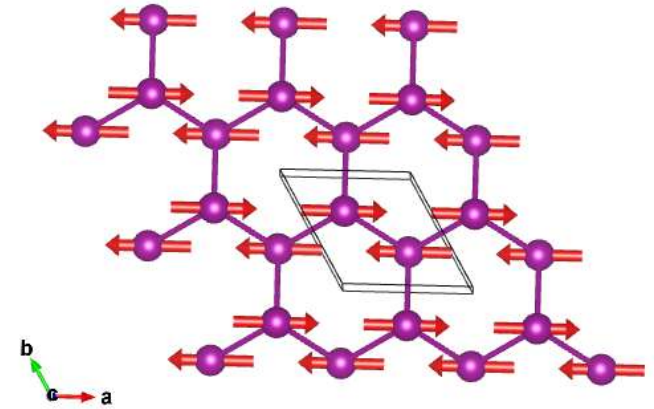
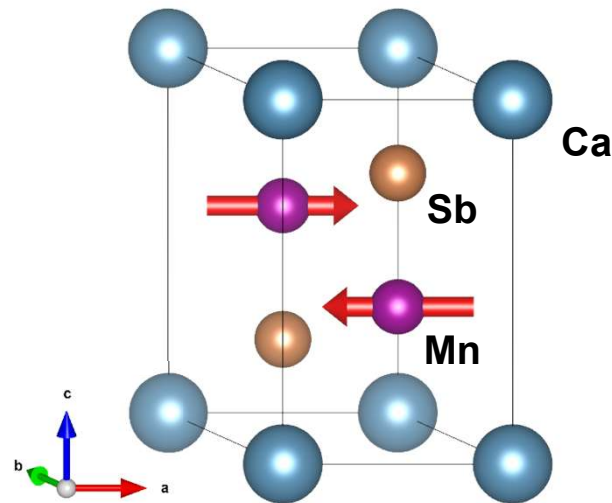
Case study for TAS Copilot workflow



Use extracted facts from a similar material

Use CaMn_2Sb_2 as a model for SrMn_2Sb_2

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

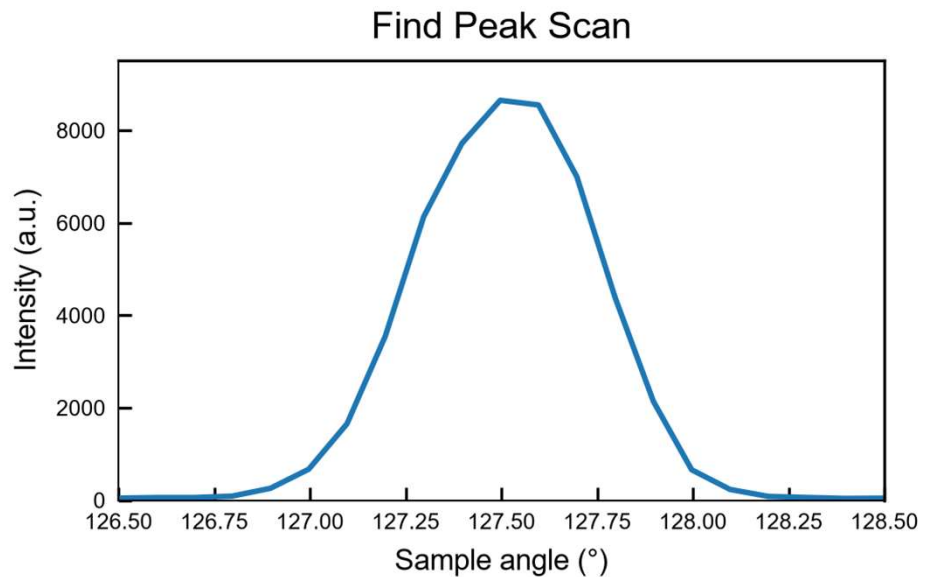
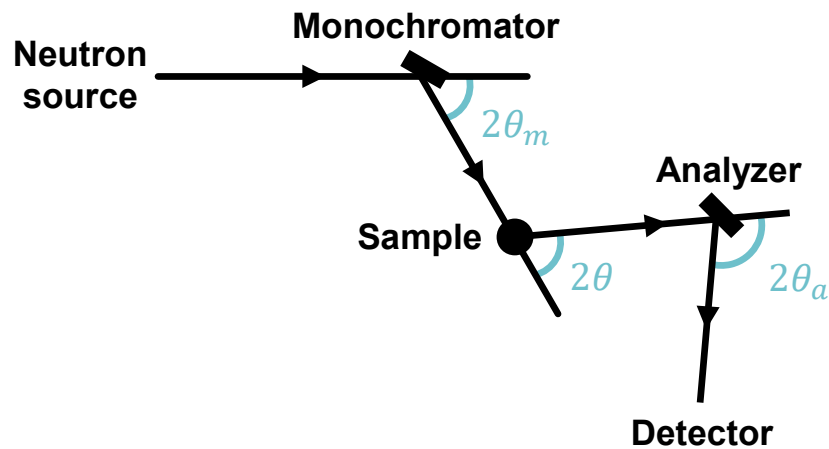


Align TAS via Bragg peaks

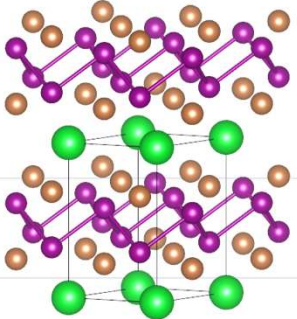
Bragg's Law: $n\lambda = 2d \sin \theta$

Bragg angle θ

Scattering angle 2θ



Choose peaks based on structure and instrument configurations



1. Structure (CIF)

Choose File

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

2. Plane, Energy, Environment

Final energy

Sample environment

Environment

Calculate

Scattering plane

Orient 1 (H K L)

Orient 2 (H K L)

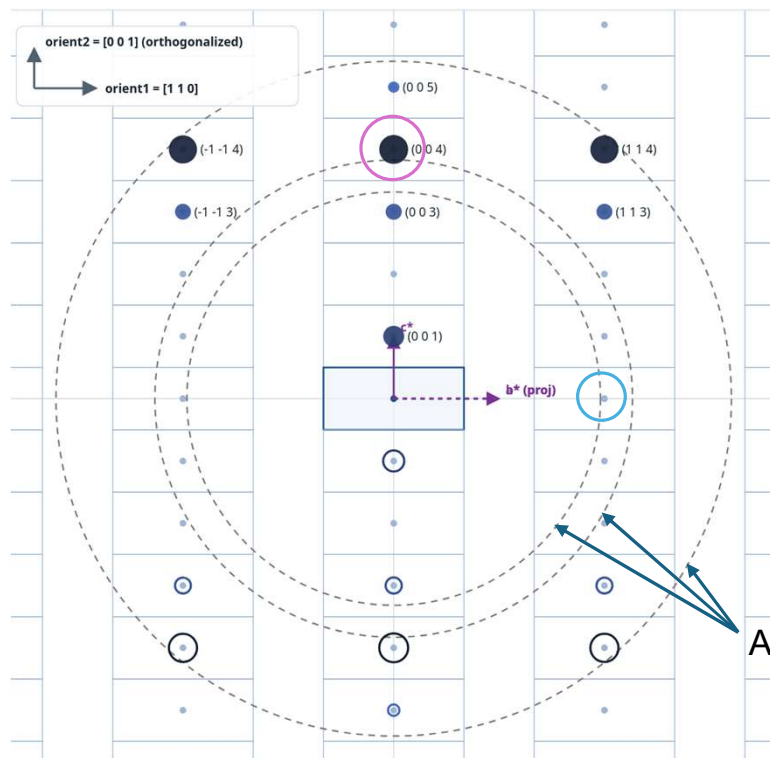
Ef (meV)

Aluminum

Copper

Orient 1 (H K L)			Orient 2 (H K L)			Ef (meV)	Environment
1	1	0	0	0	1	14.7	☒ Aluminum ☐ Copper

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

Aluminum rings

Suggested scan plans improve alignment efficiency

What scans should I try first for alignment?



Scan plan suggestions:

- A3 – sample rotation
- A4 – scattering angle
- Tilt
- Translation

Experimental alignment corresponds with suggested alignment

Scattering angle (2θ)

Sample rotation angle

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

(110)

(004) and (110) define plane

(004)

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

Type of scan

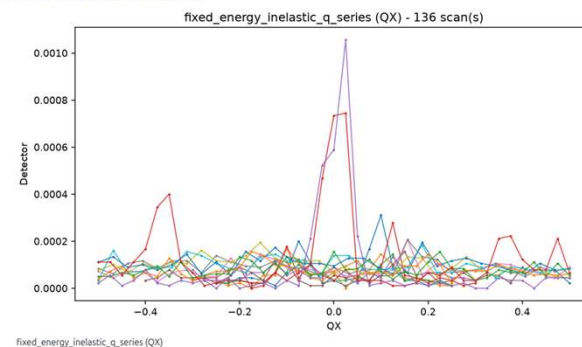
Scan Families

- `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)

Ranges measured

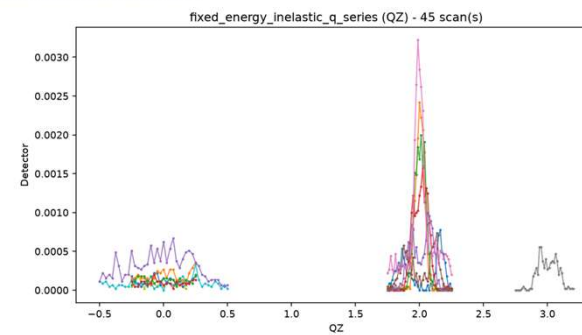
Scan Family Plots

24858-fixed_energy_inelastic_q_series-qx



fixed_energy_inelastic_q_series (QX)

24858-fixed_energy_inelastic_q_series-qz



fixed_energy_inelastic_q_series (QZ)

Next steps are suggested based on previous measurements

What to do next

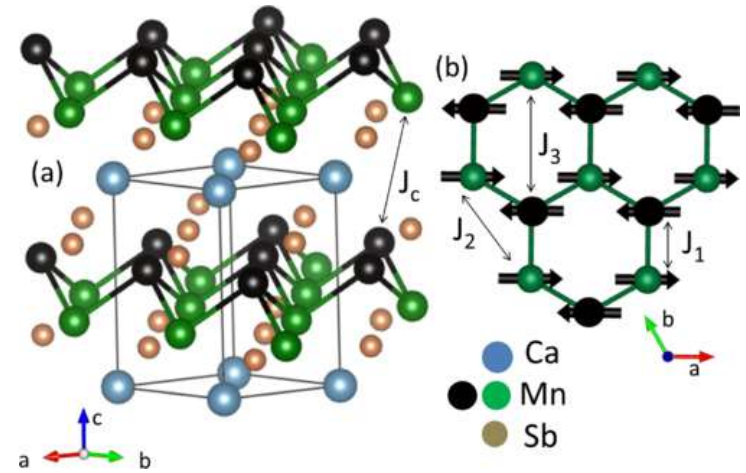
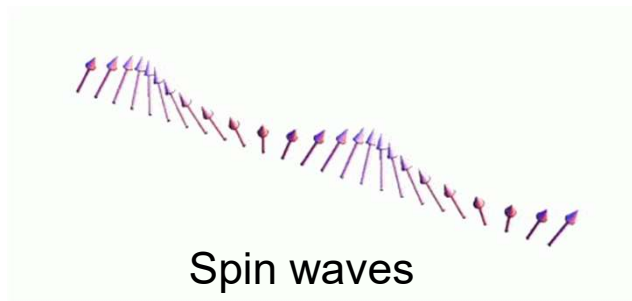
Next Actions

- [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).

Priority

Basis of suggestion

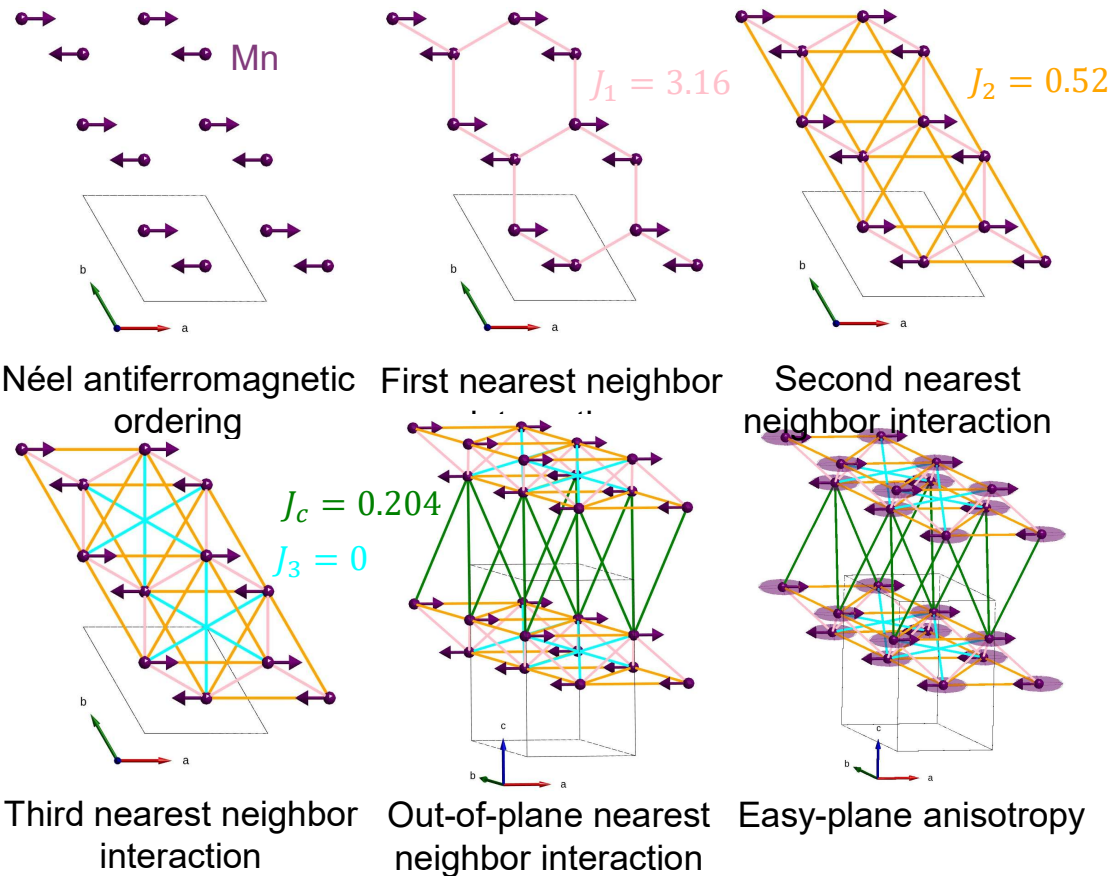
Calculate spin waves using known CaMn_2Sb_2 Hamiltonian



$$\mathcal{H} = \sum_{1NN} J_1 \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{2NN} J_2 \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{cNN} J_c \mathbf{S}_i \cdot \mathbf{S}_j$$

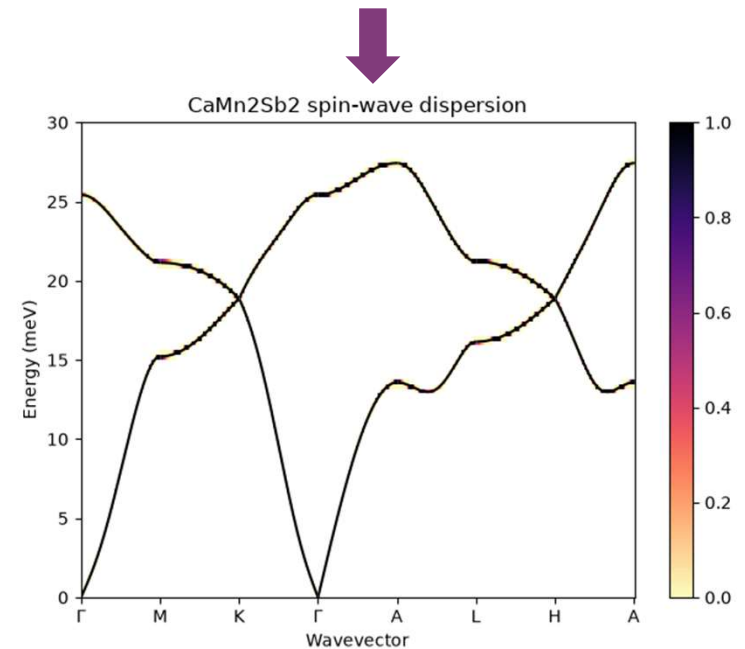
McNally et al., Phys. Rev. B 91, 180407(R), 2015.

Magnetic interactions produce magnon dispersion

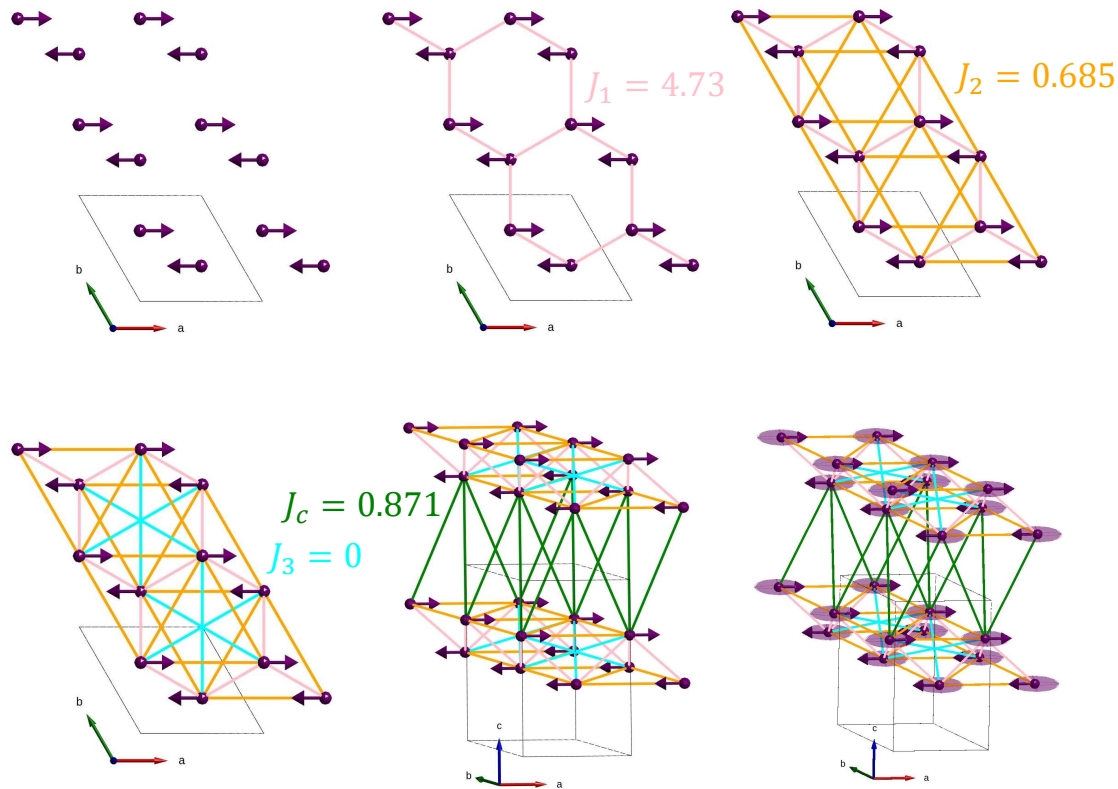


Hamiltonian describes total energy

$$\mathcal{H} = \sum_{1NN} J_1 \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{2NN} J_2 \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{CNN} J_c \mathbf{S}_i \cdot \mathbf{S}_j$$

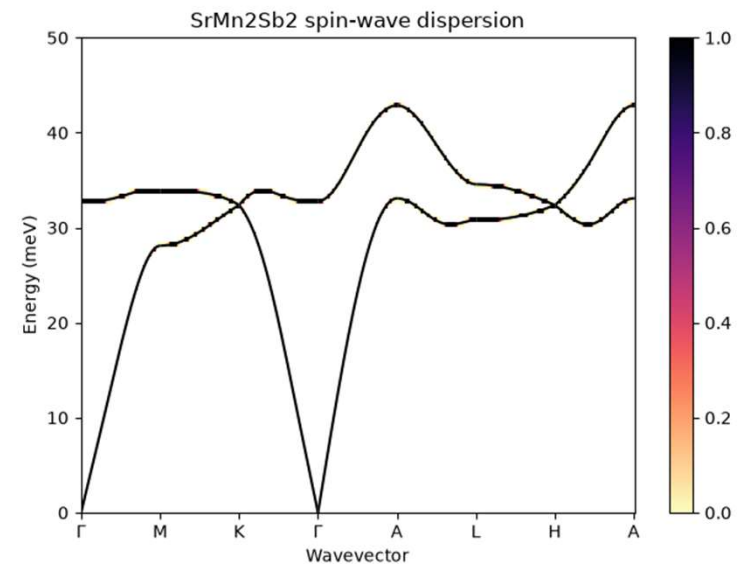


SrMn₂Sb₂ has similar magnetic interactions

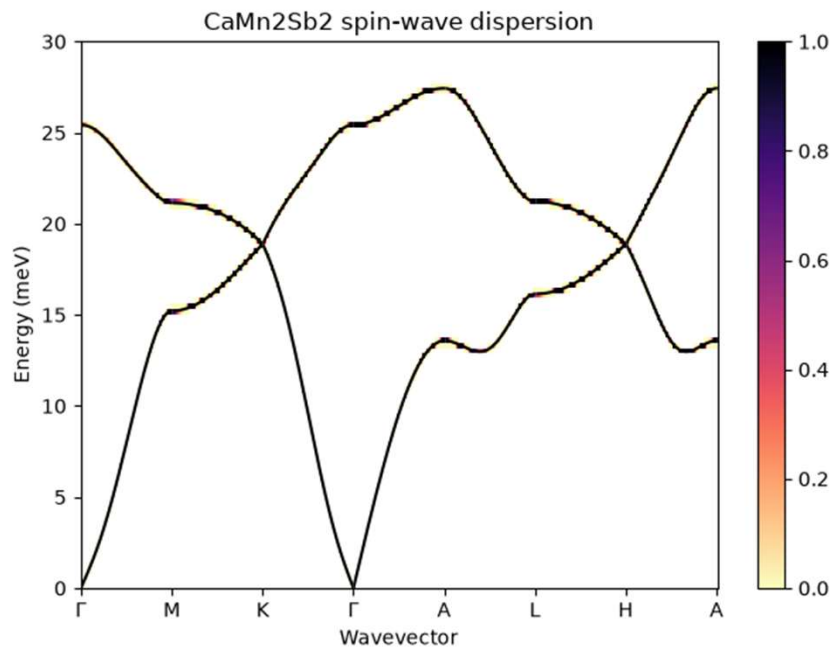


Hamiltonian describes total energy

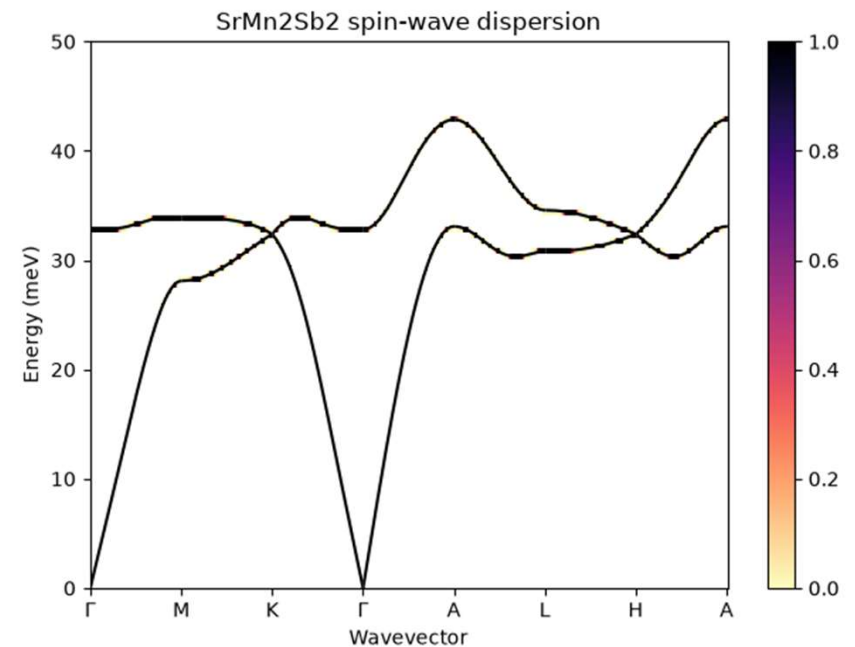
$$\mathcal{H} = \sum_{1NN} J_1 \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{2NN} J_2 \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{CNN} J_c \mathbf{S}_i \cdot \mathbf{S}_j$$



Distance and angle between magnetic atoms determine strengths of interactions



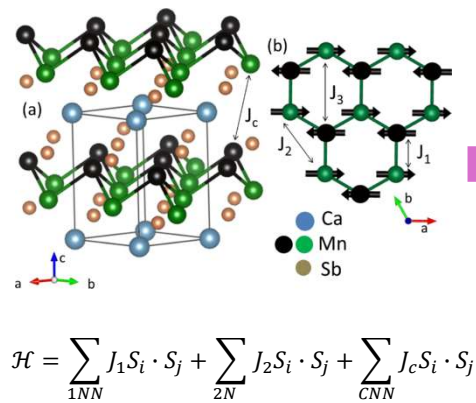
$$\begin{aligned} a &= 4.5285(4) \text{ \AA} & \alpha &= 90^\circ \\ b &= 4.5285(4) \text{ \AA} & \beta &= 90^\circ \\ c &= 7.4453(7) \text{ \AA} & \gamma &= 120^\circ \end{aligned}$$



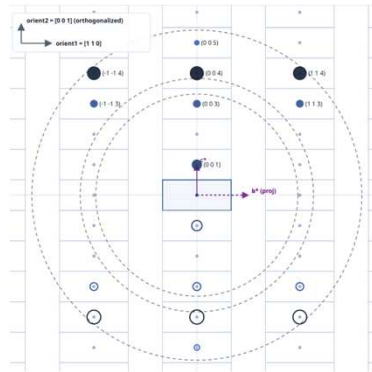
$$\begin{aligned} a &= 4.5888(2) \text{ \AA} & \alpha &= 90^\circ \\ b &= 4.5888(2) \text{ \AA} & \beta &= 90^\circ \\ c &= 7.7529(4) \text{ \AA} & \gamma &= 120^\circ \end{aligned}$$

TAS Copilot assists users with experiment planning and experiment analysis

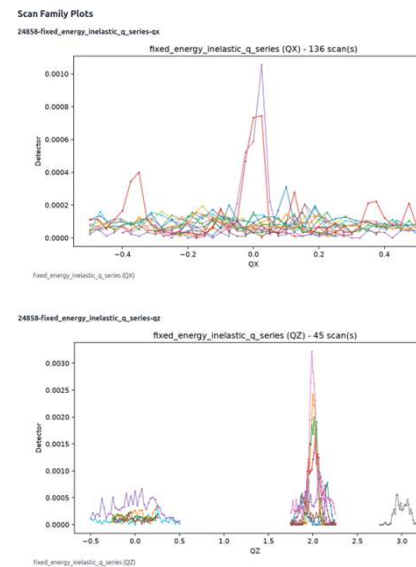
Evidence



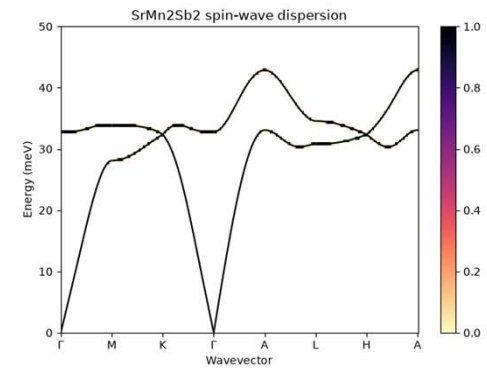
Alignment



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



Any mention of commercial products is for information only; it does not imply recommendation or endorsement by NIST.

(002) alignment

$$n\lambda = 2d \sin \theta$$

Primary scattering: $n = 1$

Pyrolytic graphite (PG) filter
removes higher order
wavelength contamination

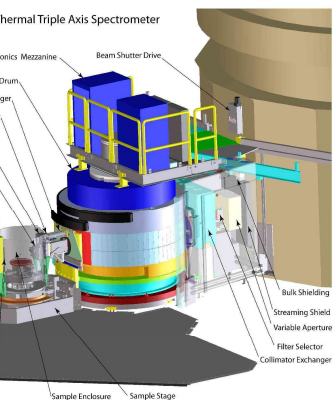
$$n\lambda = 2d \sin \theta$$

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

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



Monochromator

Sample

Analyzer

Detector

