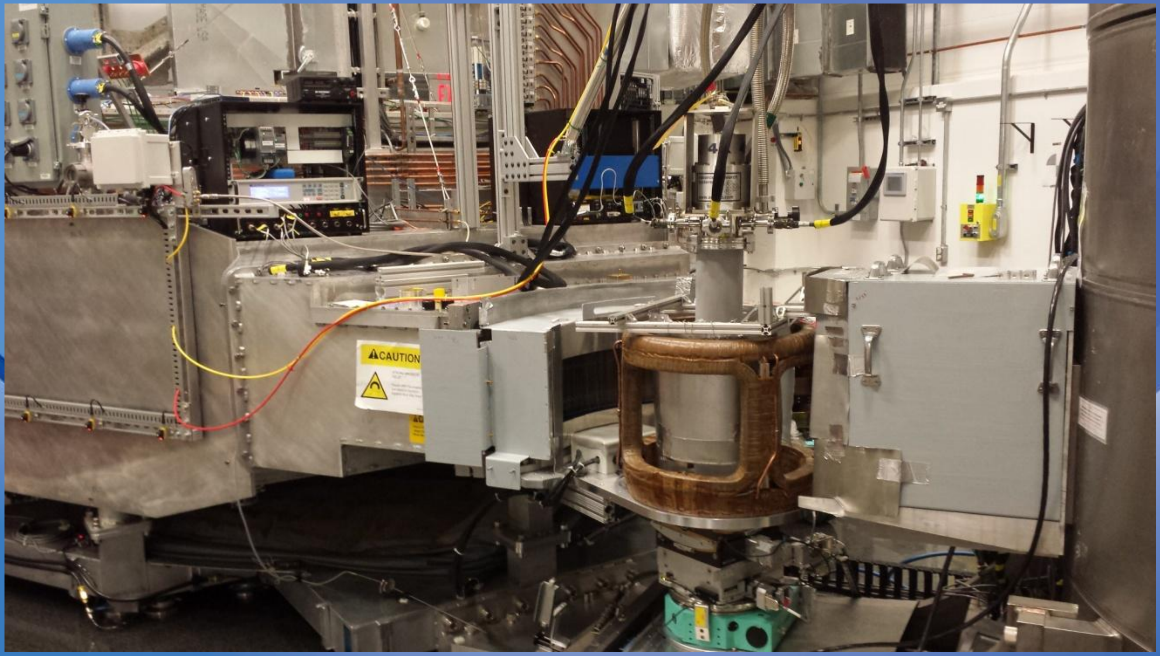
HYbrid SPECtrometer (HYSPEC) and other direct geometry instruments at SNS

Igor Zaliznyak

Condensed Matter Physics and Materials Science Division

SUSTech Symposium on Neutron Diffractometer/Spectrometer, October 10, 2016



BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

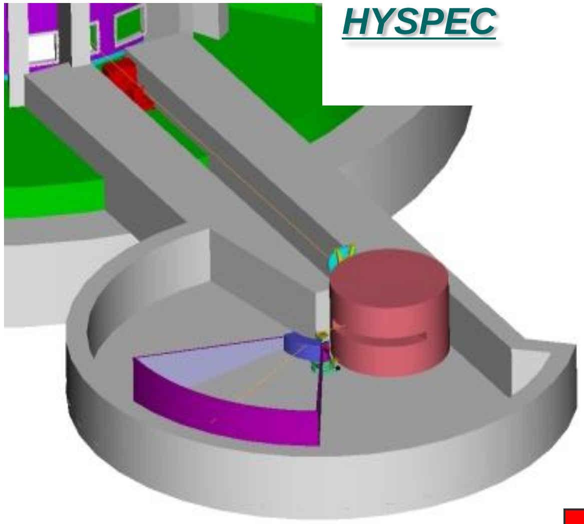
Office of Science
U.S. DEPARTMENT OF ENERGY

http://neutrons.phy.bnl.gov/HYSPEC

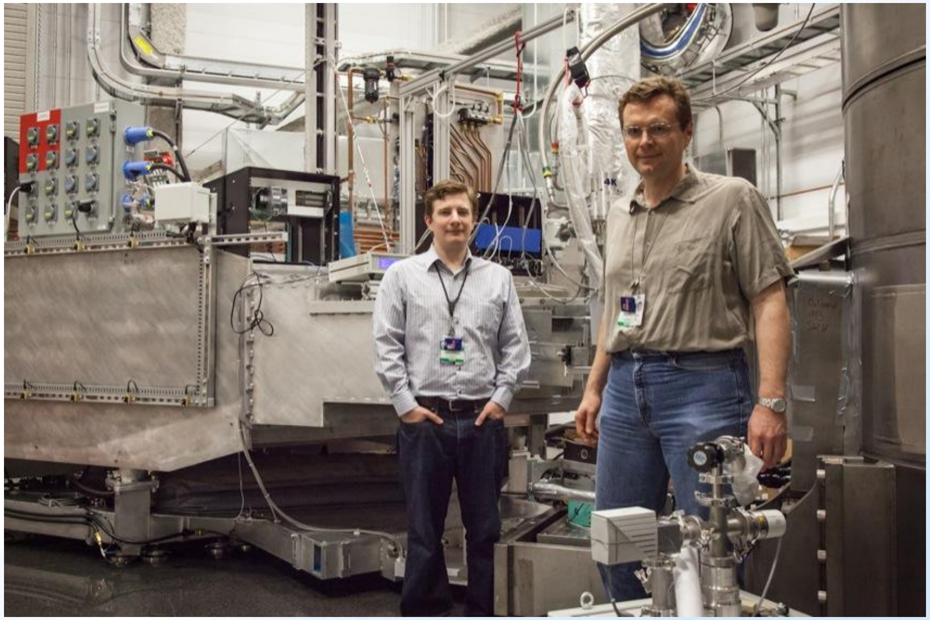
Building a spectrometer: how long and how much?

Proposal submitted to DOE,
I. Zaliznyak, S. Shapiro (2002)

HYSPEC



Commissioning Experiments,
D. Fobes and I. Zaliznyak (2012)



~ 10 - 12 years
~ 12 - 15 M$

History: HYSPEC timeline

2000
- The Concept of the Hybrid Spectrometer proposed at BNL

2001
- Direct Geometry Hybrid Spectrometer presented to SNS EFAC
- HYSPEC Instrument Development Team (IDT) formed

2002
- HYSPEC IDT filed Letter of Intent with SNS
- HYSPEC proposal submitted to DOE

2003
- DOE CD0, HYSPEC is approved as part of the SING project

2004
- HYSPEC’s placement approved on BL14B;Design&Engineering begins

2005
- DOE CD2, HYSPEC’s performance baseline approved

2006
- DOE CD3, construction begins

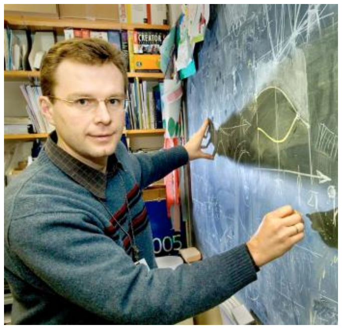
2011
- DOE CD4, HYSPEC commissioning & operation begins

2013
- HYSPEC enters SNS User Program

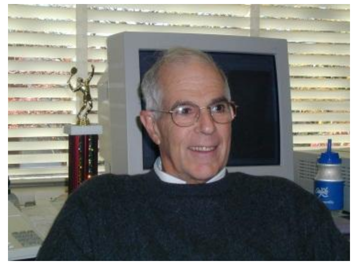
2015
- Polarized beam operation on HYSPEC is commissioned

http://neutrons.phy.bnl.gov/HYSPEC

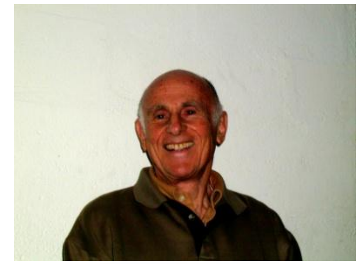
HYbrid SPECtrometer, HYSPEC: BNL Instrument Design Group



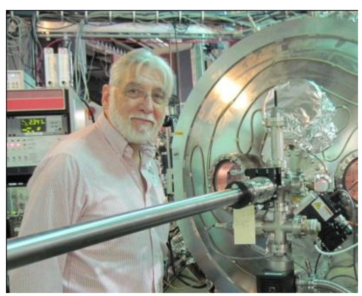
Igor Zaliznyak, PI



Steve Shapiro, co-PI



Larry Passell, advisor



Bill Leonhardt, engineer

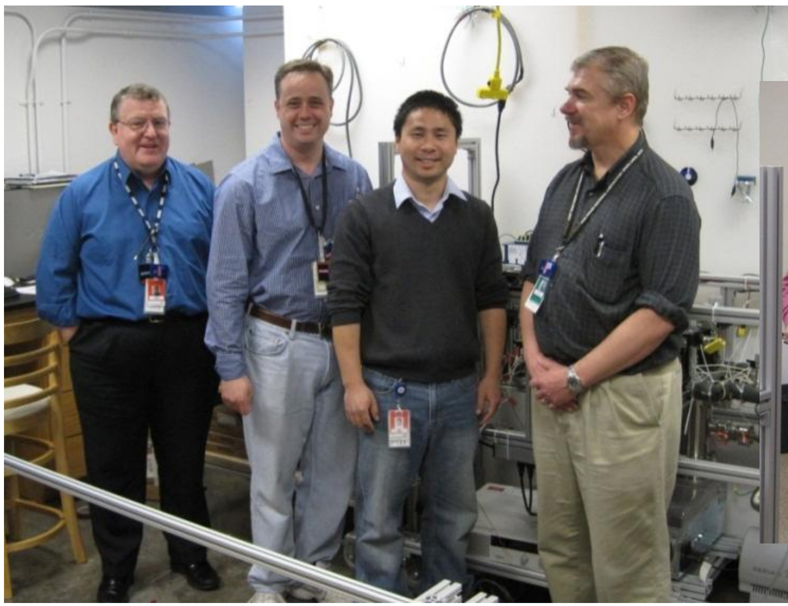
Vinita Ghosh, scientist – MC simulations

http://neutrons.phy.bnl.gov/HYSPEC

HYbrid SPECtrometer, HYSPEC – ORNL Instrument Team

HYSPEC: SNS Instrument Construction Team (… - 2013)

HYSPEC SNS Instrument Team now



Mark Hagen, Lead Scientist (now @ ESS) — Barry Winn, Scientist — Tony Tong, Scientist — David Anderson, Engineer

Melissa Graves-Brook, Science Associate

Ovidiu Garlea, Scientist, Joined in May, 2013 — Barry Winn, Scientist

HYSPEC Team - 2002

Instrument Development Team

I. Zaliznyak, co-PI	BNL
S. M. Shapiro, co-PI	BNL
G. Shirane	BNL
J. Tranquada	BNL
L. Passell	BNL
D. Abernathy	SNS
L. Daemen	Los Alamos
M. Greven	Stanford
B. Gaulin	McMaster
V. Kiryukhin	Rutgers
Y. Lee	MIT
S. Nagler	ORNL
R. Osborn	ANL
J. Rhyne	U. Missouri
C. Stassis	Ames/Iowa St.
A. Zheludev	ORNL

Instrument design team

- I. Zaliznyak (BNL)
- S. M. Shapiro (BNL)
- L. Passell (BNL)
- V. J. Ghosh (BNL) Monte-Carlo simulations
- S. Doran (SNS/ANL) Engineering design concept

http://neutrons.phy.bnl.gov/HYSPEC

HYSPEC Team - 2015

Instrument Development Team

I. Zaliznyak (co-PI, EC member	BNL
S. Shapiro (co- PI, EC member)	BNL
M. Kenzelmann (EC member)	PSI
L. Daemen	LANL
J. Fernandez-Baca	ORNL
J. Gardner	NIST/Indiana U.
B. Gaulin	McMaster U.
M. Greven	Stanford
V. Ghosh	BNL
M. Hagen	SNS =>ESS
M. Huecker	BNL
V. Kiryukhin	Rutgers
G. Lander	EITU
Y. Lee	MIT
S.-H. Lee	U. Virginia
C. Majkrzak	NIST
A. Goldman (EC member)	Ames/Iowa U.
S. Nagler	ORNL
R. Osborn	ANL
L. Passell	BNL
L. P. Regnault	CEA-Grenoble
T. Sato (EC member)	Tohoku University
J. Tranquada (EC member)	BNL
G. Xu	BNL
A. Zheludev	ETH-Zurich

IDT Executive Committee

- I. A. Zaliznyak, PI (BNL)
- S. M. Shapiro, PI (BNL)
- M. Kenzelmann (PSI)
- A. Goldman (Ames/Iowa State)
- T. Sato (Tohoku
- J. Tranquada (BNL)

http://neutrons.phy.bnl.gov/HYSPEC

HYSPEC science case: polarization first

- **Characterization of spin-dependent cross-sections by means of polarization analysis**
- **Coherent collective excitations in single crystals:**
  - lattice dynamics (phonons)
  - spin dynamics (magnons, critical scattering)
- **Structure and dynamics of partially ordered and glassy phases**
  - spin glasses
  - charge glasses
  - correlated amorphous phases
  - small angle
- **Study of the microscopic physical properties of samples in extreme environments:**
  - temperature
  - pressure
  - magnetic field

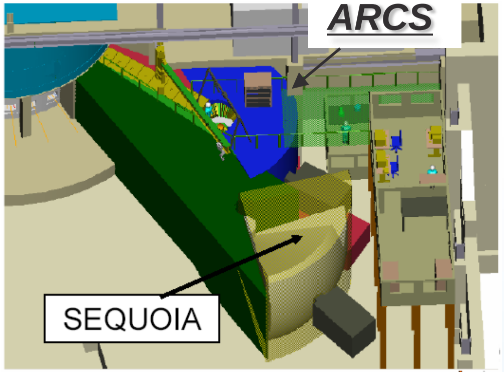
HYSPEC intended place among the SNS inelastic instruments.

epithermal

High energy transfer

10-1000 meV Fermi Chopper Spectrometer

- E = 10 - 1000 meV
- Q = 0.1 – 22 Å^{-1}

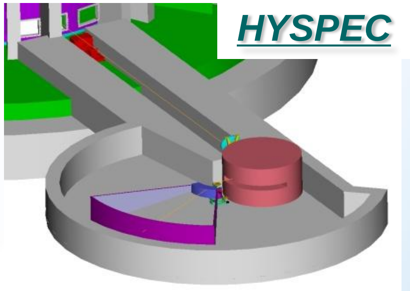


thermal

High intensity at moderate resolution and medium energy transfer + polarized beam

Crystal-Focussing Hybrid Spectrometer

- E = 3.8 - 90 meV
- Q = 0.1 – 8 Å^{-1}

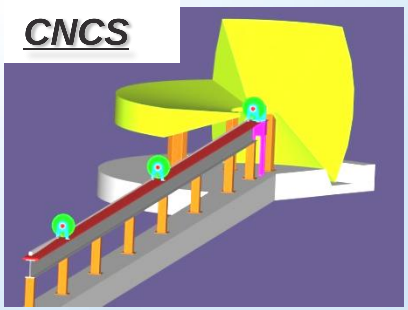


subthermal

High resolution and low energy transfer

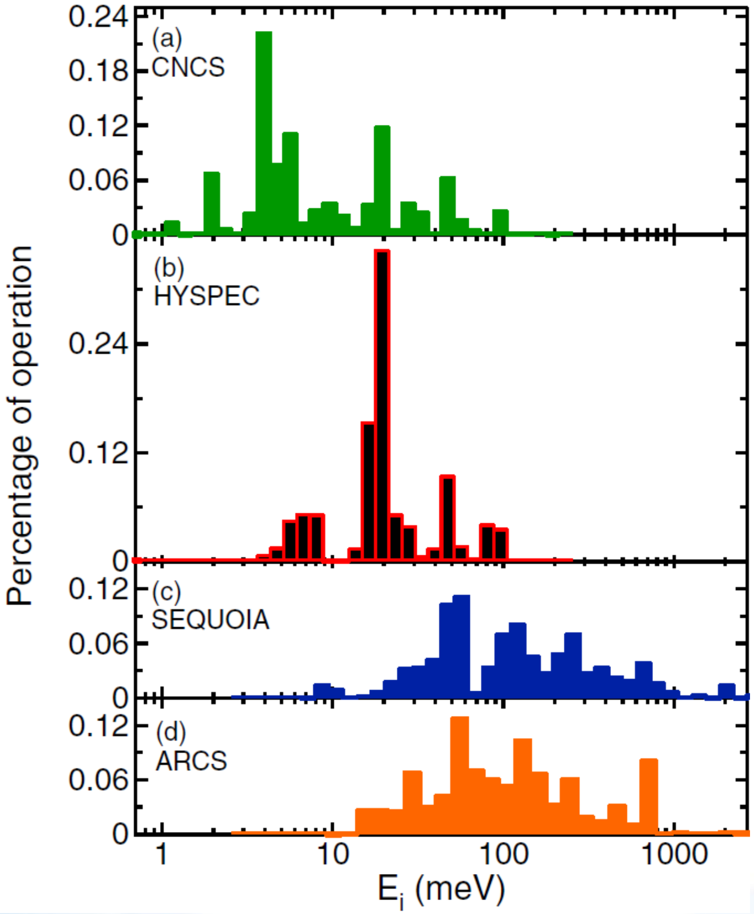
10-100 μeV Multichopper Spectrometer

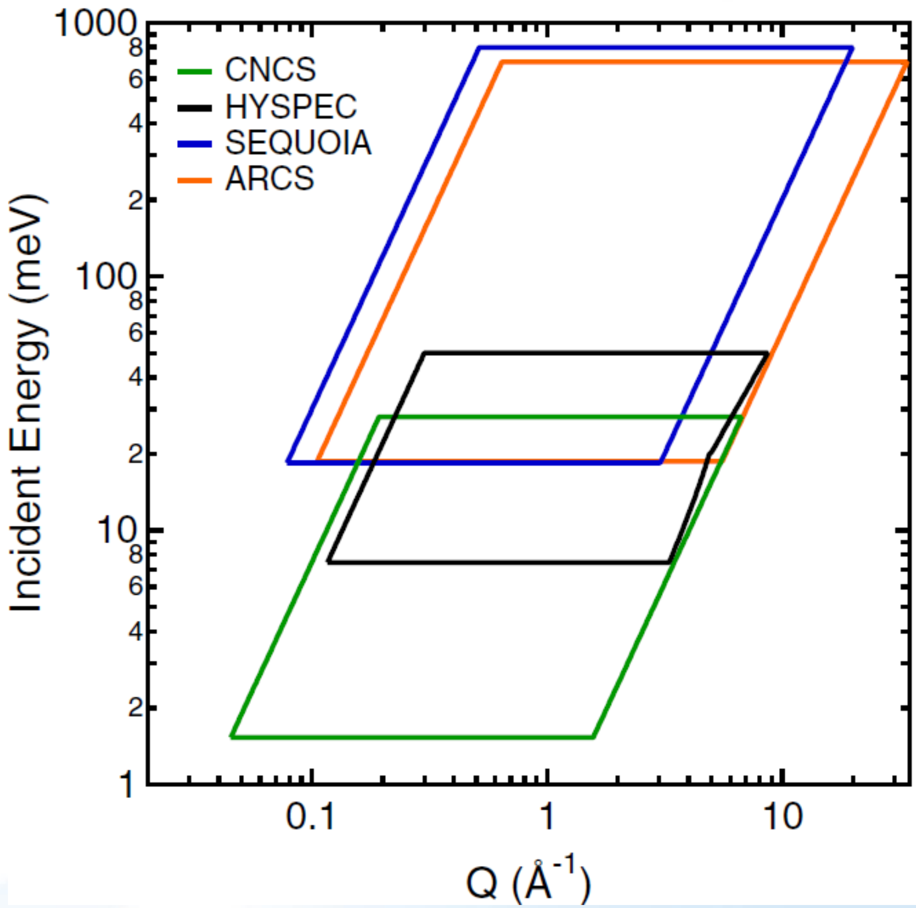
- E = 2 - 20 meV
- Q = 0.1 - 4 Å^{-1}



Direct Geometry Spectrometers at SNS

M. Stone, et. al. Rev. Sci. Instrum. 85, 045113 (2014)



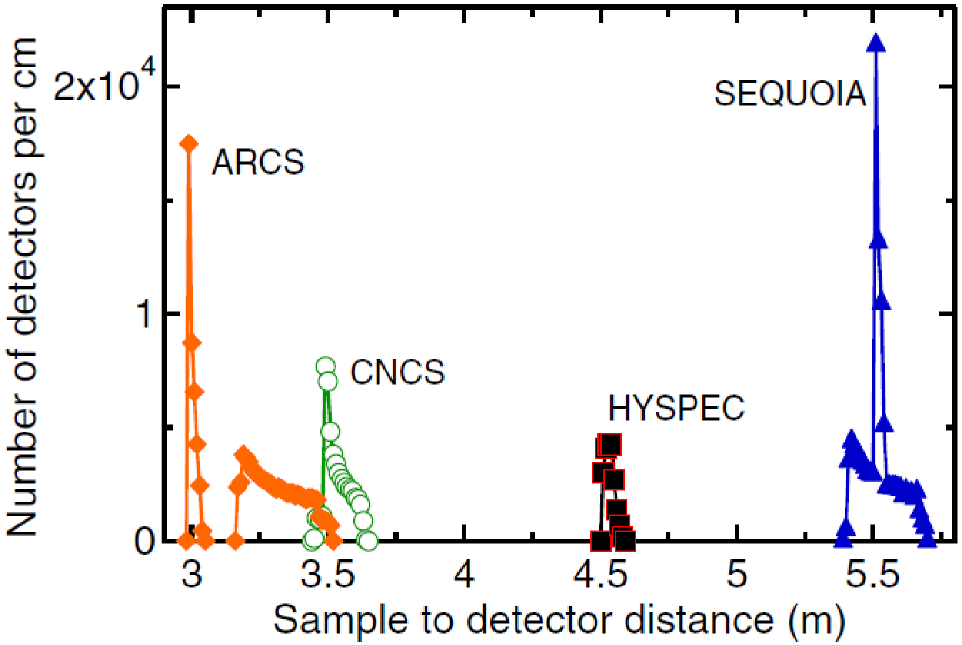


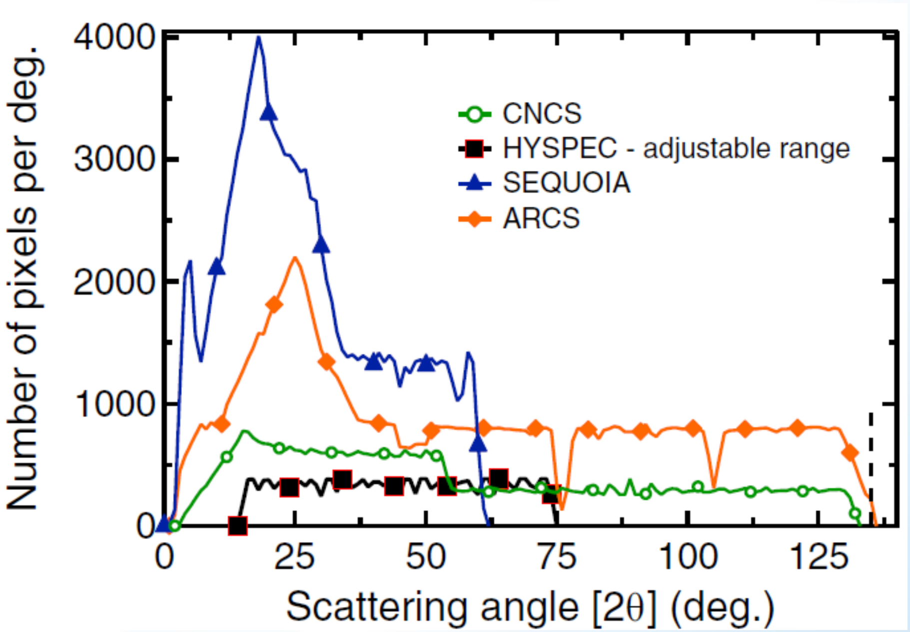
Direct Geometry Spectrometers at SNS

M. Stone, et. al. Rev. Sci. Instrum. 85, 045113 (2014)

Parameter	CNCS	HYSPEC	SEQUOIA	ARCS
Moderator	c-lH	c-lH	apd-H_2O	apd-H_2O
Source-beam monitor distance (m)	34.85	37.38	18.23	11.831
Source-downstream monitor distance (m)	n/a	n/a	29.003	18.5
Source-sample distance (m)	36.26	40.77	20.01	13.6
Height of beam at sample (cm)	5	3.5	5	5
Width of beam at sample (cm)	1.5	3.5	5	5
Detector tube diameter (cm)	2.54	2.54	2.54	2.54
Detector tube length (m)	2	1.2	1.2	1
Mean sample-detector distance (m)	3.54	4.54	5.53	3.21
Minimum equatorial scattering angle (deg.)	3.8	0[a]	2.0	2.4
Maximum equatorial scattering angle (deg.)	135	135	59.3	136.0
Maximum out of plane scattering angle (deg.)	16	7.5	19.4	27
Solid angle detector coverage[b] (Sr.)	1.606	0.226	0.863	2.196
Incident energy range (meV)[c]	1–80	4–60	8–2000	15–1500
Range of energy resolution ($\%E_i$)[d]	1–5	3–5	1–3	3–5
Radial collimator	Yes	Yes	No	Yes
Entry into user program	2009	2013	2010	2008
Reference	19		20, 34	21

Direct Geometry Spectrometers at SNS





M. Stone, et. al. Rev. Sci. Instrum. 85, 045113 (2014)

Direct Geometry Spectrometers at SNS

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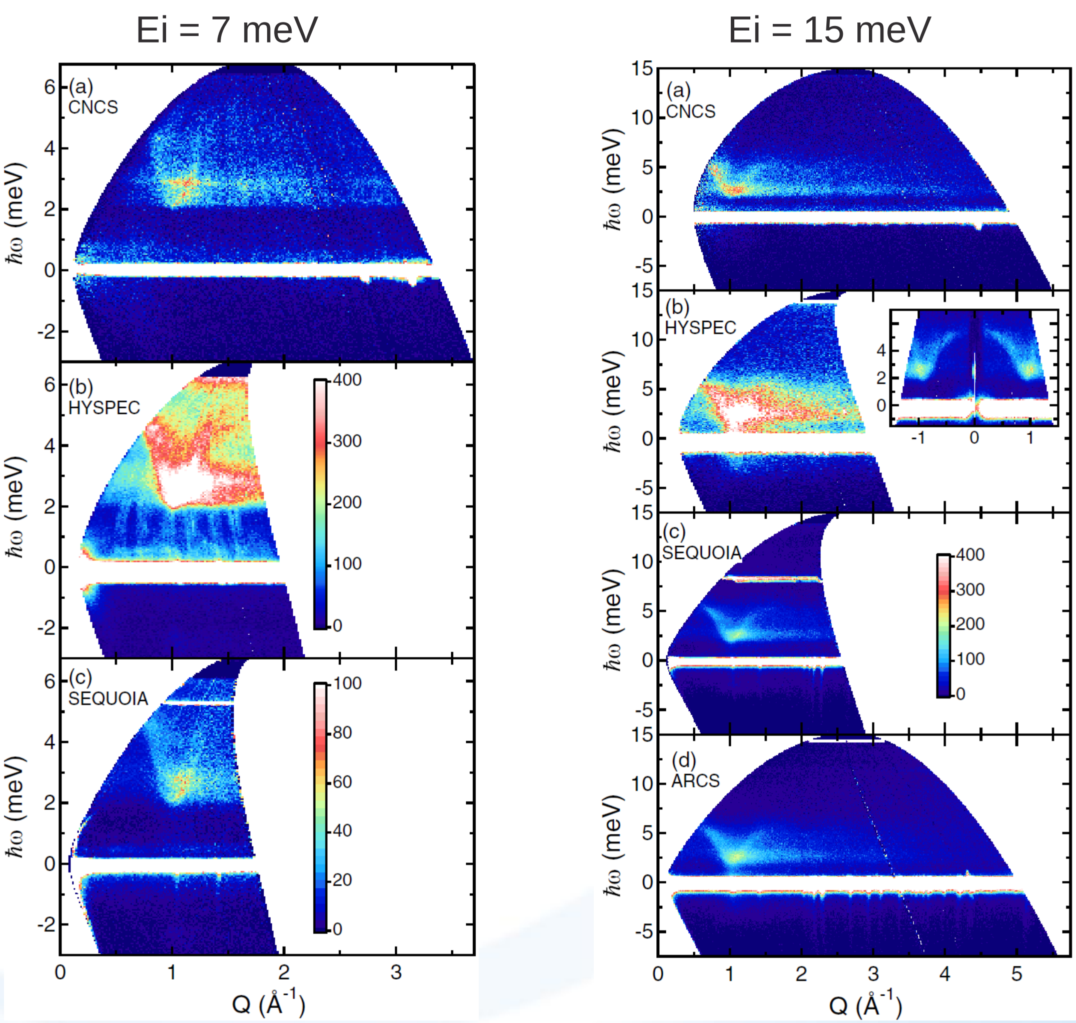
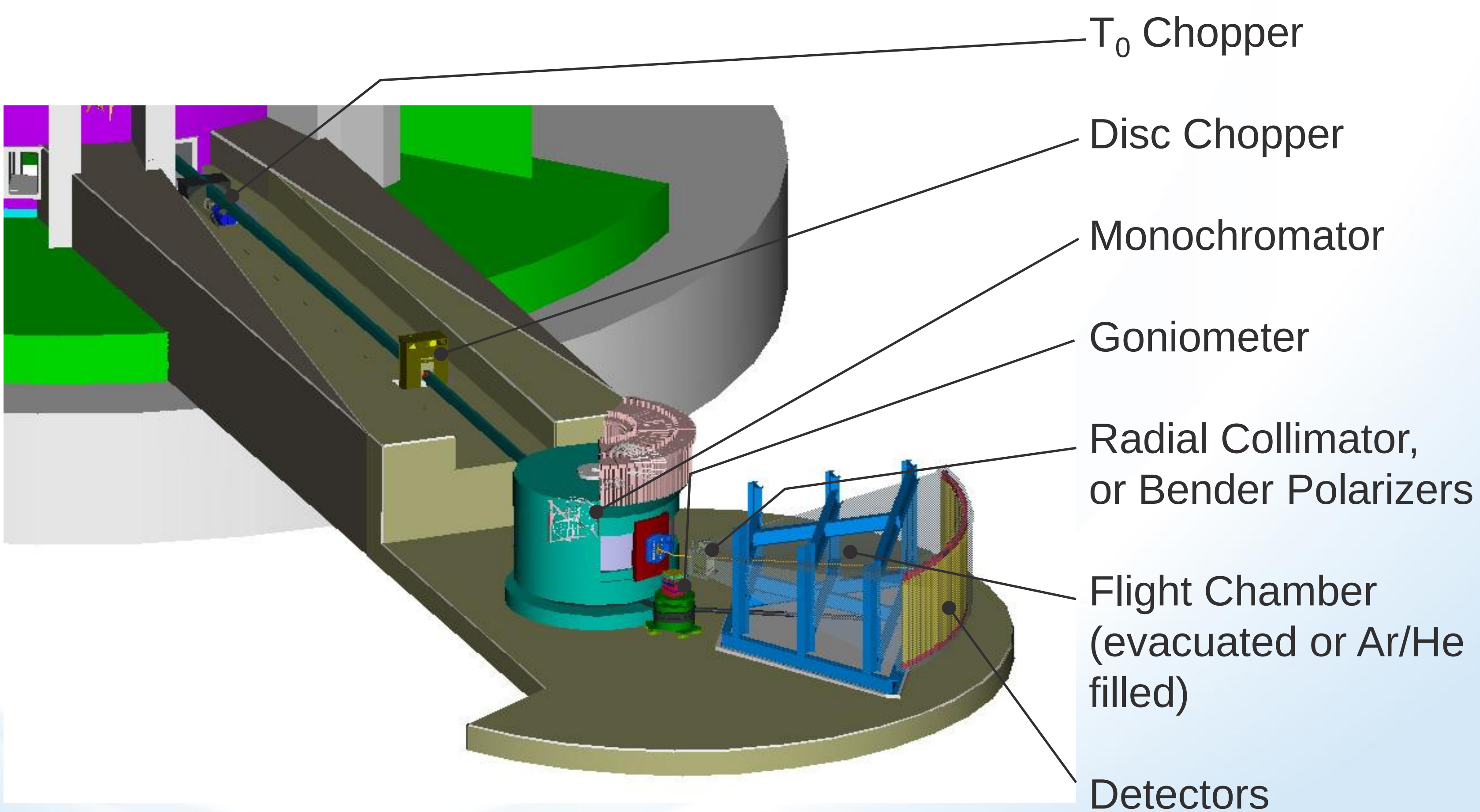


Magnetic intensity from the same powder sample of CrCl2 (Haldane gap chain S=1 antiferromagnet) measured on the four different spectrometers at two incident energies. Note the 4x larger scale for HYSPEC data at Ei = 7 meV.

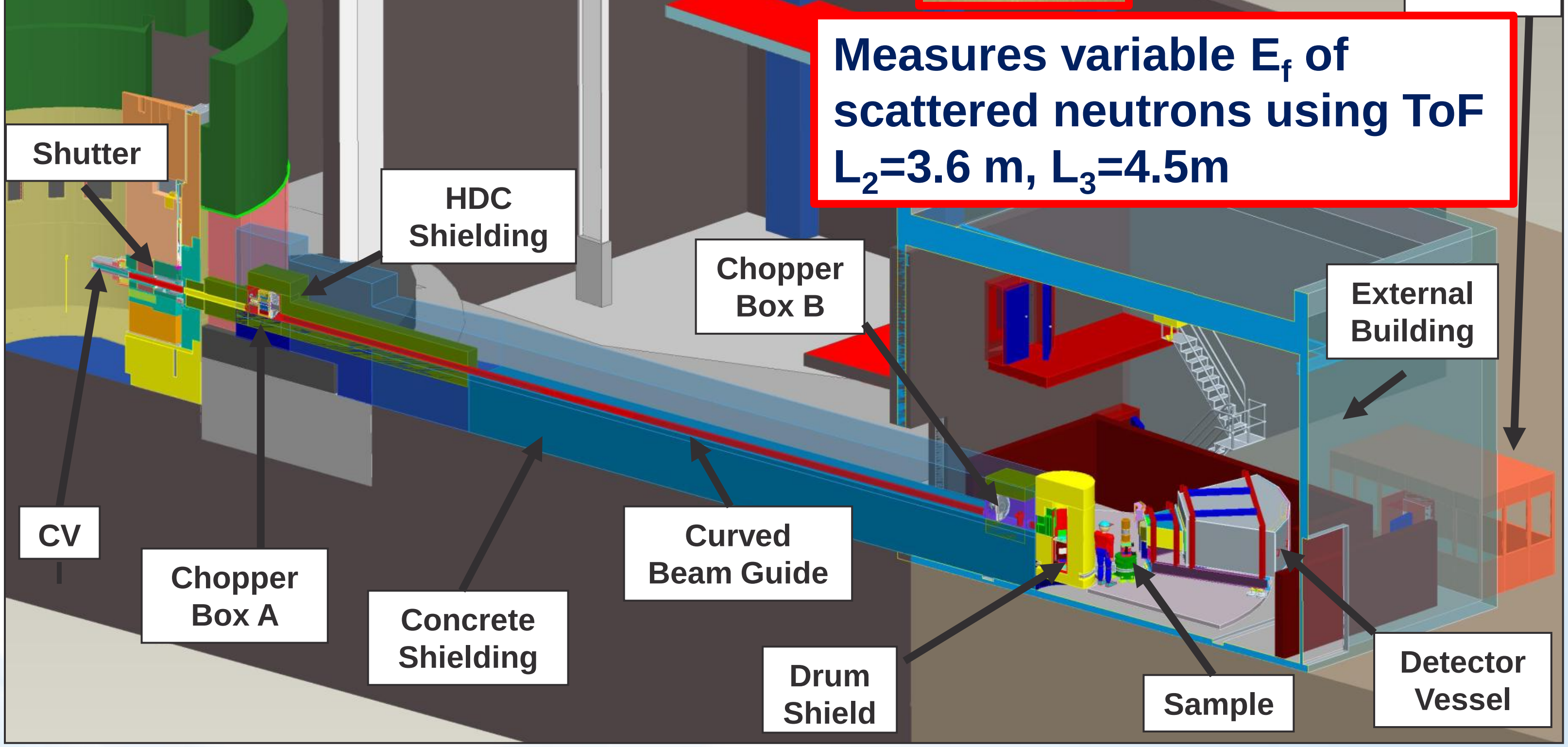
HYSPEC conceptual design - 2003



HYSPEC layout (design – 2008)

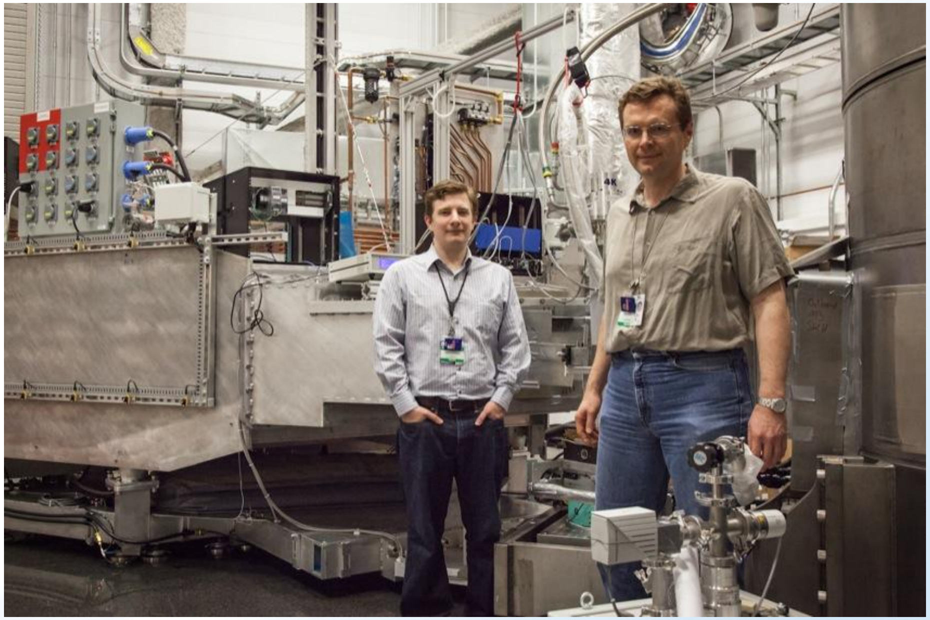
Short strait blade Fermi chopper at L_1=37.2 m to select E_i: trade off between E resolution and flux via frequency range 60-420 Hz

Measures variable E_f of scattered neutrons using ToF L_2=3.6 m, L_3=4.5m



HYSPEC in operation - 2012

Commissioning Experiments,
D. Fobes and I. Zaliznyak (2012)



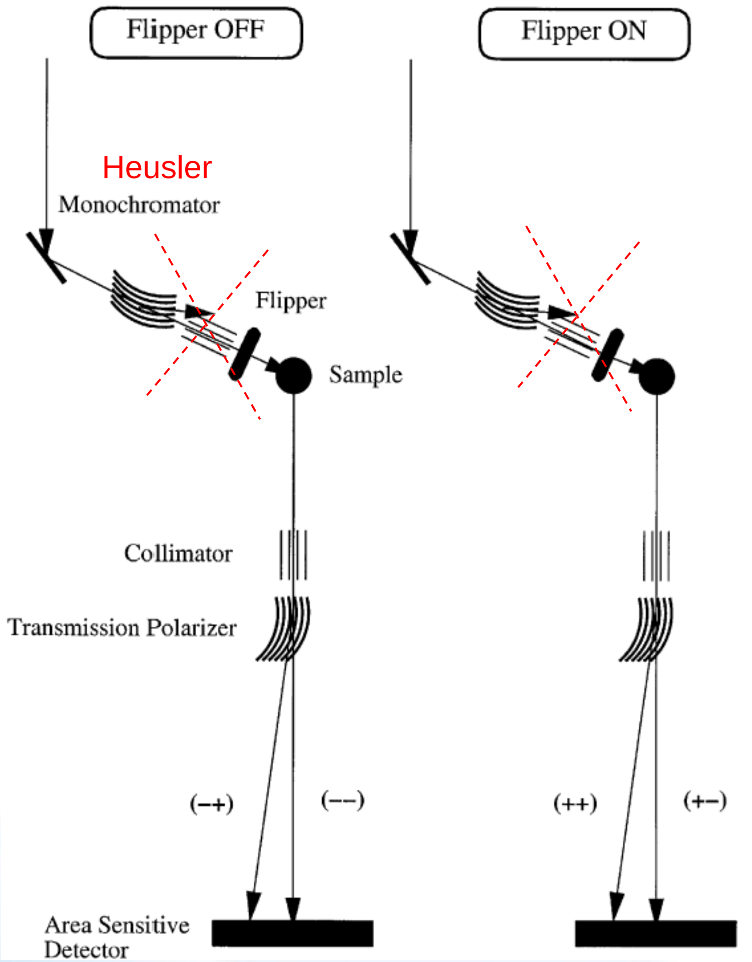
HYSPEC in operation - 2013

Tune-up complete: apertures, beam stop, shielding, shielding

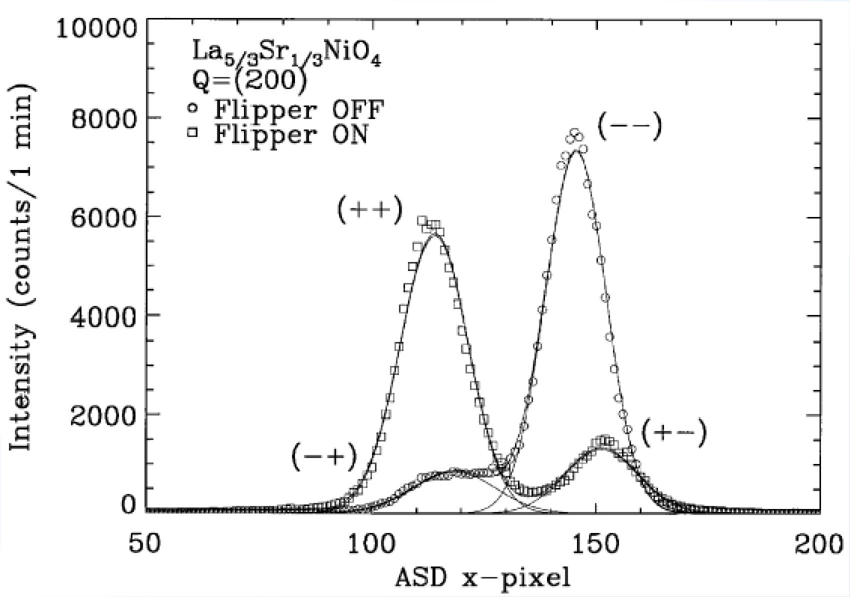
HYSPEC in operation - 2013

Tune-up complete: apertures, beam stop, shielding, shielding

Initial HYSPEC concept for polarized beam measurement with a Position Sensitive Detector (PSD)

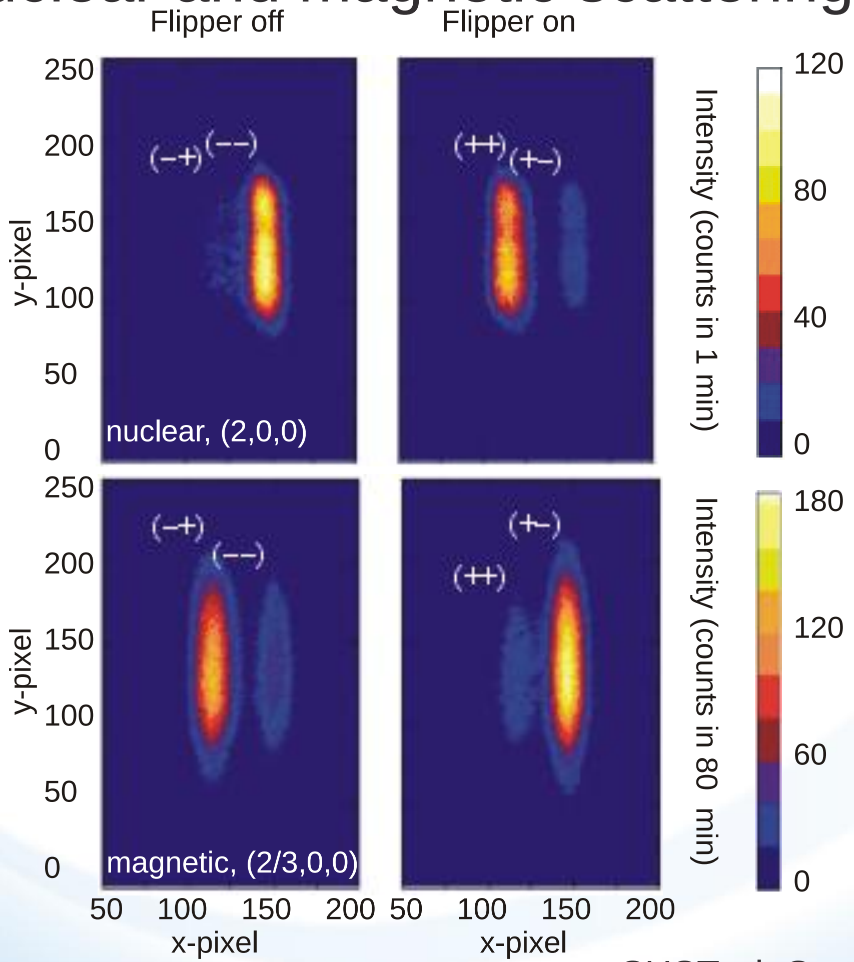


S.-H. Lee, C. F. Majkrzak, Physica B 267-268, 341 (1999)



Initial concept for HYSPEC polarization analysis: experimental demonstration with PSD on SPINS

Nuclear and magnetic scattering intensities in $La_{5/3}Sr_{1/3}NiO_4$



I. A. Zaliznyak and S.-H. Lee, in Modern Techniques for Characterizing Magnetic Materials, ed. Y. Zhu (Springer, 2005)

http://neutrons.phy.bnl.gov/HYSPEC

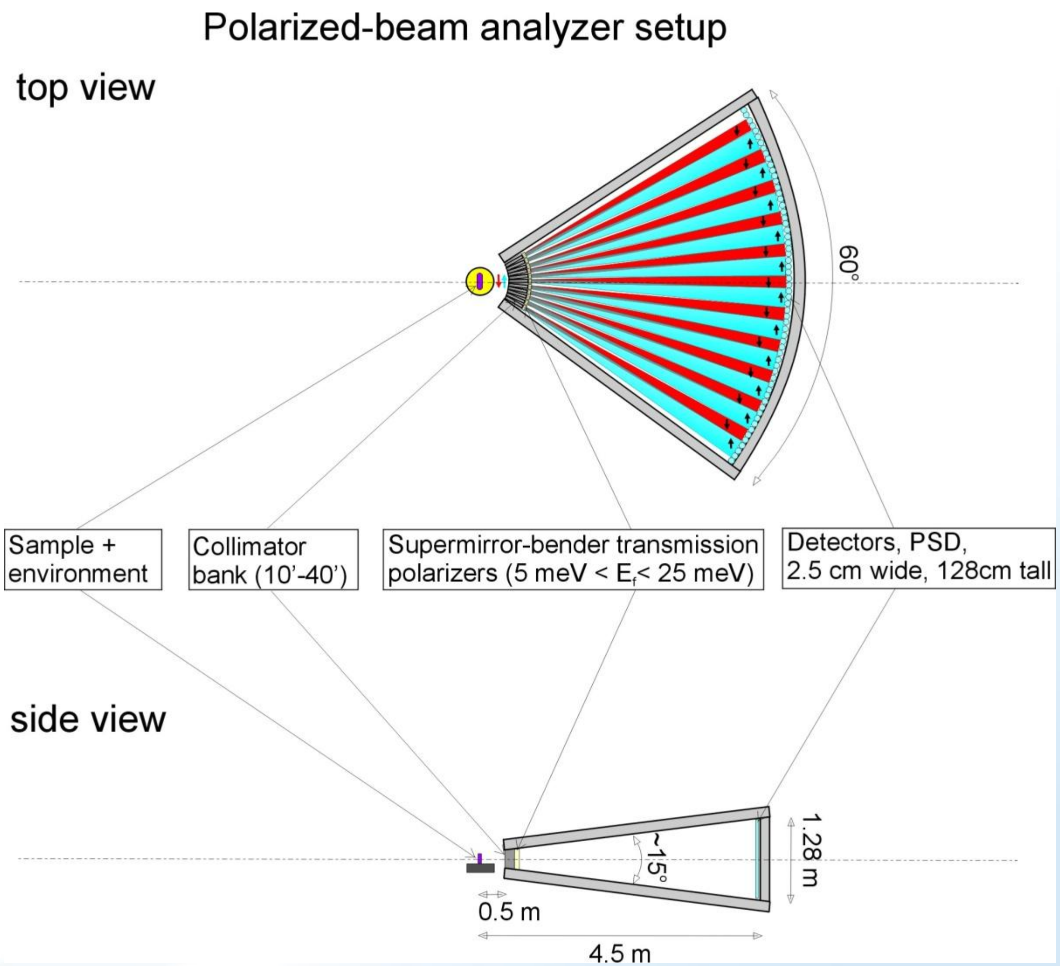
HYSPEC setup for polarization analysis (2002 design)

- Polarized incident beam is supplied by reflection from the vertically focusing Cu_2MnAl (Heusler alloy) crystal monochromator

10 meV < E_i^{pol} < 90 meV

- Polarization analysis of the scattered neutrons is performed by a set of 18-22 supermirror-bender transmission polarizers, each 2 cm wide, 5 cm thick and 15 cm high,

3.7 meV < E_f^{pol} < 15-25 meV

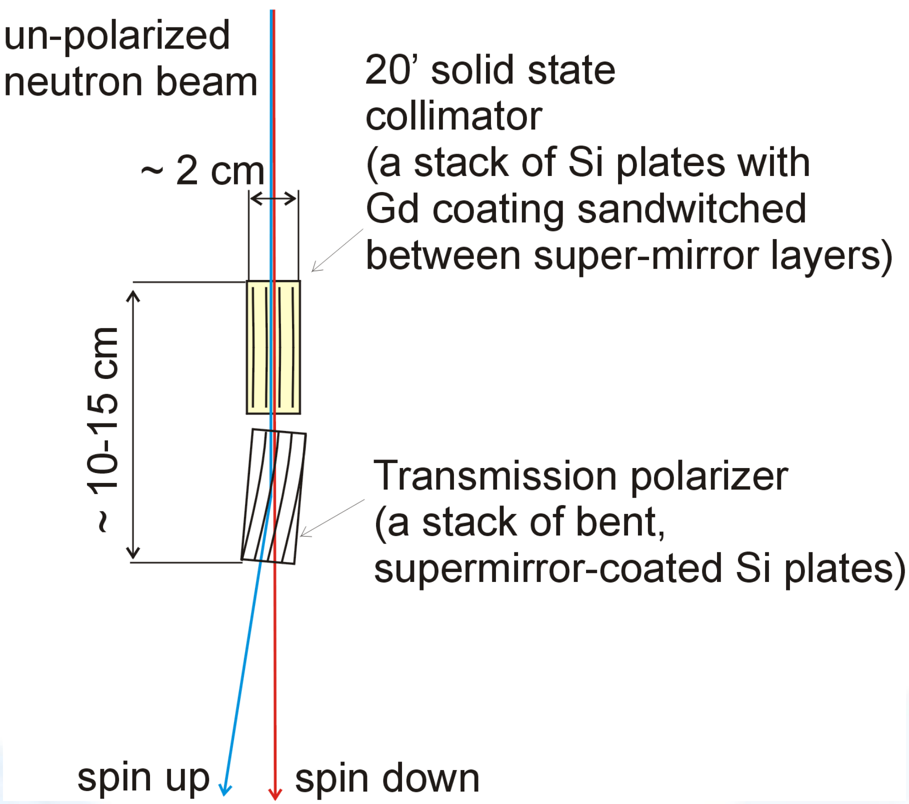


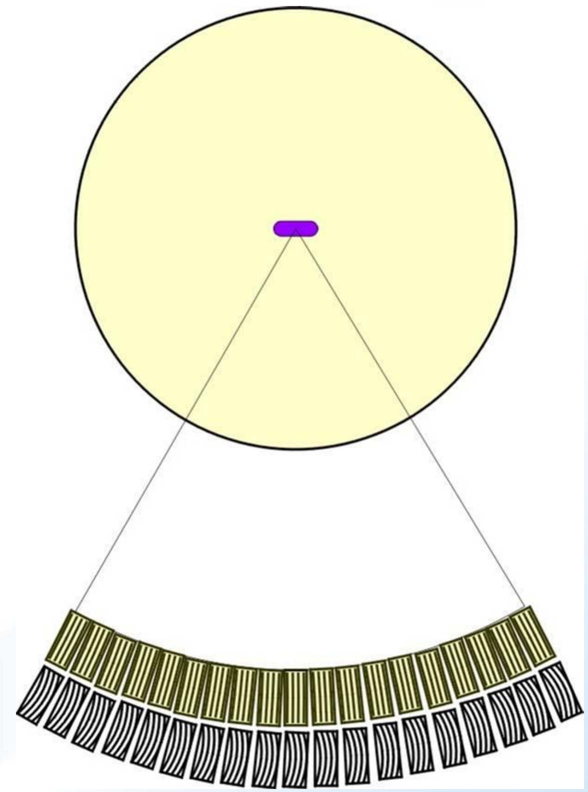
I. Zaliznyak, et. al., Physica B **356**, 150-155 (2005); cond-mat/0410040.

A supermirror-bender transmission polarizer setup for HYSPEC (2002)

A very compact device
(but needs a saturating magnetic field)

An array of 20 benders covers 60 deg. acceptance of the detector bank.

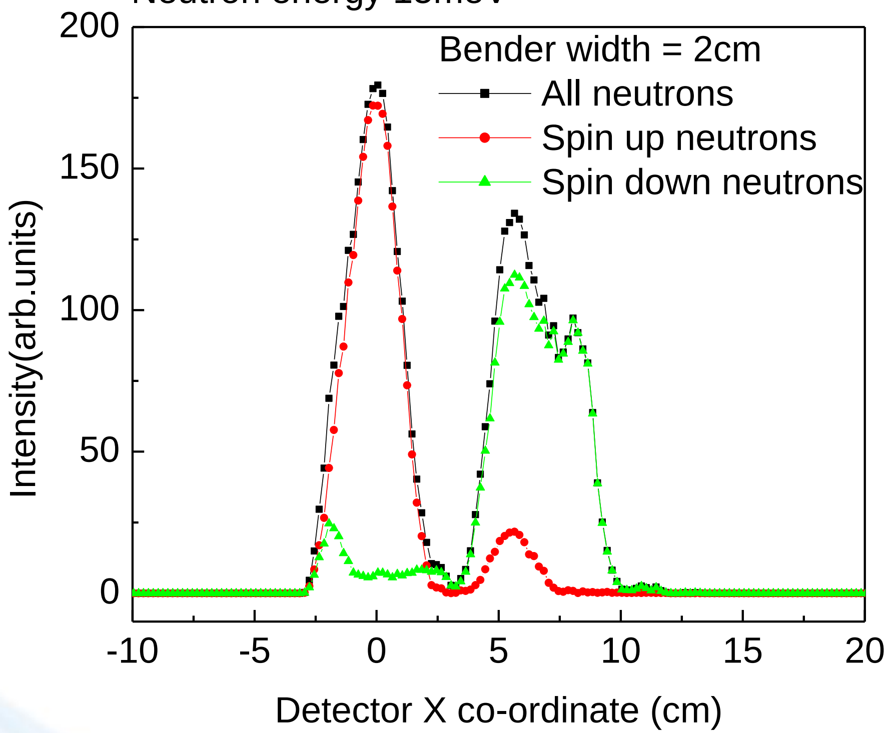


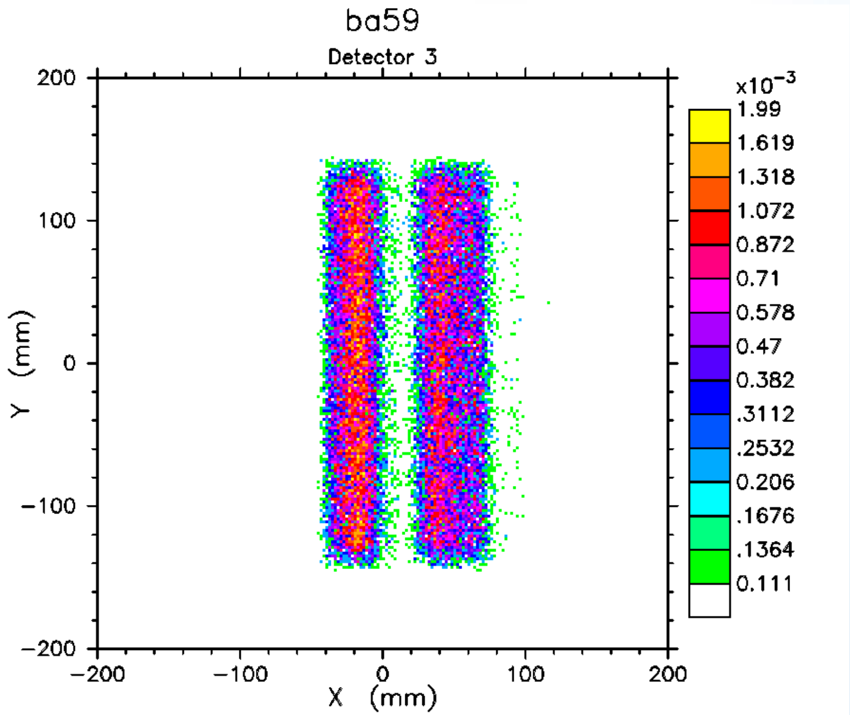


I. Zaliznyak, et. al., Physica B **356**, 150-155 (2005); cond-mat/0410040.

MC simulation (NISP) of HYSPEC operation in the polarized beam mode: beam separation

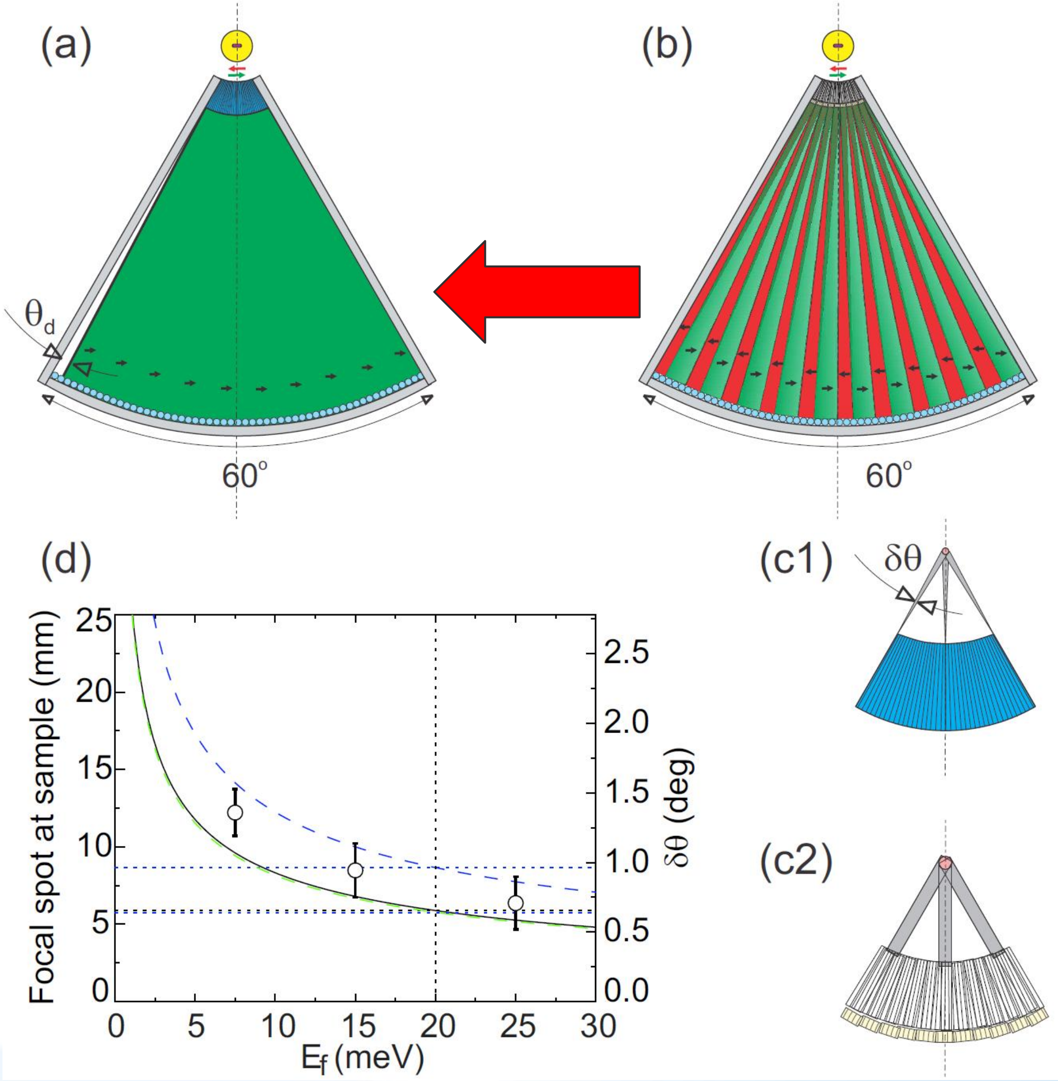
Simulation for the bender geometry optimized for E=14.7 meV (C. Majkrzak, 1995)
Sample-to-detector distance L_{SD} is 4.5 m





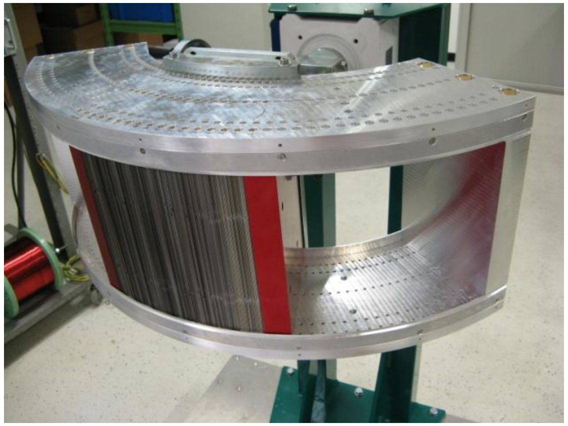
I. Zaliznyak, et. al., Physica B **356**, 150-155 (2005); cond-mat/0410040.

Change of plan: Radial Supermirror

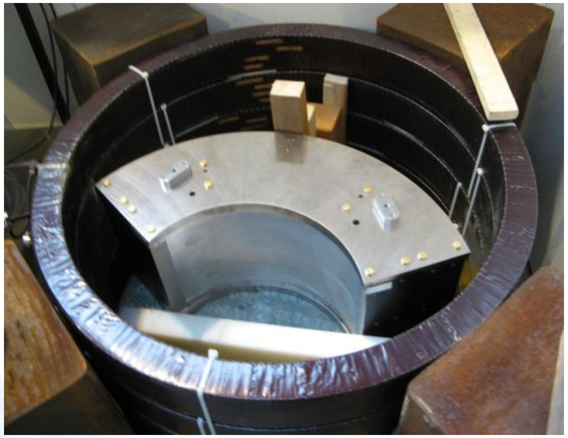


SUSTech Symposium on Neutron Diffractometer/Spectrometer.Shenzhen, Oct. 2016.

Change of plan: PSI Supermirror Polarization Analyzer

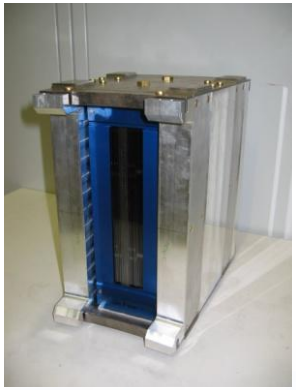


Supermirror analyzer assembled with around 200 supermirrors



supermirror analyzer inside the magnetization unit (500 G)

Prototype I (1.8 deg)

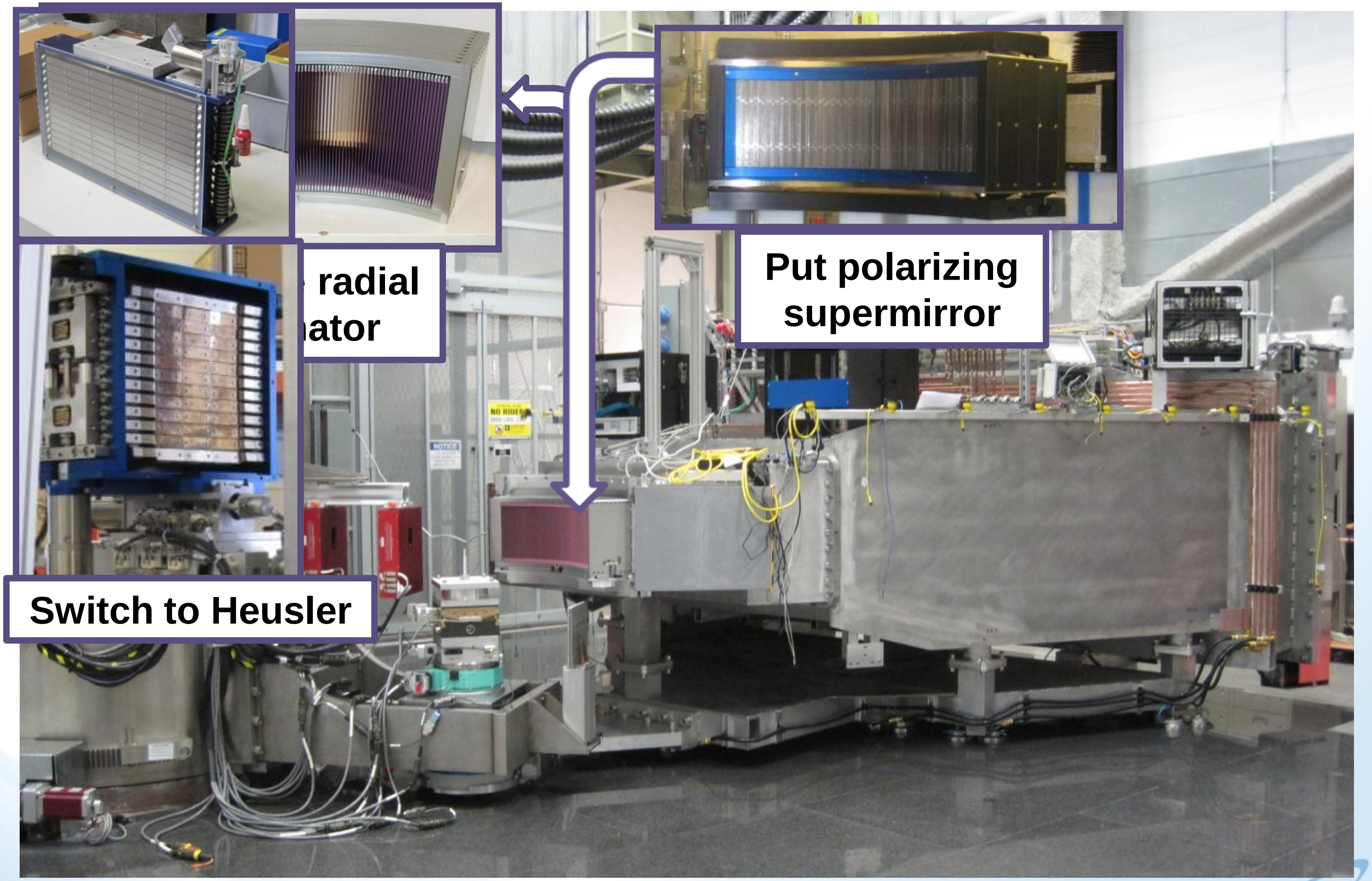


Prototype II (4.0 deg)

2011 status:

- 780 out of 960 polarizers produced
- ~100 polarizers per month
- 200 polarizers installed in housing & tested on BOA (optics beamline at SINQ, PSI)
- Anticipated completion in March 2011, followed by tests at SINQ

Polarized beam setup with the PSI Polarizing Supermirror Array (B. Winn)

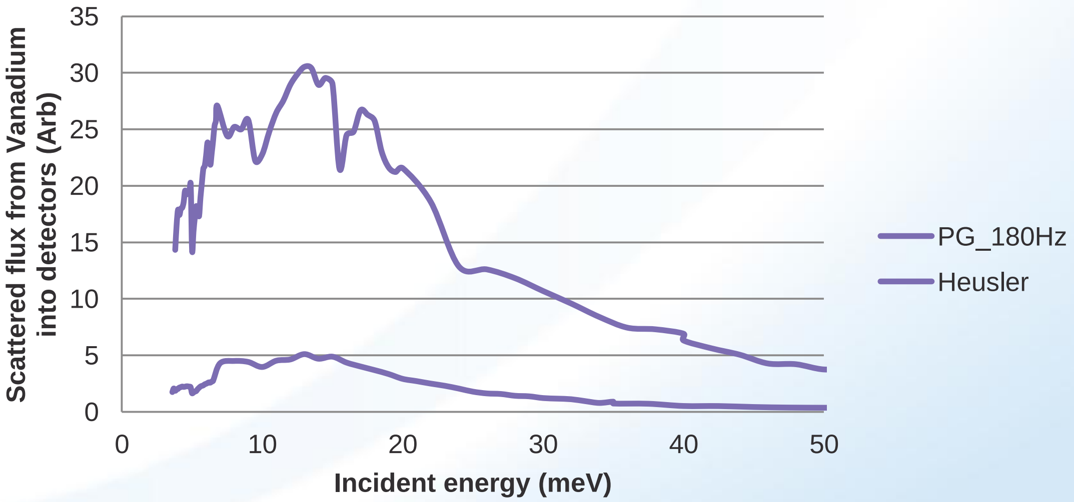


Intensity at sample, V scatterer

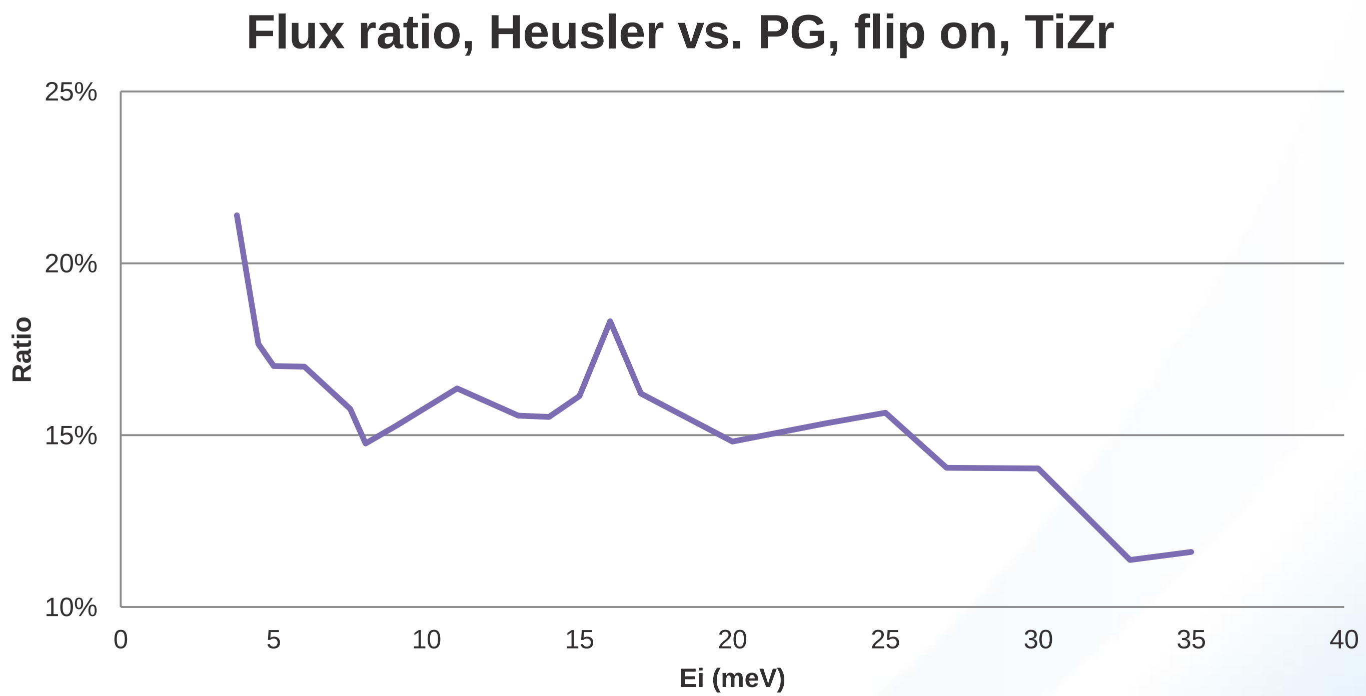
- 15 cm high beam from guide vertically focused to sample ~2.5 cm x 2.5 cm FWHM
- 4.2E5 n/s/MW/cm^2: Gold foil measurement at sample position, PG focus array to sample 1.8 m, Ei=15 meV, Fermi 180 Hz
- Plot: Vanadium incoherent isotropic scatter integrated over detector array at 40^o < 2Θ < 100^o, PG & Heusler

3.8 meV < Ei < 50 meV

Common Ei's:
3.8, 7, 15, 20, 27, 35 meV
Rare Ei: 50 meV

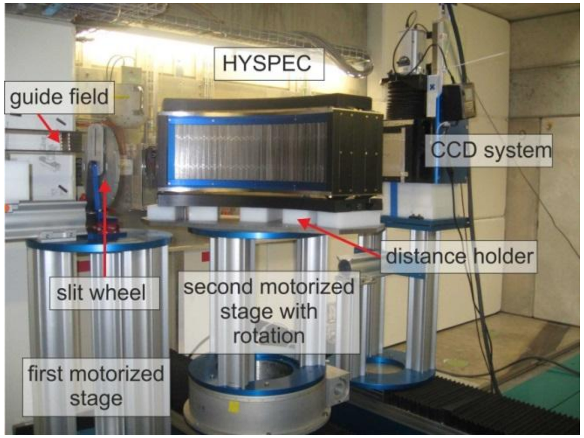


Heusler relative to PG



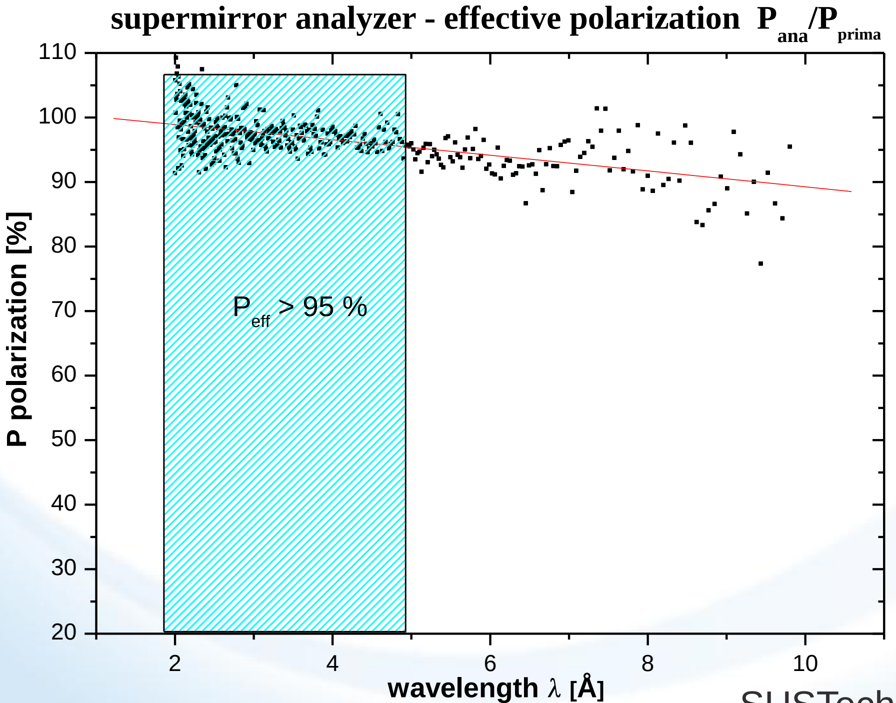
- Working energy range Ei 3.8 meV to 25 meV
- Loss in flux on sample 5 to 10 times

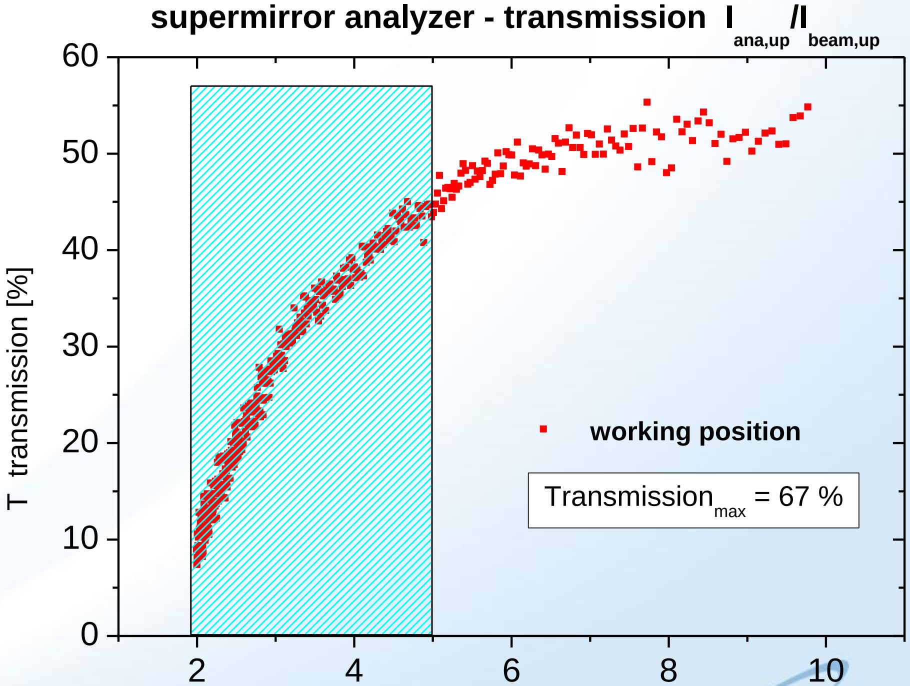
Performance of the Polarizer



960 supermirrors, 60º
U. Filges
BOA beamline at SINQ
Ready to ship

Magnetization unit at HYSPEC





Polarized beam commissioned (2015)

Neutron Sciences FUTURE FOR USERS ABOUT SCIENCE INSTRUMENTS & SUPPORT PUBLICATIONS NEWS CAR

https://neutrons.ornl.gov/news/supermirroruser

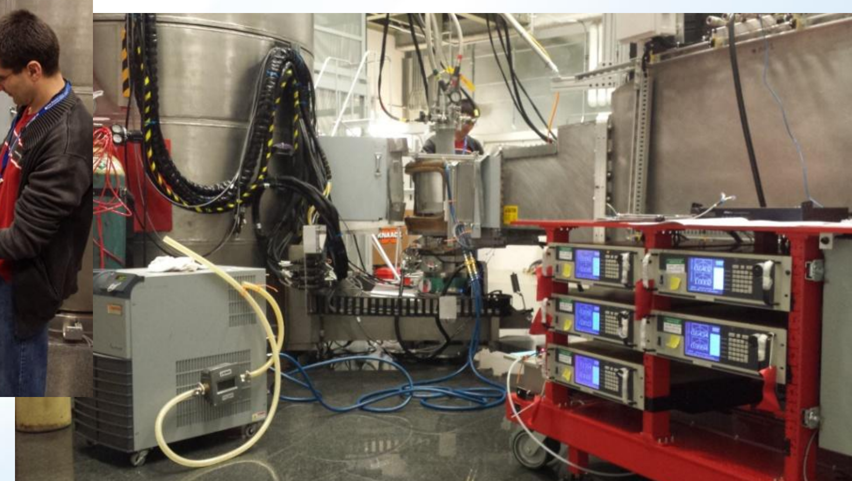
More Power to HYSPEC

November 11, 2015

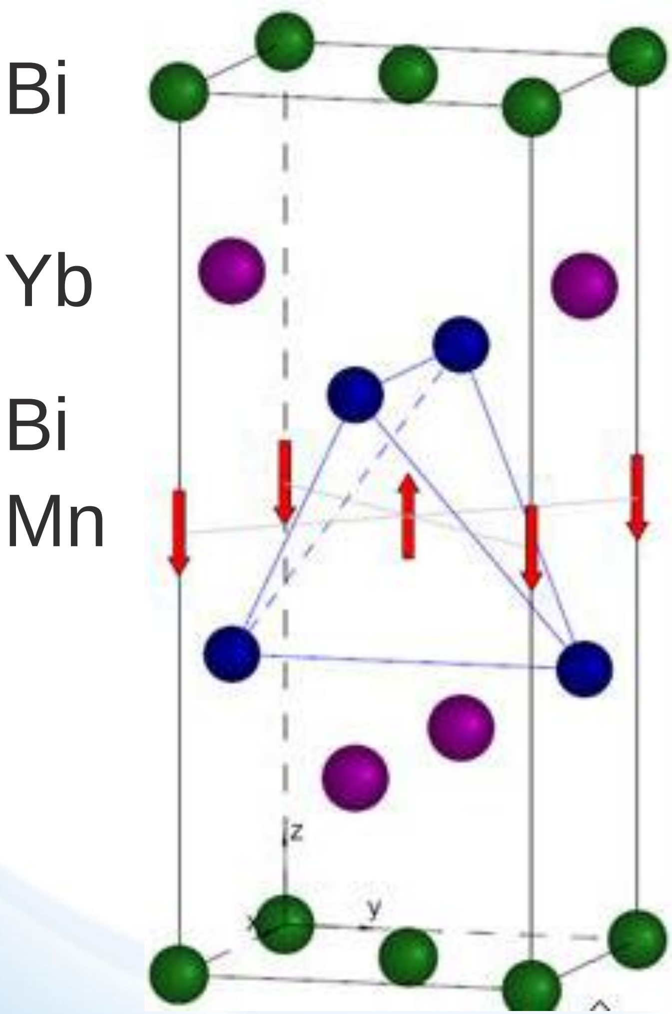
After installing the new wide-angle super mirror array at SNS's hybrid spectrometer, beam line 14B, HYSPEC is ready to tackle new problems using fully polarized neutron scattering.

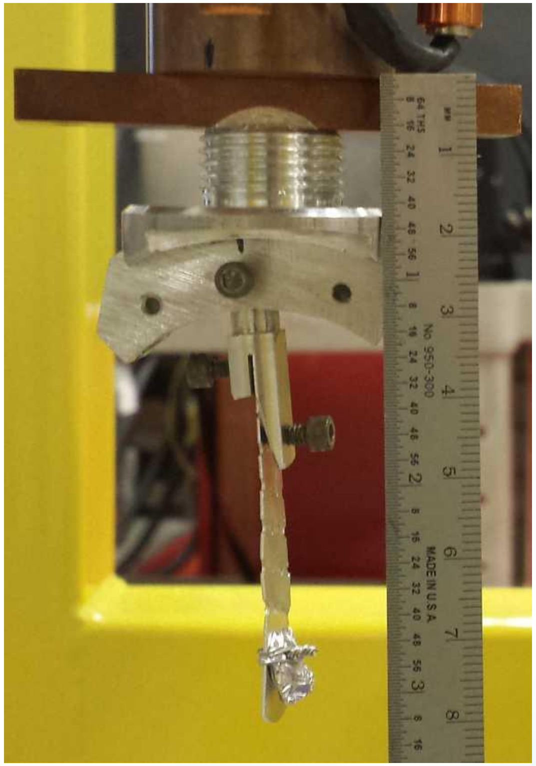

HYSPEC

HYSPEC polarized beam setup in operation



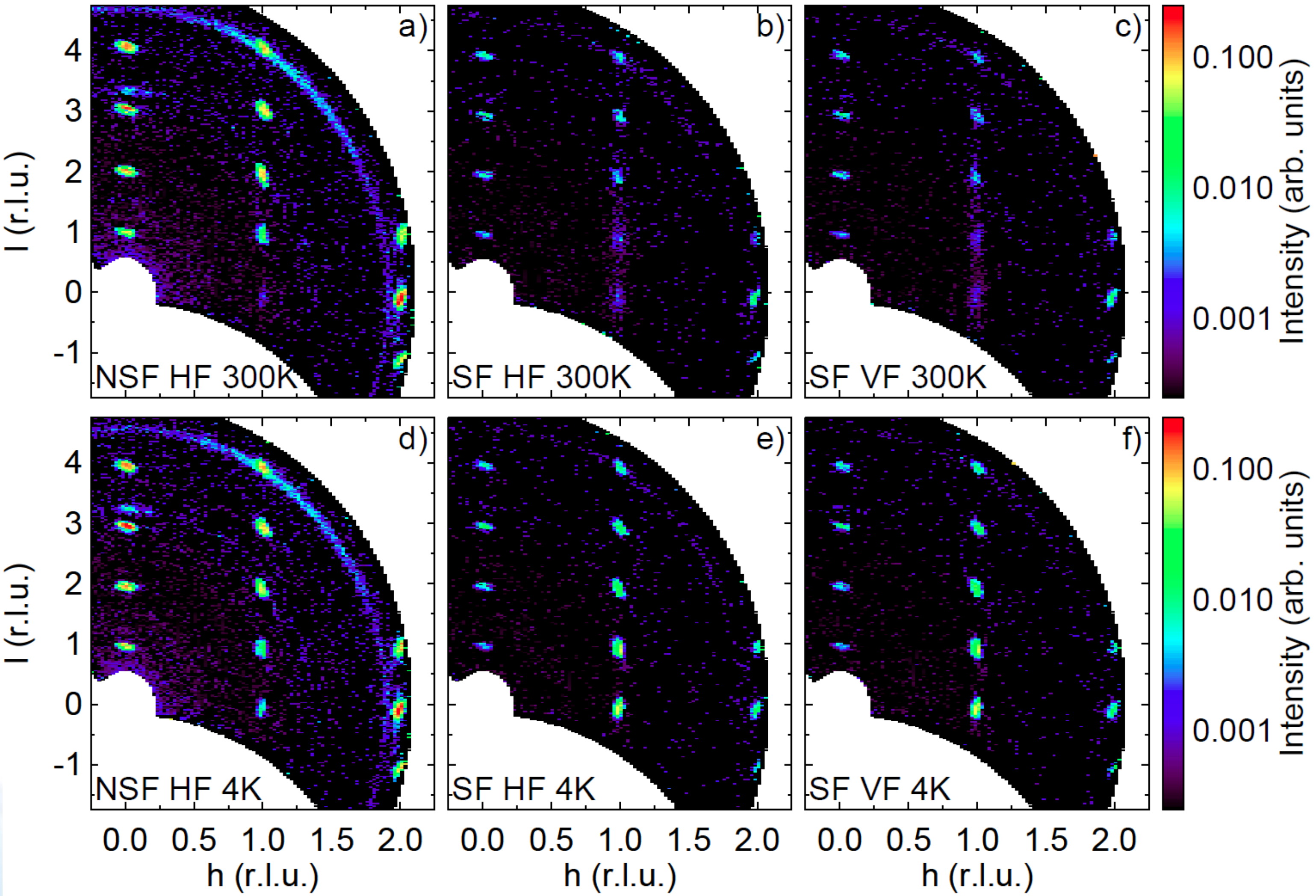
First test: antiferromagnetic structure of the layered semimetal $YbMnBi_2$



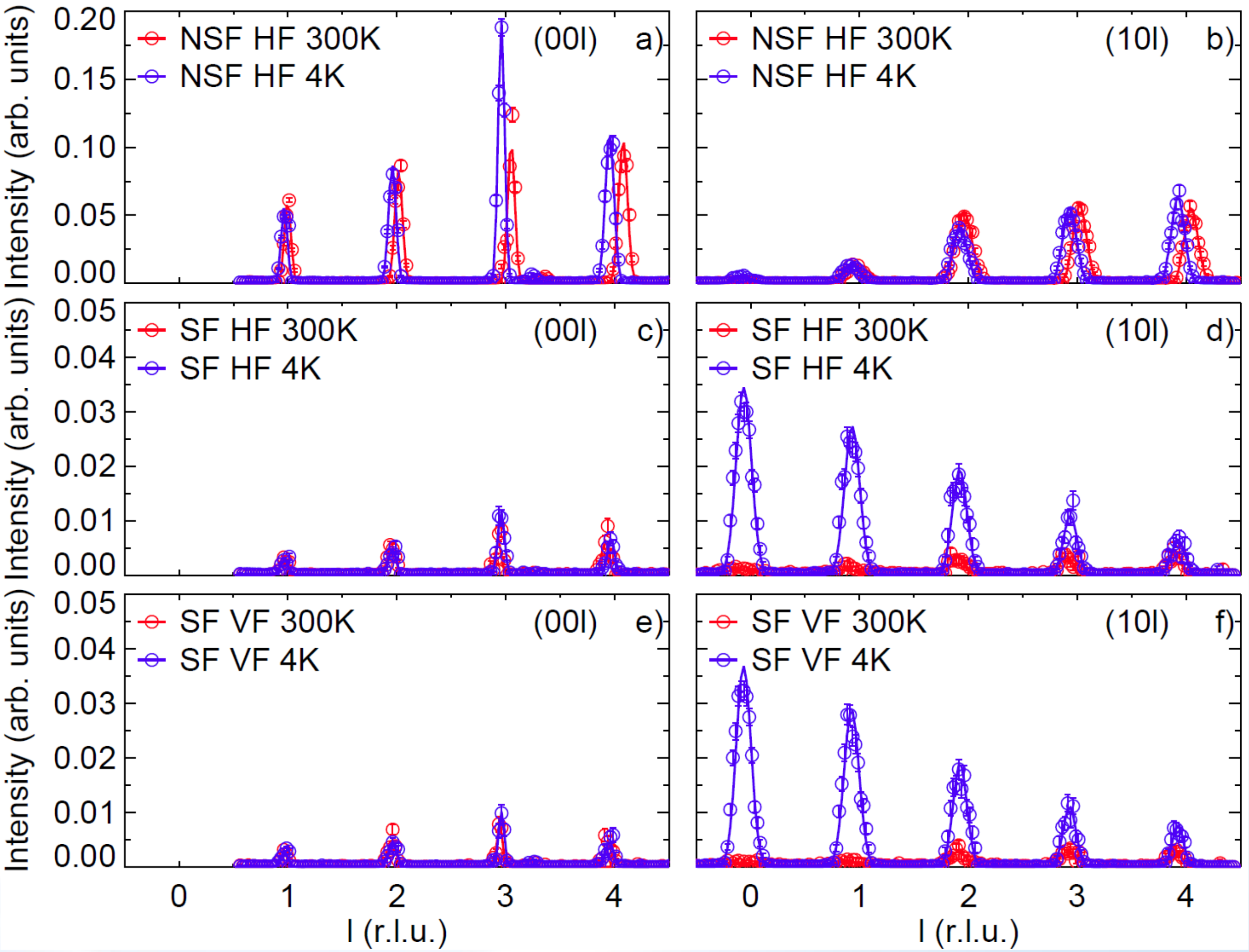


$YbMnBi_2$ (~0.5g) single crystal

Polarized diffraction measurement of $YbMnBi_2$: one night on HYSPEC



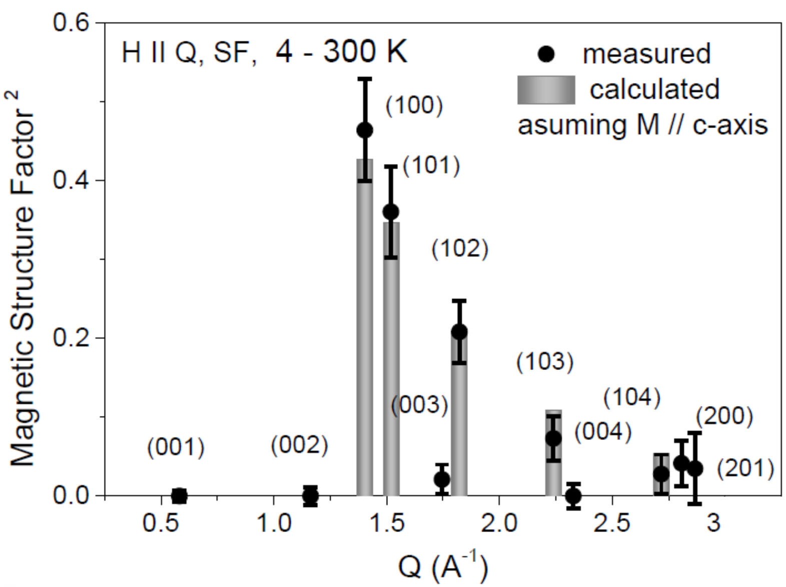
Polarized diffraction scans on $YbMnBi_2$ Bragg peaks



HYSPEC is not a diffractometer, but… can do diffraction, if needed

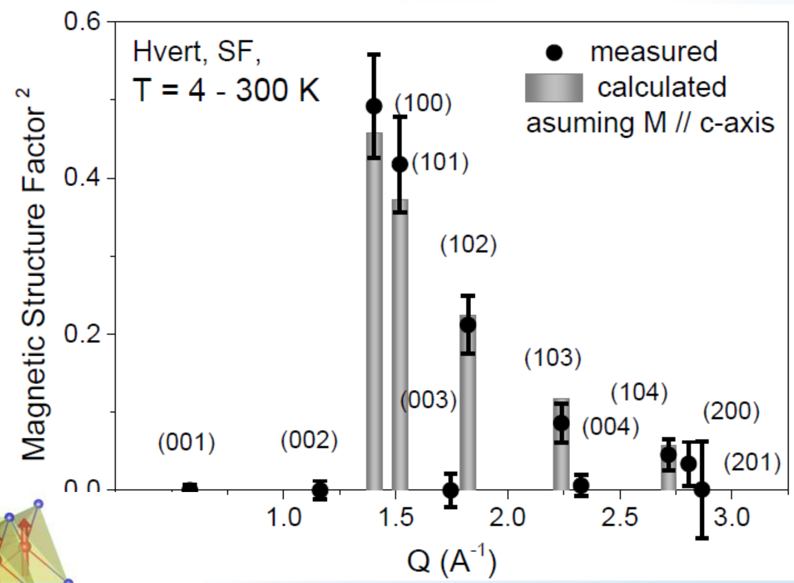
The refinement compares favorably to HB3 diffractometer

Fit of the **4K – 300 K data with P || Q**. AFM model with spins along c axis gives ordered moment amplitude of **4.37(18) μ_B**

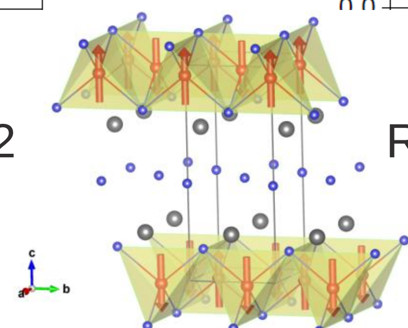


RF-factor: 25.9, χ^2(Intensity): 0.72

Fit of the **4K – 300 K data with P vertical (⊥Q)**. AFM model with spins along c axis gives ordered moment amplitude of **4.52(17) μ_B**

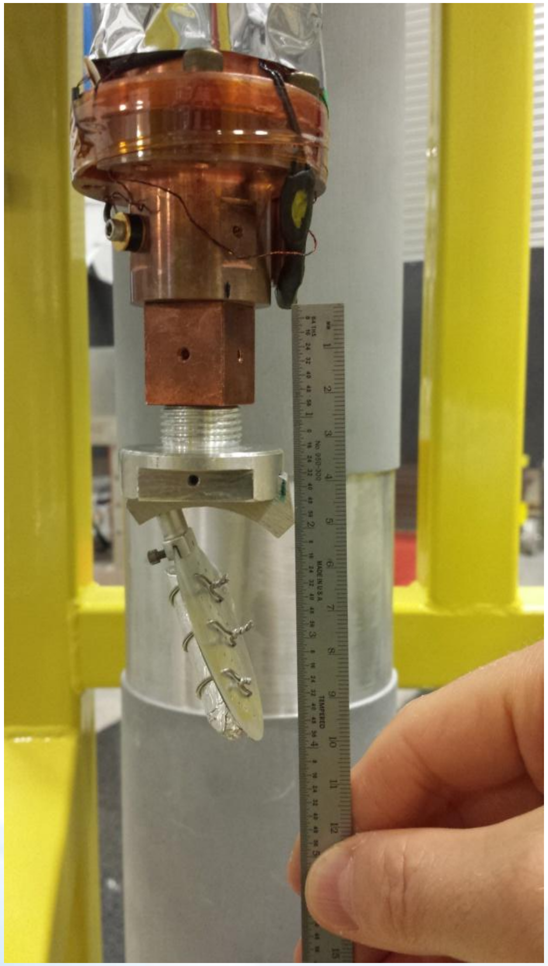


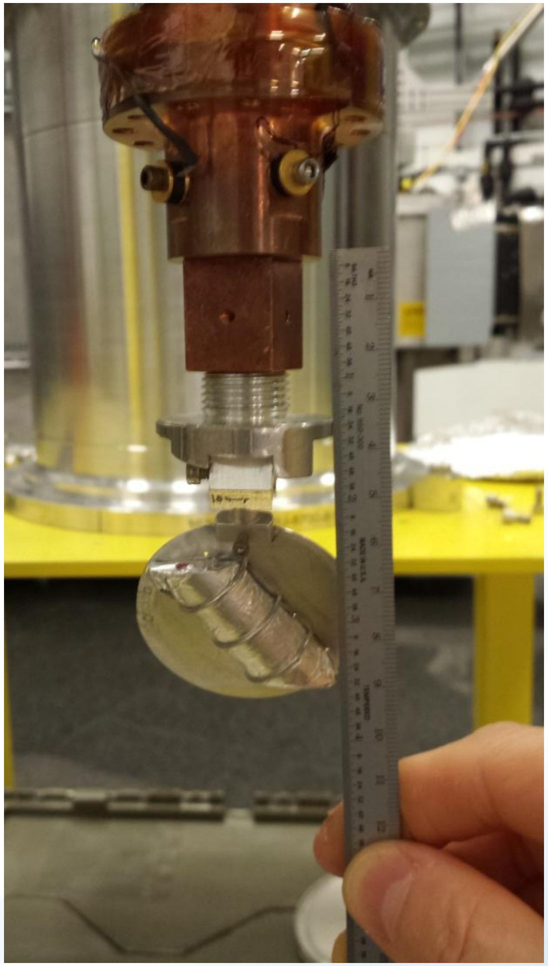
RF-factor: 17, χ^2(Intensity): 0.46

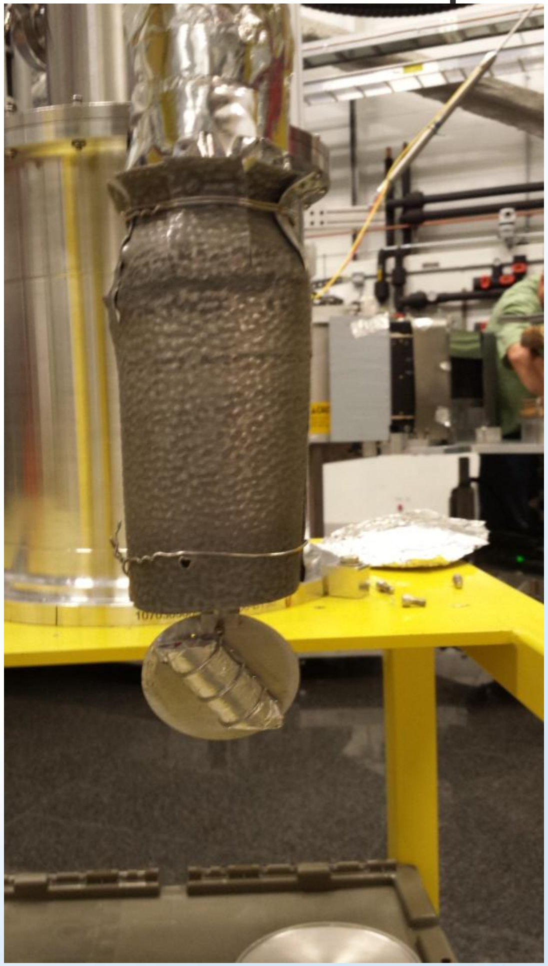


Magnetic dynamics in $FeTe_{0.45}Se_{0.55}$ superconductor: sample geometry

Large (~ 23g) bulk single crystal, irregularly mounted on Al plate



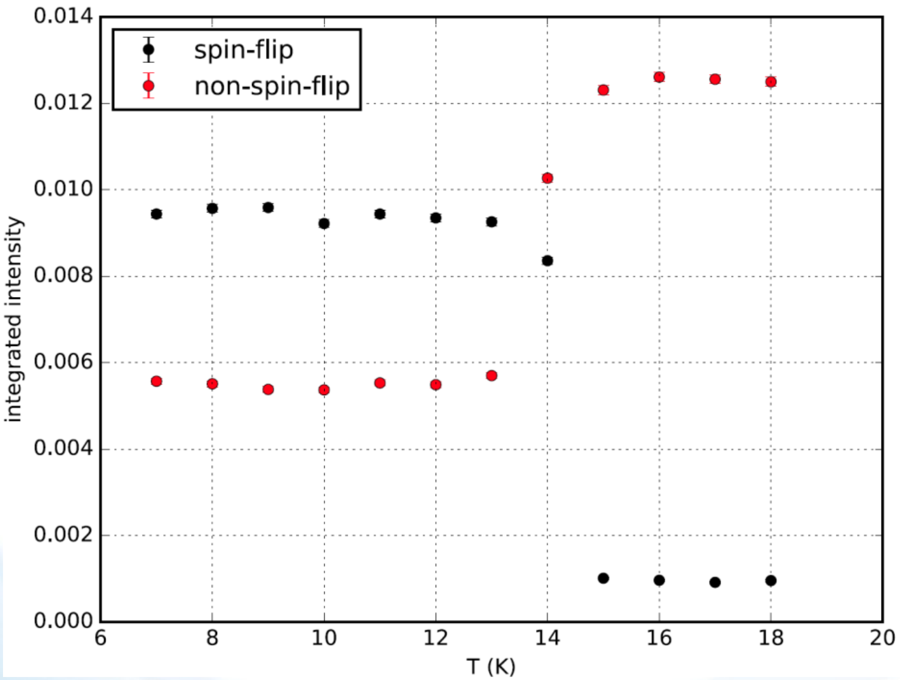


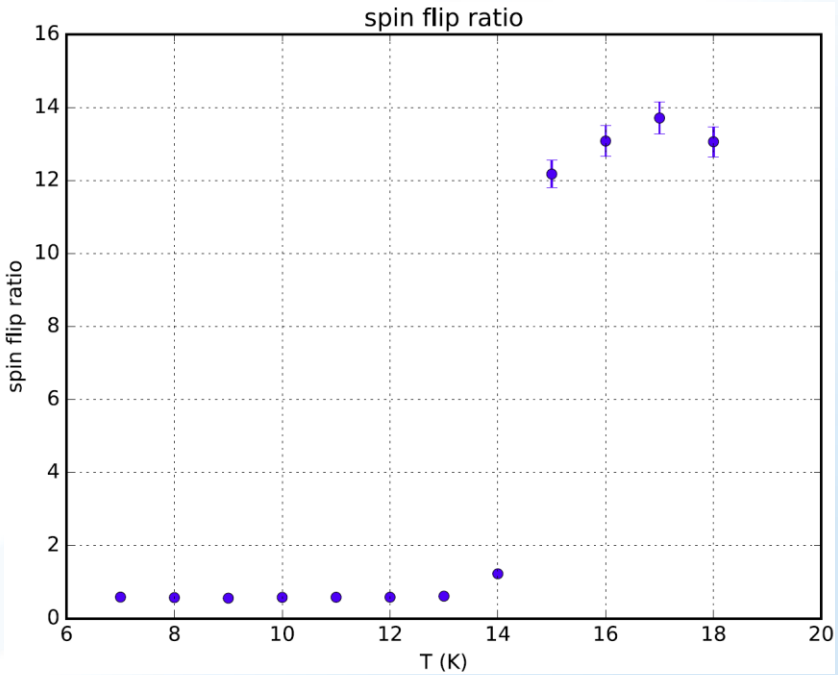


Beam depolarization in superconducting $FeTe_{0.45}Se_{0.55}$

Sample is cooled in guide field ~ 10~20G => the beam is fully depolarized at T<Tc!

Flipping Ratio (T>Tc) = 13(1)





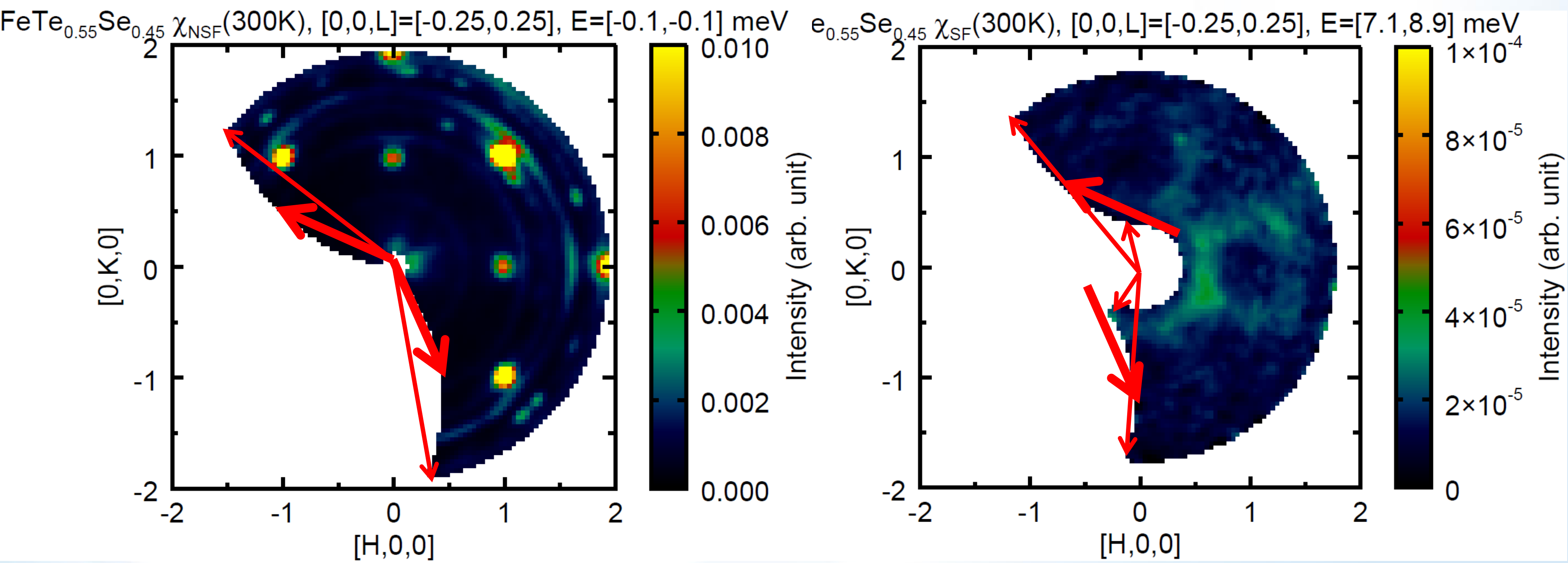
Zero field cooling: FR = 5 ~ 8

- Cooled in a mu-metal shield from 16 K to 5 K
- Cooled on the instrument sample table, in a compensating guide field providing zero field environment
- Effect is similar: flipping ratio improved.
- FR varies from 5 to 8, depending on the sample rotation angle

“P||Q” setup: align polarization with the middle of detector at E=0

Change of the mutual alignment of **P** and **Q** with energy transfer

E=0 meV   E=8.0(9) meV



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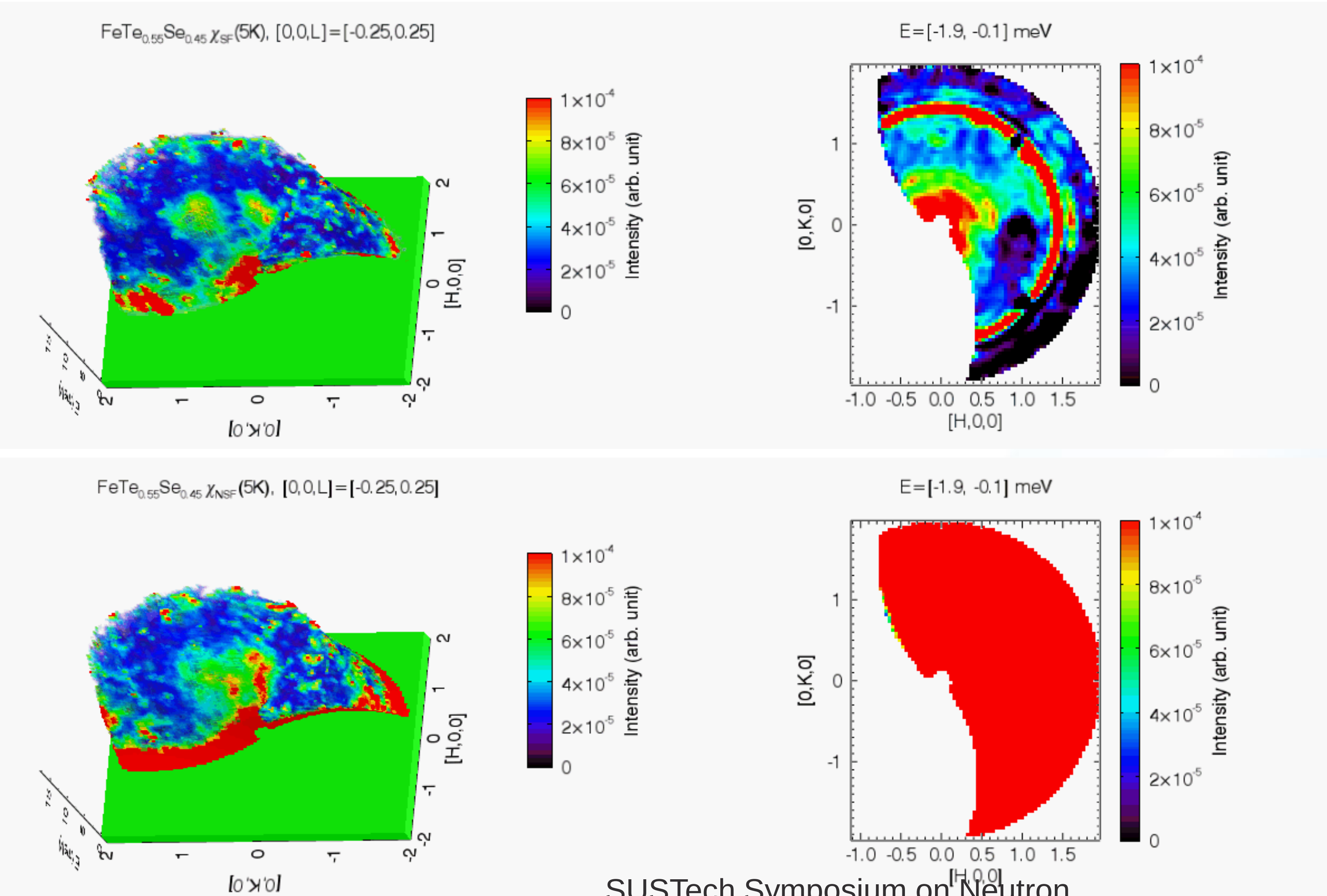
SF and NSF at 5 K



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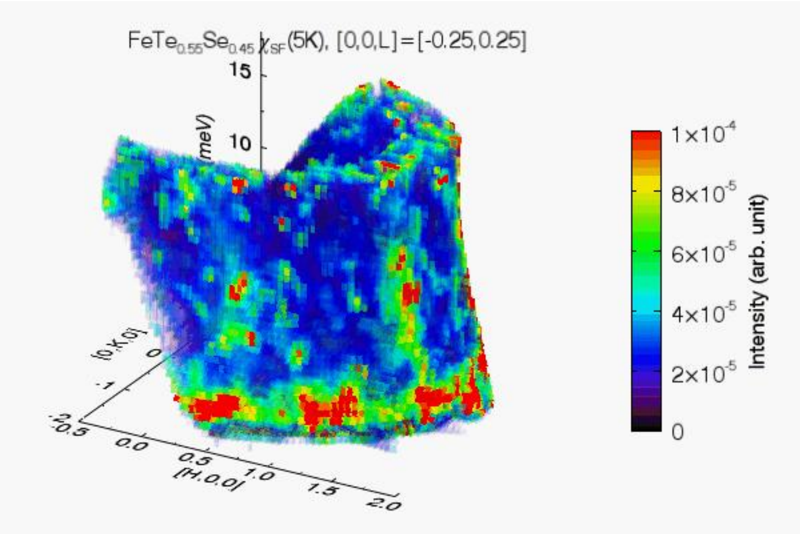
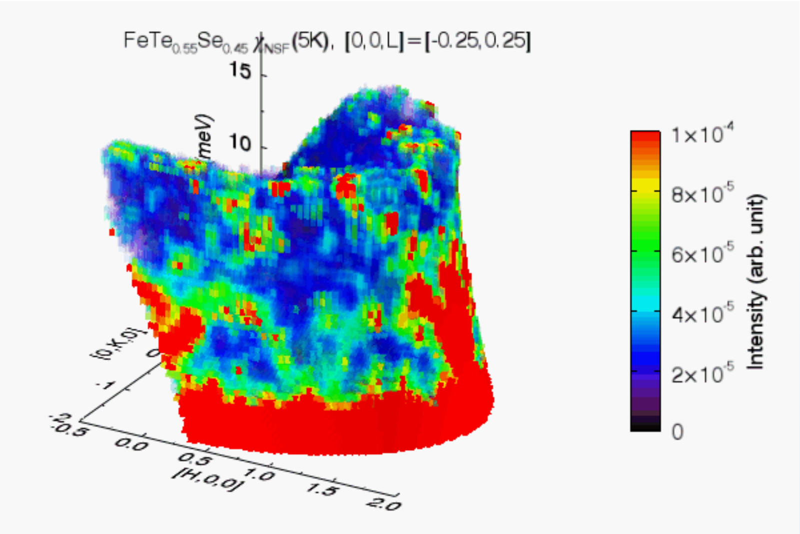
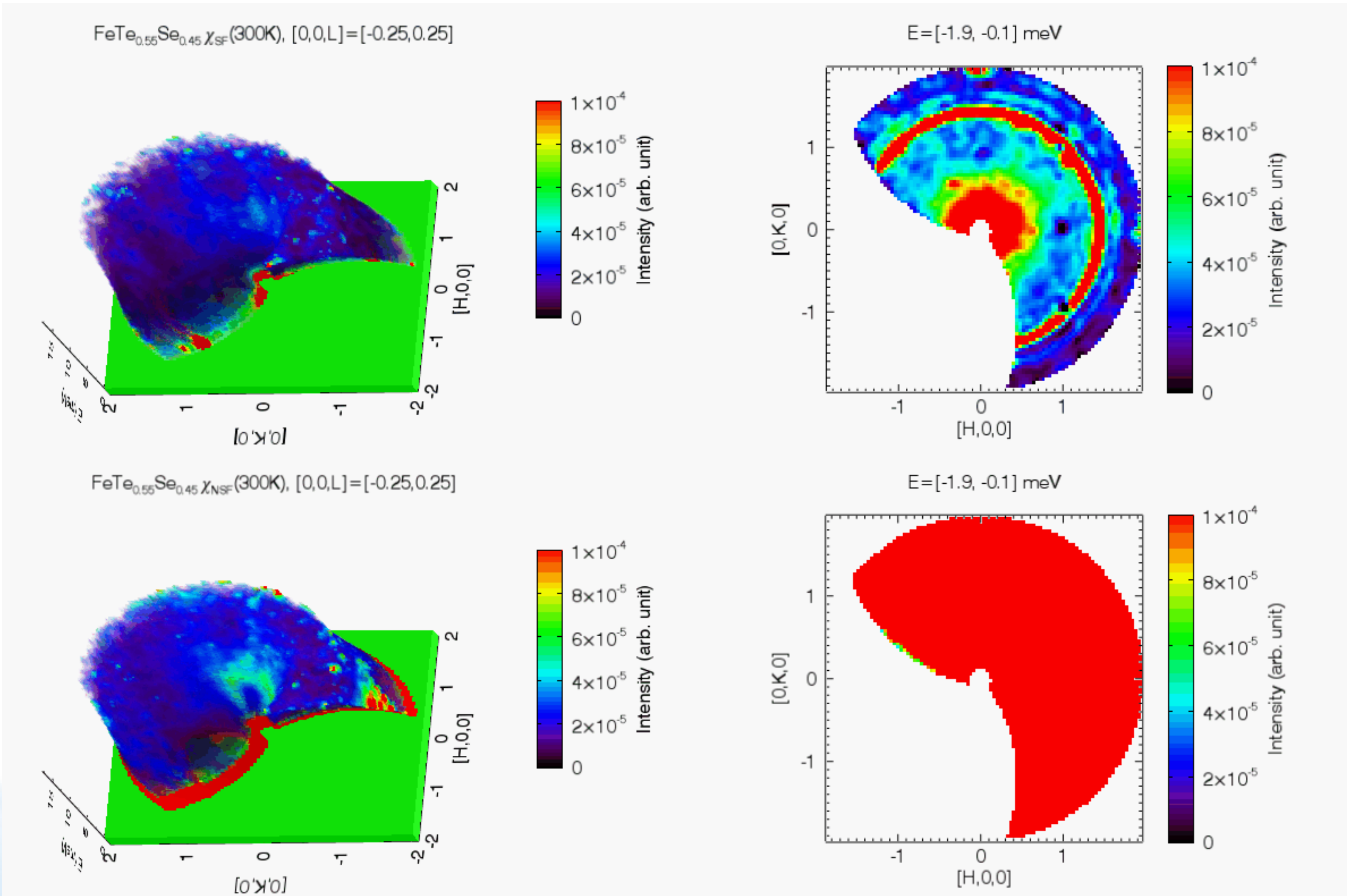




SF and NSF at 300 K

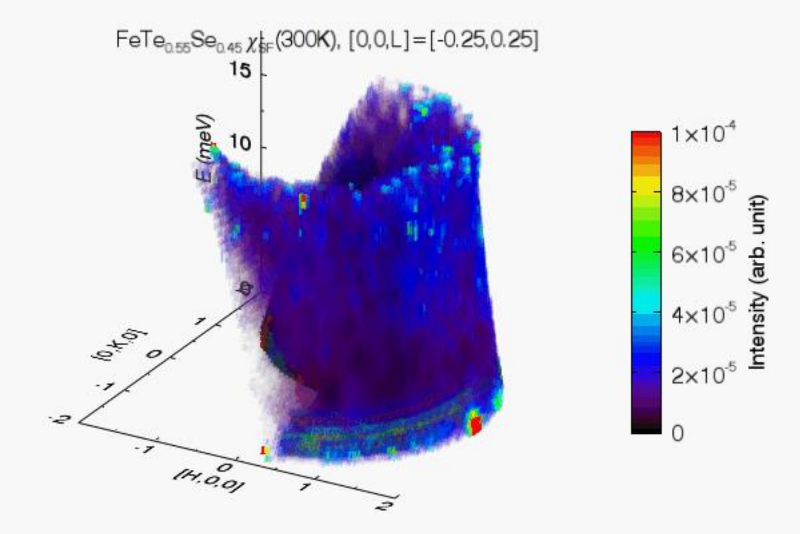


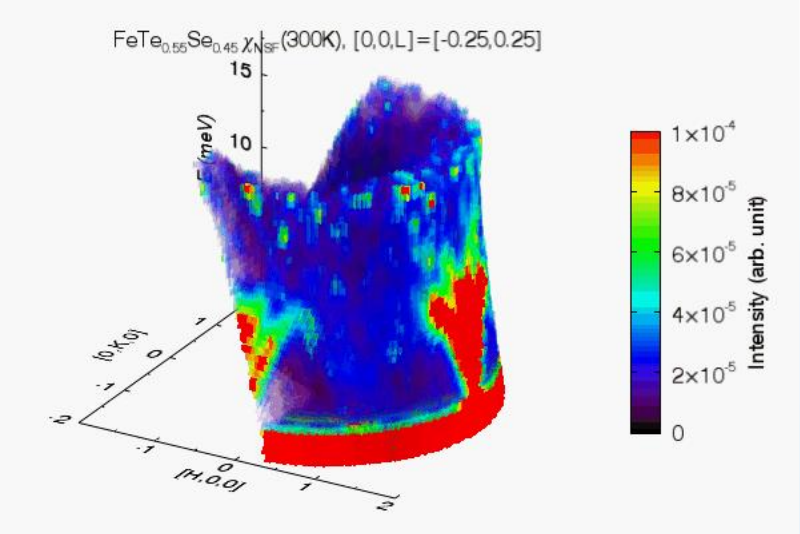
SUSTech Symposium on Neutron Diffractometer/Spectrometer.Shenzhen, Oct. 2016.

Brookhaven Science Associates

BROOKHAVEN NATIONAL LABORATORY

SF and NSF at 300 K





Magnetic and non-magnetic excitations in $FeTe_{0.55}Se_{0.45}$ by polarized neutron scattering on HYSPEC

I. Zaliznyak , O. Garlea, A. Savici, J. Schneeloch, J. Tranquada, Z. Xu , G. Xu , G. Gu

Comparison of the equivalent slices from the Spin-Flip (left) and the Non-Spin-Flip (right) data sets

Spin-Flip Scattering (magnetic)
$I_{SF}(Q,E)$ at T = 300 K

Non-Spin-Flip Scattering (phonon)
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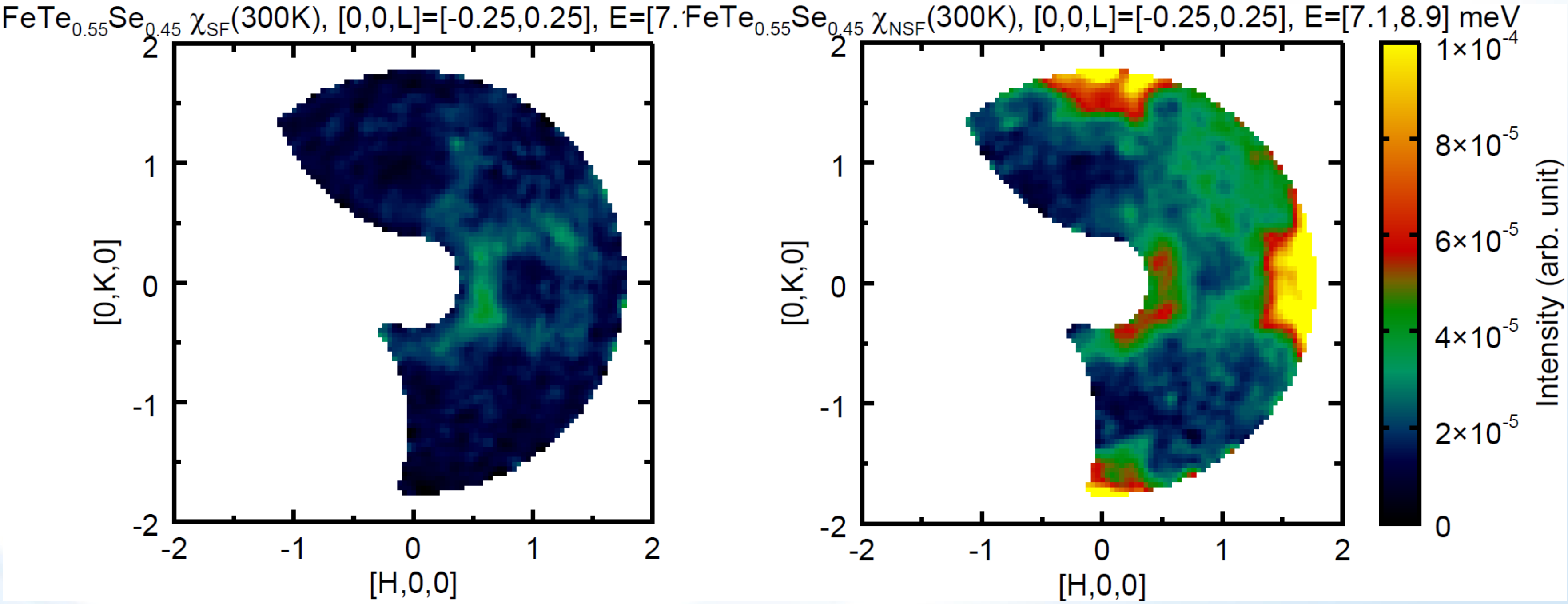

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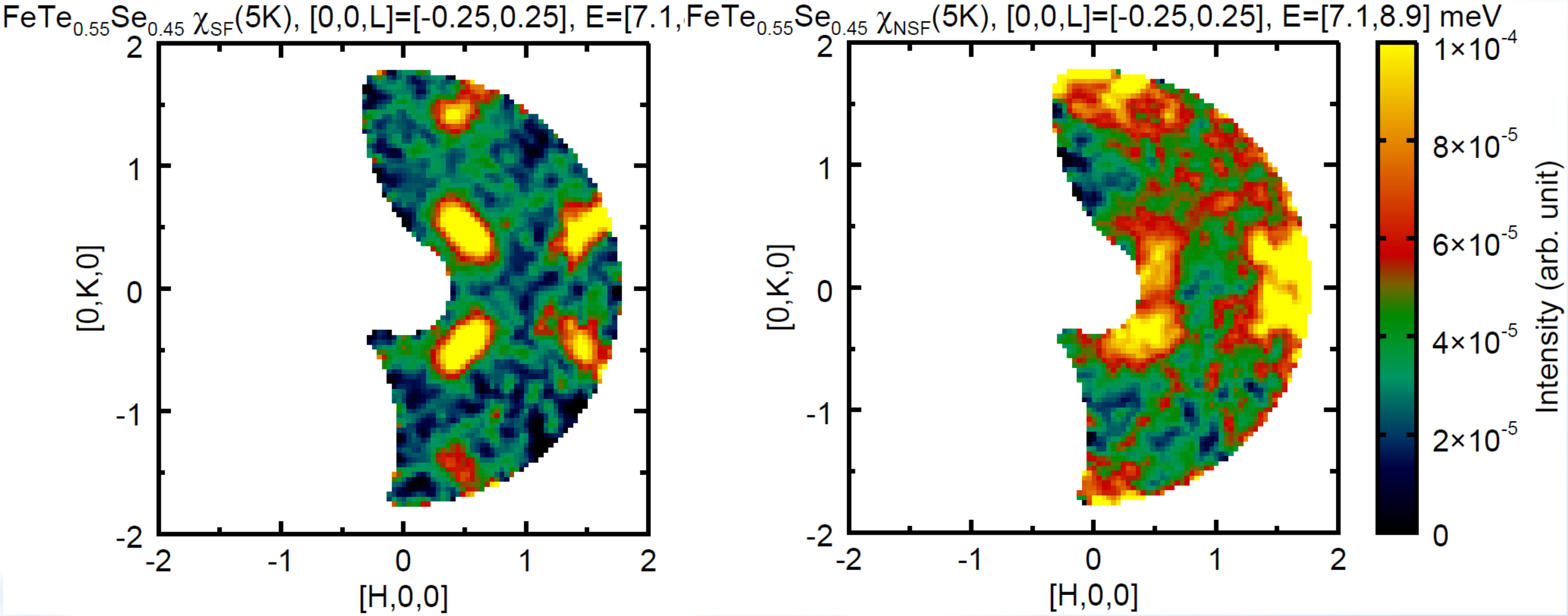

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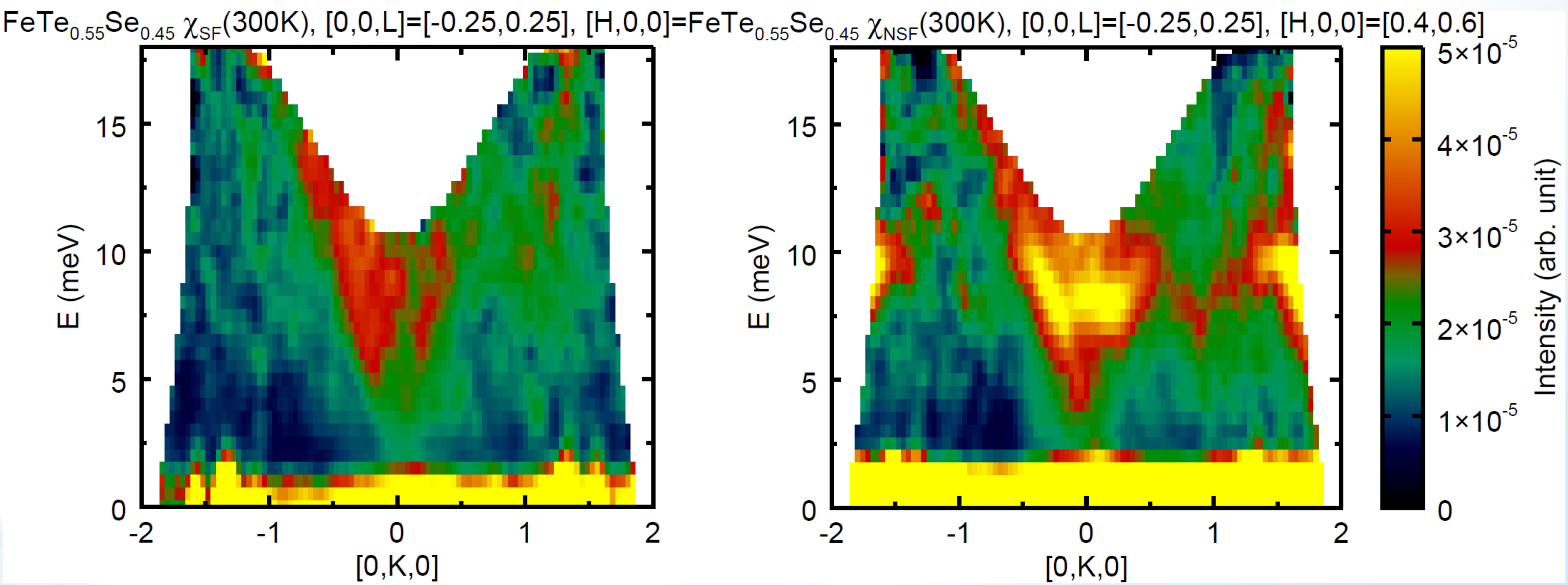

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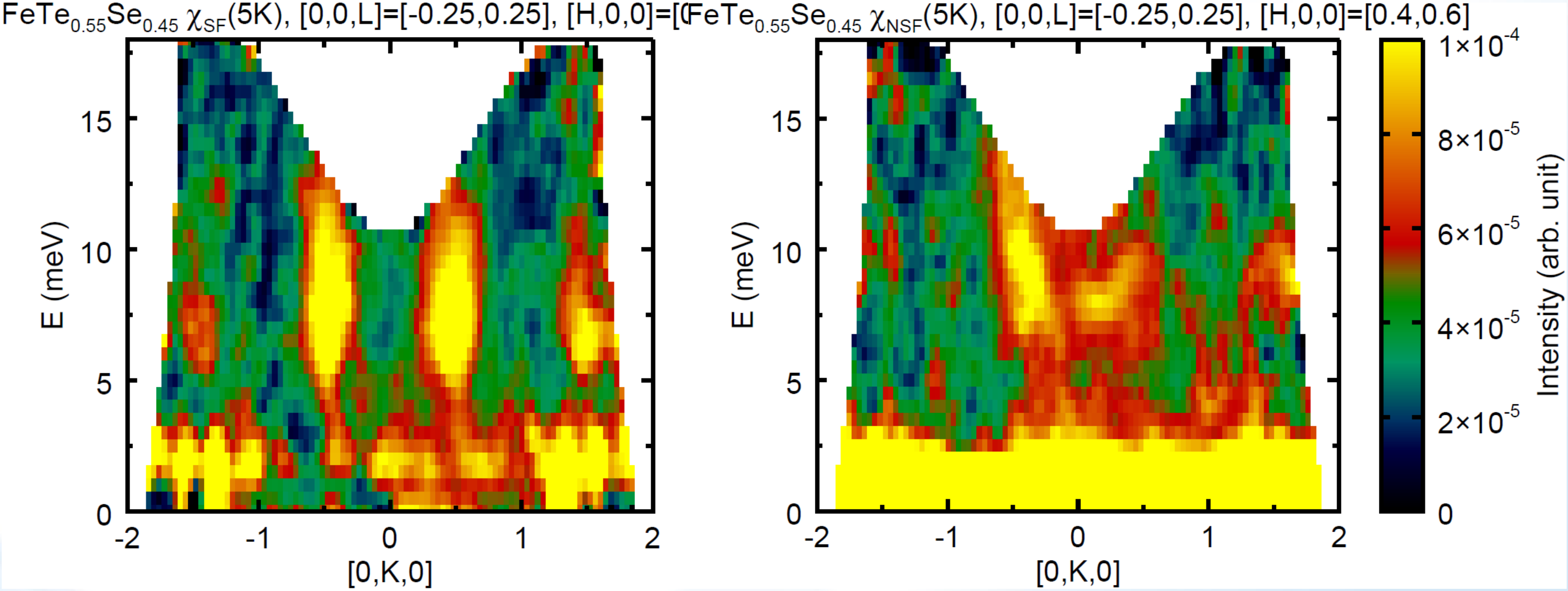

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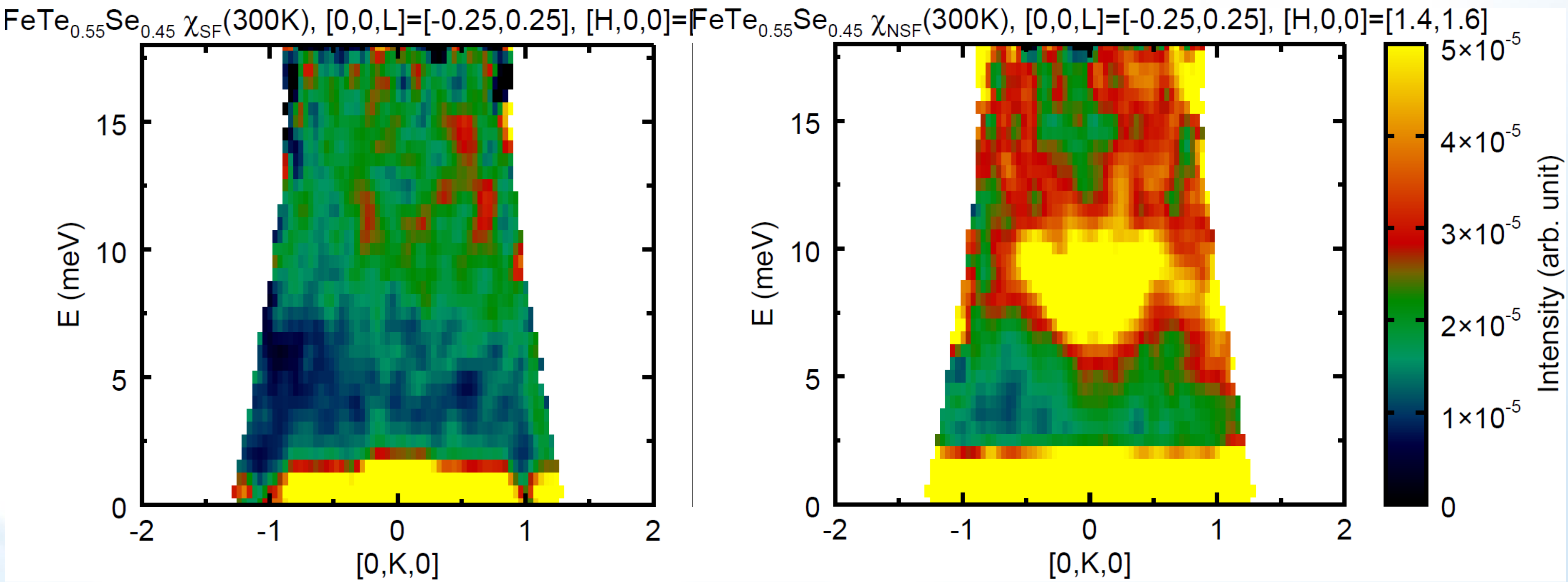

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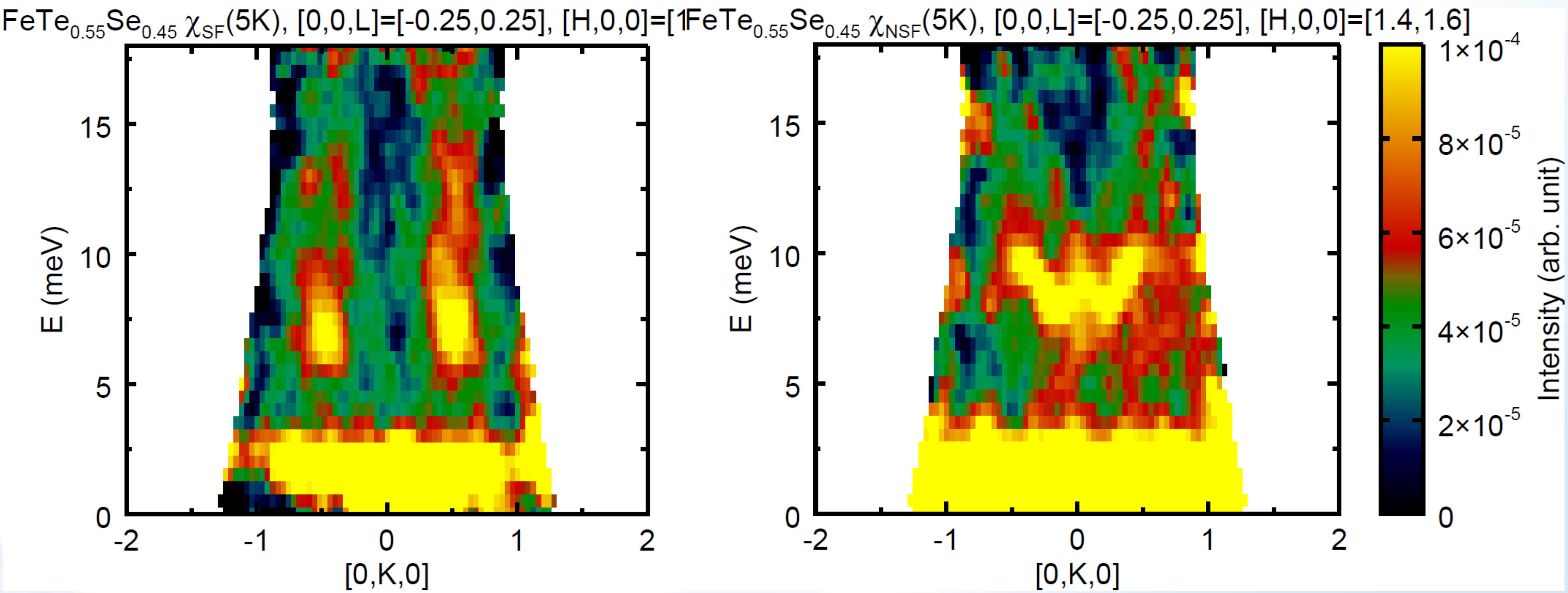

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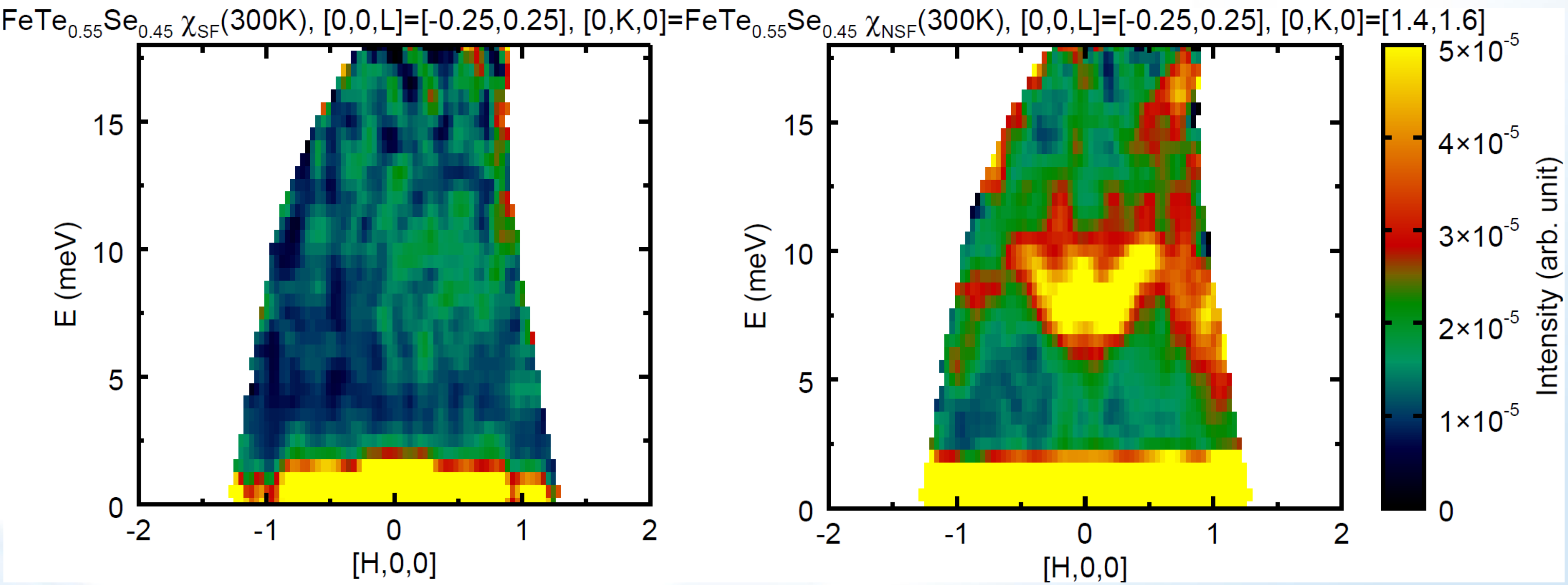

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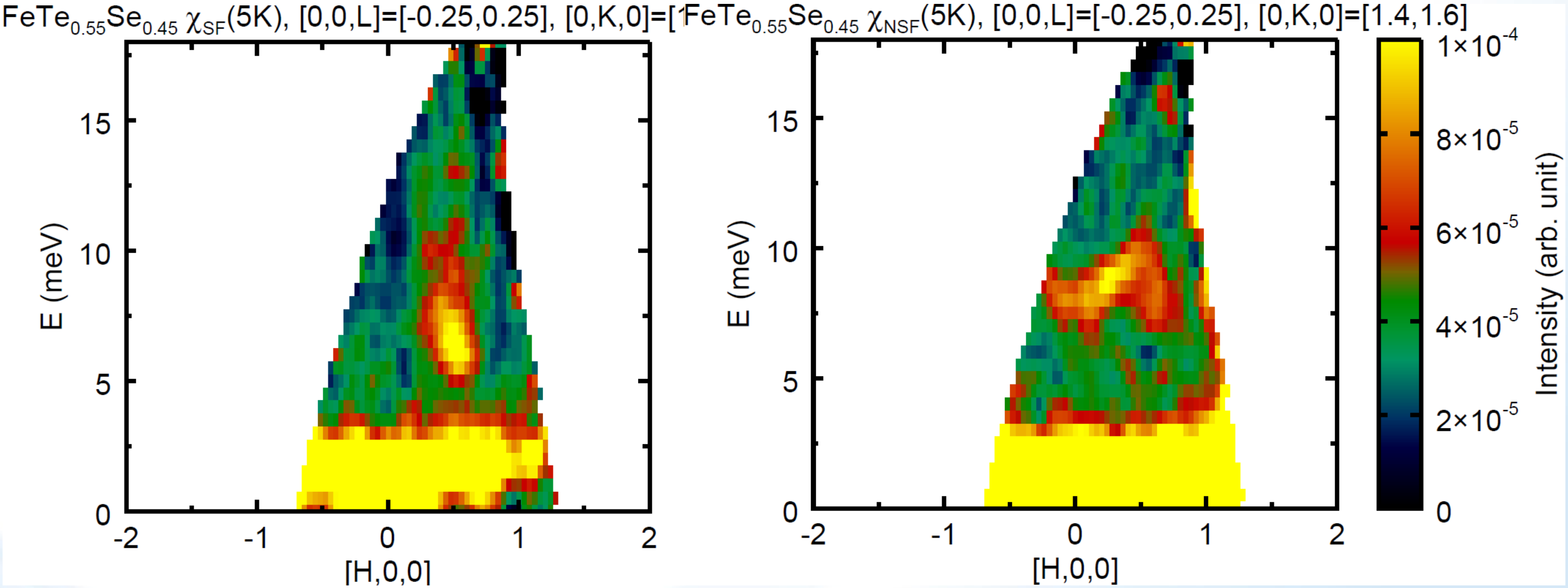

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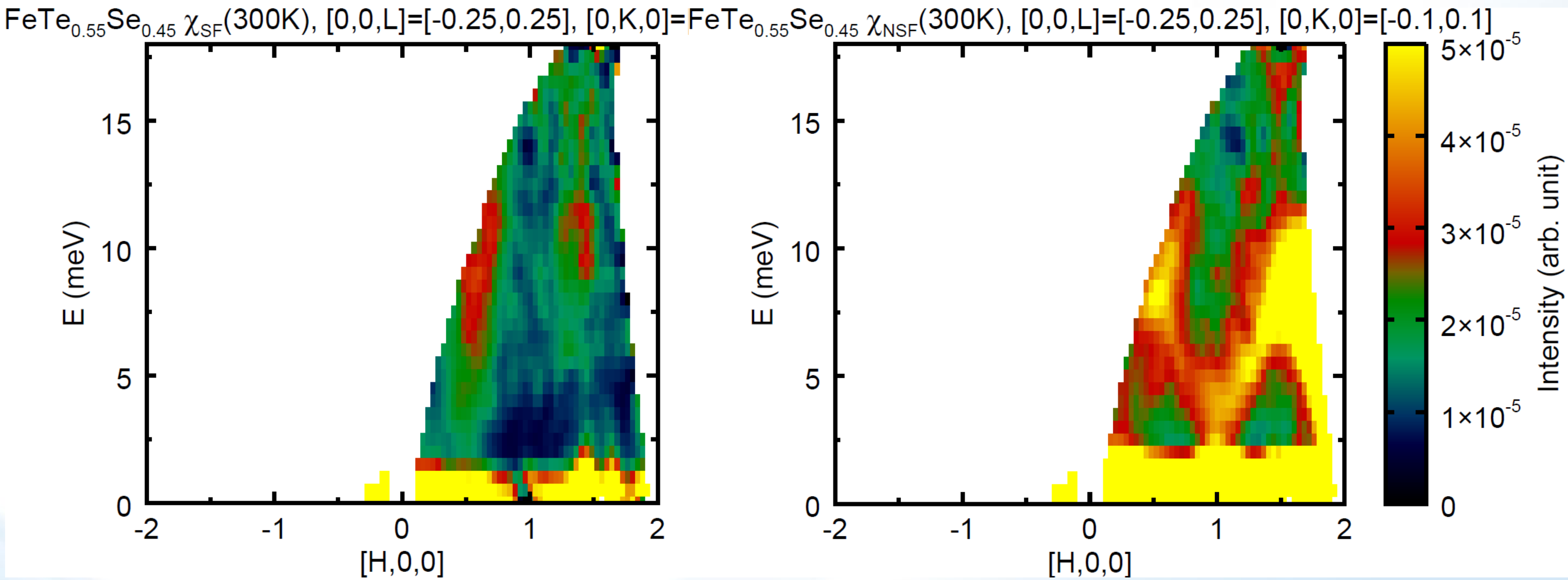

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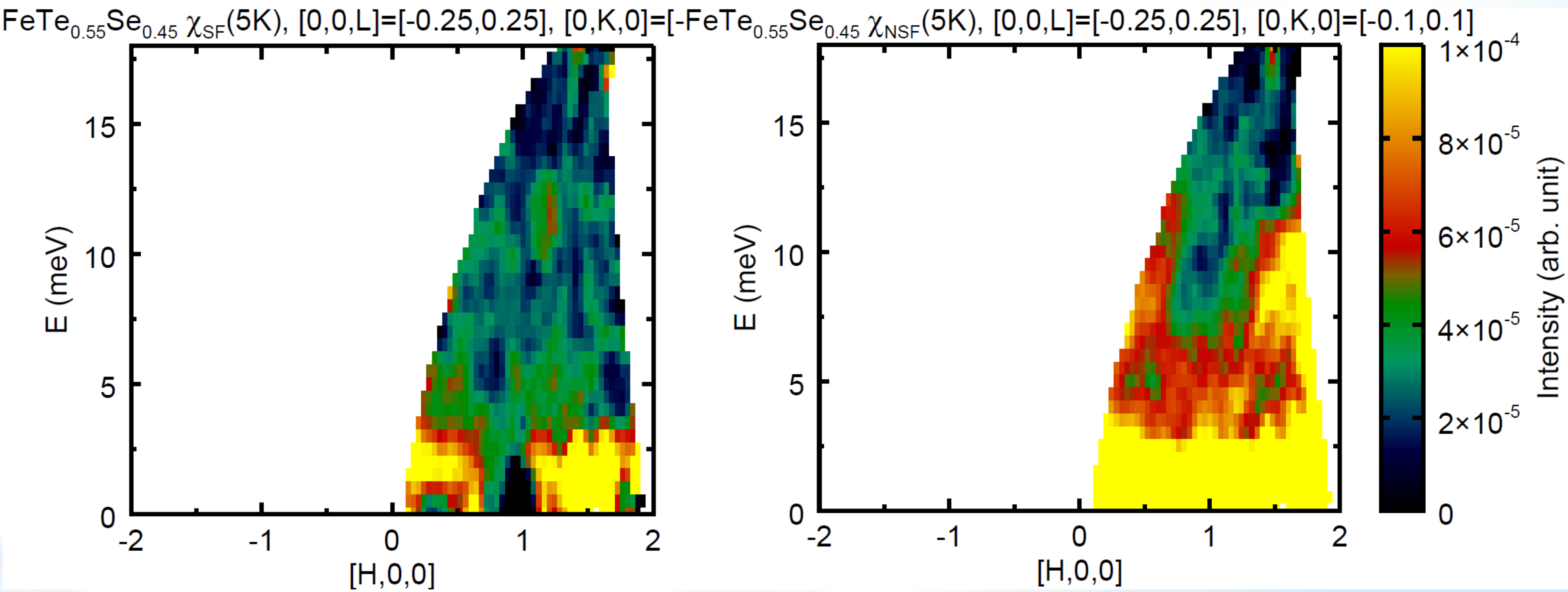

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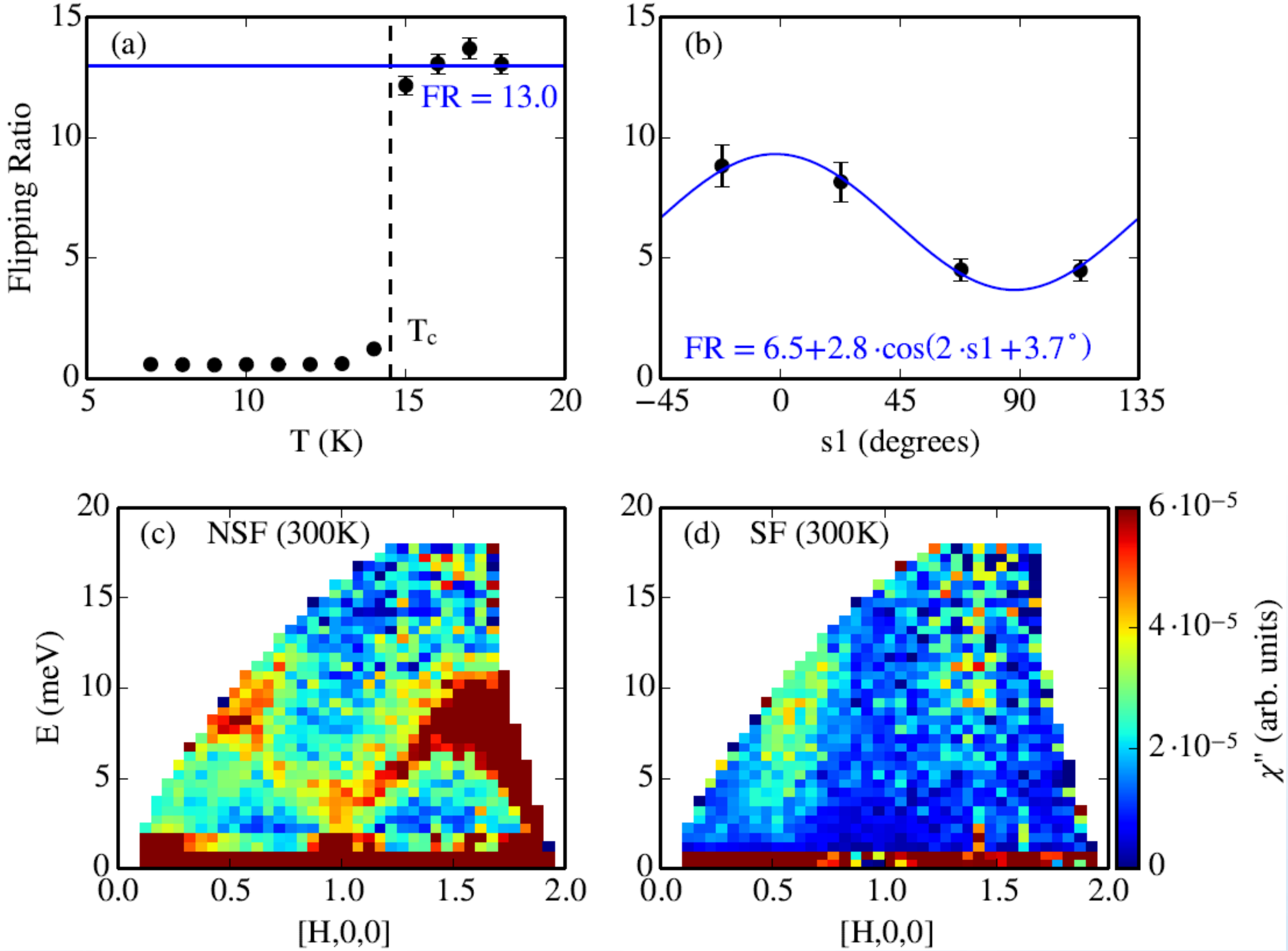

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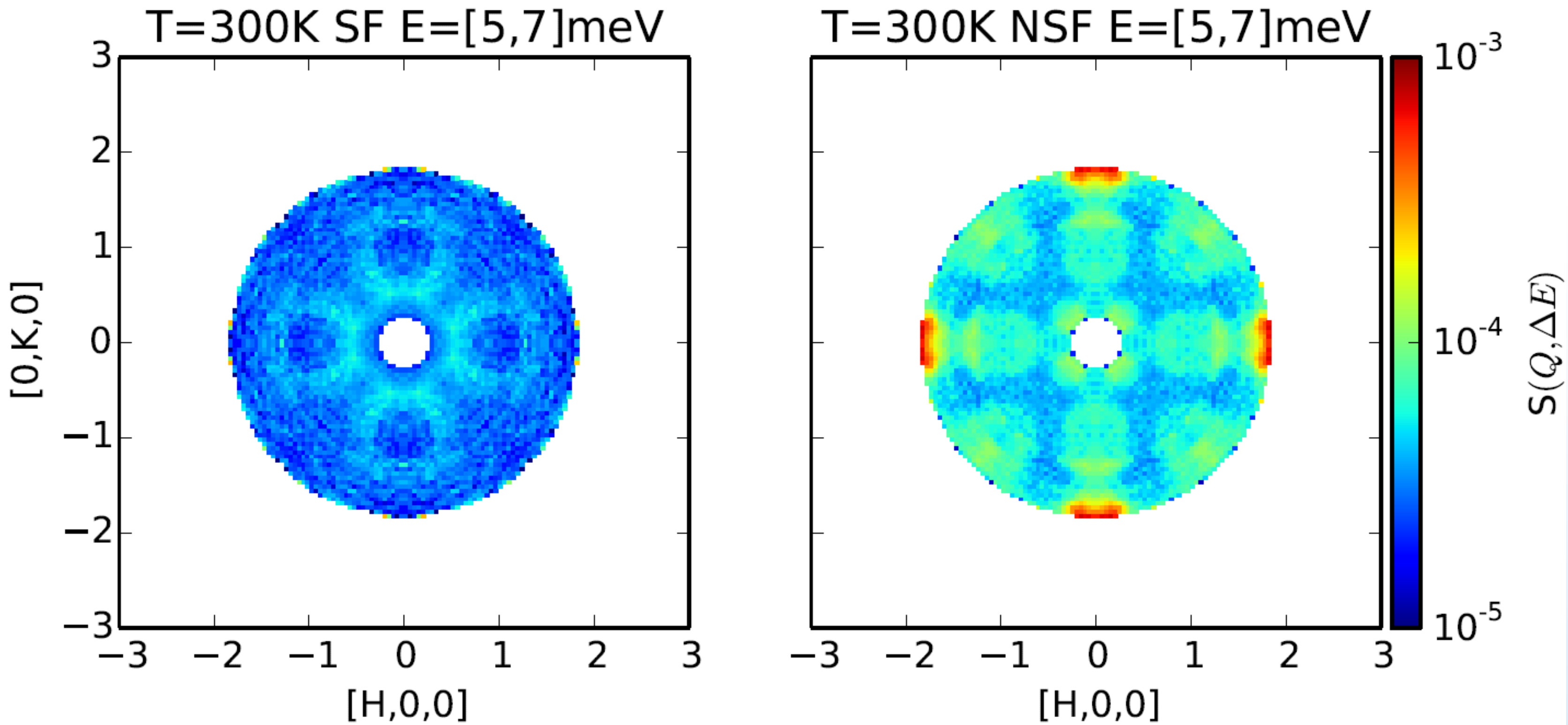

Summary and conclusions

- Direct geometry inelastic spectrometers are a “must be” in the spallation source instrument suite
  - Different instruments serve different problems!
  - Complementary instruments are optimized to serve different neutron energy range (cold, thermal, epithermal)
  - Thermal and sub-thermal neutron flux is high => intensity can be traded for resolution, small sample, and polarization
- In the hindsight: what would I do differently on HYSPEC?
  - Larger detector bank, 90º, or even 120 degrees
  - Additional 60º detector bank in a second vessel?
  - Taller detector tubes (2 – 2.5m) = larger vertical acceptance

HYSPEC Summary

- Polarized neutron surveys of a large volume of the sample's phase space are possible despite
  - Factor 20 to 80 transmission losses in the polarized setup
  - Restricted field of view at the focus of the radial supermirrotr array
  - Large number of corrections for transmission and deflection in the polarized setup (A. Savici, SNS)
- It's a miracle?
  - Careful experiment planning and execution
  - Precise instrument and sample alignment
  - Steady and maintenance-free setup
- It's a miracle!