OAK RIDGE National Laboratory

Spectroscopy Suite:

Overview and Strategy

Spectroscopy Suite Review, September 17th, 2020

Mark Lumsden

Spectroscopy Group Leader
Neutron Scattering Division

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

U.S. DEPARTMENT OF ENERGY

Spectroscopy Group

Mark Lumsden, Group Leader
Sharon Porter, Admin

Chemical Spectroscopy

BASIS & VISION

Timmy Ramirez-Cuesta, Lead
Luke Daemen
BASIS
Yongqiang Cheng
Niina Jalarvo
Naresh Osti
Matthew Ryder
Raphael Balderas*
Murillo Martins

Direct Geometry Spectroscopy

ARCS, SEQUOIA, CNCS, & HYSPEC

Doug Abernathy, Lead
Ovidiu Garlea
Garrett Granroth
Sasha Kolesnikov
Daniel Pajerowski
Andrey Podlesnyak
Andrei Savici
Matthew Stone
Barry Winn
Anjana Samarakoon*
Allen Scheie*
Tao Xie*

Triple-Axis Spectroscopy

HB-1A, HB-1, HB-3, & CTAX

Jaime Fernandez-Baca, Lead
Adam Aczel
Songxue Chi
Tao Hong
Masa Matsuda
Wei Tian
Travis Williams
Fei Li*
Depei Zhang*

Large Scale Structures Group

Volker Urban, Group Leader
Katerra Sweat, Admin

SANS / Spin Echo

NSE

William Heller, Lead
Laura Stingaciu
Piotr Zolnierczuk
(Only listing Spin Echo staff)

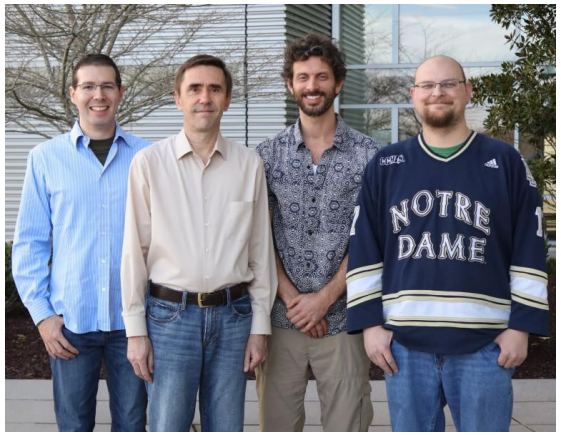
Direct Geometry Spectroscopy

SNS BL-18 (ARCS)

Doug Abernathy
Garrett Granroth
Rick Goyette (SA)

Thermal Chopper Spectrometer
with large solid angle coverage

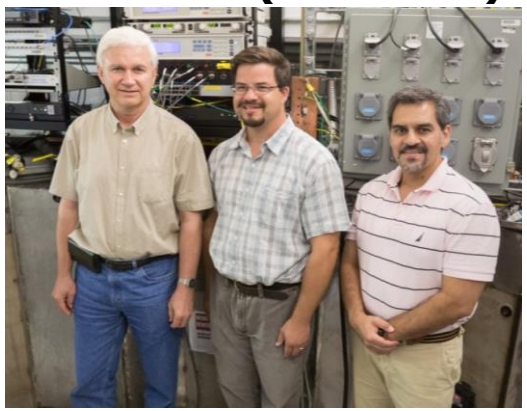
SNS BL-5 (CNCS)



Cold Neutron Chopper
Spectrometer

Daniel Pajerowski
Andrei Podlesnyak
Chris Schmitt (SA)

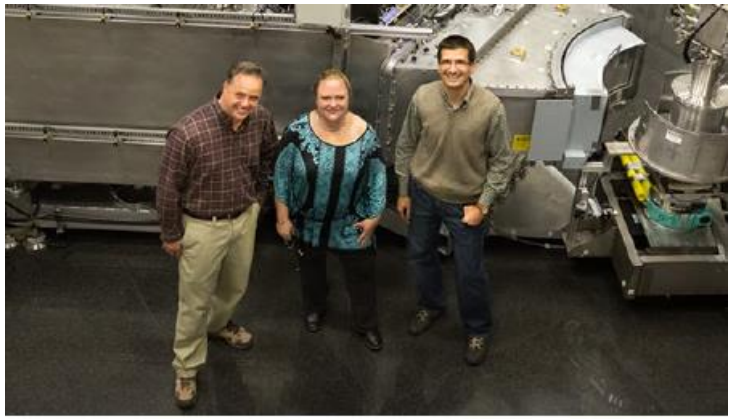
SNS BL-17 (SEQUOIA)



Matthew Stone
Sasha Kolesnikov
Victor Fanelli (SA)

Thermal Chopper Spectrometer
with fine Q and ω resolution

SNS BL-14B (HYSPEC)

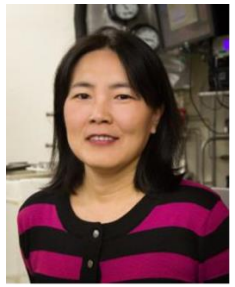


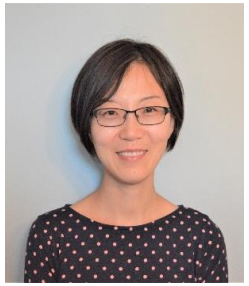
Barry Winn
Ovidiu Garlea
Melissa Graves-Brook (SA)

Versatile cold neutron spectrometer for
polarized and unpolarized measurements

Triple-Axis Spectroscopy

HFIR HB-1A (FIE-TAX)

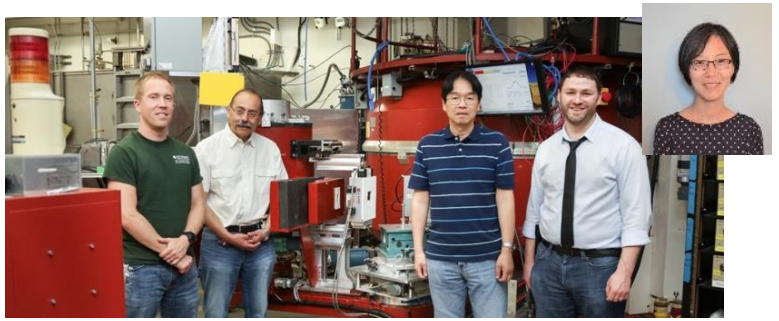




Adam Aczel
Wei Tian
Shirley Xu (SA)

Fixed incident energy triple-axis spectrometer

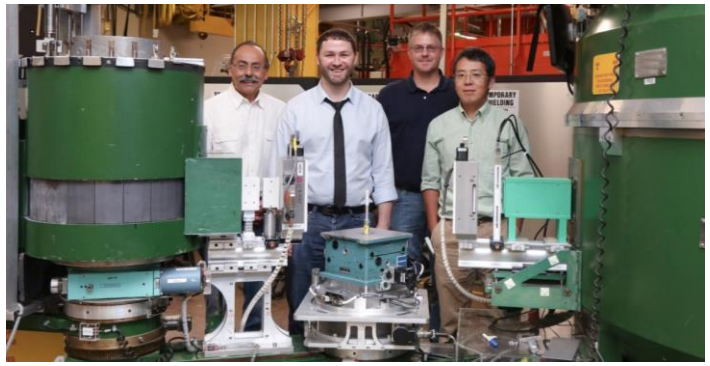
HFIR HB-1 (PTAX)



Masa Matsuda
Jaime Fernandez-Baca
Travis Williams
Shirley Xu (SA)

Polarized neutron triple-axis spectrometer

HFIR HB-3 (TAX)



Versatile thermal triple-axis spectrometer

Songxue Chi
Jaime Fernandez-Baca
Travis Williams
Mike Cox(SA)

HFIR CG-4C (CTAX)

Tao Hong
Jaime Fernandez-Baca
Travis Williams
Mike Cox(SA)

Cold neutron triple-axis spectrometer

Chemical Spectroscopy

SNS BL-2 (BASIS)

Eugene Mamontov
Niina Jalarvo
Naresh Osti
Chris Schmitt (SA)

Near-backscattering, crystal-analyzer spectrometer

Shull Fellow
Matthew Ryder

SNS BL-16B (VISION)

Indirect Geometry spectrometer optimized for measuring vibrational spectroscopy

Luke Daemen
Timmy Ramirez-Cuesta
Eric Novak (SA)

YQ Cheng (CIS)

SNS BL-15 (NSE)

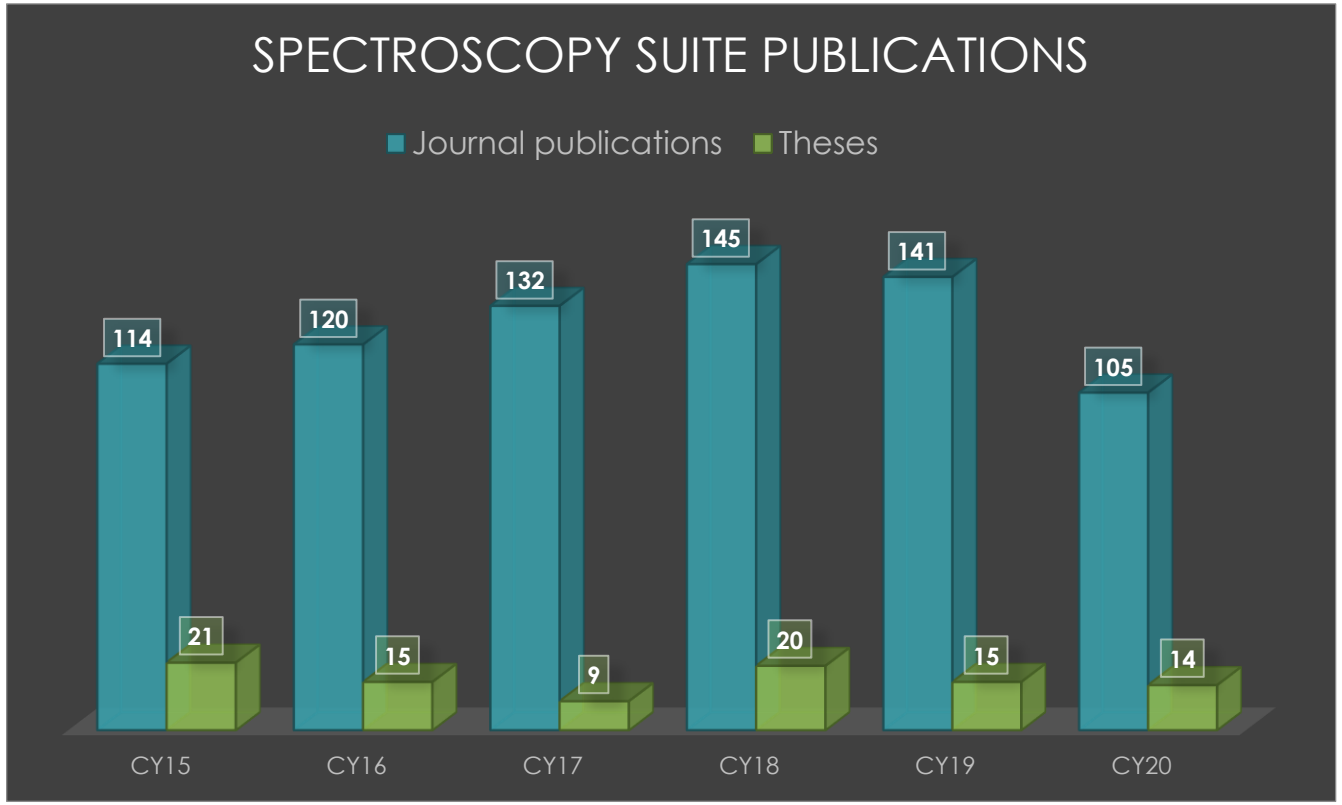
Laura Stingaciu
Piotr Zolnierczuk
Mary Odom (SA)

Time-of-flight neutron spin echo spectrometer

(Green: Supports Polarization Analysis)

	Cold Moderator: 2 meV < Ei < 100 meV	Thermal Moderator: 5 meV < Ei < 2 eV	
1-3% elastic E resolution / less flux	CNCS	SEQUOIA	Direct Geometry
3-5% elastic E resolution / high flux	HYSPEC	ARCS	Direct Geometry
Highest time-averaged flux	CTAX	HB-1A, HB-1, HB-3	Triple-Axis
High energy resolution and high flux on sample, almost constant ΔE/E	BASIS	VISION	Indirect Geometry
Ultra high-resolution spectroscopy	NSE	HB-1 (Wollaston prisms)	Spin Echo

Spectroscopy Suite Publications



- Steady publication output from 2017 – present
- **Note:** FY19 involved an unplanned 11-month HFIR shutdown and a significant reduction in SNS beam time.
- FY20: COVID-19 impact on user program.

~30-35% of instrument publications from SNS/HFIR use instruments from Spectroscopy Suite

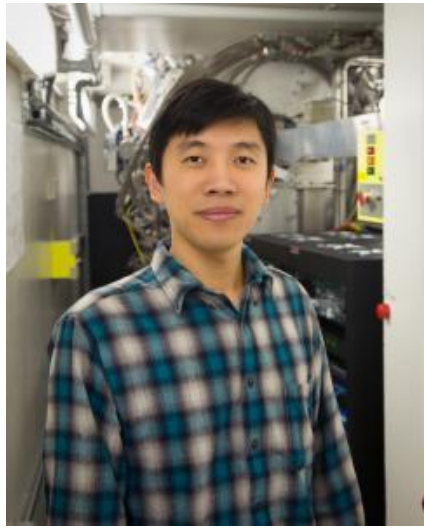
Spectroscopy Staffing

- Instrument scientist staffing changes:
  - **ARCS instrument scientist**:
    - Andrew Christianson – Arnab Banerjee – Garrett Granroth
  - **CNCS instrument scientist**:
    - Georg Ehlers – Daniel Pajerowski (this happened before 2017 review)
  - **NSE instrument scientists:**
    - Transition from Juelich staff to ORNL staff
- Added new scientific associates:
    - Mary Odom – NSE
    - Shirley Xu – HB-1A / HB-1
    - Eric Novak – VISION

Spectroscopy Staffing

- Added two new computational instrument scientists:

Andrei Savici
Direct Geometry Team
(Also providing support for TAS)

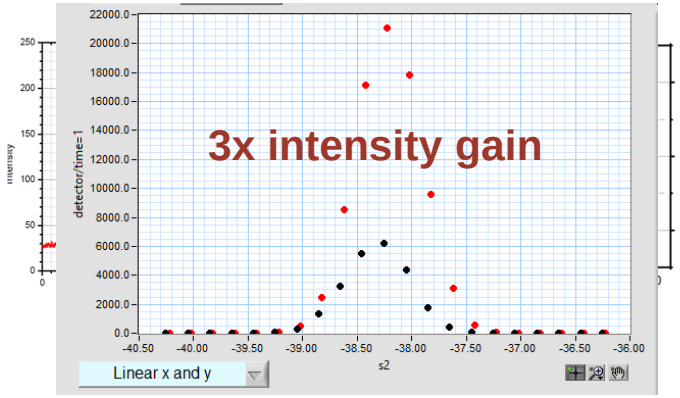


Yongqiang Cheng
Chemical Spectroscopy Team
(Also providing support for NSE)

Technique developments – collaboration with NTD

Monochromator optimization HB-1A

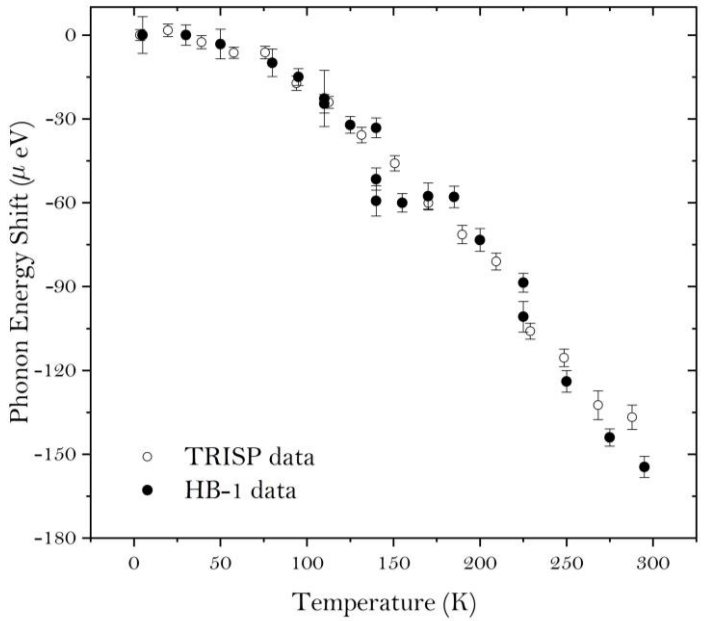
- Incorrect beam focus was analyzed, planned, corrected, & characterized in collaboration NTD staff



- Lowell Crow went to Missouri to align first monochromator and helped to characterize performance
- Lee Robertson worked with Wei Tian to model optics

Larmor diffraction & high res. spectroscopy on HB-1

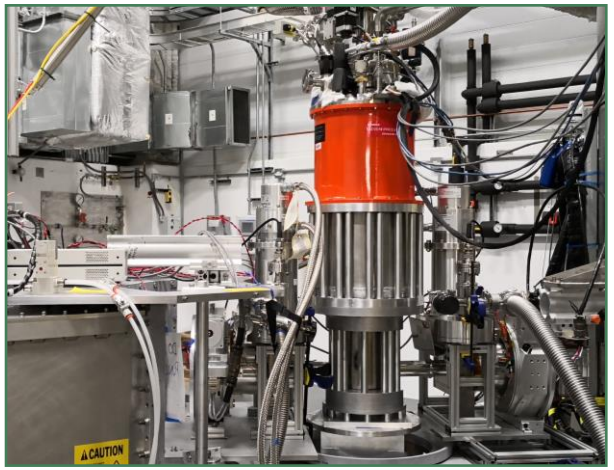
- Development of Wollaston prisms and implementation for Larmor diffraction or inelastic spin echo on HB-1 led by Fankang Li, NTD



Phonon energy shift of Ge compared with TRISP (FRM-II)

Spherical neutron polarimetry

- New design, led by Peter Jiang, uses high-Tc films combined with mu-metal.
- Initial design for HB-1; tested on HYSPEC



- DOE Early Career Award for Peter Jiang.
- Plans to develop wide angle HYSPEC SNP device

Recent highlights of instrument upgrades

- HB-1: Wollaston prisms; SNP device (underway)
- HB-1A: Upgrade of the monochromator system and drum
- HB-3: shield around sample position
- CNCS: radial collimator
- ARCS: upgrade of detector electronics
- HYSPEC: elevator / oscillator; purchased supermirror array
- BASIS: implemented use of higher order Si (333)
- VISION: addition of collimators for diffraction banks

Recent highlights of instrument upgrades

- Sample environment:
  - SNS 14T magnet
  - 6T workhorse magnet for HFIR
  - CTAX: 11T uncompensated magnet moved to HFIR
  - Liquid helium autofill (LHeF) system installed across SNS and tested at HB-1A
  - Pressure cells for spectroscopy (clamp cells, DACs, etc.)
  - Second 6T magnet for HFIR to handle demand (underway)

Planned instrument upgrades

- HB-1: upgrade of Heusler monochromator (underway)
- HB-3: Velocity selector in incident beam
- HB-1 / HB-3: new secondary spectrometers
- HB-1A: new secondary spectrometer (underway)
- SEQUOIA / CNCS: complete detector array (CNCS underway)
- SEQUOIA: radial collimator; Brillouin scattering
- HYSPEC: shielding to reduce time independent background (order submitted)
- VISION: new CCR with fast cooldown; optimized sample changer

New instruments – international context

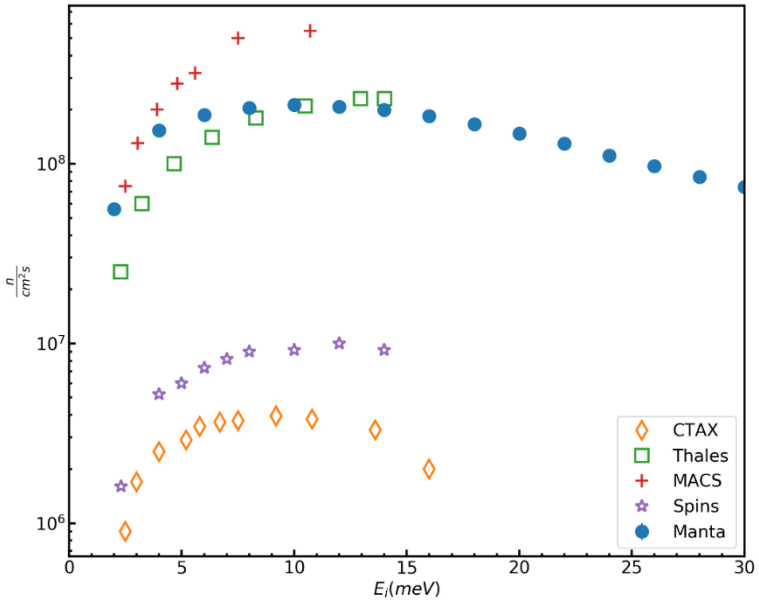
	Thermal TAS	Cold TAS	Thermal DGS	Cold DGS	Backscattering	Vibrational Spectroscopy	Spin Echo
ORNL	3	1	2	2	1	1	1
NIST	1	2	0	1	1	1	1
FRM-II	2	3	1	1	1	0	2
ISIS	0	0	3	1	2	1	0
J-PARC	0	0	0	4	1	0	1
ILL	3	2	1	2	2	1	3
PSI	1	2	0	1	0	0	0

Instrument priorities (HFIR & SNS-FTS):

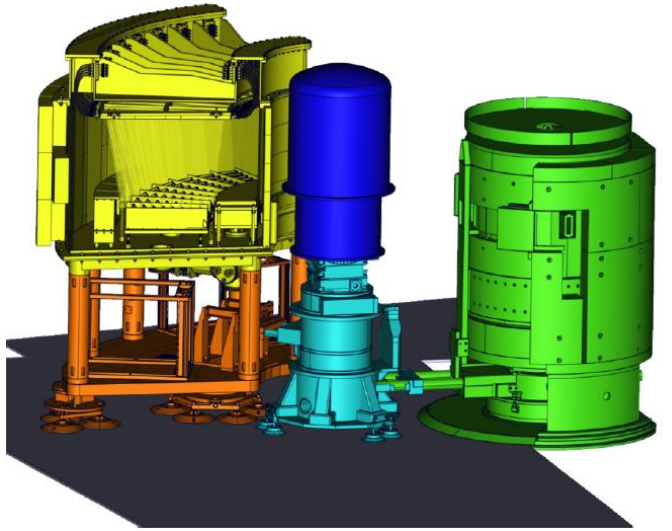
- World class cold neutron triple-axis @ HFIR
- High resolution NSE @ HFIR
- BeFAST (compliment to VISION)

New HFIR spectroscopy instruments

- **MANTA**
  - World class flux on sample
  - Interchangeable secondary spectrometer
    - CAMEA-like multianalyzer
    - Single detector (compatible with Wollaston prisms)
- **HFIR-NSE**:
  - High-flux, high-resolution NSE optimized for small samples
  - Provide measurements to Fourier times up to 500 ns with extended Q range of 0.02-2 $Å^{-1}$



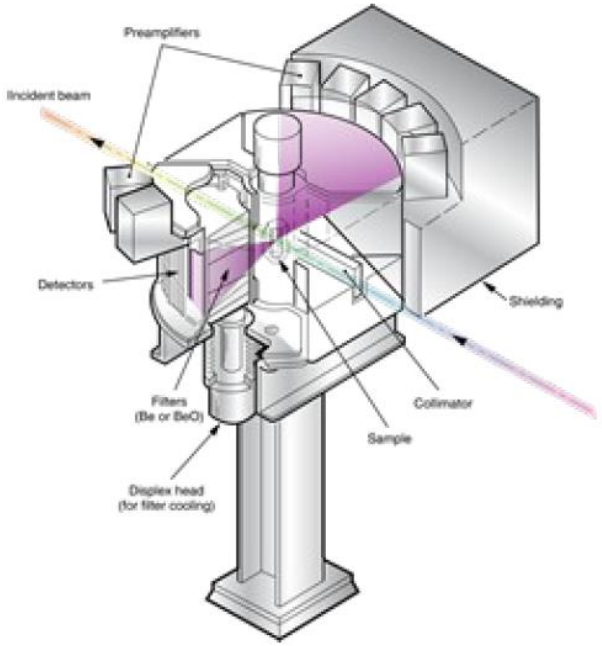
McSTAS simulation of incident flux for MANTA (G. Granroth)



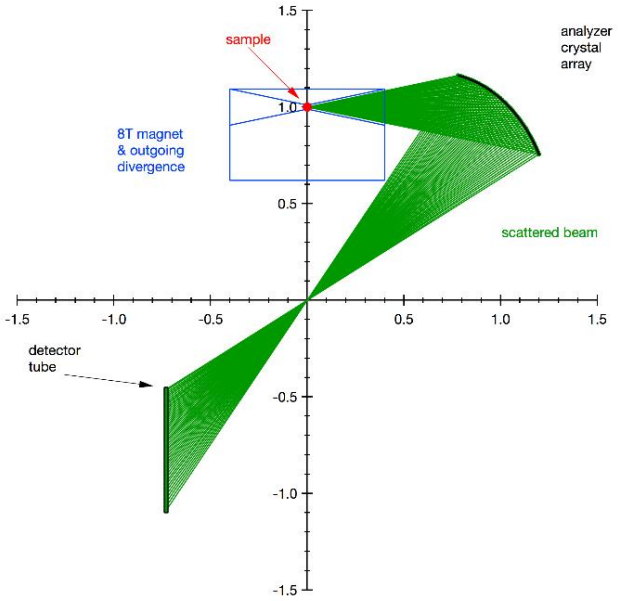
CAMEA at PSI

New SNS-FTS instruments

- **BeFAST**
  - Compact Be filter spectrometer on BL-16A; enable neutron near-IR Spectroscopy
  - Coarser resolution than VISION (up to 5 meV). Better intensity for $\Delta E > 3000$ cm^{-1}
  - Extend chemical spectroscopy capabilities with emphasis on hydrogen bonded systems.



- **HIGGS**:
  - New indirect geometry spectrometer for BL-8A (decoupled water moderator)
  - Planar array of PG analyzers scattering through common point to detectors below sample
  - Optimized for complex sample environments

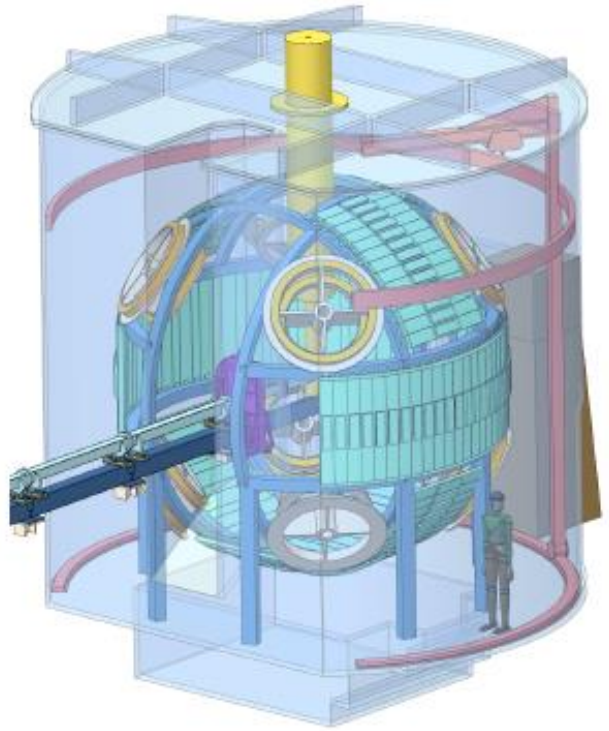


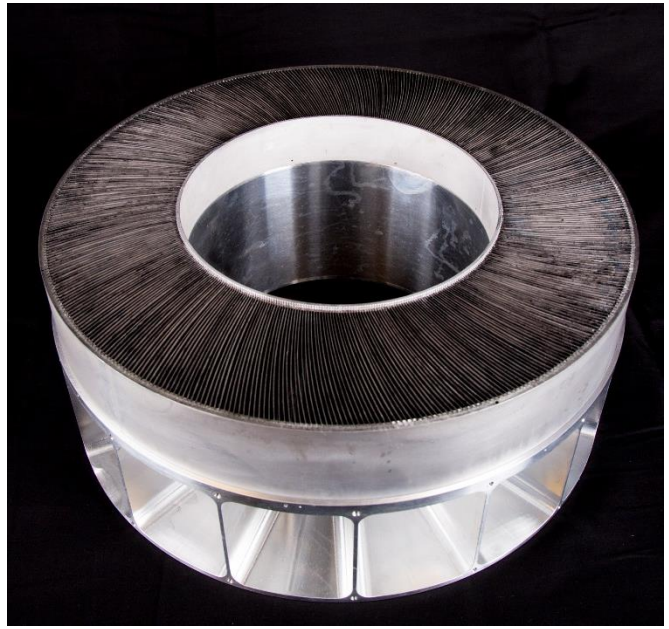
(Green: Supports Polarization Analysis)

	Cold Moderator: 2 meV < Ei < 100 meV	Thermal Moderator: 5 meV < Ei < 2 eV	
1-3% elastic E resolution / less flux	CNCS	SEQUOIA	**Direct Geometry**
3-5% elastic E resolution / high flux	**HYSPEC**	ARCS	
Highest time-averaged flux	**MANTA**	HB-1A, **HB-1**, HB-3	**Triple-Axis**
High energy resolution and high flux on sample, almost constant ΔE/E	BASIS	VISION, **BeFAST, HIGGS**	**Indirect Geometry**
Ultra high-resolution spectroscopy	**NSE, HFIR-NSE**	**HB-1 (Wollaston prisms)**	**Spin Echo**

Second Target Station

- High brightness coupled hydrogen moderators
- Spectroscopy concepts underway:
  - ***CHESS***: chopper spectrometer for small samples (Gabriele Sala)
  - ***TITAN***: extreme environment spectrometer / diffractometer (Barry Winn)
  - ***BWAVES***: indirect geometry spectrometer with high energy resolution and a very broad dynamic range of energy transfers (Eugene Mamontov)
  - ***JANUS***: Hybrid indirect/direct geometry spectrometer (Timmy Ramirez-Cuesta)
  - ***EXPANSE***: Wide angle neutron spin echo (Changwoo Do)

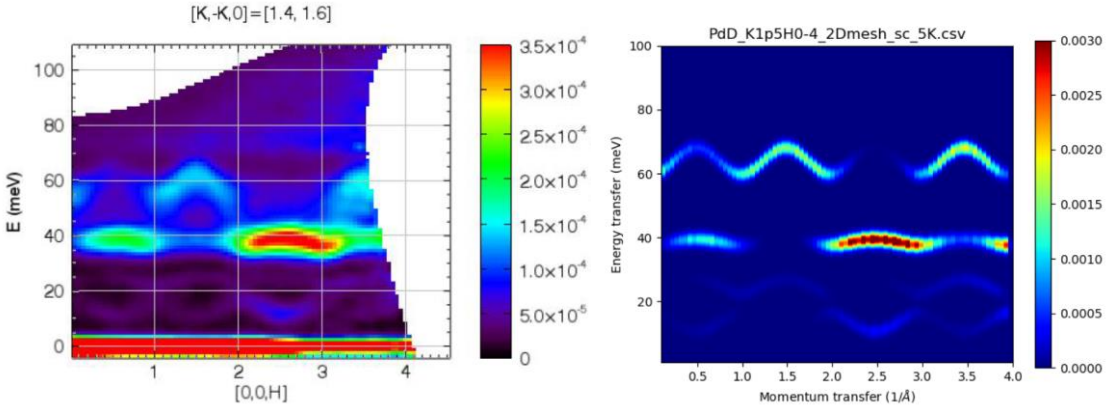




Spectroscopy data analysis software

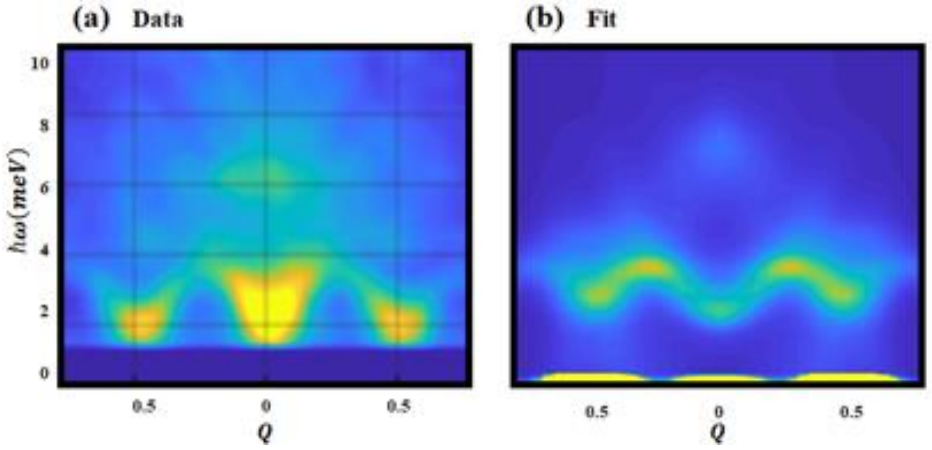
- Ongoing developments:
  - ICEMAN – workflow management software (T. Ramirez-Cuesta)
  - QCLIMAX - advanced analytical fitting of QENS data (T. Ramirez-Cuesta)
  - OCLIMAX - software for calculating phonon spectra from DFT (YQ Cheng)
  - Mantid software to visualize DGS data (A. Savici)
  - Landau-Lifshitz code to simulate classical magnetic excitations (A. Samarakoon, A. Tennant, C. Batista)

OCLIMAX Example: single crystal *phonons in PdD*



SEQUOIA OCLIMAX

Landau-Lifshitz: calculation of spectrum of α-$RuCl_3$



Spectroscopy data analysis software

- Data analysis plans developed (T. Ramirez-Cuesta & G. Granroth)
  - Expand ICEMAN concept (uses scientific workflows)
  - Enable DFT / OCLIMAX / access to HPC resources to enable modeling of large-scale systems
  - Molecular dynamics for QENS / NSE analysis
  - Extend McVINE to become a more useful analysis tool
  - Ensure long-term future of SpinW
  - Transform prototype Landau-Lifshitz code into user tool
  - Enable access to community developed codes like DMRG, DMFT, quantum Monte Carlo, etc.
  - All of these could be incorporated into an ICEMAN-like concept to provide a general data analysis framework for Spectroscopy

Specific 2017 recommendation – SE support

- Concerns about lack of adequate support for sample environment (particularly at HFIR)
- Staffing has remained constant but there are steps that have been taken to improve the situation including
  - SA and instrument scientist training on certain SE tasks
  - Cross-training and rebalancing of staff between SNS and HFIR
  - Block scheduling of equipment to minimize moves
  - Instrument hall coordinators now supporting HFIR

Specific 2017 recommendation – SE support

- Automation:
  - Auto needle valve control across HFIR & SNS
  - Liquid helium autofill deployed across SNS and being deployed at HFIR
  - Multipoint liquid helium autofill being developed
- Other steps:
  - SE steering committees are strong advocates & communication venues
  - Science productivity / midscale used to increase equipment inventory
- Concerns:
  - Demand continues to outpace equipment purchase particularly for magnets
  - Lack of helium recovery infrastructure & rising helium costs.

Summary

- Mature instrument suite with steady publication output
- Continuous improvement of instruments
- Commitment to technique development in close collaboration with staff in NTD
- Plans for new instruments at HFIR, SNS-FTS, and SNS-STS to expand spectroscopy suite
- Plans underway for advanced, integrated data analysis platform / tools

September 17, 2020

Time	Event		
8:30–8:50 am	Welcome (Paul Langan)		
8:50–9:20 am	Neutron Scattering Division Outlook & Strategy (Hans Christen)		
9:20–9:50 am	Spectroscopy Overview & Strategy (Mark Lumsden)		
9:50–10:15 am	Break		
10:15 am–12:05 pm	**Parallel Beam line presentations**		
	Direct Geometry	***Triple-Axis***	***Chemical Spectroscopy***
10:15–10:25 am	Team overview (Doug Abernathy)	Team overview (Jaime Fernandez-Baca)	Team overview (Timmy Ramirez-Cuesta)
10:25–10:50 am	CNCS (Daniel Pajerowski)	CTAX (Tao Hong)	BASIS (Eugene Mamontov)
10:50-11:15 am	HYSPEC (Barry Winn)	HB-1 (Masa Matsuda)	NSE (Laura Stingaciu)
11:15–11:40 am	SEQUOIA (Matt Stone)	HB-1A (Adam Aczel)	VISION (Luke Daemen)
11:40 am–12:05 pm	ARCS (Doug Abernathy)	HB-3 (Songxue Chi)	
12:05–1:00 pm	***LUNCH***		
1:00-1:30 pm	Direct Geometry / Triple-axis software (A. Savici)		Chemical spectroscopy software (YQ Cheng)
1:30 pm -	Committee work time and report writing		

September 18, 2020

9:00–9:30 am	Committee recap and Q&A (GL and TLs)		
9:30–11:30 am	Meet with Direct Geometry Team members	Meet with Triple-Axis Team members	Meet with Chemical Spectroscopy Team members
11:30 am-12:30 pm	Committee work time and report writing		
12:30-1:30 pm	Lunch		
1:30–2:30 pm	Committee Verbal Report and Recommendations (DD, GL, TLs, instrument teams)		
2:30 p.m.	Adjourn		